



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 11:32 AM UTC

PDB ID : 7NFE / pdb_00007nfe
EMDB ID : EMD-12301
Title : Cryo-EM structure of NHEJ super-complex (monomer)
Authors : Chaplin, A.K.; Hardwick, S.W.; Kefala Stavridi, A.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2021-02-06
Resolution : 4.29 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

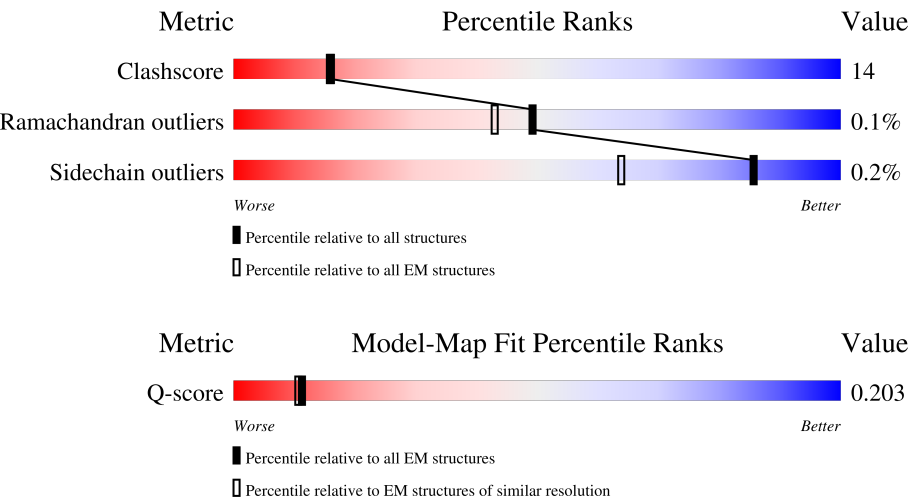
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.29 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4494 (3.79 - 4.79)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4156	59%27%14%
2	B	609	50%28%22%
3	C	732	45%25%30%
4	F	299	18% 45%19%36%

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Mol	Chain	Length	Quality of chain
4	G	299	8% 44% 22% 34%
5	H	336	10% 42% 18% 40%
5	I	336	17% 41% 16% 43%
6	J	911	17% 11% 72%
7	D	24	50% 50%
8	E	24	46% 54%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44554 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3585	Total	C	N	O	S	0	0
			27806	17851	4651	5132	172		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3673	2365	610	680	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	513	Total	C	N	O	S	0	0
			3999	2557	669	752	21		

- Molecule 4 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	190	Total	C	N	O	S	0	0
			1465	936	247	275	7		
4	G	197	Total	C	N	O	S	0	0
			1502	950	253	291	8		

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	201	Total	C	N	O	S	0	0
			1575	991	271	307	6		
5	I	193	Total	C	N	O	S	0	0
			1521	958	257	300	6		

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	258	Total	C	N	O	S	0	0
			2026	1284	345	386	11		

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*AP*TP*AP*AP*AP*CP*TP*AP*AP*AP*AP*AP*CP*TP*AP*TP*TP*AP*TP*TP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	24	Total	C	N	O	P	0	0
			493	238	92	139	24		

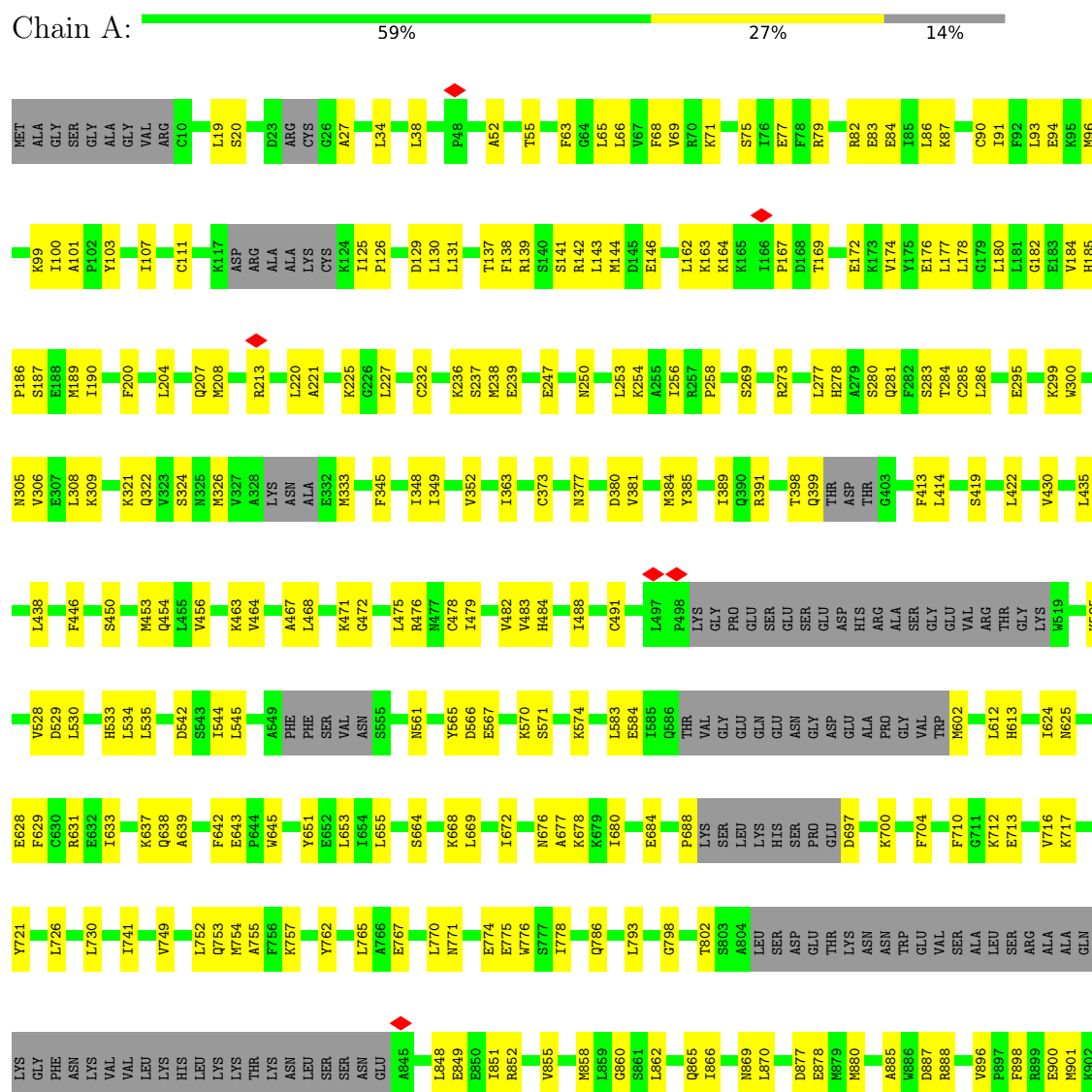
- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	24	Total	C	N	O	P	0	0
			494	240	81	149	24		

3 Residue-property plots [i](#)

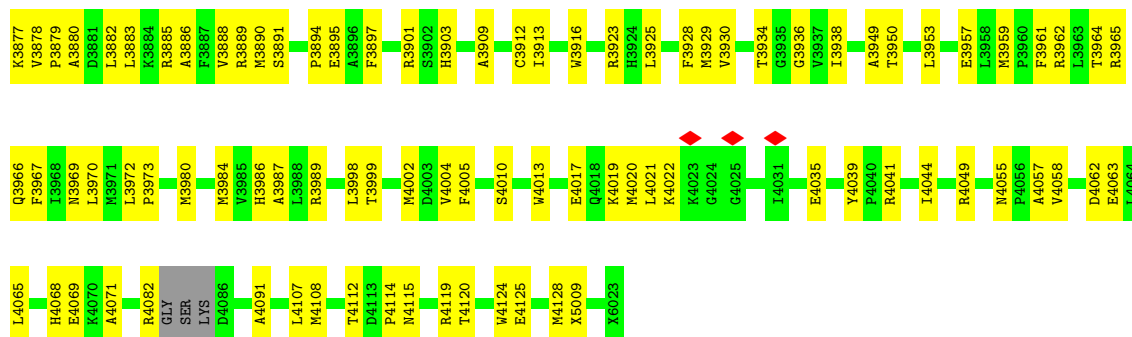
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit



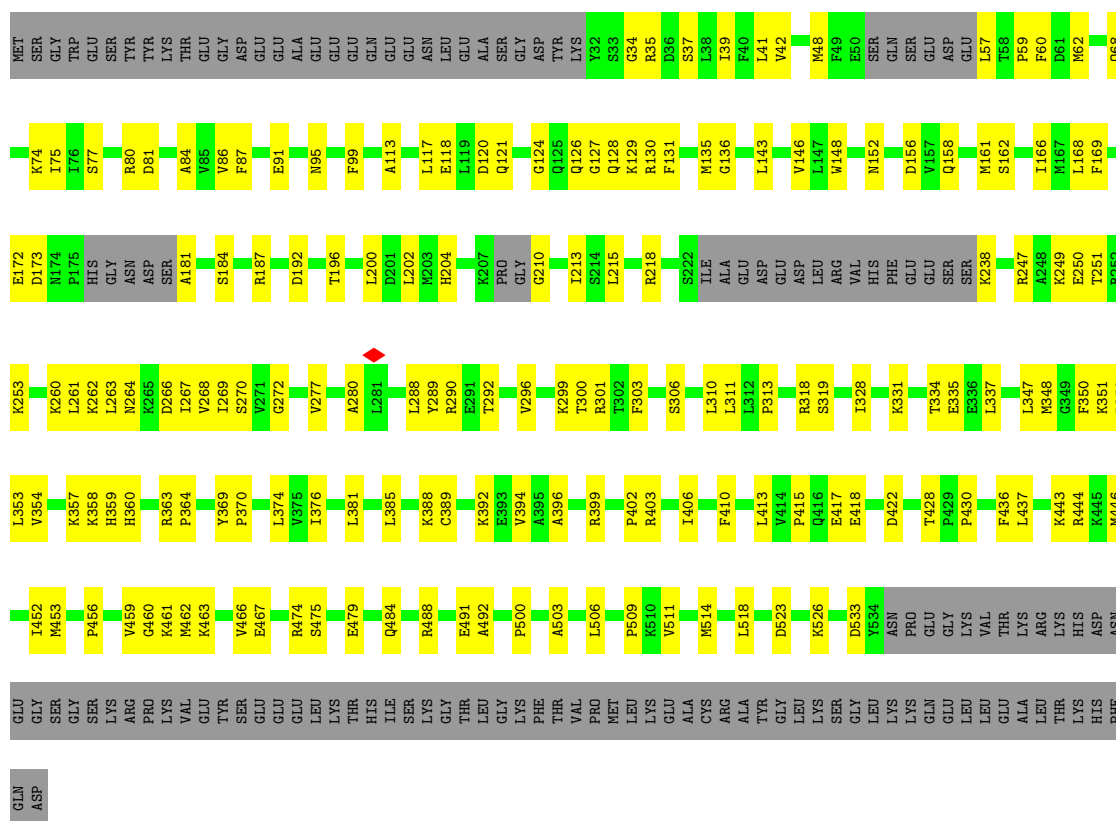
L2326	K2227	GLY	ASP	Y1802	Q1716	M1600	F1493	C1377	L1254	F1036	P903
L2327	V2230	PRO	PHE	D1809	V1719	L1601	GLY	E1378	C1255	W1039	L907
R2328	F2231	PRO	THR	P1810	GLY	D1602	ASP	P1379	L1257	Q1043	F910
V2330	V2331	GLY	GLY	R1811	M1724	Q1603	GLU	F1384	L1258	I1044	R913
MET	L2235	GLY	VAL	L1812	S1726	R1606	ARG	R1151	L1259	E1050	Y928
GLU	L2235	GLY	GLN	S1813	S1726	E1607	GLN	V1389	L1260	K1051	C931
ARG	C2244	ASP	SER	Q1817	T1733	R1608	CYS	Q1390	L1261	V1054	L934
LYS	W2245	GLY	VAL	S1818	P1734	Q1611	LEU	C1399	E1265	T1056	H935
ASN	L2251	VAL	THR	F1819	F1735	S1502	S1502	C1413	S1162	R1057	S936
ILE	P2252	VAL	THR	V1820	F1736	L1503	L1503	I1414	L1163	S1058	Y937
L2237	P2252	GLY	GLY	V1821	Y1739	Q1614	D1504	T1417	CH164	L1059	N941
E2338	R2254	VAL	VAL	R1822	Y1739	G1615	L1505	H1418	L1165	F1060	K1061
S2340	F2257	PRO	GLN	S1823	V1740	L1616	L1505	L1419	L1282	K1087	P957
L2341	F2257	ASP	MET	P1824	D1741	T1620	L1515	H1418	E1285	E1088	Y962
C2342	E2258	GLY	GLY	L1824	T1741	L1621	L1515	H1418	E1286	F1089	D977
L2349	K2259	ARG	ARG	T1825	C1742	I1622	F1519	H1418	A1286	E1092	Q978
D2356	F2260	THR	THR	L1826	K1744	L1623	R1527	H1418	Q1287	S1094	Y979
K2359	F2260	VAL	LYS	L1827	K1745	Q1624	L1528	H1418	I1301	L1095	T980
F2360	GLY	LYS	LYS	L1828	D1748	H1625	L1531	H1418	E1293	V1096	R981
N2365	ASN	LYS	LYS	W1829	H1748	H1626	L1531	H1418	A1287	E1097	Q982
K2366	ASN	LYS	LYS	S1832	L1750	K1627	L1531	H1418	E1287	Q1098	L983
V2367	LYS	GLY	GLY	D1834	E1751	S1637	L1537	H1418	E1287	F1099	Y984
T2368	D2269	GLY	GLY	V1844	Q1754	E1640	L1538	H1418	E1287	V1109	P986
F2371	N2270	GLY	GLY	L1845	E1760	T1641	S1539	H1418	E1287	F1101	L987
P2372	S2271	GLY	GLY	D1846	E1760	K1642	T1540	H1418	E1287	E1102	Y989
L2373	L2274	ALA	ALA	I1847	T1763	V1645	L1549	H1418	E1287	I1106	N998
L2374	L2277	ALA	ALA	T1848	E1764	S1687	L1551	H1418	E1287	L1111	L1009
P2377	V2280	ASN	ASN	D1849	V1765	S1687	H1552	H1418	E1287	H1115	L1013
F2378	M2281	GLY	ASP	K1852	C1767	S1660	H1552	H1418	E1287	C1127	L1014
M2379	M2281	GLY	ASP	T1862	R1768	F1661	H1552	H1418	E1287	Q1238	V1018
P2387	L2285	GLY	LEU	K1857	E1769	M1662	H1552	H1418	E1287	P1239	C1032
T2395	P2290	GLY	LEU	LEU	H1772	H1685	H1552	H1418	E1287	R1136	E1035
V2400	CYS	GLY	GLY	ASN	V1773	G1686	H1552	H1418	E1287	H1142	
L2411	ILE	GLY	GLY	E1860	E1776	S1667	H1552	H1418	E1287		
Y2412	GLN	GLY	GLY	S1861	E1776	S1667	H1552	H1418	E1287		
L2415	S2297	GLY	GLY	T1862	E1776	E1670	H1552	H1418	E1287		
K2417	E2298	GLY	GLY	Q1866	F1778	Y1675	H1552	H1418	E1287		
K2418	F2300	GLY	GLY	I1867	Q1779	Y1675	H1552	H1418	E1287		
F2420	N2306	GLN	GLY	M1871	S1780	T1694	H1552	H1418	E1287		
M2424	V2310	GLY	GLY	K1875	E1776	L1696	H1552	H1418	E1287		
R2425	V2310	GLY	GLY	I1876	F1778	L1696	H1552	H1418	E1287		
D2428	A2320	GLY	GLY	V1879	F1778	F1698	H1552	H1418	E1287		
D2429	E2321	GLY	GLY	S1879	S1790	F1699	H1552	H1418	E1287		
E2430	L2325	GLY	GLY	R1883	V1792	S1701	H1552	H1418	E1287		
		GLY	GLY	LEU	Q1794	E1709	H1552	H1418	E1287		
		GLY	GLY	LYS	V1795	R1712	H1552	H1418	E1287		
		GLY	GLY	LYS	V1795	V1713	H1552	H1418	E1287		
		GLY	GLY	D1887	L1797	V1713	H1552	H1418	E1287		
		GLY	GLY	D1888	V1797	V1713	H1552	H1418	E1287		
		GLY	GLY	V1889	V1797	V1713	H1552	H1418	E1287		





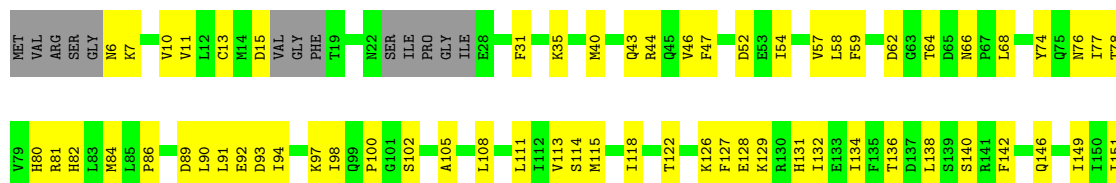
• Molecule 2: X-ray repair cross-complementing protein 6

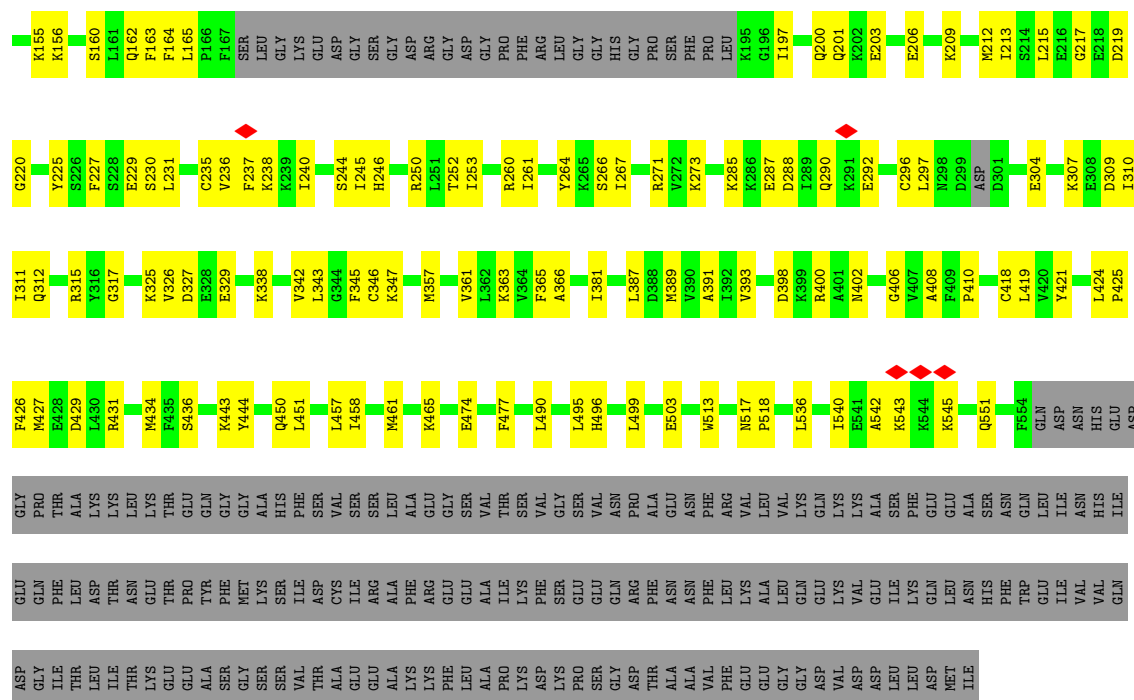
Chain B: 50% 28% 22%



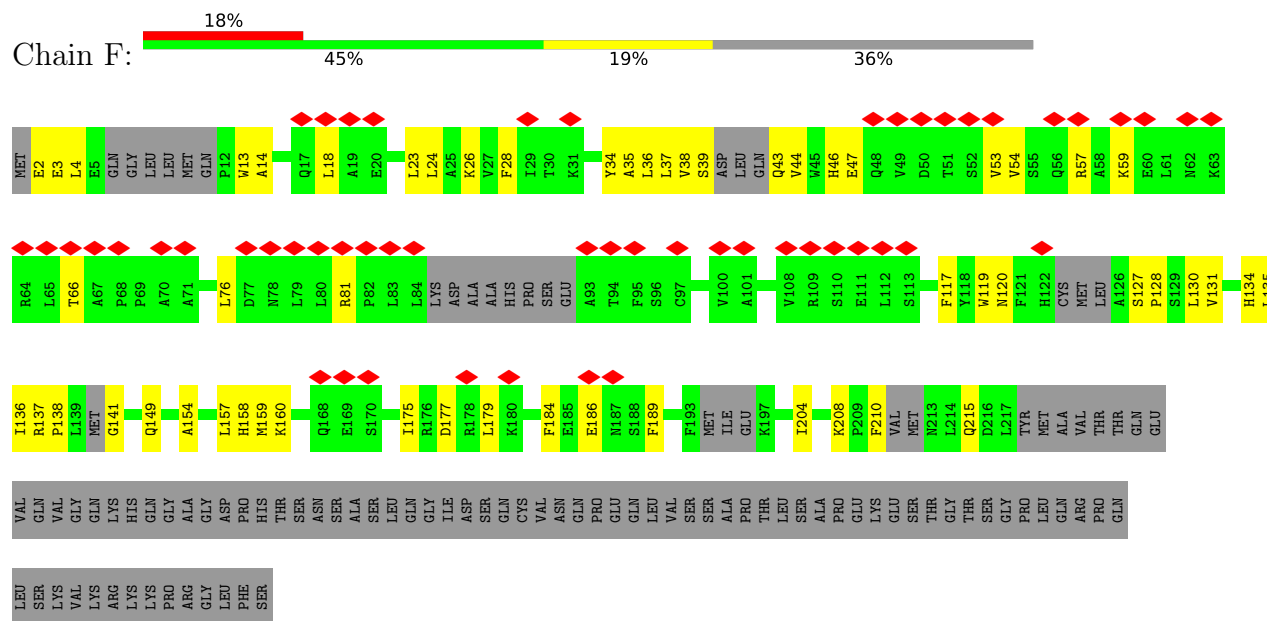
• Molecule 3: X-ray repair cross-complementing protein 5

Chain C: 45% 25% 30%

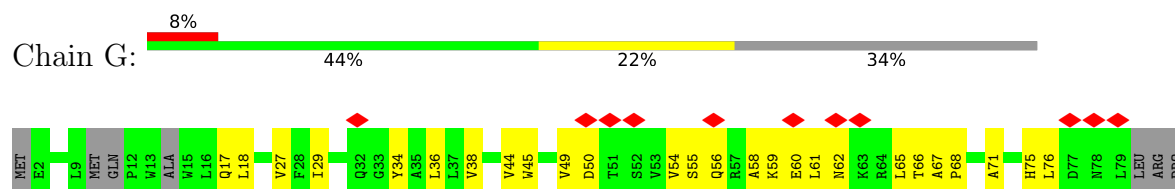


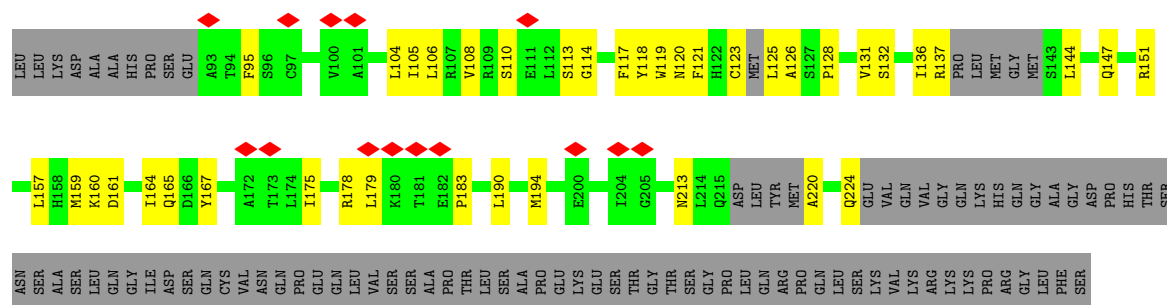


• Molecule 4: Non-homologous end-joining factor 1

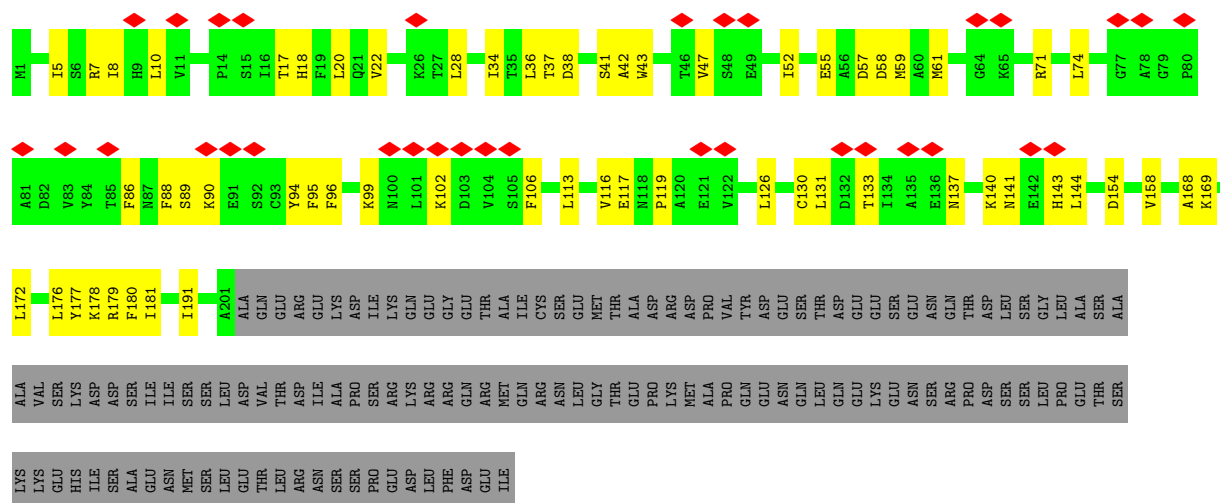
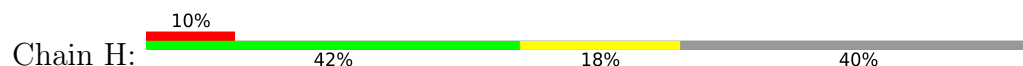


• Molecule 4: Non-homologous end-joining factor 1

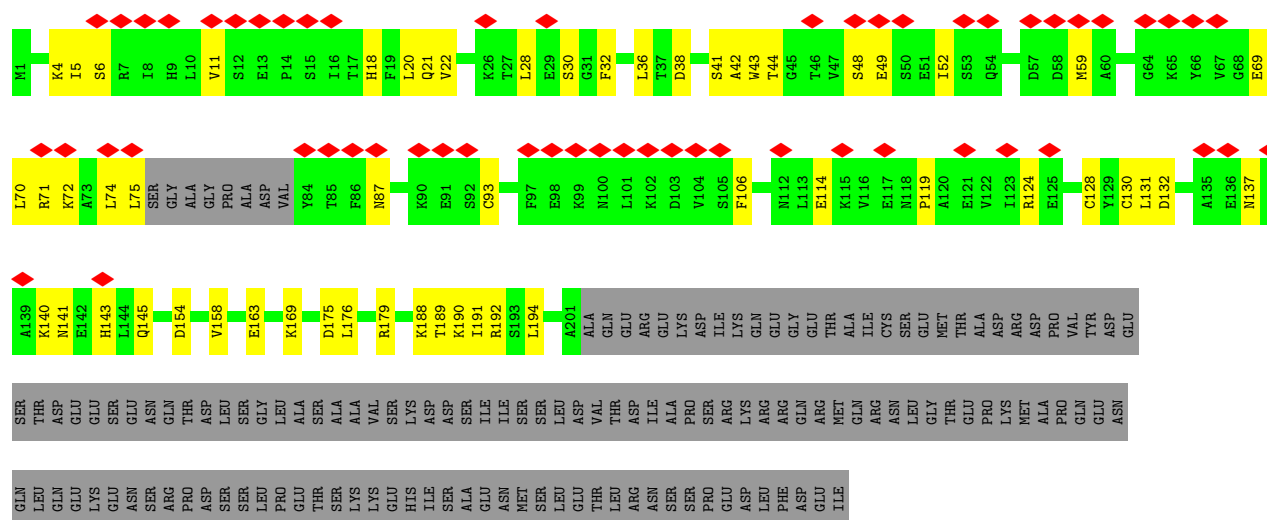




• Molecule 5: DNA repair protein XRCC4



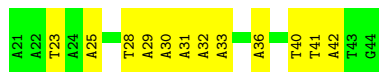
• Molecule 5: DNA repair protein XRCC4



• Molecule 6: DNA ligase 4



Chain D: 50% 50%



- Molecule 8: DNA (5'-D(P*TP*AP*AP*TP*AP*AP*TP*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*AP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45943	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.753	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/28219	0.34	4/38230 (0.0%)
2	B	0.10	0/3740	0.31	0/5053
3	C	0.15	0/4075	0.33	0/5509
4	F	0.14	0/1488	0.33	0/2015
4	G	0.15	0/1522	0.40	0/2064
5	H	0.11	0/1602	0.31	0/2159
5	I	0.12	0/1546	0.32	0/2082
6	J	0.10	0/2073	0.29	0/2807
7	D	0.27	0/554	0.47	0/852
8	E	0.21	0/552	0.47	0/851
All	All	0.14	0/45371	0.34	4/61622 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3859	TYR	N-CA-C	-7.03	103.70	111.36
1	A	3858	MET	N-CA-C	-5.80	105.30	112.90
1	A	3854	ALA	N-CA-C	-5.44	105.45	111.71
1	A	1955	VAL	CA-C-O	-5.22	118.09	122.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	27806	0	27233	743	0
2	B	3673	0	3652	131	0
3	C	3999	0	3899	141	0
4	F	1465	0	1432	48	0
4	G	1502	0	1439	62	0
5	H	1575	0	1514	62	0
5	I	1521	0	1440	47	0
6	J	2026	0	1895	75	0
7	D	493	0	273	11	0
8	E	494	0	278	14	0
All	All	44554	0	43055	1252	0

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 14.

All (1252) 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:A:3365:SER:HB3	1:A:3376:GLY:HA3	1.61	0.82
3:C:40:MET:HE3	3:C:235:CYS:HB3	1.62	0.80
1:A:3183:ILE:HG23	1:A:3238:MET:HE1	1.64	0.79
2:B:337:LEU:HD11	3:C:490:LEU:HA	1.67	0.77
4:G:128:PRO:O	4:G:132:SER:HB2	1.85	0.77
6:J:814:ARG:HD2	6:J:849:GLY:H	1.50	0.77
4:G:132:SER:HB3	4:G:137:ARG:HH21	1.51	0.76
5:I:5:ILE:HA	5:I:21:GLN:HA	1.68	0.76
1:A:901:MET:HG2	1:A:903:PRO:HD3	1.67	0.75
1:A:3728:VAL:HG22	1:A:3736:LYS:HG2	1.69	0.75
1:A:3727:THR:HB	1:A:3737:ARG:HB3	1.68	0.75
3:C:44:ARG:HD2	3:C:238:LYS:HB3	1.67	0.75
1:A:1184:ARG:NH1	1:A:1265:GLU:OE1	2.20	0.75
1:A:1257:LEU:HA	1:A:1260:LEU:HD12	1.67	0.74
1:A:2480:ILE:O	1:A:2484:TYR:HB2	1.86	0.74
2:B:269:ILE:HD11	2:B:381:LEU:HD23	1.69	0.74
1:A:3361:GLU:HB3	1:A:3366:SER:HA	1.69	0.73
1:A:1724:MET:HG2	1:A:1768:ARG:HD3	1.68	0.73
3:C:77:ILE:HG21	3:C:113:VAL:HG21	1.70	0.73
4:G:44:VAL:HA	4:G:125:LEU:HD23	1.72	0.72
1:A:1098:GLN:HG3	1:A:1151:ARG:HB3	1.71	0.72
1:A:793:LEU:HB3	1:A:870:LEU:HA	1.72	0.71
4:G:106:LEU:HB3	4:G:121:PHE:HB2	1.72	0.71
8:E:30:DT:H2'	8:E:31:DT:H71	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2449:VAL:HG23	1:A:2452:ARG:HH12	1.55	0.71
5:H:18:HIS:HD2	5:H:36:LEU:HD21	1.54	0.70
5:I:32:PHE:HE1	5:I:74:LEU:HB3	1.56	0.70
3:C:58:LEU:HB2	3:C:78:THR:HB	1.74	0.69
4:G:55:SER:OG	4:G:59:LYS:NZ	2.25	0.69
4:G:147:GLN:HB3	4:G:151:ARG:NH1	2.07	0.69
1:A:2133:LEU:HD11	1:A:2171:LEU:HD22	1.74	0.69
1:A:2428:ASP:HB3	1:A:2431:ARG:HB2	1.74	0.69
1:A:2893:LEU:HD11	1:A:2922:ARG:HB3	1.75	0.69
4:G:126:ALA:HB3	4:G:131:VAL:HG21	1.75	0.69
3:C:10:VAL:HG22	3:C:131:HIS:HB2	1.74	0.69
1:A:1361:LYS:O	1:A:1365:ASN:N	2.23	0.68
4:F:136:ILE:HA	4:G:136:ILE:HG23	1.75	0.68
5:I:141:ASN:O	5:I:145:GLN:NE2	2.26	0.68
3:C:408:ALA:HB1	3:C:419:LEU:HD21	1.76	0.68
1:A:3416:LEU:HD23	1:A:3449:LYS:HZ2	1.58	0.68
1:A:306:VAL:HA	1:A:309:LYS:HE2	1.75	0.68
3:C:391:ALA:HB3	3:C:408:ALA:HB3	1.76	0.68
4:G:45:TRP:H	4:G:125:LEU:HB3	1.60	0.67
5:I:18:HIS:HB3	5:I:36:LEU:HD11	1.76	0.67
1:A:1624:GLN:O	1:A:1627:LYS:NZ	2.27	0.67
2:B:444:ARG:NH1	3:C:244:SER:OG	2.27	0.67
4:G:161:ASP:O	4:G:165:GLN:NE2	2.28	0.67
5:H:141:ASN:ND2	5:I:141:ASN:OD1	2.27	0.67
2:B:204:HIS:NE2	2:B:210:GLY:O	2.23	0.66
2:B:396:ALA:HB3	2:B:413:LEU:HB2	1.77	0.66
4:G:147:GLN:HB3	4:G:151:ARG:HH12	1.60	0.66
1:A:213:ARG:HD2	2:B:335:GLU:HG2	1.77	0.66
3:C:151:ILE:HD11	3:C:215:LEU:HB2	1.76	0.66
1:A:4041:ARG:HA	1:A:4044:ILE:HG22	1.76	0.66
1:A:1285:GLU:HG3	1:A:1287:GLN:HG2	1.78	0.66
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	1.77	0.66
3:C:44:ARG:NH2	3:C:236:VAL:O	2.22	0.66
5:H:37:THR:HA	5:H:42:ALA:HA	1.78	0.66
1:A:352:VAL:HG11	1:A:1735:ARG:HG2	1.77	0.66
1:A:1379:PRO:HB2	1:A:1384:PHE:HB3	1.78	0.66
5:H:7:ARG:HE	5:I:131:LEU:HB2	1.60	0.66
1:A:1831:CYS:SG	1:A:1832:SER:N	2.70	0.65
1:A:3894:PRO:O	1:A:3895:GLU:HG3	1.96	0.65
1:A:2447:LYS:HG2	1:A:2449:VAL:HG12	1.77	0.65
3:C:44:ARG:HD3	3:C:238:LYS:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:18:LEU:HD11	4:F:23:LEU:HD12	1.78	0.65
2:B:523:ASP:HA	2:B:526:LYS:HE2	1.79	0.65
1:A:2281:MET:HE2	1:A:2326:ILE:HG12	1.77	0.65
4:F:76:LEU:O	4:F:81:ARG:NH2	2.31	0.64
1:A:3492:CYS:HB3	1:A:3711:PRO:HD3	1.77	0.64
1:A:1453:SER:O	1:A:1457:GLN:NE2	2.30	0.64
2:B:261:LEU:HB3	2:B:269:ILE:HB	1.78	0.64
5:H:43:TRP:HB3	5:H:113:LEU:HB3	1.79	0.64
1:A:566:ASP:OD1	1:A:645:TRP:NE1	2.28	0.64
1:A:3302:LYS:HE2	1:A:3363:SER:HB2	1.80	0.64
4:F:149:GLN:NE2	4:G:194:MET:SD	2.67	0.64
1:A:2894:GLU:HG3	1:A:3973:PRO:HG3	1.80	0.64
3:C:66:ASN:ND2	3:C:74:TYR:O	2.30	0.63
5:H:17:THR:O	5:H:18:HIS:ND1	2.30	0.63
1:A:1180:GLN:HB2	1:A:1183:CYS:HB2	1.80	0.63
1:A:2962:ARG:HA	1:A:3989:ARG:HH12	1.62	0.63
6:J:792:MET:HA	6:J:796:ILE:HB	1.79	0.63
1:A:1437:TYR:HD1	1:A:1503:LEU:HD21	1.63	0.63
1:A:1889:VAL:O	1:A:1909:ASN:N	2.31	0.63
2:B:296:VAL:HG12	3:C:297:LEU:HD23	1.81	0.63
8:E:31:DT:H2"	8:E:32:DT:C4	2.34	0.63
2:B:218:ARG:HB3	4:G:178:ARG:HH12	1.63	0.63
1:A:3766:GLN:OE1	1:A:3769:GLN:NE2	2.32	0.63
3:C:327:ASP:OD1	6:J:711:ASN:ND2	2.31	0.63
1:A:1366:THR:O	1:A:1369:MET:HB3	1.98	0.63
3:C:15:ASP:HB3	3:C:136:THR:HA	1.81	0.62
1:A:1568:ASN:HA	1:A:1600:MET:HE1	1.81	0.62
1:A:1766:LEU:O	1:A:1822:ARG:NH1	2.33	0.62
1:A:2165:LEU:HG	1:A:2169:LEU:HD23	1.80	0.62
1:A:3625:LEU:O	1:A:3630:ARG:NH1	2.32	0.62
3:C:165:LEU:O	3:C:227:PHE:N	2.33	0.62
4:F:128:PRO:HG3	4:G:44:VAL:H	1.62	0.62
1:A:529:ASP:O	1:A:533:HIS:ND1	2.29	0.62
1:A:3806:LEU:HD13	1:A:3929:MET:HE3	1.82	0.62
1:A:1789:GLY:O	1:A:1794:GLN:NE2	2.33	0.62
5:H:42:ALA:HB2	5:H:119:PRO:HB3	1.82	0.62
5:I:36:LEU:HB3	5:I:43:TRP:HB2	1.80	0.62
1:A:1769:GLU:O	1:A:1822:ARG:NH1	2.26	0.61
3:C:212:MET:HB3	3:C:220:GLY:HA3	1.81	0.61
5:I:4:LYS:O	5:I:22:VAL:N	2.31	0.61
1:A:2197:THR:HG22	1:A:5009:UNK:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3480:LEU:HD21	1:A:3510:GLN:HB3	1.82	0.61
4:F:2:GLU:HG3	4:F:46:HIS:HB2	1.82	0.61
1:A:3445:LEU:O	1:A:3449:LYS:HG2	2.00	0.61
1:A:3909:ALA:HB1	1:A:3984:MET:HE3	1.82	0.61
1:A:896:VAL:HB	1:A:903:PRO:HG2	1.82	0.61
5:I:11:VAL:HG22	5:I:87:ASN:HB3	1.83	0.61
5:I:179:ARG:NH2	6:J:781:ILE:O	2.32	0.61
6:J:719:ASP:HB3	6:J:743:MET:HE1	1.80	0.61
1:A:65:LEU:O	1:A:69:VAL:N	2.23	0.61
2:B:260:LYS:HZ3	2:B:270:SER:HB3	1.65	0.61
4:F:128:PRO:HB3	4:G:44:VAL:HG23	1.82	0.61
1:A:978:GLN:HE21	1:A:979:VAL:HG13	1.64	0.61
1:A:2574:ASN:O	1:A:2787:HIS:ND1	2.33	0.61
1:A:1389:VAL:HG22	1:A:1390:GLN:H	1.64	0.61
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.82	0.61
4:F:158:HIS:NE2	4:F:184:PHE:O	2.32	0.61
1:A:258:PRO:HG2	3:C:551:GLN:HG2	1.82	0.61
1:A:1475:LEU:HD13	1:A:1527:ARG:HG3	1.83	0.61
3:C:346:CYS:SG	3:C:347:LYS:N	2.74	0.61
1:A:1102:GLU:HG2	1:A:1154:PRO:HA	1.83	0.60
4:G:62:ASN:HB2	4:G:65:LEU:HB2	1.82	0.60
1:A:2563:LEU:HD12	1:A:2795:GLN:HB2	1.83	0.60
1:A:1662:ASN:ND2	1:A:1701:SER:O	2.34	0.60
1:A:2529:THR:OG1	1:A:2530:ARG:NH1	2.35	0.60
1:A:3593:ARG:NH1	1:A:3664:ASN:OD1	2.34	0.60
1:A:3657:SER:OG	1:A:3660:ASN:ND2	2.34	0.60
2:B:303:PHE:HA	2:B:311:LEU:H	1.66	0.60
1:A:1741:ASP:O	1:A:1745:LYS:HG2	2.02	0.60
4:G:18:LEU:HA	4:G:95:PHE:HB2	1.82	0.60
1:A:65:LEU:HA	1:A:68:PHE:HB2	1.84	0.60
1:A:672:ILE:O	1:A:676:ASN:ND2	2.34	0.60
1:A:1432:CYS:HB2	1:A:1486:LEU:HD21	1.84	0.60
1:A:1809:ASP:HB3	1:A:1811:ARG:HH12	1.65	0.60
1:A:2538:ARG:HG2	1:A:2565:MET:SD	2.41	0.60
6:J:670:THR:H	6:J:703:GLY:HA3	1.66	0.60
1:A:3796:MET:H	1:A:3801:GLY:HA2	1.67	0.60
1:A:247:GLU:HG2	1:A:285:CYS:HB3	1.83	0.59
1:A:3140:GLU:OE2	1:A:3167:ARG:NH1	2.35	0.59
1:A:3480:LEU:HD23	1:A:3513:ALA:HB2	1.82	0.59
1:A:3789:ARG:HG2	1:A:3938:ILE:HG12	1.84	0.59
2:B:351:LYS:NZ	3:C:477:PHE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:HA	1:A:422:LEU:HD12	1.85	0.59
1:A:2373:PRO:O	1:A:2377:ARG:NH1	2.35	0.59
3:C:240:ILE:HD12	3:C:273:LYS:HZ3	1.66	0.59
1:A:1175:HIS:HB3	1:A:1178:ARG:HE	1.67	0.59
1:A:1724:MET:HA	1:A:1768:ARG:HH11	1.66	0.59
1:A:3134:ALA:HB2	1:A:3182:ILE:HG22	1.83	0.59
2:B:289:TYR:HD2	2:B:292:THR:H	1.51	0.59
3:C:10:VAL:HB	3:C:54:ILE:HG22	1.84	0.59
5:I:140:LYS:HA	5:I:143:HIS:NE2	2.18	0.59
1:A:1899:VAL:HB	1:A:1911:LEU:HD13	1.85	0.59
2:B:263:LEU:HA	2:B:347:LEU:HB3	1.85	0.59
5:H:158:VAL:HG12	5:I:158:VAL:HG12	1.84	0.59
1:A:877:ASP:HA	1:A:880:MET:HG2	1.85	0.59
1:A:928:VAL:HG21	1:A:2769:VAL:HG22	1.84	0.59
1:A:678:LYS:NZ	1:A:775:GLU:OE1	2.35	0.59
1:A:3359:ILE:HA	1:A:3362:LEU:HB2	1.83	0.59
1:A:3755:GLY:N	1:A:3799:ARG:O	2.36	0.59
4:G:17:GLN:NE2	4:G:18:LEU:O	2.35	0.59
4:F:208:LYS:HE2	4:G:144:LEU:HD13	1.83	0.58
5:I:42:ALA:HB2	5:I:119:PRO:HA	1.84	0.58
1:A:1528:LEU:HD11	1:A:1571:LEU:HD21	1.85	0.58
2:B:350:PHE:HE2	3:C:458:ILE:HG12	1.66	0.58
3:C:81:ARG:HG3	3:C:90:LEU:HD11	1.85	0.58
1:A:472:GLY:O	1:A:476:ARG:NH1	2.35	0.58
1:A:1622:ILE:HA	1:A:1625:HIS:CE1	2.39	0.58
2:B:488:ARG:HH12	2:B:503:ALA:H	1.52	0.58
3:C:122:THR:HA	3:C:127:PHE:HE2	1.69	0.58
1:A:1751:GLU:O	1:A:1754:GLN:NE2	2.28	0.58
1:A:3857:LEU:HA	1:A:3860:LYS:HB2	1.85	0.58
2:B:369:TYR:OH	3:C:436:SER:O	2.20	0.58
3:C:496:HIS:NE2	3:C:503:GLU:HB3	2.18	0.58
4:G:61:LEU:HD13	4:G:120:ASN:HD21	1.68	0.58
1:A:111:CYS:HB2	1:A:130:LEU:HD22	1.86	0.58
4:F:137:ARG:O	4:F:141:GLY:N	2.37	0.58
5:I:175:ASP:OD1	5:I:176:LEU:N	2.37	0.58
1:A:1346:THR:HG21	1:A:1401:ASN:HB3	1.86	0.58
1:A:1696:LEU:O	1:A:1699:PHE:N	2.37	0.58
3:C:402:ASN:HD21	7:D:25:DA:H3'	1.67	0.58
1:A:1867:ILE:HG22	1:A:1871:MET:HE2	1.85	0.58
1:A:3041:LEU:HA	1:A:3044:MET:HE2	1.86	0.58
1:A:3240:MET:SD	1:A:3275:SER:OG	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:VAL:O	1:A:1825:LEU:N	2.32	0.57
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.86	0.57
1:A:3863:ASN:HB3	1:A:3866:GLU:HG2	1.86	0.57
4:F:175:ILE:HG22	4:F:177:ASP:H	1.69	0.57
1:A:1181:THR:HG22	1:A:1184:ARG:HH12	1.69	0.57
1:A:2443:MET:HE1	1:A:2476:ILE:HA	1.85	0.57
1:A:3744:ASP:O	1:A:3746:ARG:NH1	2.36	0.57
2:B:288:LEU:O	3:C:311:ILE:N	2.32	0.57
1:A:2277:LEU:HA	1:A:2280:VAL:HG22	1.86	0.57
1:A:3878:VAL:O	1:A:3965:ARG:NH1	2.38	0.57
3:C:410:PRO:HA	3:C:419:LEU:HA	1.86	0.57
6:J:904:GLN:OE1	6:J:908:GLN:NE2	2.37	0.57
1:A:2325:LEU:HD23	1:A:2328:ARG:HH12	1.69	0.57
2:B:48:MET:HB2	2:B:59:PRO:HB2	1.87	0.57
1:A:186:PRO:HD2	1:A:189:MET:HE1	1.86	0.57
1:A:534:LEU:O	1:A:561:ASN:ND2	2.36	0.57
1:A:1826:THR:O	1:A:1830:HIS:ND1	2.31	0.57
3:C:406:GLY:HA3	3:C:421:TYR:HE1	1.68	0.57
6:J:865:ILE:HG13	6:J:888:ILE:HG23	1.87	0.57
1:A:1844:VAL:O	1:A:1848:ILE:HG12	2.04	0.57
4:G:29:ILE:HG21	4:G:76:LEU:HB3	1.87	0.57
5:I:38:ASP:OD1	5:I:41:SER:N	2.37	0.57
6:J:747:CYS:O	6:J:751:LYS:N	2.36	0.57
1:A:2349:LEU:HB3	1:A:2360:PHE:HE1	1.70	0.57
2:B:187:ARG:HE	4:G:175:ILE:HG21	1.70	0.57
1:A:1179:PRO:HB3	1:A:1259:LEU:HD23	1.86	0.57
1:A:3867:THR:OG1	1:A:4119:ARG:NH2	2.37	0.57
4:F:39:SER:HB2	4:F:44:VAL:HA	1.86	0.57
1:A:163:LYS:H	2:B:301:ARG:HB2	1.69	0.57
2:B:75:ILE:HD11	3:C:317:GLY:HA3	1.86	0.57
2:B:251:THR:HA	3:C:431:ARG:HH12	1.69	0.57
2:B:533:ASP:OD1	3:C:250:ARG:NH2	2.33	0.57
2:B:352:PRO:HA	2:B:394:VAL:HA	1.86	0.56
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.87	0.56
1:A:3868:VAL:HG22	1:A:4114:PRO:HB2	1.85	0.56
1:A:450:SER:O	1:A:454:GLN:N	2.31	0.56
1:A:1769:GLU:HB2	1:A:1772:HIS:CD2	2.39	0.56
6:J:817:THR:OG1	6:J:884:ARG:NH2	2.38	0.56
4:F:14:ALA:H	4:F:26:LYS:HB3	1.70	0.56
4:F:57:ARG:HH22	4:F:120:ASN:HB2	1.70	0.56
4:G:56:GLN:O	4:G:60:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:THR:HG23	1:A:1736:PHE:H	1.70	0.56
1:A:3159:ARG:HA	1:A:3162:ASN:ND2	2.21	0.56
1:A:3240:MET:HE1	1:A:3279:SER:HB3	1.87	0.56
1:A:3771:MET:HE3	1:A:3998:LEU:HD13	1.88	0.56
3:C:105:ALA:O	3:C:140:SER:OG	2.24	0.56
6:J:879:ARG:HH21	6:J:880:ARG:HH12	1.54	0.56
1:A:237:SER:O	1:A:238:MET:HE2	2.04	0.56
1:A:94:GLU:HB2	1:A:96:MET:HE1	1.87	0.56
2:B:166:ILE:HB	2:B:200:LEU:HD13	1.88	0.56
3:C:64:THR:HG22	3:C:76:ASN:H	1.71	0.56
1:A:4062:ASP:HA	1:A:4065:LEU:HD12	1.88	0.56
5:H:168:ALA:HB3	6:J:810:LEU:HD21	1.87	0.56
5:I:6:SER:O	5:I:20:LEU:N	2.38	0.56
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.88	0.56
1:A:913:ARG:O	1:A:913:ARG:NH1	2.37	0.56
1:A:3627:ALA:N	1:A:3682:GLU:O	2.38	0.56
1:A:2957:LEU:HD21	1:A:2993:PHE:HZ	1.70	0.55
1:A:3751:LEU:N	1:A:3803:ILE:O	2.36	0.55
1:A:862:LEU:O	1:A:3133:GLN:NE2	2.35	0.55
1:A:3757:ASP:OD1	1:A:3759:ARG:NH1	2.39	0.55
2:B:37:SER:HB3	2:B:161:MET:HE2	1.88	0.55
2:B:363:ARG:HG3	2:B:364:PRO:HD2	1.87	0.55
3:C:94:ILE:HA	3:C:98:ILE:HD13	1.88	0.55
1:A:321:LYS:O	1:A:324:SER:OG	2.24	0.55
1:A:3798:SER:OG	1:A:3799:ARG:NH1	2.38	0.55
1:A:3855:TYR:O	1:A:3858:MET:HG3	2.06	0.55
2:B:168:LEU:HB3	2:B:202:LEU:HD12	1.88	0.55
1:A:139:ARG:HH21	1:A:182:GLY:H	1.52	0.55
2:B:42:VAL:HG22	2:B:169:PHE:HB2	1.89	0.55
3:C:111:LEU:HB3	3:C:115:MET:HE1	1.88	0.55
3:C:393:VAL:O	3:C:406:GLY:N	2.39	0.55
1:A:256:ILE:HG22	1:A:258:PRO:HD3	1.89	0.55
1:A:1802:TYR:OH	1:A:1846:ASP:OD2	2.23	0.55
1:A:3014:CYS:HA	1:A:3018:SER:HB2	1.89	0.55
1:A:1813:SER:HB3	1:A:1936:ARG:HH22	1.72	0.55
1:A:2387:PRO:HD3	1:A:2418:LYS:HD2	1.89	0.55
6:J:801:TYR:HB2	6:J:815:ARG:NH2	2.21	0.55
6:J:823:TYR:OH	6:J:854:SER:OG	2.25	0.55
1:A:172:GLU:HG2	1:A:220:LEU:HD12	1.87	0.55
1:A:1483:LEU:O	1:A:1487:VAL:HG22	2.06	0.55
1:A:1709:GLU:HG3	1:A:1712:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:PRO:HA	2:B:62:MET:SD	2.47	0.54
4:G:160:LYS:O	4:G:164:ILE:HG12	2.08	0.54
1:A:1233:SER:HB3	1:A:3695:LEU:HD23	1.90	0.54
1:A:1942:CYS:O	1:A:1946:ASN:ND2	2.40	0.54
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.39	0.54
3:C:31:PHE:CG	3:C:100:PRO:HG3	2.42	0.54
5:I:30:SER:HA	5:I:52:ILE:HG13	1.89	0.54
2:B:181:ALA:N	2:B:184:SER:HG	2.04	0.54
6:J:726:LEU:O	6:J:730:PHE:N	2.36	0.54
1:A:3101:TYR:O	1:A:3104:GLN:HG3	2.08	0.54
3:C:450:GLN:HG3	3:C:536:LEU:HD22	1.88	0.54
4:G:59:LYS:HA	4:G:66:THR:HA	1.88	0.54
6:J:844:GLU:HB3	6:J:898:ILE:HD12	1.89	0.54
1:A:2544:SER:HA	1:A:2842:ARG:HH22	1.73	0.54
1:A:3819:THR:HA	1:A:3889:ARG:HH12	1.73	0.54
1:A:1009:LEU:O	1:A:1013:ILE:HG12	2.07	0.54
4:G:27:VAL:HB	4:G:36:LEU:HA	1.89	0.54
4:G:29:ILE:HG23	4:G:34:TYR:HB3	1.89	0.54
1:A:295:GLU:HB3	1:A:299:LYS:HZ3	1.73	0.54
1:A:20:SER:HB2	1:A:69:VAL:HG21	1.90	0.54
1:A:865:GLN:HG3	1:A:866:ILE:HD12	1.89	0.54
1:A:2271:SER:HA	1:A:2274:ILE:HD12	1.89	0.54
2:B:156:ASP:O	2:B:158:GLN:NE2	2.38	0.54
1:A:3226:ASP:OD2	1:A:3229:SER:OG	2.25	0.54
2:B:350:PHE:CE2	3:C:458:ILE:HG12	2.43	0.54
2:B:402:PRO:HD2	2:B:406:ILE:HG21	1.89	0.54
3:C:450:GLN:NE2	3:C:536:LEU:O	2.33	0.54
5:H:36:LEU:HB3	5:H:43:TRP:HB2	1.90	0.54
1:A:3916:TRP:CE2	1:A:4107:LEU:HD21	2.43	0.54
6:J:818:VAL:HG12	6:J:862:HIS:HB2	1.90	0.54
1:A:741:ILE:HG21	1:A:776:TRP:CE2	2.44	0.53
1:A:1607:GLU:HG3	1:A:1611:GLN:HB2	1.90	0.53
1:A:2371:PHE:HD2	1:A:2374:LEU:HG	1.73	0.53
3:C:296:CYS:HA	3:C:304:GLU:HA	1.88	0.53
5:H:36:LEU:O	5:H:43:TRP:N	2.31	0.53
8:E:31:DT:H2"	8:E:32:DT:C5	2.43	0.53
1:A:721:TYR:HB2	1:A:726:LEU:HD13	1.91	0.53
2:B:352:PRO:HB2	2:B:354:VAL:HG22	1.90	0.53
5:H:7:ARG:HG2	5:I:131:LEU:HD12	1.90	0.53
6:J:872:VAL:HA	6:J:875:PHE:HD2	1.73	0.53
1:A:2269:ASP:CG	1:A:2270:ASN:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:PHE:H	3:C:290:GLN:HE22	1.57	0.53
1:A:3880:ALA:HA	1:A:3966:GLN:HE22	1.74	0.53
6:J:710:LYS:O	6:J:714:LEU:N	2.37	0.53
1:A:754:MET:HA	1:A:757:LYS:HG2	1.90	0.53
1:A:767:GLU:O	1:A:771:ASN:ND2	2.41	0.53
1:A:2225:HIS:ND1	1:A:2226:PRO:O	2.42	0.53
1:A:2540:LEU:HD13	1:A:2835:LYS:HD3	1.89	0.53
1:A:583:LEU:HB3	1:A:612:LEU:HD22	1.90	0.53
1:A:1175:HIS:HA	1:A:1228:GLY:HA2	1.89	0.53
1:A:1697:PRO:HG2	1:A:1749:ALA:HB1	1.91	0.53
1:A:3883:LEU:HD23	1:A:3970:LEU:HB2	1.91	0.53
2:B:410:PHE:HB3	2:B:437:LEU:HD12	1.90	0.53
5:H:38:ASP:OD1	5:H:41:SER:N	2.41	0.53
5:H:140:LYS:HA	5:H:143:HIS:CE1	2.44	0.53
7:D:41:DT:H1'	7:D:42:DA:C8	2.43	0.53
1:A:1151:ARG:NH2	1:A:1163:LEU:O	2.28	0.53
1:A:2260:PHE:HB2	1:A:2306:ASN:HD21	1.74	0.53
1:A:3858:MET:SD	1:A:4119:ARG:HB2	2.49	0.53
6:J:809:PRO:HB2	6:J:901:CYS:HB3	1.91	0.53
1:A:935:HIS:ND1	1:A:987:LEU:HD22	2.23	0.53
1:A:567:GLU:HA	1:A:570:LYS:HG2	1.90	0.53
1:A:1549:SER:OG	1:A:1550:VAL:N	2.42	0.53
6:J:823:TYR:O	6:J:871:ARG:NH2	2.39	0.53
1:A:1191:PHE:O	1:A:1195:VAL:HG23	2.09	0.52
1:A:3660:ASN:OD1	1:A:3661:ASP:N	2.42	0.52
3:C:7:LYS:HB3	3:C:128:GLU:H	1.74	0.52
6:J:722:LYS:HE2	6:J:742:PHE:HA	1.90	0.52
1:A:860:GLY:HA3	1:A:3136:THR:HG21	1.91	0.52
2:B:148:TRP:NE1	2:B:152:ASN:HD21	2.08	0.52
3:C:513:TRP:O	3:C:517:ASN:ND2	2.37	0.52
1:A:169:THR:HG21	8:E:21:DA:H5'	1.90	0.52
1:A:380:ASP:O	1:A:384:MET:HG2	2.09	0.52
1:A:1825:LEU:HD21	1:A:1875:LYS:HB3	1.92	0.52
1:A:3616:ALA:O	1:A:3629:ARG:NH2	2.42	0.52
2:B:303:PHE:HB2	2:B:310:LEU:HA	1.91	0.52
4:F:204:ILE:O	4:F:208:LYS:NZ	2.43	0.52
1:A:349:ILE:O	1:A:391:ARG:NH2	2.42	0.52
1:A:1098:GLN:HG2	1:A:1152:ARG:HG3	1.90	0.52
1:A:1264:LEU:HD21	1:A:1341:ILE:HA	1.91	0.52
1:A:1829:TRP:O	1:A:1883:ARG:NH2	2.43	0.52
1:A:3328:ILE:HD11	1:A:3412:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3781:CYS:HB2	1:A:3786:LEU:HD12	1.91	0.52
1:A:4082:ARG:HH21	1:A:4091:ALA:HA	1.75	0.52
4:F:57:ARG:NH2	4:F:120:ASN:HB2	2.24	0.52
1:A:1281:VAL:HG13	1:A:1282:LEU:HG	1.92	0.52
1:A:4019:LYS:HG2	1:A:4020:MET:HE2	1.91	0.52
2:B:331:LYS:O	2:B:334:THR:N	2.43	0.52
4:F:186:GLU:HA	4:F:189:PHE:HB3	1.91	0.52
8:E:17:DT:H2"	8:E:18:DA:C4	2.45	0.52
1:A:3813:LYS:HE2	1:A:3817:LEU:HD11	1.92	0.52
4:G:36:LEU:HG	4:G:38:VAL:HG13	1.92	0.52
1:A:295:GLU:HB3	1:A:299:LYS:NZ	2.25	0.52
1:A:1039:TRP:O	1:A:1043:GLN:N	2.42	0.52
1:A:3266:SER:HA	1:A:3272:TRP:HB3	1.92	0.52
4:G:110:SER:H	4:G:117:PHE:HB3	1.74	0.52
5:H:8:ILE:HB	5:H:86:PHE:CG	2.44	0.52
5:I:163:GLU:O	6:J:846:ARG:NH2	2.43	0.52
6:J:720:VAL:HB	6:J:745:HIS:HB3	1.92	0.52
1:A:1926:ASN:HB2	1:A:1974:ASN:HD21	1.75	0.52
5:H:130:CYS:O	5:H:133:THR:OG1	2.25	0.52
5:H:180:PHE:HB2	6:J:774:LEU:HD21	1.91	0.52
5:I:48:SER:OG	5:I:49:GLU:N	2.43	0.52
1:A:2773:ARG:HG3	1:A:2775:TYR:H	1.74	0.52
1:A:3897:PHE:CE2	1:A:3901:ARG:HD2	2.45	0.52
2:B:91:GLU:H	2:B:136:GLY:HA3	1.75	0.52
5:H:28:LEU:HA	5:H:71:ARG:HH21	1.75	0.52
1:A:1058:SER:HA	1:A:1061:LYS:HE2	1.91	0.51
1:A:1064:TYR:HA	1:A:1106:ILE:HG21	1.92	0.51
1:A:2395:THR:OG1	1:A:2431:ARG:NH1	2.43	0.51
1:A:1657:SER:OG	1:A:1660:SER:OG	2.22	0.51
1:A:2474:TYR:HD2	1:A:2517:LEU:HD11	1.74	0.51
1:A:19:LEU:HD22	1:A:34:LEU:HA	1.93	0.51
1:A:143:LEU:HB3	1:A:144:MET:HE2	1.92	0.51
1:A:1667:SER:O	1:A:1667:SER:OG	2.28	0.51
1:A:1772:HIS:CE1	1:A:1773:VAL:HG13	2.45	0.51
2:B:95:ASN:HD21	2:B:99:PHE:H	1.58	0.51
6:J:798:ASP:HA	6:J:801:TYR:HB3	1.92	0.51
1:A:2501:LEU:O	1:A:2505:VAL:HG22	2.11	0.51
1:A:3809:THR:OG1	1:A:3930:VAL:O	2.29	0.51
1:A:3380:ARG:O	1:A:3384:HIS:ND1	2.44	0.51
6:J:667:MET:HE1	6:J:708:ARG:HG3	1.92	0.51
1:A:269:SER:HB3	1:A:308:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3819:THR:HG23	1:A:3889:ARG:HH12	1.76	0.51
2:B:456:PRO:HA	2:B:459:VAL:HG22	1.92	0.51
1:A:934:LEU:HA	1:A:937:MET:HG2	1.93	0.51
1:A:2839:ASP:O	1:A:2842:ARG:HG2	2.10	0.51
4:F:2:GLU:N	4:F:47:GLU:O	2.44	0.51
4:F:3:GLU:HG2	4:F:4:LEU:H	1.76	0.51
1:A:467:ALA:O	1:A:471:LYS:NZ	2.40	0.51
3:C:40:MET:O	3:C:43:GLN:HG2	2.11	0.51
3:C:62:ASP:OD1	3:C:102:SER:N	2.41	0.51
5:H:88:PHE:HA	5:H:95:PHE:HA	1.93	0.51
6:J:730:PHE:O	6:J:733:LYS:NZ	2.34	0.51
1:A:1097:GLU:HB2	1:A:1151:ARG:HD3	1.92	0.51
1:A:2379:MET:SD	1:A:2379:MET:N	2.83	0.51
1:A:2094:MET:HA	1:A:2097:LEU:HD12	1.92	0.51
1:A:4013:TRP:CE2	1:A:4035:GLU:HB2	2.46	0.51
2:B:350:PHE:HB3	2:B:394:VAL:HB	1.92	0.51
7:D:23:DT:H3	8:E:33:DA:H2	1.59	0.51
7:D:36:DA:N6	8:E:22:DG:H1	2.09	0.51
1:A:1694:THR:HB	1:A:1745:LYS:HB3	1.93	0.50
1:A:2189:ILE:O	1:A:2192:THR:OG1	2.29	0.50
1:A:3159:ARG:HA	1:A:3162:ASN:HD21	1.76	0.50
1:A:3183:ILE:HD12	1:A:3238:MET:HE2	1.93	0.50
3:C:315:ARG:NE	3:C:317:GLY:O	2.44	0.50
6:J:792:MET:SD	6:J:796:ILE:HD12	2.50	0.50
1:A:798:GLY:O	1:A:802:THR:OG1	2.24	0.50
1:A:1148:ALA:O	1:A:1162:SER:OG	2.29	0.50
1:A:1519:PHE:HB3	1:A:1570:GLU:OE1	2.11	0.50
1:A:1169:VAL:HG21	1:A:1198:LEU:HD21	1.93	0.50
1:A:1675:TYR:CE1	1:A:1696:LEU:HG	2.45	0.50
1:A:1818:SER:HA	1:A:1821:ASP:HB2	1.93	0.50
1:A:4017:GLU:O	1:A:4021:LEU:HG	2.11	0.50
3:C:44:ARG:HG3	3:C:235:CYS:SG	2.52	0.50
6:J:746:MET:O	6:J:751:LYS:NZ	2.42	0.50
1:A:2145:PHE:CZ	1:A:2149:LEU:HD11	2.46	0.50
1:A:3451:LEU:HD13	1:A:3486:GLU:HB2	1.94	0.50
3:C:58:LEU:N	3:C:78:THR:O	2.37	0.50
5:H:43:TRP:HH2	5:H:90:LYS:HE3	1.76	0.50
1:A:2547:SER:HB3	1:A:2550:ILE:HG12	1.94	0.50
1:A:3845:LYS:HD2	1:A:3846:MET:HG2	1.92	0.50
4:F:26:LYS:HD3	4:F:37:LEU:HD12	1.94	0.50
4:G:66:THR:N	5:H:57:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:O	1:A:185:HIS:NE2	2.44	0.50
1:A:752:LEU:HD22	1:A:776:TRP:CZ3	2.46	0.50
1:A:1258:ASP:HA	1:A:1261:LEU:HD12	1.93	0.50
1:A:1338:VAL:O	1:A:1342:MET:HG2	2.12	0.50
1:A:1725:GLN:OE1	1:A:1726:SER:N	2.44	0.50
2:B:264:ASN:ND2	2:B:266:ASP:OD1	2.44	0.50
4:F:154:ALA:O	4:F:158:HIS:ND1	2.45	0.50
4:G:104:LEU:HD21	4:G:106:LEU:HD13	1.92	0.50
5:H:140:LYS:HA	5:H:143:HIS:ND1	2.26	0.50
1:A:221:ALA:O	1:A:225:LYS:HG2	2.11	0.50
1:A:1920:TYR:HA	1:A:1923:PHE:CE1	2.47	0.50
1:A:2461:PHE:HA	1:A:2464:HIS:HE2	1.76	0.50
3:C:342:VAL:HG12	3:C:393:VAL:HG13	1.94	0.50
4:G:213:ASN:O	4:G:220:ALA:N	2.45	0.50
5:I:30:SER:OG	5:I:49:GLU:OE1	2.29	0.50
6:J:752:GLU:O	6:J:756:ARG:N	2.44	0.50
1:A:204:LEU:HB3	1:A:208:MET:HE1	1.92	0.50
5:H:176:LEU:HA	5:H:179:ARG:HD2	1.93	0.50
6:J:843:LEU:O	6:J:847:PHE:N	2.45	0.50
1:A:602:MET:O	1:A:1087:ARG:NH1	2.39	0.50
2:B:202:LEU:O	2:B:238:LYS:NZ	2.45	0.50
4:F:36:LEU:HG	4:F:38:VAL:H	1.77	0.50
4:G:58:ALA:HB1	4:G:67:ALA:HB3	1.93	0.50
6:J:819:TYR:HB2	6:J:860:VAL:HG13	1.93	0.50
1:A:137:THR:O	1:A:141:SER:N	2.38	0.49
1:A:2567:SER:HA	1:A:2572:TYR:CG	2.47	0.49
1:A:2839:ASP:HA	1:A:2842:ARG:HE	1.77	0.49
1:A:3156:PRO:O	1:A:3159:ARG:HG3	2.12	0.49
2:B:126:GLN:HA	2:B:129:LYS:HG2	1.93	0.49
3:C:6:ASN:ND2	3:C:128:GLU:OE1	2.41	0.49
6:J:864:ILE:HD12	6:J:893:TRP:HB3	1.93	0.49
2:B:460:GLY:HA2	2:B:463:LYS:HE3	1.94	0.49
1:A:542:ASP:HA	1:A:545:LEU:HG	1.94	0.49
1:A:684:GLU:OE1	1:A:684:GLU:N	2.43	0.49
1:A:2105:HIS:CE1	1:A:2156:VAL:HA	2.48	0.49
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.80	0.49
1:A:1093:GLU:HA	1:A:1096:VAL:HB	1.94	0.49
1:A:1363:LEU:O	1:A:1367:HIS:ND1	2.27	0.49
2:B:348:MET:SD	3:C:518:PRO:HD3	2.53	0.49
4:G:54:VAL:HA	4:G:119:TRP:CZ3	2.47	0.49
5:H:55:GLU:HA	5:H:58:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:LYS:O	1:A:2106:ARG:HG2	2.12	0.49
2:B:290:ARG:HD2	3:C:309:ASP:HA	1.94	0.49
2:B:300:THR:OG1	3:C:292:GLU:O	2.26	0.49
2:B:417:GLU:O	2:B:428:THR:OG1	2.29	0.49
2:B:462:MET:HE3	2:B:462:MET:HA	1.95	0.49
4:F:13:TRP:HB3	4:F:215:GLN:NE2	2.27	0.49
5:I:18:HIS:NE2	5:I:38:ASP:HB3	2.28	0.49
1:A:373:CYS:SG	1:A:381:VAL:HG22	2.52	0.49
1:A:713:GLU:HB2	1:A:717:LYS:HE3	1.95	0.49
1:A:774:GLU:HG2	1:A:858:MET:SD	2.53	0.49
1:A:3490:VAL:HG21	1:A:3493:TRP:CE3	2.48	0.49
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.45	0.49
1:A:3820:MET:HE1	1:A:3828:TYR:CE2	2.48	0.49
2:B:488:ARG:HH12	2:B:503:ALA:N	2.10	0.49
3:C:13:CYS:HB3	3:C:59:PHE:HE2	1.78	0.49
3:C:93:ASP:HB3	3:C:97:LYS:HD2	1.94	0.49
6:J:720:VAL:HG12	6:J:744:ILE:HD12	1.95	0.49
1:A:141:SER:O	1:A:141:SER:OG	2.28	0.49
1:A:3455:LYS:HA	1:A:3491:PRO:HB3	1.94	0.49
1:A:3640:PHE:O	1:A:3644:PHE:HB3	2.13	0.49
2:B:124:GLY:O	2:B:128:GLN:N	2.45	0.49
3:C:219:ASP:OD1	3:C:219:ASP:N	2.45	0.49
4:F:43:GLN:HG2	4:G:128:PRO:HB2	1.93	0.49
6:J:694:GLY:O	6:J:718:HIS:NE2	2.45	0.49
1:A:3617:LEU:HB2	1:A:3632:PHE:HE2	1.78	0.49
2:B:261:LEU:HD23	2:B:269:ILE:HD12	1.95	0.49
2:B:422:ASP:OD1	2:B:422:ASP:N	2.44	0.49
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.78	0.49
1:A:1014:LEU:O	1:A:1018:VAL:HG12	2.13	0.49
1:A:2219:LEU:O	1:A:2223:VAL:N	2.45	0.49
5:H:172:LEU:O	5:H:176:LEU:HG	2.13	0.49
6:J:841:LYS:HD3	6:J:864:ILE:HB	1.95	0.49
1:A:176:GLU:HA	1:A:227:LEU:HB2	1.95	0.48
1:A:2244:CYS:HG	1:A:2245:TRP:CG	2.31	0.48
1:A:2365:ASN:HA	1:A:2368:THR:HG22	1.94	0.48
1:A:3980:MET:SD	1:A:3980:MET:N	2.86	0.48
5:H:140:LYS:HA	5:H:143:HIS:HD1	1.78	0.48
6:J:725:TRP:NE1	6:J:736:VAL:O	2.32	0.48
1:A:27:ALA:HB1	1:A:77:GLU:HG3	1.95	0.48
1:A:3161:LEU:O	1:A:3165:THR:HG23	2.13	0.48
3:C:285:LYS:HB2	3:C:287:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:4:LEU:HD12	4:F:28:PHE:HB3	1.93	0.48
5:H:18:HIS:HB3	5:H:36:LEU:HD11	1.94	0.48
7:D:40:DT:H5"	7:D:41:DT:C4	2.48	0.48
1:A:2104:MET:HE2	1:A:2108:LEU:HD12	1.95	0.48
1:A:2443:MET:SD	1:A:2476:ILE:HG23	2.53	0.48
1:A:3759:ARG:HH21	1:A:4010:SER:HA	1.78	0.48
1:A:3835:PRO:HG3	1:A:3877:LYS:HB3	1.94	0.48
6:J:829:LEU:HD11	6:J:855:CYS:HB3	1.95	0.48
1:A:139:ARG:NH2	1:A:182:GLY:H	2.10	0.48
1:A:1377:CYS:SG	1:A:1378:GLU:N	2.86	0.48
1:A:3367:SER:HB2	1:A:3372:LYS:HE3	1.94	0.48
1:A:3964:THR:H	1:A:3967:PHE:HD2	1.62	0.48
3:C:13:CYS:HB3	3:C:59:PHE:CE2	2.49	0.48
3:C:131:HIS:ND1	3:C:160:SER:OG	2.46	0.48
3:C:250:ARG:HG2	3:C:260:ARG:HD3	1.95	0.48
4:F:28:PHE:HB2	4:F:35:ALA:HB3	1.96	0.48
6:J:759:ASP:HB3	6:J:765:TYR:CZ	2.48	0.48
1:A:1933:LEU:O	1:A:1937:ARG:N	2.43	0.48
3:C:44:ARG:CD	3:C:238:LYS:HE3	2.44	0.48
1:A:1069:HIS:CG	1:A:1074:LYS:HD2	2.48	0.48
1:A:1949:ILE:HG23	1:A:2100:LEU:HD22	1.94	0.48
1:A:2098:THR:C	1:A:2102:LYS:HZ2	2.21	0.48
2:B:357:LYS:HG3	2:B:360:HIS:CE1	2.49	0.48
3:C:457:LEU:O	3:C:461:MET:HG2	2.14	0.48
4:G:178:ARG:HH21	4:G:179:LEU:HD11	1.79	0.48
1:A:363:ILE:HD12	1:A:413:PHE:HA	1.96	0.48
1:A:1052:SER:O	1:A:1056:THR:N	2.47	0.48
1:A:1132:ASP:HB3	1:A:1136:ARG:HH21	1.78	0.48
1:A:1765:VAL:HA	1:A:1768:ARG:NE	2.28	0.48
1:A:3284:SER:HB2	1:A:3301:LEU:HD21	1.94	0.48
1:A:3821:SER:OG	1:A:3823:GLU:OE1	2.29	0.48
6:J:739:GLN:OE1	6:J:741:ARG:NH2	2.47	0.48
1:A:84:GLU:O	1:A:87:LYS:HG3	2.14	0.48
1:A:232:CYS:HB3	1:A:278:HIS:CE1	2.49	0.48
1:A:1112:ALA:O	1:A:1180:GLN:NE2	2.47	0.48
1:A:1568:ASN:OD1	1:A:1569:THR:N	2.46	0.48
1:A:1616:LEU:O	1:A:1620:THR:HG23	2.14	0.48
1:A:1766:LEU:HD13	1:A:1778:PHE:CD2	2.49	0.48
1:A:3583:LEU:HB3	1:A:3733:ARG:HH11	1.79	0.48
1:A:3759:ARG:O	1:A:3763:ARG:HG2	2.14	0.48
5:H:178:LYS:HA	5:H:181:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:817:THR:OG1	6:J:859:GLY:O	2.25	0.48
1:A:3082:TYR:O	1:A:3086:LEU:HG	2.14	0.48
4:F:59:LYS:HG2	4:F:66:THR:HB	1.96	0.48
1:A:885:ALA:O	1:A:888:ARG:NH2	2.47	0.48
1:A:2562:LEU:O	1:A:2566:THR:HG23	2.14	0.48
1:A:2814:SER:O	1:A:2818:LYS:HG2	2.14	0.48
2:B:357:LYS:O	2:B:358:LYS:HG2	2.14	0.48
3:C:434:MET:HA	3:C:434:MET:HE2	1.95	0.48
1:A:237:SER:OG	1:A:280:SER:O	2.29	0.47
1:A:483:VAL:HG21	1:A:567:GLU:HG2	1.96	0.47
1:A:2461:PHE:HA	1:A:2464:HIS:NE2	2.29	0.47
1:A:542:ASP:N	1:A:542:ASP:OD1	2.44	0.47
1:A:566:ASP:OD2	1:A:570:LYS:NZ	2.42	0.47
1:A:631:ARG:HD3	1:A:668:LYS:HB3	1.96	0.47
1:A:941:MET:HE1	1:A:962:TYR:CE1	2.49	0.47
1:A:2425:ARG:HH11	1:A:2457:PRO:HB2	1.79	0.47
3:C:338:LYS:HB3	3:C:398:ASP:HA	1.95	0.47
4:F:43:GLN:HB3	4:F:131:VAL:HG21	1.96	0.47
1:A:399:GLN:OE1	1:A:1744:LYS:NZ	2.48	0.47
1:A:2429:ASP:OD1	1:A:2429:ASP:N	2.48	0.47
6:J:659:PHE:CZ	6:J:729:CYS:HB3	2.49	0.47
1:A:1586:SER:HA	1:A:1593:VAL:HG21	1.96	0.47
1:A:1603:GLN:HE22	1:A:1606:ARG:HH22	1.61	0.47
1:A:2415:LEU:HB3	1:A:2420:PHE:HB3	1.96	0.47
1:A:2773:ARG:HD2	1:A:2789:SER:HB2	1.96	0.47
1:A:3175:PRO:HG2	1:A:3178:ILE:HG12	1.95	0.47
1:A:3784:ARG:HH12	1:A:3986:HIS:CD2	2.32	0.47
3:C:200:GLN:O	3:C:203:GLU:HG2	2.13	0.47
5:H:144:LEU:HD11	5:I:145:GLN:OE1	2.15	0.47
1:A:896:VAL:N	1:A:903:PRO:O	2.40	0.47
1:A:1225:GLU:HB3	1:A:1236:LEU:HB2	1.95	0.47
1:A:2425:ARG:NH1	1:A:2457:PRO:O	2.47	0.47
2:B:348:MET:HE3	2:B:399:ARG:HG3	1.97	0.47
2:B:492:ALA:HB2	2:B:500:PRO:HD3	1.95	0.47
4:F:53:VAL:O	4:F:57:ARG:HB2	2.14	0.47
1:A:254:LYS:O	1:A:300:TRP:NE1	2.42	0.47
1:A:645:TRP:CZ3	1:A:1505:LEU:HD13	2.50	0.47
1:A:651:TYR:CZ	1:A:655:LEU:HD11	2.49	0.47
1:A:770:LEU:HD11	1:A:858:MET:HG3	1.96	0.47
1:A:982:GLN:OE1	1:A:2589:TYR:OH	2.20	0.47
1:A:1783:ARG:HG2	1:A:1830:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:LYS:C	1:A:1962:TYR:H	2.22	0.47
1:A:2320:ALA:HB1	1:A:2367:VAL:HB	1.95	0.47
1:A:2589:TYR:HD1	1:A:2777:HIS:CE1	2.33	0.47
1:A:3298:LEU:HD11	1:A:3336:ILE:HG22	1.97	0.47
1:A:3389:VAL:O	1:A:3393:GLU:HG2	2.14	0.47
2:B:74:LYS:HD2	2:B:81:ASP:HB2	1.96	0.47
2:B:262:LYS:HA	2:B:268:VAL:HG12	1.95	0.47
3:C:292:GLU:N	3:C:292:GLU:OE1	2.47	0.47
3:C:400:ARG:NH2	8:E:33:DA:O4'	2.48	0.47
4:F:136:ILE:HG12	4:G:136:ILE:HD13	1.97	0.47
6:J:893:TRP:HA	6:J:904:GLN:HB2	1.96	0.47
1:A:453:MET:HA	1:A:456:VAL:HG22	1.96	0.47
1:A:1675:TYR:CD1	1:A:1696:LEU:HG	2.50	0.47
1:A:2527:HIS:HD2	1:A:2529:THR:H	1.63	0.47
2:B:272:GLY:N	2:B:369:TYR:O	2.38	0.47
3:C:52:ASP:N	3:C:52:ASP:OD1	2.48	0.47
3:C:266:SER:OG	3:C:363:LYS:HG2	2.15	0.47
5:I:188:LYS:HD2	5:I:191:ILE:HD12	1.96	0.47
1:A:75:SER:O	1:A:79:ARG:N	2.48	0.47
1:A:1560:TYR:O	1:A:1564:SER:OG	2.22	0.47
1:A:1748:ASP:OD1	1:A:1749:ALA:N	2.48	0.47
1:A:2792:THR:OG1	1:A:2793:PRO:HD3	2.15	0.47
1:A:3113:ASN:O	1:A:3117:ILE:HG13	2.15	0.47
2:B:42:VAL:HB	2:B:87:PHE:CE1	2.49	0.47
1:A:90:CYS:HA	1:A:93:LEU:HG	1.96	0.47
2:B:523:ASP:OD1	2:B:523:ASP:N	2.48	0.47
3:C:54:ILE:HG12	3:C:86:PRO:HG3	1.97	0.47
3:C:108:LEU:HD22	3:C:146:GLN:HB2	1.96	0.47
6:J:800:GLU:O	6:J:805:TRP:N	2.46	0.47
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.97	0.46
1:A:3772:ASN:ND2	1:A:3788:LEU:O	2.42	0.46
1:A:4039:TYR:HB3	1:A:4041:ARG:HD3	1.98	0.46
5:H:130:CYS:HB3	5:I:130:CYS:HB3	1.97	0.46
1:A:998:ASN:HB3	1:A:1044:ILE:HG13	1.96	0.46
1:A:3118:ASP:HB3	1:A:3121:LEU:HG	1.97	0.46
2:B:280:ALA:N	3:C:429:ASP:OD1	2.48	0.46
2:B:369:TYR:CD1	2:B:370:PRO:HD2	2.51	0.46
3:C:13:CYS:HA	3:C:57:VAL:O	2.15	0.46
3:C:132:ILE:O	3:C:162:GLN:N	2.34	0.46
1:A:3700:GLU:OE1	1:A:3700:GLU:N	2.48	0.46
1:A:571:SER:HA	1:A:574:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1614:GLN:OE1	1:A:1614:GLN:N	2.48	0.46
1:A:3459:ASN:O	1:A:3463:LEU:HG	2.15	0.46
2:B:446:MET:HE2	2:B:446:MET:HA	1.97	0.46
3:C:246:HIS:HB3	3:C:264:TYR:CZ	2.51	0.46
4:G:75:HIS:HB2	5:H:102:LYS:HZ3	1.80	0.46
6:J:667:MET:SD	6:J:668:SER:N	2.89	0.46
1:A:238:MET:SD	1:A:284:THR:OG1	2.69	0.46
1:A:2442:MET:HE1	1:A:2446:LEU:HD13	1.97	0.46
1:A:3761:ASP:HB2	1:A:3793:VAL:HG11	1.96	0.46
2:B:34:GLY:O	2:B:253:LYS:NZ	2.49	0.46
3:C:7:LYS:HG2	3:C:126:LYS:O	2.16	0.46
1:A:322:GLN:HB3	1:A:326:MET:HE1	1.98	0.46
1:A:385:TYR:O	1:A:389:ILE:HG12	2.16	0.46
1:A:2967:GLU:OE1	1:A:2967:GLU:N	2.45	0.46
1:A:3735:PRO:HB3	1:A:3753:LYS:HD3	1.97	0.46
2:B:48:MET:HG2	2:B:60:PHE:HB2	1.97	0.46
3:C:43:GLN:HA	3:C:46:VAL:HG22	1.96	0.46
6:J:792:MET:O	6:J:797:ALA:N	2.46	0.46
1:A:100:ILE:HD12	1:A:141:SER:HA	1.98	0.46
1:A:629:PHE:O	1:A:633:ILE:HG12	2.16	0.46
1:A:3571:PHE:CE2	1:A:3575:LEU:HD11	2.51	0.46
3:C:342:VAL:HG12	3:C:393:VAL:HG22	1.97	0.46
4:F:135:LEU:C	4:F:138:PRO:HD2	2.40	0.46
1:A:430:VAL:HG11	1:A:1640:GLU:HB2	1.97	0.46
1:A:565:TYR:HE1	1:A:642:PHE:HB2	1.81	0.46
2:B:35:ARG:N	2:B:162:SER:H	2.14	0.46
3:C:164:PHE:CD2	3:C:225:TYR:HB2	2.51	0.46
3:C:213:ILE:HA	3:C:217:GLY:HA2	1.97	0.46
4:G:220:ALA:O	4:G:224:GLN:HG2	2.16	0.46
5:H:89:SER:OG	5:H:94:TYR:O	2.33	0.46
1:A:1111:LEU:HB2	1:A:1127:CYS:SG	2.56	0.46
1:A:1285:GLU:OE2	1:A:1286:ALA:N	2.45	0.46
1:A:2891:ARG:O	1:A:2895:GLU:HG2	2.15	0.46
1:A:2893:LEU:HD21	1:A:2922:ARG:O	2.16	0.46
1:A:3083:SER:OG	1:A:3102:TYR:O	2.34	0.46
1:A:3460:GLU:H	1:A:3460:GLU:CD	2.24	0.46
3:C:542:ALA:O	3:C:545:LYS:NZ	2.49	0.46
6:J:759:ASP:OD1	6:J:760:CYS:N	2.41	0.46
1:A:749:VAL:O	1:A:753:GLN:HG3	2.16	0.46
1:A:3495:PHE:HB3	1:A:3502:MET:CE	2.45	0.46
4:G:54:VAL:HA	4:G:119:TRP:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:190:LYS:HE3	5:I:194:LEU:HD11	1.98	0.46
1:A:87:LYS:O	1:A:91:ILE:HG12	2.16	0.45
1:A:305:ASN:O	1:A:309:LYS:HG3	2.16	0.45
1:A:1260:LEU:HD13	1:A:1297:PHE:CE1	2.51	0.45
1:A:1297:PHE:HA	1:A:1301:ILE:HG12	1.98	0.45
1:A:1475:LEU:HD23	1:A:1475:LEU:H	1.81	0.45
1:A:1834:ASP:OD1	1:A:1834:ASP:N	2.47	0.45
1:A:3131:SER:O	1:A:3135:LEU:HG	2.17	0.45
1:A:3854:ALA:O	1:A:3858:MET:N	2.49	0.45
1:A:4115:ASN:OD1	1:A:4119:ARG:NE	2.36	0.45
2:B:35:ARG:O	2:B:162:SER:N	2.49	0.45
2:B:77:SER:HA	2:B:249:LYS:O	2.17	0.45
3:C:156:LYS:HA	3:C:156:LYS:HD3	1.66	0.45
3:C:271:ARG:H	3:C:271:ARG:HD3	1.81	0.45
4:G:34:TYR:H	4:G:49:VAL:HG21	1.81	0.45
5:I:140:LYS:HA	5:I:143:HIS:CD2	2.51	0.45
1:A:99:LYS:HD2	1:A:99:LYS:HA	1.75	0.45
1:A:2531:LEU:HG	1:A:2538:ARG:NE	2.31	0.45
1:A:2575:PRO:HA	1:A:2786:LYS:HA	1.97	0.45
1:A:2860:ASP:OD1	1:A:2861:ILE:N	2.49	0.45
1:A:2923:TRP:CD2	1:A:2946:GLU:HG3	2.51	0.45
2:B:403:ARG:NH1	7:D:31:DA:O3'	2.49	0.45
3:C:47:PHE:HZ	3:C:495:LEU:HB2	1.81	0.45
4:F:160:LYS:NZ	4:G:183:PRO:HA	2.32	0.45
5:H:179:ARG:HB3	6:J:805:TRP:CZ2	2.51	0.45
7:D:29:DA:H2''	7:D:30:DA:C8	2.51	0.45
1:A:468:LEU:HB3	1:A:479:ILE:HD11	1.99	0.45
1:A:491:CYS:HA	1:A:625:ASN:HD22	1.81	0.45
1:A:1454:ALA:O	1:A:1458:LEU:HG	2.17	0.45
1:A:3839:TYR:OH	1:A:4120:THR:O	2.33	0.45
1:A:4013:TRP:NE1	1:A:4017:GLU:OE2	2.50	0.45
3:C:89:ASP:O	3:C:92:GLU:HG2	2.16	0.45
3:C:151:ILE:O	3:C:155:LYS:HG2	2.16	0.45
5:H:36:LEU:N	5:H:43:TRP:O	2.44	0.45
5:I:22:VAL:HG11	5:I:75:LEU:HA	1.99	0.45
6:J:863:VAL:HG23	6:J:886:PHE:HB2	1.98	0.45
8:E:33:DA:H2'	8:E:34:DT:C5	2.52	0.45
1:A:1260:LEU:HD13	1:A:1297:PHE:CZ	2.51	0.45
1:A:1760:GLU:O	1:A:1764:GLU:HG2	2.16	0.45
1:A:3495:PHE:HB3	1:A:3502:MET:HE3	1.98	0.45
1:A:3588:TRP:HE1	1:A:3610:TYR:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3886:ALA:O	1:A:3890:MET:HG2	2.16	0.45
1:A:4055:ASN:ND2	1:A:4057:ALA:HB3	2.31	0.45
3:C:146:GLN:HB3	3:C:149:ILE:HD11	1.97	0.45
1:A:697:ASP:HB2	1:A:700:LYS:HG3	1.97	0.45
1:A:1050:GLU:C	1:A:1053:PRO:HD2	2.42	0.45
1:A:2424:MET:HG2	1:A:2461:PHE:CZ	2.52	0.45
1:A:2532:PRO:HB2	1:A:2537:ASP:OD1	2.16	0.45
1:A:3490:VAL:HG21	1:A:3493:TRP:CD2	2.52	0.45
4:G:117:PHE:CZ	4:G:119:TRP:HB2	2.51	0.45
1:A:977:ASP:O	1:A:981:ARG:HG2	2.17	0.45
1:A:1896:ILE:HG22	1:A:1899:VAL:HG13	1.99	0.45
1:A:2412:TYR:O	1:A:2416:LYS:HG2	2.16	0.45
1:A:3097:ASP:N	1:A:3097:ASP:OD1	2.49	0.45
2:B:247:ARG:NH1	2:B:491:GLU:OE1	2.49	0.45
2:B:318:ARG:NH2	2:B:331:LYS:HE3	2.32	0.45
2:B:385:LEU:O	2:B:389:CYS:N	2.46	0.45
3:C:206:GLU:HA	3:C:209:LYS:HG2	1.98	0.45
5:I:36:LEU:N	5:I:43:TRP:O	2.46	0.45
8:E:25:DT:H2"	8:E:26:DT:H5"	1.99	0.45
1:A:1101:PHE:HD2	1:A:1163:LEU:HD12	1.82	0.45
1:A:1215:GLU:HB2	1:A:1219:PHE:CD2	2.52	0.45
1:A:2130:HIS:HE1	1:A:2164:TRP:HA	1.82	0.45
1:A:2880:CYS:HB3	1:A:2886:GLN:HA	1.99	0.45
1:A:3949:ALA:HB1	1:A:3953:LEU:HD12	1.99	0.45
3:C:35:LYS:NZ	3:C:98:ILE:O	2.48	0.45
4:G:68:PRO:HG2	5:H:106:PHE:HE1	1.81	0.45
6:J:665:CYS:HB2	6:J:697:THR:HG21	1.98	0.45
1:A:639:ALA:HB1	1:A:642:PHE:HB3	1.99	0.45
1:A:1095:LEU:HB3	1:A:1099:PHE:CE2	2.52	0.45
1:A:2773:ARG:HE	1:A:2774:SER:N	2.14	0.45
1:A:3253:SER:HA	1:A:3256:MET:SD	2.56	0.45
1:A:3860:LYS:HA	1:A:3860:LYS:HD3	1.45	0.45
2:B:148:TRP:CD1	2:B:152:ASN:HD21	2.35	0.45
3:C:206:GLU:HA	3:C:209:LYS:HE3	1.98	0.45
3:C:495:LEU:HD12	3:C:495:LEU:HA	1.74	0.45
5:I:59:MET:O	5:I:59:MET:HG2	2.17	0.45
1:A:478:CYS:O	1:A:482:VAL:HG23	2.17	0.45
1:A:770:LEU:O	1:A:774:GLU:HG3	2.17	0.45
1:A:900:GLU:N	1:A:900:GLU:OE1	2.49	0.45
1:A:1239:PRO:HG2	1:A:1243:TYR:HE2	1.81	0.45
1:A:1457:GLN:HA	1:A:1460:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1763:THR:HA	1:A:1766:LEU:HB3	1.99	0.45
1:A:3298:LEU:HD22	1:A:3333:THR:HG23	1.99	0.45
1:A:3455:LYS:NZ	1:A:3489:SER:O	2.24	0.45
1:A:4115:ASN:O	1:A:4119:ARG:HG2	2.17	0.45
2:B:35:ARG:C	2:B:161:MET:HE3	2.41	0.45
2:B:277:VAL:HG21	3:C:357:MET:HE3	1.99	0.45
1:A:52:ALA:HA	1:A:55:THR:HG22	1.98	0.45
1:A:345:PHE:HA	1:A:348:ILE:HG12	1.99	0.45
1:A:1102:GLU:OE1	1:A:1152:ARG:NH2	2.50	0.45
1:A:1324:PRO:HB2	1:A:1325:GLN:H	1.62	0.45
1:A:3389:VAL:O	1:A:3393:GLU:N	2.50	0.45
3:C:40:MET:O	3:C:44:ARG:HG2	2.17	0.45
5:H:179:ARG:NH1	6:J:805:TRP:HB3	2.32	0.45
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.99	0.44
1:A:1399:CYS:O	1:A:1403:MET:HG2	2.17	0.44
1:A:1776:GLU:HA	1:A:1779:GLN:HG2	1.99	0.44
1:A:2321:GLU:O	1:A:2325:LEU:HG	2.17	0.44
2:B:289:TYR:CE1	3:C:309:ASP:HB3	2.53	0.44
3:C:363:LYS:HD2	3:C:418:CYS:SG	2.57	0.44
3:C:543:LYS:HD3	3:C:545:LYS:HZ3	1.82	0.44
5:H:47:VAL:HG11	5:H:52:ILE:HD12	1.99	0.44
5:H:59:MET:HE1	5:H:99:LYS:H	1.82	0.44
5:H:94:TYR:CE2	5:H:96:PHE:HB3	2.52	0.44
5:H:158:VAL:HG22	6:J:840:ILE:HD11	2.00	0.44
1:A:624:ILE:O	1:A:628:GLU:HG2	2.17	0.44
1:A:2820:MET:SD	1:A:2829:LYS:HG2	2.57	0.44
2:B:374:LEU:O	3:C:540:ILE:HG13	2.18	0.44
5:H:131:LEU:HD23	5:H:131:LEU:HA	1.79	0.44
1:A:475:LEU:O	1:A:479:ILE:HD13	2.17	0.44
1:A:1115:HIS:CE1	1:A:1181:THR:H	2.35	0.44
1:A:1871:MET:HG2	1:A:1940:TYR:HA	2.00	0.44
1:A:3174:ASP:HB3	1:A:3179:TRP:HE1	1.82	0.44
4:F:158:HIS:CE1	4:F:184:PHE:HB3	2.52	0.44
4:G:105:ILE:HD11	4:G:120:ASN:ND2	2.33	0.44
1:A:1215:GLU:HB2	1:A:1219:PHE:HD2	1.81	0.44
1:A:2424:MET:HG2	1:A:2461:PHE:HZ	1.82	0.44
1:A:2787:HIS:O	1:A:2791:ILE:HG12	2.18	0.44
1:A:3570:ASP:OD2	1:A:3686:TRP:NE1	2.50	0.44
1:A:3880:ALA:HB2	1:A:3965:ARG:CZ	2.48	0.44
2:B:131:PHE:CE1	2:B:135:MET:HG3	2.52	0.44
5:H:22:VAL:HG23	5:H:34:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:18:HIS:HE2	5:I:38:ASP:HB3	1.83	0.44
1:A:535:LEU:HD13	1:A:565:TYR:HD2	1.82	0.44
1:A:3923:ARG:HB3	1:A:3928:PHE:HE1	1.83	0.44
3:C:118:ILE:O	3:C:122:THR:HG23	2.17	0.44
6:J:696:ASP:OD1	6:J:696:ASP:N	2.50	0.44
6:J:721:VAL:HG22	6:J:743:MET:SD	2.57	0.44
1:A:849:GLU:HA	1:A:852:ARG:HD3	1.99	0.44
1:A:851:ILE:O	1:A:855:VAL:HG23	2.17	0.44
1:A:2454:LEU:O	1:A:2458:VAL:HG23	2.18	0.44
1:A:2799:GLN:OE1	1:A:2800:ARG:NH1	2.50	0.44
1:A:3008:TRP:NE1	1:A:3054:GLN:HE22	2.15	0.44
6:J:663:GLU:OE2	6:J:697:THR:OG1	2.30	0.44
1:A:162:LEU:HD21	2:B:299:LYS:HB3	2.00	0.44
1:A:1637:SER:O	1:A:1642:LYS:NZ	2.42	0.44
1:A:2474:TYR:OH	1:A:2512:ASP:OD2	2.24	0.44
1:A:2825:THR:O	1:A:2829:LYS:HG3	2.17	0.44
1:A:3029:LYS:HA	1:A:3064:PHE:HE1	1.82	0.44
1:A:3897:PHE:CZ	1:A:3901:ARG:HD2	2.53	0.44
2:B:118:GLU:O	2:B:121:GLN:HG2	2.18	0.44
3:C:86:PRO:HB3	3:C:90:LEU:HD23	2.00	0.44
4:F:24:LEU:N	4:F:38:VAL:HA	2.33	0.44
1:A:189:MET:SD	1:A:189:MET:N	2.91	0.44
2:B:418:GLU:HB3	2:B:430:PRO:HD3	1.99	0.44
7:D:32:DA:H2"	7:D:33:DA:C8	2.53	0.44
1:A:1403:MET:HB3	1:A:1463:LEU:HD12	1.99	0.44
1:A:1471:GLN:OE1	1:A:1477:HIS:N	2.51	0.44
1:A:3891:SER:O	1:A:3891:SER:OG	2.34	0.44
2:B:68:GLN:HE22	2:B:120:ASP:HA	1.82	0.44
5:I:69:GLU:HG3	5:I:106:PHE:HZ	1.83	0.44
5:I:71:ARG:HE	5:I:75:LEU:HD11	1.83	0.44
1:A:79:ARG:O	1:A:83:GLU:HG2	2.18	0.43
1:A:273:ARG:O	1:A:277:LEU:HG	2.17	0.43
1:A:1009:LEU:HD13	1:A:1036:PHE:CE2	2.53	0.43
1:A:1142:HIS:CG	1:A:1197:LEU:HD12	2.53	0.43
1:A:2125:TRP:O	1:A:2129:LEU:HG	2.18	0.43
1:A:2460:GLU:OE1	1:A:2460:GLU:N	2.50	0.43
3:C:465:LYS:N	3:C:474:GLU:O	2.47	0.43
5:H:10:LEU:HD21	5:H:18:HIS:HB2	2.00	0.43
1:A:877:ASP:OD1	1:A:878:GLU:N	2.49	0.43
1:A:907:LEU:HA	1:A:910:PHE:HD2	1.83	0.43
1:A:1857:LYS:NZ	1:A:1860:GLU:HG3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1876:ILE:HA	1:A:1879:VAL:HG22	2.00	0.43
1:A:2492:ASP:N	1:A:2492:ASP:OD1	2.51	0.43
6:J:809:PRO:HG2	6:J:810:LEU:HD12	1.99	0.43
6:J:821:ASP:OD2	6:J:871:ARG:NH1	2.50	0.43
1:A:484:HIS:CE1	1:A:488:ILE:HD11	2.53	0.43
1:A:913:ARG:HD2	1:A:913:ARG:HA	1.71	0.43
1:A:1413:ASP:OD1	1:A:1414:ILE:N	2.48	0.43
1:A:1824:LEU:O	1:A:1828:LEU:HD23	2.19	0.43
1:A:1860:GLU:OE1	1:A:1861:SER:N	2.52	0.43
1:A:2773:ARG:HH11	1:A:2785:ILE:HB	1.84	0.43
1:A:3588:TRP:CG	1:A:3613:MET:HG3	2.53	0.43
1:A:3828:TYR:HA	1:A:3835:PRO:HD2	2.00	0.43
1:A:3959:MET:HG3	1:A:4124:TRP:CZ2	2.54	0.43
5:H:5:ILE:HG12	5:H:126:LEU:HG	2.00	0.43
6:J:663:GLU:HA	6:J:688:TYR:HB3	1.99	0.43
1:A:144:MET:HE2	1:A:144:MET:N	2.34	0.43
1:A:898:PHE:HB2	1:A:901:MET:O	2.18	0.43
1:A:913:ARG:NE	1:A:2803:ILE:HD11	2.32	0.43
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.19	0.43
1:A:1779:GLN:OE1	1:A:1826:THR:HG21	2.18	0.43
1:A:1985:LYS:HD2	1:A:2183:HIS:HB2	2.00	0.43
1:A:2553:HIS:O	1:A:2557:LEU:HG	2.17	0.43
1:A:3129:LEU:O	1:A:3132:VAL:HG12	2.17	0.43
2:B:462:MET:O	2:B:466:VAL:HG12	2.19	0.43
1:A:1568:ASN:ND2	1:A:1603:GLN:HE21	2.16	0.43
1:A:1627:LYS:HA	1:A:1670:GLU:OE2	2.18	0.43
1:A:2475:ASN:HA	1:A:2478:MET:HG2	1.99	0.43
1:A:2486:ASP:OD1	1:A:2486:ASP:N	2.50	0.43
1:A:3155:VAL:HG22	1:A:3156:PRO:HD3	2.01	0.43
1:A:3544:ASP:OD1	1:A:3548:GLY:N	2.51	0.43
1:A:3722:PHE:HD1	1:A:3740:ILE:HG12	1.83	0.43
1:A:4055:ASN:O	1:A:4058:VAL:HG12	2.18	0.43
2:B:143:LEU:HA	2:B:146:VAL:HG22	2.01	0.43
3:C:203:GLU:HA	3:C:206:GLU:HG3	2.00	0.43
3:C:245:ILE:HD12	3:C:245:ILE:HA	1.90	0.43
3:C:267:ILE:H	3:C:361:VAL:HB	1.83	0.43
3:C:357:MET:HE3	3:C:425:PRO:HB3	2.00	0.43
1:A:584:GLU:N	1:A:613:HIS:O	2.39	0.43
1:A:1051:LYS:HA	1:A:1054:VAL:HG12	1.99	0.43
1:A:1255:CYS:O	1:A:1259:LEU:HG	2.17	0.43
1:A:1428:ILE:HG12	1:A:1451:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2500:LYS:HA	1:A:2503:LYS:NZ	2.33	0.43
1:A:3164:TRP:O	1:A:3186:ARG:NH1	2.52	0.43
1:A:3638:LYS:O	1:A:3642:LYS:HG2	2.18	0.43
1:A:3821:SER:O	1:A:3825:LYS:HG3	2.19	0.43
1:A:3879:PRO:HG2	1:A:3882:LEU:HD21	2.01	0.43
3:C:543:LYS:HD3	3:C:543:LYS:HA	1.85	0.43
4:F:44:VAL:H	4:F:131:VAL:HG22	1.83	0.43
6:J:889:LEU:HD11	6:J:906:GLU:HG2	2.00	0.43
1:A:38:LEU:HB3	1:A:84:GLU:HG2	2.01	0.43
1:A:200:PHE:CE1	1:A:227:LEU:HD21	2.53	0.43
1:A:463:LYS:HG3	1:A:544:ILE:HG21	2.01	0.43
1:A:677:ALA:HA	1:A:680:ILE:HG12	2.00	0.43
1:A:2223:VAL:O	1:A:2223:VAL:HG13	2.19	0.43
1:A:3451:LEU:HD11	1:A:3483:MET:HA	2.01	0.43
3:C:80:HIS:O	3:C:81:ARG:HD2	2.18	0.43
1:A:138:PHE:O	1:A:142:ARG:HG2	2.19	0.43
1:A:913:ARG:HE	1:A:2803:ILE:HD11	1.83	0.43
1:A:1369:MET:HE3	1:A:1418:HIS:HB2	2.01	0.43
1:A:1849:ASP:HA	1:A:1852:LYS:HG2	1.99	0.43
1:A:2544:SER:HA	1:A:2842:ARG:NH2	2.34	0.43
1:A:3301:LEU:HA	1:A:3304:VAL:HG22	2.00	0.43
1:A:3627:ALA:HA	1:A:3630:ARG:HB2	2.00	0.43
2:B:173:ASP:OD1	2:B:173:ASP:N	2.52	0.43
2:B:266:ASP:OD1	2:B:267:ILE:N	2.52	0.43
2:B:479:GLU:HB3	3:C:427:MET:HG3	2.01	0.43
2:B:509:PRO:HB3	3:C:343:LEU:HA	2.00	0.43
3:C:225:TYR:HB3	3:C:230:SER:OG	2.19	0.43
5:H:117:GLU:OE1	5:H:117:GLU:N	2.51	0.43
1:A:887:ASP:OD1	1:A:887:ASP:N	2.50	0.43
1:A:1102:GLU:O	1:A:1106:ILE:HG12	2.19	0.43
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.52	0.43
1:A:1623:LEU:HD13	1:A:1661:PHE:CG	2.52	0.43
1:A:1661:PHE:HA	1:A:1665:HIS:HB2	2.00	0.43
1:A:1780:SER:HB2	1:A:1784:ARG:HH12	1.82	0.43
1:A:3259:LEU:O	1:A:3276:TRP:NE1	2.35	0.43
1:A:3913:ILE:HD13	1:A:3987:ALA:HB3	2.01	0.43
2:B:192:ASP:O	2:B:196:THR:HG23	2.18	0.43
2:B:463:LYS:HG2	3:C:387:LEU:HD11	2.00	0.43
2:B:474:ARG:HD2	2:B:474:ARG:HA	1.69	0.43
1:A:710:PHE:HA	1:A:713:GLU:CD	2.43	0.43
1:A:1055:ASN:O	1:A:1059:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1965:PHE:HE2	1:A:1973:LYS:HZ1	1.66	0.43
1:A:2514:ASN:OD1	1:A:2517:LEU:N	2.40	0.43
1:A:2586:PHE:CD1	1:A:2782:ASP:HB2	2.54	0.43
1:A:2832:ILE:O	1:A:2835:LYS:HG3	2.18	0.43
1:A:2962:ARG:HA	1:A:3989:ARG:NH1	2.30	0.43
1:A:2995:GLU:O	1:A:2999:LEU:HG	2.19	0.43
1:A:3139:GLN:O	1:A:3139:GLN:NE2	2.52	0.43
1:A:4002:MET:O	1:A:4005:PHE:HB3	2.18	0.43
2:B:357:LYS:O	2:B:359:HIS:ND1	2.52	0.43
4:F:54:VAL:HG22	4:F:119:TRP:CH2	2.54	0.43
1:A:225:LYS:HE2	1:A:253:LEU:HD22	2.01	0.42
1:A:688:PRO:HG3	1:A:704:PHE:HE2	1.84	0.42
1:A:865:GLN:H	1:A:3169:PRO:HA	1.84	0.42
1:A:1465:HIS:CE1	1:A:1476:HIS:HE1	2.37	0.42
1:A:2452:ARG:NH2	1:A:2453:GLU:OE2	2.52	0.42
1:A:3361:GLU:N	1:A:3361:GLU:OE1	2.52	0.42
1:A:4065:LEU:HA	1:A:4069:GLU:HB2	2.00	0.42
5:I:43:TRP:HD1	5:I:93:CYS:SG	2.42	0.42
8:E:21:DA:C8	8:E:21:DA:H5"	2.54	0.42
1:A:525:LYS:O	1:A:528:VAL:HG22	2.19	0.42
1:A:1056:THR:O	1:A:1059:LEU:HG	2.19	0.42
1:A:2578:GLU:HA	1:A:2784:GLN:HG3	2.00	0.42
1:A:3014:CYS:SG	1:A:3015:SER:N	2.92	0.42
1:A:3101:TYR:O	1:A:3105:ASN:ND2	2.52	0.42
1:A:3669:LYS:HA	1:A:3672:LYS:HD2	1.99	0.42
2:B:474:ARG:HH11	2:B:475:SER:H	1.67	0.42
4:F:210:PHE:N	4:F:215:GLN:HB3	2.34	0.42
1:A:1178:ARG:HH22	1:A:1183:CYS:HB3	1.84	0.42
1:A:1597:LEU:O	1:A:1601:LEU:HG	2.19	0.42
1:A:1948:ALA:O	1:A:1952:ILE:HG12	2.18	0.42
1:A:3636:PHE:CE2	1:A:3640:PHE:HB2	2.54	0.42
1:A:3912:CYS:HB3	1:A:3961:PHE:CG	2.55	0.42
2:B:95:ASN:ND2	2:B:99:PHE:H	2.16	0.42
3:C:7:LYS:O	3:C:129:LYS:N	2.52	0.42
3:C:365:PHE:CE1	3:C:418:CYS:HB3	2.53	0.42
4:G:34:TYR:H	4:G:49:VAL:HG11	1.83	0.42
5:H:168:ALA:HB1	6:J:810:LEU:HD11	2.01	0.42
6:J:673:GLN:HG2	6:J:681:ARG:HH22	1.82	0.42
1:A:3337:ILE:HG23	1:A:3377:LEU:HD13	2.01	0.42
2:B:127:GLY:HA2	2:B:130:ARG:HG2	2.01	0.42
3:C:345:PHE:HB3	3:C:389:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:175:ILE:HG13	4:G:167:TYR:HE1	1.82	0.42
6:J:711:ASN:HA	6:J:714:LEU:HB2	2.00	0.42
8:E:35:DT:H6	8:E:35:DT:H2'	1.63	0.42
1:A:172:GLU:OE1	1:A:172:GLU:N	2.42	0.42
1:A:1261:LEU:HD22	1:A:1340:ARG:HG3	2.01	0.42
1:A:1482:GLU:O	1:A:1486:LEU:HB2	2.19	0.42
1:A:1791:CYS:O	1:A:1795:VAL:HG23	2.18	0.42
1:A:2168:LEU:HD11	1:A:2189:ILE:HG23	2.01	0.42
1:A:2873:PRO:HG3	1:A:2922:ARG:NH1	2.34	0.42
3:C:381:ILE:HB	3:C:410:PRO:HB3	2.02	0.42
4:F:157:LEU:HD21	4:G:157:LEU:HB2	2.02	0.42
4:F:179:LEU:HD13	4:G:159:MET:SD	2.60	0.42
4:G:45:TRP:HB3	4:G:123:CYS:HB3	2.01	0.42
4:G:132:SER:HA	4:G:136:ILE:HB	2.01	0.42
1:A:986:PRO:HA	1:A:989:MET:HE2	2.01	0.42
1:A:1253:THR:O	1:A:1257:LEU:HG	2.18	0.42
1:A:1790:SER:C	1:A:1794:GLN:HE21	2.28	0.42
1:A:1899:VAL:HB	1:A:1911:LEU:HD22	2.01	0.42
1:A:2215:LEU:O	1:A:2219:LEU:HG	2.20	0.42
1:A:2411:LEU:O	1:A:2415:LEU:HG	2.20	0.42
1:A:2537:ASP:HA	1:A:2540:LEU:HB3	2.02	0.42
1:A:2855:VAL:O	1:A:2859:GLN:HG3	2.20	0.42
1:A:3617:LEU:O	1:A:3633:ILE:HG12	2.19	0.42
1:A:3772:ASN:OD1	1:A:3788:LEU:N	2.53	0.42
1:A:3820:MET:HG3	1:A:3824:GLU:OE1	2.20	0.42
2:B:353:LEU:HD11	2:B:415:PRO:HD2	2.01	0.42
4:F:76:LEU:HD13	4:F:117:PHE:HB2	2.01	0.42
4:G:61:LEU:HD23	4:G:118:TYR:HB3	2.01	0.42
5:H:169:LYS:HB2	5:I:169:LYS:HG3	2.02	0.42
6:J:706:ASN:OD1	6:J:708:ARG:HG2	2.19	0.42
6:J:717:LYS:HG3	6:J:718:HIS:CE1	2.55	0.42
1:A:125:ILE:HB	1:A:126:PRO:HD3	2.02	0.42
1:A:414:LEU:HD11	1:A:464:VAL:HG11	2.02	0.42
1:A:1235:ILE:HD12	1:A:1238:GLN:O	2.20	0.42
1:A:2358:ASP:OD1	1:A:2358:ASP:N	2.53	0.42
1:A:2794:LEU:HD21	1:A:2808:LEU:HD13	2.02	0.42
1:A:3969:ASN:HD22	1:A:3972:LEU:HD13	1.85	0.42
2:B:514:MET:SD	2:B:518:LEU:HD23	2.60	0.42
3:C:406:GLY:HA2	3:C:424:LEU:H	1.85	0.42
5:H:7:ARG:NE	5:I:128:CYS:HA	2.35	0.42
1:A:236:LYS:HE2	1:A:236:LYS:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:H	1:A:239:GLU:CD	2.26	0.42
1:A:491:CYS:HA	1:A:625:ASN:ND2	2.34	0.42
1:A:1539:SER:HB2	1:A:1552:HIS:CD2	2.54	0.42
1:A:2145:PHE:O	1:A:2149:LEU:HG	2.20	0.42
1:A:2257:PHE:CE1	1:A:2299:TYR:HA	2.54	0.42
1:A:3037:GLN:O	1:A:3041:LEU:HG	2.20	0.42
1:A:3386:SER:O	1:A:3390:GLN:OE1	2.38	0.42
1:A:3537:SER:HA	1:A:3540:TYR:CG	2.54	0.42
2:B:57:LEU:HD23	2:B:62:MET:HE3	2.02	0.42
2:B:247:ARG:HB3	2:B:484:GLN:HE22	1.85	0.42
2:B:463:LYS:O	2:B:467:GLU:HG2	2.19	0.42
5:H:42:ALA:H	5:H:116:VAL:HG22	1.85	0.42
1:A:131:LEU:HD22	1:A:177:LEU:HG	2.01	0.42
1:A:174:VAL:HA	1:A:177:LEU:HB2	2.02	0.42
1:A:793:LEU:HD22	1:A:869:ASN:HB2	2.01	0.42
1:A:1366:THR:HB	1:A:1370:ARG:HH12	1.83	0.42
1:A:2970:LYS:HE3	1:A:2970:LYS:HB3	1.92	0.42
1:A:3407:ALA:O	1:A:3410:ILE:HG12	2.19	0.42
1:A:3474:ARG:HE	1:A:3474:ARG:HB2	1.67	0.42
1:A:3950:THR:HG23	1:A:3957:GLU:H	1.85	0.42
2:B:113:ALA:O	2:B:117:LEU:HG	2.20	0.42
2:B:215:LEU:HA	2:B:218:ARG:HE	1.85	0.42
3:C:91:LEU:HD21	3:C:499:LEU:HD11	2.00	0.42
5:I:28:LEU:O	5:I:71:ARG:NH1	2.52	0.42
5:I:189:THR:O	5:I:192:ARG:HG3	2.20	0.42
6:J:879:ARG:O	6:J:885:LYS:NZ	2.49	0.42
6:J:889:LEU:HD13	6:J:893:TRP:CD1	2.55	0.42
1:A:1165:LEU:O	1:A:1169:VAL:HG23	2.20	0.42
1:A:3023:ASN:HB2	1:A:3031:TRP:CH2	2.55	0.42
1:A:3100:LYS:HA	1:A:3103:ILE:HG22	2.01	0.42
1:A:3350:GLU:OE1	1:A:3350:GLU:N	2.53	0.42
1:A:3544:ASP:OD1	1:A:3547:THR:N	2.51	0.42
1:A:3858:MET:HE2	1:A:3858:MET:HB2	1.65	0.42
2:B:41:LEU:HD12	2:B:86:VAL:O	2.20	0.42
4:F:130:LEU:O	4:F:134:HIS:HB2	2.20	0.42
4:G:113:SER:O	4:G:113:SER:OG	2.36	0.42
7:D:28:DT:H2"	7:D:29:DA:C8	2.55	0.42
1:A:187:SER:HA	1:A:190:ILE:HB	2.02	0.41
1:A:2325:LEU:HD22	1:A:2328:ARG:HH22	1.85	0.41
2:B:39:ILE:HG22	2:B:84:ALA:HB3	2.02	0.41
2:B:509:PRO:HB2	2:B:511:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:20:LEU:HD23	5:H:74:LEU:HA	2.01	0.41
1:A:82:ARG:O	1:A:86:LEU:HD23	2.20	0.41
1:A:200:PHE:CE2	1:A:227:LEU:HD11	2.55	0.41
1:A:250:ASN:C	1:A:254:LYS:HZ1	2.27	0.41
1:A:435:LEU:O	1:A:438:LEU:HG	2.20	0.41
1:A:446:PHE:CE2	1:A:530:LEU:HB2	2.54	0.41
1:A:529:ASP:OD1	1:A:529:ASP:N	2.52	0.41
1:A:1092:GLU:OE2	1:A:1094:SER:OG	2.38	0.41
1:A:1101:PHE:CD2	1:A:1163:LEU:HD12	2.55	0.41
1:A:1212:LEU:HD13	1:A:1220:LEU:HD22	2.02	0.41
1:A:1527:ARG:HH12	1:A:1531:LEU:HG	1.86	0.41
1:A:1739:TYR:O	1:A:1743:MET:HG2	2.20	0.41
1:A:2227:LYS:O	1:A:2230:VAL:HG12	2.20	0.41
1:A:2300:PHE:CD1	1:A:2341:LEU:HD21	2.55	0.41
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.55	0.41
1:A:3605:ASN:HA	1:A:3608:LYS:HG2	2.02	0.41
4:F:3:GLU:HG2	4:F:4:LEU:N	2.34	0.41
4:F:34:TYR:HD2	4:F:36:LEU:HB3	1.85	0.41
4:G:50:ASP:O	4:G:54:VAL:HG23	2.20	0.41
5:I:140:LYS:HD2	5:I:143:HIS:NE2	2.36	0.41
6:J:670:THR:N	6:J:703:GLY:HA3	2.33	0.41
1:A:71:LYS:HE3	1:A:71:LYS:HB2	1.78	0.41
1:A:778:ILE:HD13	1:A:778:ILE:HA	1.91	0.41
1:A:848:LEU:HA	1:A:851:ILE:HD12	2.01	0.41
1:A:1092:GLU:O	1:A:1096:VAL:HG23	2.20	0.41
1:A:1487:VAL:HG11	1:A:1515:LEU:HD21	2.00	0.41
1:A:3027:LEU:HD13	1:A:3064:PHE:HB2	2.02	0.41
1:A:3903:HIS:HE1	1:A:3936:GLY:HA2	1.86	0.41
2:B:319:SER:HB3	2:B:328:ILE:HA	2.01	0.41
2:B:388:LYS:NZ	3:C:451:LEU:HB3	2.34	0.41
4:G:190:LEU:HA	4:G:194:MET:HG2	2.02	0.41
5:I:69:GLU:HA	5:I:72:LYS:HG2	2.01	0.41
1:A:63:PHE:O	1:A:66:LEU:HB2	2.21	0.41
1:A:1596:VAL:O	1:A:1600:MET:HG2	2.20	0.41
1:A:1862:THR:O	1:A:1866:GLN:OE1	2.39	0.41
1:A:2840:PHE:O	1:A:2844:LEU:HG	2.21	0.41
1:A:3353:GLU:HG2	1:A:3356:ALA:H	1.86	0.41
1:A:3572:ILE:HA	1:A:3575:LEU:HD12	2.03	0.41
1:A:3578:LEU:O	1:A:3736:LYS:HE3	2.19	0.41
1:A:3805:TRP:CD1	1:A:3807:GLU:H	2.38	0.41
1:A:4013:TRP:NE1	1:A:4035:GLU:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:HA	2:B:247:ARG:HD2	1.87	0.41
2:B:360:HIS:CE1	2:B:443:LYS:HE2	2.56	0.41
2:B:479:GLU:HA	3:C:426:PHE:HB3	2.01	0.41
4:G:71:ALA:HB2	5:H:106:PHE:HZ	1.84	0.41
6:J:858:GLU:OE1	6:J:883:LYS:N	2.49	0.41
1:A:19:LEU:HB3	1:A:34:LEU:HD13	2.03	0.41
1:A:565:TYR:CE1	1:A:642:PHE:HB2	2.56	0.41
1:A:570:LYS:HB3	1:A:645:TRP:CH2	2.55	0.41
1:A:786:GLN:OE1	1:A:786:GLN:N	2.49	0.41
1:A:1089:PHE:HE1	1:A:1099:PHE:HD2	1.68	0.41
1:A:1146:ASN:C	1:A:1146:ASN:HD22	2.27	0.41
1:A:1186:LYS:HD2	1:A:1186:LYS:HA	1.82	0.41
1:A:1212:LEU:HA	1:A:1215:GLU:HG2	2.03	0.41
1:A:2094:MET:HB3	1:A:2145:PHE:HE1	1.84	0.41
1:A:3026:ASP:OD1	1:A:3026:ASP:N	2.53	0.41
1:A:3061:LEU:O	1:A:3065:ILE:HG12	2.19	0.41
1:A:3163:THR:O	1:A:3167:ARG:HG3	2.21	0.41
1:A:3828:TYR:HD1	1:A:3835:PRO:HD2	1.85	0.41
2:B:301:ARG:NH1	2:B:313:PRO:HD3	2.35	0.41
3:C:134:ILE:HB	3:C:163:PHE:HD1	1.85	0.41
3:C:402:ASN:ND2	7:D:25:DA:H3'	2.34	0.41
4:G:108:VAL:O	4:G:108:VAL:HG13	2.21	0.41
5:H:154:ASP:O	5:H:158:VAL:HG23	2.20	0.41
6:J:891:GLU:HB3	6:J:895:THR:HB	2.02	0.41
1:A:164:LYS:C	1:A:167:PRO:HD2	2.45	0.41
1:A:574:LYS:HB2	1:A:574:LYS:HE3	1.86	0.41
1:A:1430:GLU:O	1:A:1434:VAL:HG13	2.20	0.41
1:A:2133:LEU:HD23	1:A:2164:TRP:HZ3	1.85	0.41
1:A:2259:LYS:HE2	1:A:2259:LYS:HB2	1.91	0.41
1:A:2486:ASP:HB2	1:A:2488:GLU:CD	2.45	0.41
1:A:3232:ARG:NH2	1:A:3268:THR:OG1	2.54	0.41
1:A:3494:GLN:HA	1:A:3709:GLY:HA2	2.01	0.41
1:A:3499:ILE:HA	1:A:3502:MET:HE2	2.03	0.41
1:A:3758:LEU:HD13	1:A:3801:GLY:HA3	2.03	0.41
1:A:570:LYS:O	1:A:574:LYS:HG3	2.20	0.41
1:A:639:ALA:O	1:A:643:GLU:N	2.54	0.41
1:A:865:GLN:HB3	1:A:3170:ASP:HB2	2.02	0.41
1:A:2251:ILE:HD11	1:A:2285:LEU:HD13	2.01	0.41
1:A:2492:ASP:O	1:A:2495:SER:OG	2.27	0.41
1:A:3298:LEU:HD13	1:A:3337:ILE:HB	2.02	0.41
1:A:3330:LEU:HD23	1:A:3384:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3347:CYS:SG	1:A:3348:LEU:N	2.93	0.41
1:A:3856:MET:N	1:A:3856:MET:SD	2.94	0.41
3:C:82:HIS:CE1	3:C:84:MET:HB3	2.55	0.41
5:H:191:ILE:HD13	6:J:765:TYR:CD1	2.56	0.41
1:A:100:ILE:HB	1:A:141:SER:HB2	2.01	0.41
1:A:101:ALA:HA	1:A:144:MET:HG3	2.02	0.41
1:A:637:LYS:HD3	1:A:638:GLN:O	2.21	0.41
1:A:664:SER:O	1:A:668:LYS:HG3	2.21	0.41
1:A:2338:GLU:OE2	1:A:2340:SER:OG	2.29	0.41
2:B:35:ARG:HD2	2:B:80:ARG:NE	2.36	0.41
3:C:11:VAL:HG21	3:C:114:SER:HB2	2.03	0.41
3:C:197:ILE:HB	3:C:201:GLN:HB2	2.03	0.41
3:C:261:ILE:HA	3:C:366:ALA:HA	2.02	0.41
4:F:46:HIS:NE2	4:F:127:SER:HB2	2.36	0.41
5:I:154:ASP:O	5:I:158:VAL:HG23	2.21	0.41
1:A:86:LEU:HD12	1:A:129:ASP:HB2	2.03	0.41
1:A:174:VAL:O	1:A:178:LEU:HG	2.21	0.41
1:A:653:LEU:HD11	1:A:669:LEU:HG	2.03	0.41
1:A:712:LYS:O	1:A:716:VAL:HG23	2.21	0.41
1:A:1032:CYS:O	1:A:1035:GLU:HG2	2.21	0.41
1:A:1260:LEU:HD22	1:A:1293:ALA:HB1	2.03	0.41
1:A:1419:LEU:O	1:A:1423:ILE:N	2.49	0.41
1:A:1572:LEU:HA	1:A:1575:LEU:HD21	2.03	0.41
1:A:1608:ARG:HA	1:A:1611:GLN:O	2.21	0.41
1:A:1817:GLN:HG3	1:A:1821:ASP:OD2	2.20	0.41
1:A:2086:ASP:O	1:A:2090:ARG:NE	2.50	0.41
1:A:2252:PRO:C	1:A:2254:ARG:H	2.29	0.41
1:A:2368:THR:HG21	1:A:2400:VAL:HG22	2.03	0.41
1:A:2447:LYS:HE2	1:A:2447:LYS:HB2	1.96	0.41
1:A:3324:ARG:HB3	1:A:3391:ALA:HB3	2.02	0.41
1:A:3583:LEU:HD13	1:A:3733:ARG:HD2	2.02	0.41
2:B:363:ARG:HB3	2:B:436:PHE:CD1	2.56	0.41
2:B:452:ILE:C	2:B:453:MET:HE2	2.46	0.41
3:C:138:LEU:HA	3:C:142:PHE:HE2	1.85	0.41
3:C:164:PHE:CD2	3:C:231:LEU:HD22	2.56	0.41
3:C:326:VAL:HA	3:C:329:GLU:CD	2.45	0.41
3:C:443:LYS:HG3	3:C:444:TYR:CD2	2.56	0.41
5:H:10:LEU:HD11	5:H:18:HIS:CG	2.55	0.41
5:H:17:THR:C	5:H:18:HIS:HD1	2.28	0.41
6:J:865:ILE:N	6:J:889:LEU:O	2.45	0.41
1:A:204:LEU:O	1:A:207:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:HG23	1:A:399:GLN:HG2	2.03	0.41
1:A:1713:VAL:HA	1:A:1716:GLN:NE2	2.36	0.41
1:A:1923:PHE:HA	1:A:1941:HIS:HD2	1.85	0.41
1:A:2098:THR:HA	1:A:2101:VAL:HG22	2.03	0.41
1:A:2274:ILE:HA	1:A:2277:LEU:CD2	2.51	0.41
1:A:3885:ARG:HA	1:A:3888:VAL:HB	2.03	0.41
1:A:4022:LYS:HE2	1:A:4022:LYS:HB2	1.92	0.41
1:A:4055:ASN:HD21	1:A:4057:ALA:HB3	1.86	0.41
5:H:17:THR:HB	5:I:124:ARG:CG	2.50	0.41
1:A:377:ASN:O	1:A:381:VAL:HG23	2.21	0.40
1:A:1793:THR:O	1:A:1797:LEU:HG	2.22	0.40
1:A:3104:GLN:NE2	1:A:3105:ASN:OD1	2.54	0.40
1:A:3233:SER:HA	1:A:3272:TRP:HZ2	1.86	0.40
1:A:3573:ASN:O	1:A:3577:GLN:HG2	2.21	0.40
1:A:3962:ARG:HD2	1:A:3962:ARG:HA	1.93	0.40
1:A:3999:THR:HG23	1:A:4044:ILE:HD11	2.03	0.40
2:B:461:LYS:HE3	2:B:461:LYS:HB3	1.96	0.40
3:C:68:LEU:HD12	3:C:68:LEU:HA	1.96	0.40
4:G:114:GLY:HA3	5:H:61:MET:C	2.46	0.40
5:H:131:LEU:HB3	5:I:4:LYS:HZ2	1.85	0.40
6:J:668:SER:O	6:J:670:THR:HG23	2.21	0.40
6:J:879:ARG:HE	6:J:880:ARG:NH1	2.19	0.40
7:D:40:DT:O2	8:E:18:DA:H8	2.04	0.40
1:A:146:GLU:HB2	1:A:184:VAL:H	1.85	0.40
1:A:283:SER:O	1:A:286:LEU:HG	2.21	0.40
1:A:730:LEU:HD13	1:A:755:ALA:HB2	2.03	0.40
1:A:2990:GLU:HG2	1:A:2994:TRP:CE2	2.56	0.40
1:A:3274:VAL:HG13	1:A:3315:TYR:CD1	2.56	0.40
3:C:236:VAL:HG13	3:C:237:PHE:HD1	1.86	0.40
3:C:307:LYS:O	3:C:310:ILE:HG12	2.21	0.40
4:F:26:LYS:HG2	4:F:37:LEU:HB2	2.04	0.40
4:G:34:TYR:N	4:G:49:VAL:HG11	2.37	0.40
4:G:128:PRO:O	4:G:132:SER:CB	2.61	0.40
1:A:65:LEU:O	1:A:69:VAL:HG22	2.21	0.40
1:A:931:CYS:O	1:A:984:TYR:OH	2.35	0.40
1:A:2185:MET:O	1:A:2189:ILE:HG12	2.22	0.40
1:A:2367:VAL:O	1:A:2371:PHE:N	2.50	0.40
1:A:2508:GLN:HG2	1:A:2549:LYS:HD2	2.03	0.40
1:A:2818:LYS:HD3	1:A:2818:LYS:HA	1.83	0.40
1:A:3190:LEU:HB2	1:A:3235:LYS:HE3	2.02	0.40
1:A:3903:HIS:ND1	1:A:3934:THR:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HD23	2:B:168:LEU:HD13	2.03	0.40
2:B:376:ILE:HG12	3:C:540:ILE:HG12	2.03	0.40
2:B:506:LEU:O	3:C:343:LEU:HD22	2.22	0.40
4:F:159:MET:HE1	4:F:160:LYS:NZ	2.37	0.40
4:G:54:VAL:HG22	4:G:119:TRP:CH2	2.56	0.40
5:H:7:ARG:NH2	5:I:132:ASP:OD1	2.53	0.40
1:A:1642:LYS:HA	1:A:1645:VAL:HG12	2.03	0.40
1:A:1923:PHE:HA	1:A:1941:HIS:CD2	2.57	0.40
1:A:2231:PHE:O	1:A:2235:LEU:HG	2.21	0.40
1:A:2342:CYS:HB2	1:A:2374:LEU:HD21	2.03	0.40
1:A:2438:ILE:O	1:A:2442:MET:HG3	2.21	0.40
1:A:3369:ASP:O	1:A:3373:VAL:HG23	2.21	0.40
1:A:3493:TRP:HZ3	1:A:3520:GLU:HB3	1.85	0.40
1:A:3834:ALA:O	1:A:3838:GLU:N	2.39	0.40
1:A:3909:ALA:O	1:A:3984:MET:HE1	2.21	0.40
1:A:4068:HIS:HB3	1:A:4071:ALA:HB3	2.04	0.40
2:B:350:PHE:HD1	2:B:396:ALA:HA	1.86	0.40
4:F:128:PRO:HG3	4:G:44:VAL:N	2.32	0.40
5:H:18:HIS:HA	5:H:37:THR:O	2.22	0.40
5:H:137:ASN:HB3	5:I:137:ASN:HB3	2.02	0.40
5:I:70:LEU:O	5:I:74:LEU:HB2	2.21	0.40
1:A:103:TYR:O	1:A:107:ILE:HG12	2.22	0.40
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	2.03	0.40
1:A:2310:VAL:HB	1:A:2359:LYS:NZ	2.37	0.40
1:A:2492:ASP:O	1:A:2495:SER:N	2.53	0.40
1:A:2773:ARG:HE	1:A:2774:SER:H	1.68	0.40
1:A:2806:LYS:HG3	1:A:2857:CYS:SG	2.61	0.40
1:A:3609:MET:O	1:A:3612:ARG:HG3	2.21	0.40
1:A:3950:THR:HB	1:A:4063:GLU:OE2	2.22	0.40
1:A:4108:MET:O	1:A:4112:THR:HG22	2.22	0.40
1:A:4125:GLU:HB3	1:A:4128:MET:HG2	2.04	0.40
2:B:172:GLU:HG3	2:B:213:ILE:HG21	2.03	0.40
2:B:250:GLU:C	3:C:431:ARG:HH22	2.29	0.40
2:B:306:SER:N	3:C:288:ASP:OD1	2.54	0.40
2:B:392:LYS:HB2	2:B:394:VAL:HG22	2.04	0.40
3:C:312:GLN:HG2	3:C:325:LYS:NZ	2.36	0.40
5:H:177:TYR:HE1	6:J:778:PHE:HD2	1.69	0.40
5:I:44:THR:N	5:I:114:GLU:O	2.55	0.40
8:E:22:DG:C5	8:E:23:DT:C4	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	3483/4156 (84%)	3321 (95%)	160 (5%)	2 (0%)	48	83
2	B	465/609 (76%)	440 (95%)	25 (5%)	0	100	100
3	C	503/732 (69%)	479 (95%)	23 (5%)	1 (0%)	43	77
4	F	174/299 (58%)	159 (91%)	15 (9%)	0	100	100
4	G	183/299 (61%)	164 (90%)	19 (10%)	0	100	100
5	H	199/336 (59%)	192 (96%)	7 (4%)	0	100	100
5	I	189/336 (56%)	178 (94%)	11 (6%)	0	100	100
6	J	256/911 (28%)	237 (93%)	19 (7%)	0	100	100
All	All	5452/7678 (71%)	5170 (95%)	279 (5%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	MET
1	A	3563	ASP
3	C	229	GLU

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 PDB entries followed by that with respect to all EM entries.

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	2961/3671 (81%)	2954 (100%)	7 (0%)	87	85
2	B	392/548 (72%)	392 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	428/649 (66%)	426 (100%)	2 (0%)	81	81
4	F	157/262 (60%)	157 (100%)	0	100	100
4	G	159/262 (61%)	159 (100%)	0	100	100
5	H	166/303 (55%)	166 (100%)	0	100	100
5	I	161/303 (53%)	161 (100%)	0	100	100
6	J	212/808 (26%)	212 (100%)	0	100	100
All	All	4636/6806 (68%)	4627 (100%)	9 (0%)	85	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1537	VAL
1	A	1955	VAL
1	A	3567	VAL
1	A	3568	ILE
1	A	3856	MET
1	A	3858	MET
1	A	3860	LYS
3	C	252	THR
3	C	253	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	109	ASN
1	A	638	GLN
1	A	771	ASN
1	A	783	HIS
1	A	978	GLN
1	A	1043	GLN
1	A	1048	GLN
1	A	1125	GLN
1	A	1287	GLN
1	A	1442	GLN
1	A	1465	HIS
1	A	1603	GLN
1	A	1625	HIS
1	A	1691	GLN

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Mol	Chain	Res	Type
1	A	1771	GLN
1	A	1941	HIS
1	A	2130	HIS
1	A	2141	ASN
1	A	2152	ASN
1	A	2176	ASN
1	A	2177	ASN
1	A	2234	ASN
1	A	2306	ASN
1	A	2348	GLN
1	A	2354	ASN
1	A	2432	GLN
1	A	2472	GLN
1	A	2508	GLN
1	A	2518	GLN
1	A	2523	ASN
1	A	2527	HIS
1	A	2543	ASN
1	A	2784	GLN
1	A	2830	ASN
1	A	3054	GLN
1	A	3093	GLN
1	A	3250	ASN
1	A	3291	GLN
1	A	3423	GLN
1	A	3457	ASN
1	A	3573	ASN
1	A	3590	ASN
1	A	3634	GLN
1	A	3671	ASN
1	A	3679	ASN
1	A	3748	HIS
1	A	3863	ASN
1	A	3969	ASN
1	A	4018	GLN
1	A	4042	GLN
1	A	4087	HIS
1	A	4092	GLN
2	B	98	ASN
2	B	152	ASN
2	B	360	HIS
3	C	82	HIS

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Mol	Chain	Res	Type
3	C	402	ASN
3	C	411	HIS
3	C	492	GLN
4	F	75	HIS
4	F	133	GLN
4	G	42	GLN
4	G	78	ASN
4	G	120	ASN
4	G	215	GLN
5	H	100	ASN
5	H	137	ASN
5	H	141	ASN
5	I	137	ASN
5	I	156	ASN
5	I	185	ASN
5	I	200	ASN
6	J	711	ASN
6	J	753	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	97.03
1	A	5016:UNK	C	6004:UNK	N	48.85

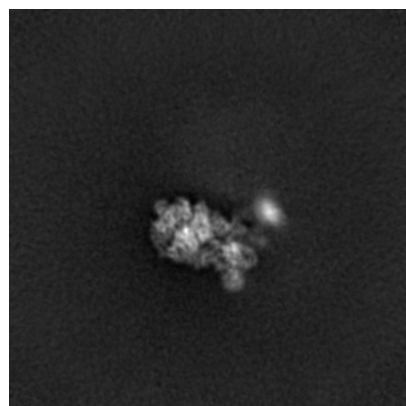
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12301. These allow visual inspection of the internal detail of the map and identification of artifacts.

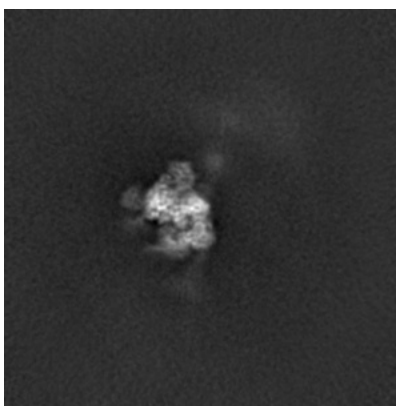
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

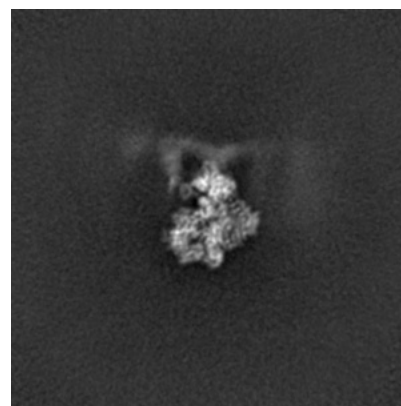
6.1.1 Primary map



X

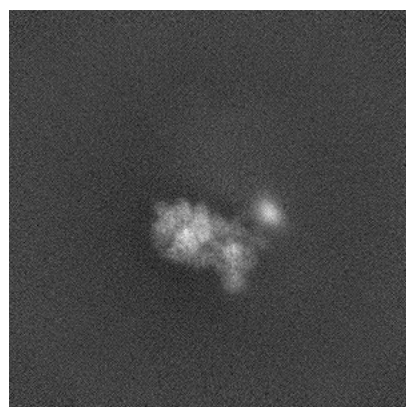


Y



Z

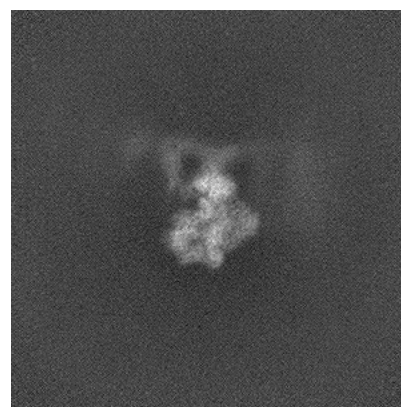
6.1.2 Raw map



X



Y

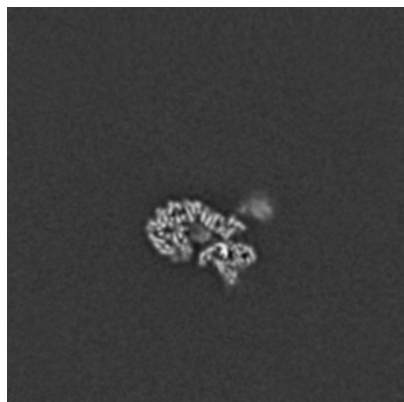


Z

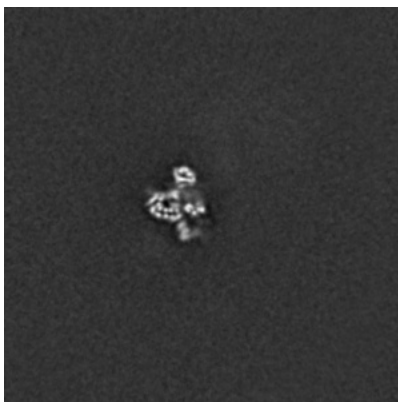
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

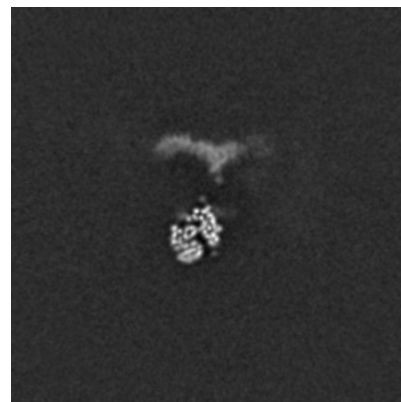
6.2.1 Primary map



X Index: 270

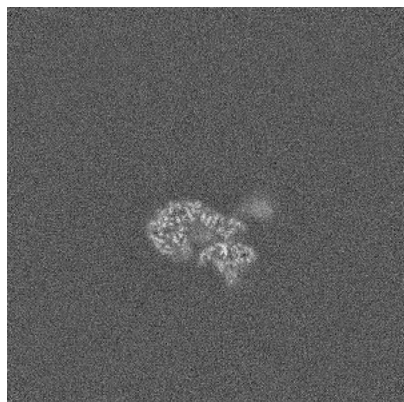


Y Index: 270

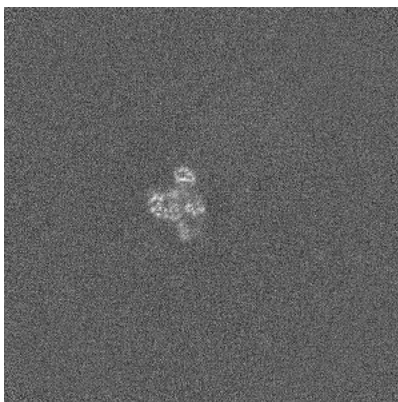


Z Index: 270

6.2.2 Raw map



X Index: 270



Y Index: 270

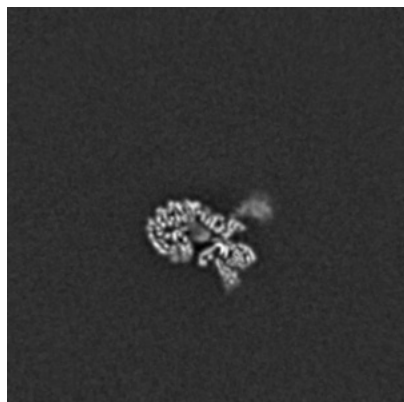


Z Index: 270

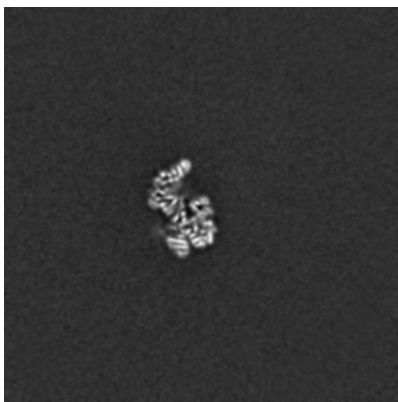
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

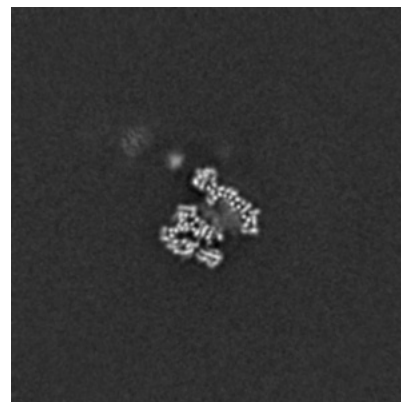
6.3.1 Primary map



X Index: 272

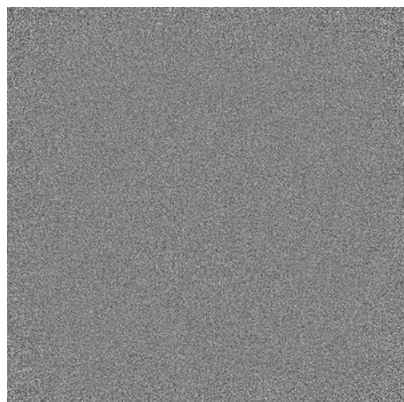


Y Index: 238

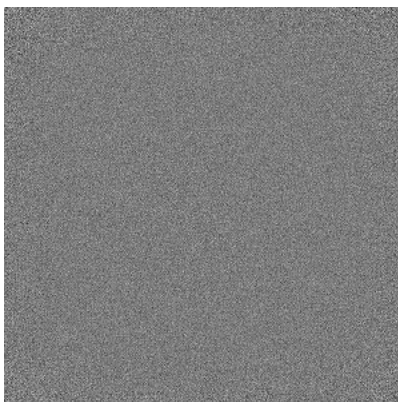


Z Index: 241

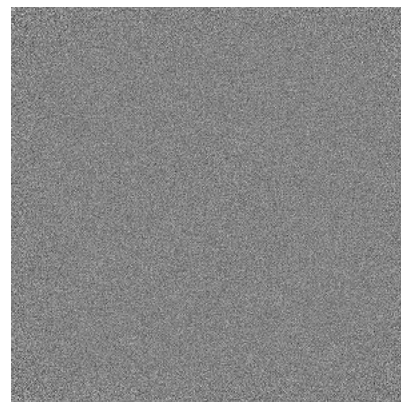
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

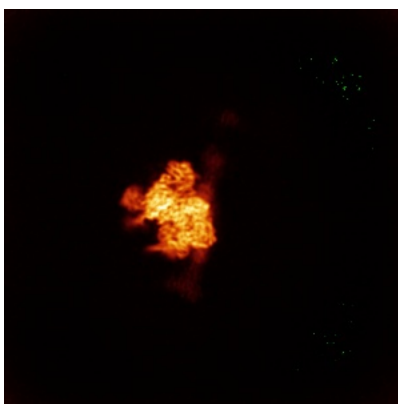
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

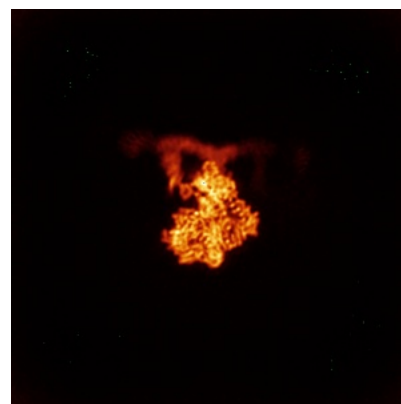
6.4.1 Primary map



X

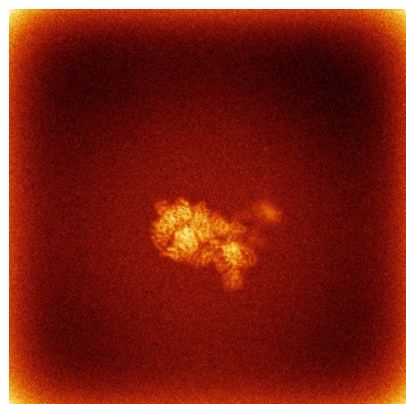


Y

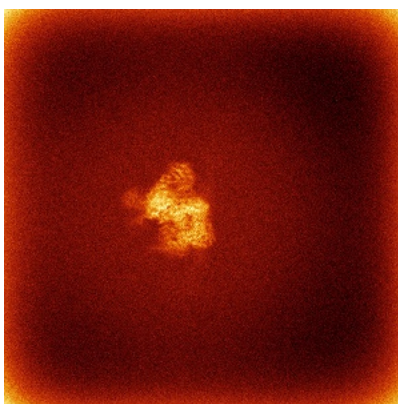


Z

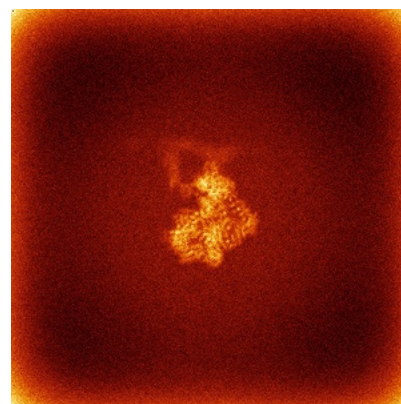
6.4.2 Raw map



X



Y

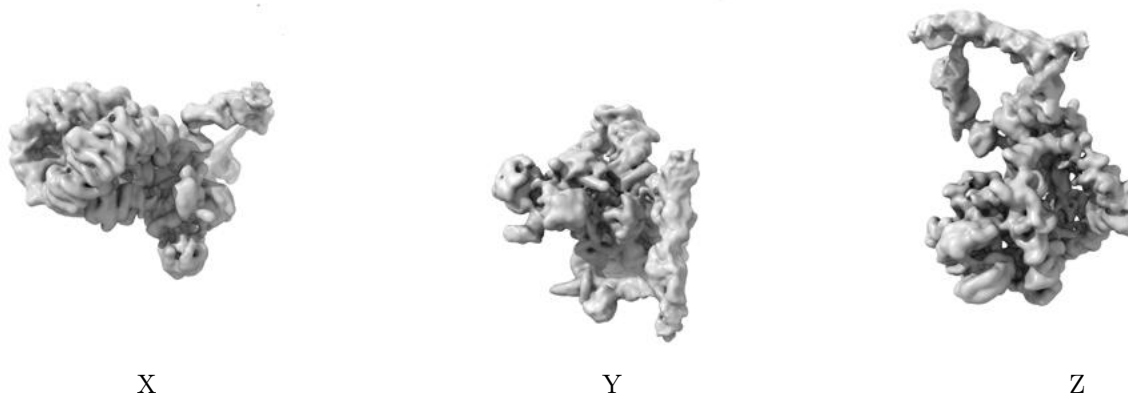


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

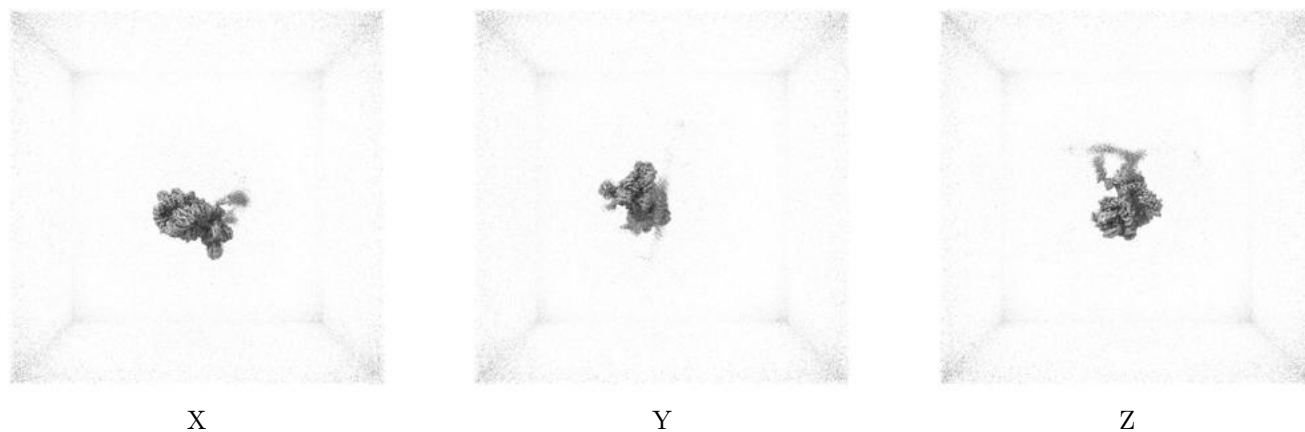
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

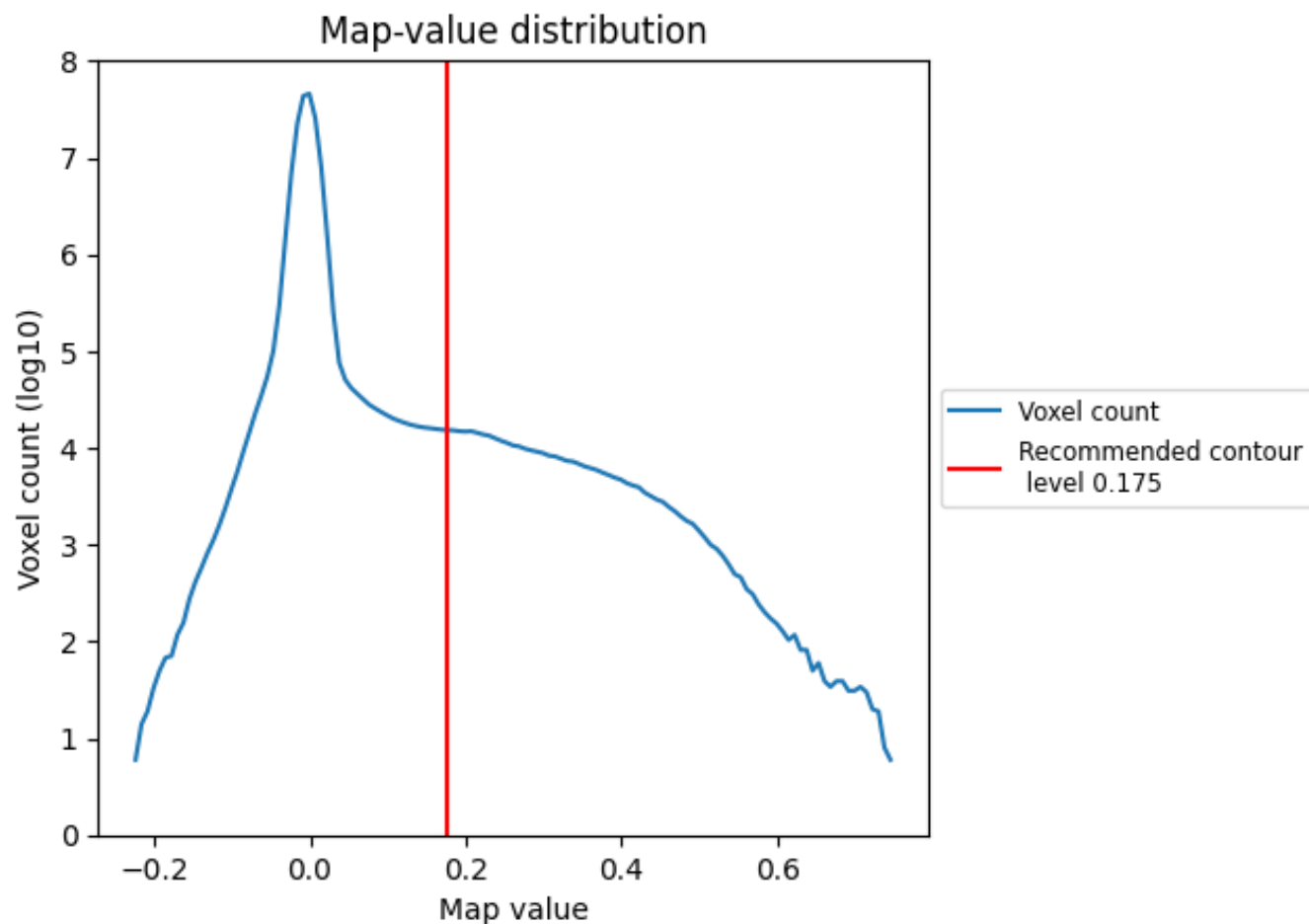
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

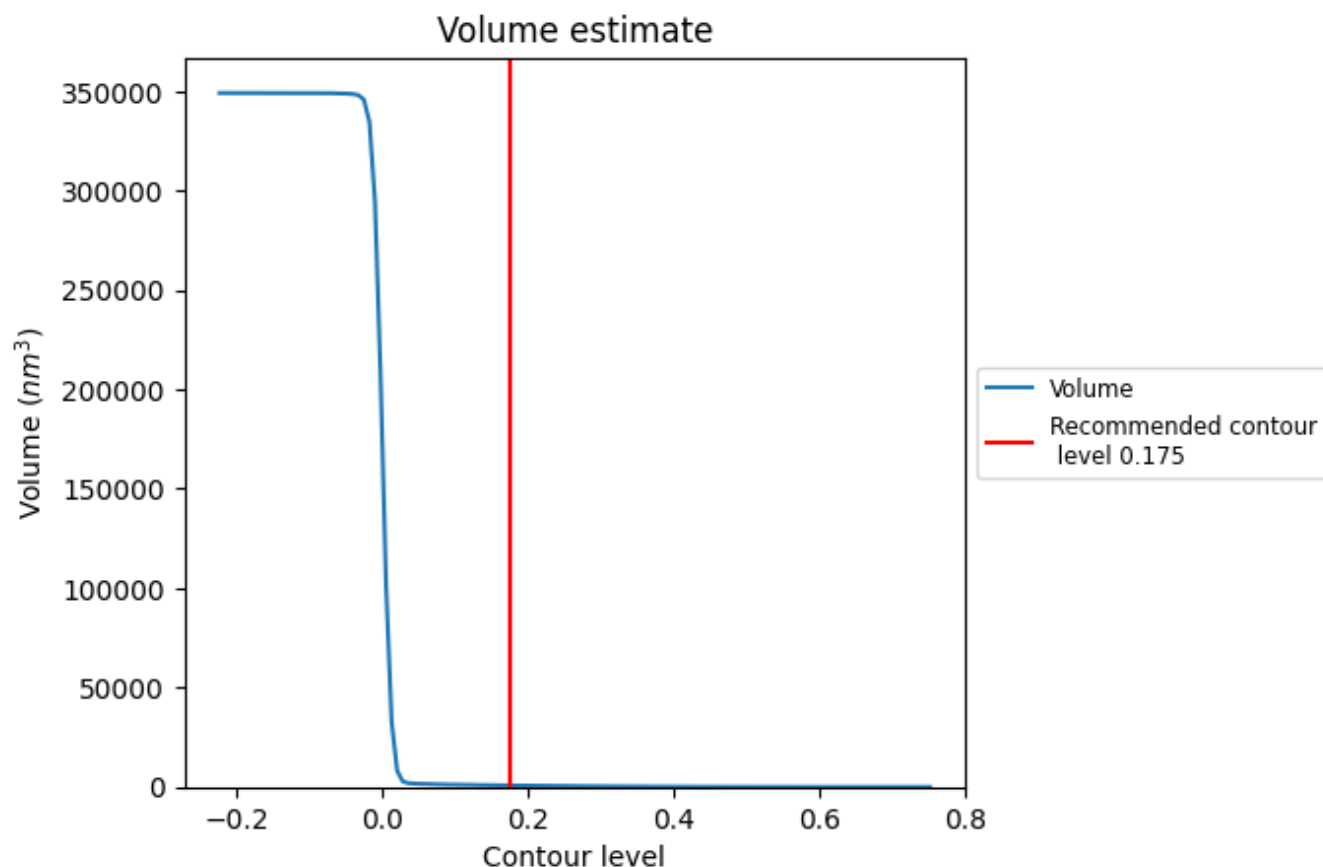
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

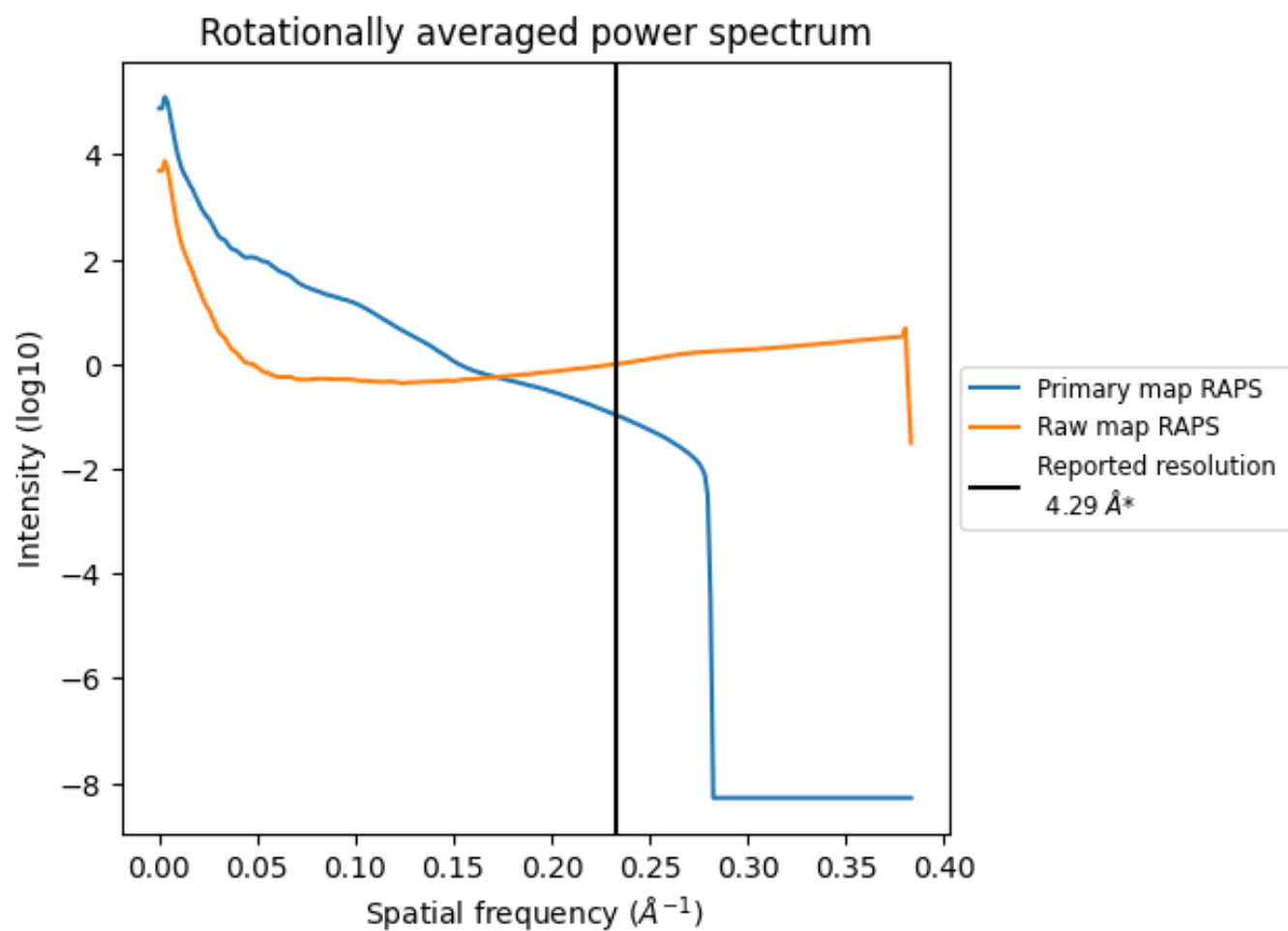
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 758 nm^3 ; this corresponds to an approximate mass of 685 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

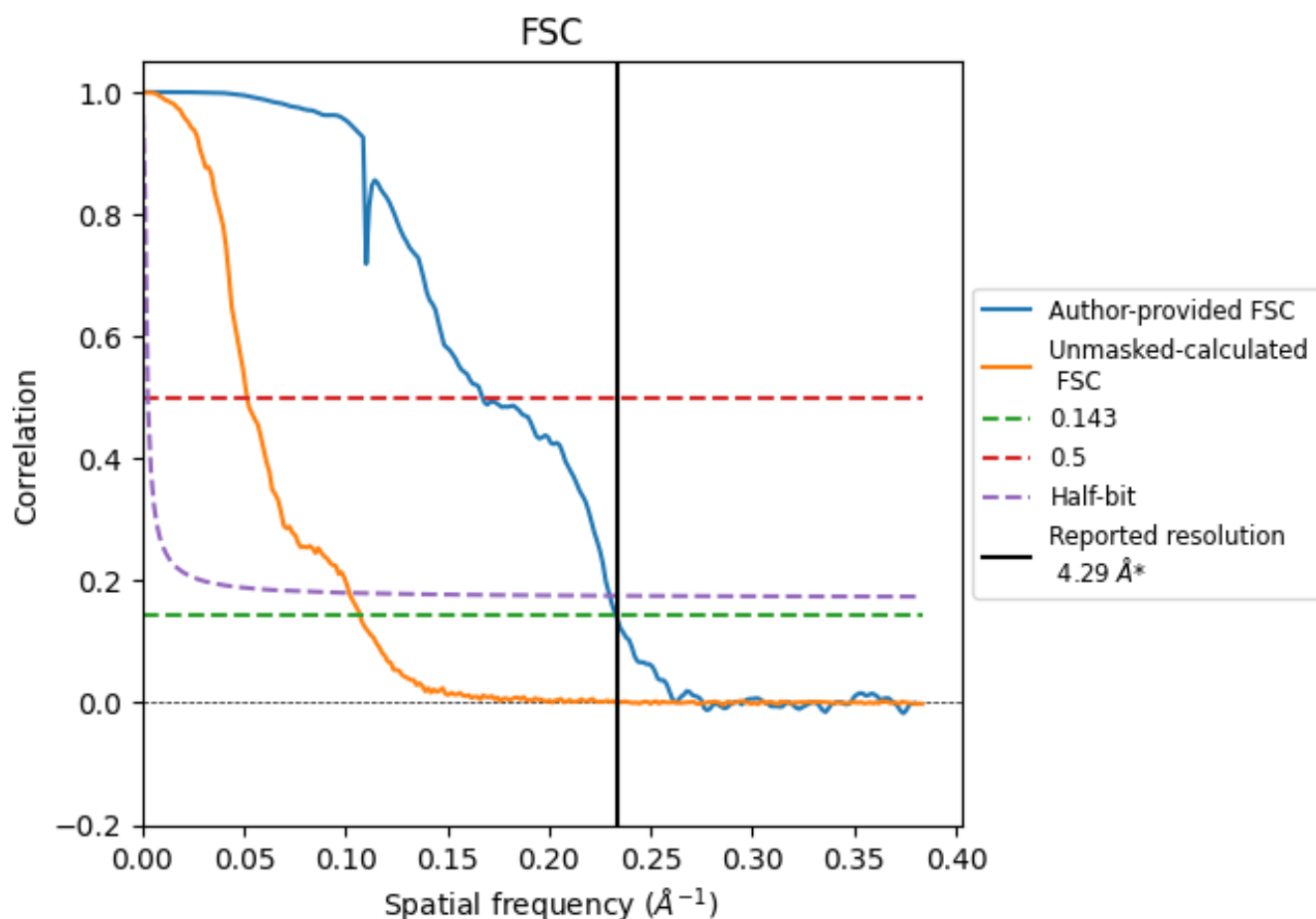


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.29	5.98	4.35
Unmasked-calculated*	9.34	19.38	9.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.34 differs from the reported value 4.29 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-12301 and PDB model 7NFE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

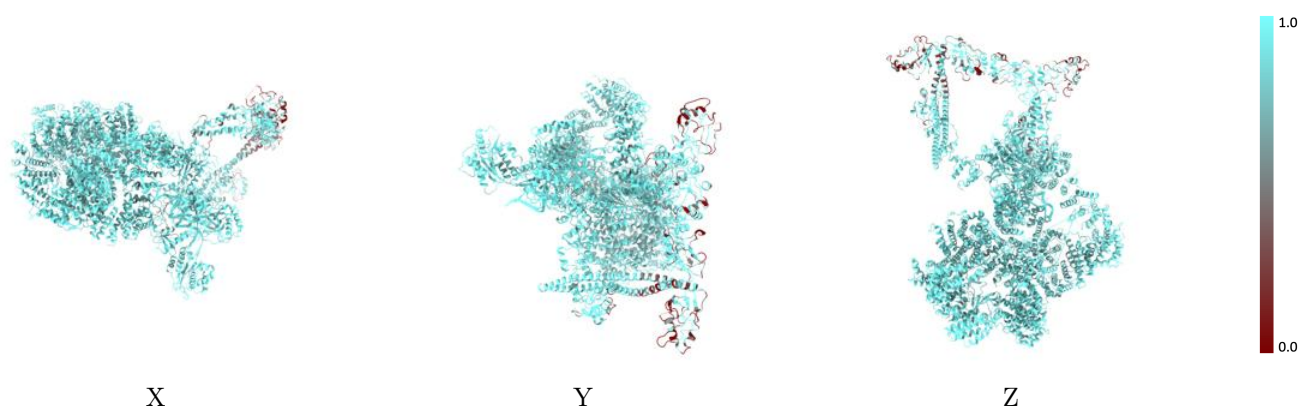
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



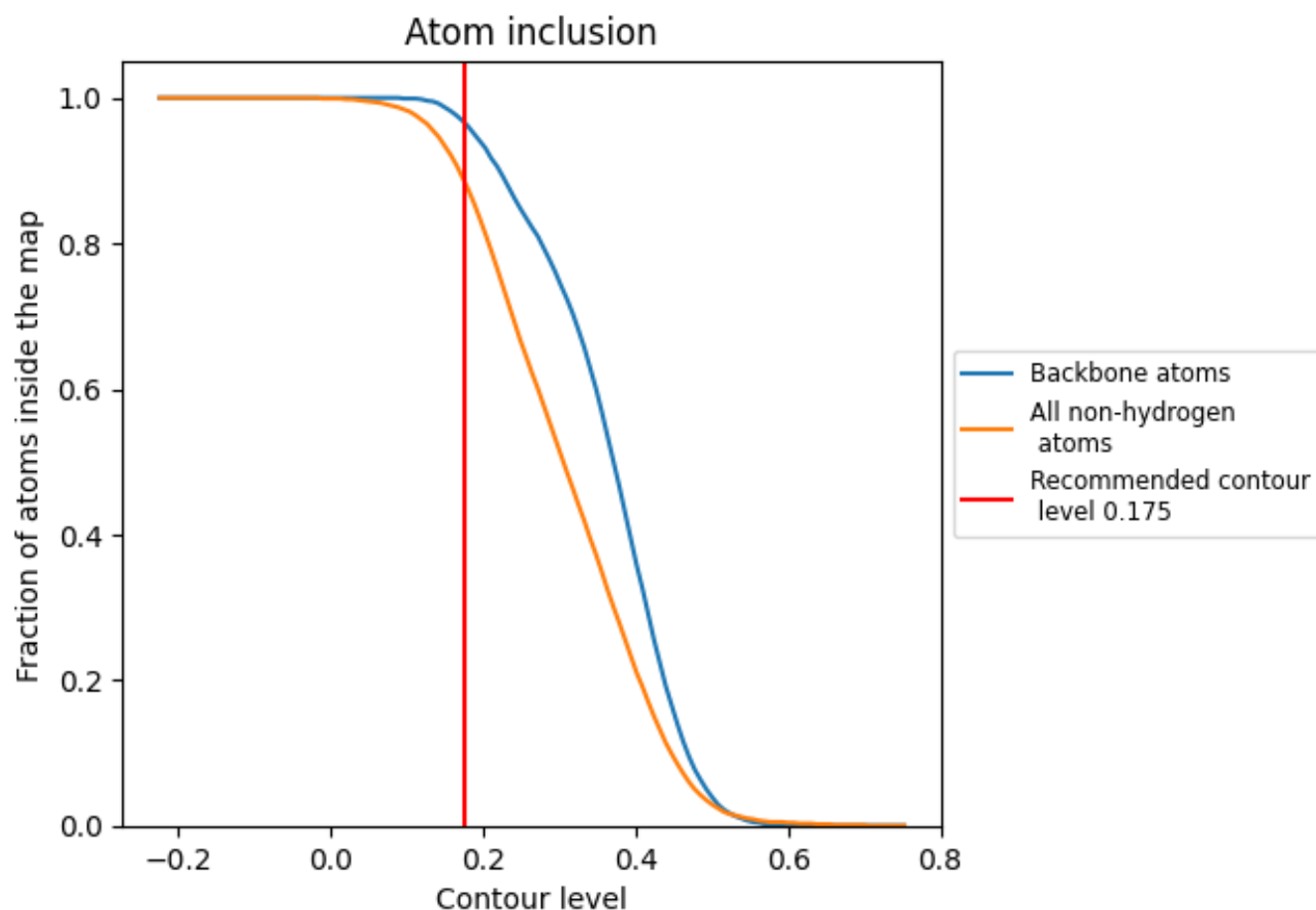
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.2030
A	0.9110	0.2140
B	0.9100	0.2270
C	0.9210	0.2180
D	0.9820	0.2580
E	0.9920	0.2600
F	0.6520	0.1300
G	0.8050	0.1390
H	0.7620	0.1350
I	0.6490	0.1360
J	0.8950	0.1560

1.0

0.0

<0.0