



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 06:51 am BST

PDB ID : 6QL9 / pdb_00006ql9
Title : Structure of Fatty acid synthase complex from *Saccharomyces cerevisiae* at 2.9 Angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

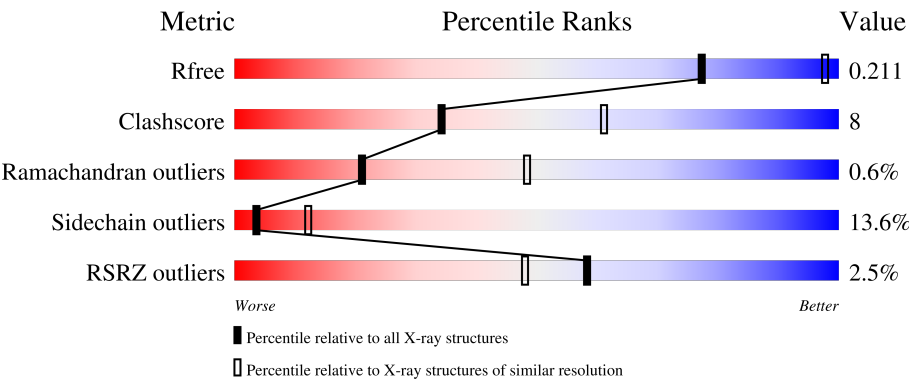
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	3% 72%18%7%
1	B	1887	2% 71%18%7%
1	C	1887	2% 71%18%7%
1	D	1887	3% 72%18%6%

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Mol	Chain	Length	Quality of chain
1	E	1887	
1	F	1887	
2	G	2051	
2	J	2051	
3	H	2051	
3	I	2051	
3	K	2051	
3	L	2051	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MLI	J	2102	-	-	X	-
8	ACT	C	1903	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 179453 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1760	Total	C	N	O	S	0	0	0
			13686	8661	2308	2665	52			
1	B	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	C	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	D	1765	Total	C	N	O	S	0	0	0
			13729	8688	2314	2675	52			
1	E	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	F	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			

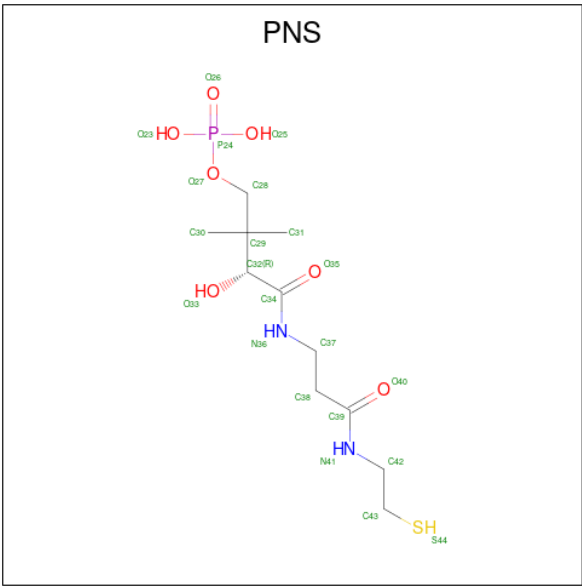
- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2036	Total	C	N	O	S	0	1	0
			16028	10271	2666	3035	56			
2	J	2035	Total	C	N	O	S	0	1	0
			16025	10272	2665	3032	56			

- Molecule 3 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	2035	Total	C	N	O	S	0	1	0
			16028	10274	2664	3034	56			
3	I	2034	Total	C	N	O	S	0	1	0
			16019	10266	2664	3033	56			
3	K	2035	Total	C	N	O	S	0	0	0
			16021	10269	2662	3034	56			
3	L	2036	Total	C	N	O	S	0	1	0
			16040	10280	2666	3038	56			

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	B	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	C	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	D	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	E	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
4	F	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

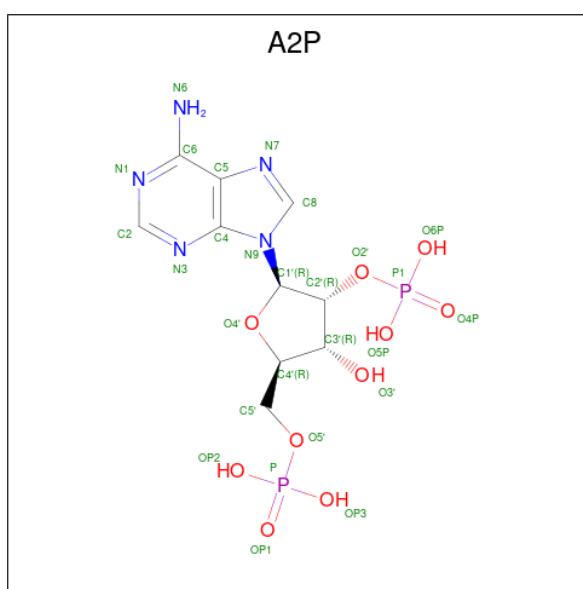
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Na 6 6	0	0
6	B	5	Total Na 5 5	0	0
6	C	4	Total Na 4 4	0	0
6	D	8	Total Na 8 8	0	0
6	E	3	Total Na 3 3	0	0
6	F	2	Total Na 2 2	0	0
6	G	2	Total Na 2 2	0	0
6	H	2	Total Na 2 2	0	0

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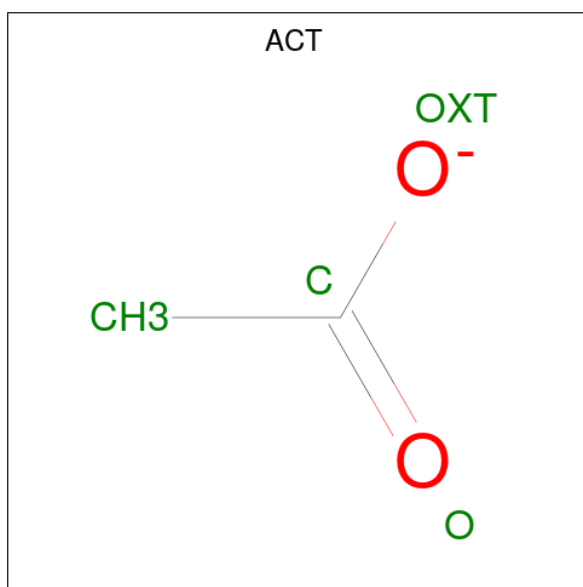
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Na	0	0
			1	1		
6	J	2	Total	Na	0	0
			2	2		
6	K	2	Total	Na	0	0
			2	2		
6	L	2	Total	Na	0	0
			2	2		

- Molecule 7 is ADENOSINE-2'-5'-DIPHOSPHATE (CCD ID: A2P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



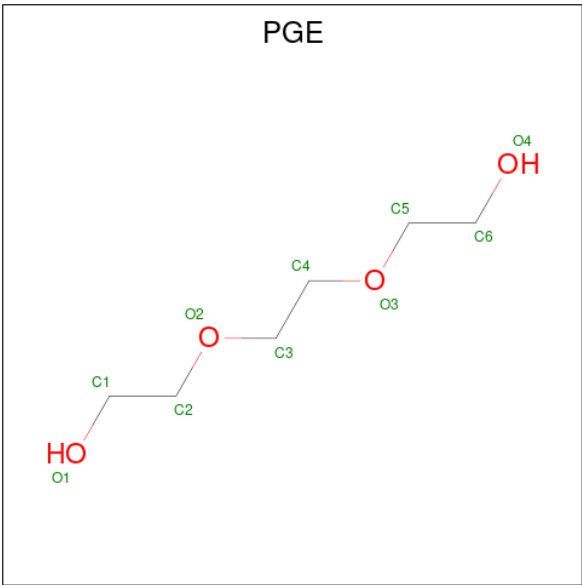
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



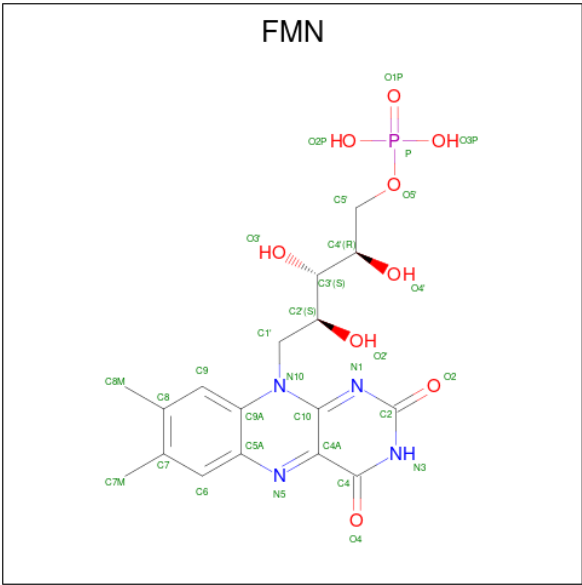
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



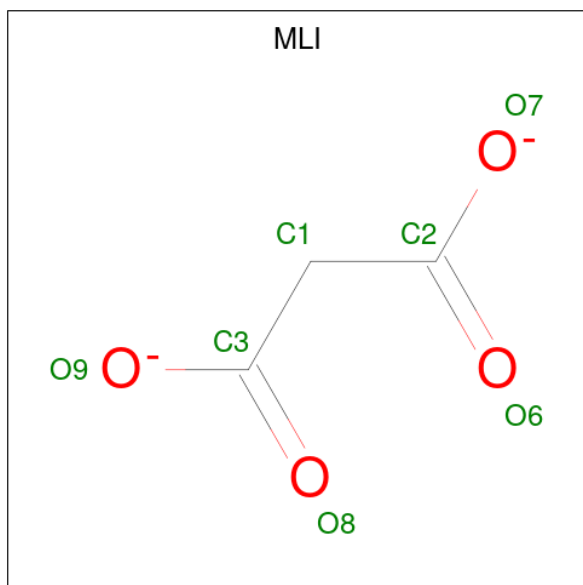
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	O	0	0
			7	3	4		
11	J	1	Total	C	O	0	0
			7	3	4		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	42	Total	O	0	0
			42	42		
12	B	36	Total	O	0	0
			36	36		
12	C	42	Total	O	0	0
			42	42		
12	D	60	Total	O	0	0
			60	60		

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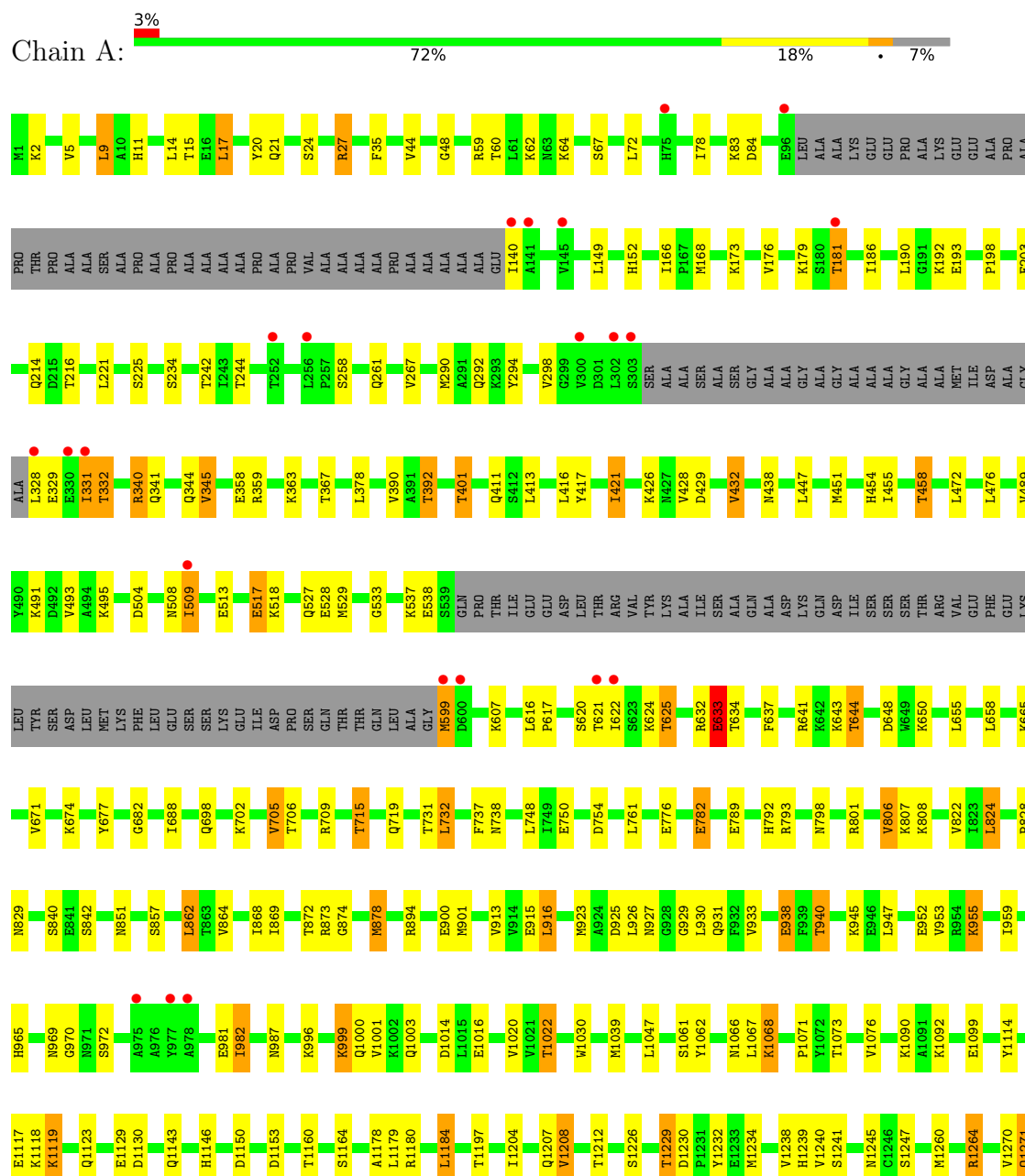
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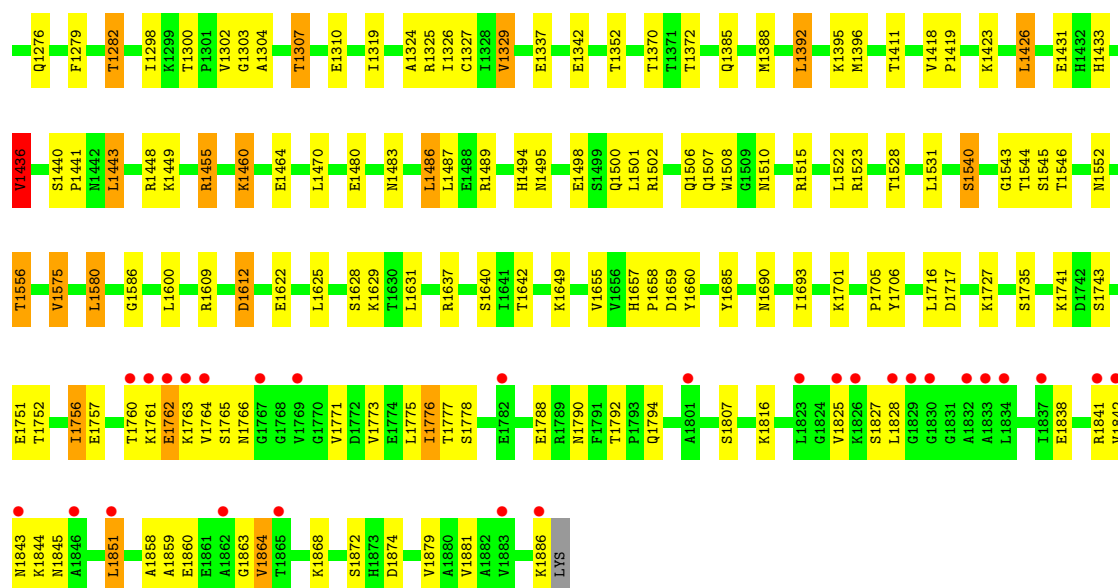
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	30	Total 30	O 30	0	0
12	F	24	Total 24	O 24	0	0
12	G	19	Total 19	O 19	0	0
12	H	24	Total 24	O 24	0	0
12	I	17	Total 17	O 17	0	0
12	J	17	Total 17	O 17	0	0
12	K	5	Total 5	O 5	0	0
12	L	12	Total 12	O 12	0	0

3 Residue-property plots

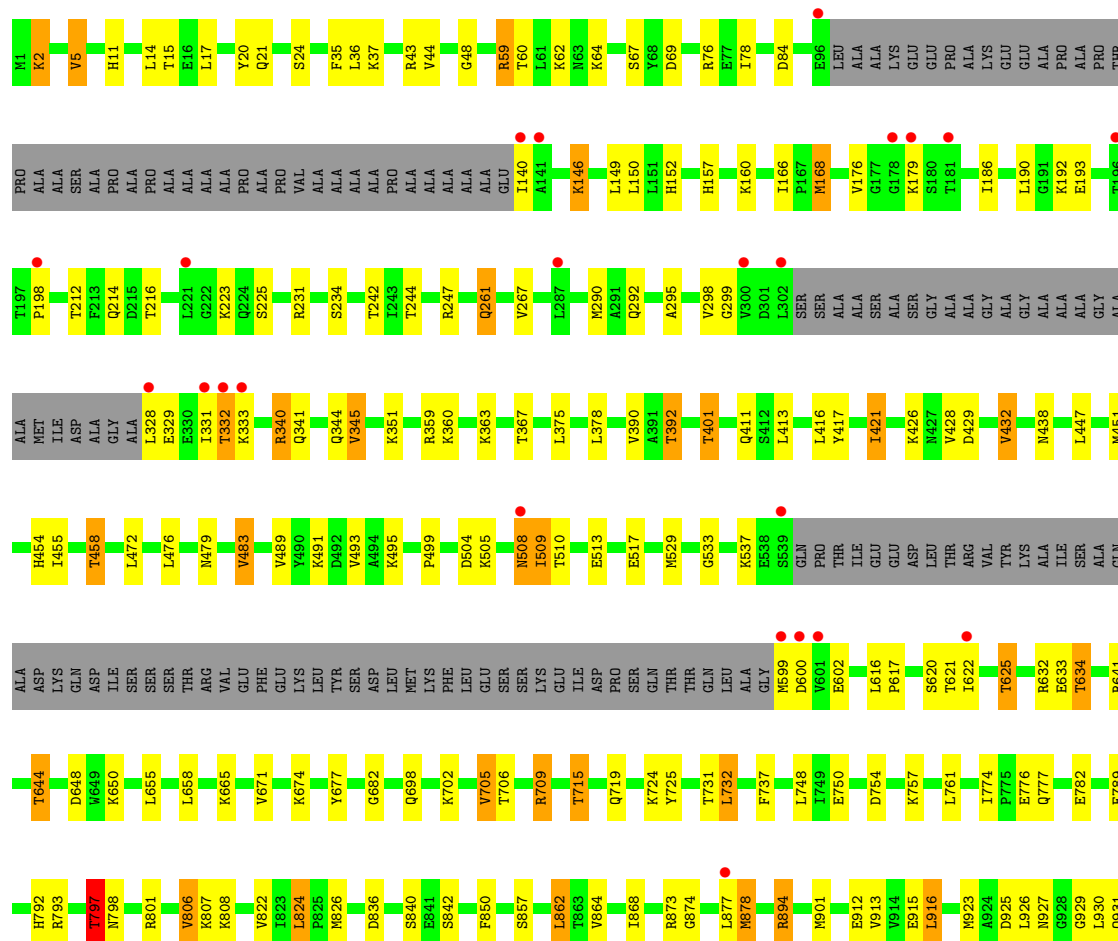
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

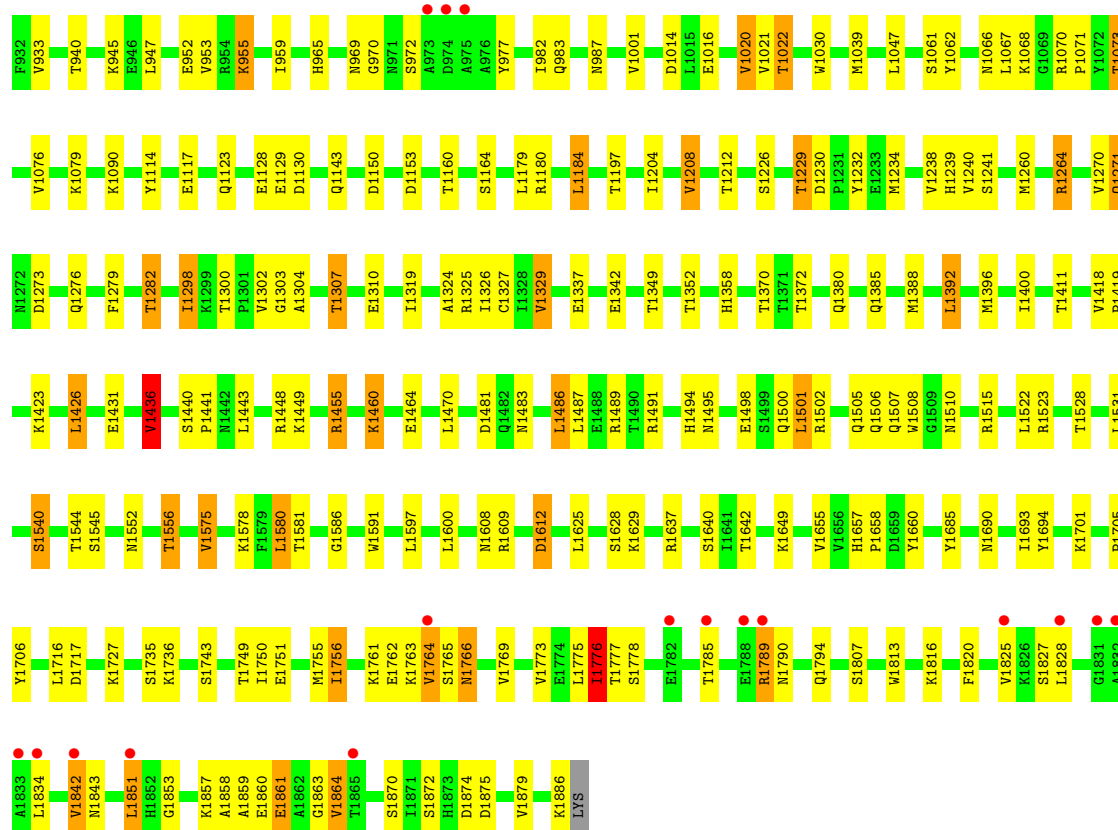
- Molecule 1: Fatty acid synthase subunit alpha



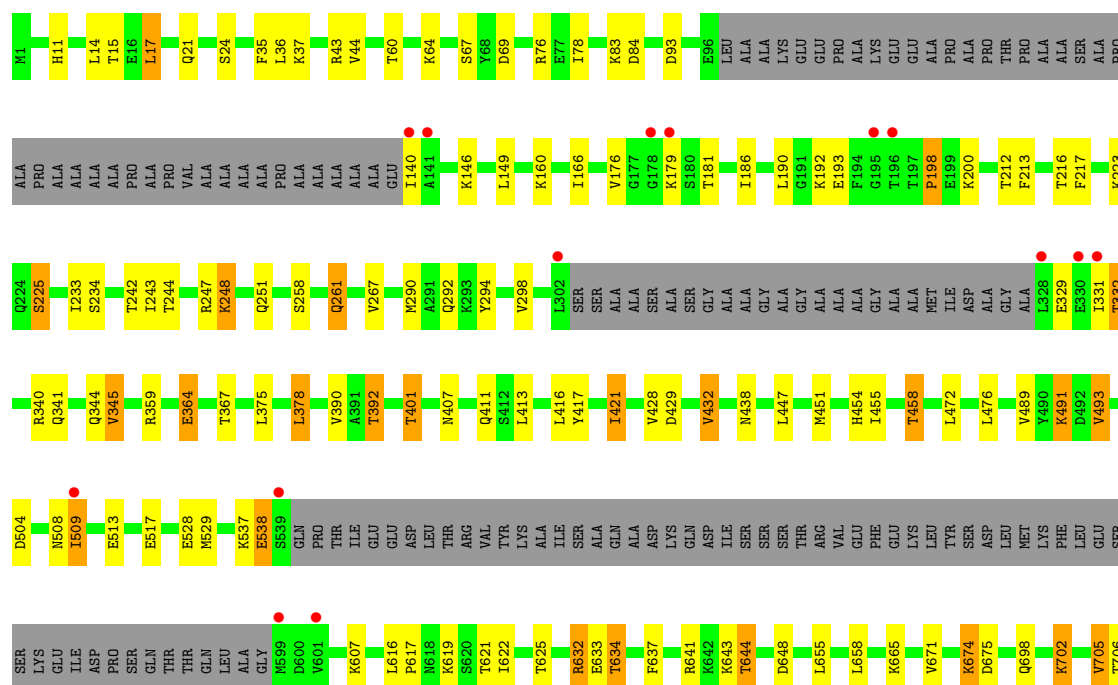


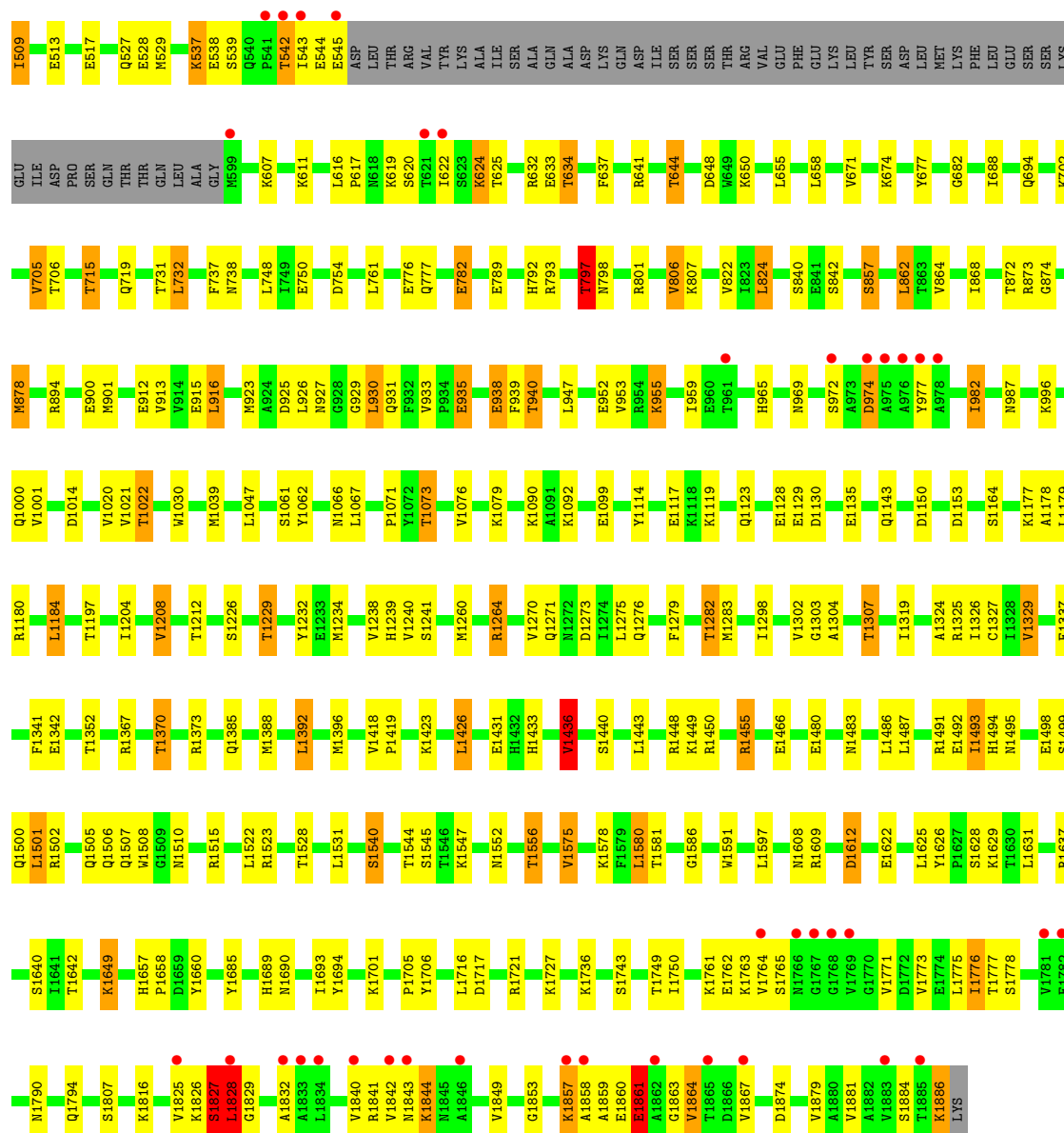
• Molecule 1: Fatty acid synthase subunit alpha



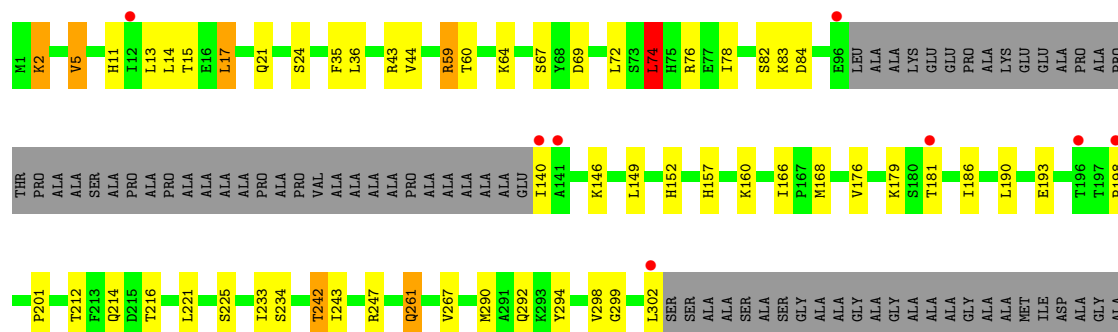


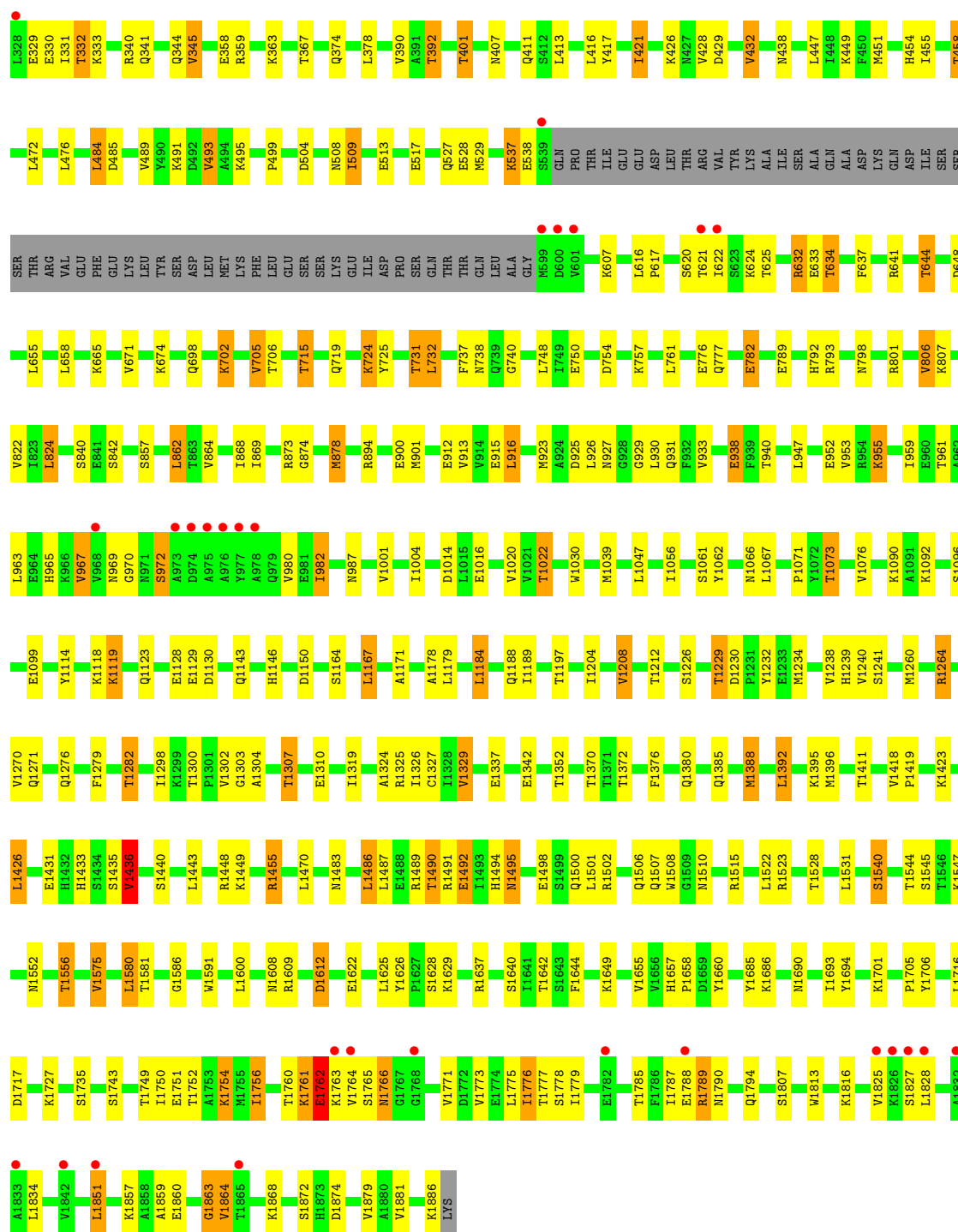
• Molecule 1: Fatty acid synthase subunit alpha





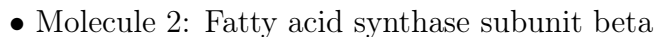
• Molecule 1: Fatty acid synthase subunit alpha

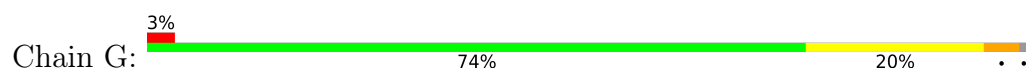




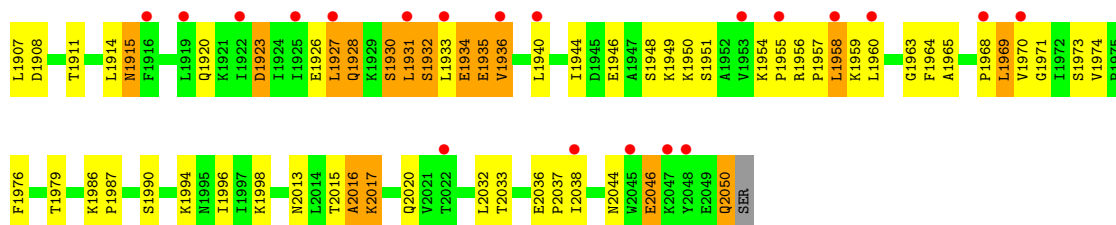
- Molecule 1: Fatty acid synthase subunit alpha





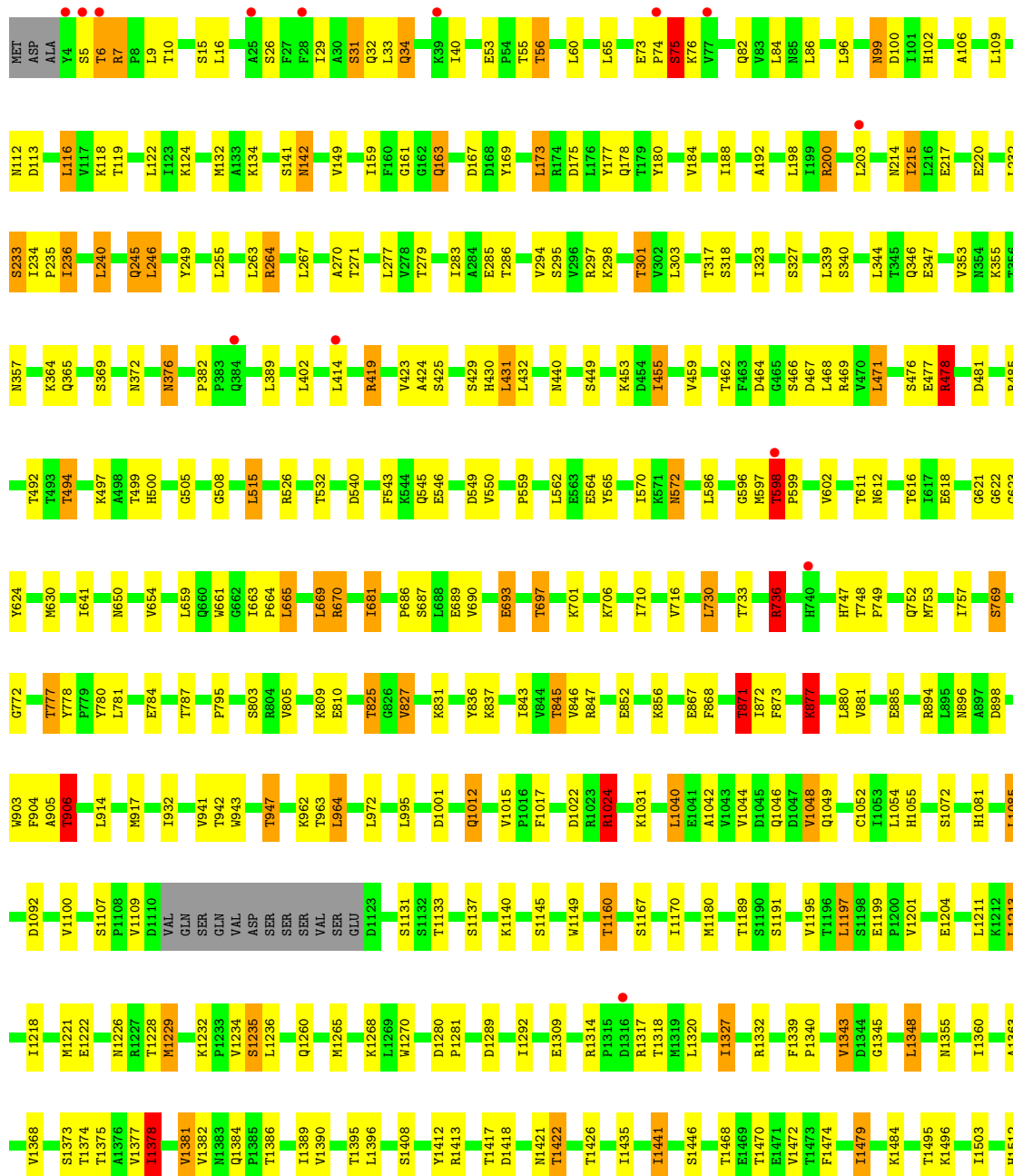


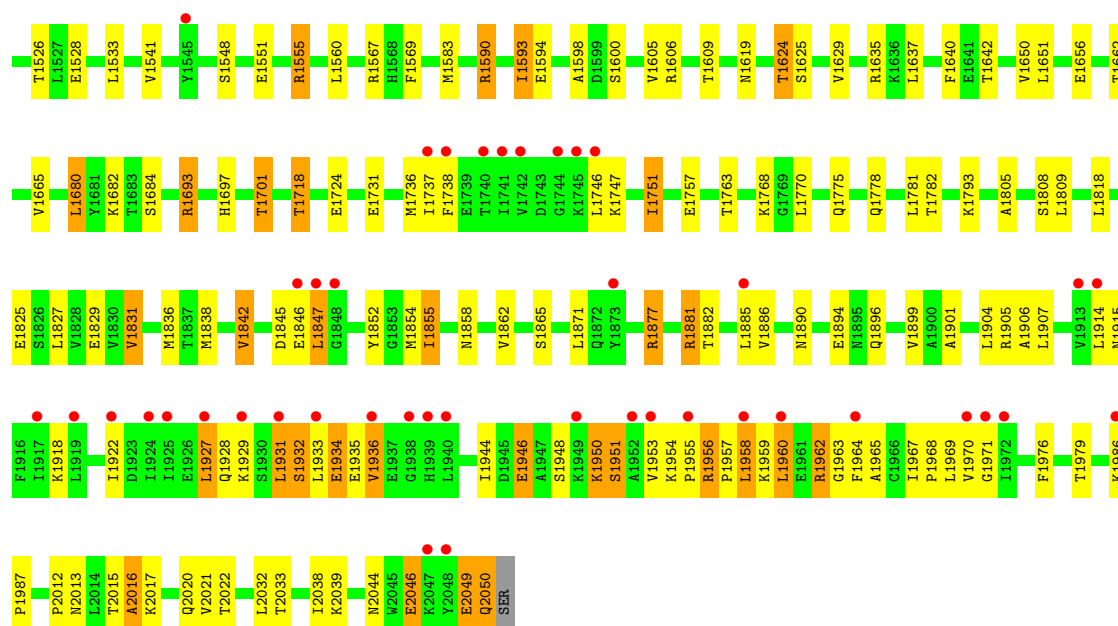
VAL	ASP	ALA	TVR	SE	T6	R7	P6	T10	L9	T11	S15	L16	L21	T24	A25	S26	F27	T28	I29	A30	S31	Q32	L33	Q34	F37	L41	E53	R174	P54	T55	T56	L60	V68	P74	S75	K76	V77	G78	Q79	F80	D81	O82	V83	L84	N85	L86	L96	N99	D100	L101
H102	A106	E111	N112	D113	T114	T115	L116	V117	L118	T119	K120	E121	T122	N142	S26	V149	I159	F160	G161	G162	Q163	D167	V169	L173	R174	D175	Y180	V184	I188	L198	I199	R200	L203	N214	I215	L232	S233	P234	P235	L236	L240	Q245	L246							
Y249	L255	L263	R264	L267	A270	T271	A424	K425	S429	H430	L431	L432	D437	L438	G439	N440	S449	K453	D454	L455	Q456	V459	Y460	T461	Y462	F463	D464	G465	S466	D467	L468	R469	V470	L471	S476	E477	N353	N354	K355	T356	N357	Q365	T492	T493	G621	G622	M630	H500	Y778	
L389	K397	K413	S417	R418	R419	V423	A424	S425	S429	H430	L431	L432	D437	L438	G439	N440	S449	K453	D454	L455	Q456	V459	Y460	T461	Y462	F463	D464	G465	S466	D467	L468	R469	V470	L471	S476	E477	N353	N354	K355	T356	N357	Q365	T492	T493	G621	G622	M630	H500	Y778	
G505	G508	L515	T516	H517	K520	R526	A530	G531	T532	D540	F543	K544	K545	L562	Y565	I570	K571	N572	K576	L586	G596	M597	T598	P599	V602	T611	N612	T616	I617	E618	G621	G622	M630	H500	Y778															
N650	V654	L659	Q660	W661	I663	P664	L665	L666	L669	R670	I681	G684	V685	P686	S687	V690	E693	T697	L698	G699	L700	K706	V716	K721	L730	T733	H740	H747	T748	P749	Q752	M753	I757	S769	G772	T777	Y778													
P779	Y780	L781	T787	P795	S803	R804	V805	K809	E810	V827	Y836	I843	V844	T845	V846	M850	K856	E867	L868	G869	L700	K706	V716	K721	L730	T733	H740	H747	T748	P749	Q752	M753	I757	S769	G772	T777	Y778													
T947	R953	Y954	E955	K962	T963	L964	S965	L972	L995	Q1012	V1015	F1016	P1017	D1022	R1023	R1024	L1040	E1041	A1042	V1043	I1044	D1045	Q1046	V1048	Q1049	C1052	I1053	L1054	H1055	S1072	H1081	L1085	D1092	V1100	S1107	P1108	V1109	D1110	VAL	GLN	GLN									
VAL	ASP	SER	SER	VAL	S1121	S1131	P1132	T1133	S1137	S1145	V1149	S1157	T1160	Q1161	D1162	K1163	S1167	T1170	R1171	K1172	M1180	T1189	S1190	S1191	V1195	T1196	L1197	S1198	E1199	P1200	V1201	L1211	L1212	L1213	E1216	I1217	I1218	M1221	E1222	M1226	R1227	T1228	M1229							
S1285	L1236	Q1260	M1285	K1268	L1269	W1270	D1280	P1281	D1289	T1292	E1309	R1314	T1317	D1318	M1319	L1320	I1327	R1344	T1345	K1346	F1339	P1340	V1343	D1344	G1345	L1347	D1348	N1355	K1358	M1359	L1360	A1363	L1366	Q1367	V1368	V1371	V1372	S1373	T1374											
T1375	A1376	V1377	T1378	V1381	V1382	H1383	Q1384	P1385	T1386	I1389	V1390	T1395	S1408	Y1412	R1413	T1417	D1418	M1421	T1422	T1426	I1435	K1436	T1441	S1446	T1468	E1469	T1470	E1471	V1472	T1473	F1474	T1479	K1484	C1485	T1495	K1496	I1503	L1507	H1512	T1526										
L1527	E1528	L1533	V1541	S1548	E1551	L1560	R1567	H1568	F1569	M1583	R1590	I1593	E1594	A1598	D1599	S1600	S1603	R1604	V1605	R1606	T1609	N1619	K1623	T1624	S1625	V1629	R1635	K1636	L1637	I1638	K1639	F1640	F1641	T1642	V1650	L1651	E1656	V1665	F1666	T1667										
L1680	Y1681	K1692	T1693	S1694	L1701	T1701	T1718	E1724	K1727	E1731	M1736	I1737	E1738	E1739	T1740	I1741	V1742	K1745	L1746	K1747	T1748	E1749	K1750	F1751	F1752	K1753	L1770	Q1775	Q1778	L1781	T1782	K1793	A1805	G1806	H1807	S1808	L1818	R1905	L1906											
S1826	L1827	V1828	E1829	V1830	V1831	M1836	T1837	M1838	V1842	D1845	E1846	L1847	G1848	R1849	Y1852	G1853	M1854	I1855	M1858	P1859	G1860	V1861	A1862	A1863	A1864	Q1868	E1869	A1870	L1871	Q1872	Y1873	R1877	R1881	V1884	L1885	V1886	I1887	L1888	V1889	M1890	Q1896	V1899	A1900	A1901	L1904	R1905	L1906			



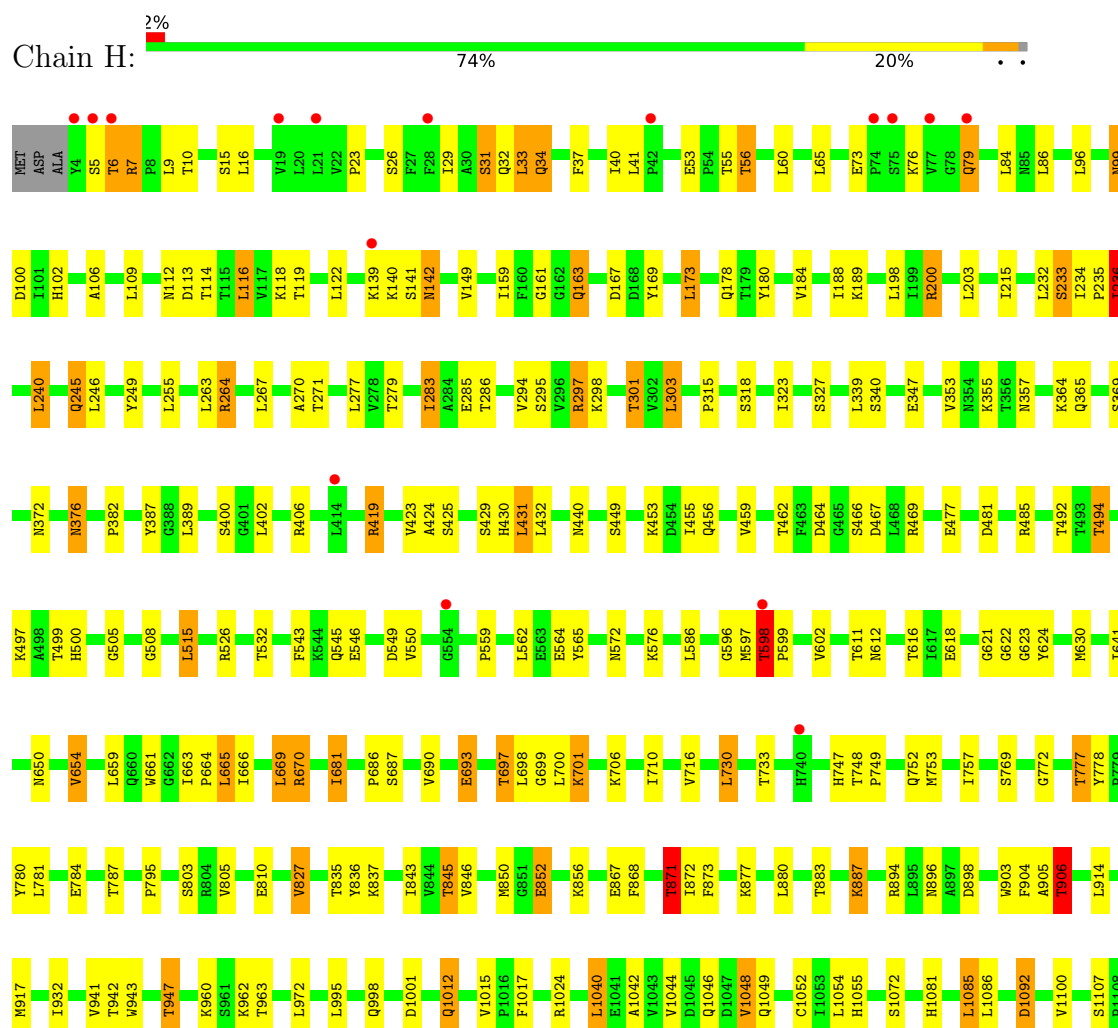
• Molecule 2: Fatty acid synthase subunit beta

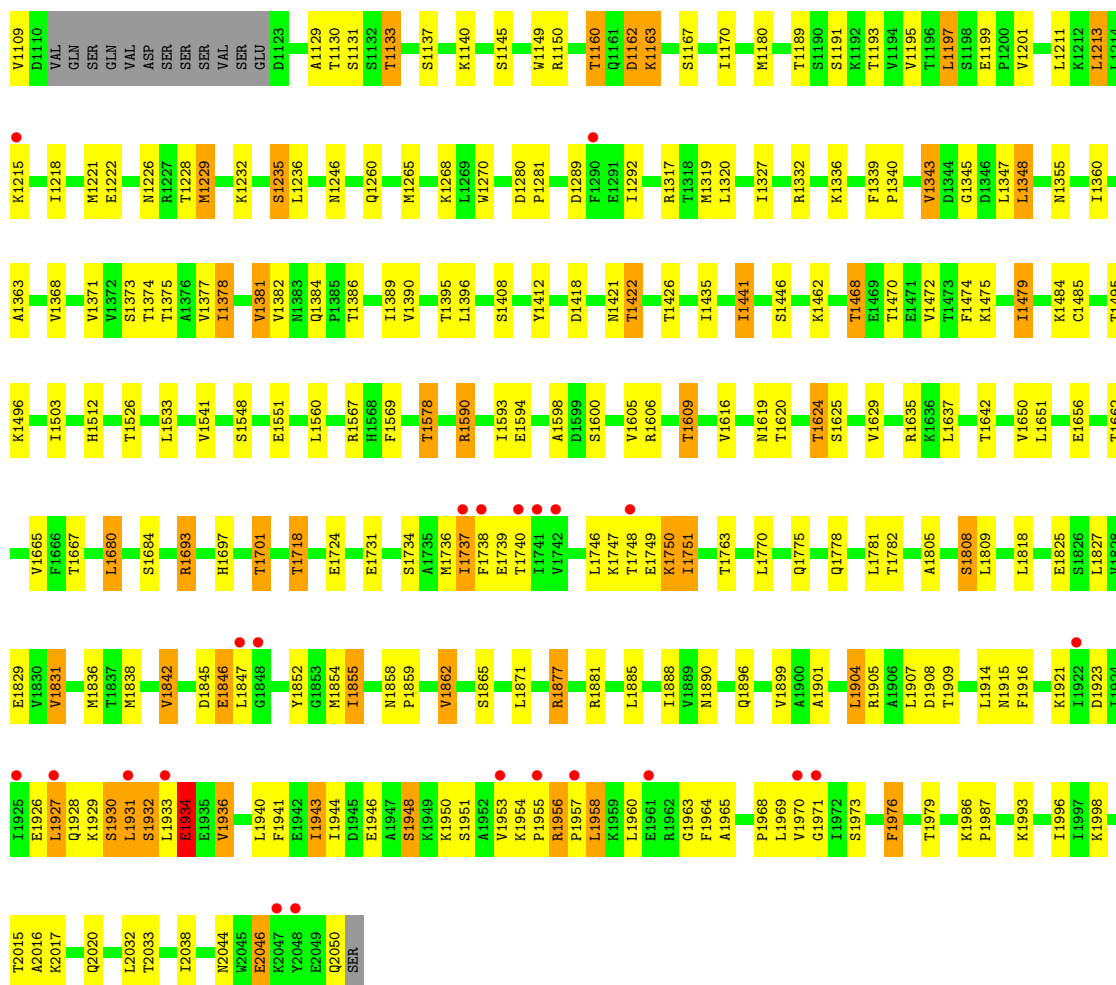
Chain J: 3% 74% 20%



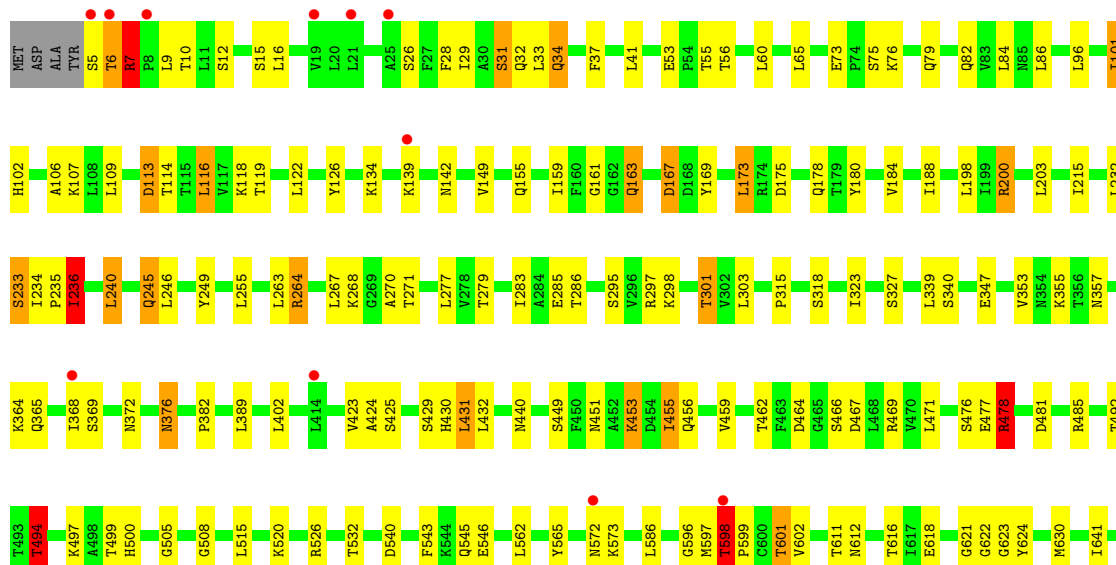


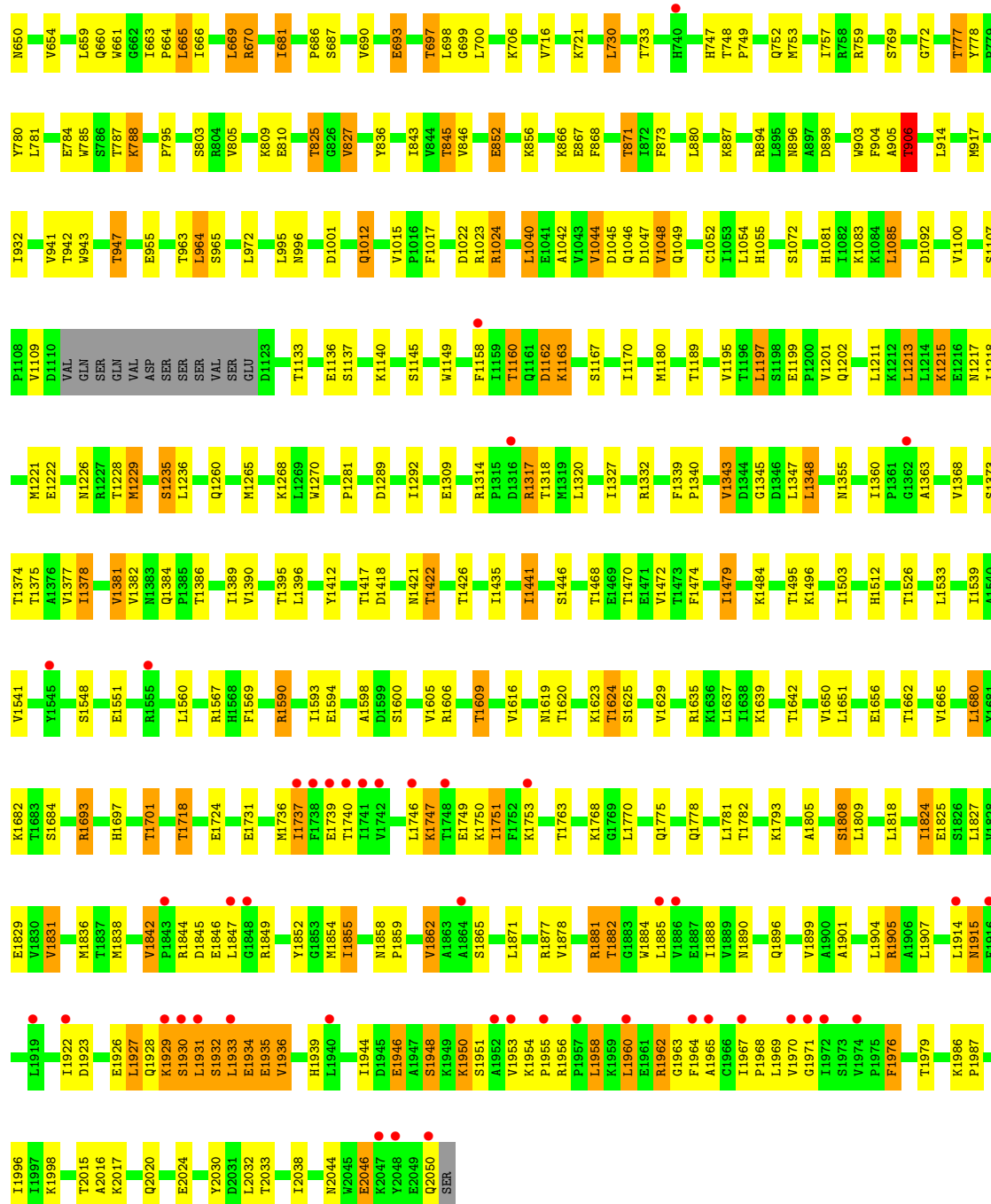
• Molecule 3: Fatty acid synthase subunit beta





• Molecule 3: Fatty acid synthase subunit beta



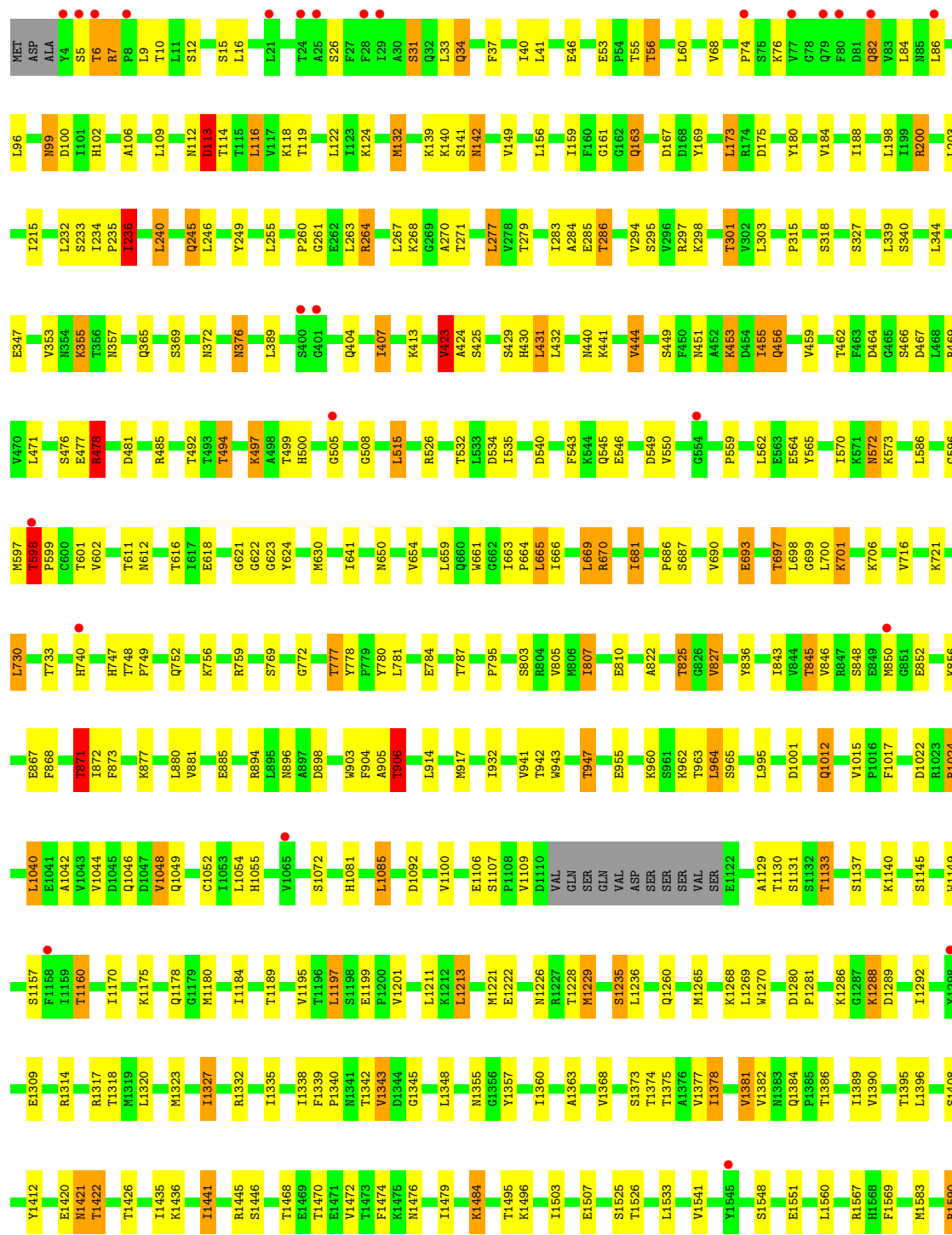


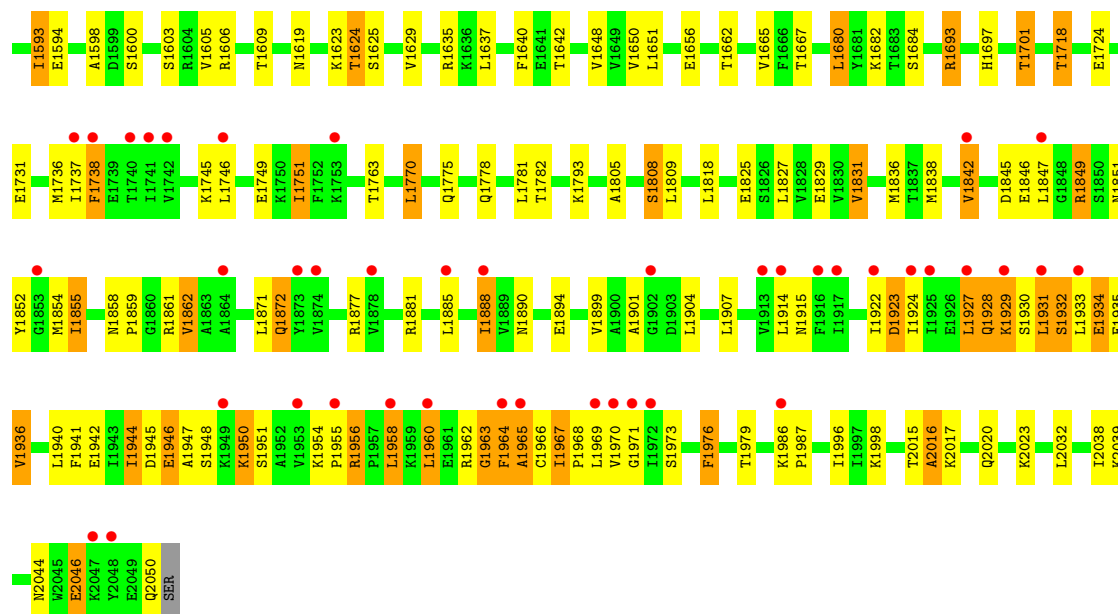


SER

• Molecule 3: Fatty acid synthase subunit beta

Chain L: 3% 73% 21% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	217.62Å 347.60Å 265.27Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	191.50 – 2.82 191.50 – 2.82	Depositor EDS
% Data completeness (in resolution range)	78.6 (191.50-2.82) 78.7 (191.50-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.211 0.194 , 0.211	Depositor DCC
R_{free} test set	35171 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	179453	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: J8W, ACT, FMN, PNS, MLI, NA, PGE, EDO, A2P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	1/13939 (0.0%)	1.49	16/18837 (0.1%)
1	B	1.01	1/13933 (0.0%)	1.49	21/18829 (0.1%)
1	C	1.00	1/13933 (0.0%)	1.48	22/18829 (0.1%)
1	D	1.01	1/13983 (0.0%)	1.50	19/18898 (0.1%)
1	E	1.00	1/13933 (0.0%)	1.49	26/18829 (0.1%)
1	F	1.00	1/13933 (0.0%)	1.48	12/18829 (0.1%)
2	G	1.01	1/16394 (0.0%)	1.47	32/22244 (0.1%)
2	J	1.01	1/16392 (0.0%)	1.47	26/22242 (0.1%)
3	H	1.01	1/16385 (0.0%)	1.47	24/22231 (0.1%)
3	I	1.01	1/16372 (0.0%)	1.47	29/22213 (0.1%)
3	K	1.02	1/16374 (0.0%)	1.47	25/22216 (0.1%)
3	L	1.02	2/16394 (0.0%)	1.47	23/22243 (0.1%)
All	All	1.01	13/181965 (0.0%)	1.48	275/246440 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	1
3	I	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1689	HIS	CE1-NE2	5.64	1.38	1.32
1	C	166	ILE	N-CA	5.41	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1842	VAL	N-CA	5.37	1.50	1.46
3	K	1842	VAL	N-CA	5.33	1.50	1.46
1	E	166	ILE	N-CA	5.31	1.50	1.46
2	G	1842	VAL	N-CA	5.31	1.50	1.46
1	A	166	ILE	N-CA	5.30	1.50	1.46
3	H	1842	VAL	N-CA	5.30	1.50	1.46
3	L	1842	VAL	N-CA	5.19	1.50	1.46
3	I	1842	VAL	N-CA	5.14	1.50	1.46
1	F	166	ILE	N-CA	5.13	1.50	1.46
3	L	1044	VAL	C-O	5.06	1.28	1.23
1	B	166	ILE	N-CA	5.05	1.50	1.46

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1150	ASP	CA-CB-CG	9.99	122.59	112.60
3	I	1158	PHE	CA-CB-CG	8.82	122.62	113.80
1	B	1886	LYS	CA-C-O	8.76	135.69	120.80
1	D	1229	THR	CA-CB-OG1	-8.53	96.81	109.60
1	B	1229	THR	CA-CB-OG1	-8.48	96.88	109.60
2	G	1751	ILE	N-CA-C	-8.33	98.83	109.58
1	D	974	ASP	CA-CB-CG	8.28	120.88	112.60
1	A	1229	THR	CA-CB-OG1	-8.19	97.31	109.60
1	C	1229	THR	CA-CB-OG1	-8.19	97.31	109.60
1	E	1229	THR	CA-CB-OG1	-8.15	97.38	109.60
1	F	1229	THR	CA-CB-OG1	-8.10	97.45	109.60
1	A	633	GLU	CB-CA-C	7.69	121.65	110.04
1	C	1612	ASP	CA-CB-CG	7.23	119.83	112.60
1	D	1612	ASP	CA-CB-CG	7.16	119.76	112.60
3	L	1964	PHE	CB-CA-C	7.16	124.66	110.42
1	B	1612	ASP	CA-CB-CG	7.12	119.72	112.60
2	G	1868	GLN	N-CA-C	-7.11	99.14	109.59
1	E	1612	ASP	CA-CB-CG	7.09	119.69	112.60
2	G	28	PHE	CA-CB-CG	7.07	120.87	113.80
1	A	1612	ASP	CA-CB-CG	6.93	119.53	112.60
3	L	807	ILE	N-CA-CB	-6.89	103.21	112.16
1	A	625	THR	CB-CA-C	6.87	118.25	109.80
3	I	142	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	1886	LYS	CA-C-O	6.85	132.45	120.80
1	E	1264	ARG	CG-CD-NE	-6.83	96.96	112.00
1	A	1264	ARG	CG-CD-NE	-6.81	97.01	112.00
1	B	1264	ARG	CG-CD-NE	-6.80	97.03	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1612	ASP	CA-CB-CG	6.75	119.36	112.60
1	D	1886	LYS	CA-C-O	6.74	132.26	120.80
2	J	1024	ARG	CB-CG-CD	6.69	126.69	111.30
1	C	1264	ARG	CG-CD-NE	-6.69	97.28	112.00
1	D	1721	ARG	CG-CD-NE	-6.67	97.33	112.00
1	E	392	THR	CA-CB-OG1	-6.63	99.65	109.60
1	D	1264	ARG	CG-CD-NE	-6.51	97.68	112.00
1	C	392	THR	CA-CB-OG1	-6.46	99.91	109.60
1	B	600	ASP	CA-CB-CG	6.44	119.04	112.60
2	G	1868	GLN	CB-CA-C	6.39	119.85	110.26
1	B	392	THR	CA-CB-OG1	-6.38	100.03	109.60
1	E	201	PRO	CA-C-N	6.37	128.82	120.28
1	E	201	PRO	C-N-CA	6.37	128.82	120.28
2	J	827	VAL	CB-CA-C	6.35	115.56	109.33
3	L	827	VAL	CB-CA-C	6.27	115.48	109.33
1	B	797	THR	CB-CA-C	6.25	121.16	110.79
2	J	598	THR	CA-CB-OG1	-6.25	100.23	109.60
3	I	827	VAL	CB-CA-C	6.22	115.43	109.33
2	G	598	THR	CA-CB-OG1	-6.21	100.28	109.60
2	G	1417	THR	CA-CB-OG1	-6.19	100.31	109.60
1	D	392	THR	CA-CB-OG1	-6.19	100.32	109.60
1	B	401	THR	CB-CA-C	6.18	120.02	110.14
3	L	1963	GLY	CA-C-O	-6.07	115.23	121.61
1	B	600	ASP	CB-CA-C	6.06	119.75	109.75
1	D	401	THR	CB-CA-C	6.06	119.83	110.14
3	K	827	VAL	CB-CA-C	6.04	115.25	109.33
2	J	494	THR	CB-CA-C	6.02	120.39	111.06
1	F	715	THR	CA-CB-OG1	-6.00	100.60	109.60
1	F	392	THR	CA-CB-OG1	-5.99	100.62	109.60
3	K	494	THR	CB-CA-C	5.99	120.34	111.06
1	B	970	GLY	CA-C-O	-5.98	117.07	122.57
3	H	598	THR	CA-CB-OG1	-5.98	100.63	109.60
1	E	35	PHE	CA-CB-CG	5.96	119.76	113.80
1	D	715	THR	CA-CB-OG1	-5.95	100.68	109.60
2	G	494	THR	CB-CA-C	5.95	120.28	111.06
3	I	494	THR	CB-CA-C	5.94	120.27	111.06
3	I	1160	THR	CA-CB-OG1	-5.92	100.73	109.60
3	L	494	THR	CB-CA-C	5.92	120.23	111.06
1	A	392	THR	CA-CB-OG1	-5.91	100.73	109.60
1	F	1150	ASP	CB-CA-C	-5.91	98.66	110.42
3	K	1160	THR	CA-CB-OG1	-5.90	100.75	109.60
3	H	494	THR	CB-CA-C	5.90	120.20	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	827	VAL	CB-CA-C	5.89	115.10	109.33
1	C	715	THR	CA-CB-OG1	-5.88	100.78	109.60
1	C	35	PHE	CA-CB-CG	5.88	119.67	113.80
2	G	885	GLU	CB-CG-CD	5.88	122.59	112.60
1	C	401	THR	CB-CA-C	5.86	119.52	110.14
1	A	970	GLY	CA-C-O	-5.85	117.55	122.29
3	I	1882	THR	CA-CB-OG1	-5.84	100.84	109.60
3	H	1160	THR	CA-CB-OG1	-5.84	100.84	109.60
2	J	736	ARG	CB-CG-CD	5.84	124.72	111.30
3	L	598	THR	CA-CB-OG1	-5.83	100.86	109.60
1	A	401	THR	CB-CA-C	5.82	119.45	110.14
1	D	977	TYR	CA-CB-CG	5.82	124.38	113.90
1	E	401	THR	CB-CA-C	5.81	119.44	110.14
1	F	35	PHE	CA-CB-CG	5.81	119.61	113.80
1	C	1886	LYS	CA-C-O	5.79	130.65	120.80
2	J	787	THR	CA-CB-OG1	-5.79	100.92	109.60
2	J	478	ARG	CG-CD-NE	5.78	124.72	112.00
1	F	401	THR	CB-CA-C	5.78	119.38	110.14
1	C	797	THR	CB-CA-C	5.77	120.38	110.79
1	D	35	PHE	CA-CB-CG	5.76	119.56	113.80
1	D	1150	ASP	CB-CA-C	-5.75	99.31	110.46
1	A	1150	ASP	CB-CA-C	-5.73	99.01	110.42
1	D	797	THR	CB-CA-C	5.72	120.28	110.79
3	L	1160	THR	CA-CB-OG1	-5.69	101.06	109.60
1	E	970	GLY	CA-C-O	-5.69	117.33	122.57
2	G	827	VAL	CB-CA-C	5.69	114.90	109.33
3	H	787	THR	CA-CB-OG1	-5.69	101.07	109.60
1	D	1827	SER	CA-C-N	5.68	132.39	121.54
1	D	1827	SER	C-N-CA	5.68	132.39	121.54
3	L	478	ARG	CG-CD-NE	5.68	124.49	112.00
3	I	1162	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	35	PHE	CA-CB-CG	5.66	119.46	113.80
3	I	598	THR	CA-CB-OG1	-5.66	101.10	109.60
2	G	787	THR	CA-CB-OG1	-5.65	101.12	109.60
3	L	423	VAL	CA-CB-CG2	5.64	119.98	110.40
2	J	661	TRP	CA-C-N	5.63	126.08	119.94
2	J	661	TRP	C-N-CA	5.63	126.08	119.94
1	B	715	THR	CA-CB-OG1	-5.63	101.15	109.60
3	I	1881	ARG	CB-CG-CD	5.62	124.23	111.30
1	B	625	THR	CB-CA-C	5.59	116.68	109.80
1	A	715	THR	CA-CB-OG1	-5.59	101.21	109.60
1	A	35	PHE	CA-CB-CG	5.57	119.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	787	THR	CA-CB-OG1	-5.57	101.25	109.60
3	H	871	THR	CA-CB-OG1	-5.56	101.25	109.60
2	G	871	THR	CA-CB-OG1	-5.54	101.29	109.60
2	J	871	THR	CA-CB-OG1	-5.54	101.29	109.60
3	L	787	THR	CA-CB-OG1	-5.53	101.30	109.60
1	C	251	GLN	CB-CG-CD	5.51	121.97	112.60
2	G	544	LYS	CA-CB-CG	5.50	125.10	114.10
1	F	493	VAL	N-CA-C	-5.49	107.63	112.90
2	J	1738	PHE	CA-CB-CG	5.49	119.29	113.80
1	E	1825	VAL	CA-C-N	5.49	127.57	120.44
1	E	1825	VAL	C-N-CA	5.49	127.57	120.44
3	I	200	ARG	CA-C-N	5.48	127.57	120.44
3	I	200	ARG	C-N-CA	5.48	127.57	120.44
3	K	1555	ARG	CB-CG-CD	5.47	123.88	111.30
3	I	233	SER	CA-C-N	5.46	123.68	120.24
3	I	233	SER	C-N-CA	5.46	123.68	120.24
3	K	1162	ASP	CA-CB-CG	5.45	118.05	112.60
3	K	871	THR	CA-CB-OG1	-5.44	101.43	109.60
3	L	661	TRP	CA-C-N	5.44	125.87	119.94
3	L	661	TRP	C-N-CA	5.44	125.87	119.94
2	J	1160	THR	CA-CB-OG1	-5.43	101.45	109.60
3	H	233	SER	CA-C-N	5.43	123.66	120.24
3	H	233	SER	C-N-CA	5.43	123.66	120.24
3	I	1417	THR	CA-CB-OG1	-5.42	101.46	109.60
1	A	938	GLU	CB-CG-CD	5.42	121.82	112.60
3	K	598	THR	CA-CB-OG1	-5.42	101.47	109.60
2	G	200	ARG	CA-C-N	5.42	127.49	120.44
2	G	200	ARG	C-N-CA	5.42	127.49	120.44
3	I	661	TRP	CA-C-N	5.42	125.85	119.94
3	I	661	TRP	C-N-CA	5.42	125.85	119.94
3	K	787	THR	CA-CB-OG1	-5.42	101.48	109.60
1	E	1762	GLU	CB-CG-CD	5.41	121.80	112.60
2	J	113	ASP	CA-CB-CG	5.41	118.01	112.60
3	L	871	THR	CA-CB-OG1	-5.41	101.49	109.60
1	B	1776	ILE	CA-C-O	-5.40	115.43	121.05
2	G	661	TRP	CA-C-N	5.39	125.81	119.94
2	G	661	TRP	C-N-CA	5.39	125.81	119.94
1	A	940	THR	CA-CB-OG1	-5.39	101.52	109.60
3	I	1976	PHE	CA-CB-CG	5.38	119.18	113.80
2	G	1160	THR	CA-CB-OG1	-5.37	101.54	109.60
3	H	661	TRP	CA-C-N	5.37	125.79	119.94
3	H	661	TRP	C-N-CA	5.37	125.79	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1881	ARG	CA-C-O	-5.36	115.17	120.80
2	J	200	ARG	CA-C-N	5.36	127.41	120.44
2	J	200	ARG	C-N-CA	5.36	127.41	120.44
1	C	1273	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	970	GLY	CA-C-O	-5.33	117.66	122.57
3	H	200	ARG	CA-C-N	5.32	127.35	120.44
3	H	200	ARG	C-N-CA	5.32	127.35	120.44
3	H	1609	THR	CA-CB-OG1	-5.31	101.63	109.60
3	H	1976	PHE	CA-CB-CG	5.31	119.11	113.80
2	G	233	SER	CA-C-N	5.30	123.58	120.24
2	G	233	SER	C-N-CA	5.30	123.58	120.24
2	J	1417	THR	CA-CB-OG1	-5.29	101.67	109.60
1	B	1300	THR	CB-CA-C	5.28	115.71	110.33
2	G	1024	ARG	CB-CG-CD	5.27	123.42	111.30
3	L	236	ILE	CB-CA-C	5.27	115.70	111.06
3	I	478	ARG	CG-CD-NE	5.26	123.57	112.00
1	C	493	VAL	N-CA-C	-5.26	107.85	112.90
3	I	1609	THR	CA-CB-OG1	-5.26	101.72	109.60
1	E	493	VAL	N-CA-C	-5.25	107.18	112.17
3	K	684	GLY	CA-C-O	-5.25	118.61	122.23
1	C	972	SER	CA-C-N	5.25	127.57	120.38
1	C	972	SER	C-N-CA	5.25	127.57	120.38
2	G	684	GLY	CA-C-O	-5.25	118.61	122.23
1	E	938	GLU	CB-CG-CD	5.24	121.51	112.60
1	E	1761	LYS	CA-C-N	5.23	127.24	120.44
1	E	1761	LYS	C-N-CA	5.23	127.24	120.44
1	F	1760	THR	CA-C-O	-5.23	115.92	121.94
2	J	65	LEU	CA-C-N	5.23	125.74	119.94
2	J	65	LEU	C-N-CA	5.23	125.74	119.94
1	B	836	ASP	CA-CB-CG	5.22	117.82	112.60
3	I	906	THR	CB-CA-C	5.22	118.18	110.14
1	C	1073	THR	CA-CB-OG1	-5.22	101.77	109.60
2	G	113	ASP	CA-CB-CG	5.21	117.81	112.60
3	I	236	ILE	CB-CA-C	5.21	115.65	111.06
3	I	1044	VAL	CA-C-O	-5.21	115.85	121.27
3	H	906	THR	CB-CA-C	5.21	118.16	110.14
2	J	825	THR	N-CA-C	-5.21	102.14	109.96
1	C	1376	PHE	CA-CB-CG	5.20	119.00	113.80
1	D	1073	THR	CA-CB-OG1	-5.20	101.80	109.60
2	J	906	THR	CB-CA-C	5.20	118.15	110.14
2	J	781	LEU	CA-C-N	5.20	127.24	120.28
2	J	781	LEU	C-N-CA	5.20	127.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1073	THR	CA-CB-OG1	-5.20	101.81	109.60
2	G	460	TYR	CA-C-N	5.20	128.09	120.71
2	G	460	TYR	C-N-CA	5.20	128.09	120.71
3	I	781	LEU	CA-C-N	5.20	127.24	120.28
3	I	781	LEU	C-N-CA	5.20	127.24	120.28
3	K	1976	PHE	CA-CB-CG	5.20	119.00	113.80
3	L	1738	PHE	CA-CB-CG	5.19	118.99	113.80
1	B	1349	THR	CA-CB-OG1	5.19	117.38	109.60
1	C	1056	ILE	O-C-N	5.19	127.13	121.94
3	I	825	THR	N-CA-C	-5.19	102.18	109.96
3	K	1044	VAL	CA-C-O	-5.18	115.88	121.27
1	E	74	LEU	CB-CA-C	5.18	119.38	111.76
3	H	1162	ASP	CA-CB-CG	5.18	117.78	112.60
3	L	200	ARG	CA-C-N	5.17	127.17	120.44
3	L	200	ARG	C-N-CA	5.17	127.17	120.44
1	A	517	GLU	N-CA-C	-5.16	102.22	109.96
1	E	972	SER	CA-C-N	5.15	127.44	120.38
1	E	972	SER	C-N-CA	5.15	127.44	120.38
3	H	781	LEU	CA-C-N	5.15	127.18	120.28
3	H	781	LEU	C-N-CA	5.15	127.18	120.28
2	J	540	ASP	CA-CB-CG	5.15	117.75	112.60
2	G	517	HIS	CA-CB-CG	-5.15	108.65	113.80
3	K	1609	THR	CA-CB-OG1	-5.15	101.88	109.60
3	L	113	ASP	CA-CB-CG	5.14	117.75	112.60
3	H	65	LEU	CA-C-N	5.14	125.65	119.94
3	H	65	LEU	C-N-CA	5.14	125.65	119.94
3	K	200	ARG	CA-C-N	5.14	127.12	120.44
3	K	200	ARG	C-N-CA	5.14	127.12	120.44
2	G	781	LEU	CA-C-N	5.14	127.16	120.28
2	G	781	LEU	C-N-CA	5.14	127.16	120.28
1	A	1300	THR	CB-CA-C	5.13	115.57	110.33
1	E	1300	THR	CB-CA-C	5.13	115.56	110.33
3	K	1738	PHE	CA-CB-CG	5.13	118.93	113.80
1	F	1056	ILE	O-C-N	5.13	127.07	121.94
3	L	781	LEU	CA-C-N	5.13	127.15	120.28
3	L	781	LEU	C-N-CA	5.13	127.15	120.28
1	C	538	GLU	CB-CA-C	5.12	118.99	110.74
3	K	661	TRP	CA-C-N	5.12	125.53	119.94
3	K	661	TRP	C-N-CA	5.12	125.53	119.94
2	G	906	THR	CB-CA-C	5.12	118.03	110.14
1	B	1273	ASP	CA-CB-CG	5.12	117.72	112.60
3	H	1934	GLU	CA-C-N	5.12	127.65	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1934	GLU	C-N-CA	5.12	127.65	120.28
3	L	1976	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	938	GLU	CB-CG-CD	5.11	121.29	112.60
3	K	906	THR	CB-CA-C	5.11	118.00	110.14
3	I	65	LEU	CA-C-N	5.10	125.64	119.98
3	I	65	LEU	C-N-CA	5.10	125.64	119.98
1	F	1325	ARG	N-CA-C	-5.10	107.61	113.88
1	B	1481	ASP	CB-CA-C	-5.10	100.84	110.01
3	K	781	LEU	CA-C-N	5.09	127.11	120.28
3	K	781	LEU	C-N-CA	5.09	127.11	120.28
2	G	236	ILE	CB-CA-C	5.09	115.54	111.06
3	K	65	LEU	CA-C-N	5.09	125.59	119.94
3	K	65	LEU	C-N-CA	5.09	125.59	119.94
2	G	1609	THR	CA-CB-OG1	-5.08	101.97	109.60
1	E	1376	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	1279	PHE	CA-CB-CG	5.08	118.88	113.80
1	E	715	THR	CA-CB-OG1	-5.08	101.98	109.60
1	E	1388	MET	N-CA-CB	-5.07	102.52	111.39
2	J	233	SER	CA-C-N	5.06	123.43	120.24
2	J	233	SER	C-N-CA	5.06	123.43	120.24
3	K	233	SER	CA-C-N	5.06	123.43	120.24
3	K	233	SER	C-N-CA	5.06	123.43	120.24
3	L	825	THR	N-CA-C	-5.06	102.38	109.96
1	B	1073	THR	CA-CB-OG1	-5.05	102.02	109.60
1	D	1273	ASP	CA-CB-CG	5.05	117.65	112.60
2	G	1923	ASP	CA-C-N	5.05	127.01	120.70
2	G	1923	ASP	C-N-CA	5.05	127.01	120.70
1	D	940	THR	CA-CB-OG1	-5.04	102.04	109.60
3	K	1417	THR	CA-CB-OG1	-5.04	102.04	109.60
1	D	1861	GLU	N-CA-CB	5.03	118.03	110.53
1	B	1150	ASP	CB-CA-C	-5.03	100.41	110.42
1	C	940	THR	CA-CB-OG1	-5.02	102.07	109.60
2	J	1378	ILE	CB-CA-C	5.02	118.17	111.19
3	H	236	ILE	CB-CA-C	5.01	115.47	111.06
1	E	1056	ILE	O-C-N	5.01	126.95	121.94
3	H	1738	PHE	CA-CB-CG	5.01	118.81	113.80
1	E	1073	THR	CA-CB-OG1	-5.00	102.10	109.60
3	L	906	THR	CB-CA-C	5.00	117.84	110.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1207	GLN	Peptide
1	C	1841	ARG	Peptide
1	C	538	GLU	Peptide
1	D	1828	LEU	Peptide
3	I	1844	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13686	0	13661	221	2
1	B	13680	0	13658	223	0
1	C	13680	0	13658	229	0
1	D	13729	0	13701	218	2
1	E	13680	0	13658	224	0
1	F	13680	0	13658	219	0
2	G	16028	0	15999	249	0
2	J	16025	0	15997	257	0
3	H	16028	0	15993	254	0
3	I	16019	0	15983	256	0
3	K	16021	0	15986	268	0
3	L	16040	0	15998	304	0
4	A	21	0	21	1	0
4	B	21	0	21	1	0
4	C	21	0	21	0	0
4	D	21	0	21	0	0
4	E	21	0	21	0	0
4	F	21	0	21	2	0
5	A	40	0	60	0	0
5	B	40	0	60	4	0
5	C	36	0	54	1	0
5	D	52	0	78	1	0
5	E	48	0	72	0	0
5	F	32	0	48	0	0
5	H	4	0	6	0	0
5	J	16	0	24	2	0
6	A	6	0	0	0	0
6	B	5	0	0	0	0
6	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	8	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	1	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
7	A	27	0	11	3	0
7	B	27	0	11	5	0
7	C	27	0	11	1	0
7	D	27	0	11	3	0
7	E	27	0	11	2	0
7	F	27	0	11	1	0
8	B	4	0	3	1	0
8	C	8	0	6	2	0
8	H	12	0	9	0	0
9	E	10	0	14	0	0
10	G	31	0	19	5	0
10	H	31	0	19	5	0
10	I	31	0	19	6	0
10	J	31	0	19	8	0
10	K	31	0	19	5	0
10	L	31	0	19	6	0
11	G	7	0	2	1	0
11	J	7	0	2	2	0
12	A	42	0	0	1	0
12	B	36	0	0	0	0
12	C	42	0	0	0	0
12	D	60	0	0	1	0
12	E	30	0	0	0	0
12	F	24	0	0	1	0
12	G	19	0	0	1	0
12	H	24	0	0	2	0
12	I	17	0	0	1	0
12	J	17	0	0	0	0
12	K	5	0	0	0	0
12	L	12	0	0	0	0
All	All	179453	0	178694	2704	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2704) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASP:OD2	1:B:508:ASN:OD1	1.53	1.21
3:K:1904:LEU:HD22	3:K:1960:LEU:HD23	1.32	1.12
1:B:508:ASN:C	1:B:508:ASN:HD22	1.61	1.09
3:I:867:GLU:O	3:I:871:THR:OG1	1.69	1.08
1:C:1486:LEU:O	1:C:1490:THR:HG22	1.55	1.06
1:B:193:GLU:OE2	1:B:225:SER:OG	1.72	1.06
1:E:1486:LEU:O	1:E:1490:THR:HG22	1.56	1.05
1:C:1471:LYS:HD3	1:C:1759:MET:HE3	1.36	1.03
3:I:1922:ILE:HB	3:I:1927:LEU:HD21	1.40	1.02
2:J:180:TYR:O	2:J:184:VAL:HG22	1.60	1.01
1:D:1135:GLU:OE2	1:E:242:THR:HG21	1.62	0.98
3:K:154:ALA:HA	3:K:499:THR:HG21	1.41	0.98
1:B:792:HIS:HE1	1:E:792:HIS:HE1	1.04	0.96
1:C:792:HIS:HE1	1:D:792:HIS:HE1	1.08	0.96
1:A:340:ARG:HH12	1:A:344:GLN:HE21	1.13	0.95
3:K:110:GLN:HG2	3:K:535:ILE:HD13	1.47	0.94
2:G:79:GLN:HE21	2:G:79:GLN:H	1.15	0.94
1:D:192:LYS:HG2	1:D:224:GLN:HB2	1.50	0.94
2:J:1946:GLU:O	2:J:1950:LYS:HD3	1.67	0.94
1:E:340:ARG:NH1	1:E:344:GLN:HE21	1.65	0.93
1:E:340:ARG:HH12	1:E:344:GLN:NE2	1.67	0.92
1:F:340:ARG:NH1	1:F:344:GLN:HE21	1.66	0.92
1:A:792:HIS:HE1	1:F:792:HIS:HE1	1.07	0.92
3:I:1946:GLU:O	3:I:1950:LYS:HD3	1.68	0.91
1:D:1119:LYS:HE3	1:D:1341:PHE:CD1	2.03	0.91
1:C:1486:LEU:O	1:C:1490:THR:CG2	2.17	0.91
1:A:340:ARG:NH1	1:A:344:GLN:HE21	1.69	0.90
1:C:340:ARG:NH1	1:C:344:GLN:HE21	1.68	0.90
1:F:340:ARG:HH12	1:F:344:GLN:NE2	1.68	0.90
1:E:1486:LEU:O	1:E:1490:THR:CG2	2.19	0.89
1:D:340:ARG:NH1	1:D:344:GLN:HE21	1.69	0.89
1:C:1851:LEU:HD22	1:C:1851:LEU:H	1.35	0.89
1:B:1851:LEU:H	1:B:1851:LEU:HD23	1.35	0.89
3:L:404:GLN:HA	3:L:407:ILE:HD13	1.50	0.89
1:B:508:ASN:O	1:B:508:ASN:ND2	2.03	0.89
3:L:261:GLY:O	3:L:264:ARG:NH1	2.04	0.89
1:B:340:ARG:HH12	1:B:344:GLN:HE21	1.20	0.88
1:B:340:ARG:NH1	1:B:344:GLN:HE21	1.70	0.88
3:K:438:LEU:O	3:K:442:ASP:OD1	1.92	0.88
2:G:964:LEU:HD23	2:G:964:LEU:H	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ARG:HH12	1:C:344:GLN:HE21	0.88	0.88
1:C:340:ARG:HH12	1:C:344:GLN:NE2	1.71	0.87
3:I:964:LEU:HD23	3:I:964:LEU:H	1.40	0.87
3:K:2037:PRO:O	3:K:2041:ILE:HD12	1.75	0.86
3:L:1420:GLU:HG2	3:L:1421:ASN:ND2	1.88	0.86
3:L:1915:ASN:ND2	3:L:1964:PHE:H	1.74	0.86
2:G:856:LYS:NZ	2:G:1052:CYS:SG	2.49	0.86
1:D:340:ARG:HH12	1:D:344:GLN:HE21	1.19	0.85
1:B:1380:GLN:HE22	5:B:1906:EDO:H11	1.41	0.85
3:L:856:LYS:NZ	3:L:1052:CYS:SG	2.50	0.84
3:H:856:LYS:NZ	3:H:1052:CYS:SG	2.50	0.84
3:L:534:ASP:C	3:L:535:ILE:HD12	2.03	0.84
2:J:598:THR:HG22	2:J:622:GLY:HA3	1.59	0.84
2:J:856:LYS:NZ	2:J:1052:CYS:SG	2.49	0.84
3:K:598:THR:HG22	3:K:622:GLY:HA3	1.59	0.84
3:I:856:LYS:NZ	3:I:1052:CYS:SG	2.51	0.84
2:J:192:ALA:HB2	2:J:215:ILE:CD1	2.07	0.84
3:K:856:LYS:NZ	3:K:1052:CYS:SG	2.50	0.84
3:L:1922:ILE:HB	3:L:1927:LEU:HD11	1.58	0.84
3:I:597:MET:H	3:I:601:THR:CG2	1.90	0.83
3:I:598:THR:HG22	3:I:622:GLY:HA3	1.60	0.83
1:C:1471:LYS:HD3	1:C:1759:MET:CE	2.08	0.83
3:L:1421:ASN:N	3:L:1421:ASN:HD22	1.75	0.83
3:H:598:THR:HG22	3:H:622:GLY:HA3	1.62	0.82
2:J:871:THR:HG22	2:J:872:ILE:HG13	1.61	0.82
2:G:598:THR:HG22	2:G:622:GLY:HA3	1.62	0.82
3:L:451:ASN:HD22	3:L:453:LYS:CE	1.93	0.82
3:H:871:THR:HG22	3:H:872:ILE:HG13	1.61	0.82
3:L:598:THR:HG22	3:L:622:GLY:HA3	1.63	0.81
1:D:1303:GLY:HA2	1:D:1649:LYS:CD	2.11	0.81
1:E:724:LYS:HG2	1:E:725:TYR:CD2	2.16	0.81
3:I:597:MET:H	3:I:601:THR:HG23	1.44	0.81
3:L:1861:ARG:HB2	3:L:1965:ALA:CB	2.11	0.80
1:B:504:ASP:OD2	1:B:508:ASN:CG	2.24	0.80
1:A:738:ASN:HD22	7:A:1918:A2P:HN62	1.29	0.80
1:E:724:LYS:HG2	1:E:725:TYR:CE2	2.17	0.80
3:K:451:ASN:HD22	3:K:453:LYS:HE3	1.45	0.79
1:E:1279:PHE:HB2	1:E:1282:THR:HG23	1.65	0.79
3:L:1946:GLU:C	3:L:1950:LYS:HE3	2.07	0.79
1:B:1279:PHE:HB2	1:B:1282:THR:HG23	1.65	0.79
2:G:1858:ASN:ND2	2:G:1861:ARG:HG2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:376:ASN:HD22	2:J:376:ASN:C	1.91	0.79
3:I:376:ASN:C	3:I:376:ASN:HD22	1.91	0.79
1:C:1208:VAL:HG13	1:C:1212:THR:HB	1.65	0.78
3:H:376:ASN:C	3:H:376:ASN:HD22	1.91	0.78
3:K:195:LEU:O	3:K:199:ILE:HD12	1.83	0.78
3:K:297:ARG:O	3:K:301:THR:HG22	1.83	0.78
1:F:1208:VAL:HG13	1:F:1212:THR:HB	1.66	0.78
3:I:297:ARG:O	3:I:301:THR:HG22	1.84	0.78
1:B:1764:VAL:HG21	1:B:1769:VAL:HG13	1.63	0.78
1:F:1279:PHE:HB2	1:F:1282:THR:HG23	1.65	0.78
1:B:1208:VAL:HG13	1:B:1212:THR:HB	1.66	0.78
3:L:1942:GLU:O	3:L:1946:GLU:HG3	1.84	0.78
1:A:1208:VAL:HG13	1:A:1212:THR:HB	1.65	0.78
1:D:1279:PHE:HB2	1:D:1282:THR:HG23	1.66	0.78
1:C:935:GLU:HB3	1:C:938:GLU:HG2	1.66	0.78
1:D:1867:VAL:HG12	1:D:1884:SER:HB3	1.64	0.78
2:G:376:ASN:HD22	2:G:376:ASN:C	1.91	0.78
3:H:1916:PHE:CE2	3:H:1943:ILE:HD12	2.19	0.77
3:I:1170:ILE:HG12	3:I:1221:MET:CE	2.14	0.77
1:C:1426:LEU:HD22	1:F:1716:LEU:HD21	1.66	0.77
3:I:101:ILE:HD13	3:I:126:TYR:HB3	1.66	0.77
3:K:597:MET:HA	10:K:2101:FMN:N5	1.99	0.77
3:L:297:ARG:O	3:L:301:THR:HG22	1.84	0.77
1:A:1716:LEU:HD21	1:E:1426:LEU:HD22	1.66	0.77
3:L:871:THR:HG22	3:L:872:ILE:HG13	1.65	0.77
1:C:1716:LEU:HD21	1:F:1426:LEU:HD22	1.66	0.77
1:D:1208:VAL:HG13	1:D:1212:THR:HB	1.65	0.77
3:K:376:ASN:C	3:K:376:ASN:HD22	1.91	0.77
1:F:1303:GLY:HA2	1:F:1649:LYS:HE2	1.66	0.77
3:K:309:ARG:NH1	3:K:442:ASP:OD2	2.18	0.77
1:B:705:VAL:CG2	1:B:732:LEU:HD21	2.15	0.77
3:K:1170:ILE:HG12	3:K:1221:MET:CE	2.15	0.77
3:L:451:ASN:HD22	3:L:453:LYS:HE3	1.50	0.77
1:B:792:HIS:CE1	1:E:792:HIS:HE1	1.96	0.77
1:D:1466:GLU:HB3	1:D:1493:ILE:HD12	1.65	0.76
1:B:1303:GLY:HA2	1:B:1649:LYS:HE2	1.66	0.76
3:H:297:ARG:O	3:H:301:THR:HG22	1.85	0.76
1:B:1716:LEU:HD21	1:D:1426:LEU:HD22	1.67	0.76
2:J:53:GLU:O	2:J:118:LYS:HE2	1.86	0.76
3:K:871:THR:HG22	3:K:872:ILE:HG13	1.67	0.76
3:L:376:ASN:HD22	3:L:376:ASN:C	1.91	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1208:VAL:HG13	1:E:1212:THR:HB	1.65	0.76
1:C:1279:PHE:HB2	1:C:1282:THR:HG23	1.67	0.76
3:I:597:MET:HA	10:I:2101:FMN:N5	2.01	0.75
1:B:1380:GLN:HE22	5:B:1906:EDO:C1	1.98	0.75
3:H:455:ILE:HD11	3:H:469:ARG:HG2	1.68	0.75
2:G:297:ARG:O	2:G:301:THR:HG22	1.84	0.75
2:J:99:ASN:HD22	2:J:100:ASP:H	1.35	0.75
3:L:455:ILE:HD11	3:L:469:ARG:HG2	1.68	0.75
2:G:871:THR:HG22	2:G:872:ILE:HG13	1.69	0.75
3:I:455:ILE:HD11	3:I:469:ARG:HG2	1.68	0.75
1:A:1303:GLY:HA2	1:A:1649:LYS:HE2	1.66	0.75
2:G:455:ILE:HD11	2:G:469:ARG:HG2	1.67	0.75
1:A:1279:PHE:HB2	1:A:1282:THR:HG23	1.66	0.75
2:J:1314:ARG:NH2	3:L:315:PRO:O	2.19	0.75
3:L:99:ASN:HD22	3:L:100:ASP:H	1.34	0.75
1:A:1426:LEU:HD22	1:E:1716:LEU:HD21	1.67	0.75
2:J:297:ARG:O	2:J:301:THR:HG22	1.86	0.75
1:B:792:HIS:HE1	1:E:792:HIS:CE1	1.96	0.74
3:K:110:GLN:HG2	3:K:535:ILE:CD1	2.17	0.74
1:E:59:ARG:HG2	3:K:1896:GLN:HE22	1.51	0.74
1:F:705:VAL:CG2	1:F:732:LEU:HD21	2.16	0.74
1:B:774:ILE:HG22	7:B:1918:A2P:H2	1.69	0.74
1:C:1303:GLY:HA2	1:C:1649:LYS:HE2	1.67	0.74
2:J:1951:SER:HA	2:J:1954:LYS:HE2	1.70	0.74
1:B:1160:THR:CG2	1:C:244:THR:HG21	2.17	0.74
1:E:1303:GLY:HA2	1:E:1649:LYS:HE2	1.68	0.74
2:G:99:ASN:HD22	2:G:100:ASP:H	1.36	0.74
1:A:1276:GLN:O	1:A:1282:THR:HG21	1.87	0.74
1:D:705:VAL:CG2	1:D:732:LEU:HD21	2.18	0.74
1:E:1276:GLN:O	1:E:1282:THR:HG21	1.88	0.74
3:K:110:GLN:CG	3:K:535:ILE:HD13	2.17	0.74
1:B:451:MET:HE1	1:B:476:LEU:HG	1.69	0.73
1:C:792:HIS:HE1	1:D:792:HIS:CE1	2.00	0.73
1:C:1276:GLN:O	1:C:1282:THR:HG21	1.88	0.73
3:K:455:ILE:HD11	3:K:469:ARG:HG2	1.70	0.73
1:C:705:VAL:CG2	1:C:732:LEU:HD21	2.18	0.73
3:H:99:ASN:HD22	3:H:100:ASP:H	1.35	0.73
2:G:1054:LEU:HB2	10:G:2101:FMN:HM73	1.70	0.73
1:D:1276:GLN:O	1:D:1282:THR:HG21	1.87	0.73
3:K:451:ASN:ND2	3:K:453:LYS:HE3	2.02	0.73
1:D:1303:GLY:HA2	1:D:1649:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HH11	2:J:1896:GLN:HE22	1.37	0.73
1:A:792:HIS:CE1	1:F:792:HIS:HE1	2.00	0.73
1:A:705:VAL:CG2	1:A:732:LEU:HD21	2.19	0.72
1:B:529:MET:HE1	1:B:894:ARG:HG3	1.72	0.72
1:C:1865:THR:CB	1:C:1886:LYS:HG3	2.20	0.72
2:J:455:ILE:HD11	2:J:469:ARG:HG2	1.71	0.72
3:H:597:MET:HA	10:H:2101:FMN:N5	2.04	0.72
1:E:705:VAL:CG2	1:E:732:LEU:HD21	2.19	0.72
3:H:79:GLN:HE21	3:H:79:GLN:H	1.35	0.72
1:C:1785:THR:O	1:C:1789:ARG:HG2	1.90	0.72
1:F:1276:GLN:O	1:F:1282:THR:HG21	1.88	0.72
2:G:1217:ASN:C	2:G:1218:ILE:HD12	2.15	0.72
3:K:730:LEU:HD12	3:K:730:LEU:C	2.15	0.72
1:B:1276:GLN:O	1:B:1282:THR:HG21	1.88	0.72
1:C:789:GLU:OE1	1:D:801:ARG:NH2	2.23	0.72
1:C:792:HIS:CE1	1:D:792:HIS:HE1	2.01	0.71
3:L:264:ARG:HE	3:L:456:GLN:HB2	1.52	0.71
3:L:1420:GLU:HG2	3:L:1421:ASN:HD22	1.53	0.71
1:B:1279:PHE:HB2	1:B:1282:THR:CG2	2.21	0.71
2:G:730:LEU:C	2:G:730:LEU:HD12	2.15	0.71
2:J:1881:ARG:C	2:J:1881:ARG:HD3	2.15	0.71
3:K:110:GLN:CG	3:K:535:ILE:CD1	2.67	0.71
3:L:730:LEU:C	3:L:730:LEU:HD12	2.15	0.71
1:E:1279:PHE:HB2	1:E:1282:THR:CG2	2.20	0.71
3:I:730:LEU:C	3:I:730:LEU:HD12	2.15	0.71
3:I:1778:GLN:HB3	3:I:1831:VAL:HG13	1.73	0.71
1:A:792:HIS:HE1	1:F:792:HIS:CE1	2.00	0.71
1:E:451:MET:HE1	1:E:476:LEU:HG	1.72	0.71
2:J:1838:MET:HE3	2:J:1976:PHE:CD1	2.25	0.71
3:L:1778:GLN:HB3	3:L:1831:VAL:HG13	1.73	0.71
1:A:1760:THR:HG23	1:A:1760:THR:O	1.89	0.71
7:C:1917:A2P:H1'	7:C:1917:A2P:O6P	1.91	0.71
3:H:1923:ASP:O	3:H:1927:LEU:HD22	1.91	0.71
2:J:597:MET:HA	10:J:2101:FMN:N5	2.05	0.71
3:L:597:MET:HA	10:L:2101:FMN:N5	2.05	0.71
1:A:1039:MET:O	1:A:1609:ARG:NH2	2.24	0.71
1:E:340:ARG:HH12	1:E:344:GLN:HE21	0.83	0.71
3:H:1170:ILE:HA	3:H:1221:MET:HE1	1.72	0.71
1:E:1039:MET:O	1:E:1609:ARG:NH2	2.24	0.71
1:F:1039:MET:O	1:F:1609:ARG:NH2	2.24	0.70
2:J:730:LEU:C	2:J:730:LEU:HD12	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:MET:O	1:B:1609:ARG:NH2	2.24	0.70
1:C:1279:PHE:HB2	1:C:1282:THR:CG2	2.21	0.70
1:F:451:MET:HE1	1:F:476:LEU:HG	1.74	0.70
3:I:1878:VAL:O	3:I:1882:THR:HG22	1.91	0.70
3:H:730:LEU:C	3:H:730:LEU:HD12	2.16	0.70
3:K:1904:LEU:HD22	3:K:1960:LEU:CD2	2.15	0.70
1:A:454:HIS:O	1:A:458:THR:HG22	1.91	0.70
1:B:1426:LEU:HD22	1:D:1716:LEU:HD21	1.73	0.70
2:G:1778:GLN:HB3	2:G:1831:VAL:HG13	1.72	0.70
3:I:1217:ASN:O	3:I:1218:ILE:HD12	1.91	0.70
1:A:1279:PHE:HB2	1:A:1282:THR:CG2	2.21	0.70
1:F:340:ARG:HH12	1:F:344:GLN:HE21	0.83	0.70
1:F:529:MET:HE1	1:F:894:ARG:HG2	1.72	0.70
3:H:1778:GLN:HB3	3:H:1831:VAL:HG13	1.73	0.70
3:K:1422:THR:HG22	3:K:1474:PHE:CD1	2.27	0.70
1:E:454:HIS:O	1:E:458:THR:HG22	1.92	0.70
2:G:597:MET:HA	10:G:2101:FMN:N5	2.07	0.70
2:J:1778:GLN:HB3	2:J:1831:VAL:HG13	1.73	0.70
3:K:1778:GLN:HB3	3:K:1831:VAL:HG13	1.72	0.70
1:D:1279:PHE:HB2	1:D:1282:THR:CG2	2.21	0.70
1:E:1167:LEU:HD12	1:E:1171:ALA:CB	2.21	0.70
1:D:454:HIS:O	1:D:458:THR:HG22	1.92	0.70
3:I:1217:ASN:C	3:I:1218:ILE:HD12	2.16	0.70
3:I:1422:THR:HG22	3:I:1474:PHE:CD1	2.26	0.69
1:A:1657:HIS:CD2	1:A:1658:PRO:HD2	2.27	0.69
3:K:315:PRO:O	3:L:1314:ARG:NH2	2.26	0.69
1:D:1039:MET:O	1:D:1609:ARG:NH2	2.24	0.69
3:L:1422:THR:HG22	3:L:1474:PHE:CD1	2.26	0.69
1:D:1119:LYS:HE3	1:D:1341:PHE:CG	2.27	0.69
3:H:315:PRO:O	3:I:1314:ARG:NH2	2.25	0.69
3:I:101:ILE:HD13	3:I:126:TYR:CB	2.22	0.69
1:A:1844:LYS:HG3	1:A:1844:LYS:O	1.92	0.69
1:C:1039:MET:O	1:C:1609:ARG:NH2	2.24	0.69
3:H:1838:MET:HE3	3:H:1976:PHE:CD1	2.26	0.69
3:L:1170:ILE:HA	3:L:1221:MET:HE1	1.74	0.69
1:A:451:MET:HE1	1:A:476:LEU:HG	1.73	0.69
1:C:454:HIS:O	1:C:458:THR:HG22	1.92	0.69
1:E:1304:ALA:O	1:E:1307:THR:CG2	2.41	0.69
1:F:1279:PHE:HB2	1:F:1282:THR:CG2	2.21	0.69
3:H:1422:THR:HG22	3:H:1474:PHE:CD1	2.27	0.69
1:C:451:MET:HE1	1:C:476:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:GLU:OE1	1:C:894:ARG:NH1	2.25	0.69
1:C:1304:ALA:O	1:C:1307:THR:CG2	2.41	0.69
1:D:528:GLU:OE1	1:D:894:ARG:NH1	2.26	0.69
1:D:1304:ALA:O	1:D:1307:THR:CG2	2.41	0.69
1:D:1466:GLU:HB3	1:D:1493:ILE:CD1	2.23	0.69
1:F:13:LEU:O	1:F:17:LEU:HD12	1.92	0.69
2:G:1868:GLN:HG3	2:G:1872:GLN:NE2	2.08	0.69
3:K:99:ASN:HD22	3:K:100:ASP:H	1.39	0.69
3:K:1838:MET:HE3	3:K:1976:PHE:CD1	2.28	0.69
3:L:1054:LEU:HB2	10:L:2101:FMN:HM73	1.74	0.69
1:A:244:THR:HG21	1:C:1160:THR:CG2	2.23	0.69
1:B:454:HIS:O	1:B:458:THR:HG22	1.92	0.69
1:A:1304:ALA:O	1:A:1307:THR:CG2	2.41	0.69
1:D:1829:GLY:HA2	1:D:1832:ALA:HB3	1.74	0.69
1:E:982:ILE:HD12	3:K:965:SER:HA	1.74	0.69
2:G:1422:THR:HG22	2:G:1474:PHE:CD1	2.28	0.69
1:F:982:ILE:HD12	3:L:965:SER:HA	1.75	0.68
1:F:1304:ALA:O	1:F:1307:THR:CG2	2.42	0.68
3:L:534:ASP:O	3:L:535:ILE:HD12	1.92	0.68
3:L:1265:MET:O	3:L:1269:LEU:HD12	1.92	0.68
1:B:1304:ALA:O	1:B:1307:THR:CG2	2.41	0.68
3:K:1337:ALA:HB1	3:K:1378:ILE:HG13	1.74	0.68
1:B:793:ARG:HD2	1:E:789:GLU:OE2	1.93	0.68
2:G:1170:ILE:HA	2:G:1221:MET:HE1	1.73	0.68
2:J:736:ARG:NH1	2:J:769:SER:O	2.25	0.68
2:J:1054:LEU:HB2	10:J:2101:FMN:HM73	1.74	0.68
2:J:1422:THR:HG22	2:J:1474:PHE:CD1	2.28	0.68
1:D:1367:ARG:O	1:D:1370:THR:OG1	2.12	0.68
2:J:1170:ILE:HA	2:J:1221:MET:HE1	1.74	0.68
3:L:1838:MET:HE3	3:L:1976:PHE:CD1	2.28	0.68
1:F:1303:GLY:HA2	1:F:1649:LYS:CE	2.24	0.68
3:I:1838:MET:HE3	3:I:1976:PHE:CD1	2.28	0.68
3:K:154:ALA:HA	3:K:499:THR:CG2	2.20	0.68
3:K:155:GLN:H	3:K:499:THR:CG2	2.06	0.68
1:A:340:ARG:HH12	1:A:344:GLN:NE2	1.89	0.68
1:E:528:GLU:OE1	1:E:894:ARG:NH1	2.26	0.67
1:F:1854:ASN:O	1:F:1857:LYS:HG2	1.93	0.67
1:B:1500:GLN:HG2	1:D:1507:GLN:HE22	1.58	0.67
1:C:491:LYS:HE3	8:C:1903:ACT:H2	1.75	0.67
2:J:163:GLN:HG2	2:J:423:VAL:HG12	1.76	0.67
1:F:1826:LYS:O	1:F:1827:SER:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:GLN:HE22	1:E:1500:GLN:HG2	1.59	0.67
1:F:1794:GLN:HG2	1:F:1838:GLU:OE2	1.94	0.67
3:L:163:GLN:HG2	3:L:423:VAL:HG13	1.77	0.67
1:F:454:HIS:O	1:F:458:THR:HG22	1.93	0.67
3:H:565:TYR:HB2	3:H:795:PRO:HG2	1.75	0.67
3:L:1923:ASP:O	3:L:1927:LEU:HG	1.93	0.67
1:A:789:GLU:OE1	1:F:801:ARG:NH2	2.28	0.67
1:B:682:GLY:HA2	7:B:1918:A2P:H1'	1.76	0.67
2:G:7:ARG:NH1	3:I:28:PHE:O	2.28	0.67
3:I:1838:MET:HE3	3:I:1976:PHE:CE1	2.30	0.67
3:H:1933:LEU:O	3:H:1934:GLU:HG3	1.95	0.66
1:A:528:GLU:OE1	1:A:894:ARG:NH1	2.27	0.66
1:C:793:ARG:HA	1:C:797:THR:HG23	1.78	0.66
1:D:451:MET:HE1	1:D:476:LEU:HG	1.74	0.66
2:G:1149:TRP:CD1	2:G:1213:LEU:CD2	2.78	0.66
1:B:1303:GLY:HA2	1:B:1649:LYS:CE	2.25	0.66
1:D:1303:GLY:HA2	1:D:1649:LYS:HD2	1.77	0.66
1:E:13:LEU:O	1:E:17:LEU:HD12	1.96	0.66
3:I:1635:ARG:NH1	3:I:1656:GLU:OE1	2.28	0.66
1:A:1303:GLY:HA2	1:A:1649:LYS:CE	2.25	0.66
3:H:1916:PHE:CE2	3:H:1943:ILE:CD1	2.78	0.66
3:L:1861:ARG:CB	3:L:1965:ALA:HB2	2.26	0.66
1:C:702:LYS:HE3	1:C:731:THR:HG23	1.78	0.66
2:J:214:ASN:OD1	2:J:217:GLU:HB2	1.95	0.66
1:B:1302:VAL:CG2	1:D:1302:VAL:CG2	2.74	0.66
3:L:843:ILE:HD11	3:L:1055:HIS:HB3	1.78	0.66
1:C:1303:GLY:HA2	1:C:1649:LYS:CE	2.25	0.66
1:E:1303:GLY:HA2	1:E:1649:LYS:CE	2.25	0.66
3:H:1635:ARG:NH1	3:H:1656:GLU:OE1	2.29	0.66
2:J:1149:TRP:CD1	2:J:1213:LEU:CD2	2.79	0.66
2:J:693:GLU:O	2:J:697:THR:OG1	2.14	0.66
3:L:1929:LYS:CE	3:L:1933:LEU:HD12	2.25	0.66
2:J:1933:LEU:O	2:J:1934:GLU:HG3	1.96	0.66
2:G:565:TYR:HB2	2:G:795:PRO:HG2	1.77	0.66
3:I:565:TYR:HB2	3:I:795:PRO:HG2	1.77	0.66
1:C:1785:THR:O	1:C:1789:ARG:CG	2.44	0.65
1:E:36:LEU:O	1:E:76:ARG:NH2	2.29	0.65
3:I:106:ALA:HB2	3:I:545:GLN:HG2	1.78	0.65
1:D:13:LEU:O	1:D:17:LEU:HD12	1.95	0.65
2:G:2050:GLN:HG2	2:G:2050:GLN:O	1.95	0.65
3:H:1149:TRP:CD1	3:H:1213:LEU:CD2	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1265:MET:HE1	3:I:1569:PHE:CZ	2.31	0.65
3:K:1149:TRP:CD1	3:K:1213:LEU:CD2	2.79	0.65
3:K:1265:MET:HE1	3:K:1569:PHE:CZ	2.31	0.65
3:L:1635:ARG:NH1	3:L:1656:GLU:OE1	2.29	0.65
1:B:793:ARG:HA	1:B:797:THR:HG23	1.78	0.65
1:B:1380:GLN:NE2	5:B:1906:EDO:H11	2.12	0.65
1:F:411:GLN:HE22	1:F:1628:SER:H	1.44	0.65
2:J:1635:ARG:NH1	2:J:1656:GLU:OE1	2.28	0.65
1:D:36:LEU:O	1:D:76:ARG:NH2	2.30	0.65
2:J:565:TYR:HB2	2:J:795:PRO:HG2	1.77	0.65
3:L:1933:LEU:O	3:L:1934:GLU:HG3	1.96	0.65
3:L:565:TYR:HB2	3:L:795:PRO:HG2	1.78	0.65
1:A:1657:HIS:HD2	1:A:1659:ASP:H	1.45	0.65
2:G:1635:ARG:NH1	2:G:1656:GLU:OE1	2.29	0.65
3:I:1149:TRP:CD1	3:I:1213:LEU:CD2	2.79	0.65
3:L:1149:TRP:CD1	3:L:1213:LEU:CD2	2.79	0.65
1:C:36:LEU:O	1:C:76:ARG:NH2	2.30	0.65
1:C:1455:ARG:HD3	1:F:1455:ARG:NH2	2.12	0.65
1:A:738:ASN:ND2	7:A:1918:A2P:HN62	1.94	0.65
1:B:1030:TRP:NE1	1:B:1580:LEU:HD22	2.12	0.65
3:K:468:LEU:O	3:K:475:ILE:CD1	2.45	0.65
1:A:5:VAL:O	1:A:9:LEU:HD12	1.97	0.65
1:B:36:LEU:O	1:B:76:ARG:NH2	2.30	0.65
3:I:163:GLN:HG2	3:I:423:VAL:HG12	1.78	0.65
3:I:1170:ILE:HG12	3:I:1221:MET:HE2	1.77	0.65
3:K:565:TYR:HB2	3:K:795:PRO:HG2	1.78	0.65
3:K:1933:LEU:O	3:K:1934:GLU:HG3	1.97	0.65
2:G:163:GLN:HG2	2:G:423:VAL:HG12	1.79	0.64
3:L:1861:ARG:HB2	3:L:1965:ALA:HB3	1.79	0.64
1:A:1851:LEU:H	1:A:1851:LEU:HD22	1.61	0.64
3:I:1215:LYS:HE3	3:I:1218:ILE:HD13	1.79	0.64
2:J:964:LEU:H	2:J:964:LEU:HD22	1.63	0.64
1:B:774:ILE:CG2	7:B:1918:A2P:H2	2.27	0.64
1:E:1851:LEU:HD22	1:E:1851:LEU:H	1.62	0.64
1:F:655:LEU:HD22	1:F:916:LEU:HD11	1.79	0.64
2:J:598:THR:OG1	2:J:599:PRO:CD	2.45	0.64
3:K:108:LEU:HA	3:K:112:ASN:HD22	1.61	0.64
3:K:1635:ARG:NH1	3:K:1656:GLU:OE1	2.29	0.64
1:B:1304:ALA:O	1:B:1307:THR:HG22	1.98	0.64
1:E:1030:TRP:NE1	1:E:1580:LEU:HD22	2.12	0.64
2:G:693:GLU:O	2:G:697:THR:OG1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1838:MET:HE3	3:H:1976:PHE:CE1	2.32	0.64
3:I:1054:LEU:HB2	10:I:2101:FMN:HM73	1.78	0.64
2:J:1838:MET:HE3	2:J:1976:PHE:CE1	2.31	0.64
2:J:1886:VAL:HG23	2:J:1906:ALA:HB3	1.79	0.64
2:J:1904:LEU:HD23	2:J:1958:LEU:O	1.98	0.64
1:E:1304:ALA:O	1:E:1307:THR:HG22	1.98	0.64
3:K:693:GLU:O	3:K:697:THR:OG1	2.16	0.64
1:A:1304:ALA:O	1:A:1307:THR:HG22	1.98	0.64
1:B:411:GLN:HE22	1:B:1628:SER:H	1.44	0.64
2:J:1265:MET:HE1	2:J:1569:PHE:CZ	2.32	0.64
1:C:1477:ILE:HD12	1:C:1485:PHE:CG	2.33	0.64
1:D:1014:ASP:H	1:D:1510:ASN:HD21	1.46	0.64
1:F:1030:TRP:NE1	1:F:1580:LEU:HD22	2.12	0.64
1:F:1310:GLU:OE1	1:F:1649:LYS:HE3	1.98	0.64
2:J:102:HIS:HE1	2:J:180:TYR:OH	1.80	0.64
3:L:843:ILE:HD12	3:L:1055:HIS:O	1.98	0.64
1:C:1030:TRP:NE1	1:C:1580:LEU:HD22	2.12	0.64
3:H:102:HIS:HE1	3:H:180:TYR:OH	1.80	0.64
3:I:102:HIS:HE1	3:I:180:TYR:OH	1.80	0.64
1:A:411:GLN:HE22	1:A:1628:SER:H	1.44	0.64
1:A:1030:TRP:NE1	1:A:1580:LEU:HD22	2.12	0.64
1:B:1014:ASP:H	1:B:1510:ASN:HD21	1.46	0.64
3:K:102:HIS:HE1	3:K:180:TYR:OH	1.80	0.64
3:L:407:ILE:HD12	3:L:407:ILE:N	2.13	0.64
3:L:1838:MET:HE3	3:L:1976:PHE:CE1	2.33	0.64
1:D:411:GLN:HE22	1:D:1628:SER:H	1.45	0.63
2:G:598:THR:OG1	2:G:599:PRO:CD	2.46	0.63
3:L:102:HIS:HE1	3:L:180:TYR:OH	1.81	0.63
1:D:655:LEU:HD22	1:D:916:LEU:HD11	1.79	0.63
3:H:598:THR:OG1	3:H:599:PRO:CD	2.45	0.63
1:D:793:ARG:HA	1:D:797:THR:HG23	1.80	0.63
1:F:1014:ASP:H	1:F:1510:ASN:HD21	1.46	0.63
3:K:163:GLN:HG2	3:K:423:VAL:HG12	1.80	0.63
2:G:102:HIS:HE1	2:G:180:TYR:OH	1.81	0.63
3:I:693:GLU:O	3:I:697:THR:OG1	2.15	0.63
3:K:1054:LEU:HB2	10:K:2101:FMN:HM73	1.80	0.63
1:A:655:LEU:HD22	1:A:916:LEU:HD11	1.81	0.63
1:D:1030:TRP:NE1	1:D:1580:LEU:HD22	2.13	0.63
3:H:1265:MET:HE1	3:H:1569:PHE:CZ	2.34	0.63
3:I:598:THR:OG1	3:I:599:PRO:CD	2.46	0.63
3:K:28:PHE:O	3:L:7:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:598:THR:OG1	3:K:599:PRO:CD	2.46	0.63
1:D:1232:TYR:CZ	1:D:1701:LYS:HD2	2.34	0.63
3:K:1177:SER:N	3:K:1180:MET:HE3	2.13	0.63
3:L:1736:MET:HG2	3:L:1751:ILE:HG13	1.79	0.63
1:A:1310:GLU:OE1	1:A:1649:LYS:HE3	1.98	0.63
1:C:411:GLN:HE22	1:C:1628:SER:H	1.46	0.63
1:F:1232:TYR:CZ	1:F:1701:LYS:HD2	2.34	0.63
2:G:1265:MET:HE1	2:G:1569:PHE:CZ	2.33	0.63
3:I:597:MET:N	3:I:601:THR:CG2	2.62	0.63
3:I:1170:ILE:CG1	3:I:1221:MET:CE	2.77	0.63
3:L:693:GLU:O	3:L:697:THR:OG1	2.16	0.63
3:L:1851:ASN:ND2	3:L:1956:ARG:HH21	1.96	0.63
1:B:789:GLU:OE2	1:E:793:ARG:HD2	1.99	0.63
3:H:163:GLN:HG2	3:H:423:VAL:HG12	1.81	0.63
1:F:36:LEU:O	1:F:76:ARG:NH2	2.32	0.63
3:L:1861:ARG:CB	3:L:1965:ALA:CB	2.77	0.63
1:B:1310:GLU:OE1	1:B:1649:LYS:HE3	1.99	0.62
1:D:1304:ALA:O	1:D:1307:THR:HG22	1.99	0.62
3:K:106:ALA:HB2	3:K:545:GLN:HG2	1.79	0.62
3:K:1838:MET:HE3	3:K:1976:PHE:CE1	2.33	0.62
1:E:1232:TYR:CZ	1:E:1701:LYS:HD2	2.34	0.62
3:L:598:THR:OG1	3:L:599:PRO:CD	2.47	0.62
1:C:1014:ASP:H	1:C:1510:ASN:HD21	1.46	0.62
1:C:1304:ALA:O	1:C:1307:THR:HG22	1.98	0.62
3:H:693:GLU:O	3:H:697:THR:OG1	2.16	0.62
3:K:1904:LEU:CD1	3:K:1958:LEU:O	2.47	0.62
1:E:655:LEU:HD22	1:E:916:LEU:HD11	1.82	0.62
2:J:1624:THR:HB	2:J:1642:THR:OG1	1.99	0.62
1:A:1500:GLN:CG	1:E:1507:GLN:HE22	2.11	0.62
1:A:1757:GLU:O	1:A:1760:THR:HG22	1.98	0.62
3:L:441:LYS:O	3:L:444:VAL:HG12	1.99	0.62
1:E:1014:ASP:H	1:E:1510:ASN:HD21	1.45	0.62
1:F:1304:ALA:O	1:F:1307:THR:HG22	1.99	0.62
1:A:1245:ASN:C	1:A:1245:ASN:HD22	2.07	0.62
3:K:1170:ILE:HG12	3:K:1221:MET:HE2	1.80	0.62
1:B:1232:TYR:CZ	1:B:1701:LYS:HD2	2.34	0.62
3:L:109:LEU:HD21	3:L:116:LEU:HD22	1.81	0.62
1:E:1310:GLU:OE1	1:E:1649:LYS:HE3	2.00	0.62
3:I:1932:SER:HB3	3:I:1935:GLU:OE1	2.00	0.62
3:K:1904:LEU:CD2	3:K:1960:LEU:HD23	2.21	0.62
1:A:599:MET:N	1:A:624:LYS:HE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:MET:HE1	1:B:926:LEU:HB3	1.82	0.62
1:E:738:ASN:HD22	7:E:1917:A2P:HN62	1.48	0.62
3:L:106:ALA:HB2	3:L:545:GLN:HG2	1.82	0.62
1:B:513:GLU:OE2	1:B:873:ARG:NH1	2.32	0.61
1:C:1310:GLU:OE1	1:C:1649:LYS:HE3	1.99	0.61
1:C:1500:GLN:HA	1:F:1507:GLN:HE22	1.65	0.61
1:E:411:GLN:HE22	1:E:1628:SER:H	1.46	0.61
3:I:1927:LEU:HA	3:I:1931:LEU:HB2	1.83	0.61
3:L:451:ASN:HD22	3:L:453:LYS:HE2	1.64	0.61
1:A:1160:THR:HB	1:B:244:THR:HG21	1.81	0.61
1:D:901:MET:HE1	1:D:926:LEU:HB3	1.81	0.61
2:G:79:GLN:H	2:G:79:GLN:NE2	1.94	0.61
1:A:1232:TYR:CZ	1:A:1701:LYS:HD2	2.35	0.61
1:C:1302:VAL:CG2	1:F:1302:VAL:CG2	2.79	0.61
3:K:110:GLN:HG3	3:K:535:ILE:CD1	2.31	0.61
1:E:1863:GLY:O	1:E:1886:LYS:C	2.43	0.61
2:J:877:LYS:H	2:J:877:LYS:HE2	1.65	0.61
3:K:1161:GLN:O	3:K:1164:MET:HG2	2.00	0.61
1:A:1500:GLN:HG2	1:E:1507:GLN:HE22	1.65	0.61
1:C:455:ILE:O	1:C:458:THR:HG23	2.01	0.61
2:G:1624:THR:HB	2:G:1642:THR:OG1	2.00	0.61
3:L:1915:ASN:HD21	3:L:1964:PHE:H	1.47	0.61
1:A:1160:THR:CG2	1:B:244:THR:HG21	2.30	0.61
1:A:1507:GLN:HE22	1:E:1500:GLN:CG	2.13	0.61
1:E:702:LYS:HE3	1:E:731:THR:HG23	1.81	0.61
3:I:599:PRO:O	3:I:602:VAL:HG12	2.01	0.61
1:F:11:HIS:ND1	3:L:1998:LYS:HA	2.15	0.61
2:G:598:THR:O	2:G:599:PRO:C	2.43	0.61
3:K:1177:SER:OG	3:K:1180:MET:CE	2.49	0.61
3:K:1963:GLY:O	3:K:1965:ALA:N	2.34	0.61
1:D:1849:VAL:HB	1:D:1867:VAL:HG23	1.83	0.61
1:F:455:ILE:O	1:F:458:THR:HG23	2.00	0.61
3:H:1624:THR:HB	3:H:1642:THR:OG1	2.00	0.61
3:I:1624:THR:HB	3:I:1642:THR:OG1	2.01	0.61
3:K:1170:ILE:CG1	3:K:1221:MET:CE	2.79	0.61
3:K:1177:SER:OG	3:K:1180:MET:HE3	2.01	0.61
3:H:1923:ASP:O	3:H:1927:LEU:CD2	2.49	0.60
3:I:601:THR:O	3:I:601:THR:OG1	2.16	0.60
3:K:1170:ILE:HA	3:K:1221:MET:HE1	1.83	0.60
3:K:1624:THR:HB	3:K:1642:THR:OG1	2.01	0.60
1:A:1014:ASP:H	1:A:1510:ASN:HD21	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HE3	1:C:248:LYS:HA	1.82	0.60
2:J:1054:LEU:HB2	10:J:2101:FMN:C7M	2.30	0.60
3:K:599:PRO:O	3:K:602:VAL:HG12	2.01	0.60
1:A:455:ILE:O	1:A:458:THR:HG23	2.01	0.60
1:F:479:ASN:O	1:F:483:VAL:HG22	2.00	0.60
1:B:455:ILE:O	1:B:458:THR:HG23	2.02	0.60
1:E:982:ILE:HD13	3:K:955:GLU:CB	2.30	0.60
3:I:1962:ARG:CZ	3:I:1962:ARG:HB3	2.30	0.60
3:L:1476:ASN:HD21	3:L:1479:ILE:HD13	1.65	0.60
3:K:161:GLY:H	3:K:505:GLY:HA3	1.66	0.60
3:L:1054:LEU:HB2	10:L:2101:FMN:C7M	2.32	0.60
1:D:69:ASP:OD1	1:D:76:ARG:NH1	2.35	0.60
2:G:1854:MET:HE2	2:G:1901:ALA:HB2	1.82	0.60
3:I:1904:LEU:HD23	3:I:1958:LEU:O	2.01	0.60
2:J:1946:GLU:O	2:J:1950:LYS:CD	2.47	0.60
1:A:793:ARG:HD2	1:F:789:GLU:OE2	2.02	0.60
1:C:11:HIS:ND1	3:I:1998:LYS:HA	2.17	0.60
1:F:705:VAL:HG23	1:F:732:LEU:HD21	1.83	0.60
3:L:599:PRO:O	3:L:602:VAL:HG12	2.02	0.60
1:B:479:ASN:O	1:B:483:VAL:HG22	2.01	0.60
1:C:1232:TYR:CZ	1:C:1701:LYS:HD2	2.37	0.60
1:D:455:ILE:O	1:D:458:THR:HG23	2.01	0.60
1:F:1857:LYS:HG3	1:F:1858:ALA:N	2.17	0.60
2:G:1868:GLN:O	2:G:1869:GLU:HG2	2.01	0.60
3:I:1854:MET:HB3	3:I:1901:ALA:HB2	1.84	0.60
1:C:801:ARG:NH2	1:D:789:GLU:OE1	2.35	0.60
1:E:513:GLU:OE2	1:E:873:ARG:NH1	2.32	0.60
3:I:1170:ILE:HA	3:I:1221:MET:HE1	1.82	0.60
2:J:1962:ARG:HB3	2:J:1962:ARG:CZ	2.32	0.60
3:K:2015:THR:HG23	3:K:2028:ASP:OD2	2.02	0.60
3:K:2015:THR:O	3:K:2017:LYS:N	2.35	0.60
3:L:1854:MET:HB3	3:L:1901:ALA:HB2	1.84	0.60
3:L:1904:LEU:HD23	3:L:1958:LEU:O	2.02	0.60
1:B:69:ASP:OD1	1:B:76:ARG:NH1	2.35	0.60
1:C:655:LEU:HD22	1:C:916:LEU:HD11	1.84	0.60
1:C:789:GLU:OE2	1:D:793:ARG:HD2	2.01	0.60
1:C:901:MET:HE1	1:C:926:LEU:HB3	1.84	0.60
1:D:996:LYS:HD3	1:D:1000:GLN:NE2	2.17	0.60
1:E:901:MET:HE1	1:E:926:LEU:HB3	1.84	0.60
2:G:142:ASN:HB3	2:G:550:VAL:HG13	1.83	0.60
3:K:1343:VAL:HG22	3:K:1343:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1265:MET:HE1	3:L:1569:PHE:CZ	2.36	0.60
3:L:1343:VAL:O	3:L:1343:VAL:HG22	2.02	0.60
3:L:1624:THR:HB	3:L:1642:THR:OG1	2.01	0.59
1:B:655:LEU:HD22	1:B:916:LEU:HD11	1.84	0.59
2:J:142:ASN:HB3	2:J:550:VAL:HG13	1.83	0.59
2:G:1933:LEU:O	2:G:1934:GLU:HG3	2.03	0.59
3:K:1476:ASN:HD21	3:K:1479:ILE:HD13	1.66	0.59
3:L:1854:MET:HE2	3:L:1901:ALA:HB2	1.84	0.59
1:B:705:VAL:HG23	1:B:732:LEU:HD21	1.82	0.59
1:B:1859:ALA:O	1:B:1864:VAL:HG22	2.02	0.59
1:C:491:LYS:HE3	8:C:1903:ACT:CH3	2.31	0.59
1:F:1851:LEU:H	1:F:1851:LEU:CD2	2.14	0.59
2:G:161:GLY:H	2:G:505:GLY:HA3	1.67	0.59
3:H:1345:GLY:HA3	3:H:1412:TYR:CD1	2.38	0.59
3:H:1854:MET:HB3	3:H:1901:ALA:HB2	1.84	0.59
1:B:822:VAL:HG12	1:B:824:LEU:HD13	1.83	0.59
2:G:1343:VAL:O	2:G:1343:VAL:HG22	2.03	0.59
2:J:1854:MET:HE2	2:J:1901:ALA:HB2	1.84	0.59
3:L:807:ILE:HD11	3:L:822:ALA:HB2	1.84	0.59
1:C:822:VAL:HG12	1:C:824:LEU:HD13	1.85	0.59
1:C:901:MET:HE1	1:C:926:LEU:CB	2.33	0.59
1:E:69:ASP:OD1	1:E:76:ARG:NH1	2.35	0.59
1:F:1470:LEU:HD13	1:F:1489:ARG:HG2	1.83	0.59
3:I:1922:ILE:HB	3:I:1927:LEU:CD2	2.26	0.59
3:I:1933:LEU:O	3:I:1934:GLU:HG3	2.03	0.59
1:B:150:LEU:HD11	1:B:225:SER:OG	2.03	0.59
1:B:901:MET:HE1	1:B:926:LEU:CB	2.33	0.59
1:E:901:MET:HE1	1:E:926:LEU:CB	2.33	0.59
1:F:822:VAL:HG12	1:F:824:LEU:HD13	1.83	0.59
3:I:1824:ILE:HD13	3:I:1824:ILE:N	2.18	0.59
2:J:599:PRO:O	2:J:602:VAL:HG12	2.01	0.59
3:K:1854:MET:HE2	3:K:1901:ALA:HB2	1.84	0.59
1:A:5:VAL:HG12	1:A:9:LEU:CD1	2.33	0.59
2:G:1963:GLY:O	2:G:1965:ALA:N	2.34	0.59
3:H:2015:THR:O	3:H:2017:LYS:N	2.35	0.59
3:I:1963:GLY:O	3:I:1965:ALA:N	2.34	0.59
2:J:1963:GLY:O	2:J:1965:ALA:N	2.34	0.59
3:K:1854:MET:HB3	3:K:1901:ALA:HB2	1.84	0.59
1:A:996:LYS:HD3	1:A:1000:GLN:NE2	2.17	0.59
3:H:599:PRO:O	3:H:602:VAL:HG12	2.01	0.59
3:I:1343:VAL:HG22	3:I:1343:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:161:GLY:H	2:J:505:GLY:HA3	1.67	0.59
1:A:1470:LEU:HD13	1:A:1489:ARG:HG2	1.85	0.59
1:F:901:MET:HE1	1:F:926:LEU:CB	2.32	0.59
1:F:1863:GLY:O	1:F:1886:LYS:C	2.45	0.59
3:H:161:GLY:H	3:H:505:GLY:HA3	1.68	0.59
1:C:1515:ARG:NH2	1:F:1016:GLU:OE1	2.36	0.58
3:L:1963:GLY:O	3:L:1965:ALA:N	2.35	0.58
1:B:1448:ARG:HD2	1:B:1508:TRP:O	2.03	0.58
1:E:455:ILE:O	1:E:458:THR:HG23	2.02	0.58
2:G:612:ASN:HD21	2:G:641:ILE:HA	1.68	0.58
3:I:161:GLY:H	3:I:505:GLY:HA3	1.68	0.58
2:J:214:ASN:OD1	2:J:217:GLU:CB	2.51	0.58
1:A:67:SER:HB3	3:I:355:LYS:HE3	1.85	0.58
1:B:1160:THR:HB	1:C:244:THR:HG21	1.85	0.58
1:D:513:GLU:OE2	1:D:873:ARG:NH1	2.32	0.58
1:F:901:MET:HE1	1:F:926:LEU:HB3	1.83	0.58
2:G:1868:GLN:HG3	2:G:1872:GLN:HE21	1.66	0.58
3:H:1963:GLY:O	3:H:1965:ALA:N	2.34	0.58
3:I:236:ILE:HD12	3:I:240:LEU:HD22	1.85	0.58
3:I:1854:MET:HE2	3:I:1901:ALA:HB2	1.85	0.58
2:J:2015:THR:O	2:J:2017:LYS:N	2.35	0.58
1:A:244:THR:HG21	1:C:1160:THR:HB	1.86	0.58
1:A:901:MET:HE1	1:A:926:LEU:CB	2.34	0.58
1:B:1764:VAL:HG21	1:B:1769:VAL:CG1	2.32	0.58
1:C:1448:ARG:HD2	1:C:1508:TRP:O	2.04	0.58
2:J:236:ILE:HD12	2:J:240:LEU:HD22	1.85	0.58
3:K:598:THR:O	3:K:599:PRO:C	2.45	0.58
3:K:1345:GLY:HA3	3:K:1412:TYR:CD1	2.39	0.58
1:B:411:GLN:NE2	1:B:1628:SER:H	2.01	0.58
1:E:1448:ARG:HD2	1:E:1508:TRP:O	2.03	0.58
2:G:1889:VAL:HG23	2:G:1899:VAL:HG12	1.85	0.58
3:H:236:ILE:HD12	3:H:240:LEU:HD22	1.86	0.58
3:L:1851:ASN:HD22	3:L:1956:ARG:HH21	1.49	0.58
1:A:411:GLN:NE2	1:A:1628:SER:H	2.01	0.58
1:A:1448:ARG:HD2	1:A:1508:TRP:O	2.04	0.58
1:C:69:ASP:OD1	1:C:76:ARG:NH1	2.36	0.58
2:J:1854:MET:HB3	2:J:1901:ALA:HB2	1.84	0.58
3:K:612:ASN:HD21	3:K:641:ILE:HA	1.69	0.58
3:L:1421:ASN:ND2	3:L:1421:ASN:N	2.48	0.58
1:D:340:ARG:HH12	1:D:344:GLN:NE2	1.95	0.58
1:D:1867:VAL:HG12	1:D:1884:SER:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1343:VAL:O	3:H:1343:VAL:HG22	2.04	0.58
3:K:1775:GLN:NE2	3:K:1839:GLN:HG3	2.19	0.58
1:C:1577:GLN:HE22	1:C:1591:TRP:C	2.12	0.58
1:D:411:GLN:NE2	1:D:1628:SER:H	2.01	0.58
1:E:705:VAL:HG23	1:E:732:LEU:HD21	1.85	0.58
3:K:142:ASN:HB3	3:K:550:VAL:HG13	1.86	0.58
3:L:1946:GLU:O	3:L:1950:LYS:CD	2.51	0.58
1:A:801:ARG:NH2	1:F:789:GLU:OE1	2.37	0.58
1:B:987:ASN:ND2	1:B:1685:TYR:OH	2.37	0.58
1:C:411:GLN:NE2	1:C:1628:SER:H	2.02	0.58
1:C:1470:LEU:HD13	1:C:1489:ARG:HG2	1.86	0.58
3:H:1852:TYR:N	3:H:1904:LEU:HD23	2.18	0.58
3:H:1907:LEU:HB3	3:H:1960:LEU:HD21	1.85	0.58
3:I:1946:GLU:O	3:I:1950:LYS:CD	2.48	0.58
2:J:1343:VAL:O	2:J:1343:VAL:HG22	2.04	0.58
1:A:1859:ALA:O	1:A:1864:VAL:HG22	2.04	0.58
1:C:513:GLU:OE2	1:C:873:ARG:NH1	2.32	0.58
1:F:172:ILE:O	1:F:176:VAL:HG22	2.04	0.58
2:G:1854:MET:HB3	2:G:1901:ALA:HB2	1.86	0.58
3:H:598:THR:O	3:H:599:PRO:C	2.44	0.58
3:H:1854:MET:HE2	3:H:1901:ALA:HB2	1.85	0.58
3:I:1345:GLY:HA3	3:I:1412:TYR:CD1	2.39	0.58
1:A:901:MET:HE1	1:A:926:LEU:HB3	1.85	0.57
2:G:106:ALA:HB2	2:G:545:GLN:HG2	1.86	0.57
3:K:463:PHE:CG	3:K:486:LEU:HD23	2.39	0.57
1:D:822:VAL:HG12	1:D:824:LEU:HD13	1.85	0.57
1:E:1326:ILE:HG12	1:E:1388:MET:HG3	1.85	0.57
3:L:1922:ILE:HB	3:L:1927:LEU:CD1	2.32	0.57
1:C:1506:GLN:HA	1:C:1510:ASN:HD22	1.69	0.57
1:F:1794:GLN:HE22	1:F:1840:VAL:HA	1.67	0.57
3:H:142:ASN:HB3	3:H:550:VAL:HG13	1.85	0.57
3:K:1215:LYS:HE2	3:K:1218:ILE:HD12	1.87	0.57
3:L:161:GLY:H	3:L:505:GLY:HA3	1.68	0.57
3:L:264:ARG:HD2	3:L:284:ALA:O	2.05	0.57
1:C:644:THR:HG22	1:C:648:ASP:O	2.05	0.57
1:C:705:VAL:HG23	1:C:732:LEU:HD21	1.87	0.57
1:D:20:TYR:CE2	2:J:2033:THR:CG2	2.88	0.57
1:F:411:GLN:NE2	1:F:1628:SER:H	2.01	0.57
1:D:1448:ARG:HD2	1:D:1508:TRP:O	2.03	0.57
1:F:1448:ARG:HD2	1:F:1508:TRP:O	2.04	0.57
2:G:1807:HIS:ND1	2:G:1808:SER:OG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:73:GLU:HG2	3:H:76:LYS:HB2	1.85	0.57
2:J:1345:GLY:HA3	2:J:1412:TYR:CD1	2.39	0.57
3:L:236:ILE:HD12	3:L:240:LEU:HD22	1.85	0.57
3:L:1345:GLY:HA3	3:L:1412:TYR:CD1	2.39	0.57
1:B:1160:THR:HG21	1:C:244:THR:HG21	1.85	0.57
2:J:598:THR:O	2:J:599:PRO:C	2.45	0.57
3:K:236:ILE:HD12	3:K:240:LEU:HD22	1.85	0.57
3:H:612:ASN:HD21	3:H:641:ILE:HA	1.68	0.57
3:I:612:ASN:HD21	3:I:641:ILE:HA	1.69	0.57
3:I:2015:THR:O	3:I:2017:LYS:N	2.35	0.57
1:C:1307:THR:HG23	1:C:1586:GLY:HA2	1.86	0.57
1:D:901:MET:HE1	1:D:926:LEU:CB	2.33	0.57
2:G:1345:GLY:HA3	2:G:1412:TYR:CD1	2.39	0.57
1:B:1307:THR:HG23	1:B:1586:GLY:HA2	1.87	0.57
1:D:1307:THR:HG23	1:D:1586:GLY:HA2	1.86	0.57
3:H:106:ALA:HB2	3:H:545:GLN:HG2	1.86	0.57
3:H:1054:LEU:HB2	10:H:2101:FMN:HM73	1.87	0.57
2:J:1345:GLY:HA3	2:J:1412:TYR:CE1	2.40	0.57
3:K:1270:TRP:O	3:K:1332:ARG:NH1	2.38	0.57
1:A:67:SER:CB	3:I:355:LYS:HE3	2.35	0.57
1:A:1146:HIS:O	1:E:1118:LYS:HE2	2.05	0.57
1:C:11:HIS:HE1	3:I:1996:ILE:O	1.88	0.57
1:C:1507:GLN:HE22	1:F:1500:GLN:CG	2.18	0.57
1:F:719:GLN:HG3	1:F:1612:ASP:HA	1.87	0.57
1:F:1307:THR:HG23	1:F:1586:GLY:HA2	1.86	0.57
1:F:1506:GLN:HA	1:F:1510:ASN:HD22	1.69	0.57
2:J:612:ASN:HD21	2:J:641:ILE:HA	1.70	0.57
2:J:964:LEU:HD22	2:J:964:LEU:N	2.20	0.57
1:B:438:ASN:HD21	1:B:698:GLN:HE21	1.52	0.56
1:C:1859:ALA:O	1:C:1864:VAL:HG22	2.05	0.56
1:D:537:LYS:HE3	1:D:634:THR:OG1	2.04	0.56
1:F:927:ASN:O	1:F:929:GLY:N	2.37	0.56
2:G:964:LEU:H	2:G:964:LEU:CD2	2.14	0.56
1:B:295:ALA:O	1:B:298:VAL:O	2.22	0.56
1:B:1470:LEU:HD13	1:B:1489:ARG:HG2	1.86	0.56
1:D:719:GLN:HG3	1:D:1612:ASP:HA	1.87	0.56
1:E:1307:THR:HG23	1:E:1586:GLY:HA2	1.86	0.56
2:G:1054:LEU:HB2	10:G:2101:FMN:C7M	2.36	0.56
3:L:598:THR:O	3:L:599:PRO:C	2.46	0.56
1:A:1506:GLN:HA	1:A:1510:ASN:HD22	1.70	0.56
1:C:1431:GLU:OE2	1:C:1523:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:935:GLU:HB3	1:D:938:GLU:HG2	1.86	0.56
1:E:411:GLN:NE2	1:E:1628:SER:H	2.03	0.56
1:E:987:ASN:ND2	1:E:1685:TYR:OH	2.37	0.56
3:H:1693:ARG:NH1	3:H:1825:GLU:OE1	2.38	0.56
2:J:665:LEU:HD22	2:J:669:LEU:HD22	1.88	0.56
3:K:1234:VAL:HG13	3:K:1268:LYS:HE3	1.87	0.56
3:K:1345:GLY:HA3	3:K:1412:TYR:CE1	2.40	0.56
3:L:612:ASN:HD21	3:L:641:ILE:HA	1.69	0.56
3:L:1946:GLU:O	3:L:1950:LYS:HE3	2.04	0.56
1:A:1319:ILE:HA	1:A:1324:ALA:O	2.06	0.56
1:A:1546:THR:HG21	4:F:1901:PNS:O40	2.05	0.56
1:D:542:THR:HG22	1:D:543:ILE:HG23	1.87	0.56
2:G:236:ILE:HD12	2:G:240:LEU:HD22	1.86	0.56
3:I:598:THR:O	3:I:599:PRO:C	2.45	0.56
3:L:1944:ILE:HD13	3:L:1945:ASP:OD1	2.06	0.56
1:A:438:ASN:HD21	1:A:698:GLN:HE21	1.52	0.56
1:A:822:VAL:HG12	1:A:824:LEU:HD13	1.86	0.56
1:E:822:VAL:HG12	1:E:824:LEU:HD13	1.87	0.56
1:F:438:ASN:HD21	1:F:698:GLN:HE21	1.53	0.56
2:G:2015:THR:O	2:G:2017:LYS:N	2.35	0.56
2:J:736:ARG:HD2	2:J:769:SER:OG	2.05	0.56
3:K:597:MET:HA	10:K:2101:FMN:C5A	2.36	0.56
1:D:927:ASN:O	1:D:929:GLY:N	2.38	0.56
1:F:93:ASP:HB2	1:F:94:PRO:HD2	1.86	0.56
2:J:192:ALA:HB2	2:J:215:ILE:HD13	1.85	0.56
1:E:1486:LEU:HD11	1:E:1756:ILE:HD11	1.87	0.56
1:F:1319:ILE:HA	1:F:1324:ALA:O	2.06	0.56
3:I:1345:GLY:HA3	3:I:1412:TYR:CE1	2.40	0.56
2:J:1922:ILE:HD13	2:J:1927:LEU:HD11	1.88	0.56
3:L:1309:GLU:OE2	3:L:1314:ARG:NH1	2.39	0.56
3:L:1950:LYS:HE2	3:L:1950:LYS:H	1.70	0.56
3:L:2015:THR:O	3:L:2017:LYS:N	2.35	0.56
1:A:1016:GLU:OE1	1:E:1515:ARG:NH2	2.37	0.56
1:C:927:ASN:O	1:C:929:GLY:N	2.37	0.56
1:C:1184:LEU:HB2	1:C:1352:THR:HG21	1.88	0.56
1:C:1856:LYS:O	1:C:1860:GLU:HG2	2.06	0.56
1:E:1470:LEU:HD13	1:E:1489:ARG:HG2	1.87	0.56
1:F:1431:GLU:OE2	1:F:1523:ARG:NH1	2.38	0.56
3:K:73:GLU:O	3:K:134:LYS:NZ	2.39	0.56
1:A:509:ILE:O	1:A:878:MET:HE1	2.06	0.56
1:A:1302:VAL:CG2	1:E:1302:VAL:CG2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1431:GLU:OE2	1:D:1523:ARG:NH1	2.38	0.56
1:E:1319:ILE:HA	1:E:1324:ALA:O	2.06	0.56
3:H:1345:GLY:HA3	3:H:1412:TYR:CE1	2.41	0.56
2:J:1886:VAL:CG2	2:J:1906:ALA:HB3	2.36	0.56
3:L:264:ARG:HE	3:L:456:GLN:CB	2.18	0.56
3:L:1345:GLY:HA3	3:L:1412:TYR:CE1	2.41	0.56
1:B:1431:GLU:OE2	1:B:1523:ARG:NH1	2.39	0.56
1:B:1486:LEU:HD11	1:B:1756:ILE:HD11	1.88	0.56
1:C:1319:ILE:HA	1:C:1324:ALA:O	2.06	0.56
1:E:1431:GLU:OE2	1:E:1523:ARG:NH1	2.39	0.56
2:G:1904:LEU:HD23	2:G:1958:LEU:O	2.06	0.56
3:I:778:TYR:HE1	3:I:1085:LEU:HD13	1.71	0.56
1:B:340:ARG:HH12	1:B:344:GLN:NE2	1.96	0.55
3:L:1929:LYS:HE3	3:L:1933:LEU:HD12	1.88	0.55
1:A:1431:GLU:OE2	1:A:1523:ARG:NH1	2.39	0.55
1:C:537:LYS:HE2	1:C:634:THR:OG1	2.05	0.55
1:D:1319:ILE:HA	1:D:1324:ALA:O	2.06	0.55
3:L:1942:GLU:O	3:L:1946:GLU:CG	2.52	0.55
1:B:705:VAL:HG23	1:B:732:LEU:CD2	2.36	0.55
1:B:1160:THR:CB	1:C:244:THR:HG21	2.36	0.55
1:F:1859:ALA:O	1:F:1864:VAL:HG22	2.06	0.55
2:G:1345:GLY:HA3	2:G:1412:TYR:CE1	2.41	0.55
3:I:1309:GLU:OE2	3:I:1314:ARG:NH1	2.39	0.55
2:J:903:TRP:O	2:J:906:THR:HG22	2.06	0.55
3:L:1130:THR:H	3:L:1133:THR:HG22	1.72	0.55
1:B:509:ILE:O	1:B:878:MET:HE1	2.06	0.55
1:F:513:GLU:OE2	1:F:873:ARG:NH1	2.32	0.55
2:G:903:TRP:O	2:G:906:THR:HG22	2.06	0.55
3:L:404:GLN:CA	3:L:407:ILE:HD13	2.31	0.55
1:A:1153:ASP:OD2	1:B:359:ARG:NH1	2.39	0.55
1:B:1506:GLN:HA	1:B:1510:ASN:HD22	1.71	0.55
1:E:1552:ASN:O	1:E:1556:THR:HG23	2.07	0.55
3:I:1418:ASP:HB2	3:I:1421:ASN:HD22	1.72	0.55
1:A:789:GLU:OE2	1:F:793:ARG:HD2	2.05	0.55
1:A:1307:THR:HG23	1:A:1586:GLY:HA2	1.87	0.55
1:B:1319:ILE:HA	1:B:1324:ALA:O	2.06	0.55
1:B:1500:GLN:CG	1:D:1507:GLN:HE22	2.19	0.55
1:B:1694:TYR:OH	3:H:1001:ASP:OD2	2.23	0.55
1:E:438:ASN:HD21	1:E:698:GLN:HE21	1.54	0.55
1:F:538:GLU:HG2	1:F:635:ILE:HD11	1.89	0.55
2:G:598:THR:OG1	2:G:599:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1929:LYS:O	3:I:1929:LYS:HD3	2.05	0.55
3:K:451:ASN:HB3	3:K:453:LYS:HG2	1.89	0.55
3:L:1872:GLN:NE2	3:L:1888:ILE:HD11	2.21	0.55
1:A:1486:LEU:HD11	1:A:1756:ILE:HD11	1.89	0.55
1:C:438:ASN:HD21	1:C:698:GLN:HE21	1.55	0.55
1:C:1851:LEU:H	1:C:1851:LEU:CD2	2.15	0.55
1:D:705:VAL:HG23	1:D:732:LEU:HD21	1.87	0.55
2:G:777:THR:CG2	2:G:1081:HIS:NE2	2.70	0.55
2:G:1932:SER:HB2	2:G:1936:VAL:HG13	1.89	0.55
3:H:894:ARG:NH1	3:H:898:ASP:OD2	2.40	0.55
1:A:1460:LYS:NZ	1:A:1464:GLU:OE2	2.38	0.55
1:B:801:ARG:NH2	1:E:789:GLU:OE1	2.39	0.55
1:E:644:THR:HG22	1:E:648:ASP:O	2.06	0.55
3:K:1680:LEU:HD22	3:K:1684:SER:HB3	1.89	0.55
3:L:778:TYR:HE1	3:L:1085:LEU:HD13	1.71	0.55
1:A:719:GLN:HG3	1:A:1612:ASP:HA	1.88	0.55
1:B:927:ASN:O	1:B:929:GLY:N	2.37	0.55
1:C:793:ARG:HD2	1:D:789:GLU:OE2	2.06	0.55
1:E:963:LEU:O	1:E:967:VAL:HG12	2.07	0.55
3:L:777:THR:CG2	3:L:1081:HIS:NE2	2.70	0.55
1:B:417:TYR:OH	1:B:458:THR:HB	2.07	0.55
3:K:777:THR:CG2	3:K:1081:HIS:NE2	2.70	0.55
3:K:1855:ILE:HG22	3:K:1968:PRO:HA	1.89	0.55
1:A:705:VAL:HG23	1:A:732:LEU:HD21	1.88	0.54
1:E:1506:GLN:HA	1:E:1510:ASN:HD22	1.71	0.54
3:L:836:TYR:HA	3:L:845:THR:HG23	1.89	0.54
1:C:982:ILE:HD13	3:I:955:GLU:CB	2.37	0.54
1:D:1450:ARG:NH1	12:D:2002:HOH:O	2.39	0.54
1:F:41:THR:O	1:F:76:ARG:HD3	2.07	0.54
1:F:705:VAL:HG23	1:F:732:LEU:CD2	2.37	0.54
1:C:1486:LEU:HD11	1:C:1756:ILE:HD11	1.89	0.54
1:F:1329:VAL:HG12	1:F:1385:GLN:HB2	1.89	0.54
3:H:1680:LEU:HD22	3:H:1684:SER:HB3	1.88	0.54
3:I:1054:LEU:HB2	10:I:2101:FMN:C7M	2.37	0.54
2:J:777:THR:CG2	2:J:1081:HIS:NE2	2.70	0.54
3:K:903:TRP:O	3:K:906:THR:HG22	2.07	0.54
4:A:1901:PNS:H421	1:F:1544:THR:HG21	1.90	0.54
1:C:938:GLU:HG3	1:C:939:PHE:N	2.23	0.54
3:K:778:TYR:HE1	3:K:1085:LEU:HD13	1.72	0.54
3:L:53:GLU:O	3:L:118:LYS:HE2	2.08	0.54
1:B:11:HIS:HE1	3:H:1996:ILE:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:THR:HG22	1:B:648:ASP:O	2.07	0.54
1:B:719:GLN:HG3	1:B:1612:ASP:HA	1.88	0.54
1:C:1329:VAL:HG12	1:C:1385:GLN:HB2	1.90	0.54
1:C:1552:ASN:O	1:C:1556:THR:HG23	2.07	0.54
1:D:509:ILE:O	1:D:878:MET:HE1	2.08	0.54
1:D:644:THR:HG22	1:D:648:ASP:O	2.06	0.54
1:E:504:ASP:OD2	1:E:508:ASN:HB2	2.08	0.54
1:E:719:GLN:HG3	1:E:1612:ASP:HA	1.88	0.54
1:F:982:ILE:HD13	3:L:955:GLU:CB	2.38	0.54
2:G:1217:ASN:O	2:G:1218:ILE:HD12	2.06	0.54
3:I:894:ARG:NH1	3:I:898:ASP:OD2	2.40	0.54
3:I:1923:ASP:O	3:I:1927:LEU:HG	2.08	0.54
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.40	0.54
2:J:1680:LEU:HD22	2:J:1684:SER:HB3	1.90	0.54
2:J:1775:GLN:CG	2:J:1836:MET:HE3	2.38	0.54
3:K:1229:MET:HE2	3:K:1268:LYS:O	2.07	0.54
3:L:894:ARG:NH1	3:L:898:ASP:OD2	2.41	0.54
3:L:1693:ARG:NH1	3:L:1825:GLU:OE1	2.40	0.54
1:A:644:THR:HG22	1:A:648:ASP:O	2.06	0.54
1:A:1851:LEU:HD22	1:A:1851:LEU:N	2.23	0.54
1:F:644:THR:HG22	1:F:648:ASP:O	2.07	0.54
1:F:1552:ASN:O	1:F:1556:THR:HG23	2.08	0.54
2:G:297:ARG:O	2:G:301:THR:CG2	2.56	0.54
3:I:1693:ARG:NH1	3:I:1825:GLU:OE1	2.41	0.54
2:J:778:TYR:HE1	2:J:1085:LEU:HD13	1.73	0.54
3:L:142:ASN:HB3	3:L:550:VAL:HG13	1.90	0.54
1:A:244:THR:HG21	1:C:1160:THR:CB	2.38	0.54
2:G:778:TYR:HE1	2:G:1085:LEU:HD13	1.72	0.54
3:H:53:GLU:O	3:H:118:LYS:HE2	2.08	0.54
3:H:455:ILE:HG13	3:H:469:ARG:HD3	1.90	0.54
3:H:598:THR:OG1	3:H:599:PRO:HD3	2.07	0.54
3:H:665:LEU:HD22	3:H:669:LEU:HD22	1.90	0.54
3:I:53:GLU:O	3:I:118:LYS:HE2	2.08	0.54
3:I:777:THR:CG2	3:I:1081:HIS:NE2	2.70	0.54
2:J:903:TRP:O	2:J:906:THR:CG2	2.56	0.54
3:H:1130:THR:O	3:H:1133:THR:CG2	2.56	0.54
2:J:1855:ILE:HG22	2:J:1968:PRO:HA	1.90	0.54
3:K:451:ASN:HB3	3:K:453:LYS:CE	2.38	0.54
3:L:1420:GLU:HG2	3:L:1421:ASN:HD21	1.72	0.54
1:A:331:ILE:HD12	1:C:332:THR:HB	1.90	0.54
1:A:1552:ASN:O	1:A:1556:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1184:LEU:HB2	1:D:1352:THR:HG21	1.90	0.54
2:G:903:TRP:O	2:G:906:THR:CG2	2.56	0.54
3:K:53:GLU:O	3:K:118:LYS:HE2	2.08	0.54
1:A:417:TYR:OH	1:A:458:THR:HB	2.08	0.54
1:A:927:ASN:O	1:A:929:GLY:N	2.37	0.54
1:B:1515:ARG:HD2	1:D:1499:SER:OG	2.07	0.54
1:C:982:ILE:HD12	3:I:965:SER:HA	1.90	0.54
1:D:348:ARG:HD3	1:F:1129:GLU:OE1	2.07	0.54
1:D:417:TYR:OH	1:D:458:THR:HB	2.08	0.54
1:D:738:ASN:HD22	7:D:1923:A2P:HN62	1.56	0.54
1:E:1329:VAL:HG12	1:E:1385:GLN:HB2	1.90	0.54
3:H:698:LEU:O	3:H:700:LEU:N	2.41	0.54
3:H:1775:GLN:CG	3:H:1836:MET:HE3	2.38	0.54
3:H:1855:ILE:HG22	3:H:1968:PRO:HA	1.90	0.54
3:I:1317:ARG:O	3:I:1317:ARG:HG3	2.07	0.54
3:I:1932:SER:HB2	3:I:1936:VAL:HG13	1.89	0.54
3:K:896:ASN:HD21	3:K:906:THR:HG21	1.73	0.54
1:A:808:LYS:HE2	1:F:782:GLU:O	2.08	0.53
1:C:987:ASN:ND2	1:C:1685:TYR:OH	2.38	0.53
1:E:1851:LEU:HD22	1:E:1851:LEU:N	2.23	0.53
3:H:777:THR:CG2	3:H:1081:HIS:NE2	2.70	0.53
3:I:376:ASN:C	3:I:376:ASN:ND2	2.64	0.53
1:B:1552:ASN:O	1:B:1556:THR:HG23	2.09	0.53
1:C:1507:GLN:HE22	1:F:1500:GLN:HG2	1.73	0.53
1:E:1859:ALA:O	1:E:1864:VAL:HG22	2.08	0.53
1:F:1303:GLY:C	1:F:1307:THR:HG22	2.33	0.53
3:H:1054:LEU:HB2	10:H:2101:FMN:C7M	2.38	0.53
3:K:485:ARG:NH1	3:K:486:LEU:CD1	2.71	0.53
1:A:1118:LYS:HE2	1:E:1146:HIS:O	2.09	0.53
1:B:1184:LEU:HB2	1:B:1352:THR:HG21	1.89	0.53
1:D:987:ASN:ND2	1:D:1685:TYR:OH	2.39	0.53
2:G:836:TYR:HA	2:G:845:THR:HG23	1.90	0.53
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.41	0.53
3:H:778:TYR:HE1	3:H:1085:LEU:HD13	1.72	0.53
2:J:106:ALA:HB2	2:J:545:GLN:HG2	1.89	0.53
2:J:836:TYR:HA	2:J:845:THR:HG23	1.91	0.53
3:L:964:LEU:HD22	3:L:964:LEU:N	2.24	0.53
3:L:1881:ARG:CG	3:L:1944:ILE:HD11	2.37	0.53
1:A:11:HIS:HE1	2:G:1996:ILE:O	1.92	0.53
1:A:1184:LEU:HB2	1:A:1352:THR:HG21	1.91	0.53
1:C:719:GLN:HG3	1:C:1612:ASP:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:ASP:OD2	1:D:508:ASN:HB2	2.08	0.53
1:D:1153:ASP:OD1	1:E:359:ARG:NH1	2.42	0.53
1:F:1304:ALA:O	1:F:1307:THR:HG23	2.09	0.53
2:G:53:GLU:O	2:G:118:LYS:HE2	2.09	0.53
2:G:1680:LEU:HD22	2:G:1684:SER:HB3	1.89	0.53
3:I:903:TRP:O	3:I:906:THR:HG22	2.08	0.53
3:L:598:THR:OG1	3:L:599:PRO:HD3	2.08	0.53
1:A:1825:VAL:HG11	1:A:1858:ALA:HB1	1.91	0.53
1:C:504:ASP:OD2	1:C:508:ASN:HB2	2.09	0.53
3:I:903:TRP:O	3:I:906:THR:CG2	2.56	0.53
2:J:297:ARG:O	2:J:301:THR:CG2	2.56	0.53
3:K:155:GLN:H	3:K:499:THR:HG22	1.72	0.53
3:K:455:ILE:HG13	3:K:469:ARG:HD3	1.91	0.53
3:K:894:ARG:NH1	3:K:898:ASP:OD2	2.41	0.53
3:L:903:TRP:O	3:L:906:THR:CG2	2.57	0.53
1:D:1303:GLY:CA	1:D:1649:LYS:HD3	2.37	0.53
2:G:455:ILE:HG13	2:G:469:ARG:HD3	1.89	0.53
3:I:73:GLU:O	3:I:134:LYS:NZ	2.41	0.53
3:I:298:LYS:NZ	3:I:449:SER:O	2.42	0.53
3:L:903:TRP:O	3:L:906:THR:HG22	2.08	0.53
3:L:1940:LEU:O	3:L:1944:ILE:HG23	2.08	0.53
3:H:1319:MET:HB3	3:H:1368:VAL:HG21	1.90	0.53
3:I:1882:THR:HG23	3:I:1884:TRP:H	1.73	0.53
3:K:1378:ILE:HG22	3:K:1378:ILE:O	2.08	0.53
3:L:698:LEU:O	3:L:700:LEU:N	2.41	0.53
3:L:1881:ARG:HG3	3:L:1944:ILE:HD11	1.90	0.53
1:D:1303:GLY:C	1:D:1307:THR:HG22	2.34	0.53
2:G:597:MET:HA	10:G:2101:FMN:C5A	2.39	0.53
2:G:1309:GLU:OE2	2:G:1314:ARG:NH1	2.40	0.53
3:H:903:TRP:O	3:H:906:THR:CG2	2.57	0.53
3:I:297:ARG:O	3:I:301:THR:CG2	2.55	0.53
2:J:1418:ASP:HB2	2:J:1421:ASN:HD22	1.74	0.53
3:K:836:TYR:HA	3:K:845:THR:HG23	1.90	0.53
1:B:43:ARG:O	3:H:1662:THR:HA	2.09	0.53
3:H:903:TRP:O	3:H:906:THR:HG22	2.09	0.53
3:I:1680:LEU:HD22	3:I:1684:SER:HB3	1.90	0.53
2:J:1495:THR:O	2:J:1496:LYS:HB2	2.09	0.53
3:K:109:LEU:HD21	3:K:116:LEU:CD2	2.39	0.53
1:A:513:GLU:OE2	1:A:873:ARG:NH1	2.33	0.53
1:A:1303:GLY:C	1:A:1307:THR:HG22	2.34	0.53
1:A:1329:VAL:HG12	1:A:1385:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:ILE:HD13	3:I:955:GLU:HB2	1.90	0.53
1:D:1552:ASN:O	1:D:1556:THR:HG23	2.09	0.53
1:E:1189:ILE:H	1:E:1380:GLN:HE21	1.58	0.53
1:F:1825:VAL:HG11	1:F:1858:ALA:HB1	1.91	0.53
2:G:1149:TRP:CD1	2:G:1213:LEU:HD21	2.44	0.53
2:J:317:THR:HG23	3:K:1314:ARG:NH2	2.23	0.53
2:J:1309:GLU:OE2	2:J:1314:ARG:NH1	2.41	0.53
3:K:698:LEU:O	3:K:700:LEU:N	2.41	0.53
3:L:1775:GLN:CG	3:L:1836:MET:HE3	2.39	0.53
1:C:806:VAL:HG22	1:C:862:LEU:HD11	1.91	0.52
1:D:705:VAL:HG23	1:D:732:LEU:CD2	2.39	0.52
1:D:806:VAL:HG22	1:D:862:LEU:HD11	1.91	0.52
1:D:938:GLU:HG3	1:D:939:PHE:N	2.23	0.52
1:D:1859:ALA:O	1:D:1864:VAL:HG22	2.08	0.52
1:F:504:ASP:OD2	1:F:508:ASN:HB2	2.08	0.52
3:I:598:THR:OG1	3:I:599:PRO:HD3	2.09	0.52
3:I:1022:ASP:OD2	3:I:1024:ARG:NH1	2.43	0.52
3:K:1808:J8W:OG	3:K:1809:LEU:N	2.41	0.52
3:K:1962:ARG:HB3	3:K:1962:ARG:NH2	2.24	0.52
1:B:1303:GLY:C	1:B:1307:THR:HG22	2.33	0.52
1:E:927:ASN:O	1:E:929:GLY:N	2.38	0.52
2:G:1314:ARG:NH2	3:I:315:PRO:O	2.42	0.52
3:H:1916:PHE:CD2	3:H:1943:ILE:HD12	2.44	0.52
3:I:1697:HIS:O	3:I:1701:THR:HG23	2.09	0.52
3:K:297:ARG:O	3:K:301:THR:CG2	2.56	0.52
3:L:109:LEU:HD23	3:L:535:ILE:HD13	1.91	0.52
1:C:1016:GLU:OE1	1:F:1515:ARG:NH2	2.43	0.52
1:F:509:ILE:O	1:F:878:MET:HE1	2.08	0.52
2:G:1548:SER:HB3	2:G:1619:ASN:HD21	1.75	0.52
3:I:1548:SER:HB3	3:I:1619:ASN:HD21	1.74	0.52
2:J:245:GLN:HE21	2:J:505:GLY:HA2	1.74	0.52
3:L:297:ARG:O	3:L:301:THR:CG2	2.56	0.52
1:B:1441:PRO:HD2	1:D:1492:GLU:OE2	2.09	0.52
1:C:705:VAL:HG23	1:C:732:LEU:CD2	2.39	0.52
1:C:1271:GLN:OE1	5:C:1907:EDO:H22	2.09	0.52
1:C:1303:GLY:C	1:C:1307:THR:HG22	2.33	0.52
2:G:1022:ASP:OD1	2:G:1024:ARG:HG2	2.10	0.52
3:H:1548:SER:HB3	3:H:1619:ASN:HD21	1.74	0.52
2:J:1697:HIS:O	2:J:1701:THR:HG23	2.10	0.52
3:L:1680:LEU:HD22	3:L:1684:SER:HB3	1.90	0.52
1:A:705:VAL:HG23	1:A:732:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1460:LYS:NZ	1:B:1464:GLU:OE2	2.39	0.52
1:E:1303:GLY:C	1:E:1307:THR:HG22	2.34	0.52
1:E:1304:ALA:O	1:E:1307:THR:HG23	2.09	0.52
2:G:1693:ARG:NH1	2:G:1825:GLU:OE1	2.43	0.52
2:J:1932:SER:HB2	2:J:1936:VAL:HG13	1.92	0.52
2:J:1944:ILE:O	2:J:1948:SER:HB3	2.10	0.52
3:K:1418:ASP:HB2	3:K:1421:ASN:HD22	1.74	0.52
3:K:1693:ARG:NH1	3:K:1825:GLU:OE1	2.42	0.52
1:A:982:ILE:HD13	2:G:955:GLU:HB2	1.92	0.52
1:A:1022:THR:HG21	1:A:1388:MET:HE3	1.91	0.52
1:B:682:GLY:HA2	7:B:1918:A2P:C1'	2.39	0.52
1:B:1329:VAL:HG12	1:B:1385:GLN:HB2	1.91	0.52
1:D:21:GLN:HE21	2:J:2013:ASN:HD22	1.56	0.52
1:D:1506:GLN:HA	1:D:1510:ASN:HD22	1.74	0.52
1:E:1167:LEU:CD1	1:E:1171:ALA:CB	2.88	0.52
3:H:245:GLN:HE21	3:H:505:GLY:HA2	1.74	0.52
3:H:1149:TRP:CD1	3:H:1213:LEU:HD21	2.44	0.52
2:J:1270:TRP:O	2:J:1332:ARG:NH1	2.42	0.52
1:A:244:THR:HG21	1:C:1160:THR:HG21	1.90	0.52
1:A:517:GLU:O	1:A:518:LYS:HB2	2.10	0.52
3:I:836:TYR:HA	3:I:845:THR:HG23	1.92	0.52
3:I:1808:J8W:OG	3:I:1809:LEU:N	2.41	0.52
3:K:1697:HIS:O	3:K:1701:THR:HG23	2.09	0.52
3:L:298:LYS:NZ	3:L:449:SER:O	2.43	0.52
1:A:1153:ASP:CG	1:B:359:ARG:NH1	2.67	0.52
1:A:1245:ASN:ND2	1:A:1247:SER:H	2.07	0.52
1:D:27:ARG:HG3	2:J:2013:ASN:O	2.10	0.52
1:E:537:LYS:HE2	1:E:634:THR:OG1	2.10	0.52
3:H:1246:ASN:ND2	12:H:2201:HOH:O	2.43	0.52
3:I:245:GLN:HE21	3:I:505:GLY:HA2	1.75	0.52
3:K:665:LEU:HD22	3:K:669:LEU:HD22	1.90	0.52
3:K:903:TRP:O	3:K:906:THR:CG2	2.57	0.52
3:L:1915:ASN:HD21	3:L:1964:PHE:N	2.06	0.52
1:A:329:GLU:HA	1:A:332:THR:CG2	2.40	0.52
1:F:632:ARG:O	1:F:633:GLU:HB2	2.10	0.52
3:K:687:SER:OG	3:K:690:VAL:HG23	2.10	0.52
3:L:1129:ALA:HA	3:L:1133:THR:HG21	1.92	0.52
3:L:1270:TRP:O	3:L:1332:ARG:NH1	2.42	0.52
1:A:1304:ALA:O	1:A:1307:THR:HG23	2.08	0.52
1:C:1792:THR:HG21	1:C:1838:GLU:OE2	2.10	0.52
1:D:1329:VAL:HG12	1:D:1385:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:687:SER:OG	3:I:690:VAL:HG23	2.10	0.52
2:J:896:ASN:HD21	2:J:906:THR:HG21	1.74	0.52
2:J:1548:SER:HB3	2:J:1619:ASN:HD21	1.75	0.52
3:L:964:LEU:HD22	3:L:964:LEU:H	1.73	0.52
3:L:1932:SER:HB2	3:L:1936:VAL:HG13	1.91	0.52
1:A:504:ASP:OD2	1:A:508:ASN:HB2	2.10	0.51
1:B:789:GLU:OE1	1:E:801:ARG:NH2	2.43	0.51
1:D:59:ARG:HD3	2:J:1896:GLN:HE22	1.74	0.51
1:D:1022:THR:HG21	1:D:1388:MET:HE3	1.91	0.51
1:D:1304:ALA:O	1:D:1307:THR:HG23	2.08	0.51
1:E:146:LYS:HG2	1:E:214:GLN:NE2	2.25	0.51
1:E:705:VAL:HG23	1:E:732:LEU:CD2	2.39	0.51
1:E:982:ILE:HD12	3:K:965:SER:CA	2.41	0.51
2:G:1418:ASP:HB2	2:G:1421:ASN:HD22	1.74	0.51
3:I:101:ILE:HD13	3:I:126:TYR:CG	2.45	0.51
3:I:1495:THR:O	3:I:1496:LYS:HB2	2.09	0.51
3:I:1855:ILE:HG22	3:I:1968:PRO:HA	1.91	0.51
2:J:1149:TRP:CD1	2:J:1213:LEU:HD21	2.44	0.51
3:L:1548:SER:HB3	3:L:1619:ASN:HD21	1.75	0.51
3:L:1950:LYS:HE2	3:L:1950:LYS:N	2.25	0.51
1:A:27:ARG:HG3	2:G:2013:ASN:O	2.10	0.51
3:K:245:GLN:HE21	3:K:505:GLY:HA2	1.75	0.51
3:K:1548:SER:HB3	3:K:1619:ASN:HD21	1.75	0.51
3:L:1855:ILE:HG22	3:L:1968:PRO:HA	1.92	0.51
3:L:2020:GLN:HA	3:L:2020:GLN:HE21	1.76	0.51
1:A:706:THR:HB	1:A:737:PHE:HB3	1.91	0.51
1:B:1302:VAL:HG22	1:D:1302:VAL:CG2	2.40	0.51
1:F:1184:LEU:HB2	1:F:1352:THR:HG21	1.92	0.51
3:I:1270:TRP:O	3:I:1332:ARG:NH1	2.43	0.51
2:J:298:LYS:NZ	2:J:449:SER:O	2.43	0.51
1:A:987:ASN:ND2	1:A:1685:TYR:OH	2.40	0.51
1:A:1066:ASN:HD22	1:A:1071:PRO:HA	1.76	0.51
1:B:329:GLU:HA	1:B:332:THR:CG2	2.41	0.51
1:B:1022:THR:HG21	1:B:1388:MET:HE3	1.91	0.51
1:B:1304:ALA:O	1:B:1307:THR:HG23	2.10	0.51
1:C:1304:ALA:O	1:C:1307:THR:HG23	2.09	0.51
1:C:1694:TYR:OH	3:I:1001:ASP:OD2	2.26	0.51
1:E:1184:LEU:HB2	1:E:1352:THR:HG21	1.92	0.51
1:F:417:TYR:OH	1:F:458:THR:HB	2.09	0.51
2:G:1838:MET:HE3	2:G:1976:PHE:CE1	2.45	0.51
3:H:687:SER:OG	3:H:690:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1495:THR:O	3:H:1496:LYS:HB2	2.10	0.51
3:I:698:LEU:O	3:I:700:LEU:N	2.41	0.51
2:J:598:THR:OG1	2:J:599:PRO:HD3	2.09	0.51
2:J:1736:MET:HG2	2:J:1751:ILE:HD12	1.93	0.51
3:L:455:ILE:HG13	3:L:469:ARG:HD3	1.92	0.51
3:L:665:LEU:HD22	3:L:669:LEU:HD22	1.91	0.51
1:A:1260:MET:HG2	1:E:1342:GLU:HG3	1.93	0.51
1:A:1792:THR:HG21	1:A:1838:GLU:OE2	2.09	0.51
1:B:706:THR:HB	1:B:737:PHE:HB3	1.92	0.51
2:G:1775:GLN:CG	2:G:1836:MET:HE3	2.41	0.51
3:H:836:TYR:HA	3:H:845:THR:HG23	1.93	0.51
3:I:455:ILE:HG13	3:I:469:ARG:HD3	1.92	0.51
3:I:665:LEU:HD22	3:I:669:LEU:HD22	1.92	0.51
3:I:1775:GLN:CG	3:I:1836:MET:HE3	2.39	0.51
2:J:1693:ARG:NH1	2:J:1825:GLU:OE1	2.43	0.51
2:J:1953:VAL:O	2:J:1953:VAL:HG23	2.10	0.51
3:K:1149:TRP:CD1	3:K:1213:LEU:HD21	2.45	0.51
3:K:1337:ALA:HB1	3:K:1378:ILE:CG1	2.40	0.51
3:K:1564:HIS:O	3:K:1578:THR:OG1	2.27	0.51
3:L:285:GLU:OE1	3:L:298:LYS:HE2	2.11	0.51
3:L:1149:TRP:CD1	3:L:1213:LEU:HD21	2.44	0.51
1:B:157:HIS:O	1:B:160:LYS:HD2	2.11	0.51
1:D:20:TYR:CZ	2:J:2033:THR:CG2	2.93	0.51
1:D:682:GLY:HA2	7:D:1923:A2P:H1'	1.93	0.51
1:E:706:THR:HB	1:E:737:PHE:HB3	1.91	0.51
2:G:1170:ILE:HA	2:G:1221:MET:CE	2.41	0.51
3:H:597:MET:HA	10:H:2101:FMN:C5A	2.41	0.51
2:J:877:LYS:HE2	2:J:877:LYS:N	2.25	0.51
3:K:285:GLU:OE1	3:K:298:LYS:HE2	2.11	0.51
3:K:1904:LEU:HD13	3:K:1958:LEU:O	2.10	0.51
1:A:1160:THR:CB	1:B:244:THR:HG21	2.40	0.51
1:C:1486:LEU:O	1:C:1490:THR:HG23	2.06	0.51
1:E:509:ILE:O	1:E:878:MET:HE1	2.11	0.51
1:F:1851:LEU:H	1:F:1851:LEU:HD23	1.75	0.51
2:G:698:LEU:O	2:G:700:LEU:N	2.41	0.51
3:H:747:HIS:HE1	3:H:780:TYR:OH	1.93	0.51
3:K:1495:THR:O	3:K:1496:LYS:HB2	2.10	0.51
1:B:1491:ARG:HD3	1:B:1749:THR:HG21	1.92	0.51
1:E:1686:LYS:HD2	3:K:915:ALA:HB1	1.92	0.51
3:I:1023:ARG:HB3	3:I:1023:ARG:CZ	2.41	0.51
3:K:298:LYS:NZ	3:K:449:SER:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1507:GLN:HE22	1:D:1500:GLN:HA	1.74	0.51
1:C:1066:ASN:HD22	1:C:1071:PRO:HA	1.76	0.51
1:C:1146:HIS:O	1:F:1118:LYS:HE2	2.10	0.51
1:D:632:ARG:O	1:D:633:GLU:HB2	2.11	0.51
1:E:11:HIS:ND1	3:K:1998:LYS:HA	2.26	0.51
1:E:193:GLU:OE2	1:E:225:SER:HB2	2.11	0.51
1:F:806:VAL:HG22	1:F:862:LEU:HD11	1.93	0.51
1:F:982:ILE:HD12	3:L:965:SER:CA	2.40	0.51
1:F:1234:MET:CE	1:F:1326:ILE:HG21	2.41	0.51
1:F:1694:TYR:OH	3:L:1001:ASP:OD2	2.23	0.51
3:H:1150:ARG:HD2	3:H:1193:THR:HG21	1.93	0.51
3:H:1697:HIS:O	3:H:1701:THR:HG23	2.11	0.51
2:J:357:ASN:HB3	2:J:365:GLN:OE1	2.11	0.51
3:K:1337:ALA:O	3:K:1378:ILE:HD11	2.10	0.51
3:L:747:HIS:HE1	3:L:780:TYR:OH	1.94	0.51
3:L:1697:HIS:O	3:L:1701:THR:HG23	2.11	0.51
1:A:999:LYS:HE3	1:A:1003:GLN:HE21	1.76	0.51
1:A:1760:THR:HG23	1:A:1762:GLU:HG3	1.91	0.51
1:B:504:ASP:CG	1:B:508:ASN:CG	2.78	0.51
1:C:417:TYR:OH	1:C:458:THR:HB	2.09	0.51
1:C:1866:ASP:HB3	1:C:1885:THR:HG22	1.92	0.51
1:F:792:HIS:HD2	1:F:842:SER:OG	1.93	0.51
2:G:33:LEU:HD23	2:G:68:VAL:HG22	1.93	0.51
2:G:665:LEU:HD22	2:G:669:LEU:HD22	1.92	0.51
3:H:896:ASN:HD21	3:H:906:THR:HG21	1.76	0.51
1:A:11:HIS:ND1	2:G:1998:LYS:HA	2.25	0.50
1:C:193:GLU:OE2	1:C:225:SER:HB2	2.11	0.50
1:C:706:THR:HB	1:C:737:PHE:HB3	1.92	0.50
1:E:1637:ARG:HG2	1:E:1660:TYR:OH	2.11	0.50
1:E:1694:TYR:OH	3:K:1001:ASP:OD2	2.29	0.50
1:F:67:SER:CB	3:K:355:LYS:HE2	2.41	0.50
3:I:896:ASN:HD21	3:I:906:THR:HG21	1.76	0.50
2:J:747:HIS:HE1	2:J:780:TYR:OH	1.94	0.50
3:L:687:SER:OG	3:L:690:VAL:HG23	2.11	0.50
3:L:1495:THR:O	3:L:1496:LYS:HB2	2.10	0.50
3:L:1946:GLU:O	3:L:1950:LYS:HD2	2.10	0.50
1:A:193:GLU:OE2	1:A:225:SER:HB2	2.11	0.50
1:A:982:ILE:HD13	2:G:955:GLU:CB	2.41	0.50
1:B:792:HIS:HD2	1:B:842:SER:OG	1.94	0.50
1:D:706:THR:HB	1:D:737:PHE:HB3	1.92	0.50
1:D:792:HIS:HD2	1:D:842:SER:OG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:SER:HB3	2:J:355:LYS:HE3	1.92	0.50
1:E:1754:LYS:HA	1:E:1754:LYS:HE3	1.92	0.50
1:F:982:ILE:HD13	3:L:955:GLU:HB2	1.94	0.50
1:F:1066:ASN:HD22	1:F:1071:PRO:HA	1.75	0.50
12:F:2013:HOH:O	2:G:1727:LYS:HE3	2.11	0.50
2:G:357:ASN:HB3	2:G:365:GLN:OE1	2.12	0.50
3:H:285:GLU:OE1	3:H:298:LYS:HE2	2.10	0.50
3:I:785:TRP:O	3:I:788:LYS:HD3	2.11	0.50
3:I:964:LEU:HD23	3:I:964:LEU:N	2.17	0.50
3:K:1932:SER:HB2	3:K:1936:VAL:HG13	1.93	0.50
3:L:245:GLN:HE21	3:L:505:GLY:HA2	1.76	0.50
1:D:17:LEU:CD2	2:J:2012:PRO:HG2	2.41	0.50
2:G:245:GLN:HE21	2:G:505:GLY:HA2	1.75	0.50
2:G:298:LYS:NZ	2:G:449:SER:O	2.42	0.50
2:G:1697:HIS:O	2:G:1701:THR:HG23	2.11	0.50
3:H:1270:TRP:O	3:H:1332:ARG:NH1	2.43	0.50
2:J:687:SER:OG	2:J:690:VAL:HG23	2.12	0.50
1:A:792:HIS:HD2	1:A:842:SER:OG	1.94	0.50
1:F:1022:THR:HG21	1:F:1388:MET:HE3	1.94	0.50
3:H:298:LYS:NZ	3:H:449:SER:O	2.43	0.50
3:I:285:GLU:OE1	3:I:298:LYS:HE2	2.11	0.50
3:K:598:THR:OG1	3:K:599:PRO:HD3	2.12	0.50
1:B:1298:ILE:HG13	1:D:1649:LYS:HE3	1.93	0.50
1:D:193:GLU:OE2	1:D:225:SER:HB2	2.10	0.50
1:F:417:TYR:CE2	1:F:421:ILE:CD1	2.94	0.50
2:G:687:SER:OG	2:G:690:VAL:HG23	2.11	0.50
2:G:1270:TRP:O	2:G:1332:ARG:NH1	2.41	0.50
2:G:1855:ILE:HG22	2:G:1968:PRO:HA	1.92	0.50
3:I:747:HIS:HE1	3:I:780:TYR:OH	1.94	0.50
3:I:777:THR:HG23	3:I:1081:HIS:NE2	2.27	0.50
3:L:497:LYS:HD3	3:L:497:LYS:H	1.76	0.50
3:L:777:THR:HG23	3:L:1081:HIS:NE2	2.27	0.50
3:L:1941:PHE:HA	3:L:1944:ILE:HD12	1.93	0.50
1:A:78:ILE:HD12	1:A:78:ILE:N	2.27	0.50
1:B:267:VAL:HG12	1:B:290:MET:HE3	1.94	0.50
1:B:658:LEU:HD21	1:B:912:GLU:HB3	1.93	0.50
1:B:1302:VAL:CG2	1:D:1302:VAL:HG22	2.40	0.50
1:E:417:TYR:OH	1:E:458:THR:HB	2.10	0.50
2:G:1926:GLU:O	2:G:1930:SER:OG	2.24	0.50
2:J:1107:SER:OG	2:J:1109:VAL:HG22	2.12	0.50
2:J:2020:GLN:HE21	2:J:2020:GLN:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:2020:GLN:HA	3:K:2020:GLN:HE21	1.76	0.50
3:L:1170:ILE:HA	3:L:1221:MET:CE	2.40	0.50
1:B:247:ARG:HD3	1:B:261:GLN:NE2	2.27	0.50
1:B:677:TYR:CZ	1:B:702:LYS:HD2	2.47	0.50
1:D:1790:ASN:O	1:D:1816:LYS:NZ	2.42	0.50
1:E:1760:THR:O	1:E:1762:GLU:HG3	2.12	0.50
3:H:109:LEU:HD21	3:H:116:LEU:HD13	1.94	0.50
3:I:357:ASN:HB3	3:I:365:GLN:OE1	2.11	0.50
1:B:1066:ASN:HD22	1:B:1071:PRO:HA	1.77	0.50
1:B:1842:VAL:O	1:B:1842:VAL:HG22	2.12	0.50
1:E:982:ILE:HD13	3:K:955:GLU:HB2	1.93	0.50
2:G:747:HIS:HE1	2:G:780:TYR:OH	1.95	0.50
2:J:1881:ARG:HD3	2:J:1882:THR:N	2.27	0.50
3:L:357:ASN:HB3	3:L:365:GLN:OE1	2.12	0.50
1:A:981:GLU:CD	2:G:962:LYS:HE2	2.37	0.50
1:A:1637:ARG:HG2	1:A:1660:TYR:OH	2.12	0.50
1:D:658:LEU:HD21	1:D:912:GLU:HB3	1.94	0.50
1:F:706:THR:HB	1:F:737:PHE:HB3	1.92	0.50
3:H:376:ASN:C	3:H:376:ASN:ND2	2.65	0.50
3:H:1170:ILE:HA	3:H:1221:MET:CE	2.41	0.50
3:I:1852:TYR:N	3:I:1904:LEU:HD13	2.27	0.50
1:B:793:ARG:HA	1:B:797:THR:CG2	2.42	0.49
1:C:792:HIS:HD2	1:C:842:SER:OG	1.94	0.49
1:F:193:GLU:OE2	1:F:225:SER:HB2	2.12	0.49
3:H:576:LYS:HE2	12:H:2219:HOH:O	2.12	0.49
3:K:1736:MET:HG2	3:K:1751:ILE:HD12	1.94	0.49
3:L:499:THR:OG1	3:L:500:HIS:HD2	1.95	0.49
1:A:267:VAL:HG12	1:A:290:MET:CE	2.42	0.49
1:A:417:TYR:CE2	1:A:421:ILE:CD1	2.95	0.49
2:G:419:ARG:CZ	2:G:419:ARG:HB2	2.43	0.49
2:G:1590:ARG:NH2	2:G:1594:GLU:OE2	2.44	0.49
2:G:1782:THR:HG21	2:G:1827:LEU:HG	1.94	0.49
3:K:1946:GLU:O	3:K:1946:GLU:HG2	2.11	0.49
3:L:896:ASN:HD21	3:L:906:THR:HG21	1.76	0.49
3:L:1107:SER:OG	3:L:1109:VAL:HG22	2.12	0.49
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.47	0.49
1:B:1234:MET:CE	1:B:1326:ILE:HG21	2.42	0.49
1:B:1637:ARG:HG2	1:B:1660:TYR:OH	2.12	0.49
1:B:1851:LEU:H	1:B:1851:LEU:CD2	2.13	0.49
1:F:267:VAL:HG12	1:F:290:MET:CE	2.43	0.49
3:H:1418:ASP:HB2	3:H:1421:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:ASN:HD22	1:A:1247:SER:H	1.60	0.49
1:A:1760:THR:O	1:A:1762:GLU:HG3	2.12	0.49
1:B:417:TYR:CE2	1:B:421:ILE:CD1	2.95	0.49
1:B:1016:GLU:OE1	1:D:1515:ARG:NH2	2.46	0.49
1:C:780:GLU:OE1	1:D:857:SER:OG	2.29	0.49
1:D:417:TYR:CE2	1:D:421:ILE:CD1	2.95	0.49
1:E:806:VAL:HG22	1:E:862:LEU:HD11	1.94	0.49
2:G:1852:TYR:N	2:G:1904:LEU:HD13	2.27	0.49
2:G:2020:GLN:HA	2:G:2020:GLN:HE21	1.76	0.49
3:H:297:ARG:O	3:H:301:THR:CG2	2.56	0.49
3:H:1890:ASN:HB2	3:H:1899:VAL:HB	1.94	0.49
3:K:1107:SER:OG	3:K:1109:VAL:HG22	2.12	0.49
1:A:267:VAL:HG12	1:A:290:MET:HE3	1.94	0.49
1:D:267:VAL:HG12	1:D:290:MET:CE	2.42	0.49
1:D:1857:LYS:O	1:D:1861:GLU:HG3	2.12	0.49
1:E:1066:ASN:HD22	1:E:1071:PRO:HA	1.77	0.49
2:G:467:ASP:OD1	2:G:469:ARG:HG3	2.12	0.49
2:G:2036:GLU:HB2	2:G:2037:PRO:HD3	1.94	0.49
3:H:357:ASN:HB3	3:H:365:GLN:OE1	2.12	0.49
3:I:2020:GLN:HA	3:I:2020:GLN:HE21	1.76	0.49
2:J:777:THR:HG23	2:J:1081:HIS:NE2	2.28	0.49
2:J:1852:TYR:N	2:J:1904:LEU:HD13	2.27	0.49
3:L:109:LEU:CD2	3:L:535:ILE:HD13	2.43	0.49
3:L:1852:TYR:N	3:L:1904:LEU:HD13	2.28	0.49
1:A:48:GLY:HA3	2:G:1667:THR:OG1	2.12	0.49
1:A:1790:ASN:O	1:A:1816:LYS:NZ	2.42	0.49
1:D:738:ASN:ND2	7:D:1923:A2P:HN62	2.10	0.49
1:E:1813:TRP:CZ3	1:E:1834:LEU:HD12	2.47	0.49
2:G:1990:SER:O	2:G:1994:LYS:HD3	2.13	0.49
3:H:1932:SER:HB2	3:H:1936:VAL:HG13	1.93	0.49
1:C:793:ARG:HA	1:C:797:THR:CG2	2.43	0.49
1:C:1264:ARG:NH1	1:C:1270:VAL:HB	2.28	0.49
1:C:1577:GLN:NE2	1:C:1591:TRP:HB3	2.27	0.49
1:D:1066:ASN:HD22	1:D:1071:PRO:HA	1.76	0.49
2:G:1944:ILE:O	2:G:1948:SER:HB3	2.12	0.49
3:I:455:ILE:HG13	3:I:455:ILE:O	2.12	0.49
3:I:1107:SER:OG	3:I:1109:VAL:HG22	2.12	0.49
3:I:1149:TRP:CD1	3:I:1213:LEU:HD21	2.46	0.49
3:I:1953:VAL:HG23	3:I:1953:VAL:O	2.13	0.49
3:L:1590:ARG:NH2	3:L:1594:GLU:OE2	2.43	0.49
1:A:806:VAL:HG22	1:A:862:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:TYR:CE2	1:C:421:ILE:CD1	2.96	0.49
2:G:530:ALA:O	2:G:544:LYS:HE3	2.12	0.49
2:G:1107:SER:OG	2:G:1109:VAL:HG22	2.12	0.49
3:H:173:LEU:HD21	3:H:188:ILE:HD12	1.95	0.49
3:H:1339:PHE:N	3:H:1340:PRO:CD	2.76	0.49
3:H:1740:THR:OG1	3:H:1747:LYS:HE3	2.12	0.49
3:H:2020:GLN:HA	3:H:2020:GLN:HE21	1.77	0.49
3:I:499:THR:OG1	3:I:500:HIS:HD2	1.96	0.49
3:L:33:LEU:HD23	3:L:68:VAL:HG22	1.95	0.49
1:A:1234:MET:CE	1:A:1326:ILE:HG21	2.43	0.49
1:E:792:HIS:HD2	1:E:842:SER:OG	1.95	0.49
1:F:527:GLN:HE22	1:F:599:MET:HB2	1.77	0.49
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.76	0.49
3:I:1170:ILE:HA	3:I:1221:MET:CE	2.42	0.49
3:I:1590:ARG:NH2	3:I:1594:GLU:OE2	2.44	0.49
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.75	0.49
3:K:357:ASN:HB3	3:K:365:GLN:OE1	2.12	0.49
3:L:264:ARG:NE	3:L:456:GLN:HB2	2.26	0.49
3:L:1808:J8W:OG	3:L:1809:LEU:N	2.41	0.49
1:A:677:TYR:CZ	1:A:702:LYS:HD2	2.48	0.49
1:A:1264:ARG:NH1	1:A:1270:VAL:HB	2.28	0.49
1:E:157:HIS:O	1:E:160:LYS:HD2	2.13	0.49
1:E:267:VAL:HG12	1:E:290:MET:HE3	1.94	0.49
1:E:417:TYR:CE2	1:E:421:ILE:CD1	2.96	0.49
1:F:247:ARG:HD3	1:F:261:GLN:NE2	2.28	0.49
2:G:777:THR:HG23	2:G:1081:HIS:NE2	2.28	0.49
2:G:1495:THR:O	2:G:1496:LYS:HB2	2.11	0.49
3:H:777:THR:HG23	3:H:1081:HIS:NE2	2.28	0.49
3:H:1953:VAL:HG23	3:H:1953:VAL:O	2.13	0.49
3:I:597:MET:HA	10:I:2101:FMN:C5A	2.43	0.49
2:J:376:ASN:C	2:J:376:ASN:ND2	2.64	0.49
3:L:467:ASP:OD1	3:L:469:ARG:HG3	2.13	0.49
3:L:1890:ASN:HB2	3:L:1899:VAL:HB	1.93	0.49
1:B:806:VAL:HG22	1:B:862:LEU:HD11	1.95	0.48
1:C:267:VAL:HG12	1:C:290:MET:CE	2.43	0.48
1:C:1022:THR:HG21	1:C:1388:MET:HE3	1.94	0.48
1:D:59:ARG:HD3	2:J:1896:GLN:NE2	2.27	0.48
1:D:1373:ARG:O	1:D:1547:LYS:HE3	2.13	0.48
1:D:1637:ARG:HG2	1:D:1660:TYR:OH	2.12	0.48
2:G:430:HIS:CE1	2:G:431:LEU:HD13	2.48	0.48
3:H:1129:ALA:HA	3:H:1133:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:467:ASP:OD1	3:K:469:ARG:HG3	2.13	0.48
3:K:747:HIS:HE1	3:K:780:TYR:OH	1.94	0.48
1:A:1544:THR:O	1:A:1545:SER:HB3	2.13	0.48
1:B:1857:LYS:O	1:B:1861:GLU:HG3	2.13	0.48
1:C:1234:MET:CE	1:C:1326:ILE:HG21	2.43	0.48
1:C:1302:VAL:HG22	1:F:1302:VAL:CG2	2.43	0.48
1:C:1637:ARG:HG2	1:C:1660:TYR:OH	2.13	0.48
1:E:17:LEU:CD2	3:K:2012:PRO:HG2	2.43	0.48
1:F:1540:SER:HA	1:F:1575:VAL:HG22	1.95	0.48
3:H:481:ASP:OD2	3:H:485:ARG:NH1	2.46	0.48
3:H:1107:SER:OG	3:H:1109:VAL:HG22	2.12	0.48
3:I:1339:PHE:N	3:I:1340:PRO:CD	2.76	0.48
3:I:1890:ASN:HB2	3:I:1899:VAL:HB	1.95	0.48
2:J:499:THR:OG1	2:J:500:HIS:HD2	1.96	0.48
2:J:1890:ASN:HB2	2:J:1899:VAL:HB	1.93	0.48
3:K:1022:ASP:OD2	3:K:1024:ARG:NH1	2.46	0.48
3:K:1170:ILE:HA	3:K:1221:MET:CE	2.43	0.48
3:L:234:ILE:N	3:L:235:PRO:CD	2.76	0.48
3:L:1738:PHE:CE1	3:L:1751:ILE:HD13	2.48	0.48
1:A:782:GLU:O	1:F:808:LYS:HE2	2.13	0.48
1:B:1531:LEU:HD21	1:B:1660:TYR:CZ	2.48	0.48
1:F:267:VAL:HG12	1:F:290:MET:HE3	1.95	0.48
1:F:1637:ARG:HG2	1:F:1660:TYR:OH	2.13	0.48
2:G:77:VAL:HG23	2:G:81:ASP:OD2	2.13	0.48
3:H:1590:ARG:NH2	3:H:1594:GLU:OE2	2.44	0.48
3:K:481:ASP:OD2	3:K:485:ARG:NH1	2.46	0.48
1:B:632:ARG:O	1:B:633:GLU:HB2	2.14	0.48
1:D:1234:MET:CE	1:D:1326:ILE:HG21	2.42	0.48
2:G:499:THR:OG1	2:G:500:HIS:HD2	1.96	0.48
3:H:621:GLY:HA2	3:H:630:MET:HE1	1.96	0.48
2:J:1775:GLN:HG3	2:J:1836:MET:HE3	1.95	0.48
3:L:1054:LEU:CB	10:L:2101:FMN:HM73	2.42	0.48
1:B:1342:GLU:HG3	1:D:1260:MET:HG2	1.95	0.48
1:C:632:ARG:O	1:C:633:GLU:HB2	2.13	0.48
1:C:1657:HIS:ND1	1:C:1658:PRO:HD2	2.29	0.48
3:I:964:LEU:H	3:I:964:LEU:CD2	2.18	0.48
2:J:1962:ARG:HB3	2:J:1962:ARG:NH2	2.28	0.48
3:L:376:ASN:C	3:L:376:ASN:ND2	2.64	0.48
3:L:455:ILE:HG13	3:L:455:ILE:O	2.13	0.48
3:L:1962:ARG:NH2	3:L:1967:ILE:HD12	2.28	0.48
1:B:267:VAL:HG12	1:B:290:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:HG12	1:C:290:MET:HE3	1.95	0.48
1:F:43:ARG:O	3:L:1662:THR:HA	2.14	0.48
2:G:1890:ASN:HB2	2:G:1899:VAL:HB	1.95	0.48
2:G:1976:PHE:CD2	11:G:2102:MLI:H12	2.48	0.48
3:H:455:ILE:HG13	3:H:455:ILE:O	2.13	0.48
2:J:1886:VAL:HG23	2:J:1906:ALA:CB	2.42	0.48
3:K:159:ILE:HA	3:K:271:THR:O	2.14	0.48
3:L:481:ASP:OD2	3:L:485:ARG:NH1	2.46	0.48
1:B:67:SER:OG	2:G:355:LYS:HE3	2.14	0.48
1:C:1302:VAL:CG2	1:F:1302:VAL:HG22	2.44	0.48
1:C:1507:GLN:HE22	1:F:1500:GLN:HA	1.79	0.48
1:D:67:SER:HB3	3:L:355:LYS:HE3	1.95	0.48
1:E:1531:LEU:HD21	1:E:1660:TYR:CZ	2.48	0.48
1:F:1857:LYS:HG3	1:F:1858:ALA:H	1.77	0.48
3:H:467:ASP:OD1	3:H:469:ARG:HG3	2.13	0.48
3:H:1229:MET:HE2	3:H:1268:LYS:O	2.13	0.48
3:I:1736:MET:HG2	3:I:1751:ILE:HD12	1.95	0.48
2:J:285:GLU:OE1	2:J:298:LYS:HE2	2.13	0.48
2:J:467:ASP:OD1	2:J:469:ARG:HG3	2.13	0.48
2:J:1808:SER:OG	2:J:1809:LEU:N	2.41	0.48
2:J:1886:VAL:CG2	2:J:1906:ALA:CB	2.91	0.48
3:K:1175:LYS:O	3:K:1180:MET:HE1	2.13	0.48
1:A:359:ARG:NH1	1:C:1153:ASP:OD2	2.46	0.48
1:A:807:LYS:HD3	1:A:807:LYS:C	2.39	0.48
1:B:508:ASN:C	1:B:508:ASN:ND2	2.33	0.48
1:E:1790:ASN:O	1:E:1816:LYS:NZ	2.40	0.48
2:G:494:THR:HG23	2:G:520:LYS:NZ	2.29	0.48
2:G:896:ASN:HD21	2:G:906:THR:HG21	1.78	0.48
3:H:234:ILE:N	3:H:235:PRO:CD	2.77	0.48
3:I:159:ILE:HA	3:I:271:THR:O	2.13	0.48
2:J:481:ASP:OD2	2:J:485:ARG:NH1	2.47	0.48
2:J:1590:ARG:NH2	2:J:1594:GLU:OE2	2.43	0.48
3:L:1697:HIS:HE1	3:L:1829:GLU:OE1	1.97	0.48
1:A:21:GLN:NE2	2:G:1808:SER:O	2.47	0.48
1:C:329:GLU:HB2	1:C:332:THR:CG2	2.44	0.48
2:G:1162:ASP:O	2:G:1163:LYS:HB2	2.13	0.48
3:H:159:ILE:HA	3:H:271:THR:O	2.14	0.48
3:K:455:ILE:HG13	3:K:455:ILE:O	2.13	0.48
3:K:526:ARG:NH2	3:K:546:GLU:OE2	2.46	0.48
3:K:777:THR:HG23	3:K:1081:HIS:NE2	2.27	0.48
3:K:1339:PHE:N	3:K:1340:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1593:ILE:HD11	3:K:1640:PHE:CD1	2.49	0.48
1:A:1271:GLN:HG2	12:A:2025:HOH:O	2.14	0.48
1:A:1546:THR:CG2	4:F:1901:PNS:O40	2.61	0.48
1:B:1657:HIS:ND1	1:B:1658:PRO:HD2	2.29	0.48
1:D:267:VAL:HG12	1:D:290:MET:HE3	1.95	0.48
1:D:1544:THR:O	1:D:1545:SER:HB3	2.14	0.48
1:E:247:ARG:HD3	1:E:261:GLN:NE2	2.29	0.48
1:E:807:LYS:C	1:E:807:LYS:HD3	2.39	0.48
1:E:1234:MET:CE	1:E:1326:ILE:HG21	2.44	0.48
1:F:1544:THR:O	1:F:1545:SER:HB3	2.14	0.48
2:G:159:ILE:HA	2:G:271:THR:O	2.13	0.48
2:G:1697:HIS:HE1	2:G:1829:GLU:OE1	1.97	0.48
3:I:1932:SER:CB	3:I:1935:GLU:OE1	2.62	0.48
2:J:177:TYR:OH	2:J:220:GLU:OE2	2.31	0.48
2:J:1808:SER:OG	11:J:2102:MLI:C2	2.61	0.48
3:K:1162:ASP:O	3:K:1163:LYS:HB2	2.14	0.48
1:A:1342:GLU:HG3	1:E:1260:MET:HG2	1.94	0.47
1:B:1271:GLN:OE1	5:B:1910:EDO:H11	2.13	0.47
1:C:808:LYS:HE2	1:D:782:GLU:O	2.13	0.47
1:D:329:GLU:HA	1:D:332:THR:CG2	2.44	0.47
1:E:1544:THR:O	1:E:1545:SER:HB3	2.13	0.47
2:G:285:GLU:OE1	2:G:298:LYS:HE2	2.14	0.47
2:G:526:ARG:NH2	2:G:546:GLU:OE2	2.47	0.47
3:H:99:ASN:HD21	3:H:549:ASP:HA	1.79	0.47
3:H:1881:ARG:NH2	3:H:1941:PHE:CG	2.82	0.47
2:J:234:ILE:N	2:J:235:PRO:CD	2.77	0.47
3:K:1890:ASN:HB2	3:K:1899:VAL:HB	1.94	0.47
3:L:285:GLU:HG3	3:L:455:ILE:HG22	1.96	0.47
1:A:808:LYS:HE3	1:F:782:GLU:HB2	1.95	0.47
1:B:533:GLY:O	1:B:537:LYS:HE3	2.14	0.47
1:B:724:LYS:HD3	1:B:725:TYR:CZ	2.49	0.47
1:C:724:LYS:HD3	1:C:725:TYR:CZ	2.49	0.47
3:H:1697:HIS:HE1	3:H:1829:GLU:OE1	1.97	0.47
3:H:1927:LEU:HA	3:H:1931:LEU:HB2	1.96	0.47
3:I:467:ASP:OD1	3:I:469:ARG:HG3	2.13	0.47
3:I:730:LEU:C	3:I:730:LEU:CD1	2.87	0.47
3:I:2015:THR:O	3:I:2015:THR:OG1	2.26	0.47
1:C:1260:MET:HG2	1:F:1342:GLU:HG3	1.95	0.47
1:F:807:LYS:C	1:F:807:LYS:HD3	2.40	0.47
3:H:1162:ASP:O	3:H:1163:LYS:HB2	2.14	0.47
3:H:1578:THR:O	3:H:1578:THR:OG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:621:GLY:HA2	3:I:630:MET:HE1	1.96	0.47
2:J:159:ILE:HA	2:J:271:THR:O	2.14	0.47
2:J:173:LEU:HD21	2:J:188:ILE:HD12	1.96	0.47
2:J:681:ILE:HG21	2:J:686:PRO:HD3	1.95	0.47
3:K:785:TRP:O	3:K:788:LYS:HD3	2.13	0.47
3:L:159:ILE:HA	3:L:271:THR:O	2.14	0.47
3:L:1339:PHE:N	3:L:1340:PRO:CD	2.77	0.47
1:A:11:HIS:CE1	2:G:1996:ILE:O	2.66	0.47
1:B:807:LYS:C	1:B:807:LYS:HD3	2.39	0.47
1:E:267:VAL:HG12	1:E:290:MET:CE	2.44	0.47
1:E:1188:GLN:HA	1:E:1380:GLN:HE21	1.79	0.47
2:G:1775:GLN:HG3	2:G:1836:MET:HE3	1.96	0.47
3:K:730:LEU:C	3:K:730:LEU:CD1	2.87	0.47
1:C:1544:THR:O	1:C:1545:SER:HB3	2.14	0.47
1:D:1694:TYR:OH	2:J:1001:ASP:OD2	2.29	0.47
1:F:987:ASN:ND2	1:F:1685:TYR:OH	2.40	0.47
1:F:1531:LEU:HD21	1:F:1660:TYR:CZ	2.49	0.47
2:G:234:ILE:N	2:G:235:PRO:CD	2.77	0.47
3:H:681:ILE:HG21	3:H:686:PRO:HD3	1.97	0.47
3:H:1782:THR:HG21	3:H:1827:LEU:HG	1.96	0.47
2:J:430:HIS:CE1	2:J:431:LEU:HD13	2.50	0.47
1:C:364:GLU:OE2	1:D:365:LYS:HG3	2.14	0.47
1:C:1531:LEU:HD21	1:C:1660:TYR:CZ	2.49	0.47
1:D:1531:LEU:HD21	1:D:1660:TYR:CZ	2.49	0.47
1:E:982:ILE:HD13	3:K:955:GLU:HB3	1.97	0.47
1:F:43:ARG:HB3	3:L:1662:THR:HG22	1.96	0.47
1:F:1790:ASN:O	1:F:1816:LYS:NZ	2.43	0.47
1:F:1794:GLN:CG	1:F:1838:GLU:OE2	2.61	0.47
2:G:572:ASN:OD1	2:G:576:LYS:N	2.46	0.47
3:H:264:ARG:HA	3:H:267:LEU:HD22	1.96	0.47
2:J:1222:GLU:HG2	2:J:1235:SER:OG	2.14	0.47
3:K:670:ARG:HA	3:K:670:ARG:NE	2.30	0.47
3:K:905:ALA:HA	3:K:917:MET:SD	2.55	0.47
1:D:807:LYS:HD3	1:D:807:LYS:C	2.40	0.47
1:E:1657:HIS:ND1	1:E:1658:PRO:HD2	2.29	0.47
2:G:670:ARG:NE	2:G:670:ARG:HA	2.30	0.47
3:H:23:PRO:CD	3:H:86:LEU:CD1	2.93	0.47
3:H:499:THR:OG1	3:H:500:HIS:HD2	1.96	0.47
3:I:1852:TYR:C	3:I:1904:LEU:CD1	2.88	0.47
2:J:99:ASN:HD21	2:J:549:ASP:HA	1.79	0.47
2:J:596:GLY:N	2:J:618:GLU:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1782:THR:HG21	2:J:1827:LEU:HG	1.96	0.47
2:J:1842:VAL:O	2:J:1842:VAL:HG23	2.15	0.47
2:J:1852:TYR:C	2:J:1904:LEU:CD1	2.87	0.47
3:K:234:ILE:N	3:K:235:PRO:CD	2.77	0.47
3:K:376:ASN:C	3:K:376:ASN:ND2	2.64	0.47
3:K:430:HIS:CE1	3:K:431:LEU:HD13	2.50	0.47
3:K:1697:HIS:HE1	3:K:1829:GLU:OE1	1.98	0.47
3:K:1926:GLU:O	3:K:1930:SER:OG	2.21	0.47
3:K:1962:ARG:NH2	3:K:1967:ILE:HG12	2.29	0.47
3:L:596:GLY:N	3:L:618:GLU:HB2	2.30	0.47
1:B:1825:VAL:HG11	1:B:1858:ALA:HB1	1.97	0.47
1:F:1657:HIS:ND1	1:F:1658:PRO:HD2	2.30	0.47
2:G:543:PHE:HB2	2:G:545:GLN:OE1	2.14	0.47
2:G:596:GLY:N	2:G:618:GLU:HB2	2.30	0.47
2:G:1054:LEU:CB	10:G:2101:FMN:HM73	2.43	0.47
2:G:1852:TYR:C	2:G:1904:LEU:CD1	2.88	0.47
3:H:1319:MET:HB3	3:H:1368:VAL:CG2	2.45	0.47
3:H:1775:GLN:HG3	3:H:1836:MET:HE3	1.97	0.47
3:I:526:ARG:NH2	3:I:546:GLU:OE2	2.47	0.47
3:I:1775:GLN:HG3	3:I:1836:MET:HE3	1.97	0.47
2:J:264:ARG:HA	2:J:267:LEU:HD22	1.97	0.47
2:J:1697:HIS:HE1	2:J:1829:GLU:OE1	1.97	0.47
3:L:99:ASN:HD21	3:L:549:ASP:HA	1.80	0.47
1:B:1540:SER:HA	1:B:1575:VAL:HG22	1.97	0.47
1:D:1494:HIS:HE1	1:D:1874:ASP:OD2	1.98	0.47
1:D:1657:HIS:ND1	1:D:1658:PRO:HD2	2.30	0.47
1:E:1436:VAL:HG13	1:E:1436:VAL:O	2.14	0.47
1:F:1494:HIS:HE1	1:F:1874:ASP:OD2	1.98	0.47
2:G:455:ILE:HG13	2:G:455:ILE:O	2.13	0.47
2:G:867:GLU:O	2:G:871:THR:HB	2.15	0.47
2:G:1222:GLU:HG2	2:G:1235:SER:OG	2.14	0.47
3:H:430:HIS:CE1	3:H:431:LEU:HD13	2.50	0.47
3:I:1697:HIS:HE1	3:I:1829:GLU:OE1	1.98	0.47
3:L:905:ALA:HA	3:L:917:MET:SD	2.55	0.47
3:L:1852:TYR:C	3:L:1904:LEU:CD1	2.88	0.47
1:B:808:LYS:HE2	1:E:782:GLU:O	2.15	0.47
1:C:247:ARG:HD3	1:C:261:GLN:NE2	2.30	0.47
1:C:1540:SER:HA	1:C:1575:VAL:HG22	1.96	0.47
1:D:1264:ARG:NH1	1:D:1270:VAL:HB	2.30	0.47
1:F:157:HIS:O	1:F:160:LYS:HD2	2.15	0.47
2:G:598:THR:O	2:G:602:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:621:GLY:HA2	2:G:630:MET:HE1	1.96	0.47
3:I:481:ASP:OD2	3:I:485:ARG:NH1	2.47	0.47
2:J:543:PHE:HB2	2:J:545:GLN:OE1	2.15	0.47
3:K:167:ASP:OD1	3:K:167:ASP:N	2.45	0.47
3:L:597:MET:HA	10:L:2101:FMN:C5A	2.45	0.47
3:L:670:ARG:NE	3:L:670:ARG:HA	2.29	0.47
3:L:1775:GLN:HG3	3:L:1836:MET:HE3	1.97	0.47
3:L:1946:GLU:CA	3:L:1950:LYS:HE3	2.44	0.47
1:A:982:ILE:HD12	2:G:965:SER:HA	1.97	0.46
1:F:724:LYS:HD3	1:F:725:TYR:CZ	2.50	0.46
7:F:1912:A2P:H1'	7:F:1912:A2P:O4P	2.14	0.46
3:H:526:ARG:NH2	3:H:546:GLU:OE2	2.47	0.46
2:J:29:ILE:HD13	2:J:82:GLN:NE2	2.29	0.46
2:J:285:GLU:HG3	2:J:455:ILE:HG22	1.97	0.46
3:K:155:GLN:HG3	3:K:268:LYS:HE3	1.97	0.46
1:B:1436:VAL:O	1:B:1436:VAL:HG13	2.15	0.46
1:F:1436:VAL:HG13	1:F:1436:VAL:O	2.14	0.46
3:H:1736:MET:HG2	3:H:1751:ILE:HD12	1.96	0.46
3:I:543:PHE:HB2	3:I:545:GLN:OE1	2.15	0.46
2:J:881:VAL:O	2:J:885:GLU:HG3	2.15	0.46
2:J:1281:PRO:O	2:J:1378:ILE:HG23	2.15	0.46
3:K:1782:THR:HG21	3:K:1827:LEU:HG	1.97	0.46
3:L:543:PHE:HB2	3:L:545:GLN:OE1	2.15	0.46
1:B:789:GLU:OE1	1:E:793:ARG:NH1	2.48	0.46
1:B:1455:ARG:HD2	1:B:1455:ARG:HA	1.78	0.46
1:C:807:LYS:C	1:C:807:LYS:HD3	2.39	0.46
1:D:1436:VAL:O	1:D:1436:VAL:HG13	2.15	0.46
1:E:1264:ARG:NH1	1:E:1270:VAL:HB	2.30	0.46
1:F:294:TYR:CE1	1:F:298:VAL:HG21	2.51	0.46
3:H:1916:PHE:HE2	3:H:1943:ILE:CD1	2.26	0.46
3:I:234:ILE:N	3:I:235:PRO:CD	2.77	0.46
3:I:264:ARG:HA	3:I:267:LEU:HD22	1.98	0.46
3:I:670:ARG:NE	3:I:670:ARG:HA	2.30	0.46
2:J:1479:ILE:HD11	2:J:1512:HIS:CE1	2.51	0.46
3:K:1842:VAL:HG23	3:K:1842:VAL:O	2.14	0.46
1:B:2:LYS:HD3	3:H:2050:GLN:HA	1.96	0.46
1:B:1114:TYR:CE1	1:B:1337:GLU:HG3	2.50	0.46
1:B:1544:THR:O	1:B:1545:SER:HB3	2.14	0.46
1:C:1755:MET:HG2	1:C:1870:SER:HB3	1.97	0.46
1:D:247:ARG:HD3	1:D:261:GLN:NE2	2.30	0.46
1:D:793:ARG:HA	1:D:797:THR:CG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1189:ILE:H	1:E:1380:GLN:NE2	2.12	0.46
1:E:1540:SER:HA	1:E:1575:VAL:HG22	1.96	0.46
2:G:1842:VAL:O	2:G:1842:VAL:HG23	2.15	0.46
3:H:543:PHE:HB2	3:H:545:GLN:OE1	2.15	0.46
3:H:1808:J8W:OG	3:H:1809:LEU:N	2.41	0.46
2:J:1593:ILE:HD11	2:J:1640:PHE:CD1	2.50	0.46
3:K:1775:GLN:CG	3:K:1836:MET:HE3	2.46	0.46
1:A:1540:SER:HA	1:A:1575:VAL:HG22	1.97	0.46
1:C:1455:ARG:HA	1:C:1455:ARG:HD2	1.77	0.46
3:H:596:GLY:N	3:H:618:GLU:HB2	2.30	0.46
3:H:1842:VAL:HG23	3:H:1842:VAL:O	2.16	0.46
3:K:110:GLN:HG3	3:K:535:ILE:HD11	1.96	0.46
3:L:1927:LEU:HA	3:L:1931:LEU:HB2	1.97	0.46
1:A:1068:LYS:CD	1:A:1068:LYS:N	2.79	0.46
1:A:1436:VAL:O	1:A:1436:VAL:HG13	2.14	0.46
1:B:20:TYR:CE2	3:H:2033:THR:CG2	2.99	0.46
1:C:1500:GLN:CG	1:F:1507:GLN:HE22	2.28	0.46
1:E:1167:LEU:CD1	1:E:1171:ALA:HB1	2.46	0.46
2:G:214:ASN:C	2:G:214:ASN:HD22	2.22	0.46
3:H:670:ARG:HA	3:H:670:ARG:NE	2.30	0.46
3:I:596:GLY:N	3:I:618:GLU:HB2	2.30	0.46
2:J:526:ARG:NH2	2:J:546:GLU:OE2	2.48	0.46
2:J:905:ALA:HA	2:J:917:MET:SD	2.55	0.46
3:K:264:ARG:HA	3:K:267:LEU:HD22	1.98	0.46
3:K:1170:ILE:HG12	3:K:1221:MET:HE3	1.96	0.46
3:K:1177:SER:N	3:K:1180:MET:CE	2.77	0.46
3:L:1323:MET:HE2	3:L:1590:ARG:HE	1.80	0.46
1:B:1875:ASP:OD1	1:B:1875:ASP:N	2.45	0.46
1:D:1825:VAL:HG11	1:D:1858:ALA:HB1	1.98	0.46
1:E:1114:TYR:CE1	1:E:1337:GLU:HG3	2.51	0.46
2:G:173:LEU:HD21	2:G:188:ILE:HD12	1.98	0.46
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.48	0.46
3:H:663:ILE:HB	3:H:664:PRO:HD3	1.98	0.46
2:J:867:GLU:O	2:J:871:THR:HB	2.15	0.46
2:J:1054:LEU:CB	10:J:2101:FMN:HM73	2.42	0.46
3:K:598:THR:OG1	3:K:599:PRO:HD2	2.15	0.46
3:K:867:GLU:O	3:K:871:THR:HB	2.16	0.46
3:L:663:ILE:HB	3:L:664:PRO:HD3	1.98	0.46
1:B:2:LYS:O	1:B:5:VAL:HG23	2.15	0.46
1:B:479:ASN:O	1:B:483:VAL:CG2	2.64	0.46
1:B:1500:GLN:HG2	1:D:1507:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:878:MET:HE2	1:F:878:MET:HB2	1.87	0.46
1:F:1232:TYR:CZ	1:F:1705:PRO:HD3	2.51	0.46
2:G:376:ASN:C	2:G:376:ASN:ND2	2.64	0.46
2:G:1915:ASN:N	2:G:1915:ASN:HD22	2.14	0.46
2:G:1927:LEU:HD13	2:G:1931:LEU:HD22	1.98	0.46
3:I:430:HIS:CE1	3:I:431:LEU:HD13	2.51	0.46
3:I:905:ALA:HA	3:I:917:MET:SD	2.56	0.46
3:L:430:HIS:CE1	3:L:431:LEU:HD13	2.50	0.46
1:A:793:ARG:NH1	1:F:789:GLU:OE1	2.48	0.46
1:B:1790:ASN:O	1:B:1816:LYS:NZ	2.43	0.46
1:B:1842:VAL:O	1:B:1842:VAL:CG2	2.64	0.46
1:E:724:LYS:CG	1:E:725:TYR:CD2	2.94	0.46
3:I:1162:ASP:O	3:I:1163:LYS:HB2	2.14	0.46
3:I:1435:ILE:CG2	3:I:1441:ILE:HG22	2.46	0.46
2:J:1954:LYS:HB3	2:J:1955:PRO:HD2	1.98	0.46
2:J:1955:PRO:O	2:J:1958:LEU:HB3	2.15	0.46
3:K:173:LEU:HD21	3:K:188:ILE:HD12	1.98	0.46
3:L:621:GLY:HA2	3:L:630:MET:HE1	1.97	0.46
1:C:833:PHE:O	1:C:937:LYS:NZ	2.42	0.46
1:E:616:LEU:N	1:E:617:PRO:HD2	2.31	0.46
1:E:1129:GLU:O	1:E:1130:ASP:C	2.59	0.46
3:I:1054:LEU:CB	10:I:2101:FMN:HM73	2.46	0.46
3:I:1718:THR:HB	3:I:1763:THR:OG1	2.16	0.46
3:I:1782:THR:HG21	3:I:1827:LEU:HG	1.97	0.46
2:J:1170:ILE:HA	2:J:1221:MET:CE	2.42	0.46
3:K:681:ILE:HG21	3:K:686:PRO:HD3	1.98	0.46
3:K:1054:LEU:HB2	10:K:2101:FMN:C7M	2.45	0.46
1:A:632:ARG:O	1:A:633:GLU:HB3	2.17	0.45
1:B:20:TYR:CG	3:H:2033:THR:HG23	2.52	0.45
1:B:1358:HIS:NE2	8:B:1902:ACT:H3	2.31	0.45
1:C:413:LEU:C	1:C:413:LEU:HD13	2.41	0.45
1:C:658:LEU:HD21	1:C:912:GLU:HB3	1.97	0.45
1:C:1204:ILE:O	1:C:1208:VAL:HB	2.16	0.45
2:G:1281:PRO:O	2:G:1378:ILE:HG23	2.16	0.45
2:G:1651:LEU:HD23	2:G:1651:LEU:HA	1.87	0.45
3:H:1040:LEU:HD21	3:H:1048:VAL:HG13	1.99	0.45
3:H:1926:GLU:O	3:H:1930:SER:OG	2.21	0.45
3:K:596:GLY:N	3:K:618:GLU:HB2	2.30	0.45
3:K:1775:GLN:HE22	3:K:1839:GLN:HG3	1.80	0.45
3:L:407:ILE:N	3:L:407:ILE:CD1	2.78	0.45
1:A:1494:HIS:HE1	1:A:1874:ASP:OD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1264:ARG:NH1	1:B:1270:VAL:HB	2.31	0.45
2:G:264:ARG:HA	2:G:267:LEU:HD22	1.97	0.45
3:H:372:ASN:HB3	3:H:515:LEU:HD21	1.98	0.45
3:H:932:ILE:HD12	3:H:1042:ALA:HA	1.97	0.45
3:I:109:LEU:HD21	3:I:116:LEU:HD13	1.97	0.45
2:J:670:ARG:NE	2:J:670:ARG:HA	2.32	0.45
3:L:113:ASP:OD1	3:L:113:ASP:N	2.49	0.45
3:L:730:LEU:C	3:L:730:LEU:CD1	2.87	0.45
1:A:1776:ILE:HG13	1:A:1807:SER:HA	1.97	0.45
1:B:411:GLN:HE22	1:B:1628:SER:N	2.14	0.45
1:C:1342:GLU:HG3	1:F:1260:MET:HG2	1.97	0.45
1:E:1494:HIS:HE1	1:E:1874:ASP:OD2	1.99	0.45
3:I:6:THR:O	3:I:7:ARG:CB	2.65	0.45
3:I:904:PHE:HB2	3:I:1017:PHE:CD2	2.52	0.45
3:I:943:TRP:O	3:I:947:THR:HG23	2.17	0.45
3:K:113:ASP:N	3:K:113:ASP:OD1	2.50	0.45
3:L:1022:ASP:OD2	3:L:1024:ARG:NH1	2.49	0.45
3:L:1966:CYS:C	3:L:1967:ILE:HD13	2.41	0.45
1:A:20:TYR:CD1	2:G:2033:THR:HG23	2.51	0.45
1:A:1515:ARG:NH2	1:E:1016:GLU:OE1	2.47	0.45
1:B:360:LYS:NZ	1:E:358:GLU:OE2	2.45	0.45
1:C:1494:HIS:HE1	1:C:1874:ASP:OD2	2.00	0.45
1:D:1014:ASP:N	1:D:1510:ASN:HD21	2.14	0.45
1:D:1114:TYR:CE1	1:D:1337:GLU:HG3	2.51	0.45
1:D:1540:SER:HA	1:D:1575:VAL:HG22	1.99	0.45
1:E:1766:ASN:N	1:E:1766:ASN:OD1	2.50	0.45
1:F:1826:LYS:C	1:F:1827:SER:O	2.59	0.45
3:H:867:GLU:O	3:H:871:THR:HB	2.16	0.45
3:H:905:ALA:HA	3:H:917:MET:SD	2.57	0.45
3:I:173:LEU:HD21	3:I:188:ILE:HD12	1.99	0.45
2:J:109:LEU:HD21	2:J:116:LEU:CD2	2.46	0.45
10:J:2101:FMN:O3P	10:J:2101:FMN:O4'	2.30	0.45
3:K:31:SER:HA	3:K:34:GLN:HB3	1.99	0.45
3:K:99:ASN:HD21	3:K:549:ASP:HA	1.81	0.45
3:L:1782:THR:HG21	3:L:1827:LEU:HG	1.97	0.45
1:B:1483:ASN:HD21	1:B:1487:LEU:HD11	1.82	0.45
1:B:1766:ASN:N	1:B:1766:ASN:OD1	2.48	0.45
1:C:1436:VAL:HG13	1:C:1436:VAL:O	2.16	0.45
3:H:23:PRO:HG2	3:H:86:LEU:HD11	1.99	0.45
2:J:602:VAL:HG23	2:J:624:TYR:CE2	2.51	0.45
3:K:701:LYS:HD2	3:K:701:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:526:ARG:NH2	3:L:546:GLU:OE2	2.48	0.45
3:L:848:SER:OG	3:L:852:GLU:HG2	2.16	0.45
3:L:867:GLU:O	3:L:871:THR:HB	2.16	0.45
3:L:1288:LYS:N	3:L:1288:LYS:HD3	2.32	0.45
1:A:1483:ASN:HD21	1:A:1487:LEU:HD11	1.81	0.45
1:B:413:LEU:HD13	1:B:413:LEU:C	2.42	0.45
1:C:1022:THR:CG2	1:C:1226:SER:OG	2.65	0.45
1:D:694:GLN:HE21	5:D:1910:EDO:C1	2.29	0.45
1:E:1239:HIS:HD2	1:E:1241:SER:OG	1.99	0.45
1:F:868:ILE:HD11	1:F:923:MET:HE3	1.98	0.45
2:G:1593:ILE:HD11	2:G:1640:PHE:CD1	2.52	0.45
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.46	0.45
3:H:666:ILE:O	3:H:670:ARG:HB2	2.17	0.45
3:I:1842:VAL:HG23	3:I:1842:VAL:O	2.15	0.45
2:J:99:ASN:ND2	2:J:100:ASP:H	2.09	0.45
3:K:285:GLU:HG3	3:K:455:ILE:HG22	1.98	0.45
3:K:2046:GLU:CD	3:K:2046:GLU:N	2.75	0.45
3:L:666:ILE:O	3:L:670:ARG:HB2	2.17	0.45
3:L:1947:ALA:HA	3:L:1950:LYS:HG2	1.99	0.45
1:A:1441:PRO:HD2	1:E:1492:GLU:OE2	2.17	0.45
1:B:616:LEU:N	1:B:617:PRO:HD2	2.32	0.45
1:B:1129:GLU:O	1:B:1130:ASP:C	2.59	0.45
1:D:1455:ARG:HD2	1:D:1455:ARG:HA	1.78	0.45
1:E:868:ILE:HD11	1:E:923:MET:HE3	1.99	0.45
1:E:1776:ILE:HG13	1:E:1807:SER:HA	1.98	0.45
3:H:1852:TYR:C	3:H:1904:LEU:CD2	2.90	0.45
3:I:1363:ALA:O	3:I:1606:ARG:NH2	2.50	0.45
2:J:2050:GLN:HE21	2:J:2050:GLN:HB2	1.59	0.45
3:K:1590:ARG:NH2	3:K:1594:GLU:OE2	2.43	0.45
3:K:1651:LEU:HD23	3:K:1651:LEU:HA	1.86	0.45
3:L:681:ILE:HG21	3:L:686:PRO:HD3	1.97	0.45
3:L:1842:VAL:HG23	3:L:1842:VAL:O	2.16	0.45
1:A:359:ARG:NH1	1:C:1153:ASP:CG	2.75	0.45
1:A:413:LEU:C	1:A:413:LEU:HD13	2.42	0.45
1:A:1114:TYR:CE1	1:A:1337:GLU:HG3	2.52	0.45
1:B:11:HIS:CE1	3:H:1996:ILE:O	2.69	0.45
1:B:1776:ILE:HG13	1:B:1807:SER:HA	1.99	0.45
1:C:1790:ASN:O	1:C:1816:LYS:NZ	2.43	0.45
1:D:868:ILE:HD11	1:D:923:MET:HE3	1.98	0.45
1:D:1483:ASN:HD21	1:D:1487:LEU:HD11	1.81	0.45
1:F:1114:TYR:CE1	1:F:1337:GLU:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:270:ALA:O	2:G:459:VAL:HA	2.17	0.45
2:G:932:ILE:HD12	2:G:1042:ALA:HA	1.99	0.45
2:J:109:LEU:HD21	2:J:116:LEU:HD22	1.99	0.45
2:J:1348:LEU:HD12	2:J:1348:LEU:HA	1.90	0.45
2:J:2020:GLN:HA	2:J:2020:GLN:NE2	2.32	0.45
3:K:543:PHE:HB2	3:K:545:GLN:OE1	2.17	0.45
3:K:881:VAL:O	3:K:885:GLU:HG3	2.17	0.45
3:L:1782:THR:CG2	3:L:1827:LEU:HD21	2.46	0.45
1:A:173:LYS:NZ	1:A:203:GLU:OE2	2.50	0.45
1:C:1129:GLU:O	1:C:1130:ASP:C	2.59	0.45
1:C:1483:ASN:HD21	1:C:1487:LEU:HD11	1.82	0.45
1:D:413:LEU:C	1:D:413:LEU:HD13	2.42	0.45
1:D:545:GLU:OE1	1:D:545:GLU:N	2.48	0.45
1:D:1129:GLU:O	1:D:1130:ASP:C	2.59	0.45
1:D:1239:HIS:HD2	1:D:1241:SER:OG	2.00	0.45
1:E:1014:ASP:N	1:E:1510:ASN:HD21	2.14	0.45
1:E:1491:ARG:HD3	1:E:1749:THR:HG21	1.99	0.45
2:G:285:GLU:HG3	2:G:455:ILE:HG22	1.98	0.45
2:G:455:ILE:HD11	2:G:469:ARG:CG	2.43	0.45
3:H:285:GLU:HG3	3:H:455:ILE:HG22	1.99	0.45
3:H:904:PHE:HB2	3:H:1017:PHE:CD2	2.52	0.45
3:H:943:TRP:O	3:H:947:THR:HG23	2.17	0.45
3:H:1040:LEU:O	3:H:1046:GLN:HA	2.17	0.45
3:H:1381:VAL:HG13	3:H:1390:VAL:HG22	1.99	0.45
3:I:748:THR:HB	3:I:749:PRO:HD3	1.98	0.45
2:J:270:ALA:O	2:J:459:VAL:HA	2.17	0.45
2:J:943:TRP:O	2:J:947:THR:HG23	2.17	0.45
2:J:1435:ILE:CG2	2:J:1441:ILE:HG22	2.47	0.45
2:J:1904:LEU:HG	2:J:1960:LEU:HD23	1.98	0.45
3:K:372:ASN:HB3	3:K:515:LEU:HD21	1.99	0.45
1:A:533:GLY:O	1:A:537:LYS:NZ	2.50	0.45
1:A:1129:GLU:O	1:A:1130:ASP:C	2.59	0.45
1:A:1232:TYR:CZ	1:A:1705:PRO:HD3	2.52	0.45
1:B:146:LYS:HG2	1:B:214:GLN:NE2	2.32	0.45
1:B:1022:THR:CG2	1:B:1226:SER:OG	2.65	0.45
1:B:1153:ASP:CG	1:C:359:ARG:NH1	2.75	0.45
1:B:1204:ILE:O	1:B:1208:VAL:HB	2.17	0.45
1:D:1232:TYR:CZ	1:D:1705:PRO:HD3	2.51	0.45
2:G:1363:ALA:O	2:G:1606:ARG:NH2	2.50	0.45
2:G:2046:GLU:CD	2:G:2046:GLU:N	2.75	0.45
3:H:602:VAL:HG23	3:H:624:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1955:PRO:O	3:H:1958:LEU:HB3	2.17	0.45
3:H:2020:GLN:HA	3:H:2020:GLN:NE2	2.32	0.45
3:I:681:ILE:HG21	3:I:686:PRO:HD3	1.99	0.45
3:I:1229:MET:HE2	3:I:1268:LYS:O	2.16	0.45
3:I:2046:GLU:N	3:I:2046:GLU:CD	2.75	0.45
3:L:1229:MET:HE2	3:L:1268:LYS:O	2.17	0.45
1:B:1232:TYR:CZ	1:B:1705:PRO:HD3	2.52	0.44
1:C:1491:ARG:HD3	1:C:1749:THR:HG21	1.98	0.44
1:E:658:LEU:HD21	1:E:912:GLU:HB3	1.99	0.44
1:E:1232:TYR:CZ	1:E:1705:PRO:HD3	2.52	0.44
1:F:413:LEU:C	1:F:413:LEU:HD13	2.42	0.44
1:F:1239:HIS:HD2	1:F:1241:SER:OG	2.00	0.44
2:G:6:THR:OG1	2:G:7:ARG:N	2.50	0.44
2:G:666:ILE:O	2:G:670:ARG:HB2	2.17	0.44
2:G:1736:MET:HG2	2:G:1751:ILE:HD12	1.99	0.44
2:G:2020:GLN:HA	2:G:2020:GLN:NE2	2.32	0.44
3:H:270:ALA:O	3:H:459:VAL:HA	2.17	0.44
3:H:1479:ILE:HD11	3:H:1512:HIS:CE1	2.52	0.44
3:H:1718:THR:HB	3:H:1763:THR:OG1	2.17	0.44
3:H:1782:THR:CG2	3:H:1827:LEU:HD21	2.47	0.44
3:H:2046:GLU:CD	3:H:2046:GLU:N	2.75	0.44
3:I:285:GLU:HG3	3:I:455:ILE:HG22	1.99	0.44
3:I:1955:PRO:O	3:I:1958:LEU:HB3	2.17	0.44
3:I:1962:ARG:HB3	3:I:1962:ARG:NH2	2.31	0.44
2:J:2046:GLU:CD	2:J:2046:GLU:N	2.75	0.44
3:K:1363:ALA:O	3:K:1606:ARG:NH2	2.50	0.44
3:L:270:ALA:O	3:L:459:VAL:HA	2.17	0.44
3:L:1422:THR:CG2	3:L:1474:PHE:CD1	2.99	0.44
3:L:1738:PHE:HE1	3:L:1751:ILE:HD13	1.82	0.44
1:A:529:MET:HE3	1:A:637:PHE:CB	2.47	0.44
1:A:1204:ILE:O	1:A:1208:VAL:HB	2.17	0.44
1:C:509:ILE:O	1:C:878:MET:HE1	2.17	0.44
1:C:1114:TYR:CE1	1:C:1337:GLU:HG3	2.52	0.44
1:D:894:ARG:NH2	1:D:900:GLU:OE1	2.50	0.44
1:E:67:SER:CB	2:J:355:LYS:HE3	2.47	0.44
1:E:413:LEU:HD13	1:E:413:LEU:C	2.42	0.44
1:E:1129:GLU:OE1	1:F:348:ARG:HD3	2.18	0.44
1:F:1491:ARG:HD3	1:F:1749:THR:HG21	1.99	0.44
1:F:1717:ASP:C	1:F:1717:ASP:OD1	2.61	0.44
2:G:1213:LEU:HD13	2:G:1213:LEU:HA	1.85	0.44
3:I:1213:LEU:HD13	3:I:1213:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:372:ASN:HB3	2:J:515:LEU:HD21	1.99	0.44
2:J:1040:LEU:HD21	2:J:1048:VAL:HG13	1.99	0.44
2:J:1292:ILE:O	2:J:1368:VAL:O	2.36	0.44
3:K:943:TRP:O	3:K:947:THR:HG23	2.17	0.44
3:K:1222:GLU:HG2	3:K:1235:SER:OG	2.17	0.44
3:L:173:LEU:HD21	3:L:188:ILE:HD12	1.97	0.44
3:L:1130:THR:O	3:L:1178:GLN:NE2	2.50	0.44
3:L:1946:GLU:O	3:L:1950:LYS:CE	2.65	0.44
1:A:1153:ASP:OD1	1:B:359:ARG:NH1	2.49	0.44
1:B:20:TYR:CD1	3:H:2033:THR:HG23	2.52	0.44
1:B:198:PRO:HG3	1:B:212:THR:HG21	1.99	0.44
1:B:1239:HIS:HD2	1:B:1241:SER:OG	2.00	0.44
1:C:43:ARG:O	3:I:1662:THR:HA	2.17	0.44
1:C:248:LYS:HE3	1:C:248:LYS:CA	2.48	0.44
1:C:641:ARG:NH2	1:C:925:ASP:OD2	2.51	0.44
1:E:198:PRO:HG3	1:E:212:THR:HG21	1.99	0.44
1:E:1022:THR:CG2	1:E:1226:SER:OG	2.65	0.44
1:E:1204:ILE:O	1:E:1208:VAL:HB	2.17	0.44
2:G:113:ASP:N	2:G:113:ASP:OD1	2.50	0.44
2:G:905:ALA:HA	2:G:917:MET:SD	2.58	0.44
3:H:31:SER:HA	3:H:34:GLN:HB3	2.00	0.44
3:H:1363:ALA:O	3:H:1606:ARG:NH2	2.50	0.44
3:I:2020:GLN:HA	3:I:2020:GLN:NE2	2.32	0.44
3:L:1363:ALA:O	3:L:1606:ARG:NH2	2.50	0.44
1:C:868:ILE:HD11	1:C:923:MET:HE3	1.98	0.44
1:D:616:LEU:N	1:D:617:PRO:HD2	2.33	0.44
1:F:1022:THR:CG2	1:F:1226:SER:OG	2.65	0.44
2:G:31:SER:HA	2:G:34:GLN:HB3	1.99	0.44
3:H:2015:THR:O	3:H:2015:THR:OG1	2.26	0.44
3:I:1292:ILE:O	3:I:1368:VAL:O	2.36	0.44
3:K:663:ILE:HB	3:K:664:PRO:HD3	1.99	0.44
3:L:701:LYS:O	3:L:701:LYS:HD3	2.17	0.44
1:A:1239:HIS:HD2	1:A:1241:SER:OG	2.00	0.44
1:B:868:ILE:HD11	1:B:923:MET:HE3	1.98	0.44
1:D:529:MET:HE3	1:D:637:PHE:CB	2.47	0.44
1:D:1022:THR:CG2	1:D:1226:SER:OG	2.65	0.44
1:D:1153:ASP:CG	1:E:359:ARG:NH1	2.75	0.44
1:D:1776:ILE:HG13	1:D:1807:SER:HA	1.98	0.44
1:F:1129:GLU:O	1:F:1130:ASP:C	2.60	0.44
2:G:1877:ARG:HG3	2:G:1940:LEU:HD23	1.99	0.44
2:G:1955:PRO:O	2:G:1958:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1737:ILE:HG21	3:H:1748:THR:HG23	2.00	0.44
2:J:621:GLY:HA2	2:J:630:MET:HE1	2.00	0.44
2:J:1555:ARG:N	2:J:1555:ARG:HD2	2.32	0.44
3:K:451:ASN:HB3	3:K:453:LYS:HE2	1.99	0.44
3:K:748:THR:HB	3:K:749:PRO:HD3	1.99	0.44
3:K:1718:THR:HB	3:K:1763:THR:OG1	2.17	0.44
3:K:2020:GLN:HA	3:K:2020:GLN:NE2	2.32	0.44
3:L:6:THR:OG1	3:L:7:ARG:N	2.50	0.44
3:L:1180:MET:HE3	3:L:1197:LEU:HD11	2.00	0.44
1:A:682:GLY:HA2	7:A:1918:A2P:H1'	2.00	0.44
1:A:1022:THR:CG2	1:A:1226:SER:OG	2.65	0.44
1:A:1741:LYS:HE3	1:E:1435:SER:OG	2.18	0.44
1:C:1232:TYR:CZ	1:C:1705:PRO:HD3	2.52	0.44
1:D:20:TYR:CD1	2:J:2033:THR:HG23	2.53	0.44
1:D:543:ILE:HD12	1:D:543:ILE:O	2.17	0.44
1:E:1483:ASN:HD21	1:E:1487:LEU:HD11	1.83	0.44
1:F:152:HIS:CD2	1:F:168:MET:HE3	2.53	0.44
1:F:1264:ARG:NH1	1:F:1270:VAL:HB	2.33	0.44
2:G:99:ASN:HD21	2:G:549:ASP:HA	1.82	0.44
2:G:856:LYS:HD3	2:G:1052:CYS:SG	2.58	0.44
3:I:270:ALA:O	3:I:459:VAL:HA	2.17	0.44
3:I:372:ASN:HB3	3:I:515:LEU:HD21	1.99	0.44
3:I:663:ILE:HB	3:I:664:PRO:HD3	1.99	0.44
2:J:904:PHE:HB2	2:J:1017:PHE:CD2	2.52	0.44
2:J:1976:PHE:CD2	11:J:2102:MLI:H11	2.52	0.44
3:K:621:GLY:HA2	3:K:630:MET:HE1	1.99	0.44
3:L:264:ARG:HA	3:L:267:LEU:HD22	1.99	0.44
3:L:868:PHE:HB3	3:L:873:PHE:CE2	2.52	0.44
3:L:1222:GLU:HG2	3:L:1235:SER:OG	2.18	0.44
3:L:1718:THR:HB	3:L:1763:THR:OG1	2.17	0.44
1:D:411:GLN:HE22	1:D:1628:SER:N	2.14	0.44
1:E:538:GLU:O	1:E:633:GLU:HG3	2.17	0.44
1:F:1204:ILE:O	1:F:1208:VAL:HB	2.18	0.44
2:G:2044:ASN:C	2:G:2046:GLU:H	2.25	0.44
3:H:559:PRO:HB3	3:H:564:GLU:HG3	1.99	0.44
3:I:602:VAL:HG23	3:I:624:TYR:CE2	2.53	0.44
3:I:666:ILE:O	3:I:670:ARG:HB2	2.18	0.44
2:J:1782:THR:CG2	2:J:1827:LEU:HD21	2.48	0.44
1:A:181:THR:HG21	1:C:1273:ASP:HB3	2.00	0.44
1:A:1022:THR:HG23	1:A:1226:SER:OG	2.18	0.44
1:B:1494:HIS:HE1	1:B:1874:ASP:OD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:558:ASN:HD22	2:G:558:ASN:HA	1.59	0.44
2:G:1479:ILE:HD11	2:G:1512:HIS:CE1	2.52	0.44
3:H:1680:LEU:HD22	3:H:1684:SER:CB	2.48	0.44
3:I:31:SER:HA	3:I:34:GLN:HB3	2.00	0.44
3:I:464:ASP:HB3	3:I:466:SER:H	1.82	0.44
3:I:1782:THR:CG2	3:I:1827:LEU:HD21	2.48	0.44
3:K:6:THR:O	3:K:7:ARG:CB	2.65	0.44
3:K:270:ALA:O	3:K:459:VAL:HA	2.17	0.44
3:K:1435:ILE:CG2	3:K:1441:ILE:HG22	2.47	0.44
3:K:1908:ASP:OD2	3:K:1954:LYS:HE3	2.18	0.44
3:L:1040:LEU:O	3:L:1046:GLN:HA	2.18	0.44
3:L:1381:VAL:HG13	3:L:1390:VAL:HG22	2.00	0.44
3:L:1736:MET:O	3:L:1751:ILE:HG13	2.17	0.44
3:L:1960:LEU:HD13	3:L:1960:LEU:HA	1.89	0.44
3:L:2020:GLN:HA	3:L:2020:GLN:NE2	2.32	0.44
1:A:1014:ASP:N	1:A:1510:ASN:HD21	2.15	0.44
1:A:1068:LYS:N	1:A:1068:LYS:HD2	2.33	0.44
1:D:20:TYR:CE1	2:J:2033:THR:HG23	2.53	0.44
1:D:624:LYS:CG	1:D:624:LYS:O	2.66	0.44
1:E:1418:VAL:N	1:E:1419:PRO:CD	2.81	0.44
1:E:1423:LYS:O	1:E:1426:LEU:HB2	2.18	0.44
3:H:1201:VAL:HG11	3:H:1226:ASN:HB2	2.00	0.44
3:H:1479:ILE:HD13	3:H:1479:ILE:N	2.33	0.44
2:J:598:THR:OG1	2:J:599:PRO:HD2	2.17	0.44
2:J:1854:MET:HA	2:J:1907:LEU:HD21	1.99	0.44
3:K:464:ASP:HB3	3:K:466:SER:H	1.83	0.44
3:K:1172:LYS:HB2	3:K:1172:LYS:HE3	1.82	0.44
3:K:1854:MET:HA	3:K:1907:LEU:HD21	1.99	0.44
1:A:1771:VAL:HG22	1:A:1881:VAL:HG22	2.00	0.43
1:C:411:GLN:HE22	1:C:1628:SER:N	2.14	0.43
1:C:894:ARG:NH2	1:C:900:GLU:OE1	2.51	0.43
1:C:1696:LYS:HB3	1:C:1696:LYS:HE2	1.79	0.43
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.51	0.43
1:D:1431:GLU:CG	1:D:1433:HIS:CE1	3.01	0.43
1:E:2:LYS:O	1:E:5:VAL:HG23	2.18	0.43
2:G:681:ILE:HG21	2:G:686:PRO:HD3	2.00	0.43
2:G:748:THR:HB	2:G:749:PRO:HD3	1.99	0.43
2:G:1858:ASN:OD1	2:G:1896:GLN:HA	2.18	0.43
3:H:455:ILE:HD11	3:H:469:ARG:CG	2.44	0.43
3:H:654:VAL:CG1	3:H:850:MET:HE1	2.48	0.43
3:I:856:LYS:HD3	3:I:1052:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1201:VAL:HG11	3:I:1226:ASN:HB2	2.00	0.43
3:I:1479:ILE:HD11	3:I:1512:HIS:CE1	2.52	0.43
2:J:1327:ILE:HG12	2:J:1583:MET:HE2	2.00	0.43
1:A:1431:GLU:CG	1:A:1433:HIS:CE1	3.01	0.43
1:B:429:ASP:O	1:B:432:VAL:HG13	2.18	0.43
1:C:1014:ASP:N	1:C:1510:ASN:HD21	2.15	0.43
1:E:1717:ASP:C	1:E:1717:ASP:OD1	2.61	0.43
1:F:616:LEU:N	1:F:617:PRO:HD2	2.33	0.43
1:F:1785:THR:O	1:F:1789:ARG:HB2	2.18	0.43
2:G:1292:ILE:O	2:G:1368:VAL:O	2.37	0.43
2:J:440:ASN:HD21	2:J:477:GLU:HA	1.83	0.43
2:J:730:LEU:C	2:J:730:LEU:CD1	2.87	0.43
2:J:932:ILE:HD12	2:J:1042:ALA:HA	2.00	0.43
2:J:1289:ASP:OD1	2:J:1373:SER:HB3	2.18	0.43
2:J:1422:THR:CG2	2:J:1474:PHE:CD1	2.99	0.43
3:K:1040:LEU:O	3:K:1046:GLN:HA	2.19	0.43
3:K:1422:THR:CG2	3:K:1474:PHE:CD1	2.99	0.43
3:K:1927:LEU:HD13	3:K:1931:LEU:HD22	2.00	0.43
3:L:881:VAL:O	3:L:885:GLU:HG2	2.18	0.43
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.51	0.43
1:D:677:TYR:CZ	1:D:702:LYS:HD2	2.52	0.43
1:E:152:HIS:CD2	1:E:168:MET:HE3	2.53	0.43
1:E:529:MET:HE3	1:E:637:PHE:CB	2.47	0.43
1:F:429:ASP:O	1:F:432:VAL:HG13	2.18	0.43
1:F:479:ASN:O	1:F:483:VAL:CG2	2.65	0.43
2:G:120:LYS:HD3	2:G:175:ASP:OD2	2.18	0.43
2:G:464:ASP:HB3	2:G:466:SER:H	1.83	0.43
2:G:904:PHE:HB2	2:G:1017:PHE:CD2	2.53	0.43
2:G:1969:LEU:O	2:G:1971:GLY:N	2.51	0.43
3:H:701:LYS:O	3:H:701:LYS:HD2	2.18	0.43
3:H:1915:ASN:HD21	3:H:1963:GLY:HA3	1.83	0.43
3:I:455:ILE:HD11	3:I:469:ARG:CG	2.45	0.43
3:I:601:THR:OG1	3:I:618:GLU:O	2.26	0.43
3:I:1281:PRO:O	3:I:1378:ILE:HG23	2.19	0.43
2:J:748:THR:HB	2:J:749:PRO:HD3	1.99	0.43
2:J:942:THR:HB	2:J:1012:GLN:HB2	2.00	0.43
2:J:1718:THR:HB	2:J:1763:THR:OG1	2.17	0.43
3:K:602:VAL:HG23	3:K:624:TYR:CE2	2.53	0.43
3:K:666:ILE:O	3:K:670:ARG:HB2	2.18	0.43
3:K:1680:LEU:HD22	3:K:1684:SER:CB	2.48	0.43
3:L:1915:ASN:ND2	3:L:1964:PHE:N	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:GLN:HE22	3:H:962:LYS:HD2	1.82	0.43
1:B:1153:ASP:OD2	1:C:359:ARG:NH1	2.50	0.43
1:B:1423:LYS:O	1:B:1426:LEU:HB2	2.18	0.43
1:B:1717:ASP:C	1:B:1717:ASP:OD1	2.60	0.43
1:D:1022:THR:HG23	1:D:1226:SER:OG	2.18	0.43
1:D:1204:ILE:O	1:D:1208:VAL:HB	2.17	0.43
1:E:1431:GLU:OE2	1:E:1433:HIS:HE1	2.01	0.43
1:F:1776:ILE:HG13	1:F:1807:SER:HA	1.99	0.43
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.99	0.43
2:G:868:PHE:HB3	2:G:873:PHE:CE2	2.53	0.43
2:G:1378:ILE:HD11	2:G:1381:VAL:HG22	2.01	0.43
2:G:1435:ILE:CG2	2:G:1441:ILE:HG22	2.48	0.43
3:H:1281:PRO:O	3:H:1378:ILE:HG23	2.17	0.43
3:I:113:ASP:OD1	3:I:113:ASP:N	2.50	0.43
3:I:868:PHE:HB3	3:I:873:PHE:CE2	2.53	0.43
3:I:887:LYS:HE3	12:I:2215:HOH:O	2.18	0.43
3:I:1265:MET:CE	3:I:1569:PHE:CZ	3.01	0.43
2:J:249:TYR:CZ	2:J:263:LEU:HD23	2.54	0.43
2:J:868:PHE:HB3	2:J:873:PHE:CE2	2.53	0.43
3:K:1040:LEU:HD21	3:K:1048:VAL:HG13	2.01	0.43
3:L:904:PHE:HB2	3:L:1017:PHE:CD2	2.52	0.43
3:L:1736:MET:HG2	3:L:1751:ILE:CG1	2.47	0.43
3:L:1955:PRO:O	3:L:1958:LEU:HB3	2.18	0.43
10:L:2101:FMN:O1P	10:L:2101:FMN:O4'	2.30	0.43
1:A:643:LYS:NZ	1:A:851:ASN:HD21	2.17	0.43
1:A:1431:GLU:OE2	1:A:1433:HIS:HE1	2.02	0.43
1:A:1455:ARG:HD2	1:A:1455:ARG:HA	1.78	0.43
1:B:48:GLY:HA3	3:H:1667:THR:OG1	2.17	0.43
1:C:529:MET:HE3	1:C:637:PHE:CB	2.48	0.43
1:C:616:LEU:N	1:C:617:PRO:HD2	2.33	0.43
1:C:1498:GLU:O	1:C:1502:ARG:HG3	2.19	0.43
1:E:641:ARG:NH2	1:E:925:ASP:OD2	2.52	0.43
1:E:738:ASN:ND2	7:E:1917:A2P:HN62	2.15	0.43
1:E:1486:LEU:HD12	1:E:1486:LEU:HA	1.85	0.43
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.51	0.43
1:F:1418:VAL:N	1:F:1419:PRO:CD	2.81	0.43
2:G:169:TYR:C	2:G:169:TYR:CD2	2.97	0.43
3:H:1180:MET:HE3	3:H:1197:LEU:HD11	2.00	0.43
3:I:1040:LEU:O	3:I:1046:GLN:HA	2.18	0.43
3:I:1381:VAL:HG13	3:I:1390:VAL:HG22	2.00	0.43
3:I:1915:ASN:HD22	3:I:1915:ASN:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:559:PRO:HB3	2:J:564:GLU:HG3	2.00	0.43
3:K:233:SER:HA	3:K:424:ALA:CB	2.49	0.43
3:L:6:THR:O	3:L:7:ARG:CB	2.66	0.43
3:L:500:HIS:HA	3:L:526:ARG:O	2.19	0.43
3:L:932:ILE:HD12	3:L:1042:ALA:HA	2.01	0.43
3:L:1040:LEU:HD21	3:L:1048:VAL:HG13	2.01	0.43
3:L:2046:GLU:N	3:L:2046:GLU:CD	2.75	0.43
1:C:429:ASP:O	1:C:432:VAL:HG13	2.18	0.43
1:D:1498:GLU:O	1:D:1502:ARG:HG3	2.17	0.43
2:G:943:TRP:O	2:G:947:THR:HG23	2.18	0.43
2:G:1265:MET:CE	2:G:1569:PHE:CZ	3.02	0.43
3:H:6:THR:OG1	3:H:7:ARG:N	2.50	0.43
3:H:233:SER:HA	3:H:424:ALA:CB	2.48	0.43
3:H:730:LEU:C	3:H:730:LEU:CD1	2.88	0.43
3:H:1292:ILE:O	3:H:1368:VAL:O	2.35	0.43
3:H:1846:GLU:OE2	3:H:1957:PRO:HB3	2.19	0.43
3:I:1680:LEU:HD22	3:I:1684:SER:CB	2.48	0.43
2:J:1201:VAL:HG11	2:J:1226:ASN:HB2	1.99	0.43
2:J:1915:ASN:HD22	2:J:1915:ASN:N	2.15	0.43
3:K:558:ASN:HD22	3:K:558:ASN:HA	1.62	0.43
3:K:1775:GLN:HG3	3:K:1836:MET:HE3	2.01	0.43
3:K:1954:LYS:HB3	3:K:1955:PRO:HD2	2.00	0.43
3:L:372:ASN:HB3	3:L:515:LEU:HD21	2.01	0.43
3:L:478:ARG:HA	3:L:478:ARG:HD3	1.92	0.43
3:L:1281:PRO:O	3:L:1378:ILE:HG23	2.17	0.43
1:A:294:TYR:CE1	1:A:298:VAL:HG21	2.54	0.43
1:A:529:MET:HE3	1:A:637:PHE:HB2	2.01	0.43
1:B:152:HIS:CD2	1:B:168:MET:HE3	2.54	0.43
1:C:341:GLN:O	1:C:345:VAL:HG13	2.18	0.43
1:C:1495:ASN:HD22	1:F:1515:ARG:HG2	1.84	0.43
1:D:6:GLU:CG	2:J:2021:VAL:HG11	2.48	0.43
1:D:529:MET:HE3	1:D:637:PHE:HB2	2.00	0.43
1:D:1392:LEU:HD22	1:D:1396:MET:HG3	2.00	0.43
1:E:411:GLN:HE22	1:E:1628:SER:N	2.14	0.43
2:G:77:VAL:HG13	2:G:77:VAL:O	2.18	0.43
2:G:716:VAL:HG11	2:G:730:LEU:HD22	2.00	0.43
2:G:1680:LEU:HD22	2:G:1684:SER:CB	2.48	0.43
3:H:1265:MET:CE	3:H:1569:PHE:CZ	3.01	0.43
3:I:1944:ILE:O	3:I:1948:SER:HB3	2.19	0.43
3:I:2030:TYR:HA	3:I:2033:THR:OG1	2.19	0.43
2:J:1180:MET:HE3	2:J:1197:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:6:THR:OG1	3:K:7:ARG:N	2.51	0.43
3:L:740[A]:HIS:CD2	3:L:852:GLU:OE2	2.71	0.43
1:A:152:HIS:CD2	1:A:168:MET:HE3	2.53	0.43
1:A:1302:VAL:HG22	1:E:1302:VAL:CG2	2.48	0.43
1:B:375:LEU:HD21	1:E:374:GLN:OE1	2.19	0.43
1:C:1776:ILE:HG13	1:C:1807:SER:HA	2.00	0.43
1:C:1865:THR:H	1:C:1886:LYS:HB2	1.84	0.43
1:D:1423:LYS:O	1:D:1426:LEU:HB2	2.19	0.43
1:F:13:LEU:C	1:F:17:LEU:HD12	2.43	0.43
2:G:116:LEU:HA	2:G:116:LEU:HD13	1.79	0.43
2:G:1343:VAL:O	2:G:1343:VAL:CG2	2.67	0.43
2:G:1541:VAL:HG22	2:G:1625:SER:HB2	2.01	0.43
3:H:169:TYR:CD2	3:H:169:TYR:C	2.97	0.43
3:H:868:PHE:HB3	3:H:873:PHE:CE2	2.53	0.43
3:H:1347:LEU:HD12	3:H:1347:LEU:HA	1.89	0.43
3:H:1422:THR:CG2	3:H:1474:PHE:CD1	3.00	0.43
3:I:169:TYR:CD2	3:I:169:TYR:C	2.96	0.43
3:I:602:VAL:HG21	3:I:623:GLY:HA3	2.01	0.43
3:I:852:GLU:H	3:I:852:GLU:HG3	1.71	0.43
3:I:942:THR:HB	3:I:1012:GLN:HB2	2.01	0.43
3:I:1222:GLU:HG2	3:I:1235:SER:OG	2.18	0.43
3:I:1854:MET:HA	3:I:1907:LEU:HD21	2.01	0.43
3:I:1904:LEU:HG	3:I:1960:LEU:HD23	2.01	0.43
2:J:1374:THR:HG23	2:J:1396:LEU:HD12	2.01	0.43
3:L:82:GLN:H	3:L:82:GLN:HG3	1.71	0.43
3:L:233:SER:HA	3:L:424:ALA:CB	2.49	0.43
3:L:1085:LEU:HD12	3:L:1085:LEU:HA	1.86	0.43
3:L:1292:ILE:O	3:L:1368:VAL:O	2.37	0.43
1:A:1423:LYS:O	1:A:1426:LEU:HB2	2.19	0.43
1:B:341:GLN:O	1:B:345:VAL:HG13	2.19	0.43
1:B:451:MET:HE1	1:B:476:LEU:CG	2.45	0.43
1:B:793:ARG:NH1	1:E:789:GLU:OE1	2.52	0.43
1:C:1239:HIS:HD2	1:C:1241:SER:OG	2.01	0.43
1:C:1495:ASN:ND2	1:F:1515:ARG:HG2	2.33	0.43
1:C:1813:TRP:CZ3	1:C:1834:LEU:HD12	2.54	0.43
1:D:20:TYR:CZ	2:J:2033:THR:HG23	2.54	0.43
1:D:27:ARG:HB2	2:J:2016:ALA:HB2	2.01	0.43
1:F:11:HIS:CE1	3:L:1996:ILE:O	2.72	0.43
1:F:981:GLU:CD	3:L:962:LYS:HE2	2.43	0.43
2:G:1320:LEU:HD12	2:G:1366:LEU:O	2.19	0.43
2:G:1718:THR:HB	2:G:1763:THR:OG1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:155:GLN:HG3	3:I:268:LYS:HE3	2.01	0.43
3:I:440:ASN:HD21	3:I:477:GLU:HA	1.83	0.43
3:I:478:ARG:HA	3:I:478:ARG:HD3	1.93	0.43
3:I:1045:ASP:HB2	3:I:1047:ASP:HB2	2.01	0.43
3:I:1422:THR:CG2	3:I:1474:PHE:CD1	3.00	0.43
2:J:74:PRO:O	2:J:75:SER:HB3	2.17	0.43
2:J:99:ASN:HD22	2:J:100:ASP:N	2.10	0.43
2:J:602:VAL:HG21	2:J:623:GLY:HA3	2.01	0.43
3:K:440:ASN:HD21	3:K:477:GLU:HA	1.84	0.43
3:K:1327:ILE:HD13	3:K:1327:ILE:HA	1.86	0.43
3:K:1343:VAL:O	3:K:1343:VAL:CG2	2.67	0.43
3:K:1381:VAL:HG13	3:K:1390:VAL:HG22	2.00	0.43
3:L:169:TYR:CD2	3:L:169:TYR:C	2.96	0.43
3:L:1201:VAL:HG11	3:L:1226:ASN:HB2	2.01	0.43
3:L:1342:THR:HB	3:L:1421:ASN:OD1	2.18	0.43
3:L:1484:LYS:HG3	3:L:1507:GLU:HG3	2.01	0.43
1:A:1062:TYR:CG	1:A:1693:ILE:HB	2.54	0.43
1:A:1717:ASP:OD1	1:A:1717:ASP:C	2.61	0.43
1:B:186:ILE:O	1:B:190:LEU:HG	2.19	0.43
1:B:1418:VAL:N	1:B:1419:PRO:CD	2.82	0.43
4:B:1901:PNS:H422	1:E:1644:PHE:O	2.19	0.43
1:C:1295:SER:HA	1:F:1411:THR:O	2.19	0.43
1:C:1418:VAL:N	1:C:1419:PRO:CD	2.81	0.43
1:D:341:GLN:O	1:D:345:VAL:HG13	2.19	0.43
1:D:1418:VAL:N	1:D:1419:PRO:CD	2.82	0.43
1:D:1717:ASP:C	1:D:1717:ASP:OD1	2.61	0.43
1:E:186:ILE:O	1:E:190:LEU:HG	2.19	0.43
1:F:341:GLN:O	1:F:345:VAL:HG13	2.19	0.43
1:F:538:GLU:CG	1:F:635:ILE:HD11	2.48	0.43
1:F:1483:ASN:HD21	1:F:1487:LEU:HD11	1.83	0.43
1:F:1754:LYS:HE3	1:F:1754:LYS:HA	2.01	0.43
2:G:99:ASN:HD22	2:G:100:ASP:N	2.11	0.43
2:G:249:TYR:CZ	2:G:263:LEU:HD23	2.54	0.43
3:H:748:THR:HB	3:H:749:PRO:HD3	2.00	0.43
2:J:1378:ILE:HD11	2:J:1381:VAL:HG22	2.00	0.43
3:K:856:LYS:HD3	3:K:1052:CYS:SG	2.59	0.43
3:L:31:SER:HA	3:L:34:GLN:HB3	2.00	0.43
3:L:602:VAL:HG23	3:L:624:TYR:CE2	2.54	0.43
3:L:1593:ILE:HD11	3:L:1640:PHE:CD1	2.54	0.43
3:L:1854:MET:HA	3:L:1907:LEU:HD21	2.00	0.43
3:L:1944:ILE:CD1	3:L:1945:ASP:OD1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2044:ASN:C	3:L:2046:GLU:H	2.26	0.43
1:B:793:ARG:HH11	1:E:789:GLU:CD	2.27	0.42
1:C:375:LEU:HD12	1:D:375:LEU:HD12	2.01	0.42
1:C:1431:GLU:OE2	1:C:1433:HIS:HE1	2.02	0.42
1:F:1431:GLU:OE2	1:F:1433:HIS:HE1	2.02	0.42
1:F:1600:LEU:CD1	1:F:1655:VAL:HG12	2.49	0.42
2:G:1199:GLU:CD	2:G:1567:ARG:HH21	2.27	0.42
2:G:1347:LEU:HD12	2:G:1347:LEU:HA	1.87	0.42
2:G:1381:VAL:HG13	2:G:1390:VAL:HG22	2.01	0.42
2:G:1854:MET:HA	2:G:1907:LEU:HD21	2.00	0.42
3:H:803:SER:HB3	3:H:1055:HIS:CD2	2.54	0.42
3:H:1435:ILE:CG2	3:H:1441:ILE:HG22	2.50	0.42
2:J:31:SER:HA	2:J:34:GLN:HB3	2.00	0.42
2:J:233:SER:HA	2:J:424:ALA:CB	2.49	0.42
2:J:1229:MET:HE2	2:J:1268:LYS:O	2.18	0.42
3:K:932:ILE:HD12	3:K:1042:ALA:HA	2.00	0.42
3:L:1858:ASN:HB3	3:L:1965:ALA:HB1	2.01	0.42
1:A:358:GLU:OE2	1:F:360:LYS:NZ	2.48	0.42
1:A:429:ASP:O	1:A:432:VAL:HG13	2.19	0.42
1:A:1498:GLU:O	1:A:1502:ARG:HG3	2.19	0.42
1:C:1423:LYS:O	1:C:1426:LEU:HB2	2.19	0.42
1:C:1717:ASP:C	1:C:1717:ASP:OD1	2.61	0.42
1:F:186:ILE:O	1:F:190:LEU:HG	2.19	0.42
1:F:537:LYS:NZ	1:F:634:THR:OG1	2.48	0.42
2:G:6:THR:O	2:G:7:ARG:CB	2.66	0.42
2:G:1040:LEU:O	2:G:1046:GLN:HA	2.18	0.42
2:G:1629:VAL:HG11	2:G:1639:LYS:HE2	2.01	0.42
3:I:101:ILE:HD13	3:I:126:TYR:CD2	2.54	0.42
3:I:233:SER:HA	3:I:424:ALA:CB	2.48	0.42
3:I:932:ILE:HD12	3:I:1042:ALA:HA	2.01	0.42
3:I:1289:ASP:OD1	3:I:1373:SER:HB3	2.19	0.42
3:I:1348:LEU:HD12	3:I:1348:LEU:HA	1.89	0.42
3:I:1594:GLU:O	3:I:1598:ALA:HB3	2.19	0.42
3:I:1740:THR:HB	3:I:1747:LYS:HD2	2.01	0.42
3:I:1954:LYS:HB3	3:I:1955:PRO:HD2	2.00	0.42
2:J:1363:ALA:O	2:J:1606:ARG:NH2	2.51	0.42
3:K:517:HIS:CD2	3:K:517:HIS:O	2.72	0.42
3:K:1085:LEU:HD12	3:K:1085:LEU:HA	1.85	0.42
3:K:1096:LYS:HA	3:K:1096:LYS:HD2	1.88	0.42
3:K:1289:ASP:OD1	3:K:1373:SER:HB3	2.19	0.42
3:K:1782:THR:CG2	3:K:1827:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:455:ILE:HD11	3:L:469:ARG:CG	2.45	0.42
3:L:803:SER:HB3	3:L:1055:HIS:CD2	2.54	0.42
3:L:943:TRP:O	3:L:947:THR:HG23	2.19	0.42
1:B:537:LYS:HE2	1:B:634:THR:OG1	2.19	0.42
1:B:709:ARG:HD3	7:B:1918:A2P:O4P	2.19	0.42
1:B:1736:LYS:HA	1:B:1736:LYS:HD3	1.87	0.42
1:C:1392:LEU:HD22	1:C:1396:MET:HG3	2.01	0.42
1:D:1431:GLU:OE2	1:D:1433:HIS:HE1	2.01	0.42
1:D:1491:ARG:HD3	1:D:1749:THR:HG21	2.01	0.42
1:E:341:GLN:O	1:E:345:VAL:HG13	2.20	0.42
1:F:198:PRO:HG3	1:F:212:THR:HG21	2.01	0.42
2:G:372:ASN:HB3	2:G:515:LEU:HD21	2.00	0.42
2:G:440:ASN:HD21	2:G:477:GLU:HA	1.84	0.42
2:G:942:THR:HB	2:G:1012:GLN:HB2	2.01	0.42
2:G:1040:LEU:HD21	2:G:1048:VAL:HG13	2.01	0.42
3:H:6:THR:O	3:H:7:ARG:CB	2.67	0.42
3:H:896:ASN:ND2	3:H:906:THR:HG21	2.34	0.42
3:H:1854:MET:HB3	3:H:1901:ALA:CB	2.50	0.42
3:I:1040:LEU:HD21	3:I:1048:VAL:HG13	2.01	0.42
2:J:1969:LEU:O	2:J:1971:GLY:N	2.52	0.42
3:K:246:LEU:HD12	3:K:246:LEU:HA	1.89	0.42
3:K:803:SER:HB3	3:K:1055:HIS:CD2	2.55	0.42
3:K:2044:ASN:C	3:K:2046:GLU:H	2.26	0.42
3:L:896:ASN:ND2	3:L:906:THR:HG21	2.34	0.42
3:L:1199:GLU:CD	3:L:1567:ARG:HH21	2.27	0.42
3:L:1877:ARG:HG3	3:L:1940:LEU:HD23	2.01	0.42
1:A:1418:VAL:N	1:A:1419:PRO:CD	2.82	0.42
1:A:1751:GLU:HG3	1:A:1872:SER:HB2	2.00	0.42
1:B:59:ARG:HG2	3:H:1896:GLN:HE22	1.83	0.42
1:C:1022:THR:HG23	1:C:1226:SER:OG	2.19	0.42
1:E:952:GLU:OE1	1:E:952:GLU:HA	2.18	0.42
1:F:407:ASN:ND2	1:F:1626:TYR:O	2.44	0.42
1:F:952:GLU:OE1	1:F:952:GLU:HA	2.19	0.42
2:G:730:LEU:C	2:G:730:LEU:CD1	2.87	0.42
2:G:1327:ILE:HG12	2:G:1583:MET:HE2	2.00	0.42
2:G:1468:THR:HG23	2:G:1485:CYS:SG	2.60	0.42
3:I:597:MET:HB3	10:I:2101:FMN:C6	2.50	0.42
3:I:598:THR:OG1	3:I:599:PRO:HD2	2.18	0.42
2:J:598:THR:HG23	10:J:2101:FMN:O4	2.20	0.42
2:J:847:ARG:HG2	5:J:2104:EDO:C2	2.49	0.42
2:J:856:LYS:HD3	2:J:1052:CYS:SG	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1381:VAL:HG13	2:J:1390:VAL:HG22	2.00	0.42
2:J:2044:ASN:C	2:J:2046:GLU:H	2.26	0.42
3:K:868:PHE:HB3	3:K:873:PHE:CE2	2.54	0.42
3:K:1292:ILE:O	3:K:1368:VAL:O	2.36	0.42
3:L:277:LEU:HD23	3:L:277:LEU:HA	1.88	0.42
3:L:602:VAL:HG21	3:L:623:GLY:HA3	2.02	0.42
1:A:616:LEU:N	1:A:617:PRO:HD2	2.33	0.42
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.52	0.42
1:B:1813:TRP:HZ3	1:B:1834:LEU:HD13	1.83	0.42
1:C:529:MET:HE3	1:C:637:PHE:HB2	2.01	0.42
1:D:955:LYS:O	1:D:959:ILE:HG13	2.19	0.42
1:E:407:ASN:ND2	1:E:1626:TYR:O	2.45	0.42
1:E:1431:GLU:CG	1:E:1433:HIS:CE1	3.02	0.42
1:E:1498:GLU:O	1:E:1502:ARG:HG3	2.20	0.42
1:F:643:LYS:NZ	1:F:851:ASN:HD21	2.17	0.42
2:G:1358:LYS:HG3	12:G:2216:HOH:O	2.18	0.42
3:H:249:TYR:CZ	3:H:263:LEU:HD23	2.54	0.42
3:H:1908:ASP:OD2	3:H:1954:LYS:HE3	2.20	0.42
3:H:2044:ASN:C	3:H:2046:GLU:H	2.27	0.42
3:I:1199:GLU:CD	3:I:1567:ARG:HH21	2.27	0.42
3:I:1347:LEU:HD12	3:I:1347:LEU:HA	1.90	0.42
2:J:468:LEU:HA	2:J:471:LEU:CD2	2.49	0.42
2:J:468:LEU:HA	2:J:471:LEU:HD21	2.01	0.42
3:K:99:ASN:HD22	3:K:100:ASP:N	2.13	0.42
3:K:249:TYR:CZ	3:K:263:LEU:HD23	2.54	0.42
3:K:942:THR:HB	3:K:1012:GLN:HB2	2.01	0.42
3:K:1265:MET:CE	3:K:1569:PHE:CZ	3.01	0.42
3:L:1327:ILE:HG12	3:L:1583:MET:HE2	2.01	0.42
1:A:965:HIS:CE1	1:A:969:ASN:ND2	2.88	0.42
1:C:186:ILE:O	1:C:190:LEU:HG	2.19	0.42
1:C:438:ASN:HD21	1:C:698:GLN:HG3	1.84	0.42
1:D:185:GLU:CD	1:F:1272:ASN:HD22	2.26	0.42
1:D:359:ARG:NH1	1:F:1153:ASP:OD1	2.53	0.42
1:D:1794:GLN:HE22	1:D:1840:VAL:HA	1.84	0.42
1:E:632:ARG:O	1:E:633:GLU:CB	2.67	0.42
1:E:798:ASN:HA	1:E:801:ARG:HB2	2.01	0.42
2:G:803:SER:HB3	2:G:1055:HIS:CD2	2.55	0.42
2:G:1348:LEU:HD12	2:G:1348:LEU:HA	1.90	0.42
3:H:856:LYS:HD3	3:H:1052:CYS:SG	2.59	0.42
3:H:1854:MET:HA	3:H:1907:LEU:HD21	2.01	0.42
3:I:249:TYR:CZ	3:I:263:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1926:GLU:O	3:I:1930:SER:OG	2.23	0.42
2:J:6:THR:O	2:J:7:ARG:CB	2.67	0.42
2:J:852:GLU:H	2:J:852:GLU:HG2	1.71	0.42
2:J:1199:GLU:CD	2:J:1567:ARG:HH21	2.28	0.42
3:K:852:GLU:H	3:K:852:GLU:HG3	1.71	0.42
3:K:904:PHE:HB2	3:K:1017:PHE:CD2	2.54	0.42
3:K:1468:THR:HG23	3:K:1485:CYS:SG	2.59	0.42
3:K:1955:PRO:O	3:K:1958:LEU:HB3	2.18	0.42
3:L:1343:VAL:O	3:L:1343:VAL:CG2	2.67	0.42
1:A:27:ARG:HB2	2:G:2016:ALA:HB2	2.01	0.42
1:A:341:GLN:O	1:A:345:VAL:HG13	2.19	0.42
1:B:1498:GLU:O	1:B:1502:ARG:HG3	2.19	0.42
1:B:1755:MET:HG2	1:B:1870:SER:HB3	2.01	0.42
1:C:1431:GLU:CG	1:C:1433:HIS:CE1	3.02	0.42
1:C:1600:LEU:CD1	1:C:1655:VAL:HG12	2.49	0.42
1:C:1689:HIS:CE1	3:I:996:ASN:HD21	2.38	0.42
1:D:43:ARG:O	2:J:1662:THR:HA	2.20	0.42
1:D:152:HIS:CD2	1:D:168:MET:HE3	2.54	0.42
1:E:1062:TYR:CG	1:E:1693:ILE:HB	2.55	0.42
1:E:1486:LEU:O	1:E:1490:THR:HG23	2.09	0.42
1:F:93:ASP:O	1:F:95:SER:N	2.50	0.42
1:F:495:LYS:HB3	1:F:495:LYS:HE3	1.78	0.42
2:G:33:LEU:HD12	2:G:33:LEU:N	2.34	0.42
2:G:500:HIS:HA	2:G:526:ARG:O	2.19	0.42
2:G:1908:ASP:OD2	2:G:1954:LYS:HE3	2.19	0.42
2:G:1928:GLN:HE21	2:G:1928:GLN:HB2	1.67	0.42
2:G:1954:LYS:HB3	2:G:1955:PRO:HD2	2.02	0.42
3:H:1289:ASP:OD1	3:H:1373:SER:HB3	2.19	0.42
3:H:1877:ARG:HG3	3:H:1940:LEU:HD23	2.01	0.42
2:J:1877:ARG:HA	2:J:1877:ARG:HD2	1.84	0.42
3:K:500:HIS:HA	3:K:526:ARG:O	2.19	0.42
3:L:464:ASP:HB3	3:L:466:SER:H	1.85	0.42
3:L:1541:VAL:HG22	3:L:1625:SER:HB2	2.02	0.42
1:A:186:ILE:O	1:A:190:LEU:HG	2.19	0.42
1:A:1119:LYS:O	1:A:1178:ALA:HA	2.20	0.42
1:A:1752:THR:O	1:A:1756:ILE:HG23	2.19	0.42
1:B:952:GLU:OE1	1:B:952:GLU:HA	2.19	0.42
1:C:1736:LYS:HD2	1:C:1736:LYS:N	2.33	0.42
1:D:186:ILE:O	1:D:190:LEU:HG	2.19	0.42
1:E:72:LEU:HB2	1:E:74:LEU:HD23	2.02	0.42
1:E:980:VAL:HB	3:K:968:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:285:GLU:OE1	3:H:298:LYS:CE	2.68	0.42
3:H:303:LEU:HD12	3:H:303:LEU:HA	1.93	0.42
3:H:1594:GLU:O	3:H:1598:ALA:HB3	2.20	0.42
3:I:451:ASN:HB3	3:I:453:LYS:HG3	2.02	0.42
3:I:716:VAL:HG11	3:I:730:LEU:HD22	2.02	0.42
3:I:1374:THR:HG23	3:I:1396:LEU:HD12	2.01	0.42
3:I:1859:PRO:O	3:I:1862:VAL:HG13	2.20	0.42
3:I:1969:LEU:O	3:I:1971:GLY:N	2.53	0.42
2:J:169:TYR:CD2	2:J:169:TYR:C	2.97	0.42
2:J:716:VAL:HG11	2:J:730:LEU:HD22	2.01	0.42
2:J:803:SER:HB3	2:J:1055:HIS:CD2	2.55	0.42
2:J:1040:LEU:O	2:J:1046:GLN:HA	2.18	0.42
2:J:1265:MET:CE	2:J:1569:PHE:CZ	3.02	0.42
2:J:1962:ARG:NH2	2:J:1967:ILE:HG12	2.34	0.42
3:K:169:TYR:CD2	3:K:169:TYR:C	2.97	0.42
3:K:1927:LEU:HA	3:K:1931:LEU:HB2	2.01	0.42
3:L:1770:LEU:HD13	3:L:1770:LEU:HA	1.94	0.42
1:A:359:ARG:NH1	1:C:1153:ASP:OD1	2.52	0.42
1:A:1760:THR:O	1:A:1760:THR:CG2	2.58	0.42
1:B:17:LEU:O	1:B:21:GLN:HB2	2.20	0.42
1:C:1062:TYR:CG	1:C:1693:ILE:HB	2.55	0.42
1:E:17:LEU:O	1:E:21:GLN:HB2	2.20	0.42
1:F:798:ASN:HA	1:F:801:ARG:HB2	2.02	0.42
2:G:1594:GLU:O	2:G:1598:ALA:HB3	2.20	0.42
3:H:500:HIS:HA	3:H:526:ARG:O	2.20	0.42
3:H:1468:THR:HG23	3:H:1485:CYS:SG	2.60	0.42
3:I:101:ILE:CD1	3:I:126:TYR:HB3	2.44	0.42
2:J:246:LEU:HD12	2:J:246:LEU:HA	1.88	0.42
1:B:1500:GLN:CG	1:D:1507:GLN:NE2	2.81	0.42
1:D:1062:TYR:CG	1:D:1693:ILE:HB	2.55	0.42
1:E:438:ASN:HD21	1:E:698:GLN:HG3	1.85	0.42
1:F:1431:GLU:CG	1:F:1433:HIS:CE1	3.03	0.42
2:G:233:SER:HA	2:G:424:ALA:CB	2.49	0.42
3:H:419:ARG:CZ	3:H:419:ARG:HB3	2.49	0.42
3:H:1343:VAL:O	3:H:1343:VAL:CG2	2.67	0.42
3:H:1859:PRO:O	3:H:1862:VAL:HG13	2.20	0.42
3:H:1944:ILE:O	3:H:1948:SER:HB3	2.20	0.42
3:I:1737:ILE:HD13	3:I:1739:GLU:HG2	2.02	0.42
3:I:1923:ASP:OD2	3:I:1926:GLU:HB2	2.20	0.42
2:J:597:MET:HA	10:J:2101:FMN:C4A	2.50	0.42
2:J:663:ILE:HB	2:J:664:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:896:ASN:ND2	2:J:906:THR:HG21	2.34	0.42
3:K:1969:LEU:O	3:K:1971:GLY:N	2.52	0.42
3:L:1854:MET:HB3	3:L:1901:ALA:CB	2.49	0.42
3:L:1915:ASN:HD22	3:L:1915:ASN:N	2.16	0.42
3:L:1969:LEU:O	3:L:1971:GLY:N	2.53	0.42
1:B:11:HIS:ND1	3:H:1998:LYS:HA	2.34	0.41
1:B:1014:ASP:N	1:B:1510:ASN:HD21	2.14	0.41
1:C:294:TYR:CE1	1:C:298:VAL:HG21	2.55	0.41
1:C:952:GLU:OE1	1:C:952:GLU:HA	2.20	0.41
1:E:894:ARG:NH2	1:E:900:GLU:OE1	2.52	0.41
1:E:1022:THR:HG23	1:E:1226:SER:OG	2.20	0.41
1:F:1022:THR:HG23	1:F:1226:SER:OG	2.20	0.41
2:G:285:GLU:OE1	2:G:298:LYS:CE	2.68	0.41
2:G:1280:ASP:OD1	2:G:1281:PRO:HD2	2.20	0.41
3:H:1199:GLU:CD	3:H:1567:ARG:HH21	2.27	0.41
3:I:500:HIS:HA	3:I:526:ARG:O	2.19	0.41
3:I:896:ASN:ND2	3:I:906:THR:HG21	2.34	0.41
3:I:2044:ASN:C	3:I:2046:GLU:H	2.27	0.41
2:J:478:ARG:HA	2:J:478:ARG:HD3	1.91	0.41
3:K:1915:ASN:HD21	3:K:1963:GLY:HA3	1.84	0.41
3:K:2044:ASN:C	3:K:2046:GLU:N	2.79	0.41
3:L:716:VAL:HG11	3:L:730:LEU:HD22	2.01	0.41
3:L:1872:GLN:HE21	3:L:1888:ILE:HD11	1.85	0.41
1:A:868:ILE:HD11	1:A:923:MET:HE3	2.01	0.41
1:A:955:LYS:O	1:A:959:ILE:HG13	2.20	0.41
1:C:1752:THR:O	1:C:1756:ILE:HG23	2.20	0.41
1:D:688:ILE:HD11	1:D:872:THR:HG21	2.02	0.41
1:E:329:GLU:HA	1:E:332:THR:HG22	2.01	0.41
1:E:1392:LEU:HD22	1:E:1396:MET:HG3	2.01	0.41
1:E:1600:LEU:CD1	1:E:1655:VAL:HG12	2.50	0.41
1:F:1062:TYR:CG	1:F:1693:ILE:HB	2.55	0.41
1:F:1230:ASP:OD1	1:F:1230:ASP:C	2.64	0.41
1:F:1423:LYS:O	1:F:1426:LEU:HB2	2.19	0.41
1:F:1501:LEU:O	1:F:1505:GLN:HG3	2.21	0.41
2:G:79:GLN:HE21	2:G:79:GLN:N	1.98	0.41
2:J:464:ASP:HB3	2:J:466:SER:H	1.84	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.90	0.41
1:A:1515:ARG:HG2	1:E:1495:ASN:HD22	1.85	0.41
1:C:1716:LEU:HD21	1:F:1426:LEU:CD2	2.45	0.41
1:E:1230:ASP:C	1:E:1230:ASP:OD1	2.63	0.41
2:G:56:THR:HG21	2:G:112:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:998:GLN:HE21	3:H:998:GLN:HB3	1.65	0.41
3:H:1222:GLU:HG2	3:H:1235:SER:OG	2.19	0.41
3:H:1374:THR:HG23	3:H:1396:LEU:HD12	2.02	0.41
3:H:1986:LYS:N	3:H:1987:PRO:HD2	2.35	0.41
3:I:29:ILE:HD12	3:I:82:GLN:NE2	2.35	0.41
3:I:1858:ASN:ND2	3:I:1896:GLN:HA	2.36	0.41
3:L:559:PRO:HB3	3:L:564:GLU:HG3	2.02	0.41
3:L:1265:MET:CE	3:L:1569:PHE:CZ	3.03	0.41
3:L:1929:LYS:CD	3:L:1933:LEU:HD12	2.50	0.41
1:B:20:TYR:CD2	3:H:2033:THR:HG23	2.55	0.41
1:C:67:SER:HB3	3:H:355:LYS:HE3	2.02	0.41
1:C:674:LYS:O	1:C:675:ASP:HB2	2.20	0.41
1:C:1477:ILE:CD1	1:C:1485:PHE:CD1	3.03	0.41
1:D:930:LEU:HD23	1:D:930:LEU:HA	1.94	0.41
1:E:484:LEU:HD22	1:E:485:ASP:N	2.35	0.41
1:F:1794:GLN:NE2	1:F:1840:VAL:HA	2.34	0.41
3:H:602:VAL:HG21	3:H:623:GLY:HA3	2.02	0.41
2:J:1541:VAL:HG22	2:J:1625:SER:HB2	2.02	0.41
2:J:1927:LEU:HB3	2:J:1931:LEU:HD13	2.02	0.41
3:K:1201:VAL:HG11	3:K:1226:ASN:HB2	2.02	0.41
3:L:37:PHE:CZ	3:L:41:LEU:HD21	2.55	0.41
3:L:249:TYR:CZ	3:L:263:LEU:HD23	2.55	0.41
3:L:1280:ASP:OD1	3:L:1281:PRO:HD2	2.20	0.41
3:L:1881:ARG:HG2	3:L:1944:ILE:HD11	2.02	0.41
1:B:1260:MET:HG2	1:D:1342:GLU:HG3	2.01	0.41
1:F:1498:GLU:O	1:F:1502:ARG:HG3	2.21	0.41
2:G:167:ASP:OD1	2:G:167:ASP:N	2.45	0.41
2:G:753:MET:O	2:G:757:ILE:HG13	2.21	0.41
3:H:29:ILE:O	3:H:33:LEU:HD22	2.20	0.41
3:H:464:ASP:HB3	3:H:466:SER:H	1.84	0.41
3:H:942:THR:HB	3:H:1012:GLN:HB2	2.03	0.41
3:H:1734:SER:O	3:H:1750:LYS:HE2	2.20	0.41
3:I:1986:LYS:N	3:I:1987:PRO:HD2	2.36	0.41
2:J:1680:LEU:HD22	2:J:1684:SER:CB	2.50	0.41
3:K:455:ILE:HD11	3:K:469:ARG:CG	2.46	0.41
3:K:1353:LEU:HD11	3:K:1411:PHE:HB2	2.02	0.41
1:A:894:ARG:NH2	1:A:900:GLU:OE1	2.52	0.41
1:A:952:GLU:OE1	1:A:952:GLU:HA	2.21	0.41
1:A:1370:THR:HG22	1:A:1372:THR:H	1.85	0.41
1:B:1022:THR:HG23	1:B:1226:SER:OG	2.20	0.41
1:C:793:ARG:NH1	1:D:789:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:798:ASN:HA	1:C:801:ARG:HB2	2.02	0.41
1:C:1370:THR:HG22	1:C:1372:THR:H	1.86	0.41
1:C:1477:ILE:HD12	1:C:1485:PHE:CD1	2.56	0.41
1:C:1771:VAL:HG22	1:C:1881:VAL:HG22	2.02	0.41
1:D:359:ARG:NH1	1:F:1153:ASP:OD2	2.54	0.41
1:E:294:TYR:CE1	1:E:298:VAL:HG21	2.55	0.41
1:E:1785:THR:O	1:E:1789:ARG:HB2	2.20	0.41
1:F:751:PHE:CZ	1:F:761:LEU:HD13	2.55	0.41
1:F:1486:LEU:HD12	1:F:1486:LEU:HA	1.90	0.41
2:G:1229:MET:HE2	2:G:1268:LYS:O	2.20	0.41
2:G:1986:LYS:N	2:G:1987:PRO:HD2	2.36	0.41
2:G:2044:ASN:C	2:G:2046:GLU:N	2.78	0.41
3:H:1054:LEU:CB	10:H:2101:FMN:HM73	2.50	0.41
3:H:1378:ILE:HD11	3:H:1381:VAL:HG22	2.02	0.41
3:I:1343:VAL:O	3:I:1343:VAL:CG2	2.68	0.41
2:J:285:GLU:OE1	2:J:298:LYS:CE	2.69	0.41
3:K:1594:GLU:O	3:K:1598:ALA:HB3	2.20	0.41
3:L:56:THR:HG21	3:L:112:ASN:HD22	1.85	0.41
3:L:885:GLU:HA	3:L:885:GLU:OE1	2.20	0.41
1:A:688:ILE:HD11	1:A:872:THR:HG21	2.03	0.41
1:A:1117:GLU:O	1:E:1146:HIS:HE1	2.03	0.41
1:A:1507:GLN:NE2	1:E:1500:GLN:CG	2.83	0.41
1:B:798:ASN:HA	1:B:801:ARG:HB2	2.02	0.41
1:B:1020:VAL:HG22	1:B:1400:ILE:HG23	2.03	0.41
1:B:1062:TYR:CG	1:B:1693:ILE:HB	2.56	0.41
1:B:1785:THR:O	1:B:1789:ARG:HB2	2.21	0.41
1:B:1820:PHE:CD1	1:B:1820:PHE:C	2.99	0.41
1:C:198:PRO:HG3	1:C:212:THR:HG21	2.02	0.41
1:C:1581:THR:HB	1:C:1591:TRP:CZ3	2.56	0.41
1:C:1825:VAL:HG11	1:C:1858:ALA:HB1	2.03	0.41
1:D:407:ASN:ND2	1:D:1626:TYR:O	2.45	0.41
1:D:1119:LYS:O	1:D:1178:ALA:HA	2.21	0.41
1:D:1431:GLU:HG3	1:D:1433:HIS:CE1	2.55	0.41
1:E:955:LYS:O	1:E:959:ILE:HG13	2.20	0.41
1:F:677:TYR:CZ	1:F:702:LYS:HD2	2.55	0.41
1:F:1766:ASN:OD1	1:F:1766:ASN:N	2.52	0.41
2:G:1180:MET:HE3	2:G:1197:LEU:HD11	2.02	0.41
2:G:1201:VAL:HG11	2:G:1226:ASN:HB2	2.03	0.41
2:G:1289:ASP:OD1	2:G:1373:SER:HB3	2.20	0.41
2:G:1858:ASN:HD22	2:G:1861:ARG:HG2	1.77	0.41
2:G:1932:SER:HB3	2:G:1935:GLU:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1969:LEU:O	3:H:1971:GLY:N	2.53	0.41
3:I:1884:TRP:CZ3	3:I:1905:ARG:HB3	2.56	0.41
2:J:500:HIS:HA	2:J:526:ARG:O	2.20	0.41
2:J:1280:ASP:OD1	2:J:1281:PRO:HD2	2.21	0.41
2:J:1854:MET:HB3	2:J:1901:ALA:CB	2.50	0.41
2:J:1858:ASN:ND2	2:J:1896:GLN:HA	2.35	0.41
3:L:748:THR:HB	3:L:749:PRO:HD3	2.02	0.41
1:A:17:LEU:O	1:A:21:GLN:HB2	2.21	0.41
1:A:1443:LEU:HD23	1:A:1443:LEU:HA	1.94	0.41
1:B:1370:THR:HG22	1:B:1372:THR:H	1.86	0.41
1:C:1119:LYS:O	1:C:1178:ALA:HA	2.20	0.41
1:C:1230:ASP:OD1	1:C:1230:ASP:C	2.64	0.41
1:D:20:TYR:CG	2:J:2033:THR:HG23	2.55	0.41
1:D:1771:VAL:HG22	1:D:1881:VAL:HG22	2.02	0.41
1:E:233:ILE:HG21	1:E:243:ILE:N	2.36	0.41
1:E:429:ASP:O	1:E:432:VAL:HG13	2.20	0.41
1:E:1752:THR:O	1:E:1756:ILE:HG23	2.21	0.41
1:F:1119:LYS:O	1:F:1178:ALA:HA	2.21	0.41
2:G:1737:ILE:HD13	2:G:1739:GLU:HG2	2.03	0.41
3:H:56:THR:HG21	3:H:112:ASN:HD22	1.86	0.41
3:H:99:ASN:HD22	3:H:100:ASP:N	2.10	0.41
3:H:1348:LEU:HD12	3:H:1348:LEU:HA	1.90	0.41
3:H:1737:ILE:HD13	3:H:1739:GLU:HG2	2.02	0.41
3:H:1858:ASN:ND2	3:H:1896:GLN:HA	2.36	0.41
3:I:167:ASP:OD1	3:I:167:ASP:N	2.45	0.41
3:I:494:THR:HG23	3:I:520:LYS:HE3	2.03	0.41
3:I:1852:TYR:CA	3:I:1904:LEU:HD13	2.51	0.41
3:I:1962:ARG:NH2	3:I:1967:ILE:HG12	2.35	0.41
2:J:6:THR:O	2:J:7:ARG:HB2	2.20	0.41
2:J:29:ILE:O	2:J:32:GLN:HB3	2.21	0.41
3:K:896:ASN:ND2	3:K:906:THR:HG21	2.34	0.41
3:L:109:LEU:HD21	3:L:116:LEU:CD2	2.50	0.41
3:L:856:LYS:HD3	3:L:1052:CYS:SG	2.61	0.41
3:L:1374:THR:HG23	3:L:1396:LEU:HD12	2.02	0.41
3:L:2044:ASN:C	3:L:2046:GLU:N	2.78	0.41
1:A:1600:LEU:CD1	1:A:1655:VAL:HG12	2.50	0.41
1:A:1762:GLU:OE1	1:A:1763:LYS:N	2.50	0.41
1:B:499:PRO:HB3	1:B:873:ARG:HD3	2.02	0.41
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.90	0.41
1:B:1230:ASP:OD1	1:B:1230:ASP:C	2.63	0.41
1:B:1501:LEU:O	1:B:1505:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1441:PRO:HD2	1:F:1492:GLU:OE2	2.20	0.41
1:C:1785:THR:O	1:C:1789:ARG:HG3	2.20	0.41
1:D:20:TYR:CD2	2:J:2033:THR:HG23	2.56	0.41
1:D:359:ARG:NH1	1:F:1153:ASP:CG	2.78	0.41
1:D:798:ASN:HA	1:D:801:ARG:HB2	2.02	0.41
1:E:529:MET:HE3	1:E:637:PHE:HB2	2.03	0.41
1:E:1370:THR:HG22	1:E:1372:THR:H	1.84	0.41
1:E:1771:VAL:HG22	1:E:1881:VAL:HG22	2.01	0.41
1:F:11:HIS:HE1	3:L:1996:ILE:O	2.04	0.41
1:F:48:GLY:HA3	3:L:1667:THR:OG1	2.21	0.41
1:F:213:PHE:O	1:F:217:PHE:HB2	2.21	0.41
1:F:451:MET:HE1	1:F:476:LEU:CG	2.49	0.41
1:F:1014:ASP:N	1:F:1510:ASN:HD21	2.14	0.41
1:F:1534:ASP:CG	1:F:1567:SER:HG	2.29	0.41
1:F:1771:VAL:HG22	1:F:1881:VAL:HG22	2.01	0.41
1:F:1813:TRP:CZ3	1:F:1834:LEU:HD12	2.55	0.41
2:G:1422:THR:CG2	2:G:1474:PHE:CD1	3.00	0.41
2:G:1479:ILE:HD13	2:G:1479:ILE:N	2.35	0.41
2:G:1859:PRO:O	2:G:1862:VAL:HG13	2.19	0.41
3:H:323:ILE:HG12	3:H:387:TYR:CE2	2.56	0.41
3:H:440:ASN:HD21	3:H:477:GLU:HA	1.84	0.41
3:H:753:MET:O	3:H:757:ILE:HG13	2.21	0.41
3:H:1085:LEU:HD12	3:H:1085:LEU:HA	1.87	0.41
3:H:1541:VAL:HG22	3:H:1625:SER:CB	2.51	0.41
3:H:1907:LEU:HD23	3:H:1960:LEU:CD2	2.51	0.41
3:I:1180:MET:HE3	3:I:1197:LEU:HD11	2.02	0.41
3:I:1378:ILE:HD11	3:I:1381:VAL:HG22	2.03	0.41
3:I:1479:ILE:HD13	3:I:1479:ILE:N	2.36	0.41
2:J:346:GLN:HE22	5:J:2105:EDO:H22	1.84	0.41
2:J:364:LYS:HA	2:J:382:PRO:HG2	2.02	0.41
2:J:964:LEU:H	2:J:964:LEU:CD2	2.33	0.41
2:J:1022:ASP:OD1	2:J:1024:ARG:HG3	2.21	0.41
3:K:364:LYS:HA	3:K:382:PRO:HG2	2.02	0.41
3:K:1374:THR:HG23	3:K:1396:LEU:HD12	2.02	0.41
3:K:1479:ILE:H	3:K:1479:ILE:HD12	1.85	0.41
3:L:1289:ASP:OD1	3:L:1373:SER:HB3	2.20	0.41
3:L:1479:ILE:H	3:L:1479:ILE:HD12	1.86	0.41
3:L:1594:GLU:O	3:L:1598:ALA:HB3	2.20	0.41
3:L:1665:VAL:HA	3:L:1805:ALA:O	2.21	0.41
1:A:438:ASN:HD21	1:A:698:GLN:HG3	1.86	0.41
1:A:828:PRO:HG2	1:A:829:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ASN:ND2	1:C:1626:TYR:O	2.45	0.41
1:C:751:PHE:CZ	1:C:761:LEU:HD13	2.56	0.41
1:D:982:ILE:O	2:J:962:LYS:HA	2.21	0.41
1:D:1827:SER:O	1:D:1828:LEU:HB2	2.21	0.41
1:E:1167:LEU:HD11	1:E:1171:ALA:HB1	2.03	0.41
1:F:438:ASN:HD21	1:F:698:GLN:HG3	1.86	0.41
3:H:249:TYR:CE2	3:H:283:ILE:HD12	2.56	0.41
3:I:37:PHE:CZ	3:I:41:LEU:HD21	2.56	0.41
3:I:1541:VAL:HG22	3:I:1625:SER:CB	2.51	0.41
3:I:1665:VAL:HA	3:I:1805:ALA:O	2.21	0.41
3:I:2044:ASN:C	3:I:2046:GLU:N	2.79	0.41
2:J:597:MET:HA	10:J:2101:FMN:C5A	2.49	0.41
2:J:1594:GLU:O	2:J:1598:ALA:HB3	2.21	0.41
3:K:716:VAL:HG11	3:K:730:LEU:HD22	2.02	0.41
3:K:1858:ASN:ND2	3:K:1896:GLN:HA	2.35	0.41
3:K:2030:TYR:HA	3:K:2033:THR:OG1	2.21	0.41
3:L:942:THR:HB	3:L:1012:GLN:HB2	2.03	0.41
3:L:1954:LYS:HB3	3:L:1955:PRO:HD2	2.02	0.41
1:A:798:ASN:HA	1:A:801:ARG:HB2	2.02	0.40
1:A:1230:ASP:C	1:A:1230:ASP:OD1	2.63	0.40
1:A:1515:ARG:HG2	1:E:1495:ASN:ND2	2.36	0.40
1:B:1021:VAL:HG11	1:B:1597:LEU:HD11	2.03	0.40
1:C:17:LEU:O	1:C:21:GLN:HB2	2.21	0.40
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.90	0.40
1:E:221:LEU:HD23	1:E:221:LEU:HA	1.91	0.40
1:F:329:GLU:HA	1:F:332:THR:HG22	2.03	0.40
1:F:688:ILE:HD11	1:F:872:THR:HG21	2.03	0.40
1:F:1079:LYS:HA	1:F:1079:LYS:HE3	2.03	0.40
1:F:1581:THR:HB	1:F:1591:TRP:CZ3	2.56	0.40
2:G:37:PHE:CZ	2:G:41:LEU:HD21	2.56	0.40
2:G:896:ASN:ND2	2:G:906:THR:HG21	2.36	0.40
2:G:1911:THR:O	2:G:1915:ASN:ND2	2.54	0.40
3:H:37:PHE:CZ	3:H:41:LEU:HD21	2.56	0.40
3:H:835:THR:C	3:H:845:THR:HG22	2.46	0.40
3:H:1130:THR:N	3:H:1133:THR:HG22	2.36	0.40
3:H:1665:VAL:HA	3:H:1805:ALA:O	2.21	0.40
3:H:1956:ARG:N	3:H:1957:PRO:HD2	2.36	0.40
3:H:2044:ASN:C	3:H:2046:GLU:N	2.79	0.40
3:I:285:GLU:OE1	3:I:298:LYS:CE	2.68	0.40
2:J:1956:ARG:N	2:J:1957:PRO:HD2	2.36	0.40
2:J:1986:LYS:N	2:J:1987:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:285:GLU:OE1	3:K:298:LYS:CE	2.68	0.40
3:K:1986:LYS:N	3:K:1987:PRO:HD2	2.36	0.40
3:L:285:GLU:OE1	3:L:298:LYS:CE	2.68	0.40
3:L:740[B]:HIS:CE1	3:L:852:GLU:HB2	2.56	0.40
3:L:1861:ARG:HG3	3:L:1965:ALA:HB2	2.03	0.40
3:L:1904:LEU:HG	3:L:1960:LEU:HD23	2.03	0.40
1:B:360:LYS:CE	1:E:358:GLU:OE2	2.69	0.40
1:B:826:MET:HE1	1:B:850:PHE:CE2	2.56	0.40
1:B:965:HIS:CE1	1:B:969:ASN:ND2	2.89	0.40
1:C:965:HIS:CE1	1:C:969:ASN:ND2	2.89	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.86	0.40
1:D:1021:VAL:HG11	1:D:1597:LEU:HD11	2.04	0.40
1:E:1119:LYS:O	1:E:1178:ALA:HA	2.20	0.40
1:E:1600:LEU:HD11	1:E:1655:VAL:HG12	2.03	0.40
1:F:1751:GLU:HG3	1:F:1872:SER:HB2	2.02	0.40
2:G:1849:ARG:NH1	2:G:1957:PRO:HG3	2.36	0.40
3:H:29:ILE:O	3:H:32:GLN:HB3	2.21	0.40
3:H:364:LYS:HA	3:H:382:PRO:HG2	2.03	0.40
3:H:852:GLU:H	3:H:852:GLU:HG3	1.75	0.40
3:H:883:THR:O	3:H:887:LYS:HG2	2.21	0.40
3:H:1280:ASP:OD1	3:H:1281:PRO:HD2	2.21	0.40
3:H:1541:VAL:HG22	3:H:1625:SER:HB2	2.02	0.40
3:H:1740:THR:OG1	3:H:1747:LYS:CE	2.69	0.40
3:I:29:ILE:O	3:I:32:GLN:HB3	2.21	0.40
2:J:419:ARG:CZ	2:J:419:ARG:HB3	2.51	0.40
2:J:753:MET:O	2:J:757:ILE:HG13	2.21	0.40
2:J:1541:VAL:HG22	2:J:1625:SER:CB	2.52	0.40
3:K:37:PHE:CZ	3:K:41:LEU:HD21	2.56	0.40
3:K:597:MET:HB3	10:K:2101:FMN:C6	2.51	0.40
3:K:1665:VAL:HA	3:K:1805:ALA:O	2.20	0.40
3:K:1854:MET:HB3	3:K:1901:ALA:CB	2.49	0.40
3:K:1871:LEU:HD23	3:K:1871:LEU:HA	1.92	0.40
3:L:1335:ILE:O	3:L:1338:ILE:HG12	2.22	0.40
3:L:1541:VAL:HG22	3:L:1625:SER:CB	2.52	0.40
3:L:1986:LYS:N	3:L:1987:PRO:HD2	2.36	0.40
1:B:955:LYS:O	1:B:959:ILE:HG13	2.21	0.40
1:B:1342:GLU:HB3	1:D:1275:LEU:HB2	2.04	0.40
1:C:213:PHE:O	1:C:217:PHE:HB2	2.22	0.40
1:C:998:TYR:CE2	1:C:1002:LYS:HD3	2.56	0.40
1:C:1181:PHE:CZ	1:C:1341:PHE:HA	2.56	0.40
1:C:1501:LEU:O	1:C:1505:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:CD1	2:J:1894:GLU:N	2.85	0.40
1:D:429:ASP:O	1:D:432:VAL:HG13	2.20	0.40
1:D:632:ARG:O	1:D:633:GLU:CB	2.69	0.40
1:D:1581:THR:HB	1:D:1591:TRP:CZ3	2.57	0.40
1:E:738:ASN:ND2	1:E:740:GLY:H	2.20	0.40
1:E:878:MET:HE2	1:E:878:MET:HB2	1.90	0.40
1:E:1303:GLY:HA2	1:E:1649:LYS:HE3	2.02	0.40
1:E:1431:GLU:HG3	1:E:1433:HIS:CE1	2.56	0.40
1:E:1455:ARG:HD2	1:E:1455:ARG:HA	1.77	0.40
1:E:1581:THR:HB	1:E:1591:TRP:CZ3	2.56	0.40
1:F:30:GLU:HB2	3:L:2016:ALA:CB	2.51	0.40
1:F:290:MET:HE3	1:F:290:MET:HA	2.03	0.40
2:G:1974:VAL:HB	2:G:1976:PHE:CE1	2.56	0.40
3:H:598:THR:OG1	3:H:599:PRO:HD2	2.19	0.40
3:I:803:SER:HB3	3:I:1055:HIS:CD2	2.56	0.40
2:J:2049:GLU:O	2:J:2050:GLN:C	2.64	0.40
3:K:1878:VAL:O	3:K:1882:THR:OG1	2.34	0.40
3:L:1435:ILE:CG2	3:L:1441:ILE:HG22	2.51	0.40
3:L:1849:ARG:HD2	3:L:1849:ARG:N	2.36	0.40
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.91	0.40
1:A:1657:HIS:CD2	1:A:1658:PRO:CD	3.01	0.40
1:C:329:GLU:HB2	1:C:332:THR:HG23	2.03	0.40
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.87	0.40
1:C:643:LYS:NZ	1:C:851:ASN:HD21	2.19	0.40
1:D:17:LEU:O	1:D:21:GLN:HB2	2.21	0.40
1:D:233:ILE:HG21	1:D:243:ILE:N	2.37	0.40
1:D:294:TYR:CE1	1:D:298:VAL:HG21	2.56	0.40
1:D:965:HIS:CE1	1:D:969:ASN:ND2	2.89	0.40
1:D:1153:ASP:OD2	1:E:359:ARG:NH1	2.55	0.40
1:D:1501:LEU:O	1:D:1505:GLN:HG3	2.21	0.40
1:E:43:ARG:HD3	3:K:1660:PRO:HG2	2.03	0.40
1:E:1751:GLU:HG3	1:E:1872:SER:HB2	2.03	0.40
1:F:807:LYS:HG3	1:F:858:TRP:HB3	2.03	0.40
1:F:826:MET:HE1	1:F:850:PHE:CE2	2.57	0.40
1:F:1181:PHE:CZ	1:F:1341:PHE:HA	2.57	0.40
1:F:1736:LYS:HA	1:F:1736:LYS:HD3	1.92	0.40
2:G:1085:LEU:HD12	2:G:1085:LEU:HA	1.86	0.40
2:G:1884:TRP:CD1	2:G:1905:ARG:HH11	2.40	0.40
3:H:716:VAL:HG11	3:H:730:LEU:HD22	2.02	0.40
3:I:753:MET:O	3:I:757:ILE:HG13	2.21	0.40
3:I:1854:MET:HB3	3:I:1901:ALA:CB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:490:TRP:CH2	3:K:512:LEU:HD21	2.57	0.40
3:K:1217:ASN:HD22	3:K:1217:ASN:HA	1.62	0.40
3:L:440:ASN:HD21	3:L:477:GLU:HA	1.86	0.40
3:L:1924:ILE:O	3:L:1928:GLN:HB2	2.22	0.40
1:A:793:ARG:HH11	1:F:789:GLU:CD	2.30	0.40
1:A:1302:VAL:CG2	1:E:1302:VAL:HG22	2.51	0.40
1:A:1392:LEU:HD22	1:A:1396:MET:HG3	2.02	0.40
1:B:1392:LEU:HD22	1:B:1396:MET:HG3	2.03	0.40
1:B:1581:THR:HB	1:B:1591:TRP:CZ3	2.56	0.40
1:B:1600:LEU:CD1	1:B:1655:VAL:HG12	2.51	0.40
1:B:1751:GLU:HG3	1:B:1872:SER:HB2	2.04	0.40
1:C:233:ILE:HG21	1:C:243:ILE:N	2.36	0.40
1:C:1181:PHE:CE2	1:C:1183:ARG:HB2	2.56	0.40
1:D:20:TYR:CE2	2:J:2033:THR:HG23	2.56	0.40
1:D:499:PRO:HB3	1:D:873:ARG:HD3	2.03	0.40
1:D:952:GLU:OE1	1:D:952:GLU:HA	2.20	0.40
1:E:13:LEU:C	1:E:17:LEU:HD12	2.46	0.40
1:E:499:PRO:HB3	1:E:873:ARG:HD3	2.03	0.40
1:E:965:HIS:CE1	1:E:969:ASN:ND2	2.90	0.40
1:F:955:LYS:O	1:F:959:ILE:HG13	2.21	0.40
1:F:1167:LEU:HD12	1:F:1167:LEU:HA	1.94	0.40
1:F:1370:THR:HG22	1:F:1372:THR:H	1.86	0.40
1:F:1395:LYS:HE3	1:F:1395:LYS:HB2	1.93	0.40
2:G:249:TYR:CE2	2:G:283:ILE:HD12	2.57	0.40
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.21	0.40
3:H:1086:LEU:HG	3:H:1092:ASP:HA	2.03	0.40
3:H:1905:ARG:O	3:H:1909:THR:HG23	2.22	0.40
3:H:1954:LYS:HB3	3:H:1955:PRO:HD2	2.03	0.40
3:I:364:LYS:HA	3:I:382:PRO:HG2	2.03	0.40
3:I:1858:ASN:C	3:I:1858:ASN:HD22	2.30	0.40
2:J:56:THR:HG21	2:J:112:ASN:HD22	1.86	0.40
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.21	0.40
3:K:29:ILE:O	3:K:33:LEU:HD22	2.22	0.40
3:K:1944:ILE:O	3:K:1948:SER:HB3	2.21	0.40
3:L:74:PRO:HB3	3:L:132:MET:HE3	2.02	0.40
3:L:260:PRO:HB2	3:L:286:THR:HG23	2.03	0.40
3:L:497:LYS:H	3:L:497:LYS:CD	2.35	0.40
3:L:1778:GLN:CB	3:L:1831:VAL:HG13	2.49	0.40
3:L:1859:PRO:O	3:L:1862:VAL:HG13	2.21	0.40
3:L:1967:ILE:HD13	3:L:1967:ILE:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:ASN:O	1:D:1843:ASN:O[1_655]	1.70	0.50
1:A:1845:ASN:OD1	1:D:1844:LYS:O[1_655]	1.96	0.24

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1752/1887 (93%)	1667 (95%)	77 (4%)	8 (0%)	24	53
1	B	1751/1887 (93%)	1663 (95%)	77 (4%)	11 (1%)	21	48
1	C	1751/1887 (93%)	1661 (95%)	80 (5%)	10 (1%)	21	48
1	D	1757/1887 (93%)	1664 (95%)	81 (5%)	12 (1%)	18	45
1	E	1751/1887 (93%)	1667 (95%)	75 (4%)	9 (0%)	24	53
1	F	1751/1887 (93%)	1662 (95%)	79 (4%)	10 (1%)	21	48
2	G	2033/2051 (99%)	1915 (94%)	105 (5%)	13 (1%)	21	48
2	J	2032/2051 (99%)	1914 (94%)	101 (5%)	17 (1%)	16	41
3	H	2031/2051 (99%)	1913 (94%)	105 (5%)	13 (1%)	21	48
3	I	2030/2051 (99%)	1911 (94%)	106 (5%)	13 (1%)	21	48
3	K	2030/2051 (99%)	1909 (94%)	109 (5%)	12 (1%)	21	48
3	L	2032/2051 (99%)	1912 (94%)	107 (5%)	13 (1%)	21	48
All	All	22701/23628 (96%)	21458 (94%)	1102 (5%)	141 (1%)	21	48

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1843	ASN
1	D	539	SER
1	F	1827	SER
2	G	7	ARG

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Mol	Chain	Res	Type
2	G	1869	GLU
2	G	1970	VAL
3	H	7	ARG
3	H	1865	SER
3	H	1970	VAL
3	I	7	ARG
3	I	1865	SER
3	I	1970	VAL
2	J	7	ARG
2	J	1865	SER
2	J	1970	VAL
3	K	7	ARG
3	K	1970	VAL
3	L	7	ARG
3	L	1970	VAL
1	A	874	GLY
1	A	1436	VAL
1	B	874	GLY
1	B	1436	VAL
1	B	1765	SER
1	C	874	GLY
1	C	1436	VAL
1	D	874	GLY
1	D	1436	VAL
1	D	1828	LEU
1	E	874	GLY
1	E	1436	VAL
1	E	1765	SER
1	F	874	GLY
1	F	1436	VAL
1	F	1885	THR
2	G	769	SER
2	G	1092	ASP
2	G	1964	PHE
3	H	769	SER
3	H	1092	ASP
3	H	1964	PHE
3	I	769	SER
3	I	1092	ASP
3	I	1964	PHE
2	J	769	SER
2	J	1092	ASP

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Mol	Chain	Res	Type
2	J	1928	GLN
2	J	1964	PHE
2	J	2049	GLU
3	K	769	SER
3	K	1092	ASP
3	K	1964	PHE
3	L	769	SER
3	L	1092	ASP
3	L	1965	ALA
1	B	517	GLU
1	C	517	GLU
1	C	1765	SER
1	D	517	GLU
1	D	1764	VAL
1	E	517	GLU
1	F	517	GLU
1	F	1764	VAL
1	F	1765	SER
2	G	2016	ALA
3	H	1928	GLN
3	I	1928	GLN
3	I	2016	ALA
2	J	75	SER
2	J	2016	ALA
3	K	1928	GLN
3	L	1928	GLN
1	A	1764	VAL
1	A	1765	SER
1	C	1764	VAL
1	D	1765	SER
1	E	1764	VAL
2	G	203	LEU
2	G	598	THR
3	H	203	LEU
3	H	2016	ALA
3	I	203	LEU
3	I	598	THR
2	J	203	LEU
2	J	598	THR
3	K	203	LEU
3	K	598	THR
3	K	1864	ALA

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Mol	Chain	Res	Type
3	L	598	THR
3	L	2016	ALA
1	C	1608	ASN
1	D	1608	ASN
2	G	508	GLY
2	G	699	GLY
3	H	598	THR
3	I	699	GLY
2	J	508	GLY
3	K	699	GLY
3	L	203	LEU
3	L	508	GLY
3	L	699	GLY
1	A	198	PRO
1	B	1608	ASN
1	E	1608	ASN
2	G	1163	LYS
3	H	699	GLY
3	I	508	GLY
2	J	572	ASN
2	J	877	LYS
2	J	1847	LEU
3	L	572	ASN
1	A	1298	ILE
1	B	299	GLY
1	B	1298	ILE
1	B	1764	VAL
1	B	1863	GLY
1	C	1298	ILE
1	C	1863	GLY
1	D	1298	ILE
1	E	1298	ILE
1	E	1863	GLY
1	F	1298	ILE
3	H	508	GLY
3	K	508	GLY
1	D	198	PRO
1	F	198	PRO
1	A	1863	GLY
1	B	1853	GLY
1	C	198	PRO
1	C	1853	GLY

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Mol	Chain	Res	Type
1	D	1853	GLY
1	E	299	GLY
1	F	1863	GLY
2	J	772	GLY
3	K	772	GLY
3	L	772	GLY
1	A	1543	GLY
1	D	1863	GLY
2	G	772	GLY
3	H	772	GLY
3	I	772	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1484/1566 (95%)	1301 (88%)	183 (12%)	4	15
1	B	1483/1566 (95%)	1297 (88%)	186 (12%)	4	15
1	C	1483/1566 (95%)	1302 (88%)	181 (12%)	5	15
1	D	1489/1566 (95%)	1306 (88%)	183 (12%)	4	15
1	E	1483/1566 (95%)	1292 (87%)	191 (13%)	4	14
1	F	1483/1566 (95%)	1299 (88%)	184 (12%)	4	15
2	G	1776/1789 (99%)	1519 (86%)	257 (14%)	3	10
2	J	1775/1789 (99%)	1517 (86%)	258 (14%)	3	10
3	H	1774/1788 (99%)	1527 (86%)	247 (14%)	3	11
3	I	1773/1788 (99%)	1510 (85%)	263 (15%)	3	9
3	K	1773/1788 (99%)	1508 (85%)	265 (15%)	3	9
3	L	1775/1788 (99%)	1505 (85%)	270 (15%)	3	9
All	All	19551/20126 (97%)	16883 (86%)	2668 (14%)	3	12

All (2668) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	9	LEU
1	A	14	LEU
1	A	15	THR
1	A	17	LEU
1	A	24	SER
1	A	27	ARG
1	A	44	VAL
1	A	59	ARG
1	A	60	THR
1	A	62	LYS
1	A	64	LYS
1	A	72	LEU
1	A	83	LYS
1	A	84	ASP
1	A	140	ILE
1	A	149	LEU
1	A	176	VAL
1	A	179	LYS
1	A	181	THR
1	A	192	LYS
1	A	214	GLN
1	A	216	THR
1	A	234	SER
1	A	242	THR
1	A	258	SER
1	A	261	GLN
1	A	292	GLN
1	A	328	LEU
1	A	331	ILE
1	A	332	THR
1	A	340	ARG
1	A	345	VAL
1	A	363	LYS
1	A	367	THR
1	A	378	LEU
1	A	390	VAL
1	A	392	THR
1	A	401	THR
1	A	416	LEU
1	A	421	ILE
1	A	426	LYS
1	A	428	VAL

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Mol	Chain	Res	Type
1	A	432	VAL
1	A	447	LEU
1	A	458	THR
1	A	472	LEU
1	A	489	VAL
1	A	491	LYS
1	A	493	VAL
1	A	495	LYS
1	A	509	ILE
1	A	527	GLN
1	A	538	GLU
1	A	599	MET
1	A	607	LYS
1	A	620	SER
1	A	621	THR
1	A	622	ILE
1	A	625	THR
1	A	633	GLU
1	A	634	THR
1	A	644	THR
1	A	650	LYS
1	A	658	LEU
1	A	665	LYS
1	A	671	VAL
1	A	674	LYS
1	A	705	VAL
1	A	709	ARG
1	A	715	THR
1	A	731	THR
1	A	732	LEU
1	A	748	LEU
1	A	750	GLU
1	A	754	ASP
1	A	761	LEU
1	A	776	GLU
1	A	782	GLU
1	A	806	VAL
1	A	824	LEU
1	A	840	SER
1	A	857	SER
1	A	862	LEU
1	A	864	VAL

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Mol	Chain	Res	Type
1	A	869	ILE
1	A	878	MET
1	A	913	VAL
1	A	915	GLU
1	A	916	LEU
1	A	930	LEU
1	A	931	GLN
1	A	933	VAL
1	A	938	GLU
1	A	940	THR
1	A	945	LYS
1	A	947	LEU
1	A	953	VAL
1	A	955	LYS
1	A	972	SER
1	A	982	ILE
1	A	999	LYS
1	A	1001	VAL
1	A	1020	VAL
1	A	1022	THR
1	A	1047	LEU
1	A	1061	SER
1	A	1067	LEU
1	A	1068	LYS
1	A	1073	THR
1	A	1076	VAL
1	A	1090	LYS
1	A	1092	LYS
1	A	1099	GLU
1	A	1119	LYS
1	A	1123	GLN
1	A	1143	GLN
1	A	1164	SER
1	A	1179	LEU
1	A	1180	ARG
1	A	1184	LEU
1	A	1197	THR
1	A	1208	VAL
1	A	1229	THR
1	A	1238	VAL
1	A	1240	VAL
1	A	1271	GLN

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Mol	Chain	Res	Type
1	A	1282	THR
1	A	1307	THR
1	A	1325	ARG
1	A	1327	CYS
1	A	1329	VAL
1	A	1392	LEU
1	A	1395	LYS
1	A	1411	THR
1	A	1426	LEU
1	A	1436	VAL
1	A	1440	SER
1	A	1443	LEU
1	A	1449	LYS
1	A	1455	ARG
1	A	1460	LYS
1	A	1480	GLU
1	A	1486	LEU
1	A	1495	ASN
1	A	1501	LEU
1	A	1522	LEU
1	A	1528	THR
1	A	1540	SER
1	A	1556	THR
1	A	1575	VAL
1	A	1580	LEU
1	A	1622	GLU
1	A	1625	LEU
1	A	1629	LYS
1	A	1631	LEU
1	A	1640	SER
1	A	1642	THR
1	A	1690	ASN
1	A	1706	TYR
1	A	1727	LYS
1	A	1735	SER
1	A	1743	SER
1	A	1756	ILE
1	A	1761	LYS
1	A	1762	GLU
1	A	1766	ASN
1	A	1773	VAL
1	A	1775	LEU

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Mol	Chain	Res	Type
1	A	1776	ILE
1	A	1777	THR
1	A	1778	SER
1	A	1788	GLU
1	A	1794	GLN
1	A	1827	SER
1	A	1828	LEU
1	A	1841	ARG
1	A	1842	VAL
1	A	1851	LEU
1	A	1860	GLU
1	A	1864	VAL
1	A	1868	LYS
1	A	1879	VAL
1	B	2	LYS
1	B	5	VAL
1	B	14	LEU
1	B	15	THR
1	B	24	SER
1	B	37	LYS
1	B	44	VAL
1	B	59	ARG
1	B	60	THR
1	B	62	LYS
1	B	64	LYS
1	B	78	ILE
1	B	84	ASP
1	B	140	ILE
1	B	146	LYS
1	B	149	LEU
1	B	168	MET
1	B	176	VAL
1	B	179	LYS
1	B	192	LYS
1	B	216	THR
1	B	223	LYS
1	B	231	ARG
1	B	234	SER
1	B	242	THR
1	B	261	GLN
1	B	292	GLN
1	B	328	LEU

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Mol	Chain	Res	Type
1	B	331	ILE
1	B	332	THR
1	B	333	LYS
1	B	340	ARG
1	B	345	VAL
1	B	351	LYS
1	B	363	LYS
1	B	367	THR
1	B	378	LEU
1	B	390	VAL
1	B	392	THR
1	B	401	THR
1	B	416	LEU
1	B	421	ILE
1	B	426	LYS
1	B	428	VAL
1	B	432	VAL
1	B	447	LEU
1	B	458	THR
1	B	472	LEU
1	B	483	VAL
1	B	489	VAL
1	B	491	LYS
1	B	493	VAL
1	B	495	LYS
1	B	505	LYS
1	B	508	ASN
1	B	509	ILE
1	B	510	THR
1	B	599	MET
1	B	602	GLU
1	B	620	SER
1	B	621	THR
1	B	622	ILE
1	B	625	THR
1	B	634	THR
1	B	644	THR
1	B	650	LYS
1	B	665	LYS
1	B	671	VAL
1	B	674	LYS
1	B	705	VAL

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Mol	Chain	Res	Type
1	B	709	ARG
1	B	715	THR
1	B	731	THR
1	B	732	LEU
1	B	748	LEU
1	B	750	GLU
1	B	754	ASP
1	B	757	LYS
1	B	761	LEU
1	B	776	GLU
1	B	777	GLN
1	B	782	GLU
1	B	797	THR
1	B	806	VAL
1	B	824	LEU
1	B	840	SER
1	B	857	SER
1	B	862	LEU
1	B	864	VAL
1	B	877	LEU
1	B	878	MET
1	B	894	ARG
1	B	913	VAL
1	B	915	GLU
1	B	916	LEU
1	B	930	LEU
1	B	931	GLN
1	B	933	VAL
1	B	940	THR
1	B	945	LYS
1	B	947	LEU
1	B	953	VAL
1	B	955	LYS
1	B	972	SER
1	B	977	TYR
1	B	982	ILE
1	B	1001	VAL
1	B	1020	VAL
1	B	1022	THR
1	B	1047	LEU
1	B	1061	SER
1	B	1067	LEU

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Mol	Chain	Res	Type
1	B	1068	LYS
1	B	1070	ARG
1	B	1073	THR
1	B	1076	VAL
1	B	1079	LYS
1	B	1090	LYS
1	B	1117	GLU
1	B	1123	GLN
1	B	1128	GLU
1	B	1143	GLN
1	B	1164	SER
1	B	1179	LEU
1	B	1180	ARG
1	B	1184	LEU
1	B	1197	THR
1	B	1208	VAL
1	B	1229	THR
1	B	1238	VAL
1	B	1240	VAL
1	B	1271	GLN
1	B	1282	THR
1	B	1307	THR
1	B	1325	ARG
1	B	1327	CYS
1	B	1329	VAL
1	B	1392	LEU
1	B	1411	THR
1	B	1426	LEU
1	B	1436	VAL
1	B	1440	SER
1	B	1443	LEU
1	B	1449	LYS
1	B	1455	ARG
1	B	1460	LYS
1	B	1486	LEU
1	B	1495	ASN
1	B	1501	LEU
1	B	1522	LEU
1	B	1528	THR
1	B	1540	SER
1	B	1556	THR
1	B	1575	VAL

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Mol	Chain	Res	Type
1	B	1578	LYS
1	B	1580	LEU
1	B	1625	LEU
1	B	1629	LYS
1	B	1640	SER
1	B	1642	THR
1	B	1690	ASN
1	B	1706	TYR
1	B	1727	LYS
1	B	1735	SER
1	B	1743	SER
1	B	1750	ILE
1	B	1756	ILE
1	B	1761	LYS
1	B	1762	GLU
1	B	1763	LYS
1	B	1766	ASN
1	B	1773	VAL
1	B	1775	LEU
1	B	1776	ILE
1	B	1777	THR
1	B	1778	SER
1	B	1789	ARG
1	B	1794	GLN
1	B	1827	SER
1	B	1828	LEU
1	B	1842	VAL
1	B	1851	LEU
1	B	1860	GLU
1	B	1861	GLU
1	B	1864	VAL
1	B	1879	VAL
1	C	14	LEU
1	C	15	THR
1	C	17	LEU
1	C	24	SER
1	C	37	LYS
1	C	44	VAL
1	C	60	THR
1	C	64	LYS
1	C	78	ILE
1	C	83	LYS

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Mol	Chain	Res	Type
1	C	84	ASP
1	C	93	ASP
1	C	140	ILE
1	C	146	LYS
1	C	149	LEU
1	C	160	LYS
1	C	176	VAL
1	C	179	LYS
1	C	181	THR
1	C	192	LYS
1	C	200	LYS
1	C	216	THR
1	C	223	LYS
1	C	225	SER
1	C	234	SER
1	C	242	THR
1	C	248	LYS
1	C	258	SER
1	C	261	GLN
1	C	292	GLN
1	C	331	ILE
1	C	332	THR
1	C	345	VAL
1	C	364	GLU
1	C	367	THR
1	C	378	LEU
1	C	390	VAL
1	C	392	THR
1	C	401	THR
1	C	416	LEU
1	C	421	ILE
1	C	428	VAL
1	C	432	VAL
1	C	447	LEU
1	C	458	THR
1	C	472	LEU
1	C	489	VAL
1	C	491	LYS
1	C	493	VAL
1	C	509	ILE
1	C	607	LYS
1	C	619	LYS

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Mol	Chain	Res	Type
1	C	621	THR
1	C	622	ILE
1	C	625	THR
1	C	632	ARG
1	C	634	THR
1	C	644	THR
1	C	665	LYS
1	C	671	VAL
1	C	674	LYS
1	C	702	LYS
1	C	705	VAL
1	C	709	ARG
1	C	715	THR
1	C	731	THR
1	C	732	LEU
1	C	748	LEU
1	C	750	GLU
1	C	754	ASP
1	C	761	LEU
1	C	776	GLU
1	C	777	GLN
1	C	782	GLU
1	C	797	THR
1	C	806	VAL
1	C	824	LEU
1	C	840	SER
1	C	857	SER
1	C	862	LEU
1	C	864	VAL
1	C	869	ILE
1	C	890	LYS
1	C	893	VAL
1	C	913	VAL
1	C	915	GLU
1	C	916	LEU
1	C	930	LEU
1	C	931	GLN
1	C	933	VAL
1	C	938	GLU
1	C	940	THR
1	C	945	LYS
1	C	947	LEU

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Mol	Chain	Res	Type
1	C	953	VAL
1	C	961	THR
1	C	972	SER
1	C	982	ILE
1	C	1001	VAL
1	C	1020	VAL
1	C	1022	THR
1	C	1039	MET
1	C	1047	LEU
1	C	1061	SER
1	C	1067	LEU
1	C	1073	THR
1	C	1076	VAL
1	C	1090	LYS
1	C	1092	LYS
1	C	1099	GLU
1	C	1117	GLU
1	C	1119	LYS
1	C	1123	GLN
1	C	1128	GLU
1	C	1143	GLN
1	C	1151	LYS
1	C	1164	SER
1	C	1179	LEU
1	C	1180	ARG
1	C	1184	LEU
1	C	1197	THR
1	C	1208	VAL
1	C	1229	THR
1	C	1238	VAL
1	C	1240	VAL
1	C	1271	GLN
1	C	1282	THR
1	C	1307	THR
1	C	1325	ARG
1	C	1327	CYS
1	C	1329	VAL
1	C	1392	LEU
1	C	1395	LYS
1	C	1411	THR
1	C	1426	LEU
1	C	1436	VAL

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Mol	Chain	Res	Type
1	C	1440	SER
1	C	1443	LEU
1	C	1449	LYS
1	C	1455	ARG
1	C	1477	ILE
1	C	1480	GLU
1	C	1486	LEU
1	C	1490	THR
1	C	1495	ASN
1	C	1501	LEU
1	C	1522	LEU
1	C	1528	THR
1	C	1540	SER
1	C	1556	THR
1	C	1575	VAL
1	C	1580	LEU
1	C	1625	LEU
1	C	1640	SER
1	C	1642	THR
1	C	1690	ASN
1	C	1706	TYR
1	C	1735	SER
1	C	1736	LYS
1	C	1743	SER
1	C	1756	ILE
1	C	1761	LYS
1	C	1762	GLU
1	C	1763	LYS
1	C	1766	ASN
1	C	1773	VAL
1	C	1775	LEU
1	C	1776	ILE
1	C	1777	THR
1	C	1778	SER
1	C	1788	GLU
1	C	1794	GLN
1	C	1827	SER
1	C	1841	ARG
1	C	1843	ASN
1	C	1844	LYS
1	C	1851	LEU
1	C	1857	LYS

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Mol	Chain	Res	Type
1	C	1864	VAL
1	C	1879	VAL
1	C	1886	LYS
1	D	14	LEU
1	D	15	THR
1	D	17	LEU
1	D	24	SER
1	D	27	ARG
1	D	44	VAL
1	D	60	THR
1	D	64	LYS
1	D	78	ILE
1	D	83	LYS
1	D	84	ASP
1	D	140	ILE
1	D	149	LEU
1	D	160	LYS
1	D	168	MET
1	D	176	VAL
1	D	181	THR
1	D	192	LYS
1	D	216	THR
1	D	234	SER
1	D	242	THR
1	D	261	GLN
1	D	292	GLN
1	D	328	LEU
1	D	331	ILE
1	D	332	THR
1	D	336	LYS
1	D	340	ARG
1	D	345	VAL
1	D	367	THR
1	D	378	LEU
1	D	390	VAL
1	D	392	THR
1	D	401	THR
1	D	416	LEU
1	D	421	ILE
1	D	428	VAL
1	D	432	VAL
1	D	447	LEU

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Mol	Chain	Res	Type
1	D	458	THR
1	D	472	LEU
1	D	489	VAL
1	D	491	LYS
1	D	493	VAL
1	D	495	LYS
1	D	505	LYS
1	D	509	ILE
1	D	527	GLN
1	D	537	LYS
1	D	538	GLU
1	D	542	THR
1	D	544	GLU
1	D	607	LYS
1	D	611	LYS
1	D	619	LYS
1	D	620	SER
1	D	622	ILE
1	D	624	LYS
1	D	625	THR
1	D	634	THR
1	D	644	THR
1	D	650	LYS
1	D	671	VAL
1	D	674	LYS
1	D	705	VAL
1	D	715	THR
1	D	731	THR
1	D	732	LEU
1	D	748	LEU
1	D	750	GLU
1	D	754	ASP
1	D	761	LEU
1	D	776	GLU
1	D	777	GLN
1	D	782	GLU
1	D	797	THR
1	D	806	VAL
1	D	824	LEU
1	D	840	SER
1	D	857	SER
1	D	862	LEU

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Mol	Chain	Res	Type
1	D	864	VAL
1	D	878	MET
1	D	913	VAL
1	D	915	GLU
1	D	916	LEU
1	D	930	LEU
1	D	931	GLN
1	D	933	VAL
1	D	935	GLU
1	D	938	GLU
1	D	940	THR
1	D	947	LEU
1	D	953	VAL
1	D	955	LYS
1	D	972	SER
1	D	974	ASP
1	D	982	ILE
1	D	1001	VAL
1	D	1020	VAL
1	D	1022	THR
1	D	1047	LEU
1	D	1061	SER
1	D	1067	LEU
1	D	1073	THR
1	D	1076	VAL
1	D	1079	LYS
1	D	1090	LYS
1	D	1092	LYS
1	D	1099	GLU
1	D	1117	GLU
1	D	1123	GLN
1	D	1128	GLU
1	D	1143	GLN
1	D	1164	SER
1	D	1177	LYS
1	D	1179	LEU
1	D	1180	ARG
1	D	1184	LEU
1	D	1197	THR
1	D	1208	VAL
1	D	1229	THR
1	D	1238	VAL

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Mol	Chain	Res	Type
1	D	1240	VAL
1	D	1271	GLN
1	D	1282	THR
1	D	1283	MET
1	D	1307	THR
1	D	1325	ARG
1	D	1327	CYS
1	D	1329	VAL
1	D	1370	THR
1	D	1392	LEU
1	D	1426	LEU
1	D	1436	VAL
1	D	1440	SER
1	D	1443	LEU
1	D	1449	LYS
1	D	1455	ARG
1	D	1480	GLU
1	D	1486	LEU
1	D	1493	ILE
1	D	1495	ASN
1	D	1501	LEU
1	D	1522	LEU
1	D	1528	THR
1	D	1540	SER
1	D	1556	THR
1	D	1575	VAL
1	D	1578	LYS
1	D	1580	LEU
1	D	1622	GLU
1	D	1625	LEU
1	D	1629	LYS
1	D	1631	LEU
1	D	1640	SER
1	D	1642	THR
1	D	1649	LYS
1	D	1690	ASN
1	D	1706	TYR
1	D	1727	LYS
1	D	1736	LYS
1	D	1743	SER
1	D	1750	ILE
1	D	1761	LYS

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Mol	Chain	Res	Type
1	D	1762	GLU
1	D	1763	LYS
1	D	1773	VAL
1	D	1775	LEU
1	D	1776	ILE
1	D	1777	THR
1	D	1778	SER
1	D	1826	LYS
1	D	1827	SER
1	D	1841	ARG
1	D	1842	VAL
1	D	1844	LYS
1	D	1857	LYS
1	D	1860	GLU
1	D	1861	GLU
1	D	1864	VAL
1	D	1879	VAL
1	D	1886	LYS
1	E	2	LYS
1	E	5	VAL
1	E	14	LEU
1	E	15	THR
1	E	17	LEU
1	E	24	SER
1	E	44	VAL
1	E	59	ARG
1	E	60	THR
1	E	64	LYS
1	E	74	LEU
1	E	78	ILE
1	E	82	SER
1	E	83	LYS
1	E	84	ASP
1	E	140	ILE
1	E	149	LEU
1	E	176	VAL
1	E	179	LYS
1	E	181	THR
1	E	216	THR
1	E	234	SER
1	E	242	THR
1	E	261	GLN

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Mol	Chain	Res	Type
1	E	292	GLN
1	E	302	LEU
1	E	330	GLU
1	E	331	ILE
1	E	332	THR
1	E	333	LYS
1	E	345	VAL
1	E	363	LYS
1	E	367	THR
1	E	378	LEU
1	E	390	VAL
1	E	392	THR
1	E	401	THR
1	E	416	LEU
1	E	421	ILE
1	E	426	LYS
1	E	428	VAL
1	E	432	VAL
1	E	447	LEU
1	E	449	LYS
1	E	458	THR
1	E	472	LEU
1	E	484	LEU
1	E	489	VAL
1	E	491	LYS
1	E	493	VAL
1	E	495	LYS
1	E	509	ILE
1	E	527	GLN
1	E	537	LYS
1	E	607	LYS
1	E	620	SER
1	E	621	THR
1	E	622	ILE
1	E	624	LYS
1	E	625	THR
1	E	632	ARG
1	E	634	THR
1	E	644	THR
1	E	665	LYS
1	E	671	VAL
1	E	674	LYS

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Mol	Chain	Res	Type
1	E	702	LYS
1	E	705	VAL
1	E	715	THR
1	E	724	LYS
1	E	731	THR
1	E	732	LEU
1	E	748	LEU
1	E	750	GLU
1	E	754	ASP
1	E	757	LYS
1	E	761	LEU
1	E	776	GLU
1	E	777	GLN
1	E	782	GLU
1	E	806	VAL
1	E	824	LEU
1	E	840	SER
1	E	857	SER
1	E	862	LEU
1	E	864	VAL
1	E	869	ILE
1	E	878	MET
1	E	913	VAL
1	E	915	GLU
1	E	916	LEU
1	E	930	LEU
1	E	931	GLN
1	E	933	VAL
1	E	938	GLU
1	E	940	THR
1	E	947	LEU
1	E	953	VAL
1	E	955	LYS
1	E	961	THR
1	E	967	VAL
1	E	972	SER
1	E	982	ILE
1	E	1001	VAL
1	E	1004	ILE
1	E	1020	VAL
1	E	1022	THR
1	E	1047	LEU

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Mol	Chain	Res	Type
1	E	1061	SER
1	E	1067	LEU
1	E	1073	THR
1	E	1076	VAL
1	E	1090	LYS
1	E	1092	LYS
1	E	1096	SER
1	E	1099	GLU
1	E	1119	LYS
1	E	1123	GLN
1	E	1128	GLU
1	E	1143	GLN
1	E	1164	SER
1	E	1167	LEU
1	E	1179	LEU
1	E	1184	LEU
1	E	1197	THR
1	E	1208	VAL
1	E	1229	THR
1	E	1238	VAL
1	E	1240	VAL
1	E	1271	GLN
1	E	1282	THR
1	E	1307	THR
1	E	1325	ARG
1	E	1327	CYS
1	E	1329	VAL
1	E	1392	LEU
1	E	1395	LYS
1	E	1411	THR
1	E	1426	LEU
1	E	1436	VAL
1	E	1440	SER
1	E	1443	LEU
1	E	1449	LYS
1	E	1455	ARG
1	E	1486	LEU
1	E	1490	THR
1	E	1492	GLU
1	E	1495	ASN
1	E	1501	LEU
1	E	1522	LEU

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Mol	Chain	Res	Type
1	E	1528	THR
1	E	1540	SER
1	E	1547	LYS
1	E	1556	THR
1	E	1575	VAL
1	E	1580	LEU
1	E	1622	GLU
1	E	1625	LEU
1	E	1629	LYS
1	E	1640	SER
1	E	1642	THR
1	E	1690	ASN
1	E	1706	TYR
1	E	1727	LYS
1	E	1735	SER
1	E	1743	SER
1	E	1750	ILE
1	E	1754	LYS
1	E	1756	ILE
1	E	1761	LYS
1	E	1762	GLU
1	E	1763	LYS
1	E	1766	ASN
1	E	1773	VAL
1	E	1775	LEU
1	E	1776	ILE
1	E	1777	THR
1	E	1778	SER
1	E	1779	ILE
1	E	1787	ILE
1	E	1788	GLU
1	E	1789	ARG
1	E	1794	GLN
1	E	1827	SER
1	E	1828	LEU
1	E	1851	LEU
1	E	1857	LYS
1	E	1860	GLU
1	E	1864	VAL
1	E	1868	LYS
1	E	1879	VAL
1	F	8	GLU

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Mol	Chain	Res	Type
1	F	14	LEU
1	F	15	THR
1	F	17	LEU
1	F	24	SER
1	F	44	VAL
1	F	60	THR
1	F	64	LYS
1	F	72	LEU
1	F	84	ASP
1	F	140	ILE
1	F	146	LYS
1	F	149	LEU
1	F	161	LYS
1	F	179	LYS
1	F	181	THR
1	F	192	LYS
1	F	196	THR
1	F	200	LYS
1	F	225	SER
1	F	234	SER
1	F	242	THR
1	F	248	LYS
1	F	258	SER
1	F	261	GLN
1	F	292	GLN
1	F	328	LEU
1	F	331	ILE
1	F	332	THR
1	F	333	LYS
1	F	345	VAL
1	F	351	LYS
1	F	367	THR
1	F	378	LEU
1	F	390	VAL
1	F	392	THR
1	F	401	THR
1	F	416	LEU
1	F	421	ILE
1	F	426	LYS
1	F	428	VAL
1	F	432	VAL
1	F	447	LEU

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Mol	Chain	Res	Type
1	F	458	THR
1	F	472	LEU
1	F	483	VAL
1	F	489	VAL
1	F	491	LYS
1	F	493	VAL
1	F	509	ILE
1	F	527	GLN
1	F	538	GLU
1	F	599	MET
1	F	607	LYS
1	F	620	SER
1	F	621	THR
1	F	622	ILE
1	F	625	THR
1	F	634	THR
1	F	644	THR
1	F	650	LYS
1	F	658	LEU
1	F	665	LYS
1	F	671	VAL
1	F	674	LYS
1	F	705	VAL
1	F	715	THR
1	F	731	THR
1	F	732	LEU
1	F	748	LEU
1	F	750	GLU
1	F	754	ASP
1	F	761	LEU
1	F	776	GLU
1	F	777	GLN
1	F	782	GLU
1	F	806	VAL
1	F	824	LEU
1	F	840	SER
1	F	857	SER
1	F	862	LEU
1	F	864	VAL
1	F	869	ILE
1	F	878	MET
1	F	893	VAL

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Mol	Chain	Res	Type
1	F	913	VAL
1	F	915	GLU
1	F	916	LEU
1	F	930	LEU
1	F	931	GLN
1	F	933	VAL
1	F	938	GLU
1	F	940	THR
1	F	947	LEU
1	F	953	VAL
1	F	972	SER
1	F	982	ILE
1	F	1001	VAL
1	F	1020	VAL
1	F	1022	THR
1	F	1047	LEU
1	F	1061	SER
1	F	1067	LEU
1	F	1073	THR
1	F	1076	VAL
1	F	1079	LYS
1	F	1090	LYS
1	F	1092	LYS
1	F	1099	GLU
1	F	1117	GLU
1	F	1119	LYS
1	F	1123	GLN
1	F	1143	GLN
1	F	1164	SER
1	F	1179	LEU
1	F	1180	ARG
1	F	1184	LEU
1	F	1197	THR
1	F	1208	VAL
1	F	1229	THR
1	F	1238	VAL
1	F	1240	VAL
1	F	1264	ARG
1	F	1271	GLN
1	F	1282	THR
1	F	1283	MET
1	F	1307	THR

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Mol	Chain	Res	Type
1	F	1325	ARG
1	F	1327	CYS
1	F	1329	VAL
1	F	1392	LEU
1	F	1395	LYS
1	F	1411	THR
1	F	1426	LEU
1	F	1436	VAL
1	F	1440	SER
1	F	1443	LEU
1	F	1449	LYS
1	F	1455	ARG
1	F	1486	LEU
1	F	1495	ASN
1	F	1501	LEU
1	F	1514	LYS
1	F	1522	LEU
1	F	1528	THR
1	F	1540	SER
1	F	1556	THR
1	F	1575	VAL
1	F	1578	LYS
1	F	1580	LEU
1	F	1622	GLU
1	F	1625	LEU
1	F	1629	LYS
1	F	1640	SER
1	F	1642	THR
1	F	1690	ASN
1	F	1706	TYR
1	F	1726	LYS
1	F	1727	LYS
1	F	1735	SER
1	F	1736	LYS
1	F	1743	SER
1	F	1750	ILE
1	F	1754	LYS
1	F	1762	GLU
1	F	1763	LYS
1	F	1773	VAL
1	F	1775	LEU
1	F	1776	ILE

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Mol	Chain	Res	Type
1	F	1777	THR
1	F	1778	SER
1	F	1788	GLU
1	F	1794	GLN
1	F	1826	LYS
1	F	1827	SER
1	F	1828	LEU
1	F	1841	ARG
1	F	1842	VAL
1	F	1851	LEU
1	F	1857	LYS
1	F	1860	GLU
1	F	1864	VAL
1	F	1879	VAL
1	F	1886	LYS
2	G	6	THR
2	G	9	LEU
2	G	10	THR
2	G	15	SER
2	G	16	LEU
2	G	26	SER
2	G	31	SER
2	G	34	GLN
2	G	55	THR
2	G	56	THR
2	G	60	LEU
2	G	76	LYS
2	G	79	GLN
2	G	82	GLN
2	G	84	LEU
2	G	86	LEU
2	G	96	LEU
2	G	99	ASN
2	G	111	GLU
2	G	113	ASP
2	G	114	THR
2	G	116	LEU
2	G	119	THR
2	G	122	LEU
2	G	142	ASN
2	G	149	VAL
2	G	163	GLN

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Mol	Chain	Res	Type
2	G	167	ASP
2	G	173	LEU
2	G	174	ARG
2	G	175	ASP
2	G	184	VAL
2	G	198	LEU
2	G	200	ARG
2	G	215	ILE
2	G	232	LEU
2	G	236	ILE
2	G	240	LEU
2	G	245	GLN
2	G	246	LEU
2	G	255	LEU
2	G	264	ARG
2	G	277	LEU
2	G	279	THR
2	G	283	ILE
2	G	286	THR
2	G	294	VAL
2	G	295	SER
2	G	301	THR
2	G	303	LEU
2	G	309	ARG
2	G	318	SER
2	G	323	ILE
2	G	327	SER
2	G	339	LEU
2	G	340	SER
2	G	344	LEU
2	G	347	GLU
2	G	353	VAL
2	G	369	SER
2	G	376	ASN
2	G	389	LEU
2	G	397	LYS
2	G	413	LYS
2	G	417	SER
2	G	419	ARG
2	G	425	SER
2	G	429	SER
2	G	431	LEU

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Mol	Chain	Res	Type
2	G	432	LEU
2	G	437	ASP
2	G	438	LEU
2	G	453	LYS
2	G	456	GLN
2	G	462	THR
2	G	471	LEU
2	G	476	SER
2	G	492	THR
2	G	494	THR
2	G	532	THR
2	G	540	ASP
2	G	544	LYS
2	G	562	LEU
2	G	570	ILE
2	G	586	LEU
2	G	611	THR
2	G	616	THR
2	G	650	ASN
2	G	654	VAL
2	G	659	LEU
2	G	665	LEU
2	G	669	LEU
2	G	670	ARG
2	G	681	ILE
2	G	693	GLU
2	G	697	THR
2	G	706	LYS
2	G	721	LYS
2	G	730	LEU
2	G	733	THR
2	G	752	GLN
2	G	777	THR
2	G	805	VAL
2	G	809	LYS
2	G	810	GLU
2	G	827	VAL
2	G	843	ILE
2	G	845	THR
2	G	846	VAL
2	G	850	MET
2	G	871	THR

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Mol	Chain	Res	Type
2	G	880	LEU
2	G	887	LYS
2	G	906	THR
2	G	914	LEU
2	G	947	THR
2	G	953	ARG
2	G	963	THR
2	G	964	LEU
2	G	972	LEU
2	G	995	LEU
2	G	1012	GLN
2	G	1015	VAL
2	G	1040	LEU
2	G	1044	VAL
2	G	1048	VAL
2	G	1049	GLN
2	G	1072	SER
2	G	1085	LEU
2	G	1100	VAL
2	G	1131	SER
2	G	1133	THR
2	G	1137	SER
2	G	1145	SER
2	G	1157	SER
2	G	1160	THR
2	G	1163	LYS
2	G	1167	SER
2	G	1172	LYS
2	G	1189	THR
2	G	1191	SER
2	G	1195	VAL
2	G	1197	LEU
2	G	1211	LEU
2	G	1213	LEU
2	G	1216	GLU
2	G	1228	THR
2	G	1229	MET
2	G	1235	SER
2	G	1236	LEU
2	G	1260	GLN
2	G	1317	ARG
2	G	1318	THR

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Mol	Chain	Res	Type
2	G	1320	LEU
2	G	1327	ILE
2	G	1336	LYS
2	G	1343	VAL
2	G	1348	LEU
2	G	1355	ASN
2	G	1360	ILE
2	G	1371	VAL
2	G	1375	THR
2	G	1377	VAL
2	G	1378	ILE
2	G	1381	VAL
2	G	1382	VAL
2	G	1384	GLN
2	G	1386	THR
2	G	1389	ILE
2	G	1395	THR
2	G	1408	SER
2	G	1413	ARG
2	G	1422	THR
2	G	1426	THR
2	G	1436	LYS
2	G	1441	ILE
2	G	1446	SER
2	G	1468	THR
2	G	1470	THR
2	G	1472	VAL
2	G	1479	ILE
2	G	1484	LYS
2	G	1503	ILE
2	G	1507	GLU
2	G	1526	THR
2	G	1528	GLU
2	G	1533	LEU
2	G	1551	GLU
2	G	1560	LEU
2	G	1590	ARG
2	G	1593	ILE
2	G	1600	SER
2	G	1603	SER
2	G	1605	VAL
2	G	1609	THR

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Mol	Chain	Res	Type
2	G	1623	LYS
2	G	1624	THR
2	G	1629	VAL
2	G	1637	LEU
2	G	1650	VAL
2	G	1651	LEU
2	G	1680	LEU
2	G	1682	LYS
2	G	1693	ARG
2	G	1701	THR
2	G	1718	THR
2	G	1724	GLU
2	G	1731	GLU
2	G	1737	ILE
2	G	1746	LEU
2	G	1748	THR
2	G	1750	LYS
2	G	1751	ILE
2	G	1753	LYS
2	G	1770	LEU
2	G	1781	LEU
2	G	1793	LYS
2	G	1808	SER
2	G	1818	LEU
2	G	1831	VAL
2	G	1845	ASP
2	G	1846	GLU
2	G	1855	ILE
2	G	1862	VAL
2	G	1868	GLN
2	G	1871	LEU
2	G	1885	LEU
2	G	1899	VAL
2	G	1905	ARG
2	G	1914	LEU
2	G	1915	ASN
2	G	1920	GLN
2	G	1923	ASP
2	G	1927	LEU
2	G	1928	GLN
2	G	1930	SER
2	G	1931	LEU

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Mol	Chain	Res	Type
2	G	1932	SER
2	G	1934	GLU
2	G	1935	GLU
2	G	1936	VAL
2	G	1946	GLU
2	G	1949	LYS
2	G	1950	LYS
2	G	1951	SER
2	G	1956	ARG
2	G	1958	LEU
2	G	1959	LYS
2	G	1960	LEU
2	G	1969	LEU
2	G	1973	SER
2	G	1979	THR
2	G	2017	LYS
2	G	2032	LEU
2	G	2038	ILE
2	G	2046	GLU
2	G	2050	GLN
3	H	5	SER
3	H	6	THR
3	H	9	LEU
3	H	10	THR
3	H	15	SER
3	H	16	LEU
3	H	26	SER
3	H	31	SER
3	H	33	LEU
3	H	34	GLN
3	H	40	ILE
3	H	55	THR
3	H	56	THR
3	H	60	LEU
3	H	79	GLN
3	H	84	LEU
3	H	96	LEU
3	H	99	ASN
3	H	113	ASP
3	H	114	THR
3	H	116	LEU
3	H	119	THR

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Mol	Chain	Res	Type
3	H	122	LEU
3	H	139	LYS
3	H	140	LYS
3	H	141	SER
3	H	142	ASN
3	H	149	VAL
3	H	163	GLN
3	H	167	ASP
3	H	173	LEU
3	H	178	GLN
3	H	184	VAL
3	H	189	LYS
3	H	198	LEU
3	H	200	ARG
3	H	215	ILE
3	H	232	LEU
3	H	236	ILE
3	H	240	LEU
3	H	245	GLN
3	H	246	LEU
3	H	255	LEU
3	H	264	ARG
3	H	277	LEU
3	H	279	THR
3	H	283	ILE
3	H	286	THR
3	H	294	VAL
3	H	295	SER
3	H	297	ARG
3	H	301	THR
3	H	303	LEU
3	H	318	SER
3	H	327	SER
3	H	339	LEU
3	H	340	SER
3	H	347	GLU
3	H	353	VAL
3	H	369	SER
3	H	376	ASN
3	H	389	LEU
3	H	400	SER
3	H	402	LEU

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Mol	Chain	Res	Type
3	H	406	ARG
3	H	419	ARG
3	H	425	SER
3	H	429	SER
3	H	431	LEU
3	H	432	LEU
3	H	453	LYS
3	H	456	GLN
3	H	462	THR
3	H	492	THR
3	H	494	THR
3	H	497	LYS
3	H	515	LEU
3	H	532	THR
3	H	562	LEU
3	H	572	ASN
3	H	586	LEU
3	H	611	THR
3	H	616	THR
3	H	650	ASN
3	H	654	VAL
3	H	659	LEU
3	H	665	LEU
3	H	669	LEU
3	H	670	ARG
3	H	681	ILE
3	H	693	GLU
3	H	697	THR
3	H	701	LYS
3	H	706	LYS
3	H	710	ILE
3	H	730	LEU
3	H	733	THR
3	H	752	GLN
3	H	777	THR
3	H	784	GLU
3	H	805	VAL
3	H	810	GLU
3	H	827	VAL
3	H	837	LYS
3	H	843	ILE
3	H	845	THR

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Mol	Chain	Res	Type
3	H	846	VAL
3	H	852	GLU
3	H	871	THR
3	H	877	LYS
3	H	880	LEU
3	H	887	LYS
3	H	906	THR
3	H	914	LEU
3	H	941	VAL
3	H	947	THR
3	H	960	LYS
3	H	963	THR
3	H	972	LEU
3	H	995	LEU
3	H	1012	GLN
3	H	1015	VAL
3	H	1024	ARG
3	H	1040	LEU
3	H	1044	VAL
3	H	1048	VAL
3	H	1049	GLN
3	H	1072	SER
3	H	1085	LEU
3	H	1100	VAL
3	H	1131	SER
3	H	1133	THR
3	H	1137	SER
3	H	1140	LYS
3	H	1145	SER
3	H	1160	THR
3	H	1163	LYS
3	H	1167	SER
3	H	1189	THR
3	H	1191	SER
3	H	1195	VAL
3	H	1197	LEU
3	H	1211	LEU
3	H	1213	LEU
3	H	1215	LYS
3	H	1218	ILE
3	H	1228	THR
3	H	1229	MET

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Mol	Chain	Res	Type
3	H	1232	LYS
3	H	1235	SER
3	H	1236	LEU
3	H	1260	GLN
3	H	1317	ARG
3	H	1320	LEU
3	H	1327	ILE
3	H	1336	LYS
3	H	1343	VAL
3	H	1348	LEU
3	H	1355	ASN
3	H	1360	ILE
3	H	1371	VAL
3	H	1375	THR
3	H	1377	VAL
3	H	1378	ILE
3	H	1381	VAL
3	H	1382	VAL
3	H	1384	GLN
3	H	1386	THR
3	H	1389	ILE
3	H	1395	THR
3	H	1408	SER
3	H	1422	THR
3	H	1426	THR
3	H	1441	ILE
3	H	1446	SER
3	H	1462	LYS
3	H	1468	THR
3	H	1470	THR
3	H	1472	VAL
3	H	1475	LYS
3	H	1479	ILE
3	H	1484	LYS
3	H	1503	ILE
3	H	1526	THR
3	H	1533	LEU
3	H	1551	GLU
3	H	1560	LEU
3	H	1578	THR
3	H	1590	ARG
3	H	1593	ILE

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Mol	Chain	Res	Type
3	H	1600	SER
3	H	1605	VAL
3	H	1609	THR
3	H	1616	VAL
3	H	1620	THR
3	H	1624	THR
3	H	1629	VAL
3	H	1637	LEU
3	H	1650	VAL
3	H	1651	LEU
3	H	1680	LEU
3	H	1693	ARG
3	H	1701	THR
3	H	1718	THR
3	H	1724	GLU
3	H	1731	GLU
3	H	1737	ILE
3	H	1746	LEU
3	H	1749	GLU
3	H	1750	LYS
3	H	1751	ILE
3	H	1770	LEU
3	H	1781	LEU
3	H	1818	LEU
3	H	1831	VAL
3	H	1845	ASP
3	H	1846	GLU
3	H	1847	LEU
3	H	1855	ILE
3	H	1862	VAL
3	H	1871	LEU
3	H	1877	ARG
3	H	1885	LEU
3	H	1888	ILE
3	H	1904	LEU
3	H	1914	LEU
3	H	1921	LYS
3	H	1927	LEU
3	H	1929	LYS
3	H	1930	SER
3	H	1931	LEU
3	H	1932	SER

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Mol	Chain	Res	Type
3	H	1934	GLU
3	H	1936	VAL
3	H	1943	ILE
3	H	1946	GLU
3	H	1948	SER
3	H	1950	LYS
3	H	1951	SER
3	H	1956	ARG
3	H	1958	LEU
3	H	1973	SER
3	H	1979	THR
3	H	1993	LYS
3	H	2032	LEU
3	H	2038	ILE
3	H	2046	GLU
3	I	5	SER
3	I	6	THR
3	I	7	ARG
3	I	9	LEU
3	I	10	THR
3	I	12	SER
3	I	15	SER
3	I	16	LEU
3	I	26	SER
3	I	31	SER
3	I	33	LEU
3	I	34	GLN
3	I	55	THR
3	I	56	THR
3	I	60	LEU
3	I	75	SER
3	I	76	LYS
3	I	79	GLN
3	I	84	LEU
3	I	86	LEU
3	I	96	LEU
3	I	101	ILE
3	I	107	LYS
3	I	113	ASP
3	I	114	THR
3	I	116	LEU
3	I	119	THR

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Mol	Chain	Res	Type
3	I	122	LEU
3	I	139	LYS
3	I	149	VAL
3	I	163	GLN
3	I	167	ASP
3	I	173	LEU
3	I	175	ASP
3	I	178	GLN
3	I	184	VAL
3	I	198	LEU
3	I	200	ARG
3	I	215	ILE
3	I	232	LEU
3	I	236	ILE
3	I	240	LEU
3	I	245	GLN
3	I	246	LEU
3	I	255	LEU
3	I	264	ARG
3	I	277	LEU
3	I	279	THR
3	I	283	ILE
3	I	286	THR
3	I	295	SER
3	I	301	THR
3	I	303	LEU
3	I	318	SER
3	I	323	ILE
3	I	327	SER
3	I	339	LEU
3	I	340	SER
3	I	347	GLU
3	I	353	VAL
3	I	368	ILE
3	I	369	SER
3	I	376	ASN
3	I	389	LEU
3	I	402	LEU
3	I	425	SER
3	I	429	SER
3	I	431	LEU
3	I	432	LEU

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Mol	Chain	Res	Type
3	I	453	LYS
3	I	455	ILE
3	I	456	GLN
3	I	462	THR
3	I	471	LEU
3	I	476	SER
3	I	478	ARG
3	I	492	THR
3	I	494	THR
3	I	497	LYS
3	I	532	THR
3	I	540	ASP
3	I	562	LEU
3	I	572	ASN
3	I	573	LYS
3	I	586	LEU
3	I	601	THR
3	I	611	THR
3	I	616	THR
3	I	650	ASN
3	I	654	VAL
3	I	659	LEU
3	I	660	GLN
3	I	665	LEU
3	I	669	LEU
3	I	670	ARG
3	I	681	ILE
3	I	693	GLU
3	I	697	THR
3	I	706	LYS
3	I	721	LYS
3	I	730	LEU
3	I	733	THR
3	I	752	GLN
3	I	759	ARG
3	I	777	THR
3	I	784	GLU
3	I	788	LYS
3	I	805	VAL
3	I	809	LYS
3	I	810	GLU
3	I	825	THR

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Mol	Chain	Res	Type
3	I	827	VAL
3	I	843	ILE
3	I	845	THR
3	I	846	VAL
3	I	852	GLU
3	I	866	LYS
3	I	871	THR
3	I	880	LEU
3	I	906	THR
3	I	914	LEU
3	I	941	VAL
3	I	947	THR
3	I	963	THR
3	I	964	LEU
3	I	972	LEU
3	I	995	LEU
3	I	1012	GLN
3	I	1015	VAL
3	I	1024	ARG
3	I	1040	LEU
3	I	1044	VAL
3	I	1048	VAL
3	I	1049	GLN
3	I	1072	SER
3	I	1083	LYS
3	I	1085	LEU
3	I	1100	VAL
3	I	1133	THR
3	I	1136	GLU
3	I	1137	SER
3	I	1140	LYS
3	I	1145	SER
3	I	1160	THR
3	I	1163	LYS
3	I	1167	SER
3	I	1189	THR
3	I	1195	VAL
3	I	1197	LEU
3	I	1202	GLN
3	I	1211	LEU
3	I	1213	LEU
3	I	1215	LYS

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Mol	Chain	Res	Type
3	I	1228	THR
3	I	1229	MET
3	I	1235	SER
3	I	1236	LEU
3	I	1260	GLN
3	I	1317	ARG
3	I	1318	THR
3	I	1320	LEU
3	I	1327	ILE
3	I	1343	VAL
3	I	1348	LEU
3	I	1355	ASN
3	I	1360	ILE
3	I	1375	THR
3	I	1377	VAL
3	I	1378	ILE
3	I	1381	VAL
3	I	1382	VAL
3	I	1384	GLN
3	I	1386	THR
3	I	1389	ILE
3	I	1395	THR
3	I	1422	THR
3	I	1426	THR
3	I	1441	ILE
3	I	1446	SER
3	I	1468	THR
3	I	1470	THR
3	I	1472	VAL
3	I	1479	ILE
3	I	1484	LYS
3	I	1503	ILE
3	I	1526	THR
3	I	1533	LEU
3	I	1539	ILE
3	I	1551	GLU
3	I	1560	LEU
3	I	1590	ARG
3	I	1593	ILE
3	I	1600	SER
3	I	1605	VAL
3	I	1609	THR

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Mol	Chain	Res	Type
3	I	1616	VAL
3	I	1620	THR
3	I	1623	LYS
3	I	1624	THR
3	I	1629	VAL
3	I	1637	LEU
3	I	1639	LYS
3	I	1650	VAL
3	I	1651	LEU
3	I	1680	LEU
3	I	1682	LYS
3	I	1693	ARG
3	I	1701	THR
3	I	1718	THR
3	I	1724	GLU
3	I	1731	GLU
3	I	1737	ILE
3	I	1746	LEU
3	I	1747	LYS
3	I	1749	GLU
3	I	1750	LYS
3	I	1751	ILE
3	I	1753	LYS
3	I	1768	LYS
3	I	1770	LEU
3	I	1781	LEU
3	I	1793	LYS
3	I	1818	LEU
3	I	1824	ILE
3	I	1831	VAL
3	I	1845	ASP
3	I	1846	GLU
3	I	1847	LEU
3	I	1849	ARG
3	I	1855	ILE
3	I	1862	VAL
3	I	1871	LEU
3	I	1877	ARG
3	I	1881	ARG
3	I	1885	LEU
3	I	1888	ILE
3	I	1905	ARG

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Mol	Chain	Res	Type
3	I	1914	LEU
3	I	1915	ASN
3	I	1927	LEU
3	I	1929	LYS
3	I	1930	SER
3	I	1931	LEU
3	I	1932	SER
3	I	1933	LEU
3	I	1934	GLU
3	I	1935	GLU
3	I	1936	VAL
3	I	1939	HIS
3	I	1946	GLU
3	I	1948	SER
3	I	1950	LYS
3	I	1951	SER
3	I	1956	ARG
3	I	1958	LEU
3	I	1960	LEU
3	I	1962	ARG
3	I	1979	THR
3	I	2024	GLU
3	I	2032	LEU
3	I	2038	ILE
3	I	2046	GLU
3	I	2050	GLN
2	J	5	SER
2	J	6	THR
2	J	9	LEU
2	J	10	THR
2	J	15	SER
2	J	16	LEU
2	J	26	SER
2	J	31	SER
2	J	33	LEU
2	J	34	GLN
2	J	40	ILE
2	J	55	THR
2	J	56	THR
2	J	60	LEU
2	J	73	GLU
2	J	75	SER

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Mol	Chain	Res	Type
2	J	76	LYS
2	J	84	LEU
2	J	86	LEU
2	J	96	LEU
2	J	99	ASN
2	J	116	LEU
2	J	119	THR
2	J	122	LEU
2	J	124	LYS
2	J	132	MET
2	J	134	LYS
2	J	141	SER
2	J	142	ASN
2	J	149	VAL
2	J	163	GLN
2	J	167	ASP
2	J	173	LEU
2	J	175	ASP
2	J	178	GLN
2	J	198	LEU
2	J	200	ARG
2	J	215	ILE
2	J	232	LEU
2	J	236	ILE
2	J	240	LEU
2	J	245	GLN
2	J	246	LEU
2	J	255	LEU
2	J	264	ARG
2	J	277	LEU
2	J	279	THR
2	J	283	ILE
2	J	286	THR
2	J	294	VAL
2	J	295	SER
2	J	301	THR
2	J	303	LEU
2	J	318	SER
2	J	323	ILE
2	J	327	SER
2	J	339	LEU
2	J	340	SER

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Mol	Chain	Res	Type
2	J	344	LEU
2	J	347	GLU
2	J	353	VAL
2	J	369	SER
2	J	376	ASN
2	J	389	LEU
2	J	402	LEU
2	J	414	LEU
2	J	419	ARG
2	J	425	SER
2	J	429	SER
2	J	431	LEU
2	J	432	LEU
2	J	453	LYS
2	J	455	ILE
2	J	462	THR
2	J	471	LEU
2	J	476	SER
2	J	478	ARG
2	J	492	THR
2	J	494	THR
2	J	497	LYS
2	J	515	LEU
2	J	532	THR
2	J	562	LEU
2	J	570	ILE
2	J	572	ASN
2	J	586	LEU
2	J	611	THR
2	J	616	THR
2	J	650	ASN
2	J	654	VAL
2	J	659	LEU
2	J	665	LEU
2	J	669	LEU
2	J	670	ARG
2	J	681	ILE
2	J	689	GLU
2	J	693	GLU
2	J	697	THR
2	J	701	LYS
2	J	706	LYS

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Mol	Chain	Res	Type
2	J	710	ILE
2	J	730	LEU
2	J	733	THR
2	J	736	ARG
2	J	752	GLN
2	J	777	THR
2	J	784	GLU
2	J	805	VAL
2	J	809	LYS
2	J	810	GLU
2	J	825	THR
2	J	827	VAL
2	J	831	LYS
2	J	837	LYS
2	J	843	ILE
2	J	845	THR
2	J	846	VAL
2	J	871	THR
2	J	877	LYS
2	J	880	LEU
2	J	906	THR
2	J	914	LEU
2	J	941	VAL
2	J	947	THR
2	J	963	THR
2	J	964	LEU
2	J	972	LEU
2	J	995	LEU
2	J	1012	GLN
2	J	1015	VAL
2	J	1024	ARG
2	J	1031	LYS
2	J	1040	LEU
2	J	1044	VAL
2	J	1048	VAL
2	J	1049	GLN
2	J	1072	SER
2	J	1085	LEU
2	J	1100	VAL
2	J	1131	SER
2	J	1133	THR
2	J	1137	SER

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Mol	Chain	Res	Type
2	J	1140	LYS
2	J	1145	SER
2	J	1160	THR
2	J	1167	SER
2	J	1189	THR
2	J	1191	SER
2	J	1195	VAL
2	J	1197	LEU
2	J	1204	GLU
2	J	1211	LEU
2	J	1213	LEU
2	J	1218	ILE
2	J	1228	THR
2	J	1229	MET
2	J	1232	LYS
2	J	1234	VAL
2	J	1235	SER
2	J	1236	LEU
2	J	1260	GLN
2	J	1317	ARG
2	J	1318	THR
2	J	1320	LEU
2	J	1327	ILE
2	J	1343	VAL
2	J	1348	LEU
2	J	1355	ASN
2	J	1360	ILE
2	J	1375	THR
2	J	1377	VAL
2	J	1378	ILE
2	J	1381	VAL
2	J	1382	VAL
2	J	1384	GLN
2	J	1386	THR
2	J	1389	ILE
2	J	1395	THR
2	J	1408	SER
2	J	1413	ARG
2	J	1422	THR
2	J	1426	THR
2	J	1441	ILE
2	J	1446	SER

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Mol	Chain	Res	Type
2	J	1468	THR
2	J	1470	THR
2	J	1472	VAL
2	J	1479	ILE
2	J	1484	LYS
2	J	1503	ILE
2	J	1526	THR
2	J	1528	GLU
2	J	1533	LEU
2	J	1551	GLU
2	J	1555	ARG
2	J	1560	LEU
2	J	1590	ARG
2	J	1593	ILE
2	J	1600	SER
2	J	1605	VAL
2	J	1609	THR
2	J	1624	THR
2	J	1629	VAL
2	J	1637	LEU
2	J	1650	VAL
2	J	1651	LEU
2	J	1680	LEU
2	J	1682	LYS
2	J	1693	ARG
2	J	1701	THR
2	J	1718	THR
2	J	1724	GLU
2	J	1731	GLU
2	J	1737	ILE
2	J	1746	LEU
2	J	1747	LYS
2	J	1751	ILE
2	J	1757	GLU
2	J	1768	LYS
2	J	1770	LEU
2	J	1781	LEU
2	J	1793	LYS
2	J	1818	LEU
2	J	1831	VAL
2	J	1845	ASP
2	J	1846	GLU

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Mol	Chain	Res	Type
2	J	1847	LEU
2	J	1855	ILE
2	J	1862	VAL
2	J	1871	LEU
2	J	1877	ARG
2	J	1881	ARG
2	J	1885	LEU
2	J	1905	ARG
2	J	1914	LEU
2	J	1918	LYS
2	J	1927	LEU
2	J	1929	LYS
2	J	1931	LEU
2	J	1932	SER
2	J	1934	GLU
2	J	1935	GLU
2	J	1936	VAL
2	J	1946	GLU
2	J	1950	LYS
2	J	1951	SER
2	J	1956	ARG
2	J	1958	LEU
2	J	1959	LYS
2	J	1960	LEU
2	J	1962	ARG
2	J	1979	THR
2	J	2022	THR
2	J	2032	LEU
2	J	2038	ILE
2	J	2039	LYS
2	J	2046	GLU
2	J	2050	GLN
3	K	4	TYR
3	K	6	THR
3	K	9	LEU
3	K	10	THR
3	K	15	SER
3	K	16	LEU
3	K	26	SER
3	K	31	SER
3	K	33	LEU
3	K	34	GLN

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Mol	Chain	Res	Type
3	K	39	LYS
3	K	55	THR
3	K	56	THR
3	K	60	LEU
3	K	79	GLN
3	K	84	LEU
3	K	86	LEU
3	K	99	ASN
3	K	107	LYS
3	K	110	GLN
3	K	111	GLU
3	K	113	ASP
3	K	114	THR
3	K	116	LEU
3	K	117	VAL
3	K	119	THR
3	K	122	LEU
3	K	142	ASN
3	K	149	VAL
3	K	163	GLN
3	K	167	ASP
3	K	173	LEU
3	K	178	GLN
3	K	184	VAL
3	K	189	LYS
3	K	198	LEU
3	K	199	ILE
3	K	200	ARG
3	K	215	ILE
3	K	232	LEU
3	K	236	ILE
3	K	240	LEU
3	K	245	GLN
3	K	246	LEU
3	K	255	LEU
3	K	264	ARG
3	K	277	LEU
3	K	279	THR
3	K	283	ILE
3	K	286	THR
3	K	295	SER
3	K	297	ARG

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Mol	Chain	Res	Type
3	K	301	THR
3	K	303	LEU
3	K	318	SER
3	K	323	ILE
3	K	327	SER
3	K	339	LEU
3	K	340	SER
3	K	344	LEU
3	K	347	GLU
3	K	353	VAL
3	K	368	ILE
3	K	369	SER
3	K	376	ASN
3	K	389	LEU
3	K	397	LYS
3	K	402	LEU
3	K	417	SER
3	K	425	SER
3	K	429	SER
3	K	431	LEU
3	K	432	LEU
3	K	453	LYS
3	K	456	GLN
3	K	462	THR
3	K	471	LEU
3	K	476	SER
3	K	492	THR
3	K	494	THR
3	K	499	THR
3	K	515	LEU
3	K	540	ASP
3	K	562	LEU
3	K	572	ASN
3	K	586	LEU
3	K	611	THR
3	K	616	THR
3	K	650	ASN
3	K	654	VAL
3	K	659	LEU
3	K	665	LEU
3	K	669	LEU
3	K	670	ARG

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Mol	Chain	Res	Type
3	K	681	ILE
3	K	693	GLU
3	K	697	THR
3	K	701	LYS
3	K	706	LYS
3	K	721	LYS
3	K	730	LEU
3	K	733	THR
3	K	752	GLN
3	K	757	ILE
3	K	777	THR
3	K	784	GLU
3	K	805	VAL
3	K	810	GLU
3	K	819	LYS
3	K	825	THR
3	K	827	VAL
3	K	831	LYS
3	K	843	ILE
3	K	845	THR
3	K	846	VAL
3	K	850	MET
3	K	852	GLU
3	K	871	THR
3	K	880	LEU
3	K	906	THR
3	K	914	LEU
3	K	941	VAL
3	K	947	THR
3	K	953	ARG
3	K	962	LYS
3	K	963	THR
3	K	972	LEU
3	K	995	LEU
3	K	1012	GLN
3	K	1015	VAL
3	K	1024	ARG
3	K	1040	LEU
3	K	1044	VAL
3	K	1048	VAL
3	K	1049	GLN
3	K	1072	SER

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Mol	Chain	Res	Type
3	K	1085	LEU
3	K	1100	VAL
3	K	1131	SER
3	K	1133	THR
3	K	1137	SER
3	K	1140	LYS
3	K	1145	SER
3	K	1160	THR
3	K	1163	LYS
3	K	1167	SER
3	K	1175	LYS
3	K	1189	THR
3	K	1195	VAL
3	K	1197	LEU
3	K	1211	LEU
3	K	1213	LEU
3	K	1215	LYS
3	K	1218	ILE
3	K	1228	THR
3	K	1229	MET
3	K	1232	LYS
3	K	1235	SER
3	K	1236	LEU
3	K	1260	GLN
3	K	1268	LYS
3	K	1286	LYS
3	K	1316	ASP
3	K	1317	ARG
3	K	1318	THR
3	K	1320	LEU
3	K	1327	ILE
3	K	1343	VAL
3	K	1348	LEU
3	K	1355	ASN
3	K	1357	TYR
3	K	1360	ILE
3	K	1375	THR
3	K	1377	VAL
3	K	1378	ILE
3	K	1381	VAL
3	K	1382	VAL
3	K	1384	GLN

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Mol	Chain	Res	Type
3	K	1386	THR
3	K	1389	ILE
3	K	1395	THR
3	K	1408	SER
3	K	1422	THR
3	K	1426	THR
3	K	1439	LYS
3	K	1441	ILE
3	K	1445	ARG
3	K	1446	SER
3	K	1468	THR
3	K	1470	THR
3	K	1472	VAL
3	K	1503	ILE
3	K	1526	THR
3	K	1533	LEU
3	K	1551	GLU
3	K	1560	LEU
3	K	1578	THR
3	K	1590	ARG
3	K	1593	ILE
3	K	1600	SER
3	K	1605	VAL
3	K	1609	THR
3	K	1616	VAL
3	K	1620	THR
3	K	1624	THR
3	K	1629	VAL
3	K	1637	LEU
3	K	1639	LYS
3	K	1650	VAL
3	K	1651	LEU
3	K	1680	LEU
3	K	1682	LYS
3	K	1693	ARG
3	K	1701	THR
3	K	1718	THR
3	K	1724	GLU
3	K	1731	GLU
3	K	1737	ILE
3	K	1741	ILE
3	K	1745	LYS

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Mol	Chain	Res	Type
3	K	1749	GLU
3	K	1751	ILE
3	K	1768	LYS
3	K	1770	LEU
3	K	1775	GLN
3	K	1781	LEU
3	K	1818	LEU
3	K	1831	VAL
3	K	1845	ASP
3	K	1846	GLU
3	K	1847	LEU
3	K	1855	ILE
3	K	1862	VAL
3	K	1871	LEU
3	K	1877	ARG
3	K	1885	LEU
3	K	1888	ILE
3	K	1904	LEU
3	K	1914	LEU
3	K	1918	LYS
3	K	1921	LYS
3	K	1923	ASP
3	K	1926	GLU
3	K	1927	LEU
3	K	1929	LYS
3	K	1931	LEU
3	K	1932	SER
3	K	1934	GLU
3	K	1936	VAL
3	K	1946	GLU
3	K	1948	SER
3	K	1949	LYS
3	K	1950	LYS
3	K	1951	SER
3	K	1953	VAL
3	K	1956	ARG
3	K	1958	LEU
3	K	1960	LEU
3	K	1962	ARG
3	K	1979	THR
3	K	2032	LEU
3	K	2038	ILE

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Mol	Chain	Res	Type
3	K	2041	ILE
3	K	2046	GLU
3	K	2050	GLN
3	L	5	SER
3	L	6	THR
3	L	9	LEU
3	L	10	THR
3	L	12	SER
3	L	15	SER
3	L	16	LEU
3	L	26	SER
3	L	31	SER
3	L	34	GLN
3	L	40	ILE
3	L	46	GLU
3	L	55	THR
3	L	56	THR
3	L	60	LEU
3	L	76	LYS
3	L	82	GLN
3	L	84	LEU
3	L	86	LEU
3	L	96	LEU
3	L	99	ASN
3	L	113	ASP
3	L	114	THR
3	L	116	LEU
3	L	119	THR
3	L	122	LEU
3	L	124	LYS
3	L	132	MET
3	L	139	LYS
3	L	140	LYS
3	L	141	SER
3	L	142	ASN
3	L	149	VAL
3	L	156	LEU
3	L	163	GLN
3	L	167	ASP
3	L	173	LEU
3	L	175	ASP
3	L	184	VAL

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Mol	Chain	Res	Type
3	L	198	LEU
3	L	200	ARG
3	L	215	ILE
3	L	232	LEU
3	L	236	ILE
3	L	240	LEU
3	L	245	GLN
3	L	246	LEU
3	L	255	LEU
3	L	264	ARG
3	L	268	LYS
3	L	277	LEU
3	L	279	THR
3	L	283	ILE
3	L	286	THR
3	L	294	VAL
3	L	295	SER
3	L	301	THR
3	L	303	LEU
3	L	318	SER
3	L	327	SER
3	L	339	LEU
3	L	340	SER
3	L	344	LEU
3	L	347	GLU
3	L	353	VAL
3	L	355	LYS
3	L	369	SER
3	L	376	ASN
3	L	389	LEU
3	L	407	ILE
3	L	413	LYS
3	L	423	VAL
3	L	425	SER
3	L	429	SER
3	L	431	LEU
3	L	432	LEU
3	L	444	VAL
3	L	453	LYS
3	L	455	ILE
3	L	456	GLN
3	L	462	THR

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Mol	Chain	Res	Type
3	L	471	LEU
3	L	476	SER
3	L	478	ARG
3	L	492	THR
3	L	494	THR
3	L	497	LYS
3	L	515	LEU
3	L	532	THR
3	L	540	ASP
3	L	562	LEU
3	L	570	ILE
3	L	572	ASN
3	L	573	LYS
3	L	586	LEU
3	L	601	THR
3	L	611	THR
3	L	616	THR
3	L	650	ASN
3	L	654	VAL
3	L	659	LEU
3	L	665	LEU
3	L	669	LEU
3	L	670	ARG
3	L	681	ILE
3	L	693	GLU
3	L	697	THR
3	L	701	LYS
3	L	706	LYS
3	L	721	LYS
3	L	730	LEU
3	L	733	THR
3	L	752	GLN
3	L	756	LYS
3	L	759	ARG
3	L	777	THR
3	L	784	GLU
3	L	805	VAL
3	L	810	GLU
3	L	825	THR
3	L	827	VAL
3	L	845	THR
3	L	846	VAL

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Mol	Chain	Res	Type
3	L	850	MET
3	L	871	THR
3	L	877	LYS
3	L	880	LEU
3	L	906	THR
3	L	914	LEU
3	L	941	VAL
3	L	947	THR
3	L	960	LYS
3	L	963	THR
3	L	964	LEU
3	L	995	LEU
3	L	1012	GLN
3	L	1015	VAL
3	L	1024	ARG
3	L	1040	LEU
3	L	1048	VAL
3	L	1049	GLN
3	L	1072	SER
3	L	1085	LEU
3	L	1100	VAL
3	L	1106	GLU
3	L	1131	SER
3	L	1133	THR
3	L	1137	SER
3	L	1140	LYS
3	L	1145	SER
3	L	1157	SER
3	L	1160	THR
3	L	1175	LYS
3	L	1184	ILE
3	L	1189	THR
3	L	1195	VAL
3	L	1197	LEU
3	L	1211	LEU
3	L	1213	LEU
3	L	1228	THR
3	L	1229	MET
3	L	1235	SER
3	L	1236	LEU
3	L	1260	GLN
3	L	1286	LYS

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Mol	Chain	Res	Type
3	L	1288	LYS
3	L	1317	ARG
3	L	1318	THR
3	L	1320	LEU
3	L	1327	ILE
3	L	1343	VAL
3	L	1348	LEU
3	L	1355	ASN
3	L	1357	TYR
3	L	1360	ILE
3	L	1375	THR
3	L	1377	VAL
3	L	1378	ILE
3	L	1381	VAL
3	L	1382	VAL
3	L	1384	GLN
3	L	1386	THR
3	L	1389	ILE
3	L	1395	THR
3	L	1408	SER
3	L	1421	ASN
3	L	1422	THR
3	L	1426	THR
3	L	1436	LYS
3	L	1441	ILE
3	L	1445	ARG
3	L	1446	SER
3	L	1468	THR
3	L	1470	THR
3	L	1472	VAL
3	L	1484	LYS
3	L	1503	ILE
3	L	1525	SER
3	L	1526	THR
3	L	1533	LEU
3	L	1551	GLU
3	L	1560	LEU
3	L	1590	ARG
3	L	1593	ILE
3	L	1600	SER
3	L	1603	SER
3	L	1605	VAL

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Mol	Chain	Res	Type
3	L	1609	THR
3	L	1623	LYS
3	L	1624	THR
3	L	1629	VAL
3	L	1637	LEU
3	L	1648	VAL
3	L	1650	VAL
3	L	1651	LEU
3	L	1680	LEU
3	L	1682	LYS
3	L	1693	ARG
3	L	1701	THR
3	L	1718	THR
3	L	1724	GLU
3	L	1731	GLU
3	L	1737	ILE
3	L	1745	LYS
3	L	1746	LEU
3	L	1749	GLU
3	L	1751	ILE
3	L	1770	LEU
3	L	1781	LEU
3	L	1793	LYS
3	L	1818	LEU
3	L	1831	VAL
3	L	1845	ASP
3	L	1846	GLU
3	L	1847	LEU
3	L	1849	ARG
3	L	1855	ILE
3	L	1862	VAL
3	L	1871	LEU
3	L	1872	GLN
3	L	1885	LEU
3	L	1888	ILE
3	L	1894	GLU
3	L	1914	LEU
3	L	1923	ASP
3	L	1927	LEU
3	L	1929	LYS
3	L	1930	SER
3	L	1931	LEU

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Mol	Chain	Res	Type
3	L	1932	SER
3	L	1934	GLU
3	L	1935	GLU
3	L	1936	VAL
3	L	1944	ILE
3	L	1946	GLU
3	L	1948	SER
3	L	1950	LYS
3	L	1951	SER
3	L	1956	ARG
3	L	1958	LEU
3	L	1960	LEU
3	L	1967	ILE
3	L	1973	SER
3	L	1979	THR
3	L	2023	LYS
3	L	2032	LEU
3	L	2038	ILE
3	L	2039	LYS
3	L	2046	GLU
3	L	2050	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (578) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	40	ASN
1	A	63	ASN
1	A	183	GLN
1	A	292	GLN
1	A	335	HIS
1	A	342	GLN
1	A	344	GLN
1	A	372	GLN
1	A	379	ASN
1	A	411	GLN
1	A	438	ASN
1	A	475	GLN
1	A	506	ASN
1	A	618	ASN
1	A	719	GLN
1	A	738	ASN

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Mol	Chain	Res	Type
1	A	743	GLN
1	A	792	HIS
1	A	829	ASN
1	A	830	HIS
1	A	851	ASN
1	A	965	HIS
1	A	969	ASN
1	A	1000	GLN
1	A	1003	GLN
1	A	1064	ASN
1	A	1066	ASN
1	A	1112	ASN
1	A	1123	GLN
1	A	1146	HIS
1	A	1239	HIS
1	A	1245	ASN
1	A	1271	GLN
1	A	1272	ASN
1	A	1432	HIS
1	A	1433	HIS
1	A	1442	ASN
1	A	1483	ASN
1	A	1494	HIS
1	A	1507	GLN
1	A	1510	ASN
1	A	1552	ASN
1	A	1610	ASN
1	A	1657	HIS
1	A	1695	ASN
1	A	1780	ASN
1	A	1794	GLN
1	A	1802	GLN
1	A	1843	ASN
1	B	11	HIS
1	B	40	ASN
1	B	183	GLN
1	B	261	GLN
1	B	335	HIS
1	B	344	GLN
1	B	379	ASN
1	B	411	GLN
1	B	438	ASN

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Mol	Chain	Res	Type
1	B	475	GLN
1	B	506	ASN
1	B	508	ASN
1	B	618	ASN
1	B	669	ASN
1	B	694	GLN
1	B	719	GLN
1	B	738	ASN
1	B	743	GLN
1	B	783	HIS
1	B	792	HIS
1	B	829	ASN
1	B	830	HIS
1	B	851	ASN
1	B	898	GLN
1	B	965	HIS
1	B	969	ASN
1	B	983	GLN
1	B	1000	GLN
1	B	1064	ASN
1	B	1066	ASN
1	B	1112	ASN
1	B	1123	GLN
1	B	1146	HIS
1	B	1239	HIS
1	B	1272	ASN
1	B	1380	GLN
1	B	1432	HIS
1	B	1442	ASN
1	B	1444	ASN
1	B	1482	GLN
1	B	1483	ASN
1	B	1494	HIS
1	B	1505	GLN
1	B	1507	GLN
1	B	1510	ASN
1	B	1552	ASN
1	B	1610	ASN
1	B	1695	ASN
1	B	1780	ASN
1	B	1843	ASN
1	B	1852	HIS

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Mol	Chain	Res	Type
1	C	11	HIS
1	C	40	ASN
1	C	183	GLN
1	C	261	GLN
1	C	335	HIS
1	C	344	GLN
1	C	379	ASN
1	C	411	GLN
1	C	438	ASN
1	C	475	GLN
1	C	506	ASN
1	C	618	ASN
1	C	669	ASN
1	C	694	GLN
1	C	719	GLN
1	C	738	ASN
1	C	743	GLN
1	C	783	HIS
1	C	792	HIS
1	C	829	ASN
1	C	830	HIS
1	C	851	ASN
1	C	965	HIS
1	C	969	ASN
1	C	1000	GLN
1	C	1064	ASN
1	C	1066	ASN
1	C	1123	GLN
1	C	1146	HIS
1	C	1239	HIS
1	C	1272	ASN
1	C	1432	HIS
1	C	1433	HIS
1	C	1442	ASN
1	C	1444	ASN
1	C	1458	GLN
1	C	1482	GLN
1	C	1483	ASN
1	C	1494	HIS
1	C	1507	GLN
1	C	1510	ASN
1	C	1577	GLN

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Mol	Chain	Res	Type
1	C	1610	ASN
1	C	1695	ASN
1	C	1766	ASN
1	C	1780	ASN
1	C	1794	GLN
1	D	40	ASN
1	D	183	GLN
1	D	261	GLN
1	D	335	HIS
1	D	342	GLN
1	D	344	GLN
1	D	356	ASN
1	D	379	ASN
1	D	411	GLN
1	D	438	ASN
1	D	467	GLN
1	D	475	GLN
1	D	618	ASN
1	D	694	GLN
1	D	698	GLN
1	D	719	GLN
1	D	738	ASN
1	D	743	GLN
1	D	783	HIS
1	D	792	HIS
1	D	829	ASN
1	D	830	HIS
1	D	851	ASN
1	D	965	HIS
1	D	969	ASN
1	D	1000	GLN
1	D	1064	ASN
1	D	1066	ASN
1	D	1123	GLN
1	D	1146	HIS
1	D	1239	HIS
1	D	1271	GLN
1	D	1272	ASN
1	D	1432	HIS
1	D	1433	HIS
1	D	1442	ASN
1	D	1483	ASN

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Mol	Chain	Res	Type
1	D	1494	HIS
1	D	1507	GLN
1	D	1510	ASN
1	D	1610	ASN
1	D	1695	ASN
1	D	1780	ASN
1	D	1794	GLN
1	D	1802	GLN
1	D	1843	ASN
1	D	1852	HIS
1	E	183	GLN
1	E	261	GLN
1	E	335	HIS
1	E	342	GLN
1	E	344	GLN
1	E	356	ASN
1	E	379	ASN
1	E	411	GLN
1	E	438	ASN
1	E	475	GLN
1	E	506	ASN
1	E	618	ASN
1	E	694	GLN
1	E	719	GLN
1	E	738	ASN
1	E	743	GLN
1	E	792	HIS
1	E	829	ASN
1	E	830	HIS
1	E	851	ASN
1	E	898	GLN
1	E	965	HIS
1	E	969	ASN
1	E	1000	GLN
1	E	1064	ASN
1	E	1066	ASN
1	E	1112	ASN
1	E	1123	GLN
1	E	1146	HIS
1	E	1239	HIS
1	E	1272	ASN
1	E	1380	GLN

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Mol	Chain	Res	Type
1	E	1432	HIS
1	E	1433	HIS
1	E	1442	ASN
1	E	1458	GLN
1	E	1483	ASN
1	E	1494	HIS
1	E	1505	GLN
1	E	1507	GLN
1	E	1510	ASN
1	E	1610	ASN
1	E	1695	ASN
1	E	1780	ASN
1	E	1843	ASN
1	E	1852	HIS
1	F	40	ASN
1	F	183	GLN
1	F	261	GLN
1	F	335	HIS
1	F	341	GLN
1	F	344	GLN
1	F	356	ASN
1	F	379	ASN
1	F	411	GLN
1	F	422	HIS
1	F	438	ASN
1	F	475	GLN
1	F	506	ASN
1	F	527	GLN
1	F	618	ASN
1	F	669	ASN
1	F	694	GLN
1	F	719	GLN
1	F	738	ASN
1	F	743	GLN
1	F	792	HIS
1	F	829	ASN
1	F	830	HIS
1	F	851	ASN
1	F	965	HIS
1	F	969	ASN
1	F	979	GLN
1	F	1000	GLN

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Mol	Chain	Res	Type
1	F	1064	ASN
1	F	1066	ASN
1	F	1123	GLN
1	F	1146	HIS
1	F	1239	HIS
1	F	1432	HIS
1	F	1433	HIS
1	F	1483	ASN
1	F	1494	HIS
1	F	1507	GLN
1	F	1510	ASN
1	F	1552	ASN
1	F	1610	ASN
1	F	1695	ASN
1	F	1780	ASN
1	F	1794	GLN
1	F	1843	ASN
1	F	1852	HIS
2	G	79	GLN
2	G	99	ASN
2	G	102	HIS
2	G	112	ASN
2	G	214	ASN
2	G	354	ASN
2	G	376	ASN
2	G	404	GLN
2	G	440	ASN
2	G	500	HIS
2	G	553	ASN
2	G	558	ASN
2	G	612	ASN
2	G	650	ASN
2	G	677	GLN
2	G	718	ASN
2	G	723	HIS
2	G	747	HIS
2	G	752	GLN
2	G	900	GLN
2	G	908	ASN
2	G	936	ASN
2	G	998	GLN
2	G	1049	GLN

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Mol	Chain	Res	Type
2	G	1055	HIS
2	G	1061	GLN
2	G	1217	ASN
2	G	1352	HIS
2	G	1383	ASN
2	G	1421	ASN
2	G	1424	GLN
2	G	1512	HIS
2	G	1595	ASN
2	G	1619	ASN
2	G	1697	HIS
2	G	1712	ASN
2	G	1720	HIS
2	G	1778	GLN
2	G	1890	ASN
2	G	1915	ASN
2	G	1928	GLN
2	G	1995	ASN
2	G	2000	ASN
2	G	2020	GLN
2	G	2027	GLN
3	H	79	GLN
3	H	99	ASN
3	H	102	HIS
3	H	178	GLN
3	H	354	ASN
3	H	359	HIS
3	H	376	ASN
3	H	404	GLN
3	H	440	ASN
3	H	446	ASN
3	H	500	HIS
3	H	517	HIS
3	H	553	ASN
3	H	558	ASN
3	H	572	ASN
3	H	612	ASN
3	H	677	GLN
3	H	718	ASN
3	H	723	HIS
3	H	747	HIS
3	H	878	ASN

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Mol	Chain	Res	Type
3	H	900	GLN
3	H	936	ASN
3	H	998	GLN
3	H	1055	HIS
3	H	1061	GLN
3	H	1178	GLN
3	H	1217	ASN
3	H	1246	ASN
3	H	1352	HIS
3	H	1367	GLN
3	H	1383	ASN
3	H	1424	GLN
3	H	1512	HIS
3	H	1595	ASN
3	H	1619	ASN
3	H	1627	GLN
3	H	1697	HIS
3	H	1712	ASN
3	H	1720	HIS
3	H	1858	ASN
3	H	1890	ASN
3	H	1896	GLN
3	H	1897	GLN
3	H	1939	HIS
3	H	1995	ASN
3	H	2000	ASN
3	H	2020	GLN
3	H	2027	GLN
3	I	82	GLN
3	I	102	HIS
3	I	354	ASN
3	I	376	ASN
3	I	404	GLN
3	I	440	ASN
3	I	500	HIS
3	I	517	HIS
3	I	553	ASN
3	I	558	ASN
3	I	560	ASN
3	I	572	ASN
3	I	612	ASN
3	I	650	ASN

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Mol	Chain	Res	Type
3	I	677	GLN
3	I	718	ASN
3	I	723	HIS
3	I	747	HIS
3	I	752	GLN
3	I	760	HIS
3	I	900	GLN
3	I	936	ASN
3	I	996	ASN
3	I	998	GLN
3	I	1055	HIS
3	I	1061	GLN
3	I	1217	ASN
3	I	1246	ASN
3	I	1352	HIS
3	I	1383	ASN
3	I	1421	ASN
3	I	1424	GLN
3	I	1512	HIS
3	I	1595	ASN
3	I	1619	ASN
3	I	1697	HIS
3	I	1712	ASN
3	I	1720	HIS
3	I	1858	ASN
3	I	1890	ASN
3	I	1896	GLN
3	I	1915	ASN
3	I	1928	GLN
3	I	1995	ASN
3	I	2013	ASN
3	I	2020	GLN
3	I	2027	GLN
2	J	82	GLN
2	J	99	ASN
2	J	102	HIS
2	J	354	ASN
2	J	359	HIS
2	J	376	ASN
2	J	404	GLN
2	J	440	ASN
2	J	500	HIS

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Mol	Chain	Res	Type
2	J	517	HIS
2	J	553	ASN
2	J	558	ASN
2	J	572	ASN
2	J	612	ASN
2	J	650	ASN
2	J	677	GLN
2	J	718	ASN
2	J	723	HIS
2	J	747	HIS
2	J	834	GLN
2	J	900	GLN
2	J	936	ASN
2	J	998	GLN
2	J	1049	GLN
2	J	1055	HIS
2	J	1061	GLN
2	J	1178	GLN
2	J	1217	ASN
2	J	1246	ASN
2	J	1352	HIS
2	J	1383	ASN
2	J	1424	GLN
2	J	1432	GLN
2	J	1512	HIS
2	J	1595	ASN
2	J	1619	ASN
2	J	1697	HIS
2	J	1712	ASN
2	J	1720	HIS
2	J	1858	ASN
2	J	1890	ASN
2	J	1896	GLN
2	J	1915	ASN
2	J	1995	ASN
2	J	2013	ASN
2	J	2020	GLN
2	J	2027	GLN
2	J	2050	GLN
3	K	79	GLN
3	K	82	GLN
3	K	99	ASN

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Mol	Chain	Res	Type
3	K	102	HIS
3	K	112	ASN
3	K	178	GLN
3	K	354	ASN
3	K	359	HIS
3	K	376	ASN
3	K	384	GLN
3	K	404	GLN
3	K	440	ASN
3	K	451	ASN
3	K	500	HIS
3	K	517	HIS
3	K	553	ASN
3	K	558	ASN
3	K	572	ASN
3	K	612	ASN
3	K	650	ASN
3	K	677	GLN
3	K	723	HIS
3	K	747	HIS
3	K	752	GLN
3	K	760	HIS
3	K	878	ASN
3	K	900	GLN
3	K	908	ASN
3	K	936	ASN
3	K	996	ASN
3	K	998	GLN
3	K	1055	HIS
3	K	1061	GLN
3	K	1217	ASN
3	K	1246	ASN
3	K	1341	ASN
3	K	1352	HIS
3	K	1383	ASN
3	K	1421	ASN
3	K	1595	ASN
3	K	1619	ASN
3	K	1674	GLN
3	K	1697	HIS
3	K	1712	ASN
3	K	1720	HIS

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Mol	Chain	Res	Type
3	K	1775	GLN
3	K	1858	ASN
3	K	1890	ASN
3	K	1896	GLN
3	K	1928	GLN
3	K	2000	ASN
3	K	2020	GLN
3	K	2027	GLN
3	L	79	GLN
3	L	82	GLN
3	L	99	ASN
3	L	102	HIS
3	L	354	ASN
3	L	359	HIS
3	L	376	ASN
3	L	404	GLN
3	L	440	ASN
3	L	451	ASN
3	L	500	HIS
3	L	517	HIS
3	L	553	ASN
3	L	558	ASN
3	L	572	ASN
3	L	612	ASN
3	L	677	GLN
3	L	723	HIS
3	L	747	HIS
3	L	752	GLN
3	L	878	ASN
3	L	900	GLN
3	L	936	ASN
3	L	996	ASN
3	L	998	GLN
3	L	1055	HIS
3	L	1061	GLN
3	L	1217	ASN
3	L	1246	ASN
3	L	1352	HIS
3	L	1383	ASN
3	L	1421	ASN
3	L	1424	GLN
3	L	1432	GLN

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Mol	Chain	Res	Type
3	L	1595	ASN
3	L	1619	ASN
3	L	1627	GLN
3	L	1697	HIS
3	L	1712	ASN
3	L	1720	HIS
3	L	1851	ASN
3	L	1858	ASN
3	L	1872	GLN
3	L	1890	ASN
3	L	1915	ASN
3	L	1995	ASN
3	L	2000	ASN
3	L	2020	GLN
3	L	2027	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	J8W	L	1808	3	10,11,12	1.81	1 (10%)	9,13,15	2.03	3 (33%)
3	J8W	K	1808	3	10,11,12	1.86	1 (10%)	9,13,15	2.04	4 (44%)
3	J8W	H	1808	3	10,11,12	1.77	1 (10%)	9,13,15	1.78	2 (22%)
3	J8W	I	1808	3	10,11,12	1.99	1 (10%)	9,13,15	1.78	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	J8W	L	1808	3	-	4/9/11/13	-
3	J8W	K	1808	3	-	4/9/11/13	-
3	J8W	H	1808	3	-	4/9/11/13	-
3	J8W	I	1808	3	-	4/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1808	J8W	OG-C2	5.59	1.49	1.33
3	K	1808	J8W	OG-C2	5.35	1.49	1.33
3	L	1808	J8W	OG-C2	5.16	1.48	1.33
3	H	1808	J8W	OG-C2	4.94	1.47	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1808	J8W	CB-OG-C2	3.78	131.14	117.12
3	K	1808	J8W	CB-OG-C2	3.75	131.00	117.12
3	I	1808	J8W	CB-OG-C2	3.56	130.29	117.12
3	L	1808	J8W	CB-OG-C2	3.46	129.93	117.12
3	L	1808	J8W	OG-C2-C1	2.58	118.34	111.39
3	K	1808	J8W	O9-C3-C1	-2.31	115.32	122.08
3	K	1808	J8W	OG-C2-C1	2.31	117.60	111.39
3	I	1808	J8W	OG-C2-C1	2.28	117.52	111.39
3	H	1808	J8W	O8-C3-O9	-2.11	118.04	123.30
3	K	1808	J8W	C3-C1-C2	-2.05	105.82	113.15
3	L	1808	J8W	O9-C3-C1	-2.04	116.11	122.08
3	I	1808	J8W	C3-C1-C2	-2.02	105.94	113.15

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1808	J8W	N-CA-CB-OG
3	H	1808	J8W	C-CA-CB-OG
3	I	1808	J8W	N-CA-CB-OG
3	I	1808	J8W	C-CA-CB-OG
3	K	1808	J8W	N-CA-CB-OG
3	K	1808	J8W	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
3	L	1808	J8W	N-CA-CB-OG
3	L	1808	J8W	C-CA-CB-OG
3	H	1808	J8W	O7-C2-OG-CB
3	I	1808	J8W	O7-C2-OG-CB
3	K	1808	J8W	O7-C2-OG-CB
3	L	1808	J8W	O7-C2-OG-CB
3	H	1808	J8W	C1-C2-OG-CB
3	I	1808	J8W	C1-C2-OG-CB
3	K	1808	J8W	C1-C2-OG-CB
3	L	1808	J8W	C1-C2-OG-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1808	J8W	1	0
3	K	1808	J8W	1	0
3	H	1808	J8W	1	0
3	I	1808	J8W	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 39 are monoatomic - leaving 94 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	D	1902	-	3,3,3	0.17	0	2,2,2	0.49	0
5	EDO	F	1904	-	3,3,3	0.31	0	2,2,2	0.49	0
5	EDO	D	1913	-	3,3,3	0.13	0	2,2,2	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PNS	D	1901	1	13,20,21	0.60	0	18,26,29	1.08	1 (5%)
5	EDO	B	1903	-	3,3,3	0.10	0	2,2,2	0.18	0
7	A2P	A	1918	-	29,29,29	0.47	0	44,45,45	0.58	0
5	EDO	F	1903	-	3,3,3	0.10	0	2,2,2	0.20	0
5	EDO	A	1906	-	3,3,3	0.05	0	2,2,2	0.12	0
5	EDO	J	2105	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	D	1903	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	A	1911	-	3,3,3	0.19	0	2,2,2	0.45	0
5	EDO	E	1909	-	3,3,3	0.17	0	2,2,2	0.41	0
5	EDO	J	2103	-	3,3,3	0.08	0	2,2,2	0.14	0
7	A2P	D	1923	-	29,29,29	0.52	0	44,45,45	0.63	0
5	EDO	E	1908	-	3,3,3	0.10	0	2,2,2	0.29	0
7	A2P	E	1917	-	29,29,29	0.49	0	44,45,45	0.69	1 (2%)
5	EDO	E	1910	-	3,3,3	0.15	0	2,2,2	0.36	0
5	EDO	A	1908	-	3,3,3	0.10	0	2,2,2	0.28	0
10	FMN	J	2101	-	33,33,33	1.36	3 (9%)	48,50,50	1.39	7 (14%)
5	EDO	A	1902	-	3,3,3	0.18	0	2,2,2	0.41	0
5	EDO	D	1904	-	3,3,3	0.11	0	2,2,2	0.29	0
5	EDO	B	1906	-	3,3,3	0.16	0	2,2,2	0.49	0
4	PNS	A	1901	1	13,20,21	0.68	0	18,26,29	1.03	1 (5%)
5	EDO	C	1905	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	D	1910	-	3,3,3	0.13	0	2,2,2	0.24	0
5	EDO	D	1909	-	3,3,3	0.28	0	2,2,2	0.64	0
11	MLI	G	2102	-	6,6,6	1.36	0	7,7,7	1.05	0
5	EDO	E	1912	-	3,3,3	0.09	0	2,2,2	0.14	0
5	EDO	C	1908	-	3,3,3	0.29	0	2,2,2	0.55	0
7	A2P	C	1917	-	29,29,29	0.54	0	44,45,45	0.63	0
5	EDO	J	2104	-	3,3,3	0.10	0	2,2,2	0.34	0
10	FMN	L	2101	-	33,33,33	1.41	3 (9%)	48,50,50	1.53	10 (20%)
5	EDO	B	1912	-	3,3,3	0.11	0	2,2,2	0.22	0
5	EDO	E	1907	-	3,3,3	0.13	0	2,2,2	0.28	0
10	FMN	I	2101	-	33,33,33	1.44	4 (12%)	48,50,50	1.51	11 (22%)
8	ACT	B	1902	-	3,3,3	1.18	0	3,3,3	0.68	0
5	EDO	C	1907	-	3,3,3	0.10	0	2,2,2	0.21	0
5	EDO	A	1904	-	3,3,3	0.13	0	2,2,2	0.29	0
8	ACT	H	2103	-	3,3,3	1.12	0	3,3,3	0.83	0
5	EDO	B	1904	-	3,3,3	0.12	0	2,2,2	0.16	0
5	EDO	C	1911	-	3,3,3	0.43	0	2,2,2	0.50	0
5	EDO	E	1903	-	3,3,3	0.13	0	2,2,2	0.24	0
5	EDO	C	1910	-	3,3,3	0.11	0	2,2,2	0.23	0
8	ACT	H	2104	-	3,3,3	1.09	0	3,3,3	0.75	0
5	EDO	C	1909	-	3,3,3	0.22	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACT	C	1903	-	3,3,3	0.90	0	3,3,3	0.89	0
5	EDO	E	1902	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	B	1905	-	3,3,3	0.07	0	2,2,2	0.25	0
5	EDO	D	1907	-	3,3,3	0.13	0	2,2,2	0.32	0
5	EDO	E	1905	-	3,3,3	0.12	0	2,2,2	0.36	0
5	EDO	D	1906	-	3,3,3	0.43	0	2,2,2	0.65	0
5	EDO	A	1903	-	3,3,3	0.27	0	2,2,2	0.48	0
4	PNS	B	1901	1	13,20,21	0.61	0	18,26,29	1.23	2 (11%)
10	FMN	K	2101	-	33,33,33	1.55	5 (15%)	48,50,50	1.66	8 (16%)
5	EDO	C	1906	-	3,3,3	0.32	0	2,2,2	0.57	0
5	EDO	C	1904	-	3,3,3	0.15	0	2,2,2	0.36	0
8	ACT	H	2102	-	3,3,3	1.14	0	3,3,3	0.69	0
5	EDO	J	2106	-	3,3,3	0.07	0	2,2,2	0.35	0
5	EDO	E	1904	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	D	1911	-	3,3,3	0.19	0	2,2,2	0.32	0
5	EDO	F	1908	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	F	1905	-	3,3,3	0.19	0	2,2,2	0.41	0
5	EDO	C	1912	-	3,3,3	0.29	0	2,2,2	0.64	0
5	EDO	D	1905	-	3,3,3	0.11	0	2,2,2	0.13	0
5	EDO	F	1902	-	3,3,3	0.09	0	2,2,2	0.13	0
5	EDO	F	1909	-	3,3,3	0.23	0	2,2,2	0.52	0
5	EDO	B	1907	-	3,3,3	0.15	0	2,2,2	0.25	0
4	PNS	E	1901	1	13,20,21	0.64	0	18,26,29	1.21	1 (5%)
4	PNS	F	1901	1	13,20,21	0.86	0	18,26,29	2.65	7 (38%)
8	ACT	C	1902	-	3,3,3	1.05	0	3,3,3	0.68	0
5	EDO	F	1907	-	3,3,3	0.13	0	2,2,2	0.33	0
5	EDO	A	1905	-	3,3,3	0.29	0	2,2,2	0.48	0
4	PNS	C	1901	1	13,20,21	0.61	0	18,26,29	1.15	1 (5%)
11	MLI	J	2102	-	6,6,6	1.43	1 (16%)	7,7,7	1.15	0
9	PGE	E	1918	-	9,9,9	0.23	0	8,8,8	0.16	0
5	EDO	B	1911	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	A	1910	-	3,3,3	0.37	0	2,2,2	0.63	0
5	EDO	D	1912	-	3,3,3	0.11	0	2,2,2	0.23	0
10	FMN	G	2101	-	33,33,33	1.41	3 (9%)	48,50,50	1.53	12 (25%)
5	EDO	B	1908	-	3,3,3	0.13	0	2,2,2	0.29	0
7	A2P	B	1918	-	29,29,29	0.56	0	44,45,45	1.04	2 (4%)
5	EDO	D	1914	-	3,3,3	0.24	0	2,2,2	0.45	0
5	EDO	E	1913	-	3,3,3	0.16	0	2,2,2	0.34	0
5	EDO	H	2105	-	3,3,3	0.11	0	2,2,2	0.18	0
5	EDO	F	1906	-	3,3,3	0.23	0	2,2,2	0.38	0
5	EDO	B	1910	-	3,3,3	0.15	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	E	1911	-	3,3,3	0.19	0	2,2,2	0.41	0
5	EDO	B	1909	-	3,3,3	0.30	0	2,2,2	0.45	0
5	EDO	D	1908	-	3,3,3	0.10	0	2,2,2	0.21	0
5	EDO	A	1909	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	A	1907	-	3,3,3	0.20	0	2,2,2	0.31	0
10	FMN	H	2101	-	33,33,33	1.39	4 (12%)	48,50,50	1.37	8 (16%)
7	A2P	F	1912	-	29,29,29	0.52	0	44,45,45	0.59	0
5	EDO	E	1906	-	3,3,3	0.05	0	2,2,2	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	1902	-	-	1/1/1/1	-
5	EDO	F	1904	-	-	0/1/1/1	-
5	EDO	D	1913	-	-	0/1/1/1	-
4	PNS	D	1901	1	-	0/24/26/27	-
5	EDO	B	1903	-	-	1/1/1/1	-
7	A2P	A	1918	-	-	5/15/31/31	0/3/3/3
5	EDO	F	1903	-	-	0/1/1/1	-
5	EDO	A	1906	-	-	1/1/1/1	-
5	EDO	J	2105	-	-	0/1/1/1	-
5	EDO	D	1903	-	-	1/1/1/1	-
5	EDO	A	1911	-	-	1/1/1/1	-
5	EDO	E	1909	-	-	1/1/1/1	-
5	EDO	J	2103	-	-	0/1/1/1	-
7	A2P	D	1923	-	-	4/15/31/31	0/3/3/3
5	EDO	E	1908	-	-	1/1/1/1	-
7	A2P	E	1917	-	-	6/15/31/31	0/3/3/3
5	EDO	E	1910	-	-	0/1/1/1	-
5	EDO	A	1908	-	-	1/1/1/1	-
10	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
5	EDO	A	1902	-	-	1/1/1/1	-
5	EDO	D	1904	-	-	1/1/1/1	-
5	EDO	B	1906	-	-	0/1/1/1	-
4	PNS	A	1901	1	-	1/24/26/27	-
5	EDO	C	1905	-	-	1/1/1/1	-
5	EDO	D	1910	-	-	0/1/1/1	-
5	EDO	D	1909	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MLI	G	2102	-	-	1/4/4/4	-
5	EDO	E	1912	-	-	0/1/1/1	-
5	EDO	C	1908	-	-	1/1/1/1	-
7	A2P	C	1917	-	-	6/15/31/31	0/3/3/3
5	EDO	J	2104	-	-	0/1/1/1	-
10	FMN	L	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	B	1912	-	-	1/1/1/1	-
5	EDO	E	1907	-	-	1/1/1/1	-
10	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
5	EDO	C	1907	-	-	1/1/1/1	-
5	EDO	A	1904	-	-	0/1/1/1	-
5	EDO	B	1904	-	-	1/1/1/1	-
5	EDO	C	1911	-	-	1/1/1/1	-
5	EDO	E	1903	-	-	1/1/1/1	-
5	EDO	C	1910	-	-	1/1/1/1	-
5	EDO	C	1909	-	-	1/1/1/1	-
5	EDO	E	1902	-	-	0/1/1/1	-
5	EDO	B	1905	-	-	0/1/1/1	-
5	EDO	D	1907	-	-	1/1/1/1	-
5	EDO	E	1905	-	-	1/1/1/1	-
5	EDO	D	1906	-	-	1/1/1/1	-
5	EDO	A	1903	-	-	1/1/1/1	-
4	PNS	B	1901	1	-	1/24/26/27	-
10	FMN	K	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	C	1906	-	-	1/1/1/1	-
5	EDO	C	1904	-	-	1/1/1/1	-
5	EDO	J	2106	-	-	1/1/1/1	-
5	EDO	E	1904	-	-	0/1/1/1	-
5	EDO	D	1911	-	-	1/1/1/1	-
5	EDO	F	1908	-	-	0/1/1/1	-
5	EDO	F	1905	-	-	1/1/1/1	-
5	EDO	C	1912	-	-	1/1/1/1	-
5	EDO	D	1905	-	-	1/1/1/1	-
5	EDO	F	1902	-	-	0/1/1/1	-
5	EDO	F	1909	-	-	0/1/1/1	-
5	EDO	B	1907	-	-	0/1/1/1	-
4	PNS	E	1901	1	-	1/24/26/27	-
4	PNS	F	1901	1	-	3/24/26/27	-
5	EDO	F	1907	-	-	0/1/1/1	-
5	EDO	A	1905	-	-	1/1/1/1	-
4	PNS	C	1901	1	-	1/24/26/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MLI	J	2102	-	-	0/4/4/4	-
9	PGE	E	1918	-	-	3/7/7/7	-
5	EDO	B	1911	-	-	1/1/1/1	-
5	EDO	A	1910	-	-	1/1/1/1	-
5	EDO	D	1912	-	-	1/1/1/1	-
10	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
5	EDO	B	1908	-	-	0/1/1/1	-
7	A2P	B	1918	-	-	7/15/31/31	0/3/3/3
5	EDO	D	1914	-	-	1/1/1/1	-
5	EDO	E	1913	-	-	1/1/1/1	-
5	EDO	H	2105	-	-	1/1/1/1	-
5	EDO	F	1906	-	-	1/1/1/1	-
5	EDO	B	1910	-	-	1/1/1/1	-
5	EDO	E	1911	-	-	1/1/1/1	-
5	EDO	B	1909	-	-	0/1/1/1	-
5	EDO	D	1908	-	-	1/1/1/1	-
5	EDO	A	1909	-	-	0/1/1/1	-
5	EDO	A	1907	-	-	1/1/1/1	-
10	FMN	H	2101	-	-	2/18/18/18	0/3/3/3
7	A2P	F	1912	-	-	9/15/31/31	0/3/3/3
5	EDO	E	1906	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	2101	FMN	C9A-C5A	5.14	1.49	1.41
10	L	2101	FMN	C9A-C5A	5.08	1.49	1.41
10	H	2101	FMN	C9A-C5A	4.94	1.49	1.41
10	I	2101	FMN	C9A-C5A	4.85	1.49	1.41
10	G	2101	FMN	C9A-C5A	4.62	1.48	1.41
10	J	2101	FMN	C9A-C5A	4.54	1.48	1.41
10	I	2101	FMN	C8-C7	3.62	1.49	1.40
10	K	2101	FMN	C8-C7	3.22	1.48	1.40
10	L	2101	FMN	C8-C7	3.20	1.48	1.40
10	K	2101	FMN	C1'-C2'	3.19	1.57	1.52
10	G	2101	FMN	C8-C7	2.86	1.48	1.40
10	H	2101	FMN	C8-C7	2.80	1.47	1.40
10	J	2101	FMN	C8-C7	2.78	1.47	1.40
10	K	2101	FMN	C4A-N5	2.77	1.36	1.30
10	H	2101	FMN	C4-N3	-2.73	1.33	1.38
10	I	2101	FMN	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	2101	FMN	C4-N3	-2.42	1.34	1.38
10	K	2101	FMN	O4-C4	2.34	1.28	1.23
10	L	2101	FMN	C4-N3	-2.26	1.34	1.38
10	H	2101	FMN	C4A-N5	2.25	1.35	1.30
10	J	2101	FMN	C4-N3	-2.11	1.34	1.38
11	J	2102	MLI	O9-C3	-2.09	1.23	1.30
10	I	2101	FMN	C5A-N5	-2.02	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1901	PNS	C38-C39-N41	6.24	126.93	116.42
4	F	1901	PNS	C43-C42-N41	-5.51	99.72	112.31
10	K	2101	FMN	O2-C2-N1	-4.79	113.88	121.83
10	L	2101	FMN	O3P-P-O5'	-4.37	95.10	106.73
4	F	1901	PNS	O40-C39-N41	-4.18	115.12	123.01
7	B	1918	A2P	C2'-C1'-N9	4.10	120.43	113.53
10	K	2101	FMN	C4-C4A-N5	4.05	123.99	118.23
10	H	2101	FMN	C4-C4A-N5	3.75	123.57	118.23
10	J	2101	FMN	O2-C2-N1	-3.65	115.78	121.83
10	G	2101	FMN	C4A-C10-N10	3.60	121.75	116.48
10	H	2101	FMN	O2-C2-N1	-3.50	116.03	121.83
10	G	2101	FMN	O2-C2-N1	-3.48	116.06	121.83
10	L	2101	FMN	O2-C2-N1	-3.43	116.14	121.83
4	F	1901	PNS	C42-N41-C39	3.38	129.12	122.84
10	I	2101	FMN	C4-C4A-N5	3.38	123.04	118.23
10	K	2101	FMN	C4A-C10-N10	3.37	121.41	116.48
10	I	2101	FMN	O2-C2-N1	-3.25	116.44	121.83
10	I	2101	FMN	C4A-C10-N10	3.22	121.19	116.48
10	G	2101	FMN	C4-C4A-N5	3.21	122.80	118.23
10	J	2101	FMN	C4A-C10-N10	3.14	121.07	116.48
4	F	1901	PNS	C31-C29-C32	3.07	114.15	108.82
10	H	2101	FMN	C4A-C10-N10	3.07	120.96	116.48
10	L	2101	FMN	C4A-C10-N10	3.03	120.92	116.48
4	B	1901	PNS	C31-C29-C32	3.03	114.08	108.82
4	E	1901	PNS	C31-C29-C32	2.91	113.87	108.82
4	C	1901	PNS	C31-C29-C32	2.90	113.85	108.82
10	G	2101	FMN	C4A-C10-N1	-2.84	118.14	124.73
10	J	2101	FMN	C4-C4A-N5	2.82	122.24	118.23
10	I	2101	FMN	C4A-C10-N1	-2.77	118.31	124.73
4	A	1901	PNS	C31-C29-C32	2.73	113.56	108.82
4	D	1901	PNS	C31-C29-C32	2.71	113.52	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	2101	FMN	O5'-P-O1P	-2.68	98.97	106.47
4	F	1901	PNS	C37-C38-C39	-2.67	107.91	112.36
10	G	2101	FMN	C10-C4A-N5	-2.65	119.22	124.86
10	L	2101	FMN	C4A-C10-N1	-2.64	118.60	124.73
10	K	2101	FMN	C10-C4A-N5	-2.63	119.28	124.86
7	B	1918	A2P	C4'-O4'-C1'	-2.61	103.70	109.47
10	I	2101	FMN	C10-C4A-N5	-2.61	119.32	124.86
10	L	2101	FMN	P-O5'-C5'	2.60	125.45	118.30
10	J	2101	FMN	C10-C4A-N5	-2.56	119.42	124.86
10	H	2101	FMN	O3P-P-O5'	-2.55	99.96	106.73
10	K	2101	FMN	O3'-C3'-C4'	2.53	114.93	108.81
10	L	2101	FMN	C4-C4A-N5	2.50	121.79	118.23
10	J	2101	FMN	C4A-C10-N1	-2.46	119.01	124.73
10	K	2101	FMN	O2'-C2'-C1'	2.43	115.67	109.80
7	E	1917	A2P	C2'-C1'-N9	2.40	117.57	113.53
10	H	2101	FMN	C10-C4A-N5	-2.38	119.80	124.86
10	J	2101	FMN	N3-C2-N1	2.35	124.00	119.38
10	G	2101	FMN	C10-N1-C2	2.33	121.55	116.90
10	I	2101	FMN	C5A-N5-C4A	2.33	121.94	118.07
10	G	2101	FMN	O3P-P-O5'	-2.32	100.55	106.73
10	G	2101	FMN	O4'-C4'-C3'	2.32	114.75	109.10
10	I	2101	FMN	O5'-P-O1P	-2.32	99.97	106.47
10	G	2101	FMN	C5'-C4'-C3'	-2.31	107.75	112.20
10	I	2101	FMN	C10-N1-C2	2.30	121.49	116.90
10	G	2101	FMN	O3P-P-O2P	2.24	116.21	107.64
4	F	1901	PNS	O40-C39-C38	-2.23	117.94	122.02
10	G	2101	FMN	N3-C2-N1	2.23	123.76	119.38
10	K	2101	FMN	N3-C2-N1	2.21	123.72	119.38
10	H	2101	FMN	C4A-C10-N1	-2.17	119.70	124.73
10	J	2101	FMN	O2P-P-O5'	-2.12	101.09	106.73
10	L	2101	FMN	O2P-P-O5'	2.12	112.36	106.73
10	H	2101	FMN	N3-C2-N1	2.09	123.49	119.38
10	L	2101	FMN	C10-C4A-N5	-2.08	120.45	124.86
10	L	2101	FMN	N3-C2-N1	2.07	123.45	119.38
10	L	2101	FMN	C10-N1-C2	2.06	121.03	116.90
4	B	1901	PNS	C43-C42-N41	2.04	116.96	112.31
10	G	2101	FMN	C9A-N10-C10	-2.03	117.61	120.77
10	I	2101	FMN	O4'-C4'-C5'	-2.02	105.37	109.92
10	I	2101	FMN	N3-C2-N1	2.01	123.33	119.38
10	H	2101	FMN	C5'-C4'-C3'	-2.01	108.33	112.20
10	I	2101	FMN	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1901	PNS	C38-C39-N41-C42
4	F	1901	PNS	O40-C39-N41-C42
5	A	1910	EDO	O1-C1-C2-O2
7	A	1918	A2P	C5'-O5'-P-OP1
7	A	1918	A2P	C5'-O5'-P-OP2
7	B	1918	A2P	C5'-O5'-P-OP3
7	B	1918	A2P	C5'-O5'-P-OP2
7	B	1918	A2P	O4'-C4'-C5'-O5'
7	C	1917	A2P	C2'-O2'-P1-O6P
7	C	1917	A2P	C5'-O5'-P-OP1
7	C	1917	A2P	C5'-O5'-P-OP3
7	C	1917	A2P	C5'-O5'-P-OP2
7	D	1923	A2P	C5'-O5'-P-OP3
7	D	1923	A2P	C5'-O5'-P-OP2
7	F	1912	A2P	C5'-O5'-P-OP3
7	F	1912	A2P	O4'-C4'-C5'-O5'
7	F	1912	A2P	C1'-C2'-O2'-P1
10	L	2101	FMN	C3'-C4'-C5'-O5'
10	L	2101	FMN	O4'-C4'-C5'-O5'
10	L	2101	FMN	C4'-C5'-O5'-P
7	A	1918	A2P	O4'-C4'-C5'-O5'
7	B	1918	A2P	C3'-C4'-C5'-O5'
7	C	1917	A2P	C1'-C2'-O2'-P1
7	E	1917	A2P	C1'-C2'-O2'-P1
7	E	1917	A2P	O4'-C4'-C5'-O5'
7	E	1917	A2P	C3'-C4'-C5'-O5'
7	F	1912	A2P	C3'-C4'-C5'-O5'
5	A	1906	EDO	O1-C1-C2-O2
9	E	1918	PGE	O2-C3-C4-O3
7	A	1918	A2P	C3'-C4'-C5'-O5'
9	E	1918	PGE	O3-C5-C6-O4
7	F	1912	A2P	C3'-C2'-O2'-P1
10	K	2101	FMN	O2'-C2'-C3'-C4'
5	A	1903	EDO	O1-C1-C2-O2
5	A	1907	EDO	O1-C1-C2-O2
5	A	1908	EDO	O1-C1-C2-O2
5	B	1910	EDO	O1-C1-C2-O2
5	C	1904	EDO	O1-C1-C2-O2
5	C	1906	EDO	O1-C1-C2-O2
5	C	1908	EDO	O1-C1-C2-O2
5	C	1911	EDO	O1-C1-C2-O2
5	D	1903	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	1904	EDO	O1-C1-C2-O2
5	D	1909	EDO	O1-C1-C2-O2
5	D	1911	EDO	O1-C1-C2-O2
5	D	1912	EDO	O1-C1-C2-O2
5	D	1914	EDO	O1-C1-C2-O2
5	E	1908	EDO	O1-C1-C2-O2
5	E	1909	EDO	O1-C1-C2-O2
5	J	2106	EDO	O1-C1-C2-O2
10	J	2101	FMN	C2'-C3'-C4'-O4'
7	B	1918	A2P	C5'-O5'-P-OP1
7	D	1923	A2P	C5'-O5'-P-OP1
5	B	1912	EDO	O1-C1-C2-O2
5	F	1906	EDO	O1-C1-C2-O2
7	B	1918	A2P	O4'-C1'-N9-C4
10	I	2101	FMN	O2'-C2'-C3'-C4'
10	K	2101	FMN	C4'-C5'-O5'-P
5	B	1904	EDO	O1-C1-C2-O2
5	D	1906	EDO	O1-C1-C2-O2
5	E	1905	EDO	O1-C1-C2-O2
5	E	1907	EDO	O1-C1-C2-O2
10	I	2101	FMN	C2'-C3'-C4'-C5'
7	A	1918	A2P	C5'-O5'-P-OP3
7	E	1917	A2P	C2'-O2'-P1-O4P
7	F	1912	A2P	C5'-O5'-P-OP2
10	G	2101	FMN	C2'-C3'-C4'-O4'
7	E	1917	A2P	C4'-C5'-O5'-P
10	G	2101	FMN	C4'-C5'-O5'-P
10	H	2101	FMN	C4'-C5'-O5'-P
9	E	1918	PGE	C3-C4-O3-C5
10	J	2101	FMN	C4'-C5'-O5'-P
5	A	1905	EDO	O1-C1-C2-O2
5	B	1903	EDO	O1-C1-C2-O2
5	C	1909	EDO	O1-C1-C2-O2
5	D	1908	EDO	O1-C1-C2-O2
5	F	1905	EDO	O1-C1-C2-O2
10	I	2101	FMN	C4'-C5'-O5'-P
7	F	1912	A2P	C5'-O5'-P-OP1
5	A	1902	EDO	O1-C1-C2-O2
5	C	1905	EDO	O1-C1-C2-O2
5	C	1910	EDO	O1-C1-C2-O2
5	C	1912	EDO	O1-C1-C2-O2
5	E	1911	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	I	2101	FMN	C2'-C3'-C4'-O4'
10	K	2101	FMN	O2'-C2'-C3'-O3'
10	J	2101	FMN	C2'-C3'-C4'-C5'
5	B	1911	EDO	O1-C1-C2-O2
5	E	1906	EDO	O1-C1-C2-O2
10	I	2101	FMN	O3'-C3'-C4'-C5'
10	G	2101	FMN	C2'-C3'-C4'-C5'
7	C	1917	A2P	O4'-C4'-C5'-O5'
5	C	1907	EDO	O1-C1-C2-O2
5	D	1905	EDO	O1-C1-C2-O2
5	E	1903	EDO	O1-C1-C2-O2
4	A	1901	PNS	O33-C32-C34-O35
4	B	1901	PNS	O33-C32-C34-O35
4	C	1901	PNS	O33-C32-C34-O35
4	E	1901	PNS	O33-C32-C34-O35
4	F	1901	PNS	O33-C32-C34-O35
7	F	1912	A2P	C2'-O2'-P1-O4P
7	E	1917	A2P	C3'-C2'-O2'-P1
10	I	2101	FMN	O2'-C2'-C3'-O3'
7	B	1918	A2P	O4'-C1'-N9-C8
5	D	1902	EDO	O1-C1-C2-O2
5	E	1913	EDO	O1-C1-C2-O2
5	H	2105	EDO	O1-C1-C2-O2
7	F	1912	A2P	C2'-O2'-P1-O6P
10	J	2101	FMN	O3'-C3'-C4'-O4'
11	G	2102	MLI	C3-C1-C2-O6
10	G	2101	FMN	O3'-C3'-C4'-C5'
10	J	2101	FMN	O3'-C3'-C4'-C5'
7	D	1923	A2P	O4'-C4'-C5'-O5'
10	G	2101	FMN	O3'-C3'-C4'-O4'
5	A	1911	EDO	O1-C1-C2-O2
5	D	1907	EDO	O1-C1-C2-O2
10	H	2101	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

25 monomers are involved in 68 short contacts:

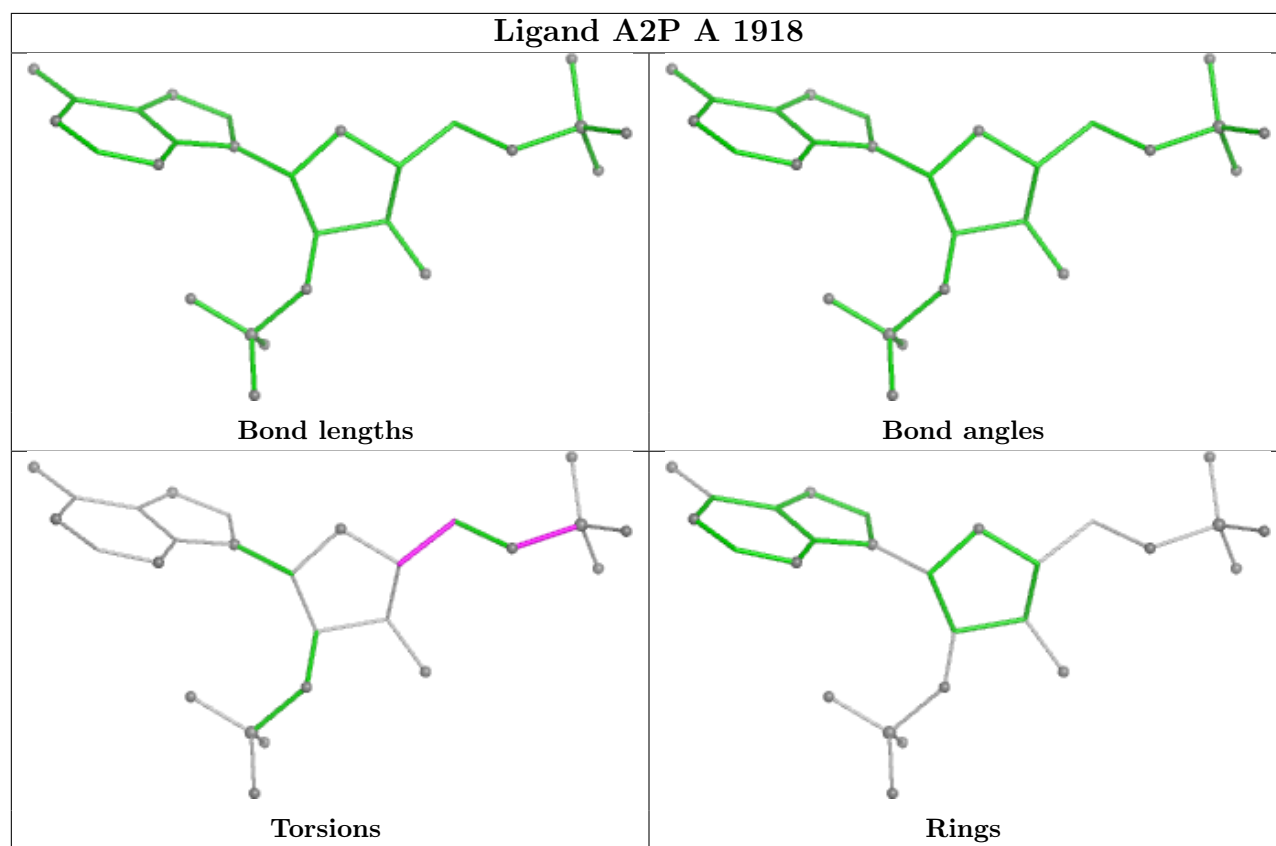
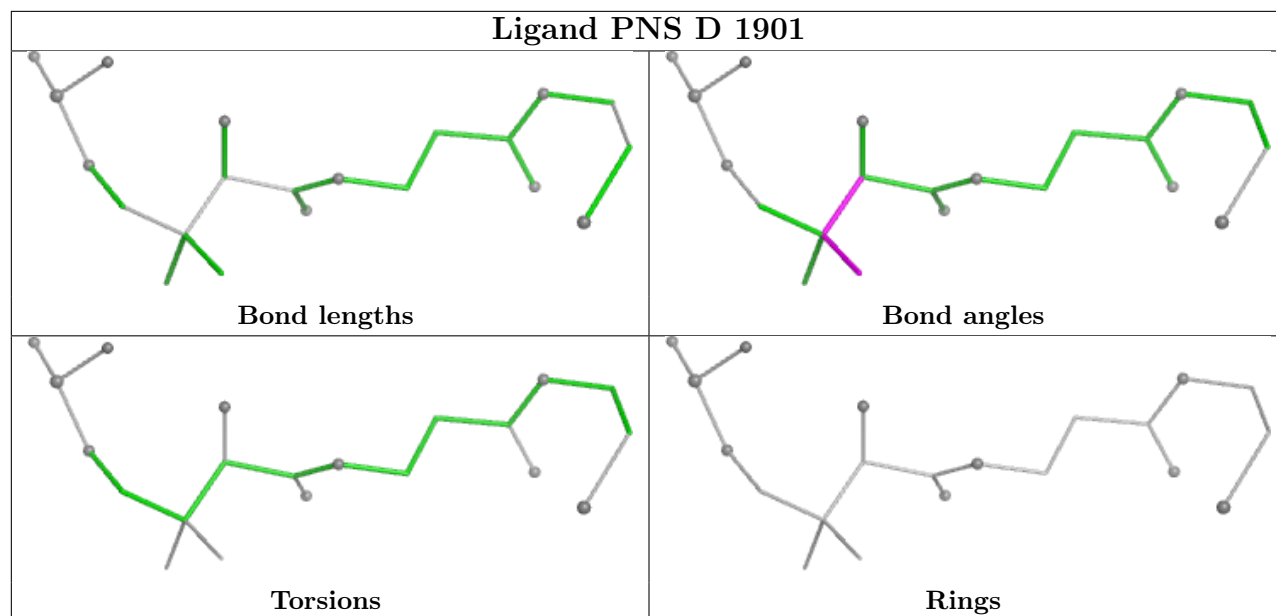
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1918	A2P	3	0
5	J	2105	EDO	1	0
7	D	1923	A2P	3	0
7	E	1917	A2P	2	0

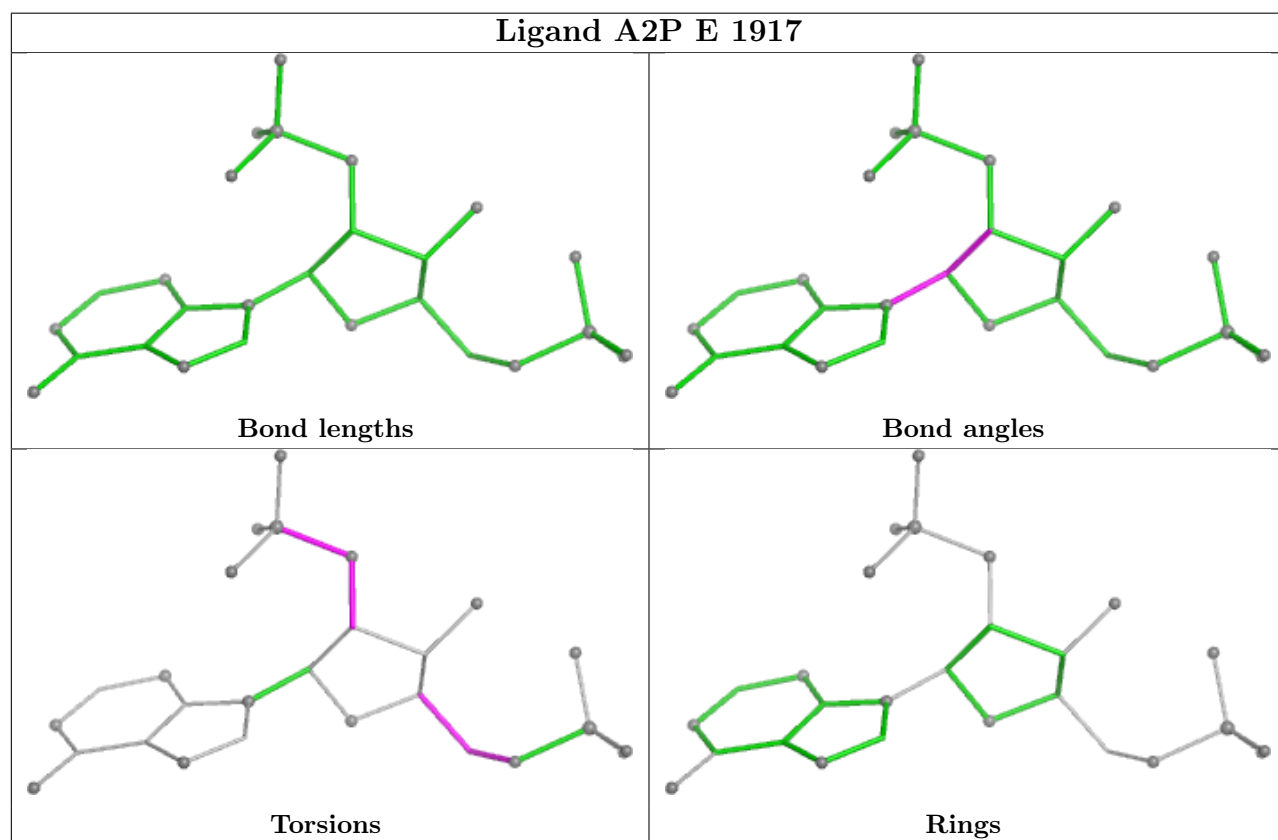
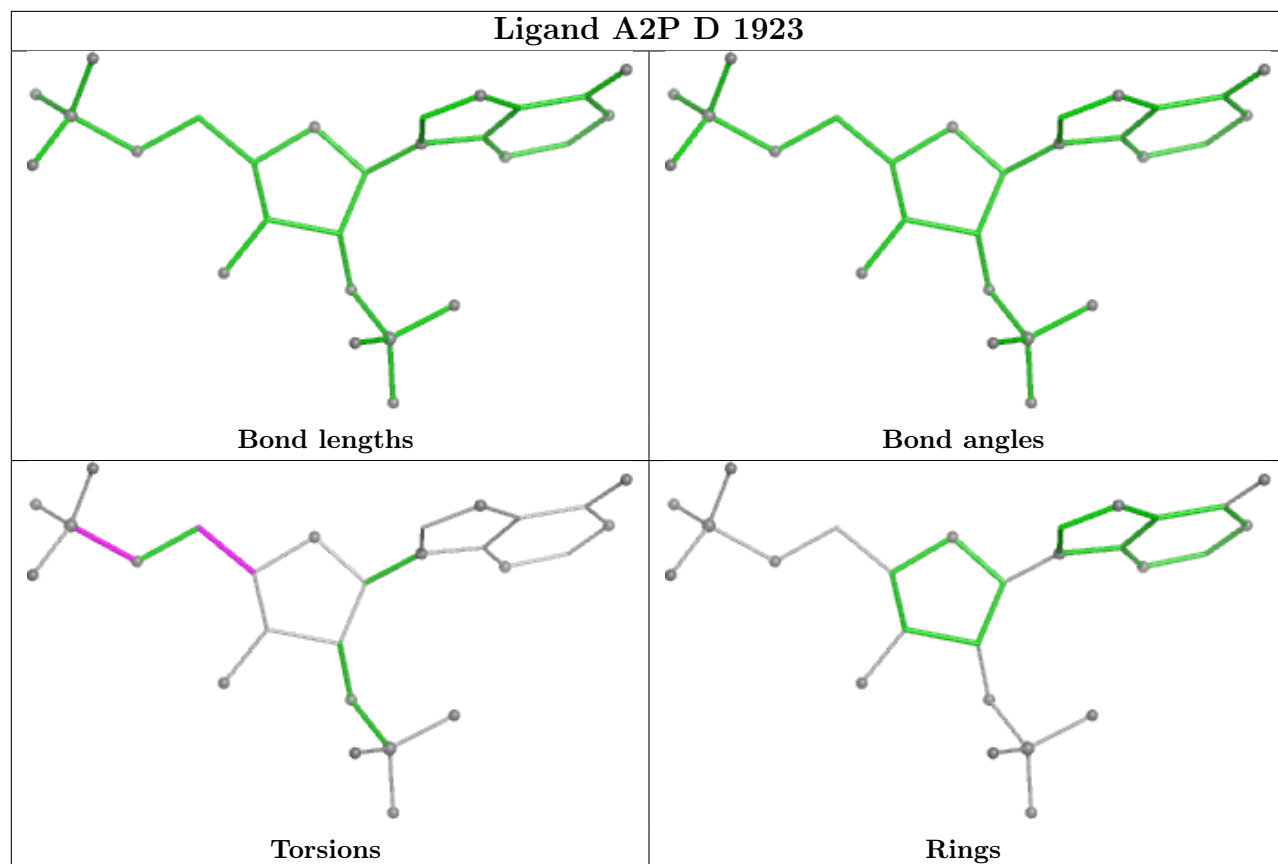
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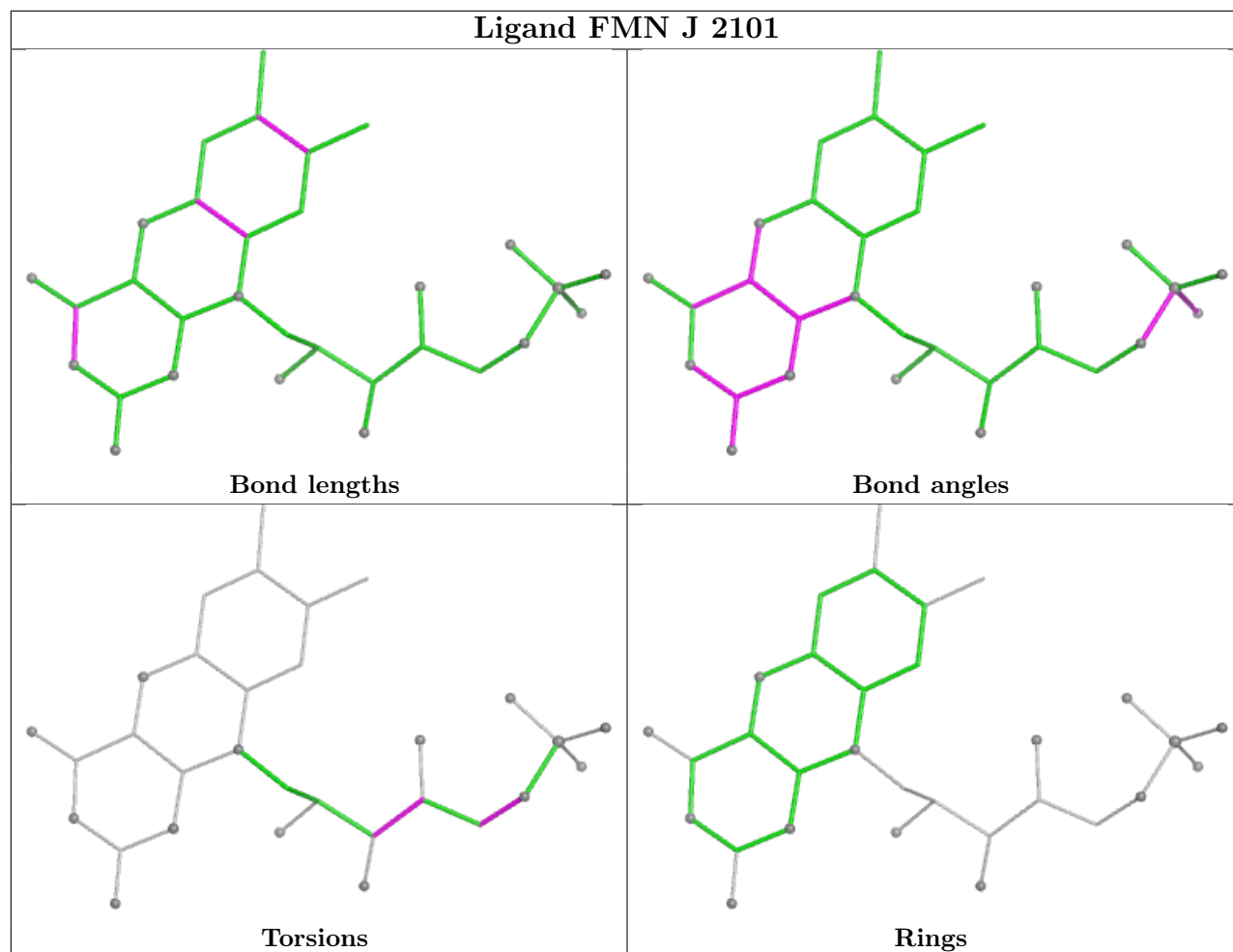
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	2101	FMN	8	0
5	B	1906	EDO	3	0
4	A	1901	PNS	1	0
5	D	1910	EDO	1	0
11	G	2102	MLI	1	0
7	C	1917	A2P	1	0
5	J	2104	EDO	1	0
10	L	2101	FMN	6	0
10	I	2101	FMN	6	0
8	B	1902	ACT	1	0
5	C	1907	EDO	1	0
8	C	1903	ACT	2	0
4	B	1901	PNS	1	0
10	K	2101	FMN	5	0
4	F	1901	PNS	2	0
11	J	2102	MLI	2	0
10	G	2101	FMN	5	0
7	B	1918	A2P	5	0
5	B	1910	EDO	1	0
10	H	2101	FMN	5	0
7	F	1912	A2P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

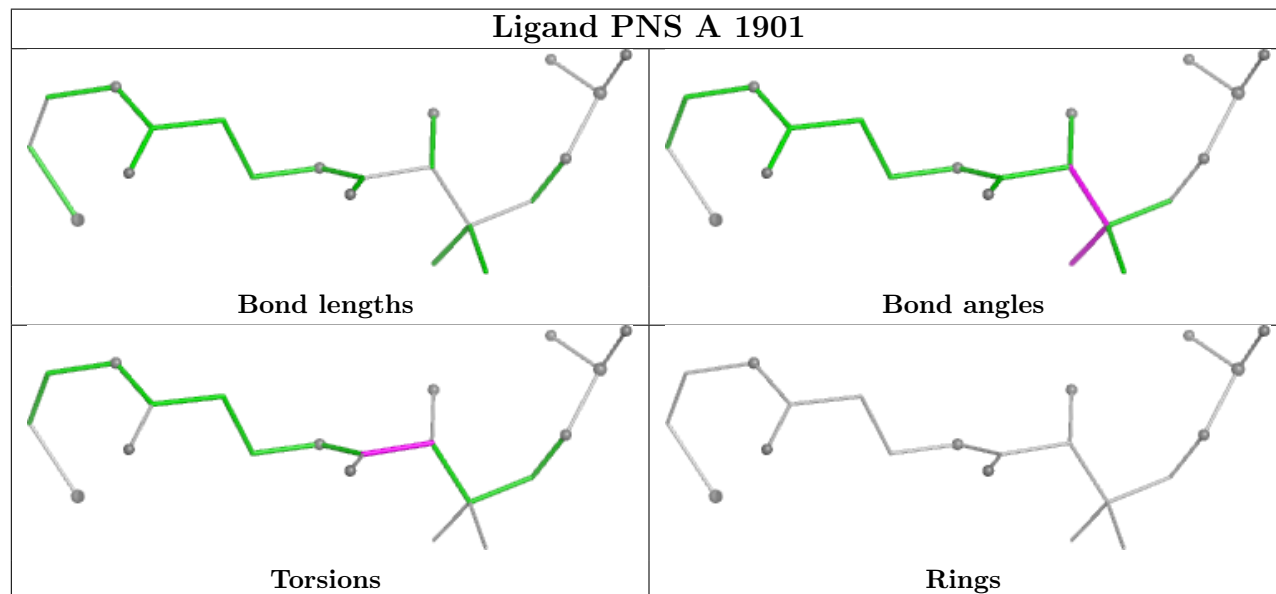


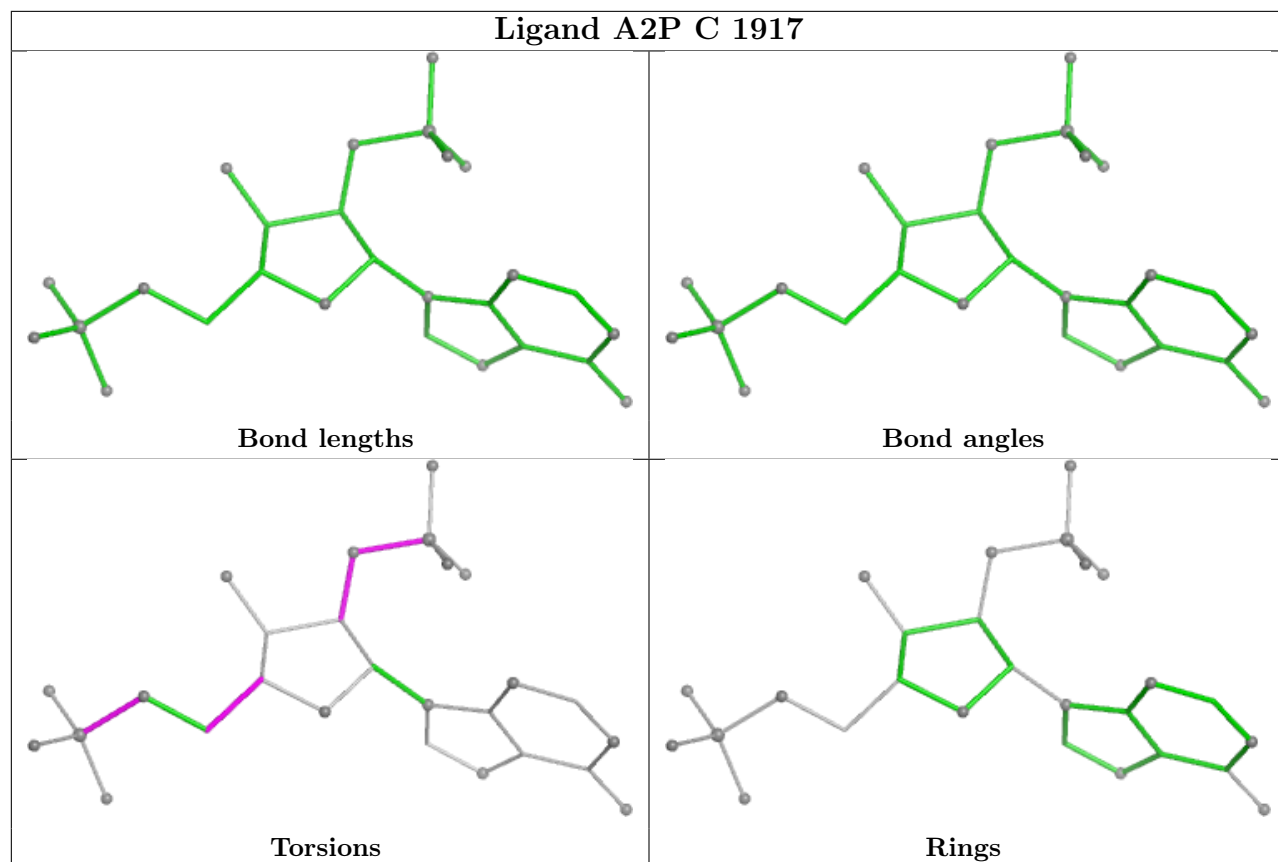


Ligand FMN J 2101

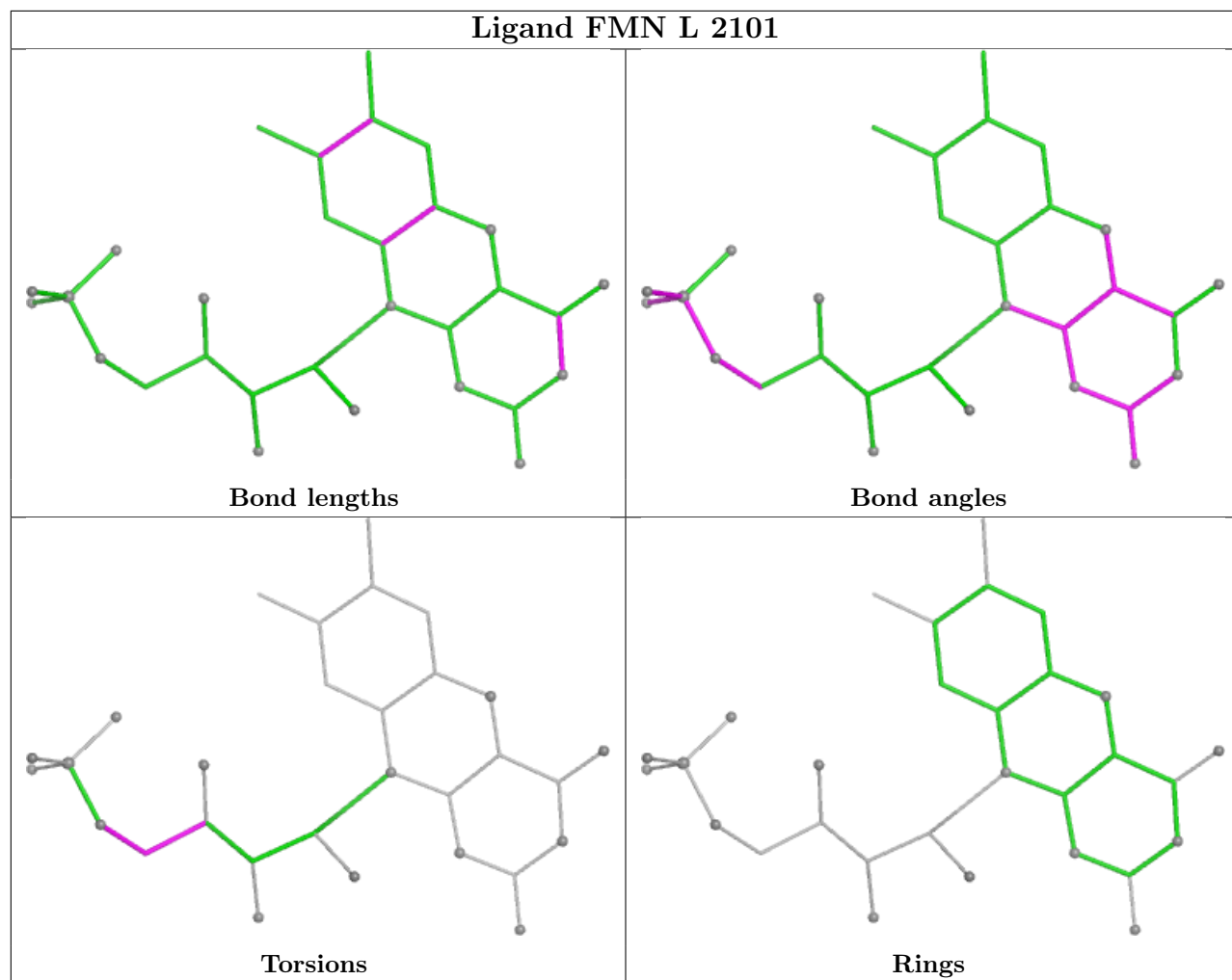


Ligand PNS A 1901

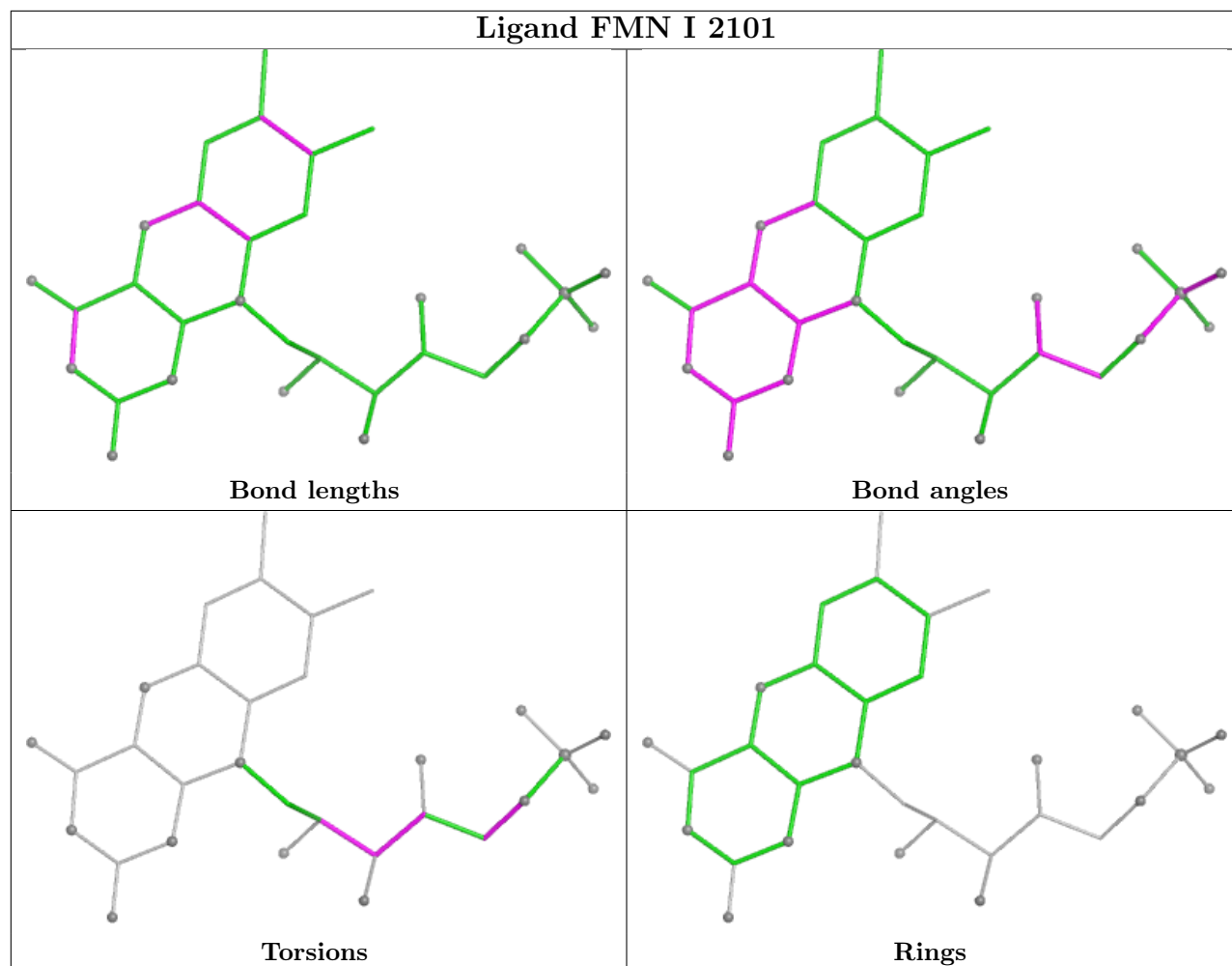




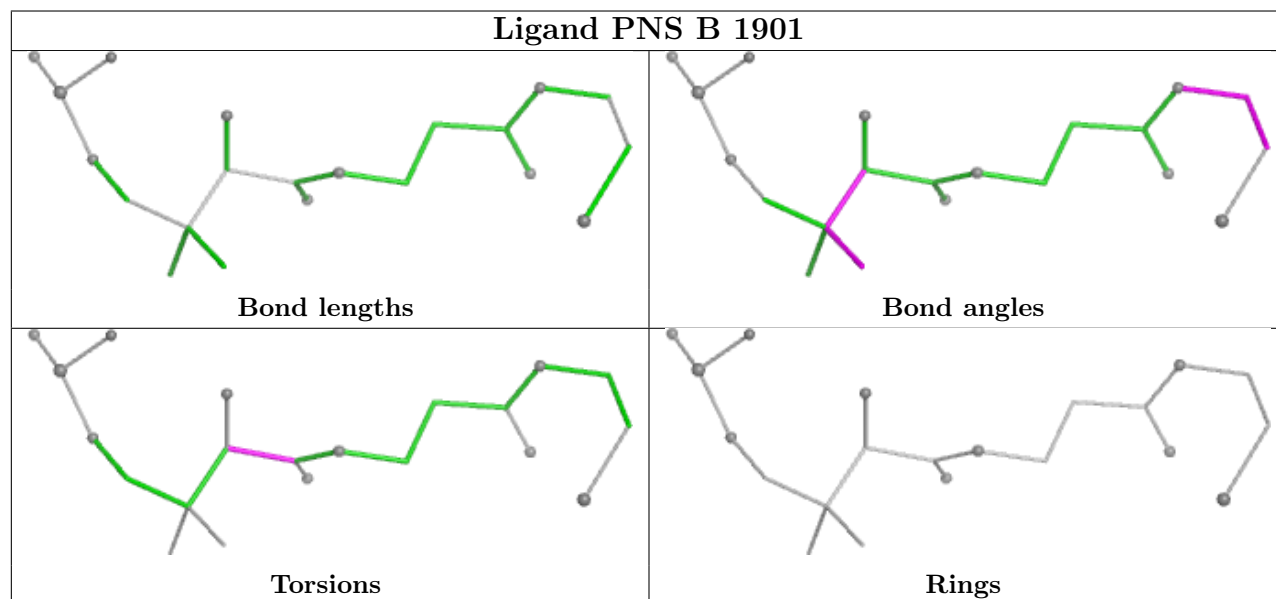
Ligand FMN L 2101



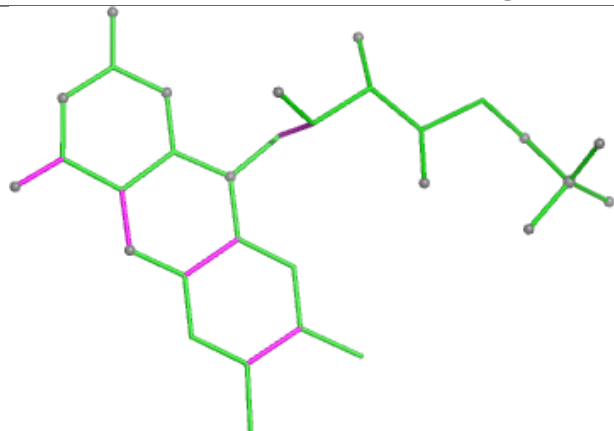
Ligand FMN I 2101



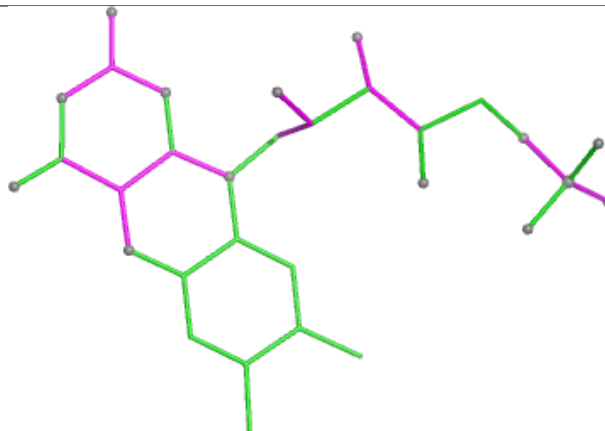
Ligand PNS B 1901



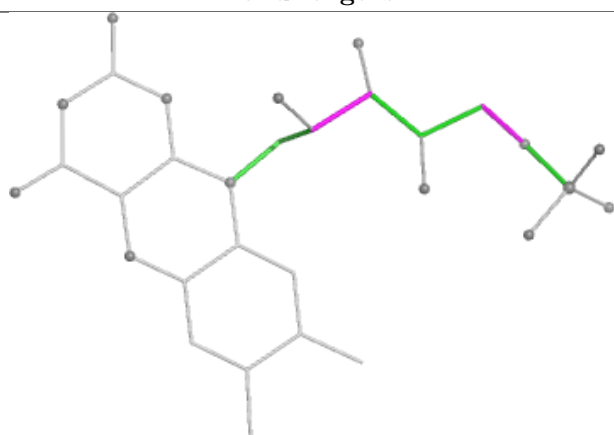
Ligand FMN K 2101



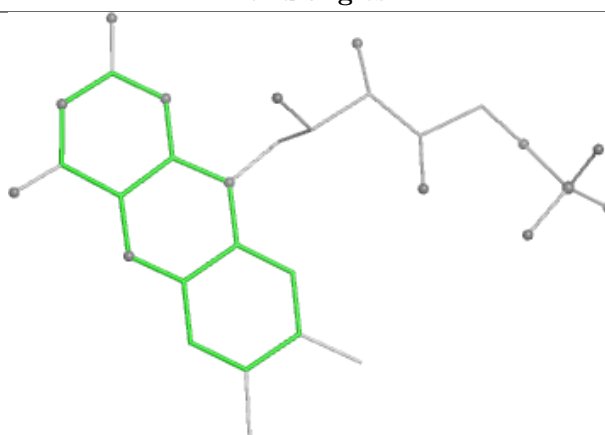
Bond lengths



Bond angles

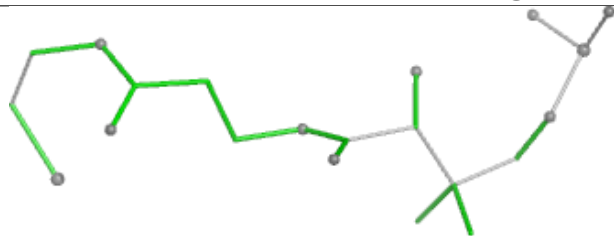


Torsions

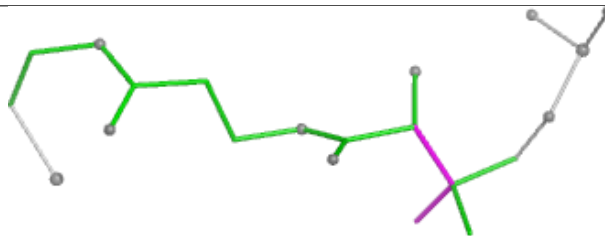


Rings

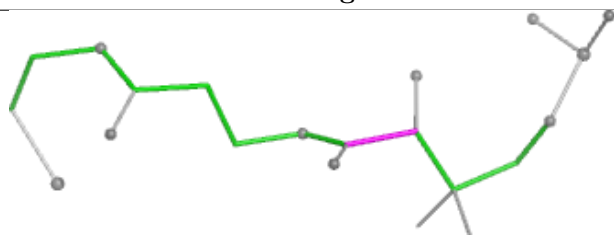
Ligand PNS E 1901



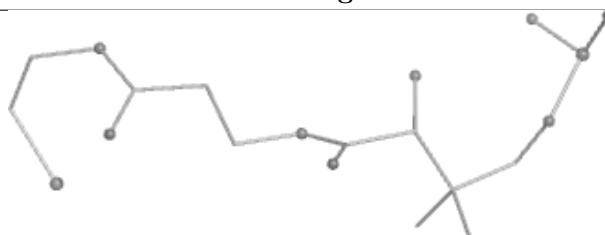
Bond lengths



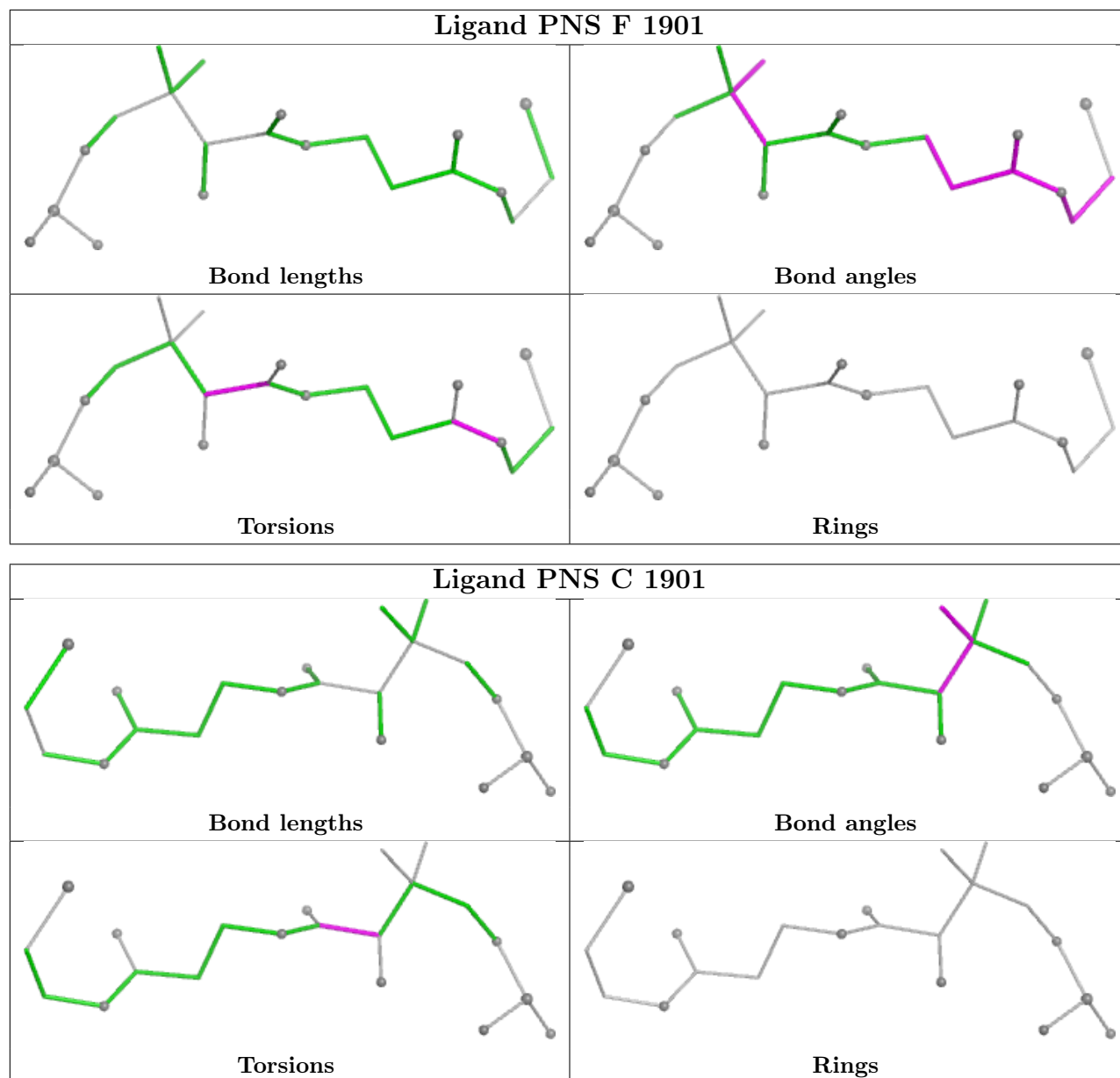
Bond angles



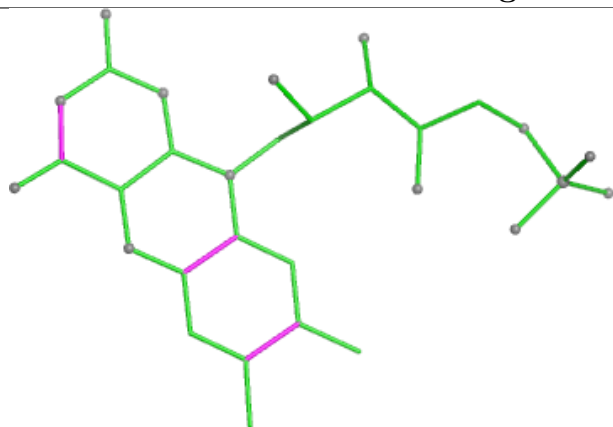
Torsions



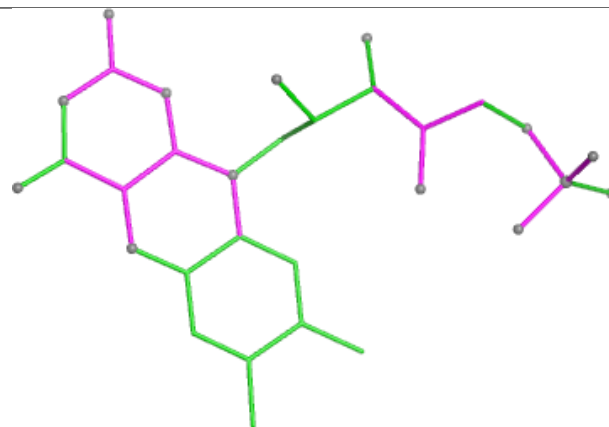
Rings



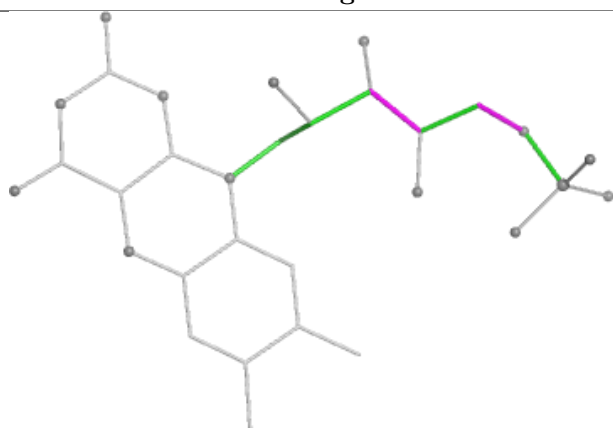
Ligand FMN G 2101



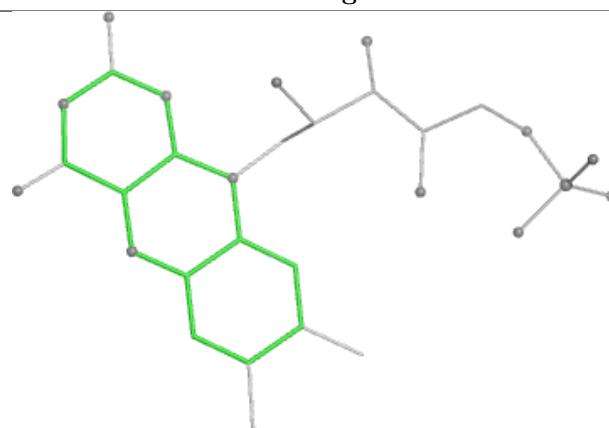
Bond lengths



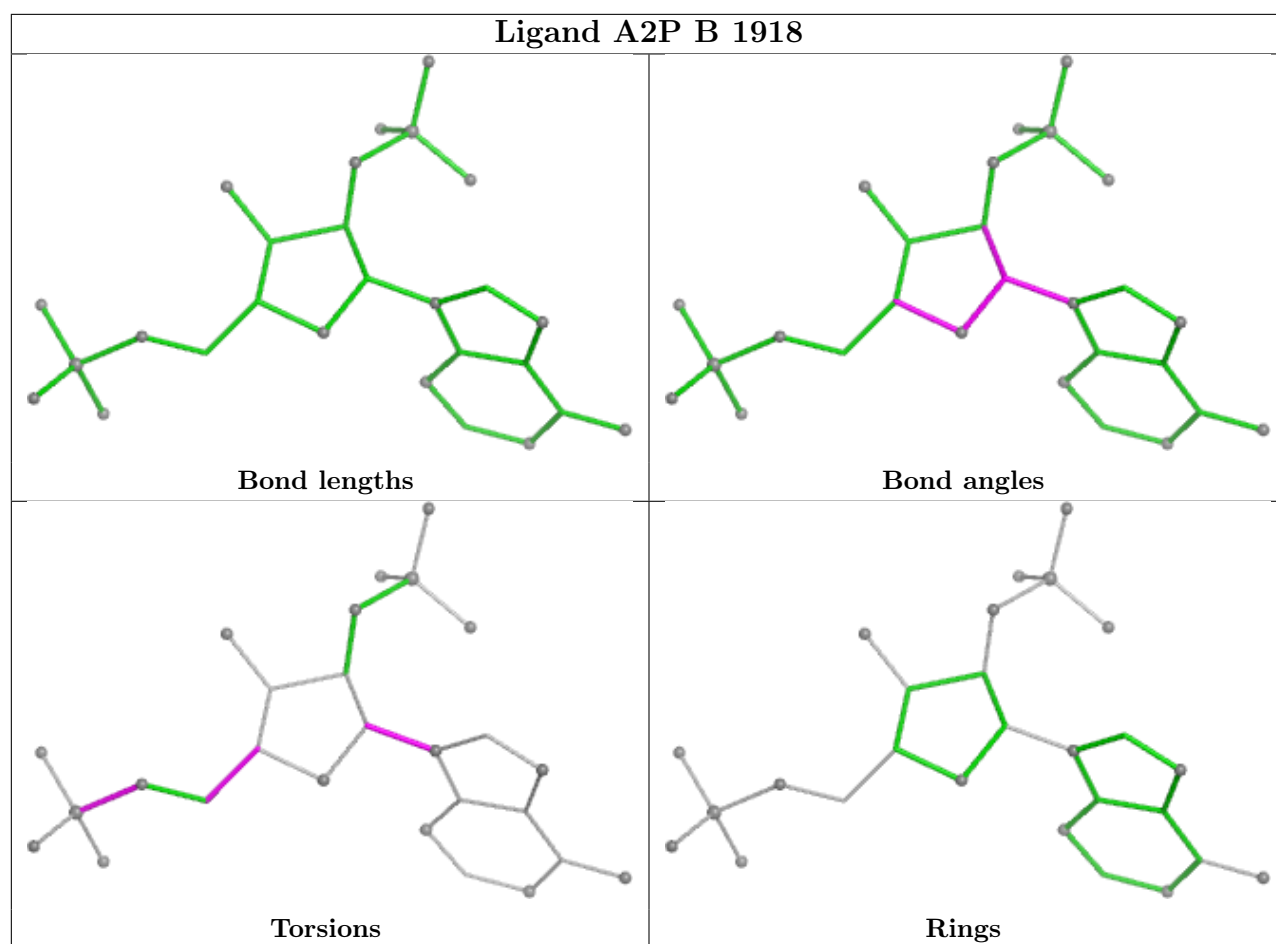
Bond angles

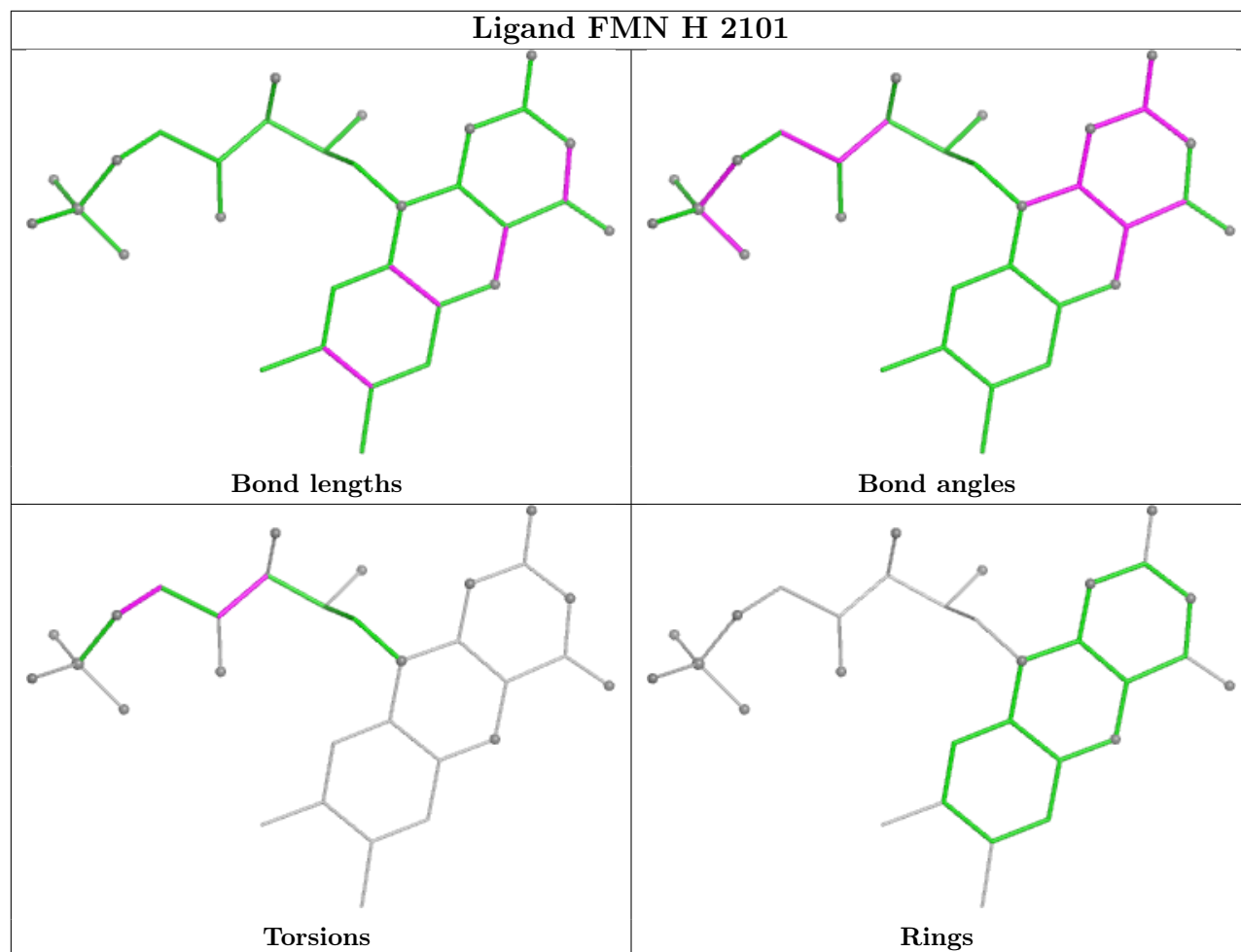


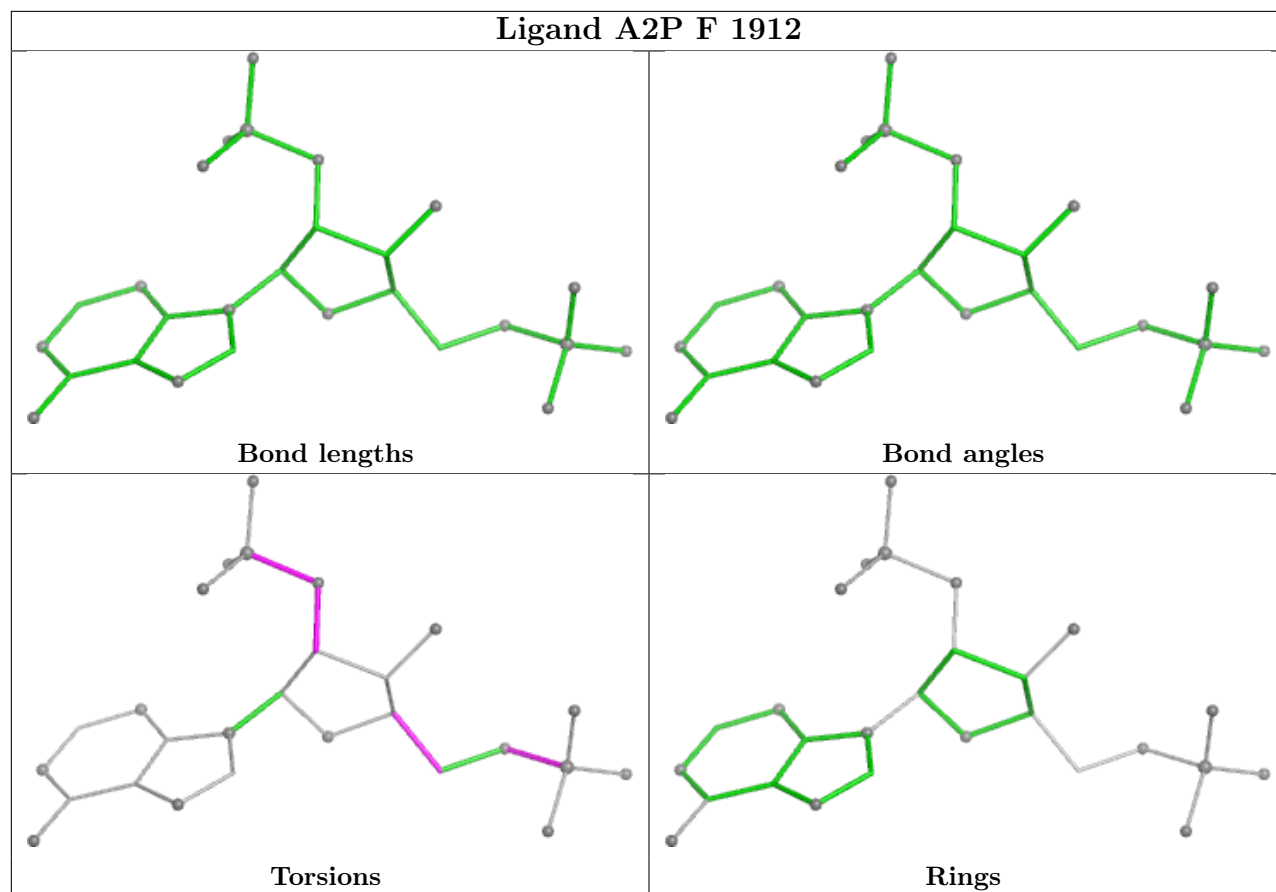
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1760/1887 (93%)	-0.06	50 (2%)	55	44	32, 54, 115, 158	0
1	B	1759/1887 (93%)	-0.18	40 (2%)	61	51	29, 53, 108, 154	0
1	C	1759/1887 (93%)	-0.14	40 (2%)	61	51	31, 53, 112, 166	0
1	D	1765/1887 (93%)	-0.13	49 (2%)	55	44	27, 47, 111, 154	0
1	E	1759/1887 (93%)	-0.12	36 (2%)	65	55	35, 57, 109, 162	0
1	F	1759/1887 (93%)	-0.10	32 (1%)	67	58	34, 59, 117, 172	0
2	G	2036/2051 (99%)	0.14	53 (2%)	57	47	30, 70, 130, 175	1 (0%)
2	J	2035/2051 (99%)	0.08	56 (2%)	55	44	28, 69, 135, 189	1 (0%)
3	H	2034/2051 (99%)	0.03	39 (1%)	66	57	34, 67, 119, 162	1 (0%)
3	I	2033/2051 (99%)	0.22	56 (2%)	55	44	38, 79, 124, 167	1 (0%)
3	K	2034/2051 (99%)	0.28	56 (2%)	55	44	57, 87, 129, 175	0
3	L	2035/2051 (99%)	0.31	68 (3%)	49	39	38, 84, 137, 191	1 (0%)
All	All	22768/23628 (96%)	0.04	575 (2%)	58	48	27, 71, 122, 191	5 (0%)

All (575) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1842	VAL	7.1
1	D	302	LEU	6.6
1	A	328	LEU	6.5
1	E	302	LEU	5.9
1	E	328	LEU	5.9
3	I	740[A]	HIS	5.9
1	C	1828	LEU	5.8
1	D	1842	VAL	5.8
1	C	328	LEU	5.8
1	A	1828	LEU	5.7
1	B	328	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	601	VAL	5.7
1	D	1828	LEU	5.5
1	F	328	LEU	5.3
3	I	1741	ILE	5.1
1	F	1828	LEU	5.1
3	I	1970	VAL	5.0
2	J	28	PHE	4.9
1	A	1833	ALA	4.9
1	D	328	LEU	4.9
1	A	140	ILE	4.9
2	G	1970	VAL	4.8
2	J	1741	ILE	4.7
1	A	303	SER	4.7
3	L	1970	VAL	4.6
2	G	28	PHE	4.6
3	L	2047	LYS	4.6
1	B	599	MET	4.5
1	C	140	ILE	4.4
1	B	302	LEU	4.4
2	J	77	VAL	4.3
3	K	4	TYR	4.3
1	A	1832	ALA	4.3
3	K	1847	LEU	4.3
3	K	1164	MET	4.3
3	K	1922	ILE	4.2
1	E	1833	ALA	4.2
1	C	1825	VAL	4.2
1	E	140	ILE	4.1
3	K	1746	LEU	4.1
1	A	1886	LYS	4.1
1	F	140	ILE	4.0
3	H	1847	LEU	4.0
2	J	1847	LEU	4.0
3	K	1741	ILE	3.9
3	L	1741	ILE	3.9
2	J	1927	LEU	3.9
3	K	1927	LEU	3.9
1	A	1883	VAL	3.9
1	D	975	ALA	3.9
3	H	28	PHE	3.9
1	A	1851	LEU	3.9
2	J	1746	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
3	L	1933	LEU	3.9
1	C	302	LEU	3.9
1	A	1825	VAL	3.9
1	D	140	ILE	3.9
3	H	1741	ILE	3.9
3	I	1742	VAL	3.8
3	K	1970	VAL	3.8
3	L	29	ILE	3.8
1	D	1825	VAL	3.8
2	G	29	ILE	3.8
1	B	601	VAL	3.7
1	F	1886	LYS	3.7
1	A	599	MET	3.7
3	I	19	VAL	3.7
3	I	5	SER	3.7
1	A	1846	ALA	3.7
3	K	1933	LEU	3.7
2	J	1970	VAL	3.7
3	H	74	PRO	3.7
2	G	1927	LEU	3.7
3	H	1970	VAL	3.7
1	A	1823	LEU	3.6
3	L	5	SER	3.6
2	J	2047	LYS	3.6
3	K	1738	PHE	3.6
2	G	1940	LEU	3.6
3	L	740[A]	HIS	3.6
1	D	972	SER	3.6
1	D	543	ILE	3.6
1	C	1842	VAL	3.6
1	F	1825	VAL	3.6
2	G	1741	ILE	3.6
3	I	1738	PHE	3.6
3	L	1913	VAL	3.6
3	I	25	ALA	3.5
1	F	302	LEU	3.5
1	B	181	THR	3.5
3	L	1738	PHE	3.5
3	L	1922	ILE	3.5
3	I	1953	VAL	3.5
1	F	599	MET	3.5
3	I	1847	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
3	K	1931	LEU	3.5
3	K	1955	PRO	3.5
3	I	1158	PHE	3.5
3	H	77	VAL	3.5
1	A	141	ALA	3.5
1	D	541	PRO	3.4
1	E	1865	THR	3.4
3	I	1931	LEU	3.4
1	B	1833	ALA	3.4
1	B	140	ILE	3.4
1	F	1885	THR	3.4
3	I	598	THR	3.4
3	I	1933	LEU	3.4
1	D	181	THR	3.4
1	F	1842	VAL	3.3
2	J	1933	LEU	3.3
2	J	1960	LEU	3.3
1	E	599	MET	3.3
3	L	1746	LEU	3.3
3	K	598	THR	3.3
1	D	977	TYR	3.3
2	G	74	PRO	3.3
3	H	1955	PRO	3.3
3	I	1746	LEU	3.3
1	B	1842	VAL	3.3
2	G	5	SER	3.3
1	A	1761	LYS	3.3
1	F	1764	VAL	3.3
2	G	598	THR	3.3
2	J	598	THR	3.2
3	L	1740	THR	3.2
1	D	622	ILE	3.2
1	D	976	ALA	3.2
3	H	598	THR	3.2
3	I	1955	PRO	3.2
3	L	1931	LEU	3.2
1	D	1832	ALA	3.2
1	D	1865	THR	3.2
1	F	1851	LEU	3.1
2	J	25	ALA	3.1
1	E	1764	VAL	3.1
2	G	1931	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	I	2048	TYR	3.1
3	I	1864	ALA	3.1
2	G	1955	PRO	3.1
2	G	1847	LEU	3.1
1	B	141	ALA	3.1
1	C	141	ALA	3.1
1	D	974	ASP	3.1
2	J	1953	VAL	3.1
3	H	19	VAL	3.1
3	I	1922	ILE	3.1
3	L	1925	ILE	3.1
2	J	1955	PRO	3.1
3	L	24	THR	3.1
1	D	1833	ALA	3.1
3	K	28	PHE	3.1
3	L	1972	ILE	3.1
3	I	21	LEU	3.1
1	A	181	THR	3.1
1	A	1764	VAL	3.0
3	L	505	GLY	3.0
1	A	1763	LYS	3.0
1	B	1828	LEU	3.0
1	C	973	ALA	3.0
1	C	976	ALA	3.0
1	A	1834	LEU	3.0
1	E	973	ALA	3.0
3	K	25	ALA	3.0
3	L	1864	ALA	3.0
3	L	1878	VAL	3.0
3	L	21	LEU	3.0
3	I	8	PRO	3.0
2	J	6	THR	3.0
2	J	1740	THR	3.0
1	E	141	ALA	3.0
2	G	1746	LEU	3.0
2	J	1958	LEU	3.0
1	B	178	GLY	2.9
2	J	74	PRO	2.9
1	B	1832	ALA	2.9
2	G	25	ALA	2.9
1	D	1883	VAL	2.9
1	E	1842	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	1742	VAL	2.9
2	J	1742	VAL	2.9
3	H	21	LEU	2.9
3	H	554	GLY	2.9
2	J	1745	LYS	2.9
2	G	1922	ILE	2.9
3	L	1917	ILE	2.9
2	G	1885	LEU	2.9
2	J	1931	LEU	2.9
3	L	1847	LEU	2.9
3	I	2047	LYS	2.9
2	G	1916	PHE	2.9
1	A	1865	THR	2.9
2	G	1919	LEU	2.9
3	L	1953	VAL	2.9
3	H	1738	PHE	2.9
3	L	1955	PRO	2.8
3	H	2047	LYS	2.8
3	K	2047	LYS	2.8
3	L	1949	LYS	2.8
1	F	978	ALA	2.8
2	J	1952	ALA	2.8
3	L	1916	PHE	2.8
2	G	740[A]	HIS	2.8
1	B	1785	THR	2.8
1	A	1830	GLY	2.8
1	C	876	GLY	2.8
1	D	141	ALA	2.8
1	F	1858	ALA	2.8
1	A	1843	ASN	2.8
1	B	877	LEU	2.8
3	K	5	SER	2.8
3	L	598	THR	2.8
1	C	599	MET	2.8
3	L	1853	GLY	2.8
1	F	96	GLU	2.8
1	E	1832	ALA	2.8
3	I	1916	PHE	2.8
2	J	1914	LEU	2.8
3	H	740[A]	HIS	2.8
1	D	599	MET	2.8
2	J	384	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	1742	VAL	2.8
2	G	21	LEU	2.8
1	B	1865	THR	2.8
1	E	974	ASP	2.8
3	I	139	LYS	2.8
1	B	1825	VAL	2.7
1	F	973	ALA	2.7
3	L	28	PHE	2.7
2	G	1888	ILE	2.7
2	J	4	TYR	2.7
3	L	4	TYR	2.7
2	G	26	SER	2.7
3	I	1957	PRO	2.7
3	I	1739	GLU	2.7
1	A	1769	VAL	2.7
1	C	1883	VAL	2.7
1	C	1862	ALA	2.7
2	J	1940	LEU	2.7
2	G	2048	TYR	2.7
3	H	1740	THR	2.7
1	C	974	ASP	2.7
1	E	539	SER	2.7
3	K	1742	VAL	2.7
3	L	77	VAL	2.7
2	J	1972	ILE	2.7
2	G	2045	TRP	2.7
1	F	974	ASP	2.7
3	K	23	PRO	2.7
2	J	5	SER	2.7
1	A	300	VAL	2.7
1	D	1764	VAL	2.7
1	B	1834	LEU	2.7
1	B	1851	LEU	2.7
1	E	622	ILE	2.7
1	F	331	ILE	2.7
3	K	1848	GLY	2.7
3	I	1974	VAL	2.7
3	L	1874	VAL	2.7
1	B	539	SER	2.7
3	L	400	SER	2.7
3	L	1914	LEU	2.7
1	D	1767	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	1848	GLY	2.6
3	I	1940	LEU	2.6
3	K	1919	LEU	2.6
3	L	1737	ILE	2.6
1	C	1833	ALA	2.6
3	I	1952	ALA	2.6
3	L	74	PRO	2.6
3	H	6	THR	2.6
1	D	1843	ASN	2.6
2	G	1953	VAL	2.6
3	K	1953	VAL	2.6
3	K	1917	ILE	2.6
1	C	1836	ASP	2.6
2	J	1738	PHE	2.6
3	H	2048	TYR	2.6
1	A	1826	LYS	2.6
1	E	621	THR	2.6
2	J	1885	LEU	2.6
2	G	1925	ILE	2.6
2	J	1922	ILE	2.6
3	I	2050	GLN	2.6
2	G	1864	ALA	2.6
2	G	1121	SER	2.6
1	C	977	TYR	2.6
2	J	2048	TYR	2.6
2	G	1958	LEU	2.6
3	H	414	LEU	2.6
3	K	21	LEU	2.6
1	E	181	THR	2.6
3	K	19	VAL	2.6
3	I	1930	SER	2.5
1	E	1826	LYS	2.5
1	A	977	TYR	2.5
1	E	1788	GLU	2.5
1	C	1858	ALA	2.5
1	E	978	ALA	2.5
1	E	1851	LEU	2.5
2	J	1971	GLY	2.5
3	L	1958	LEU	2.5
3	I	368	ILE	2.5
3	K	1924	ILE	2.5
3	K	1873	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	K	6	THR	2.5
2	J	740[A]	HIS	2.5
3	L	1929	LYS	2.5
2	G	1960	LEU	2.5
3	H	1931	LEU	2.5
3	I	1967	ILE	2.5
2	J	1913	VAL	2.5
1	C	179	LYS	2.5
3	I	414	LEU	2.5
1	A	331	ILE	2.5
1	C	331	ILE	2.5
1	E	1768	GLY	2.5
3	H	75	SER	2.5
3	I	1843	PRO	2.5
3	L	1971	GLY	2.5
1	A	1862	ALA	2.5
1	B	973	ALA	2.5
3	K	733	THR	2.5
1	C	509	ILE	2.4
2	J	1917	ILE	2.4
1	A	145	VAL	2.4
1	C	195	GLY	2.4
1	A	978	ALA	2.4
1	C	1857	LYS	2.4
1	D	1857	LYS	2.4
1	D	1885	THR	2.4
1	D	1766	ASN	2.4
3	I	1919	LEU	2.4
1	E	600	ASP	2.4
3	I	1972	ILE	2.4
3	K	368	ILE	2.4
2	G	505	GLY	2.4
3	H	1742	VAL	2.4
3	I	1362	GLY	2.4
3	K	1913	VAL	2.4
1	B	1789	ARG	2.4
1	A	1762	GLU	2.4
1	D	978	ALA	2.4
1	D	1846	ALA	2.4
1	A	256	LEU	2.4
3	H	42	PRO	2.4
1	C	1769	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1867	VAL	2.4
1	E	968	VAL	2.4
3	K	401	GLY	2.4
1	B	333	LYS	2.4
1	B	1788	GLU	2.4
1	E	1782	GLU	2.4
1	C	975	ALA	2.4
1	F	1865	THR	2.4
2	G	1740	THR	2.4
1	A	302	LEU	2.4
2	G	1933	LEU	2.4
3	H	1933	LEU	2.4
1	A	622	ILE	2.4
2	G	2038	ILE	2.4
3	K	29	ILE	2.4
3	L	80	PHE	2.4
1	C	330	GLU	2.4
3	K	374	ALA	2.4
1	C	1827	SER	2.4
2	J	1919	LEU	2.4
1	E	1825	VAL	2.3
1	A	1829	GLY	2.3
3	I	1555	ARG	2.3
3	L	401	GLY	2.3
1	D	621	THR	2.3
1	E	1828	LEU	2.3
3	H	4	TYR	2.3
3	I	1914	LEU	2.3
3	L	86	LEU	2.3
1	B	331	ILE	2.3
3	H	1737	ILE	2.3
1	C	1844	LYS	2.3
1	D	2	LYS	2.3
3	H	1957	PRO	2.3
3	K	1964	PHE	2.3
1	C	1832	ALA	2.3
2	G	1739	GLU	2.3
2	J	1873	TYR	2.3
3	I	6	THR	2.3
3	I	1740	THR	2.3
3	I	1748	THR	2.3
2	J	1986	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	1769	VAL	2.3
2	G	83	VAL	2.3
3	L	1842	VAL	2.3
1	B	1831	GLY	2.3
2	J	1938	GLY	2.3
3	L	554	GLY	2.3
1	B	508	ASN	2.3
3	K	1486	PHE	2.3
1	A	1801	ALA	2.3
1	B	975	ALA	2.3
3	I	1965	ALA	2.3
3	I	1885	LEU	2.3
1	A	509	ILE	2.3
1	A	1837	ILE	2.3
3	K	1737	ILE	2.3
3	L	6	THR	2.3
1	F	977	TYR	2.3
2	G	1873	TYR	2.3
1	B	1764	VAL	2.3
1	E	198	PRO	2.3
3	H	1953	VAL	2.3
3	L	1065	VAL	2.3
2	J	1744	GLY	2.3
3	I	1848	GLY	2.3
3	L	1964	PHE	2.3
1	A	96	GLU	2.3
1	A	600	ASP	2.3
3	H	139	LYS	2.3
1	A	75	HIS	2.3
1	C	196	THR	2.3
2	G	2022	THR	2.3
3	H	5	SER	2.3
1	D	1781	VAL	2.3
3	I	1886	VAL	2.3
1	A	1767	GLY	2.3
1	D	1768	GLY	2.3
1	A	975	ALA	2.2
1	E	976	ALA	2.2
3	L	1965	ALA	2.2
3	H	1927	LEU	2.2
3	L	1927	LEU	2.2
1	D	160	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	1763	LYS	2.2
3	H	79	GLN	2.2
3	I	1929	LYS	2.2
3	K	1750	LYS	2.2
3	K	1929	LYS	2.2
1	B	622	ILE	2.2
3	K	1972	ILE	2.2
1	F	196	THR	2.2
1	D	1769	VAL	2.2
3	L	8	PRO	2.2
1	C	878	MET	2.2
1	D	545	GLU	2.2
1	E	96	GLU	2.2
1	E	975	ALA	2.2
2	G	2047	LYS	2.2
1	F	622	ILE	2.2
2	G	1737	ILE	2.2
3	H	1925	ILE	2.2
3	L	79	GLN	2.2
1	B	600	ASP	2.2
2	J	1939	HIS	2.2
3	I	1316	ASP	2.2
1	A	1760	THR	2.2
1	B	300	VAL	2.2
1	E	1827	SER	2.2
3	K	2048	TYR	2.2
1	C	178	GLY	2.2
2	J	1848	GLY	2.2
1	F	880	ALA	2.2
3	L	82	GLN	2.2
3	K	740	HIS	2.2
1	C	967	VAL	2.2
2	J	1936	VAL	2.2
1	A	621	THR	2.2
3	K	1748	THR	2.2
1	C	1829	GLY	2.2
1	E	977	TYR	2.2
1	F	972	SER	2.2
3	H	1848	GLY	2.2
3	I	1545	TYR	2.2
3	L	1298	TYR	2.2
3	L	25	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	12	ILE	2.2
2	G	1881	ARG	2.2
3	I	1737	ILE	2.2
2	G	1936	VAL	2.2
1	E	196	THR	2.2
3	K	699	GLY	2.2
3	K	1971	GLY	2.2
2	J	1545	TYR	2.2
3	L	1885	LEU	2.2
1	F	976	ALA	2.2
2	G	1751	ILE	2.1
1	B	198	PRO	2.1
1	C	1886	LYS	2.1
3	H	1215	LYS	2.1
3	L	1753	LYS	2.1
3	K	1853	GLY	2.1
2	G	86	LEU	2.1
2	G	1738	PHE	2.1
3	H	1290	PHE	2.1
1	D	169	SER	2.1
2	G	31	SER	2.1
1	D	331	ILE	2.1
2	J	1737	ILE	2.1
1	C	601	VAL	2.1
1	B	974	ASP	2.1
1	C	1863	GLY	2.1
1	F	60	THR	2.1
2	G	24	THR	2.1
3	H	1748	THR	2.1
3	H	1971	GLY	2.1
3	K	787	THR	2.1
2	J	203	LEU	2.1
3	I	1964	PHE	2.1
1	A	1841	ARG	2.1
3	L	1873	TYR	2.1
3	K	1840	VAL	2.1
3	L	850	MET	2.1
2	G	1968	PRO	2.1
3	I	572	ASN	2.1
3	K	1885	LEU	2.1
3	L	1902	GLY	2.1
3	L	1969	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1858	ALA	2.1
1	A	1782	GLU	2.1
1	B	96	GLU	2.1
1	D	96	GLU	2.1
3	H	1961	GLU	2.1
1	B	179	LYS	2.1
1	F	1763	LYS	2.1
2	G	8	PRO	2.1
3	K	599	PRO	2.1
1	B	287	LEU	2.1
1	F	190	LEU	2.1
3	I	1960	LEU	2.1
3	K	86	LEU	2.1
3	L	1960	LEU	2.1
2	J	1964	PHE	2.1
3	I	1971	GLY	2.1
3	K	1744	GLY	2.1
1	D	542	THR	2.1
1	D	961	THR	2.1
2	J	1316	ASP	2.1
2	J	1924	ILE	2.1
2	J	1925	ILE	2.1
3	H	1922	ILE	2.1
3	L	1888	ILE	2.1
3	L	1545	TYR	2.1
2	G	1745	LYS	2.0
2	J	39	LYS	2.0
2	J	1949	LYS	2.0
3	L	1986	LYS	2.0
1	C	1764	VAL	2.0
1	D	198	PRO	2.0
1	B	221	LEU	2.0
1	F	877	LEU	2.0
2	J	414	LEU	2.0
3	K	1633	ASN	2.0
1	A	252	THR	2.0
1	B	332	THR	2.0
1	F	243	ILE	2.0
3	L	1924	ILE	2.0
1	D	1862	ALA	2.0
1	F	1832	ALA	2.0
1	D	1782	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	1846	GLU	2.0
2	J	1929	LYS	2.0
3	L	2048	TYR	2.0
1	C	539	SER	2.0
1	D	1840	VAL	2.0
2	G	1886	VAL	2.0
1	D	1834	LEU	2.0
3	K	203	LEU	2.0
3	K	414	LEU	2.0
3	L	1158	PHE	2.0
1	B	196	THR	2.0
1	C	880	ALA	2.0
1	F	1833	ALA	2.0
3	K	1133	THR	2.0
1	A	330	GLU	2.0
1	B	1782	GLU	2.0
3	I	1753	LYS	2.0
1	D	300	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	J8W	L	1808	12/13	0.89	0.13	97,105,108,110	0
3	J8W	K	1808	12/13	0.91	0.12	83,92,98,98	0
3	J8W	I	1808	12/13	0.91	0.13	79,93,103,106	0
3	J8W	H	1808	12/13	0.92	0.11	66,82,88,89	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ACT	H	2102	4/4	0.57	0.22	80,82,86,89	0
7	A2P	B	1918	27/27	0.64	0.19	87,126,138,145	0
8	ACT	B	1902	4/4	0.66	0.25	68,72,75,76	0
7	A2P	E	1917	27/27	0.70	0.18	83,114,130,138	0
7	A2P	C	1917	27/27	0.74	0.18	66,97,150,153	0
7	A2P	A	1918	27/27	0.74	0.19	87,121,166,169	0
8	ACT	H	2103	4/4	0.75	0.24	66,66,70,73	0
7	A2P	F	1912	27/27	0.76	0.18	86,121,152,158	0
7	A2P	D	1923	27/27	0.76	0.17	74,107,137,145	0
8	ACT	H	2104	4/4	0.76	0.19	81,84,84,85	0
8	ACT	C	1903	4/4	0.78	0.29	59,69,73,75	0
5	EDO	A	1911	4/4	0.79	0.33	83,84,90,91	0
5	EDO	E	1906	4/4	0.81	0.25	68,75,75,75	0
5	EDO	F	1909	4/4	0.82	0.18	54,54,56,56	0
5	EDO	H	2105	4/4	0.82	0.19	68,72,74,76	0
6	NA	D	1918	1/1	0.82	0.28	56,56,56,56	0
6	NA	F	1910	1/1	0.82	0.31	65,65,65,65	0
5	EDO	E	1908	4/4	0.82	0.16	76,79,81,82	0
5	EDO	D	1912	4/4	0.83	0.21	79,81,81,82	0
5	EDO	B	1903	4/4	0.83	0.24	70,76,77,79	0
5	EDO	E	1912	4/4	0.84	0.20	91,93,93,97	0
6	NA	C	1914	1/1	0.84	0.27	60,60,60,60	0
5	EDO	C	1908	4/4	0.84	0.19	60,69,73,74	0
6	NA	F	1911	1/1	0.85	0.07	62,62,62,62	0
5	EDO	J	2104	4/4	0.85	0.17	68,70,71,71	0
9	PGE	E	1918	10/10	0.85	0.20	88,99,106,107	0
6	NA	D	1916	1/1	0.86	0.17	55,55,55,55	0
5	EDO	D	1906	4/4	0.86	0.18	51,52,58,59	0
5	EDO	F	1904	4/4	0.86	0.21	68,73,77,78	0
5	EDO	E	1910	4/4	0.86	0.20	80,82,84,85	0
5	EDO	C	1906	4/4	0.87	0.22	67,68,72,74	0
5	EDO	B	1910	4/4	0.87	0.24	69,72,76,78	0
5	EDO	F	1902	4/4	0.87	0.15	75,80,85,89	0
5	EDO	C	1911	4/4	0.88	0.23	64,65,71,71	0
5	EDO	F	1905	4/4	0.88	0.14	65,67,67,67	0
5	EDO	A	1907	4/4	0.88	0.20	69,71,74,75	0
6	NA	D	1920	1/1	0.88	0.16	45,45,45,45	0
5	EDO	A	1909	4/4	0.88	0.21	64,64,71,71	0
5	EDO	B	1906	4/4	0.88	0.19	52,54,58,65	0
5	EDO	C	1907	4/4	0.89	0.19	75,78,80,81	0
6	NA	A	1912	1/1	0.89	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	A	1916	1/1	0.89	0.17	51,51,51,51	0
6	NA	G	2104	1/1	0.89	0.11	59,59,59,59	0
6	NA	B	1917	1/1	0.89	0.26	47,47,47,47	0
5	EDO	F	1906	4/4	0.89	0.18	71,74,76,77	0
5	EDO	C	1909	4/4	0.89	0.16	72,78,79,80	0
5	EDO	E	1911	4/4	0.89	0.14	69,69,72,72	0
6	NA	D	1917	1/1	0.90	0.18	46,46,46,46	0
5	EDO	C	1910	4/4	0.90	0.20	79,83,84,86	0
5	EDO	F	1908	4/4	0.90	0.19	83,88,92,93	0
6	NA	J	2108	1/1	0.90	0.10	60,60,60,60	0
5	EDO	A	1910	4/4	0.91	0.20	64,69,70,70	0
8	ACT	C	1902	4/4	0.91	0.17	59,62,63,65	0
5	EDO	J	2105	4/4	0.91	0.12	73,77,78,79	0
5	EDO	D	1913	4/4	0.91	0.12	61,61,63,66	0
6	NA	A	1913	1/1	0.91	0.16	42,42,42,42	0
6	NA	H	2107	1/1	0.91	0.07	49,49,49,49	0
5	EDO	E	1905	4/4	0.91	0.19	64,68,70,72	0
10	FMN	K	2101	31/31	0.91	0.12	64,75,80,88	0
6	NA	E	1914	1/1	0.92	0.09	62,62,62,62	0
6	NA	A	1915	1/1	0.92	0.08	51,51,51,51	0
5	EDO	B	1904	4/4	0.92	0.12	51,53,56,62	0
6	NA	B	1916	1/1	0.92	0.13	52,52,52,52	0
5	EDO	C	1905	4/4	0.92	0.16	54,57,61,62	0
5	EDO	E	1913	4/4	0.92	0.17	78,81,86,86	0
5	EDO	D	1902	4/4	0.92	0.13	58,59,59,60	0
5	EDO	D	1903	4/4	0.92	0.14	46,52,55,56	0
4	PNS	F	1901	21/22	0.92	0.15	89,92,102,103	0
10	FMN	I	2101	31/31	0.92	0.11	66,73,78,79	0
5	EDO	D	1911	4/4	0.92	0.16	60,61,61,62	0
11	MLI	J	2102	7/7	0.92	0.10	83,86,87,96	0
6	NA	J	2107	1/1	0.93	0.10	38,38,38,38	0
4	PNS	D	1901	21/22	0.93	0.14	90,93,101,103	0
5	EDO	D	1907	4/4	0.93	0.15	56,63,70,70	0
5	EDO	B	1905	4/4	0.93	0.14	65,66,67,67	0
5	EDO	F	1903	4/4	0.93	0.12	65,66,70,70	0
4	PNS	B	1901	21/22	0.93	0.15	91,95,106,107	0
5	EDO	A	1903	4/4	0.93	0.10	56,60,60,61	0
6	NA	C	1916	1/1	0.93	0.28	61,61,61,61	0
5	EDO	E	1904	4/4	0.93	0.14	67,70,72,74	0
5	EDO	B	1912	4/4	0.93	0.15	74,78,78,80	0
5	EDO	C	1912	4/4	0.93	0.18	50,52,53,54	0
5	EDO	A	1905	4/4	0.93	0.16	57,60,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	D	1922	1/1	0.93	0.25	46,46,46,46	0
5	EDO	J	2103	4/4	0.93	0.14	69,71,71,71	0
5	EDO	E	1909	4/4	0.93	0.10	69,70,71,72	0
5	EDO	A	1906	4/4	0.93	0.13	53,58,58,59	0
5	EDO	J	2106	4/4	0.93	0.10	72,72,73,73	0
10	FMN	L	2101	31/31	0.93	0.10	54,62,68,81	0
11	MLI	G	2102	7/7	0.93	0.09	78,86,91,92	0
5	EDO	D	1904	4/4	0.93	0.14	58,63,66,68	0
4	PNS	C	1901	21/22	0.94	0.13	75,78,88,89	0
6	NA	D	1919	1/1	0.94	0.24	46,46,46,46	0
4	PNS	A	1901	21/22	0.94	0.13	86,90,101,101	0
6	NA	B	1914	1/1	0.94	0.10	43,43,43,43	0
6	NA	B	1915	1/1	0.94	0.08	49,49,49,49	0
5	EDO	C	1904	4/4	0.94	0.15	74,76,78,79	0
4	PNS	E	1901	21/22	0.94	0.14	86,88,91,92	0
6	NA	G	2103	1/1	0.94	0.07	37,37,37,37	0
5	EDO	D	1909	4/4	0.94	0.14	60,61,62,63	0
6	NA	H	2106	1/1	0.94	0.08	34,34,34,34	0
6	NA	C	1915	1/1	0.94	0.28	62,62,62,62	0
5	EDO	D	1910	4/4	0.94	0.14	59,63,64,64	0
6	NA	D	1915	1/1	0.94	0.07	49,49,49,49	0
6	NA	K	2103	1/1	0.94	0.06	69,69,69,69	0
5	EDO	B	1907	4/4	0.94	0.14	57,58,58,59	0
5	EDO	B	1908	4/4	0.94	0.11	58,62,62,62	0
6	NA	A	1917	1/1	0.95	0.22	53,53,53,53	0
5	EDO	A	1908	4/4	0.95	0.09	59,60,60,60	0
5	EDO	E	1907	4/4	0.95	0.13	69,72,73,74	0
5	EDO	A	1902	4/4	0.95	0.14	47,51,54,54	0
6	NA	K	2102	1/1	0.95	0.15	53,53,53,53	0
6	NA	D	1921	1/1	0.95	0.10	52,52,52,52	0
5	EDO	D	1914	4/4	0.95	0.11	49,52,54,56	0
10	FMN	G	2101	31/31	0.95	0.09	46,49,53,56	0
5	EDO	E	1902	4/4	0.95	0.15	51,51,51,52	0
5	EDO	E	1903	4/4	0.95	0.09	50,54,55,56	0
6	NA	A	1914	1/1	0.95	0.15	55,55,55,55	0
5	EDO	D	1905	4/4	0.95	0.14	45,46,47,49	0
5	EDO	B	1909	4/4	0.95	0.11	50,53,54,55	0
10	FMN	H	2101	31/31	0.96	0.08	43,50,54,61	0
6	NA	L	2102	1/1	0.96	0.07	46,46,46,46	0
10	FMN	J	2101	31/31	0.96	0.08	43,46,50,55	0
5	EDO	B	1911	4/4	0.96	0.13	55,57,58,59	0
5	EDO	D	1908	4/4	0.96	0.13	54,56,58,58	0

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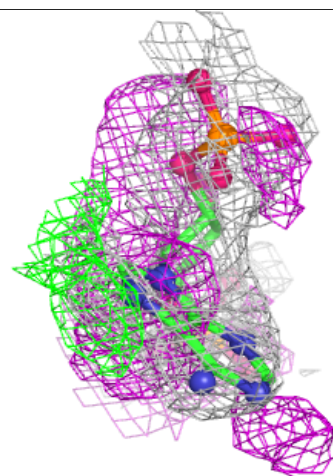
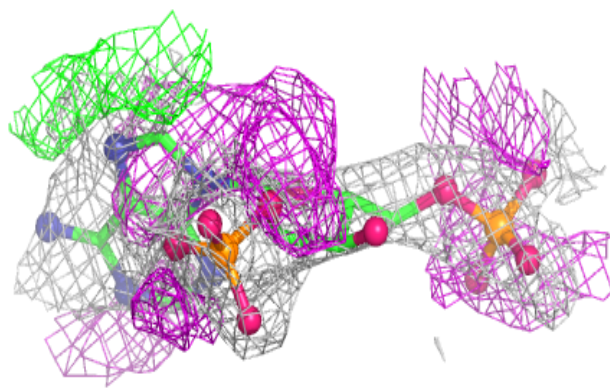
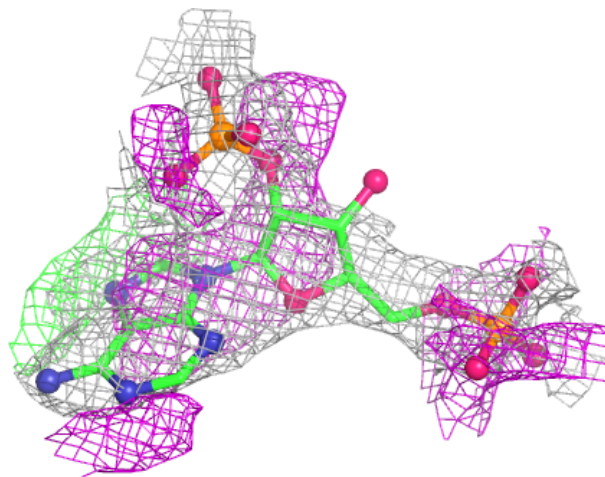
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	E	1916	1/1	0.96	0.13	51,51,51,51	0
6	NA	I	2102	1/1	0.96	0.09	84,84,84,84	0
6	NA	C	1913	1/1	0.97	0.09	56,56,56,56	0
6	NA	E	1915	1/1	0.97	0.06	50,50,50,50	0
5	EDO	F	1907	4/4	0.97	0.11	54,58,61,63	0
6	NA	L	2103	1/1	0.97	0.04	66,66,66,66	0
5	EDO	A	1904	4/4	0.97	0.11	59,63,65,65	0
6	NA	B	1913	1/1	0.98	0.05	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

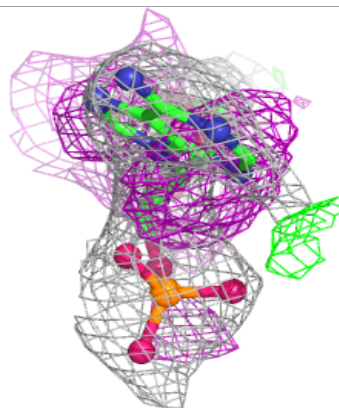
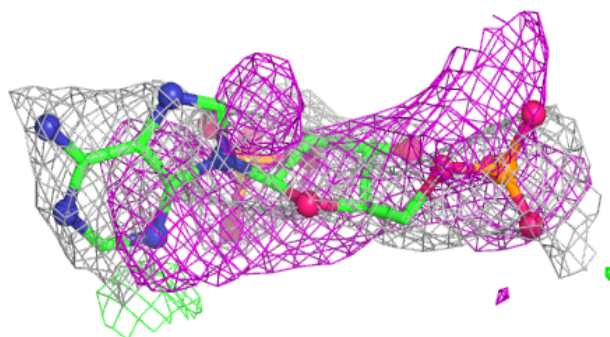
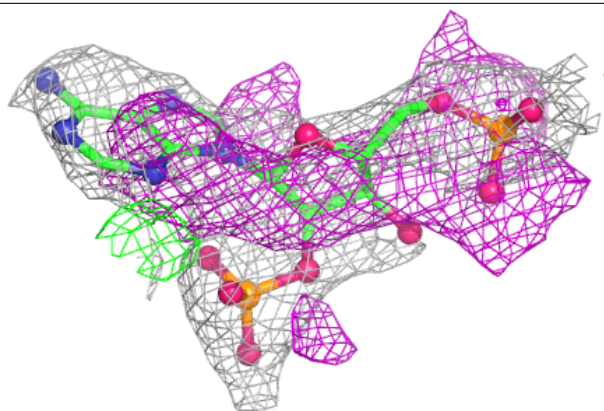
Electron density around A2P B 1918:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

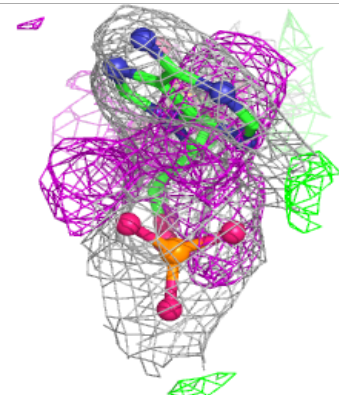
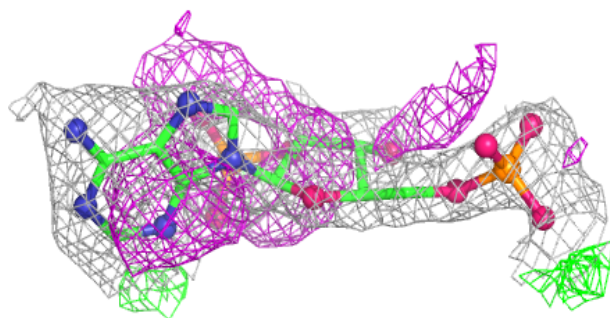
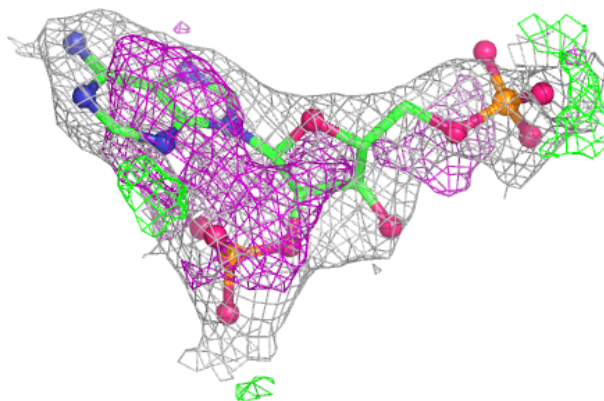


Electron density around A2P E 1917:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

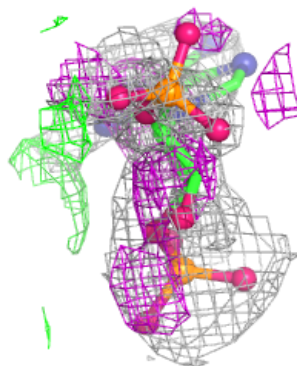
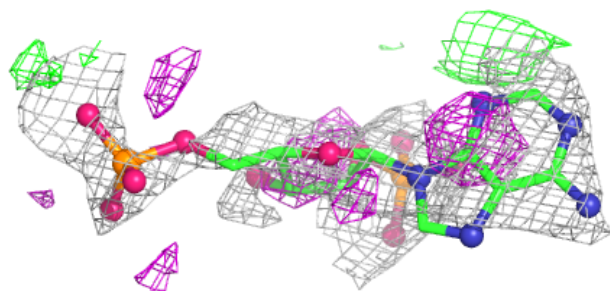
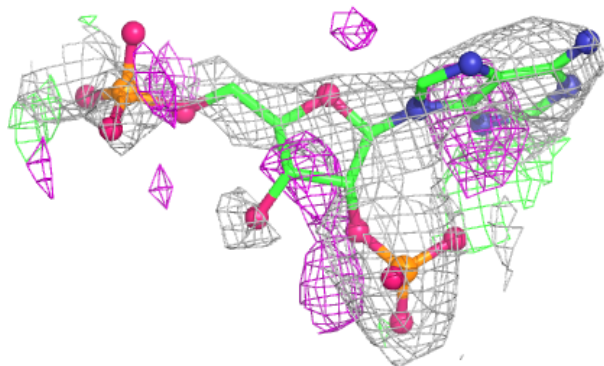
**Electron density around A2P C 1917:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

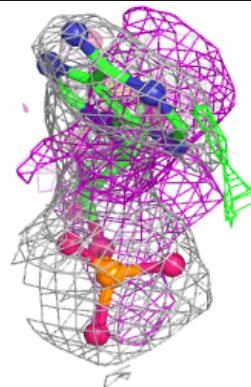
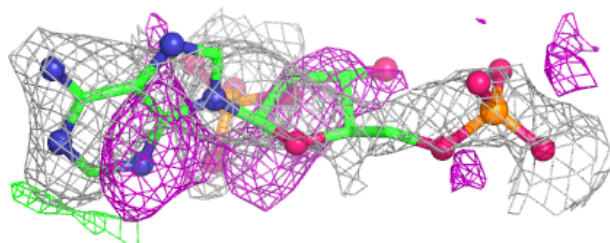
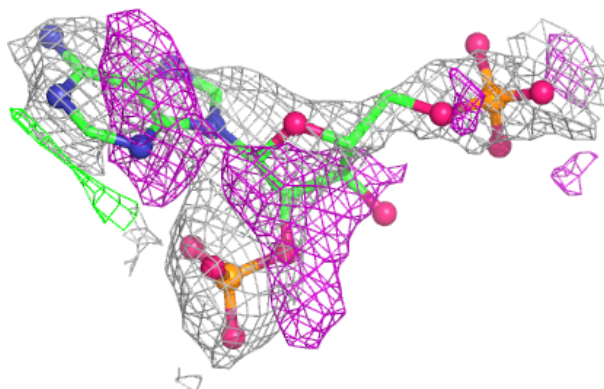


Electron density around A2P A 1918:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

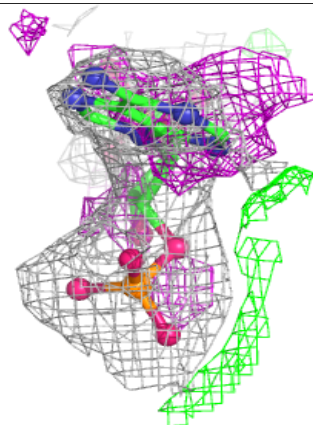
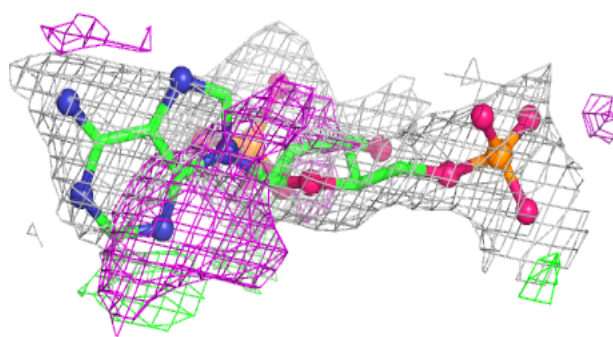
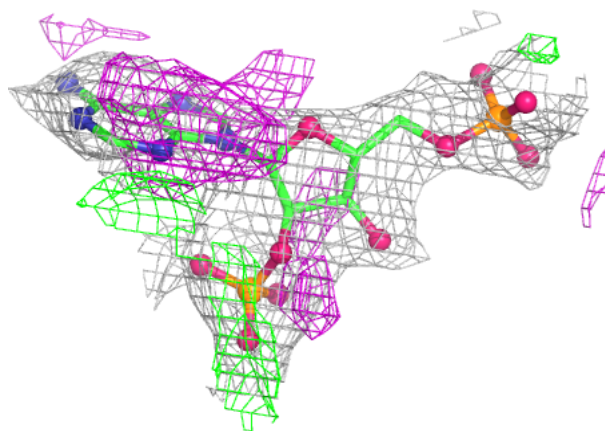
**Electron density around A2P F 1912:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



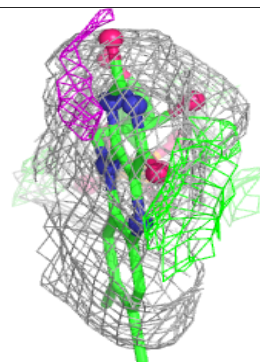
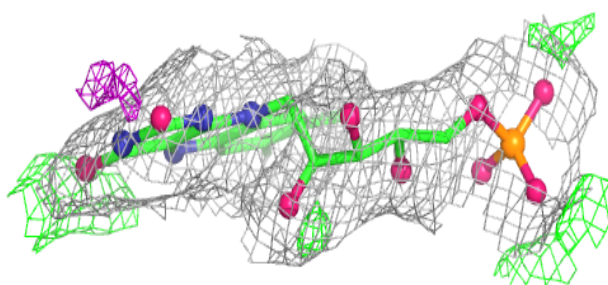
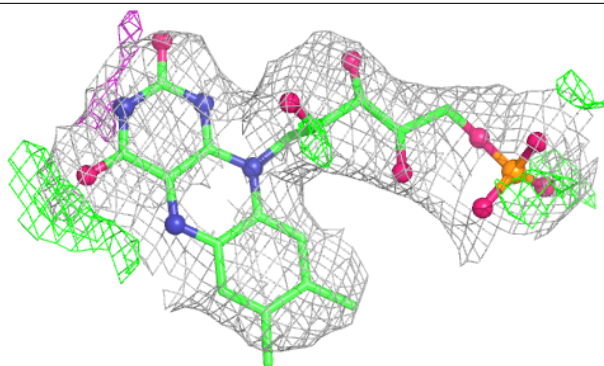
Electron density around A2P D 1923:

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and green (positive)

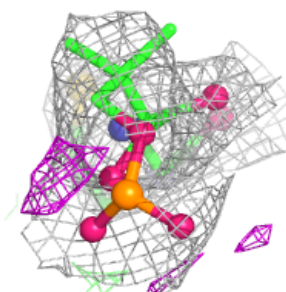
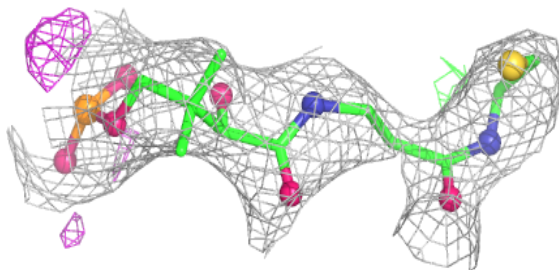
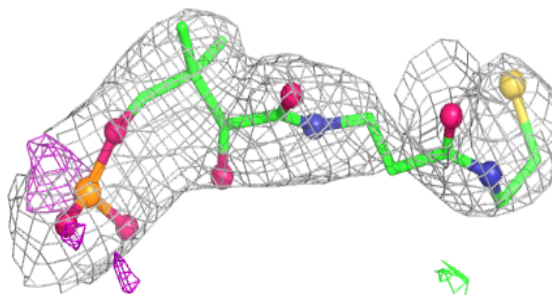


Electron density around FMN K 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

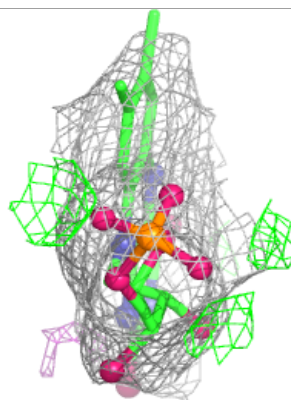
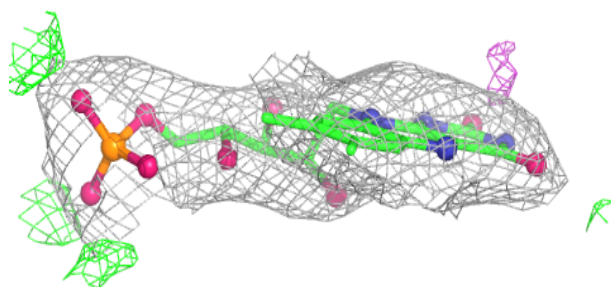
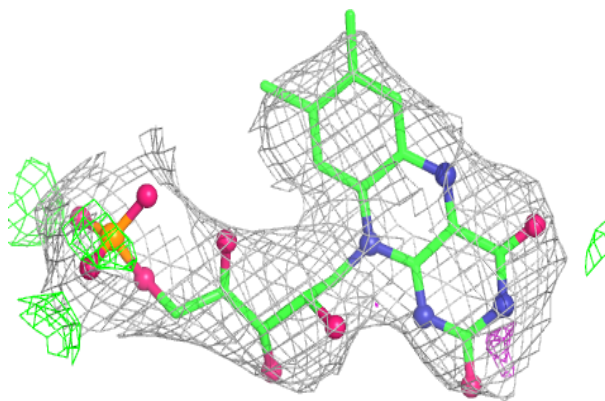
**Electron density around PNS F 1901:**

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

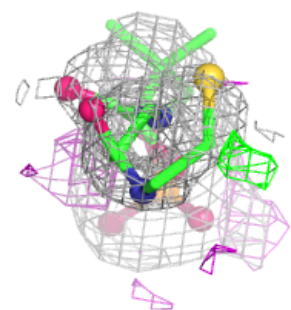
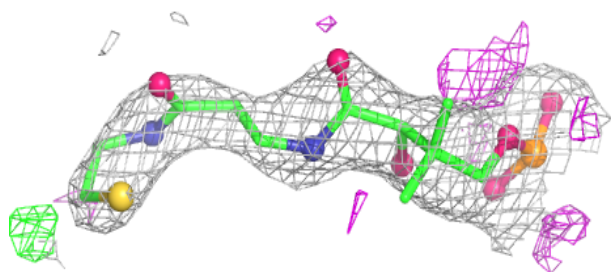
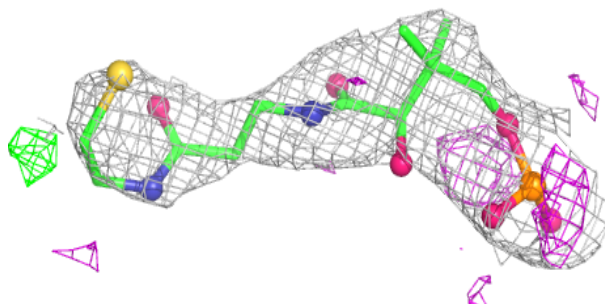


Electron density around FMN I 2101:

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and green (positive)

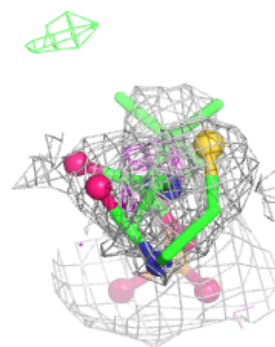
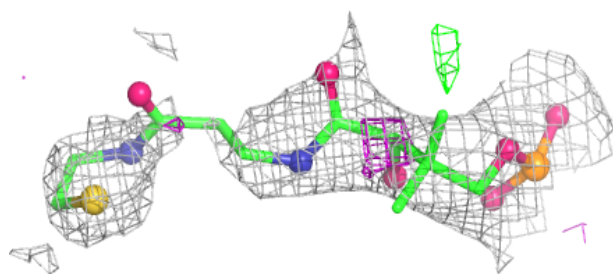
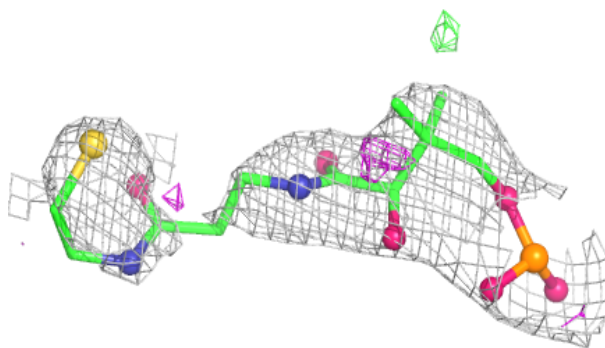
**Electron density around PNS D 1901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

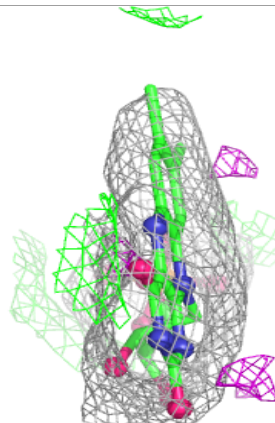
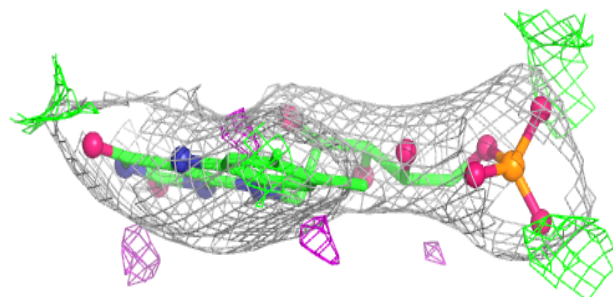
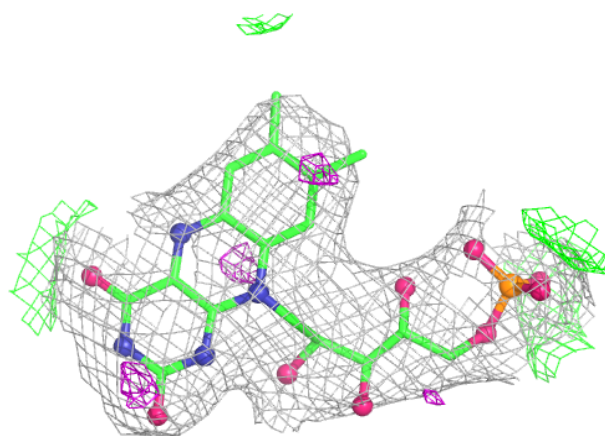


Electron density around PNS B 1901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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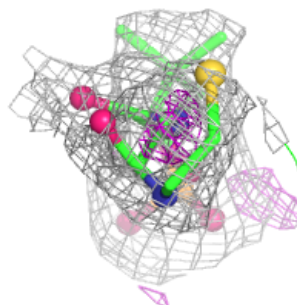
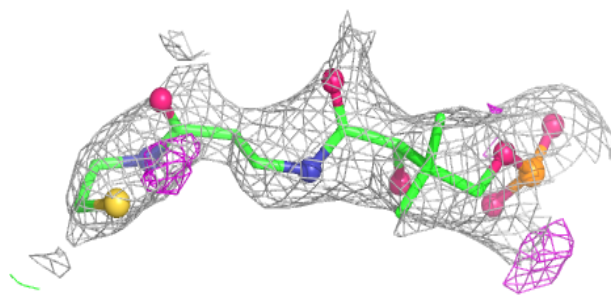
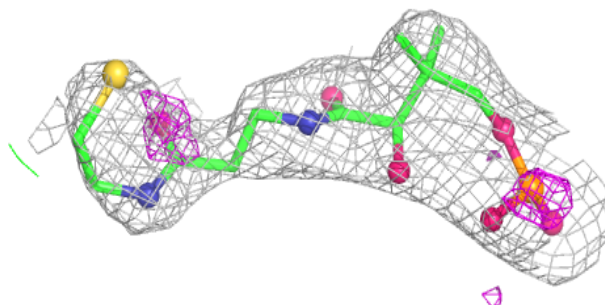
**Electron density around FMN L 2101:**

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and green (positive)

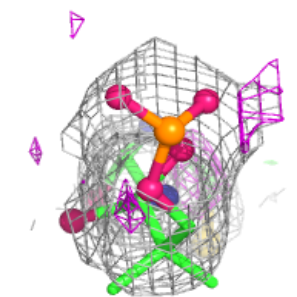
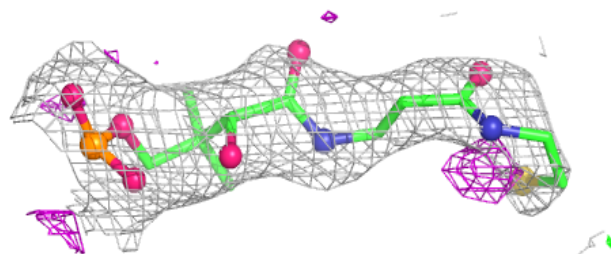
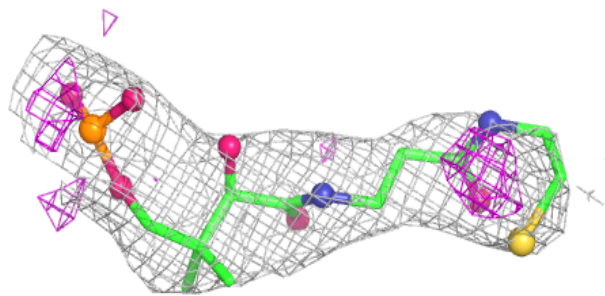


Electron density around PNS C 1901:

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and green (positive)

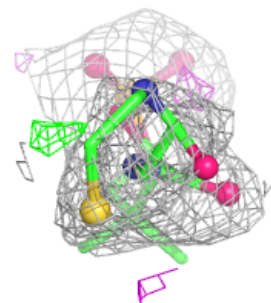
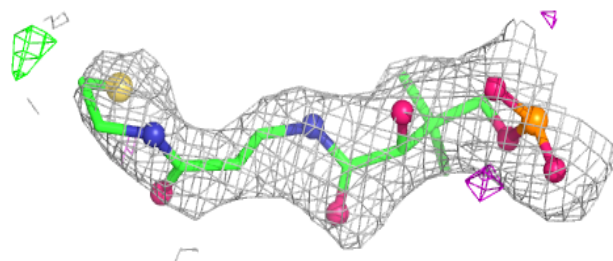
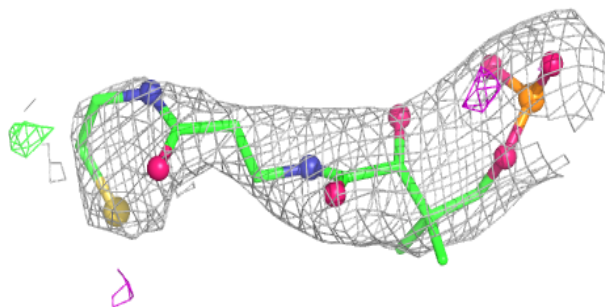
**Electron density around PNS A 1901:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

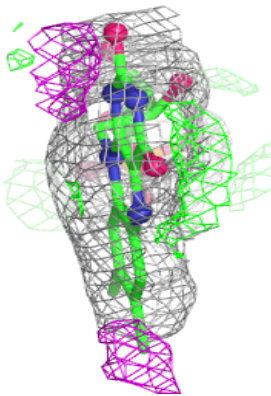
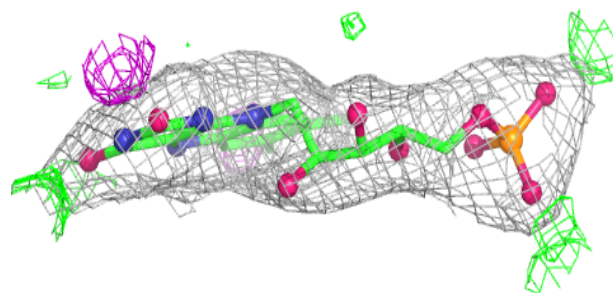
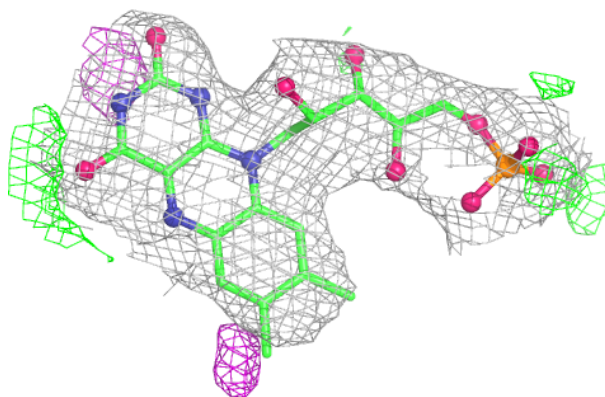


Electron density around PNS E 1901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

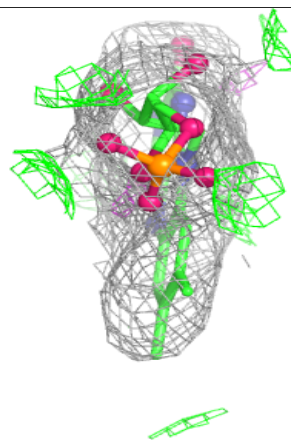
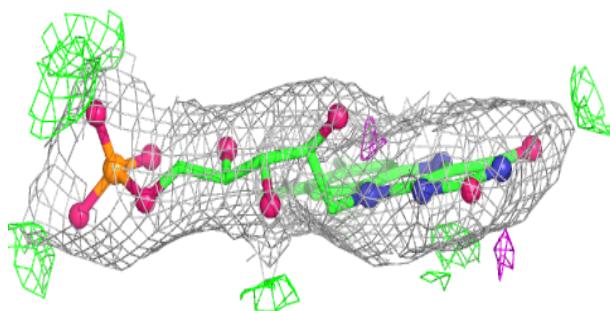
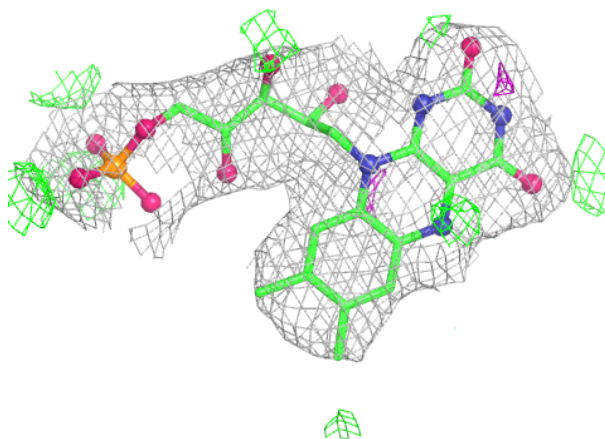
**Electron density around FMN G 2101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

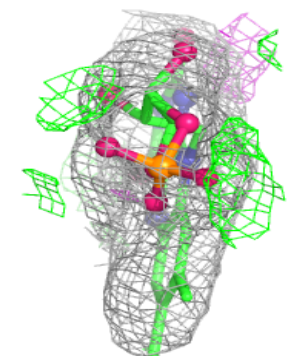
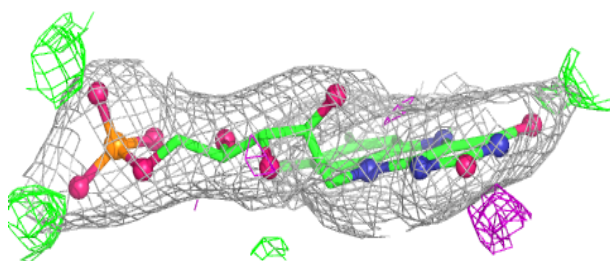
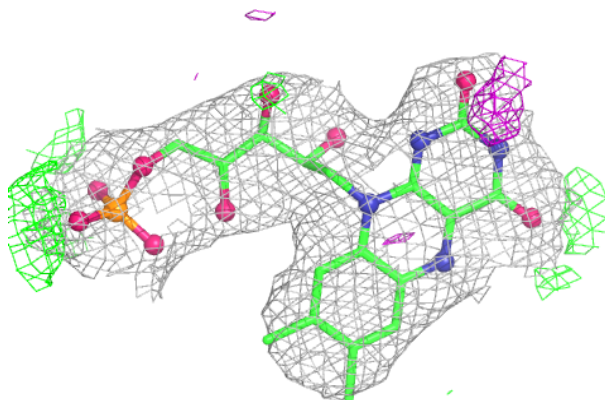


Electron density around FMN H 2101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMN J 2101:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.