



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:11 PM UTC

PDB ID : 7KEK / pdb_00007kek
EMDB ID : EMD-22840
Title : Structure of the free outer-arm dynein in pre-parallel state
Authors : Rao, Q.; Zhang, K.
Deposited on : 2020-10-11
Resolution : 8.00 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:

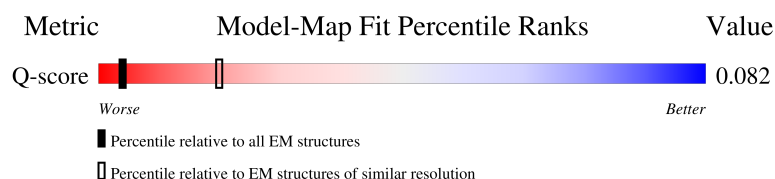
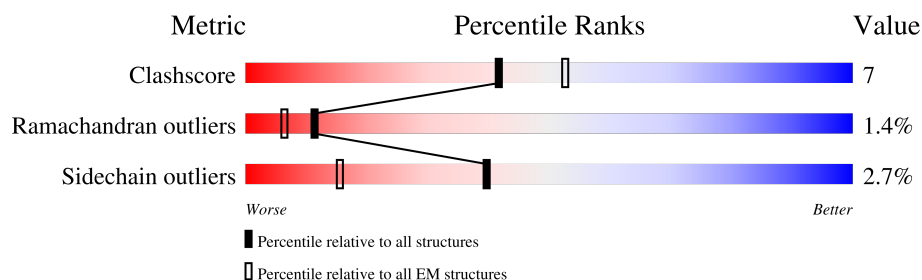
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

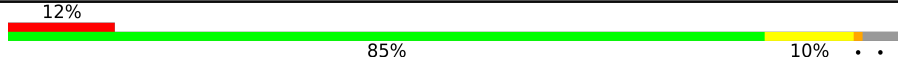
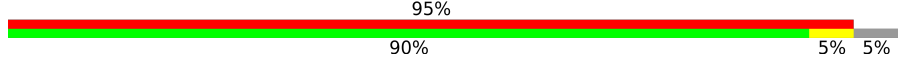
The reported resolution of this entry is 8.00 Å.

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.



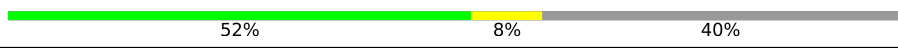
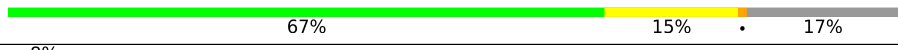
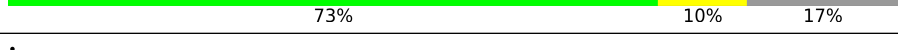
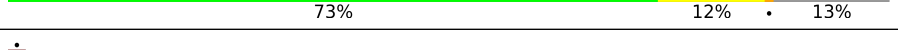
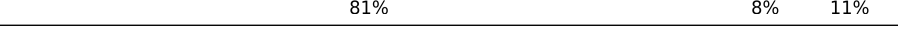
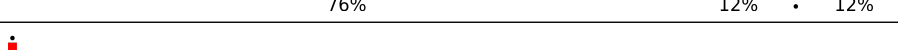
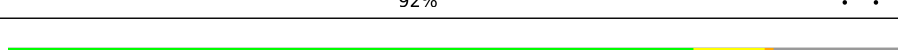
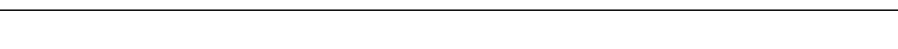
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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	4620	
2	C	4168	
3	Q	202	
4	B	4595	

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Mol	Chain	Length	Quality of chain
5	I	110	
6	H	92	
7	G	159	
8	F	133	
9	N	117	
10	O	132	
11	E	670	
12	D	667	
13	P	122	
14	L	111	
15	K	93	
16	J	111	
17	M	87	

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 117936 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 Dynein alpha heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4443	Total	C	N	O	S	0	0
			33894	21519	5788	6429	158		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4488	LYS	GLY	conflict	UNP Q22A67

- Molecule 2 is a protein called Dynein gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	3943	Total	C	N	O	S	0	0
			30436	19390	5162	5735	149		

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	192	Total	C	N	O	2	0
			1002	607	202	193		

- Molecule 4 is a protein called Dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	4516	Total	C	N	O	S	0	0
			34604	21978	5928	6547	151		

- Molecule 5 is a protein called Dynein light chain LC8_1a (LC10).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 6 is a protein called Dynein light chain LC8_1b (DLC82).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 7 is a protein called Dynein light chain roadblock LC7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock LC7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain Tctex_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain Tctex_a (LC2A).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Dynein intermediate chain DIC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain DIC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin LC3BL.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	109	Total	C	N	O	0	0
			541	323	109	109		

- Molecule 14 is a protein called Dynein light chain LC8_3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	98	Total	C	N	O	S	0	0
			783	511	132	137	3		

- Molecule 15 is a protein called Dynein light chain LC8_2a (LC8E).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

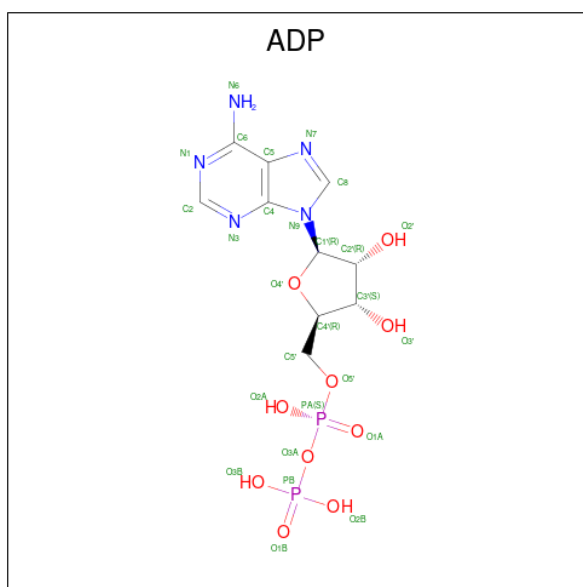
- Molecule 16 is a protein called Dynein light chain LC8_2b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	95	Total	C	N	O	S	0	0
			806	527	135	140	4		

- Molecule 17 is a protein called Dynein light chain LC8_3a.

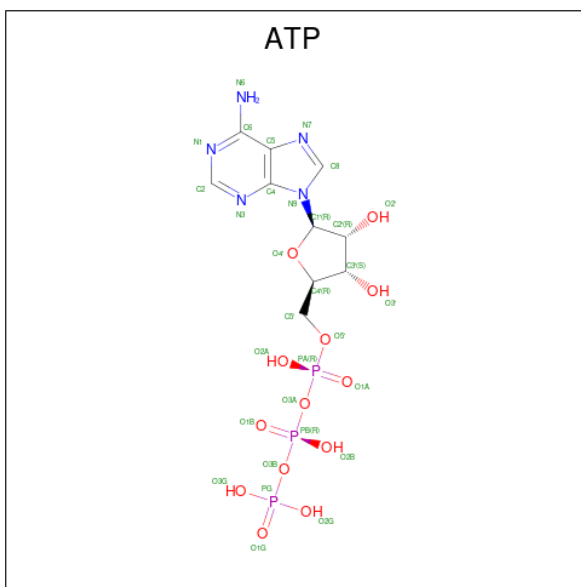
Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 27	C 10	N 5	O 10	P 2	0
18	A	1	Total 27	C 10	N 5	O 10	P 2	0
18	C	1	Total 27	C 10	N 5	O 10	P 2	0
18	C	1	Total 27	C 10	N 5	O 10	P 2	0
18	B	1	Total 27	C 10	N 5	O 10	P 2	0
18	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 31	C 10	N 5	O 13	P 3	0
19	C	1	Total 31	C 10	N 5	O 13	P 3	0
19	B	1	Total 31	C 10	N 5	O 13	P 3	0

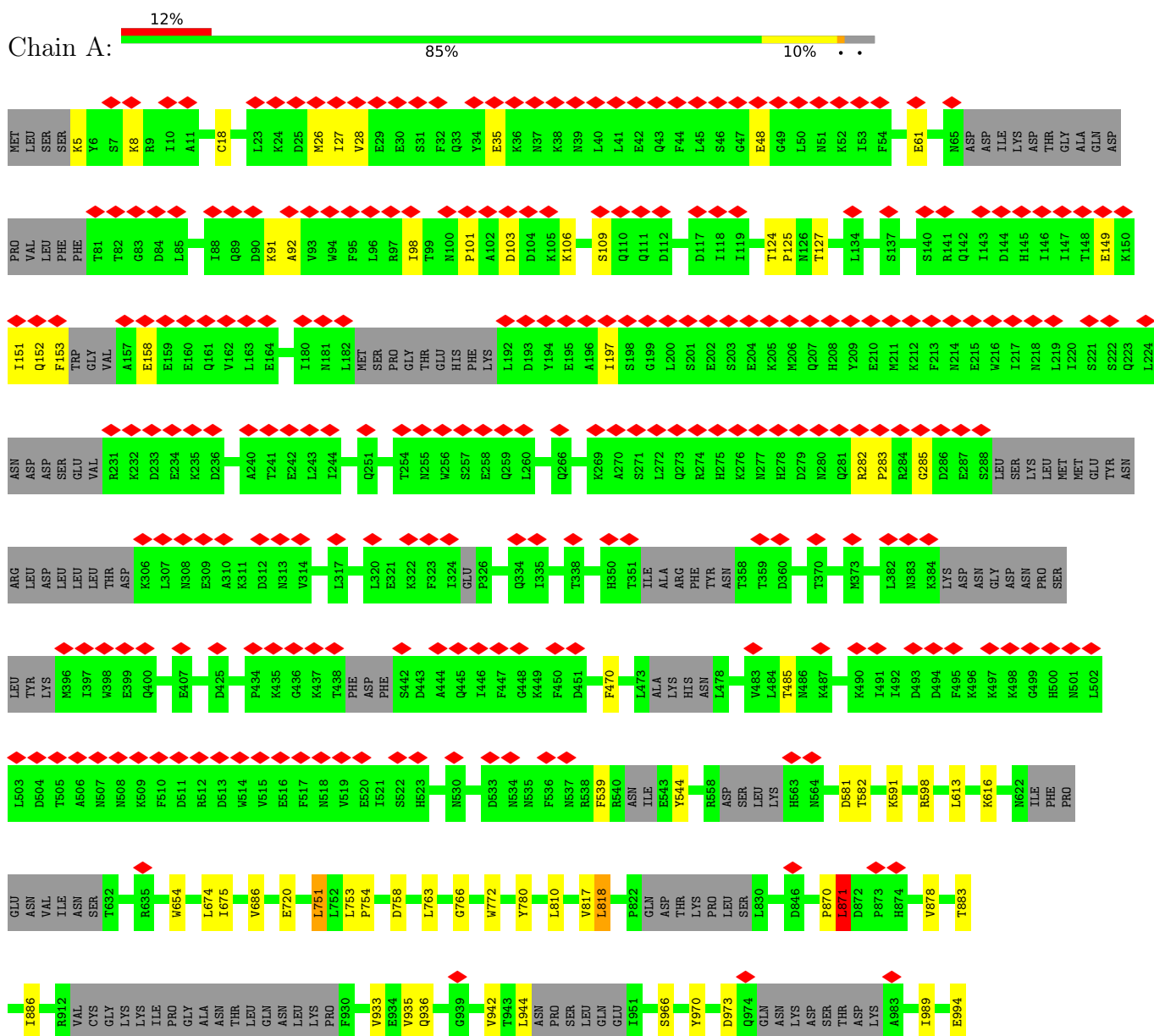
- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
20	A	3	Total Mg 3 3	0
20	C	3	Total Mg 3 3	0
20	B	3	Total Mg 3 3	0

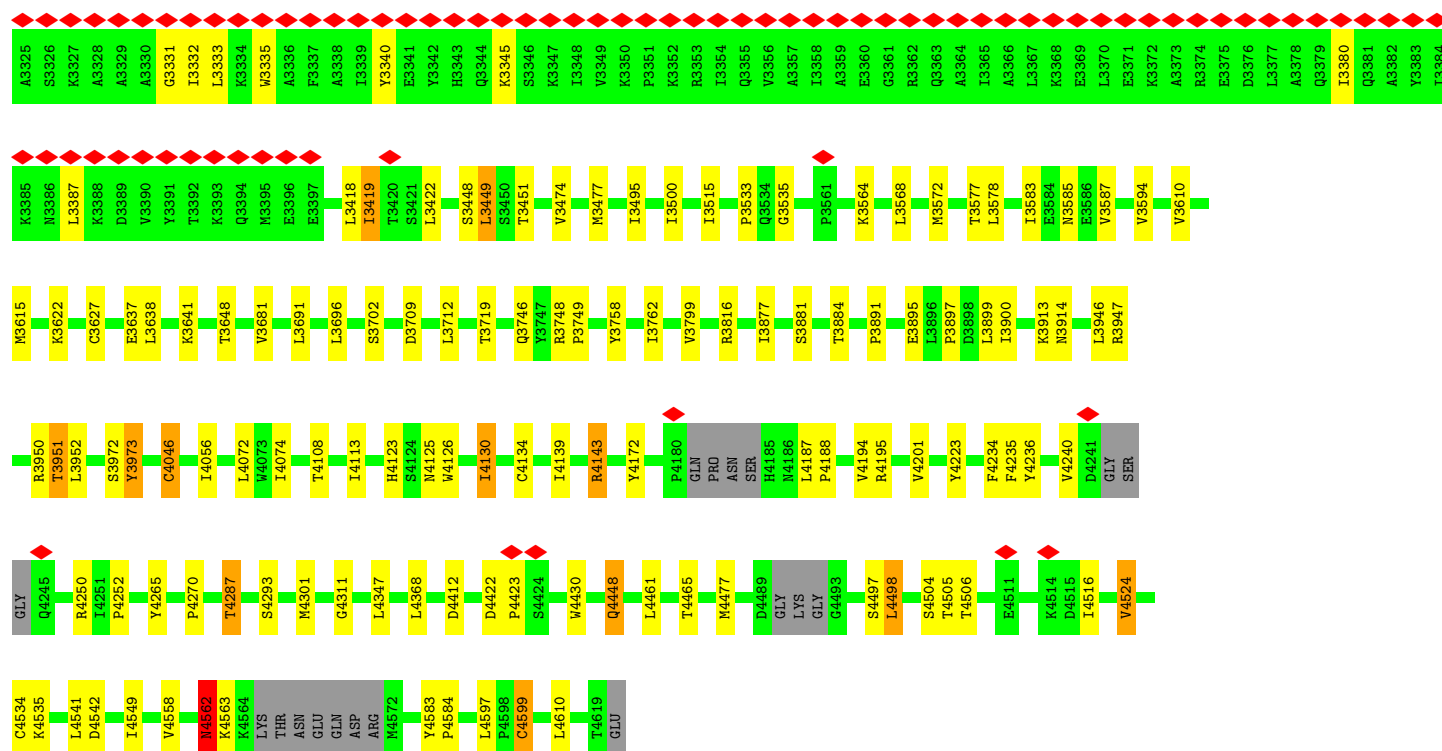
3 Residue-property plots [i](#)

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.

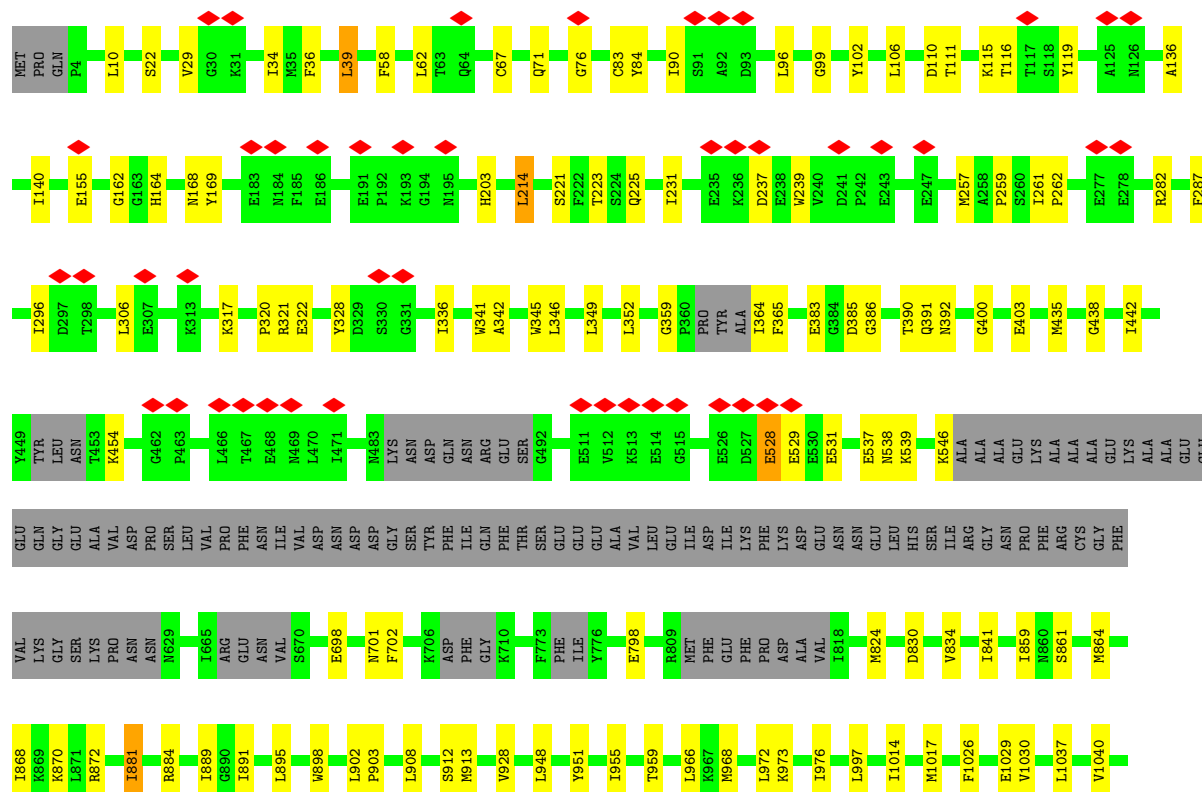
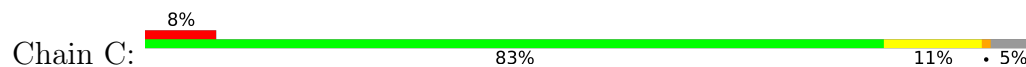
• Molecule 1: Dynein alpha heavy chain



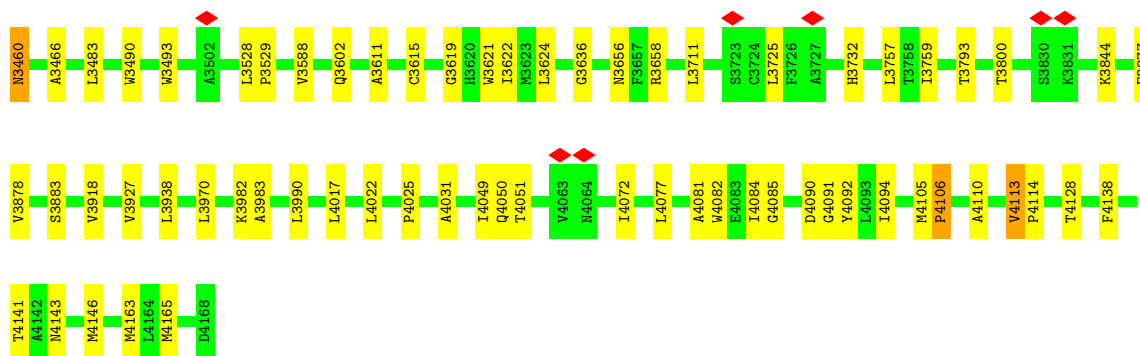
A3285	L3205	L3145	L2850	Y2389	V2010	T1786	L1830	N1482	L1275	L1149	Y998
V3266	R3206	N3146	L2866	E2400	K2011	I1787	F1631	H1486	Q1276	D1150	Y998
L3287	R3207	E3147	V2866	L2411	K2026	Q1788	D1632	V1487	K1279	M1151	T1009
F3268	A3208	A3148	T2877	L2418	F2027	V1789	I1634	Y1280	Y1281	S1161	V1013
L3269	Q3209	R2624	T2923	Q2419	L2030	Q1791	V1637	F1490	E1282	L1162	L1013
L3270	E3210	Y2656	L2923	P2420	L2033	K1792	F1639	T1500	L1283	D1163	F1016
A3211	K3151	D2659	L2935	Q2421	R2042	D1793	F1639	V1504	T1286	D1164	L1017
S3272	T3152	D2659	L2935	G2422	R2042	I1794	S1641	V1504	E1289	Y1166	F1020
Y3273	T3153	W2676	L2938	G2422	I2051	F1806	A1642	L1508	I1290	T1021	T1021
Y3274	Q3154	T2686	L2963	E2424	L2097	D1819	K1643	E1522	L1183	K1022	F1023
E3275	L3155	R2697	T2963	N2425	L2098	I1825	D1644	V1523	L1183	C1027	C1027
S3276	L3156	F2698	T2963	E2426	L2098	Y1836	K1645	F1525	W1187	S1030	S1030
G3277	A3157	L2699	T2963	T2427	I2101	E1837	K1646	T1526	L1190	I1031	I1031
G3278	N3158	L2699	T2963	V2428	I2101	F1838	N1647	L1536	L1201	L1052	L1052
G3279	L3159	K2704	T2963	Y2432	V2116	I1847	P1648	L1536	Y1201	I1065	I1065
T3280	D3160	T2708	T2963	V2433	E2117	T1857	A1649	L1536	Q1205	V1066	V1066
L3281	K3161	T2708	T2963	S2434	I2124	M1862	Q1652	K1539	Q1205	Y1069	Y1069
G3282	E3162	K2711	T2963	T2437	I2131	G1868	I1653	Q1540	Y1208	M1074	M1074
D3283	S3163	L2723	T2963	C2443	I2141	L1889	Q1655	F1541	L1209	L1076	L1076
M3284	K3164	L2727	T2963	Q2455	I2159	T1892	I1656	F1541	Y1209	I1081	I1081
N3285	K3165	L2727	T2963	Q2455	I2159	F1892	I1656	F1541	Y1209	C1082	C1082
M3287	N3167	F2728	T2963	Q2455	I2159	N1897	I1656	F1541	Y1209	S1086	S1086
K3288	K3168	L2729	T2963	Q2455	I2159	Y1915	I1656	F1541	Y1209	T1087	T1087
K3289	K3169	L2745	T2963	Q2455	I2159	G1918	I1656	F1541	Y1209	Q1096	Q1096
L3290	G3170	V2754	T2963	M2471	I2175	W1920	I1656	F1541	Y1209	L1108	L1108
K3291	E3171	E2772	T2963	W2487	I2175	G1921	I1656	F1541	Y1209	T1112	T1112
E3292	E3172	L2776	T2963	L2490	E2202	C1922	I1656	F1541	Y1209	E1113	E1113
F3293	V3173	K2776	T2963	L2490	I2203	F1926	I1656	F1541	Y1209	K1116	K1116
E3294	A3174	C2786	T2963	D2511	S2204	L1934	I1656	F1541	Y1209	M1117	M1117
K3295	A3175	C2786	T2963	P2512	S2204	I1967	I1656	F1541	Y1209	L1118	L1118
L3296	T3176	L2789	T2963	Q2513	D2205	V1970	I1656	F1541	Y1209	V1126	V1126
S3297	N3177	L2789	T2963	K2514	D2205	F1973	I1656	F1541	Y1209	ALA	ALA
I3298	K3178	V2793	T2963	M2515	W2216	I1974	I1656	F1541	Y1209	M1246	M1246
N3299	Q3179	V2793	T2963	G2544	W2216	G1979	I1656	F1541	Y1209	Y1263	Y1263
E3300	C3180	L2799	T2963	A2548	N2220	Y1980	I1656	F1541	Y1209	N1266	N1266
S3301	E3181	I2800	T2963	K2548	T2228	A1981	I1656	F1541	Y1209	F1273	F1273
T3302	I3182	E2801	T2963	K2548	T2231	V1997	I1656	F1541	Y1209	G1274	G1274
I3303	Q3183	E2802	T2963	K2548	L2254	K1764	I1656	F1541	Y1209		
E3304	A3184	E2803	T2963	M2564	N2278	L1781	I1656	F1541	Y1209		
L3305	E3185	A2804	T2963	P2565	N2278	K1780	I1656	F1541	Y1209		
L3306	Q3186	I2811	T2963	F2566	N2278	V1781	I1656	F1541	Y1209		
E3307	I3187	L2811	T2963	V2567	S2320	E1782	I1656	F1541	Y1209		
P3308	S3188	C2821	T2963	Q2573	S2320	H1760	I1656	F1541	Y1209		
Y3309	K3189	V2840	T2963	L2576	Q2340	L1764	I1656	F1541	Y1209		
L3310	E3190	L2841	T2963	L2576	M2348	K1780	I1656	F1541	Y1209		
N3311	K3191	D2844	T2963	M2602	M2348	V1781	I1656	F1541	Y1209		
Q3312	E3192		T2963	K2603	T2365	E1782	I1656	F1541	Y1209		
L3313	E3193		T2963				I1656	F1541	Y1209		
E3314	A3194		T2963				I1656	F1541	Y1209		
D3315	E3195		T2963				I1656	F1541	Y1209		
M3316	R3196		T2963				I1656	F1541	Y1209		
F3317	E3197		T2963				I1656	F1541	Y1209		
N3318	L3198		T2963				I1656	F1541	Y1209		
D3319	Y3199		T2963				I1656	F1541	Y1209		
T3320	A3200		T2963				I1656	F1541	Y1209		
F3321	A3201		T2963				I1656	F1541	Y1209		
A3322	E3262		T2963				I1656	F1541	Y1209		
T3323	G3263		T2963				I1656	F1541	Y1209		
K3324	K3264		T2963				I1656	F1541	Y1209		



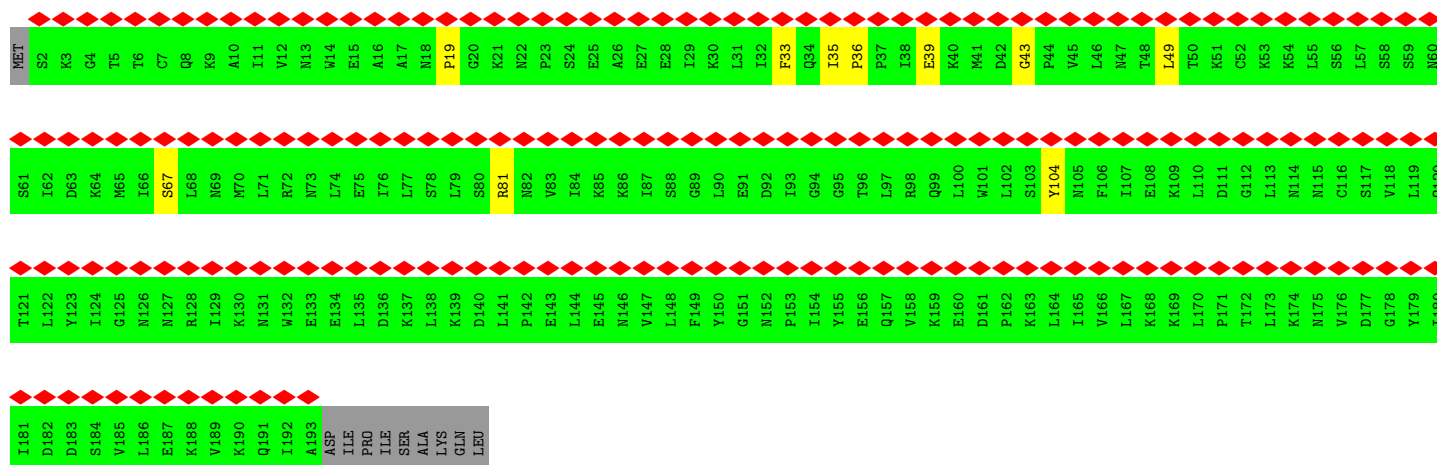
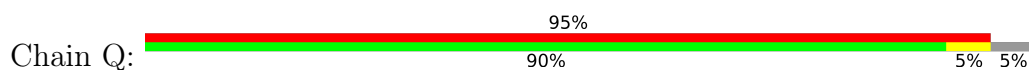
• Molecule 2: Dynein gamma heavy chain



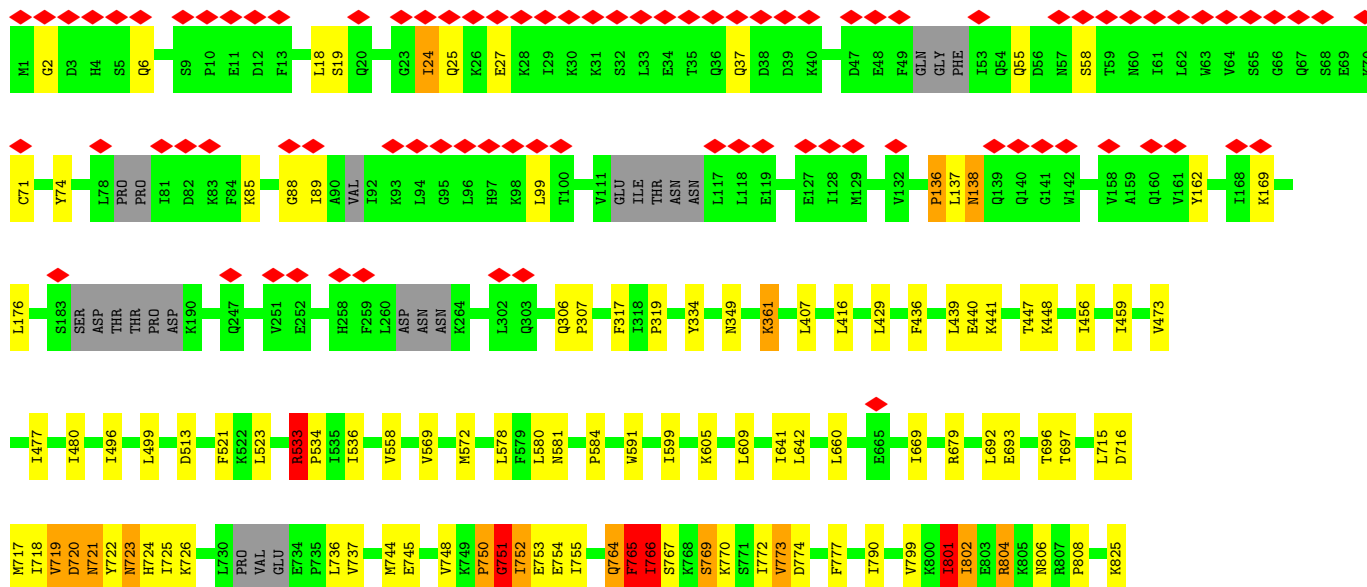
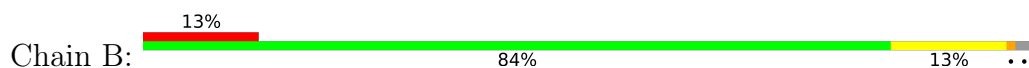


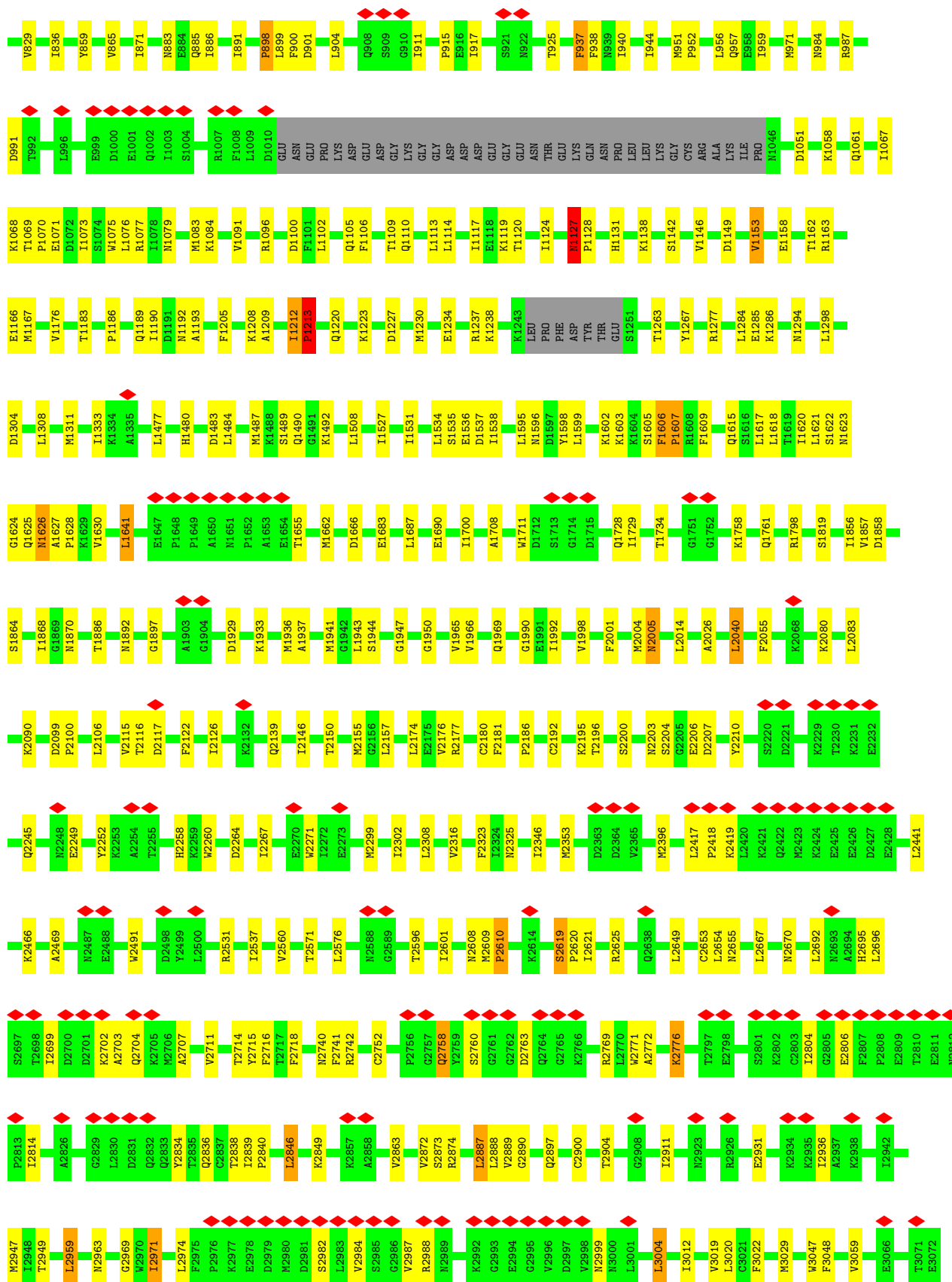


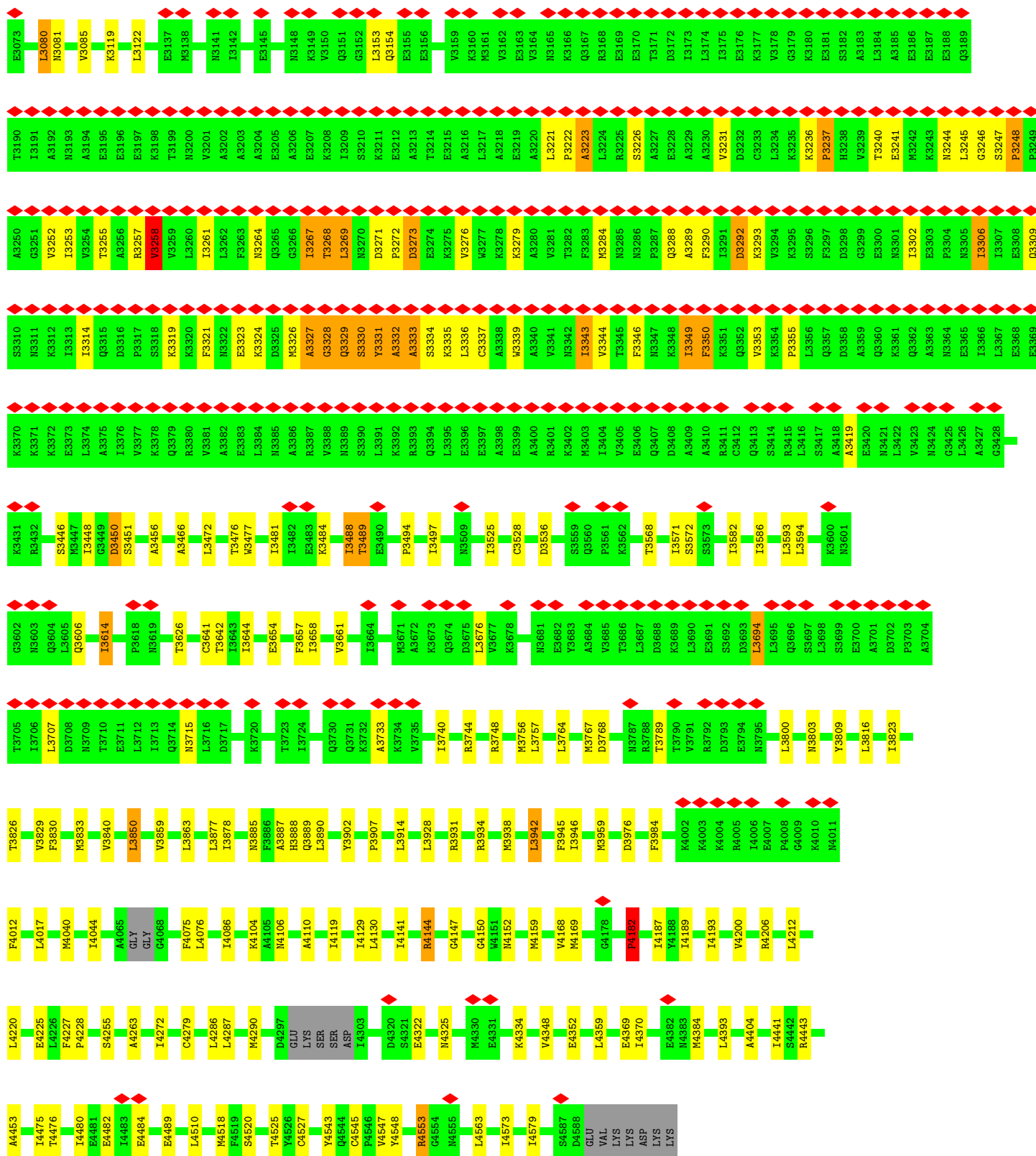
• Molecule 3: Dynein light chain 1

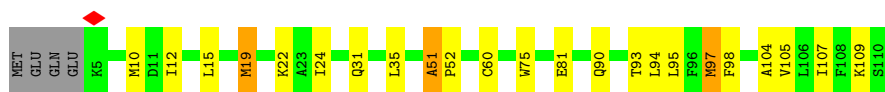


• Molecule 4: Dynein beta heavy chain

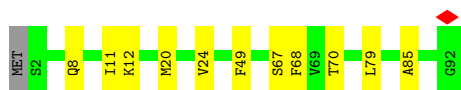
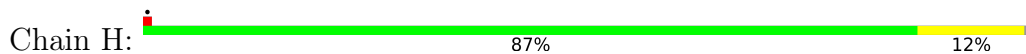




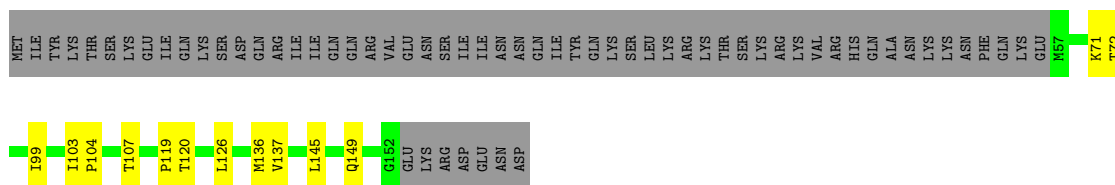




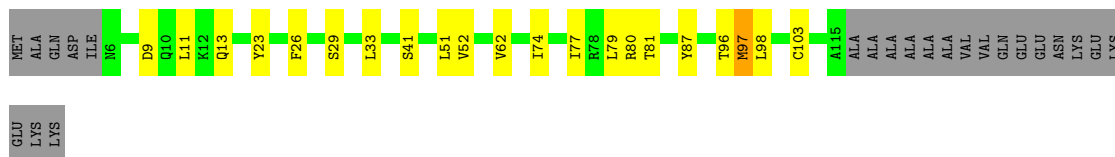
- Molecule 6: Dynein light chain LC8_1b (DLC82)



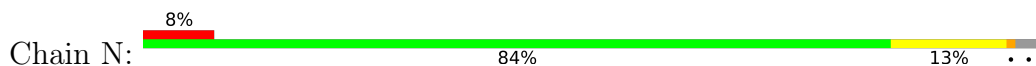
- Molecule 7: Dynein light chain roadblock LC7B



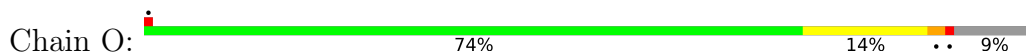
- Molecule 8: Dynein light chain roadblock LC7A



- Molecule 9: Dynein light chain Tctex_b

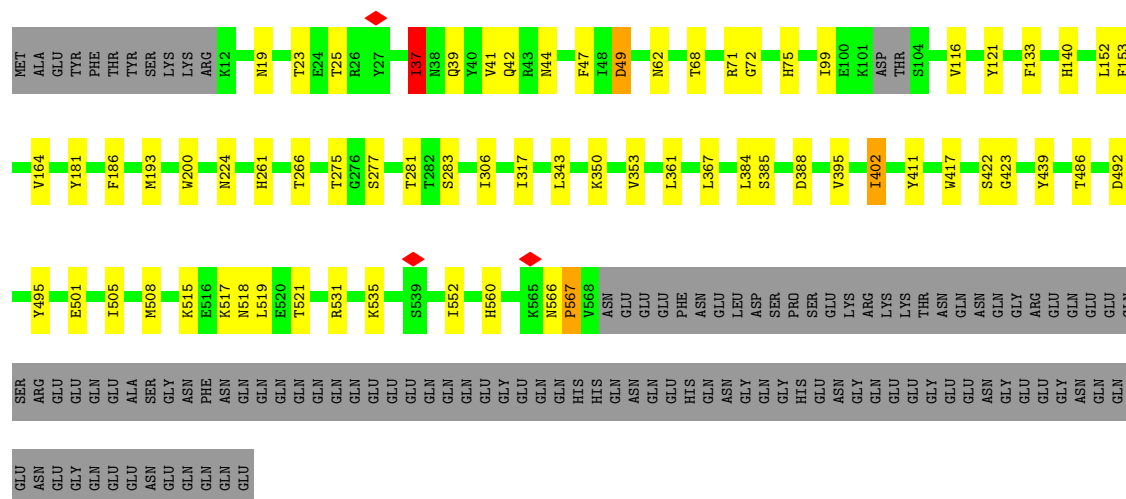


- Molecule 10: Dynein light chain Tctex_a (LC2A)



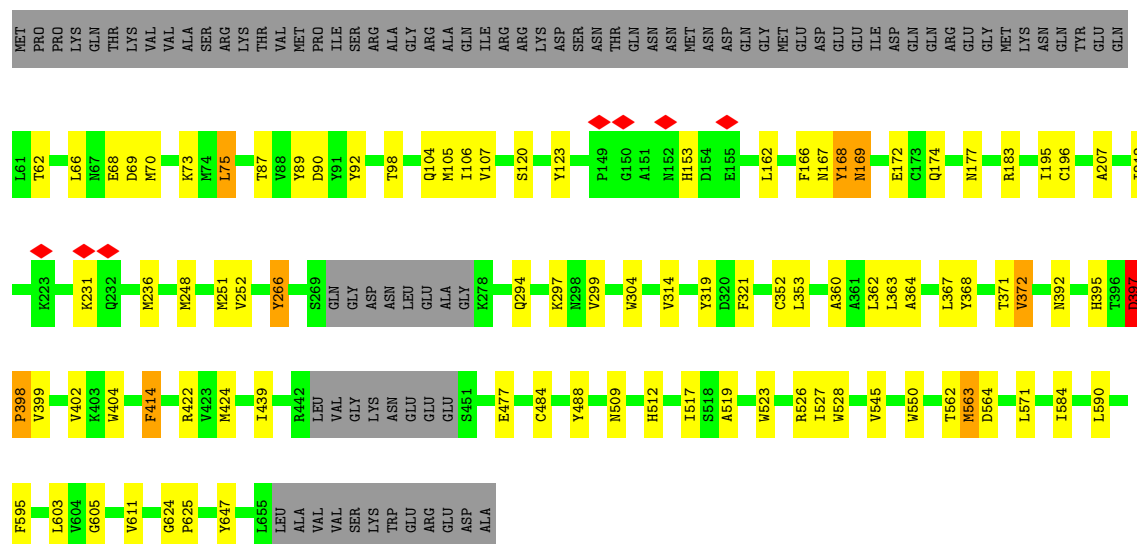
- Molecule 11: Dynein intermediate chain DIC3





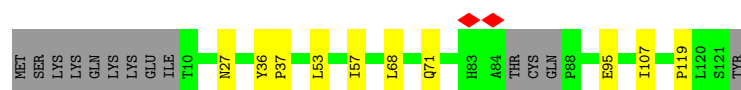
• Molecule 12: Dynein intermediate chain DIC2

Chain D: 73% 12% 13%



• Molecule 13: Thioredoxin LC3BL

Chain P: 81% 8% 11%

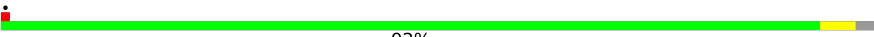


• Molecule 14: Dynein light chain LC8_3b

Chain L: 76% 12% 12%



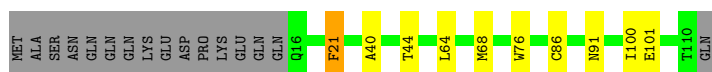
- Molecule 15: Dynein light chain LC8_2a (LC8E)

Chain K:  92%



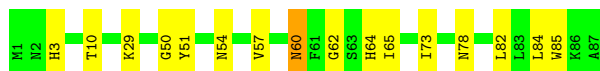
- Molecule 16: Dynein light chain LC8_2b

Chain J:  77% 8% 14%



- Molecule 17: Dynein light chain LC8_3a

Chain M:  82% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	9.863	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	1015.746, 1061.068, 970.42395	wwPDB
Map dimensions	381, 398, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.666, 2.666, 2.666	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	1.05	0/34464	1.65	14/46623 (0.0%)
2	C	1.06	1/31037 (0.0%)	1.67	15/42000 (0.0%)
3	Q	1.32	0/1005	1.76	0/1388
4	B	1.06	1/35205 (0.0%)	1.70	30/47647 (0.1%)
5	I	1.06	0/838	1.57	2/1131 (0.2%)
6	H	1.03	0/767	1.51	0/1031
7	G	1.06	0/755	1.54	0/1018
8	F	1.05	0/875	1.51	0/1178
9	N	1.06	0/867	1.54	2/1179 (0.2%)
10	O	1.01	0/1004	1.47	0/1349
11	E	1.04	0/4522	1.45	2/6114 (0.0%)
12	D	1.02	0/4772	1.44	1/6458 (0.0%)
13	P	1.33	0/538	1.83	0/746
14	L	1.03	0/800	1.50	0/1076
15	K	1.00	0/776	1.45	0/1038
16	J	0.98	0/831	1.42	0/1118
17	M	1.00	0/752	1.42	0/1006
All	All	1.05	2/119808 (0.0%)	1.65	66/162100 (0.0%)

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	2
2	C	0	3
4	B	0	4
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1136	PHE	C-N	24.82	1.65	1.34
4	B	1606	PHE	C-N	16.80	1.73	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1136	PHE	O-C-N	53.07	171.08	121.19
2	C	1136	PHE	CA-C-N	-51.88	67.16	119.56
2	C	1136	PHE	C-N-CA	-51.88	67.16	119.56
4	B	1606	PHE	CA-C-N	37.30	166.47	119.84
4	B	1606	PHE	C-N-CA	37.30	166.47	119.84
4	B	1606	PHE	O-C-N	-34.69	81.42	121.32
2	C	1136	PHE	C-N-CD	12.67	176.95	125.00
4	B	1606	PHE	C-N-CD	-12.00	75.80	125.00
4	B	3248	PRO	N-CA-CB	-7.69	95.62	103.08
4	B	765	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	1561	VAL	CA-C-N	6.95	124.62	120.24
1	A	1561	VAL	C-N-CA	6.95	124.62	120.24
4	B	3248	PRO	N-CA-C	6.85	119.06	110.70
1	A	1016	PHE	CA-CB-CG	6.60	120.40	113.80
4	B	317	PHE	CA-C-N	6.53	125.55	120.33
4	B	317	PHE	C-N-CA	6.53	125.55	120.33
4	B	533	ARG	CB-CA-C	6.38	122.75	110.17
4	B	3248	PRO	CB-CA-C	-6.11	103.47	110.92
9	N	94	ASP	CA-C-N	6.10	126.31	121.61
9	N	94	ASP	C-N-CA	6.10	126.31	121.61
2	C	2829	ASP	CA-CB-CG	6.06	118.66	112.60
4	B	2838	THR	CA-C-N	6.05	125.17	120.33
4	B	2838	THR	C-N-CA	6.05	125.17	120.33
1	A	4311	GLY	CA-C-O	-6.05	118.29	122.22
4	B	766	ILE	CA-C-N	6.00	128.32	120.28
4	B	766	ILE	C-N-CA	6.00	128.32	120.28
2	C	528	GLU	CA-C-N	5.96	132.92	121.54
2	C	528	GLU	C-N-CA	5.96	132.92	121.54
4	B	1127	ASN	CB-CA-C	5.90	121.79	110.17
1	A	285	GLY	CA-C-N	5.79	128.50	120.63
1	A	285	GLY	C-N-CA	5.79	128.50	120.63
1	A	1016	PHE	CB-CA-C	5.67	120.61	109.72
4	B	4144	ARG	CA-C-N	5.66	128.14	120.38
4	B	4144	ARG	C-N-CA	5.66	128.14	120.38
4	B	770	LYS	N-CA-C	-5.60	104.80	111.69
2	C	3636	GLY	CA-C-O	-5.56	118.44	122.45
1	A	2365	THR	CA-C-N	5.56	126.26	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2365	THR	C-N-CA	5.56	126.26	120.03
1	A	1526	THR	CA-C-N	5.47	125.30	120.10
1	A	1526	THR	C-N-CA	5.47	125.30	120.10
12	D	397	ASP	CB-CA-C	5.35	120.71	110.17
4	B	4086	ILE	CA-C-N	5.32	125.98	120.03
4	B	4086	ILE	C-N-CA	5.32	125.98	120.03
2	C	1702	ASP	CA-CB-CG	5.25	117.85	112.60
4	B	3292	ASP	N-CA-C	-5.24	104.62	111.02
2	C	1853	PHE	CA-C-N	5.23	125.79	119.98
2	C	1853	PHE	C-N-CA	5.23	125.79	119.98
1	A	3250	PRO	N-CA-CB	-5.19	97.80	103.25
2	C	1101	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	654	TRP	CA-C-N	5.11	127.40	120.65
1	A	654	TRP	C-N-CA	5.11	127.40	120.65
4	B	1213	PRO	N-CA-CB	-5.08	97.91	103.25
4	B	1158	GLU	CA-C-N	5.08	125.72	120.03
4	B	1158	GLU	C-N-CA	5.08	125.72	120.03
11	E	317	ILE	CA-C-N	5.06	125.53	120.98
11	E	317	ILE	C-N-CA	5.06	125.53	120.98
2	C	76	GLY	O-C-N	5.04	124.67	121.85
4	B	721	ASN	N-CA-C	-5.04	105.23	111.33
4	B	4182	PRO	N-CA-CB	-5.03	97.97	103.25
2	C	3493	TRP	CA-C-N	5.02	127.26	120.38
2	C	3493	TRP	C-N-CA	5.02	127.26	120.38
4	B	751	GLY	N-CA-C	-5.02	101.28	113.18
5	I	31	GLN	CA-C-N	5.01	125.64	120.03
5	I	31	GLN	C-N-CA	5.01	125.64	120.03
4	B	765	PHE	CA-C-N	-5.00	112.97	121.97
4	B	765	PHE	C-N-CA	-5.00	112.97	121.97

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
4	B	1864	SER	Peptide
4	B	2466	LYS	Peptide
4	B	3319	LYS	Peptide
4	B	3536	ASP	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	C	528	GLU	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	33894	0	32284	339	0
2	C	30436	0	29388	343	0
3	Q	1002	0	498	6	0
4	B	34604	0	33084	736	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	11	0
8	F	863	0	881	10	0
9	N	855	0	800	13	0
10	O	986	0	1002	13	0
11	E	4423	0	4291	44	0
12	D	4664	0	4484	70	0
13	P	541	0	220	2	0
14	L	783	0	811	12	0
15	K	754	0	716	3	0
16	J	806	0	769	4	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112410	1554	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 7.

All (1554) 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)
4:B:1223:LYS:HE2	4:B:1277:ARG:CB	1.23	1.63
4:B:1599:LEU:HB3	4:B:1617:LEU:CG	1.18	1.61
1:A:1219:PHE:HZ	1:A:1263:TYR:CD2	1.17	1.60
1:A:1219:PHE:CE1	1:A:1263:TYR:HA	1.26	1.60
1:A:1219:PHE:CZ	1:A:1263:TYR:CD2	1.89	1.60
4:B:1223:LYS:CE	4:B:1277:ARG:CB	1.81	1.58
4:B:1603:LYS:CG	4:B:1609:PHE:CB	1.82	1.57
2:C:1132:LYS:CE	2:C:1151:LEU:HD22	1.12	1.57
4:B:1595:LEU:HB3	4:B:1618:LEU:CD2	1.09	1.57
4:B:1606:PHE:CZ	4:B:1690:GLU:HB2	1.36	1.56
2:C:1132:LYS:HE2	2:C:1151:LEU:CD2	1.26	1.56
4:B:1599:LEU:HD23	4:B:1621:LEU:CD2	1.28	1.56
4:B:1599:LEU:HB3	4:B:1617:LEU:CD2	1.08	1.55
4:B:1599:LEU:CD2	4:B:1621:LEU:HD22	1.30	1.55
4:B:1595:LEU:CB	4:B:1618:LEU:CD2	1.80	1.54
4:B:1606:PHE:CD1	4:B:1687:LEU:HA	1.43	1.53
4:B:1212:ILE:HG23	4:B:1284:LEU:CB	1.37	1.53
1:A:1223:VAL:HG11	1:A:1282:GLU:C	1.17	1.52
4:B:808:PRO:HG2	4:B:1077:ARG:CD	1.39	1.51
4:B:1603:LYS:HG2	4:B:1609:PHE:CB	1.05	1.50
2:C:1132:LYS:CE	2:C:1151:LEU:CD2	1.81	1.50
4:B:1599:LEU:CB	4:B:1617:LEU:CD2	1.88	1.49
4:B:1599:LEU:CG	4:B:1617:LEU:HG	1.41	1.45
4:B:1602:LYS:HD2	4:B:1683:GLU:CD	1.40	1.45
4:B:1606:PHE:CE1	4:B:1687:LEU:HA	1.50	1.43
4:B:1606:PHE:C	4:B:1607:PRO:N	1.73	1.43
4:B:1599:LEU:CB	4:B:1617:LEU:CG	1.97	1.41
4:B:898:PRO:HD3	4:B:1073:ILE:CG2	1.47	1.40
2:C:364:ILE:O	2:C:365:PHE:CB	1.68	1.38
2:C:1136:PHE:HD2	2:C:1139:PHE:N	1.20	1.38
4:B:1490:GLN:CD	4:B:3614:ILE:HG21	1.48	1.38
4:B:1606:PHE:C	4:B:1607:PRO:CD	1.97	1.38
4:B:1531:ILE:CG2	4:B:1622:SER:OG	1.72	1.36
1:A:1219:PHE:HE1	1:A:1263:TYR:CA	1.36	1.36
4:B:1606:PHE:CZ	4:B:1690:GLU:CB	2.06	1.36
4:B:1603:LYS:HE2	4:B:1609:PHE:O	1.26	1.35
4:B:1603:LYS:CG	4:B:1609:PHE:HB3	1.46	1.34
1:A:1219:PHE:CZ	1:A:1263:TYR:HD2	1.30	1.33
4:B:1606:PHE:CD1	4:B:1687:LEU:CD1	2.12	1.32
4:B:1237:ARG:NE	4:B:1263:THR:CB	1.92	1.32
4:B:1606:PHE:CD1	4:B:1687:LEU:CA	2.13	1.31
1:A:1223:VAL:CG1	1:A:1282:GLU:O	1.76	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1599:LEU:CB	4:B:1617:LEU:HG	1.52	1.31
4:B:1535:SER:HB2	4:B:1622:SER:O	1.22	1.31
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.30
4:B:1595:LEU:CB	4:B:1618:LEU:HD22	1.47	1.30
4:B:1603:LYS:CG	4:B:1609:PHE:HB2	1.49	1.30
4:B:1606:PHE:CD1	4:B:1687:LEU:HD12	1.67	1.29
4:B:1603:LYS:HE2	4:B:1609:PHE:C	1.56	1.29
4:B:1220:GLN:HG2	4:B:1294:ASN:CB	1.61	1.29
4:B:1212:ILE:CG2	4:B:1284:LEU:CB	2.10	1.28
4:B:899:LEU:HD21	4:B:1075:TRP:NE1	1.47	1.28
4:B:1606:PHE:HD1	4:B:1687:LEU:CD1	1.45	1.27
4:B:1490:GLN:OE1	4:B:3614:ILE:CG2	1.82	1.27
2:C:1136:PHE:CD2	2:C:1139:PHE:N	2.05	1.24
4:B:1599:LEU:HD13	4:B:1617:LEU:CB	1.67	1.24
4:B:1490:GLN:NE2	4:B:3572:SER:CB	2.01	1.23
4:B:1212:ILE:HG12	4:B:1284:LEU:CA	1.66	1.23
4:B:1238:LYS:HE3	4:B:1308:LEU:CA	1.69	1.22
4:B:1599:LEU:HD11	4:B:1618:LEU:N	1.55	1.21
4:B:1606:PHE:HZ	4:B:1690:GLU:CB	1.43	1.21
4:B:1237:ARG:HE	4:B:1263:THR:CB	1.53	1.20
4:B:1238:LYS:CE	4:B:1308:LEU:HA	1.72	1.19
1:A:1223:VAL:HG11	1:A:1283:LEU:N	1.26	1.19
4:B:1234:GLU:OE2	4:B:1304:ASP:CB	1.90	1.19
4:B:1490:GLN:NE2	4:B:3568:THR:O	1.74	1.19
1:A:1223:VAL:CG1	1:A:1282:GLU:C	2.10	1.19
4:B:1531:ILE:O	4:B:1622:SER:HB3	1.39	1.18
1:A:1223:VAL:HG11	1:A:1282:GLU:O	1.34	1.18
4:B:1490:GLN:NE2	4:B:3572:SER:HB3	1.57	1.17
4:B:898:PRO:CD	4:B:1073:ILE:CG2	2.22	1.17
4:B:808:PRO:CG	4:B:1077:ARG:HD2	1.76	1.15
2:C:1067:VAL:HG21	2:C:1148:LEU:O	1.45	1.15
1:A:1219:PHE:CE1	1:A:1263:TYR:CA	2.18	1.15
4:B:1606:PHE:CE1	4:B:1690:GLU:HB3	1.82	1.14
4:B:1599:LEU:CD2	4:B:1617:LEU:HG	1.76	1.14
4:B:898:PRO:HB2	4:B:1077:ARG:N	1.63	1.14
4:B:1531:ILE:HG22	4:B:1622:SER:OG	1.37	1.14
4:B:764:GLN:O	4:B:766:ILE:N	1.79	1.14
2:C:1132:LYS:HE3	2:C:1151:LEU:CD2	1.70	1.13
4:B:1599:LEU:CD2	4:B:1617:LEU:O	1.97	1.13
4:B:1212:ILE:HG12	4:B:1284:LEU:HA	1.20	1.12
4:B:1602:LYS:CD	4:B:1683:GLU:CD	2.22	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1490:GLN:NE2	4:B:3572:SER:OG	1.81	1.11
2:C:1132:LYS:HG2	2:C:1151:LEU:HD11	1.18	1.11
4:B:1599:LEU:HA	4:B:1621:LEU:HD21	1.29	1.11
4:B:898:PRO:CD	4:B:1073:ILE:HG21	1.79	1.10
4:B:898:PRO:HG3	4:B:1073:ILE:HG12	1.18	1.10
4:B:900:PHE:CB	4:B:1076:LEU:HD12	1.81	1.10
4:B:1599:LEU:CB	4:B:1617:LEU:HD21	1.59	1.10
4:B:1599:LEU:HD13	4:B:1617:LEU:HB3	1.25	1.10
4:B:1606:PHE:CE1	4:B:1690:GLU:CB	2.33	1.10
4:B:900:PHE:HB3	4:B:1076:LEU:HD12	1.30	1.09
1:A:1276:GLN:HG2	12:D:153:HIS:CE1	1.87	1.08
2:C:1135:ALA:HB1	2:C:1212:GLU:CG	1.83	1.08
4:B:1602:LYS:NZ	4:B:1683:GLU:OE1	1.85	1.08
4:B:1212:ILE:HG12	4:B:1284:LEU:CB	1.83	1.08
4:B:1531:ILE:HD13	4:B:1618:LEU:HB3	1.36	1.07
1:A:1230:TYR:CB	1:A:1289:GLU:C	2.29	1.06
4:B:1531:ILE:HG23	4:B:1622:SER:OG	1.49	1.06
4:B:1606:PHE:C	4:B:1607:PRO:HD3	1.80	1.06
4:B:1238:LYS:CE	4:B:1308:LEU:CA	2.32	1.06
4:B:1602:LYS:HD2	4:B:1683:GLU:CG	1.85	1.06
2:C:454:LYS:CB	2:C:701:ASN:CB	2.33	1.06
4:B:899:LEU:HD11	4:B:1075:TRP:CZ2	1.90	1.06
4:B:1535:SER:CB	4:B:1622:SER:O	2.04	1.06
4:B:1595:LEU:HB2	4:B:1618:LEU:CD2	1.81	1.06
4:B:1490:GLN:OE1	4:B:3614:ILE:HG21	0.88	1.05
2:C:403:GLU:O	4:B:2988:ARG:NH1	1.89	1.05
4:B:808:PRO:HG2	4:B:1077:ARG:HD3	1.35	1.05
4:B:750:PRO:O	4:B:752:ILE:N	1.89	1.05
4:B:1537:ASP:HA	4:B:1625:GLN:HG3	1.36	1.05
4:B:899:LEU:HD21	4:B:1075:TRP:CD1	1.90	1.05
4:B:1535:SER:HB2	4:B:1622:SER:C	1.81	1.04
4:B:1223:LYS:HE3	4:B:1277:ARG:CB	1.82	1.04
4:B:1602:LYS:HD2	4:B:1683:GLU:OE1	1.57	1.04
4:B:1602:LYS:HB3	4:B:1683:GLU:HB3	1.33	1.04
1:A:1219:PHE:CE2	1:A:1263:TYR:HD2	1.73	1.04
2:C:1066:GLU:N	2:C:1153:ASN:OD1	1.89	1.04
4:B:1599:LEU:HB3	4:B:1617:LEU:HD21	1.11	1.03
4:B:3255:THR:OG1	4:B:3337:CYS:SG	2.13	1.03
2:C:1132:LYS:HG2	2:C:1151:LEU:CD1	1.88	1.03
4:B:1606:PHE:HD1	4:B:1687:LEU:CB	1.71	1.03
4:B:1490:GLN:HE21	4:B:3572:SER:CB	1.66	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1606:PHE:CD1	4:B:1687:LEU:CB	2.42	1.02
2:C:1136:PHE:CD2	2:C:1138:ARG:C	2.37	1.02
4:B:1595:LEU:CB	4:B:1618:LEU:HD21	1.87	1.02
2:C:1067:VAL:N	2:C:1152:SER:OG	1.92	1.02
4:B:899:LEU:H	4:B:1076:LEU:HA	1.22	1.02
4:B:1599:LEU:CD1	4:B:1617:LEU:HG	1.91	1.01
4:B:1492:LYS:HZ1	4:B:3606:GLN:HB2	1.24	1.01
4:B:1492:LYS:NZ	4:B:3606:GLN:HB2	1.74	1.01
4:B:1602:LYS:CD	4:B:1683:GLU:OE1	2.08	1.01
1:A:1230:TYR:CB	1:A:1289:GLU:O	2.09	1.01
4:B:808:PRO:CG	4:B:1077:ARG:CD	2.36	1.01
4:B:1599:LEU:CD2	4:B:1617:LEU:C	2.34	1.01
4:B:1599:LEU:HD22	4:B:1617:LEU:O	1.59	1.01
2:C:1136:PHE:CD2	2:C:1138:ARG:CA	2.21	1.00
1:A:1219:PHE:HZ	1:A:1263:TYR:CG	1.78	1.00
4:B:765:PHE:O	4:B:766:ILE:C	2.00	1.00
4:B:1537:ASP:CA	4:B:1625:GLN:HG3	1.91	1.00
1:A:1276:GLN:HG2	12:D:153:HIS:HE1	1.26	1.00
1:A:1536:LEU:CD2	4:B:3888:HIS:HB2	1.92	1.00
2:C:1132:LYS:CE	2:C:1151:LEU:HD21	1.88	1.00
4:B:1599:LEU:CD1	4:B:1618:LEU:N	2.23	1.00
2:C:539:LYS:CB	2:C:702:PHE:HA	1.92	0.99
4:B:898:PRO:CG	4:B:1073:ILE:HG12	1.93	0.99
4:B:898:PRO:HD3	4:B:1073:ILE:HG21	1.01	0.99
4:B:1599:LEU:CG	4:B:1617:LEU:CG	2.34	0.99
4:B:1603:LYS:CE	4:B:1609:PHE:O	2.10	0.99
4:B:1490:GLN:CD	4:B:3614:ILE:CG2	2.32	0.98
1:A:1219:PHE:CE2	1:A:1263:TYR:CD2	2.50	0.98
4:B:1603:LYS:HG3	4:B:1609:PHE:CB	1.92	0.97
4:B:1606:PHE:O	4:B:1607:PRO:N	1.96	0.97
4:B:1238:LYS:HE3	4:B:1308:LEU:CB	1.95	0.97
2:C:2826:VAL:O	2:C:2829:ASP:N	1.96	0.97
4:B:1599:LEU:HA	4:B:1621:LEU:CD2	1.94	0.96
4:B:1238:LYS:HE2	4:B:1308:LEU:HA	1.47	0.96
1:A:1219:PHE:HE2	1:A:1280:TYR:HA	1.29	0.95
4:B:1606:PHE:HE1	4:B:1690:GLU:HB3	1.20	0.95
4:B:898:PRO:CB	4:B:1077:ARG:N	2.28	0.95
4:B:1531:ILE:O	4:B:1622:SER:CB	2.14	0.95
4:B:1603:LYS:HG3	4:B:1609:PHE:HB3	1.49	0.94
4:B:1606:PHE:CD1	4:B:1687:LEU:HD13	2.01	0.94
4:B:1599:LEU:HD21	4:B:1617:LEU:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1136:PHE:CD2	2:C:1138:ARG:N	2.36	0.94
4:B:891:ILE:HD13	4:B:1075:TRP:HA	1.49	0.93
4:B:1531:ILE:CG2	4:B:1622:SER:HG	1.82	0.93
4:B:1598:TYR:HD2	4:B:1621:LEU:HD23	1.33	0.93
4:B:1212:ILE:CG1	4:B:1284:LEU:CA	2.36	0.93
4:B:750:PRO:O	4:B:751:GLY:C	2.09	0.93
4:B:751:GLY:O	4:B:754:GLU:N	2.01	0.93
4:B:1212:ILE:CG1	4:B:1284:LEU:CB	2.46	0.93
4:B:1602:LYS:CE	4:B:1683:GLU:OE1	2.16	0.93
1:A:1223:VAL:HG12	1:A:1282:GLU:O	1.69	0.93
1:A:1536:LEU:HD22	4:B:3888:HIS:HB2	1.51	0.92
4:B:1606:PHE:CE1	4:B:1687:LEU:CA	2.46	0.92
4:B:1599:LEU:HD13	4:B:1617:LEU:CG	1.98	0.92
4:B:1606:PHE:HD1	4:B:1687:LEU:CG	1.81	0.92
4:B:1606:PHE:CE1	4:B:1687:LEU:HD12	2.03	0.92
1:A:1276:GLN:CG	12:D:153:HIS:CE1	2.53	0.92
4:B:1238:LYS:HE3	4:B:1308:LEU:HA	1.34	0.91
4:B:898:PRO:CD	4:B:1073:ILE:HG23	1.99	0.91
4:B:1602:LYS:CB	4:B:1683:GLU:HB3	1.99	0.91
4:B:1603:LYS:N	4:B:1609:PHE:HD2	1.69	0.91
2:C:1132:LYS:CG	2:C:1151:LEU:HD21	2.00	0.91
4:B:900:PHE:HB2	4:B:1076:LEU:HB2	1.51	0.91
4:B:1490:GLN:CD	4:B:3568:THR:O	2.14	0.90
4:B:1595:LEU:HB3	4:B:1618:LEU:HD23	0.93	0.90
4:B:808:PRO:HG2	4:B:1077:ARG:HD2	0.92	0.90
4:B:716:ASP:O	4:B:717:MET:C	2.11	0.90
4:B:1599:LEU:HB2	4:B:1617:LEU:CD2	1.99	0.90
4:B:1599:LEU:HD22	4:B:1617:LEU:C	1.95	0.90
4:B:1527:ILE:CG2	4:B:1615:GLN:OE1	2.20	0.89
4:B:1603:LYS:HG2	4:B:1609:PHE:HB3	1.04	0.89
4:B:1599:LEU:HD22	4:B:1617:LEU:HG	1.52	0.89
2:C:391:GLN:HA	4:B:2596:THR:HG22	1.54	0.89
4:B:1237:ARG:NH2	4:B:1263:THR:N	2.21	0.89
4:B:1599:LEU:CB	4:B:1617:LEU:HD23	2.02	0.89
4:B:1527:ILE:HG21	4:B:1615:GLN:OE1	1.72	0.87
2:C:1067:VAL:N	2:C:1152:SER:CA	2.31	0.87
4:B:1212:ILE:CG1	4:B:1284:LEU:HA	1.97	0.87
4:B:1599:LEU:HD11	4:B:1618:LEU:CA	2.05	0.87
2:C:261:ILE:HB	2:C:385:ASP:CB	2.04	0.87
1:A:1219:PHE:CE2	1:A:1280:TYR:HA	2.10	0.86
4:B:1537:ASP:HB2	4:B:1624:GLY:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1136:PHE:HD2	2:C:1139:PHE:H	0.87	0.86
2:C:1135:ALA:HB1	2:C:1212:GLU:HG2	1.56	0.86
1:A:1223:VAL:HG13	1:A:1283:LEU:C	1.95	0.85
1:A:1219:PHE:CZ	1:A:1263:TYR:CG	2.58	0.85
4:B:1598:TYR:CD2	4:B:1621:LEU:HD23	2.11	0.85
4:B:1599:LEU:CD1	4:B:1617:LEU:CG	2.53	0.85
9:N:38:TYR:CB	9:N:75:GLN:HE22	1.89	0.85
4:B:1603:LYS:CB	4:B:1609:PHE:HB2	2.07	0.84
4:B:1599:LEU:HD22	4:B:1617:LEU:CG	2.08	0.83
4:B:1538:ILE:HB	4:B:1622:SER:O	1.78	0.83
4:B:1599:LEU:C	4:B:1617:LEU:HD21	2.02	0.83
4:B:1606:PHE:HA	4:B:1687:LEU:HD13	1.61	0.83
1:A:1209:LEU:HA	1:A:1273:PHE:CE1	2.13	0.83
4:B:900:PHE:HB2	4:B:1076:LEU:CB	2.08	0.83
4:B:1603:LYS:HG2	4:B:1609:PHE:HB2	0.83	0.83
4:B:1603:LYS:HG2	4:B:1609:PHE:CA	2.06	0.82
4:B:898:PRO:CB	4:B:1077:ARG:CA	2.57	0.82
4:B:1599:LEU:HD11	4:B:1618:LEU:HG	1.59	0.82
4:B:898:PRO:HB2	4:B:1077:ARG:CA	2.10	0.81
1:A:1276:GLN:OE1	12:D:153:HIS:CE1	2.34	0.81
4:B:898:PRO:CB	4:B:1073:ILE:HG23	2.10	0.81
2:C:1135:ALA:CB	2:C:1212:GLU:CG	2.58	0.81
2:C:1014:ILE:HD11	2:C:1037:LEU:HD12	1.62	0.81
4:B:898:PRO:CD	4:B:1073:ILE:HD13	2.11	0.81
4:B:1227:ASP:OD1	4:B:1298:LEU:HA	1.80	0.81
2:C:1132:LYS:CG	2:C:1151:LEU:HD11	2.08	0.80
4:B:1212:ILE:CB	4:B:1284:LEU:CB	2.59	0.80
4:B:1599:LEU:CA	4:B:1621:LEU:HD21	2.09	0.80
9:N:76:THR:HG21	11:E:39:GLN:HE22	1.47	0.80
4:B:2887:LEU:HD13	4:B:3020:LEU:HD11	1.62	0.80
2:C:1066:GLU:N	2:C:1153:ASN:CG	2.38	0.80
4:B:901:ASP:HA	4:B:1077:ARG:O	1.80	0.80
4:B:1234:GLU:CD	4:B:1304:ASP:CB	2.43	0.80
4:B:900:PHE:HB2	4:B:1076:LEU:HD12	1.64	0.80
4:B:1531:ILE:HG23	4:B:1622:SER:HG	1.40	0.80
4:B:349:ASN:HA	4:B:416:LEU:HD21	1.64	0.80
2:C:1066:GLU:N	2:C:1152:SER:HG	1.80	0.80
4:B:715:LEU:O	4:B:716:ASP:C	2.22	0.80
4:B:1599:LEU:CD1	4:B:1618:LEU:HG	2.12	0.80
4:B:1205:PHE:HZ	4:B:1285:GLU:CB	1.95	0.79
4:B:898:PRO:HD3	4:B:1073:ILE:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:898:PRO:HD3	4:B:1073:ILE:CG1	2.13	0.79
4:B:1237:ARG:NH2	4:B:1263:THR:H	1.79	0.79
4:B:1595:LEU:CD1	4:B:1618:LEU:HD22	2.11	0.79
4:B:660:LEU:CB	4:B:755:ILE:HD12	2.13	0.79
4:B:900:PHE:H	4:B:1076:LEU:HB2	1.47	0.79
4:B:1606:PHE:CZ	4:B:1690:GLU:CG	2.66	0.79
2:C:1069:ARG:HG2	2:C:1155:ASN:ND2	1.98	0.79
4:B:900:PHE:CB	4:B:1076:LEU:HB2	2.13	0.78
4:B:904:LEU:HG	4:B:1083:MET:HG3	1.66	0.78
4:B:1595:LEU:HB2	4:B:1618:LEU:HD22	1.46	0.78
2:C:2066:GLN:HE21	2:C:2066:GLN:HA	1.48	0.78
4:B:1599:LEU:CA	4:B:1617:LEU:HD21	2.14	0.78
4:B:1606:PHE:HB2	4:B:1687:LEU:HB2	1.66	0.78
4:B:1595:LEU:HB3	4:B:1618:LEU:HD22	1.10	0.78
4:B:1490:GLN:CB	4:B:3614:ILE:HG23	2.14	0.78
1:A:1536:LEU:HD21	4:B:3888:HIS:HB2	1.66	0.77
4:B:1599:LEU:HD23	4:B:1621:LEU:CG	2.13	0.77
1:A:1208:TYR:HD1	1:A:1273:PHE:CE2	2.03	0.77
2:C:538:ASN:O	2:C:702:PHE:CB	2.33	0.77
4:B:1534:LEU:O	4:B:1623:ASN:OD1	2.02	0.77
4:B:1599:LEU:HB3	4:B:1617:LEU:CD1	2.12	0.77
2:C:2659:ALA:HB1	2:C:2858:VAL:HG22	1.65	0.77
4:B:899:LEU:HD21	4:B:1075:TRP:CE2	2.20	0.77
4:B:1238:LYS:CE	4:B:1308:LEU:N	2.48	0.77
4:B:1237:ARG:CZ	4:B:1263:THR:CB	2.63	0.77
12:D:397:ASP:HB3	12:D:398:PRO:HD3	1.67	0.77
4:B:1599:LEU:CD2	4:B:1617:LEU:CG	2.60	0.77
2:C:391:GLN:HA	4:B:2596:THR:CG2	2.15	0.76
4:B:1595:LEU:CG	4:B:1618:LEU:HD22	2.15	0.76
4:B:1602:LYS:CE	4:B:1683:GLU:CD	2.56	0.76
4:B:1599:LEU:CA	4:B:1621:LEU:CD2	2.63	0.76
2:C:359:GLY:O	2:C:386:GLY:C	2.18	0.76
2:C:913:MET:HE1	2:C:959:THR:HG22	1.66	0.76
4:B:1537:ASP:HB3	4:B:1624:GLY:CA	2.14	0.75
4:B:1599:LEU:HD21	4:B:1617:LEU:C	2.08	0.75
2:C:10:LEU:HD12	2:C:349:LEU:HD23	1.66	0.75
4:B:899:LEU:HD11	4:B:1075:TRP:CE2	2.21	0.75
4:B:1602:LYS:HB3	4:B:1609:PHE:HE2	1.50	0.75
4:B:1603:LYS:CD	4:B:1609:PHE:HB3	2.16	0.75
2:C:2687:ALA:HB1	2:C:2830:VAL:HG22	1.67	0.75
4:B:719:VAL:O	4:B:720:ASP:C	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:900:PHE:HB2	4:B:1076:LEU:CD1	2.16	0.74
4:B:900:PHE:N	4:B:1076:LEU:HB2	2.01	0.74
2:C:1067:VAL:CG2	2:C:1148:LEU:O	2.30	0.74
4:B:1223:LYS:NZ	4:B:1277:ARG:CB	2.50	0.74
1:A:1016:PHE:CZ	1:A:1069:TYR:HB2	2.22	0.74
4:B:3253:ILE:O	4:B:3253:ILE:HG22	1.88	0.74
1:A:1212:LEU:HD21	1:A:1275:LEU:CD1	2.17	0.73
1:A:1209:LEU:HB2	1:A:1273:PHE:HE1	1.51	0.73
11:E:395:VAL:CG2	11:E:402:ILE:HD12	2.18	0.73
4:B:1599:LEU:CD1	4:B:1617:LEU:C	2.62	0.73
2:C:1067:VAL:N	2:C:1152:SER:C	2.42	0.73
1:A:933:VAL:HG11	1:A:944:LEU:HD12	1.68	0.73
1:A:1276:GLN:CD	12:D:153:HIS:CE1	2.67	0.72
2:C:2613:THR:HG21	2:C:3176:LEU:HD22	1.70	0.72
4:B:1490:GLN:CB	4:B:3614:ILE:CG2	2.66	0.72
2:C:2717:ALA:HB1	2:C:2803:MET:SD	2.29	0.72
4:B:1490:GLN:HB3	4:B:3614:ILE:HG23	1.71	0.72
2:C:1132:LYS:HG2	2:C:1151:LEU:HD21	1.71	0.72
4:B:1599:LEU:CG	4:B:1621:LEU:HD22	2.15	0.72
2:C:1128:PHE:HZ	2:C:1151:LEU:HB3	1.53	0.72
2:C:2812:GLY:O	2:C:2815:SER:N	2.23	0.72
4:B:898:PRO:HD3	4:B:1073:ILE:HD13	1.71	0.72
4:B:899:LEU:CD2	4:B:1075:TRP:NE1	2.42	0.72
4:B:900:PHE:CB	4:B:1076:LEU:CD1	2.63	0.72
2:C:898:TRP:O	2:C:902:LEU:HD13	1.90	0.72
4:B:808:PRO:HD2	4:B:1077:ARG:HH11	1.54	0.71
4:B:1537:ASP:CB	4:B:1624:GLY:N	2.52	0.71
4:B:1599:LEU:HD22	4:B:1617:LEU:CD1	2.20	0.71
4:B:898:PRO:CG	4:B:1073:ILE:HG23	2.20	0.71
4:B:891:ILE:CD1	4:B:1075:TRP:HA	2.21	0.71
1:A:1220:THR:HG23	1:A:1279:LYS:CB	2.20	0.71
4:B:2621:ILE:HG23	4:B:2667:LEU:CD1	2.20	0.71
2:C:2766:GLU:O	2:C:2769:LEU:N	2.23	0.71
1:A:3212:VAL:HG13	1:A:3335:TRP:NE1	2.06	0.70
4:B:751:GLY:O	4:B:753:GLU:N	2.24	0.70
4:B:898:PRO:CD	4:B:1073:ILE:CG1	2.69	0.70
4:B:1603:LYS:CE	4:B:1609:PHE:C	2.51	0.70
2:C:1067:VAL:N	2:C:1152:SER:CB	2.50	0.70
4:B:898:PRO:HB2	4:B:1077:ARG:HB2	1.73	0.70
4:B:1537:ASP:CB	4:B:1624:GLY:CA	2.70	0.70
2:C:2617:VAL:CG1	2:C:2900:VAL:HG22	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:LEU:CB	1:A:1273:PHE:HE1	2.04	0.70
4:B:1595:LEU:HB2	4:B:1618:LEU:HD21	1.57	0.70
2:C:1069:ARG:HG2	2:C:1155:ASN:CG	2.17	0.69
2:C:1135:ALA:CB	2:C:1212:GLU:HG3	2.22	0.69
2:C:1135:ALA:CB	2:C:1212:GLU:HG2	2.20	0.69
4:B:660:LEU:CB	4:B:752:ILE:HG23	2.22	0.69
4:B:764:GLN:O	4:B:767:SER:N	2.26	0.69
4:B:1606:PHE:HZ	4:B:1690:GLU:HB2	0.65	0.69
1:A:1212:LEU:HD21	1:A:1275:LEU:HD13	1.74	0.69
1:A:1220:THR:CG2	1:A:1279:LYS:CB	2.71	0.69
2:C:1136:PHE:CG	2:C:1138:ARG:N	2.58	0.69
4:B:1531:ILE:HD13	4:B:1618:LEU:CB	2.17	0.69
1:A:3583:ILE:HG22	1:A:3627:CYS:HA	1.74	0.69
4:B:3331:TYR:O	4:B:3334:SER:N	2.26	0.68
4:B:1230:MET:HE1	4:B:1267:TYR:HA	1.74	0.68
4:B:3273:ASP:O	4:B:3276:VAL:N	2.24	0.68
2:C:1135:ALA:HB1	2:C:1212:GLU:HG3	1.72	0.68
4:B:1220:GLN:CG	4:B:1294:ASN:CB	2.56	0.68
1:A:1500:THR:HG23	1:A:1566:GLN:HE22	1.58	0.68
2:C:2617:VAL:HG22	2:C:3183:ILE:HD13	1.75	0.68
2:C:3970:LEU:HD23	2:C:3990:LEU:HD21	1.75	0.68
4:B:2696:LEU:HD12	4:B:2707:ALA:HB2	1.74	0.68
4:B:898:PRO:HD2	4:B:1073:ILE:HD13	1.76	0.68
9:N:38:TYR:CB	9:N:75:GLN:NE2	2.57	0.68
4:B:1606:PHE:HZ	4:B:1690:GLU:CG	2.06	0.68
4:B:898:PRO:HB3	4:B:1076:LEU:C	2.18	0.68
4:B:900:PHE:CA	4:B:1076:LEU:HB2	2.24	0.67
4:B:898:PRO:HG3	4:B:1073:ILE:CG1	2.12	0.67
2:C:972:LEU:HD21	2:C:1017:MET:CE	2.25	0.67
4:B:1603:LYS:CE	4:B:1609:PHE:HB3	2.25	0.67
2:C:1135:ALA:HB1	2:C:1212:GLU:CD	2.20	0.67
2:C:2177:ILE:HG22	2:C:2233:PRO:HA	1.77	0.67
1:A:1016:PHE:CZ	1:A:1076:LEU:HD12	2.30	0.67
1:A:2443:CYS:O	1:A:2443:CYS:SG	2.53	0.67
4:B:1603:LYS:N	4:B:1609:PHE:CD2	2.58	0.67
2:C:539:LYS:CB	2:C:702:PHE:CA	2.71	0.67
2:C:1132:LYS:HE2	2:C:1151:LEU:CG	2.19	0.67
4:B:1230:MET:CE	4:B:1267:TYR:HA	2.25	0.67
4:B:1599:LEU:HD11	4:B:1618:LEU:H	1.54	0.66
4:B:899:LEU:CD2	4:B:1075:TRP:CD1	2.75	0.66
4:B:1237:ARG:CD	4:B:1263:THR:CB	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:97:MET:HE2	11:E:116:VAL:HG21	1.78	0.66
2:C:834:VAL:HG22	2:C:881:ILE:HD11	1.78	0.66
4:B:898:PRO:HG2	4:B:1077:ARG:HB2	1.77	0.66
4:B:1102:LEU:HD23	4:B:1105:GLN:HB2	1.78	0.66
2:C:1132:LYS:HG2	2:C:1151:LEU:CD2	2.26	0.66
2:C:2790:ASN:CB	2:C:2821:VAL:HG22	2.25	0.66
4:B:898:PRO:HD3	4:B:1073:ILE:CD1	2.26	0.66
4:B:1490:GLN:HB3	4:B:3614:ILE:CG2	2.26	0.66
4:B:1603:LYS:CA	4:B:1609:PHE:HD2	2.09	0.66
1:A:1013:VAL:HG13	1:A:1076:LEU:HD11	1.78	0.66
2:C:39:LEU:HD12	2:C:345:TRP:CZ2	2.31	0.66
1:A:751:LEU:HG	1:A:886:ILE:HD11	1.77	0.65
4:B:1606:PHE:CD1	4:B:1687:LEU:HB2	2.31	0.65
11:E:395:VAL:HG21	11:E:402:ILE:HD12	1.78	0.65
1:A:1634:ILE:HD13	1:A:1656:ILE:HG23	1.78	0.65
4:B:898:PRO:CD	4:B:1073:ILE:CD1	2.75	0.65
4:B:1595:LEU:CB	4:B:1618:LEU:HD23	1.86	0.65
2:C:2801:GLU:O	2:C:2804:ALA:HB3	1.96	0.65
4:B:1602:LYS:CB	4:B:1609:PHE:HE2	2.10	0.65
4:B:4168:VAL:HG11	4:B:4189:ILE:HG21	1.77	0.65
4:B:808:PRO:CG	4:B:1077:ARG:HD3	2.17	0.65
1:A:1209:LEU:CA	1:A:1273:PHE:CE1	2.80	0.65
2:C:1060:LEU:HD11	2:C:1148:LEU:HD22	1.77	0.65
1:A:3448:SER:HB3	1:A:3477:MET:HE1	1.77	0.65
2:C:1132:LYS:CD	2:C:1151:LEU:CD2	2.72	0.65
4:B:898:PRO:HA	4:B:1075:TRP:O	1.97	0.65
4:B:1238:LYS:HE2	4:B:1308:LEU:CA	2.14	0.65
4:B:898:PRO:HB2	4:B:1077:ARG:H	1.60	0.65
4:B:1537:ASP:HB2	4:B:1624:GLY:H	1.62	0.65
4:B:3289:ALA:O	4:B:3292:ASP:HB2	1.97	0.65
4:B:3326:MET:O	4:B:3327:ALA:C	2.40	0.65
4:B:898:PRO:HB2	4:B:1077:ARG:CB	2.27	0.65
2:C:2812:GLY:O	2:C:2815:SER:OG	2.08	0.64
1:A:1219:PHE:CD1	1:A:1266:ASN:CB	2.81	0.64
1:A:2418:ILE:HG22	1:A:2419:PRO:HD2	1.80	0.64
4:B:871:ILE:HD11	4:B:944:ILE:HD11	1.79	0.64
4:B:886:ILE:HA	4:B:1075:TRP:CD1	2.33	0.64
4:B:898:PRO:CB	4:B:1076:LEU:C	2.71	0.64
4:B:2157:LEU:HB2	19:B:4701:ATP:N1	2.12	0.64
5:I:94:LEU:HD21	12:D:195:ILE:HD13	1.80	0.64
1:A:1631:PHE:HB2	1:A:1634:ILE:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3290:LEU:HD22	1:A:3335:TRP:CZ2	2.33	0.64
4:B:898:PRO:CG	4:B:1077:ARG:HB2	2.28	0.64
4:B:898:PRO:HB3	4:B:1077:ARG:N	2.13	0.64
1:A:3702:SER:CB	1:A:3712:LEU:HD11	2.28	0.63
4:B:3332:ALA:O	4:B:3335:LYS:N	2.31	0.63
1:A:1219:PHE:CE1	1:A:1263:TYR:CB	2.81	0.63
1:A:1223:VAL:HG13	1:A:1283:LEU:O	1.99	0.63
4:B:1598:TYR:CE2	4:B:1621:LEU:HG	2.34	0.63
1:A:1208:TYR:CD1	1:A:1273:PHE:CE2	2.87	0.63
1:A:1212:LEU:HD13	1:A:1273:PHE:CG	2.34	0.63
2:C:391:GLN:CA	4:B:2596:THR:HG22	2.28	0.63
11:E:531:ARG:O	11:E:535:LYS:N	2.31	0.63
12:D:167:ASN:O	12:D:168:TYR:CD2	2.51	0.63
1:A:1926:PHE:HB3	1:A:1974:ILE:HG23	1.80	0.63
1:A:3128:THR:HG22	1:A:3422:LEU:HB3	1.80	0.63
2:C:1880:VAL:HA	2:C:1883:ILE:HD12	1.79	0.63
1:A:3212:VAL:HG13	1:A:3335:TRP:CD1	2.34	0.63
4:B:764:GLN:C	4:B:766:ILE:N	2.51	0.63
4:B:1531:ILE:HG23	4:B:1622:SER:CB	2.29	0.63
4:B:3878:ILE:HD11	4:B:3887:ALA:HB2	1.81	0.63
12:D:397:ASP:CB	12:D:398:PRO:HD3	2.29	0.62
2:C:903:PRO:HB3	2:C:3080:GLY:HA2	1.82	0.62
4:B:1599:LEU:HD22	4:B:1617:LEU:HD12	1.81	0.62
1:A:1219:PHE:CZ	1:A:1263:TYR:CB	2.82	0.62
4:B:1538:ILE:CB	4:B:1622:SER:O	2.40	0.62
5:I:51:ALA:HB1	5:I:52:PRO:CD	2.30	0.62
8:F:80:ARG:NH2	8:F:103:CYS:SG	2.73	0.62
1:A:1276:GLN:OE1	12:D:153:HIS:ND1	2.31	0.62
1:A:1219:PHE:CZ	1:A:1263:TYR:CA	2.80	0.62
1:A:1392:ASN:O	1:A:1396:PRO:N	2.33	0.62
4:B:1599:LEU:HD21	4:B:1618:LEU:HA	1.81	0.62
4:B:3525:ILE:HG22	4:B:3644:ILE:HD13	1.82	0.62
7:G:107:THR:HG21	7:G:137:VAL:HG11	1.81	0.62
1:A:2348:MET:HE3	1:A:2400:GLU:HG3	1.81	0.61
2:C:2431:ILE:HG23	2:C:2486:MET:HE1	1.82	0.61
4:B:898:PRO:CG	4:B:1077:ARG:CB	2.78	0.61
4:B:898:PRO:CD	4:B:1073:ILE:HG12	2.29	0.61
4:B:3314:ILE:CD1	4:B:3344:VAL:HG21	2.30	0.61
4:B:1599:LEU:HD11	4:B:1618:LEU:CG	2.31	0.61
4:B:2984:VAL:HG13	4:B:3004:LEU:HD12	1.81	0.61
2:C:1081:ILE:HD11	2:C:1117:GLN:CB	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:MET:SD	1:A:1549:MET:HA	2.39	0.61
1:A:2171:THR:O	1:A:2175:THR:HG23	1.99	0.61
4:B:900:PHE:O	4:B:1077:ARG:N	2.33	0.61
2:C:2722:VAL:HG12	2:C:2813:ILE:HD13	1.82	0.61
4:B:1602:LYS:O	4:B:1683:GLU:HB2	2.01	0.61
2:C:2738:ILE:HG22	2:C:2746:PRO:HD3	1.83	0.61
4:B:765:PHE:O	4:B:766:ILE:O	2.19	0.61
4:B:1535:SER:HB3	4:B:1623:ASN:CG	2.25	0.61
11:E:423:GLY:HA2	11:E:505:ILE:HD12	1.82	0.61
1:A:4287:THR:HG22	1:A:4549:ILE:HD12	1.82	0.61
1:A:91:LYS:CB	4:B:136:PRO:CB	2.79	0.60
2:C:1132:LYS:CD	2:C:1151:LEU:HD21	2.31	0.60
4:B:829:VAL:HG11	4:B:940:ILE:HG23	1.83	0.60
4:B:1102:LEU:HA	4:B:1105:GLN:HB2	1.84	0.60
4:B:3327:ALA:O	4:B:3329:GLN:N	2.34	0.60
5:I:24:ILE:HD11	12:D:207:ALA:HB1	1.82	0.60
1:A:1212:LEU:CD2	1:A:1275:LEU:CD1	2.79	0.60
1:A:1396:PRO:O	1:A:1400:TYR:N	2.34	0.60
1:A:1806:PHE:CD1	1:A:4194:VAL:HG22	2.36	0.60
2:C:2790:ASN:HB2	2:C:2821:VAL:HG22	1.82	0.60
4:B:723:ASN:O	4:B:726:LYS:N	2.34	0.60
1:A:3533:PRO:HD3	1:A:3648:THR:HG22	1.83	0.60
2:C:1718:VAL:HG21	2:C:1737:LEU:HD21	1.82	0.60
4:B:3153:LEU:HD13	4:B:3707:LEU:HD11	1.83	0.60
4:B:3833:MET:HE1	4:B:3945:PHE:HZ	1.66	0.60
5:I:51:ALA:HB1	5:I:52:PRO:HD2	1.83	0.60
1:A:1539:LYS:HE2	4:B:3859:VAL:CG2	2.32	0.60
1:A:1789:VAL:HG21	1:A:2010:VAL:HG22	1.83	0.60
4:B:2245:GLN:HE22	4:B:2299:MET:HE2	1.66	0.60
4:B:1598:TYR:HD2	4:B:1621:LEU:CD2	2.13	0.60
4:B:1603:LYS:HG3	4:B:1609:PHE:CD2	2.37	0.60
2:C:359:GLY:O	2:C:386:GLY:O	2.19	0.60
4:B:1598:TYR:CD2	4:B:1621:LEU:CD2	2.84	0.60
10:O:102:LEU:HD12	12:D:75:LEU:HD12	1.84	0.60
1:A:4056:ILE:HD11	1:A:4072:LEU:HD21	1.82	0.60
1:A:1031:ILE:HG21	1:A:1095:GLN:HG3	1.84	0.59
1:A:2042:ARG:HG3	1:A:2278:ASN:HA	1.84	0.59
1:A:3895:GLU:O	1:A:3899:LEU:HD13	2.02	0.59
4:B:1490:GLN:HB2	4:B:3614:ILE:HG23	1.84	0.59
4:B:3327:ALA:HA	4:B:3334:SER:HB2	1.84	0.59
1:A:3914:ASN:O	1:A:3950:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:898:PRO:CA	4:B:1073:ILE:HG23	2.32	0.59
4:B:1061:GLN:HE21	4:B:1091:VAL:HG12	1.67	0.59
4:B:4206:ARG:NH2	4:B:4573:ILE:HD13	2.17	0.59
4:B:886:ILE:HA	4:B:1075:TRP:NE1	2.18	0.59
1:A:1632:ASP:HB2	1:A:1892:PHE:CD1	2.37	0.59
4:B:1535:SER:CB	4:B:1622:SER:C	2.65	0.59
2:C:1132:LYS:HE3	2:C:1151:LEU:HD21	1.60	0.59
10:O:98:ALA:HB1	12:D:105:MET:HE2	1.84	0.59
1:A:1445:PHE:CZ	1:A:1508:LEU:HD21	2.36	0.59
4:B:1492:LYS:HZ2	4:B:3606:GLN:HB2	1.67	0.59
4:B:1599:LEU:HD13	4:B:1617:LEU:CA	2.32	0.59
12:D:352:CYS:SG	12:D:402:VAL:N	2.74	0.59
4:B:899:LEU:N	4:B:1076:LEU:HA	2.05	0.59
4:B:1606:PHE:CZ	4:B:1690:GLU:HG2	2.37	0.59
4:B:3472:LEU:O	4:B:3476:THR:OG1	2.21	0.59
1:A:539:PHE:HA	1:A:544:TYR:CB	2.33	0.59
2:C:2217:ASN:HD22	2:C:2247:THR:HG23	1.68	0.59
4:B:900:PHE:O	4:B:1077:ARG:O	2.21	0.59
1:A:1227:ARG:CB	1:A:1286:THR:HA	2.33	0.58
2:C:1067:VAL:HA	2:C:1152:SER:O	2.03	0.58
4:B:898:PRO:CB	4:B:1077:ARG:HB2	2.32	0.58
4:B:1603:LYS:CG	4:B:1609:PHE:CG	2.81	0.58
4:B:1603:LYS:HG3	4:B:1609:PHE:CG	2.37	0.58
4:B:898:PRO:HB3	4:B:1073:ILE:HG23	1.84	0.58
4:B:2174:LEU:HD11	4:B:2302:ILE:HD11	1.85	0.58
4:B:1537:ASP:HB3	4:B:1624:GLY:HA3	1.84	0.58
4:B:1603:LYS:HD2	4:B:1617:LEU:HD22	1.85	0.58
2:C:214:LEU:C	2:C:214:LEU:HD22	2.29	0.58
2:C:2722:VAL:CG1	2:C:2813:ILE:HD13	2.33	0.58
4:B:3324:LYS:O	4:B:3327:ALA:N	2.37	0.58
4:B:3528:CYS:SG	4:B:3642:THR:HG21	2.42	0.58
11:E:306:ILE:HG23	11:E:343:LEU:HD12	1.85	0.58
1:A:2033:LEU:CD2	1:A:4498:LEU:HD23	2.34	0.58
2:C:2821:VAL:O	2:C:2825:ASP:N	2.36	0.58
2:C:3732:HIS:CG	2:C:3757:LEU:HD12	2.39	0.58
4:B:898:PRO:N	4:B:1073:ILE:CG2	2.67	0.58
4:B:2740:ASN:O	4:B:2742:ARG:N	2.37	0.58
1:A:1066:VAL:HB	1:A:1069:TYR:CE1	2.38	0.58
1:A:1216:ILE:HG23	1:A:1279:LYS:CB	2.33	0.58
2:C:2534:VAL:HG21	2:C:2586:THR:HG22	1.86	0.58
1:A:936:GLN:HA	1:A:1081:ILE:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3223:LEU:HD11	1:A:3332:ILE:CD1	2.34	0.58
2:C:1738:PHE:CE2	2:C:1770:MET:HE1	2.39	0.58
2:C:1186:THR:O	2:C:1188:LEU:N	2.36	0.58
4:B:3764:LEU:HD11	4:B:3816:LEU:HD21	1.84	0.58
2:C:2555:LEU:HD22	2:C:2953:ASN:HD22	1.68	0.57
4:B:1110:GLN:O	4:B:1114:LEU:HG	2.04	0.57
4:B:3081:ASN:HD21	4:B:3484:LYS:HD3	1.69	0.57
4:B:3257:ARG:O	4:B:3258:VAL:C	2.45	0.57
10:O:102:LEU:CD1	12:D:75:LEU:HD12	2.34	0.57
2:C:1559:LEU:HD23	2:C:1607:LEU:HD21	1.86	0.57
12:D:571:LEU:HB3	12:D:647:TYR:CE2	2.40	0.57
4:B:1237:ARG:HH21	4:B:1263:THR:N	1.97	0.57
1:A:2030:LEU:HB2	1:A:2101:ILE:HD13	1.87	0.57
2:C:1081:ILE:HD11	2:C:1117:GLN:HB3	1.86	0.57
4:B:1603:LYS:CE	4:B:1617:LEU:HD22	2.34	0.57
2:C:1136:PHE:HB3	2:C:1139:PHE:CD2	2.40	0.57
1:A:1209:LEU:HB2	1:A:1273:PHE:CE1	2.35	0.57
1:A:2786:CYS:HB3	1:A:2850:LEU:HD22	1.87	0.57
4:B:3331:TYR:O	4:B:3332:ALA:C	2.47	0.57
4:B:3332:ALA:O	4:B:3333:ALA:C	2.48	0.57
4:B:3829:VAL:HG11	4:B:3946:ILE:HD13	1.86	0.57
10:O:98:ALA:HA	12:D:107:VAL:HA	1.86	0.57
2:C:1333:VAL:HG12	2:C:1340:GLN:HE21	1.68	0.57
2:C:2631:ALA:HB1	2:C:2886:ALA:HB1	1.85	0.57
1:A:1013:VAL:HG12	1:A:1017:LEU:HD12	1.86	0.56
1:A:3223:LEU:HD21	1:A:3332:ILE:CD1	2.35	0.56
2:C:136:ALA:HB2	2:C:168:ASN:HA	1.87	0.56
4:B:1209:ALA:CB	4:B:1286:LYS:CB	2.83	0.56
4:B:2264:ASP:O	4:B:2625:ARG:NH2	2.38	0.56
4:B:3984:PHE:CD2	4:B:4076:LEU:HD11	2.40	0.56
2:C:1900:TYR:O	2:C:1903:VAL:N	2.38	0.56
2:C:2718:GLY:N	2:C:2803:MET:HE1	2.19	0.56
4:B:4370:ILE:HD13	4:B:4384:MET:HB3	1.87	0.56
1:A:1525:PHE:HB2	1:A:1541:PHE:HD2	1.70	0.56
1:A:1631:PHE:CZ	1:A:1687:LEU:HD22	2.41	0.56
4:B:591:TRP:CD1	11:E:411:TYR:HH	2.22	0.56
4:B:3984:PHE:CE2	4:B:4076:LEU:HD11	2.40	0.56
1:A:1276:GLN:CD	12:D:153:HIS:ND1	2.63	0.56
4:B:1599:LEU:HD13	4:B:1617:LEU:C	2.30	0.56
11:E:439:TYR:HB3	11:E:508:MET:HE1	1.88	0.56
1:A:1544:ILE:HG12	1:A:1580:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1132:LYS:CG	2:C:1151:LEU:CD2	2.73	0.56
4:B:1603:LYS:CA	4:B:1609:PHE:CD2	2.89	0.56
4:B:3267:ILE:HD12	4:B:3279:LYS:CD	2.36	0.56
1:A:1220:THR:HG22	1:A:1279:LYS:HA	1.87	0.56
4:B:1606:PHE:CA	4:B:1607:PRO:HD3	2.35	0.56
4:B:773:VAL:O	4:B:777:PHE:HB2	2.05	0.56
1:A:4599:CYS:O	1:A:4599:CYS:SG	2.63	0.56
2:C:1541:LEU:HD13	2:C:1584:LEU:HD22	1.88	0.56
4:B:764:GLN:O	4:B:765:PHE:O	2.17	0.56
1:A:1065:ILE:HG21	1:A:1082:CYS:SG	2.46	0.56
4:B:1603:LYS:HE3	4:B:1617:LEU:HD22	1.86	0.56
1:A:3220:ILE:HD11	1:A:3290:LEU:HD12	1.89	0.56
1:A:3709:ASP:HB3	1:A:3712:LEU:HD12	1.87	0.56
2:C:34:ILE:HD12	2:C:116:THR:HG22	1.88	0.56
2:C:1136:PHE:CE2	2:C:1138:ARG:C	2.53	0.56
4:B:319:PRO:CB	11:E:552:ILE:HG22	2.36	0.56
12:D:294:GLN:HE21	12:D:297:LYS:HE2	1.71	0.55
17:M:65:ILE:HD13	17:M:85:TRP:CH2	2.40	0.55
4:B:1599:LEU:HD21	4:B:1618:LEU:CA	2.35	0.55
4:B:3267:ILE:HG23	4:B:3271:ASP:HB2	1.88	0.55
4:B:3586:ILE:HG21	4:B:3594:LEU:HD11	1.88	0.55
1:A:3018:LEU:O	1:A:3022:CYS:SG	2.64	0.55
4:B:2703:ALA:HB2	4:B:2763:ASP:HB2	1.87	0.55
9:N:38:TYR:O	9:N:75:GLN:NE2	2.39	0.55
2:C:1069:ARG:CG	2:C:1155:ASN:ND2	2.69	0.55
2:C:1128:PHE:CE2	2:C:1151:LEU:HD13	2.41	0.55
2:C:2008:LEU:HD23	2:C:2150:ILE:HD11	1.89	0.55
2:C:2790:ASN:HB3	2:C:2821:VAL:HG22	1.88	0.55
4:B:2040:LEU:CD1	4:B:2083:LEU:HD22	2.35	0.55
2:C:972:LEU:HD11	2:C:1017:MET:HE3	1.88	0.55
4:B:1531:ILE:HG23	4:B:1618:LEU:O	2.07	0.55
1:A:1500:THR:O	1:A:1504:VAL:HG23	2.06	0.55
4:B:3020:LEU:HD13	4:B:3022:PHE:CZ	2.42	0.55
1:A:1548:TRP:CZ2	1:A:1552:MET:HE2	2.41	0.55
4:B:900:PHE:H	4:B:1076:LEU:CB	2.19	0.55
4:B:1937:ALA:HB2	4:B:1969:GLN:HE22	1.72	0.55
12:D:75:LEU:HD23	12:D:75:LEU:N	2.22	0.55
1:A:942:VAL:HG21	1:A:1021:THR:HG22	1.89	0.54
2:C:1834:TRP:CD1	2:C:1884:CYS:HG	2.25	0.54
4:B:2122:PHE:CE2	4:B:2126:ILE:HD11	2.42	0.54
4:B:3314:ILE:HD12	4:B:3344:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:42:ILE:HD12	14:L:98:LEU:HD12	1.89	0.54
1:A:1183:LEU:C	1:A:1183:LEU:HD23	2.32	0.54
4:B:898:PRO:CB	4:B:1077:ARG:CB	2.84	0.54
4:B:1527:ILE:HG23	4:B:1615:GLN:CD	2.32	0.54
1:A:1016:PHE:CE2	1:A:1069:TYR:HB2	2.43	0.54
1:A:1129:ILE:HD11	1:A:1211:GLU:HB3	1.89	0.54
1:A:3235:TYR:OH	1:A:3258:PHE:CD1	2.60	0.54
2:C:2822:LYS:O	2:C:2826:VAL:HG23	2.07	0.54
1:A:2216:TRP:O	1:A:2220:ASN:ND2	2.38	0.54
2:C:955:ILE:O	2:C:959:THR:HG23	2.07	0.54
2:C:2066:GLN:HE21	2:C:2066:GLN:CA	2.17	0.54
4:B:162:TYR:CB	4:B:176:LEU:CB	2.85	0.54
4:B:1234:GLU:HB2	4:B:1308:LEU:CB	2.37	0.54
4:B:3085:VAL:HG21	4:B:3456:ALA:HB1	1.89	0.54
1:A:2432:TYR:CE1	1:A:2471:MET:HE1	2.43	0.54
1:A:3099:TYR:HA	1:A:3451:THR:HG21	1.88	0.54
2:C:539:LYS:CB	2:C:702:PHE:CB	2.84	0.54
2:C:1738:PHE:CZ	2:C:1770:MET:HE1	2.43	0.54
2:C:3460:ASN:N	2:C:3460:ASN:HD22	2.05	0.54
2:C:4077:LEU:HD13	2:C:4105:MET:HG2	1.90	0.54
4:B:1602:LYS:C	4:B:1609:PHE:CD2	2.86	0.54
12:D:174:GLN:HA	17:M:62:GLY:HA2	1.89	0.54
1:A:4125:ASN:HD21	1:A:4187:LEU:HG	1.73	0.54
4:B:1602:LYS:HA	4:B:1683:GLU:HG3	1.87	0.54
4:B:3902:TYR:O	4:B:3934:ARG:NH1	2.40	0.54
1:A:1504:VAL:HG22	1:A:1565:CYS:HB3	1.89	0.54
4:B:904:LEU:O	4:B:1083:MET:HB2	2.08	0.54
4:B:3658:ILE:HD11	4:B:3748:ARG:HE	1.72	0.54
4:B:3833:MET:HE2	4:B:3840:VAL:HG21	1.88	0.54
2:C:881:ILE:O	2:C:881:ILE:HG22	2.07	0.54
1:A:3500:ILE:HD12	1:A:3515:ILE:HG23	1.89	0.54
2:C:1067:VAL:CA	2:C:1152:SER:O	2.56	0.54
5:I:90:GLN:HB2	5:I:93:THR:HG21	1.90	0.54
1:A:1536:LEU:HD21	4:B:3888:HIS:CB	2.37	0.54
1:A:3124:ILE:O	1:A:3128:THR:HG23	2.07	0.54
1:A:3449:LEU:HD21	1:A:3474:VAL:HG22	1.90	0.54
4:B:3085:VAL:HG23	4:B:3477:TRP:CE2	2.43	0.54
12:D:120:SER:OG	12:D:123:TYR:N	2.38	0.54
1:A:2418:ILE:CG2	1:A:2428:VAL:HG22	2.38	0.53
4:B:898:PRO:CB	4:B:1077:ARG:HA	2.35	0.53
12:D:66:LEU:HB2	12:D:70:MET:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:716:ASP:O	4:B:719:VAL:N	2.41	0.53
4:B:769:SER:O	4:B:773:VAL:N	2.41	0.53
4:B:1527:ILE:HG23	4:B:1615:GLN:OE1	2.07	0.53
1:A:2745:LEU:HD11	1:A:2754:VAL:HG21	1.89	0.53
4:B:1117:ILE:HG12	4:B:1190:ILE:HD11	1.91	0.53
4:B:1484:LEU:HD12	4:B:1508:LEU:HD12	1.90	0.53
4:B:3830:PHE:HB3	4:B:4290:MET:HE1	1.89	0.53
1:A:1609:THR:HG21	1:A:1629:LYS:HE3	1.91	0.53
4:B:1477:LEU:HD22	4:B:1508:LEU:HD22	1.89	0.53
4:B:1490:GLN:OE1	4:B:3568:THR:O	2.24	0.53
2:C:912:SER:HA	2:C:966:LEU:HD22	1.91	0.53
2:C:2693:GLN:O	2:C:2696:SER:OG	2.20	0.53
9:N:90:ASP:O	9:N:93:THR:OG1	2.25	0.53
1:A:1445:PHE:CE1	1:A:1561:VAL:HG13	2.43	0.53
1:A:1487:VAL:HA	1:A:1490:PHE:CZ	2.44	0.53
1:A:1536:LEU:CD2	4:B:3888:HIS:CB	2.80	0.53
2:C:972:LEU:HD21	2:C:1017:MET:SD	2.48	0.53
4:B:718:ILE:HD11	4:B:773:VAL:HG21	1.90	0.53
12:D:364:ALA:HB2	12:D:404:TRP:NE1	2.23	0.53
1:A:3170:GLY:HA3	1:A:3380:ILE:HG21	1.91	0.53
1:A:3702:SER:HB3	1:A:3712:LEU:HD11	1.91	0.53
1:A:4505:THR:HG22	1:A:4558:VAL:HG12	1.90	0.53
2:C:2659:ALA:CB	2:C:2858:VAL:HG22	2.35	0.53
4:B:1212:ILE:HG22	4:B:1213:PRO:HD3	1.91	0.53
1:A:2567:VAL:HG22	1:A:2573:GLN:HG3	1.90	0.53
1:A:3913:LYS:O	1:A:3947:ARG:NH1	2.40	0.53
2:C:1135:ALA:O	2:C:1137:PRO:HD3	2.08	0.53
2:C:2755:LEU:O	2:C:2758:MET:N	2.41	0.53
4:B:2846:LEU:HD11	4:B:2872:VAL:HG11	1.90	0.53
1:A:1634:ILE:HD13	1:A:1656:ILE:CG2	2.39	0.53
4:B:720:ASP:O	4:B:721:ASN:C	2.52	0.53
4:B:2711:VAL:HA	4:B:2714:THR:HG22	1.91	0.53
10:O:38:ILE:HG22	10:O:67:LEU:HD11	1.91	0.53
11:E:384:LEU:HD23	11:E:417:TRP:CE2	2.43	0.53
14:L:80:LYS:HB2	17:M:60:ASN:HD21	1.73	0.53
1:A:2411:LEU:HD12	1:A:2428:VAL:HG21	1.90	0.53
1:A:4234:PHE:O	1:A:4236:TYR:N	2.42	0.53
4:B:533:ARG:HB3	4:B:534:PRO:CD	2.39	0.53
1:A:3229:PRO:HB2	1:A:3233:ILE:HG23	1.92	0.52
4:B:2696:LEU:HD23	4:B:2699:ILE:HD12	1.91	0.52
7:G:99:ILE:HG23	7:G:103:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2758:MET:O	2:C:2759:LYS:C	2.52	0.52
5:I:12:ILE:HG23	7:G:120:THR:HG23	1.90	0.52
9:N:88:TYR:HA	11:E:23:THR:HG22	1.91	0.52
10:O:76:VAL:N	10:O:77:PRO:CD	2.73	0.52
12:D:89:TYR:CD1	15:K:56:PRO:HB3	2.44	0.52
12:D:519:ALA:HB1	12:D:545:VAL:CG1	2.39	0.52
1:A:1687:LEU:C	1:A:1687:LEU:HD23	2.35	0.52
2:C:90:ILE:HD11	2:C:96:LEU:HD23	1.90	0.52
2:C:4017:LEU:HD21	2:C:4022:LEU:HD11	1.91	0.52
4:B:569:VAL:HG13	4:B:578:LEU:HD11	1.91	0.52
4:B:1102:LEU:HD23	4:B:1105:GLN:CB	2.39	0.52
2:C:1207:LEU:HD13	2:C:1214:TYR:CE1	2.44	0.52
2:C:4051:THR:HG21	2:C:4143:ASN:HD22	1.74	0.52
1:A:2676:TRP:CD2	1:A:2699:LEU:HD21	2.45	0.52
2:C:2803:MET:HE3	2:C:2810:ALA:HB1	1.91	0.52
2:C:2896:ALA:O	2:C:2900:VAL:HG23	2.10	0.52
2:C:4084:ILE:HD11	2:C:4106:PRO:HG3	1.91	0.52
4:B:721:ASN:OD1	4:B:777:PHE:CE2	2.63	0.52
4:B:1102:LEU:O	4:B:1106:PHE:N	2.35	0.52
4:B:1941:MET:HE3	4:B:1992:ILE:HD11	1.90	0.52
1:A:1422:SER:HB2	1:A:1486:HIS:CE1	2.45	0.52
2:C:2617:VAL:CG2	2:C:3183:ILE:HD13	2.40	0.52
2:C:3227:ALA:HA	2:C:3393:ILE:HG22	1.91	0.52
4:B:361:LYS:HA	4:B:477:ILE:HG23	1.90	0.52
4:B:2863:VAL:HG21	4:B:3059:VAL:HA	1.91	0.52
4:B:3020:LEU:HD13	4:B:3022:PHE:CE2	2.45	0.52
1:A:2676:TRP:CE2	1:A:2699:LEU:HD21	2.45	0.52
2:C:2096:ILE:HD11	2:C:2141:TYR:CD2	2.45	0.52
4:B:591:TRP:CD1	11:E:411:TYR:OH	2.63	0.52
4:B:716:ASP:O	4:B:718:ILE:N	2.43	0.52
4:B:1149:ASP:O	4:B:1153:VAL:N	2.43	0.52
4:B:1205:PHE:HE2	4:B:1286:LYS:HA	1.74	0.52
1:A:1052:LEU:HB3	1:A:1166:TYR:CE2	2.45	0.52
2:C:403:GLU:O	4:B:2988:ARG:CZ	2.54	0.52
7:G:71:LYS:HG3	7:G:72:THR:HG23	1.91	0.52
17:M:65:ILE:HG21	17:M:85:TRP:CE2	2.45	0.52
1:A:1208:TYR:CD1	1:A:1273:PHE:HE2	2.27	0.52
1:A:3163:SER:HA	1:A:3387:LEU:HD13	1.91	0.52
1:A:3220:ILE:CD1	1:A:3290:LEU:HD12	2.40	0.52
2:C:2007:LEU:HD11	2:C:2128:MET:HE3	1.92	0.52
4:B:825:LYS:O	4:B:829:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:898:PRO:CG	4:B:1073:ILE:CG1	2.77	0.52
4:B:1599:LEU:CD1	4:B:1617:LEU:CB	2.61	0.52
7:G:149:GLN:HE22	12:D:252:VAL:HA	1.74	0.52
1:A:1825:ILE:HD12	1:A:1889:LEU:HA	1.91	0.51
4:B:885:GLN:O	4:B:1075:TRP:HD1	1.93	0.51
4:B:1212:ILE:HG21	4:B:1285:GLU:O	2.10	0.51
4:B:1599:LEU:HB2	4:B:1617:LEU:HD23	1.75	0.51
4:B:2608:ASN:ND2	4:B:2655:ASN:O	2.42	0.51
4:B:3085:VAL:HG23	4:B:3477:TRP:CZ2	2.45	0.51
1:A:1276:GLN:CG	12:D:153:HIS:HE1	2.05	0.51
2:C:1856:TYR:HA	2:C:1934:TRP:HH2	1.75	0.51
2:C:2751:TRP:O	2:C:2754:SER:HB3	2.10	0.51
4:B:1109:THR:O	4:B:1113:LEU:HG	2.10	0.51
4:B:2150:THR:HG22	4:B:2203:ASN:HD22	1.75	0.51
4:B:2695:HIS:CG	4:B:2695:HIS:O	2.63	0.51
4:B:2889:VAL:HG21	4:B:3029:MET:HE1	1.93	0.51
10:O:19:LEU:HA	10:O:22:LEU:HD21	1.91	0.51
1:A:1135:VAL:HG13	1:A:1201:TYR:OH	2.11	0.51
1:A:3170:GLY:HA2	1:A:3380:ILE:HD13	1.91	0.51
2:C:3438:HIS:HD1	2:C:3443:LYS:HB2	1.75	0.51
4:B:1595:LEU:HD13	4:B:1618:LEU:HD22	1.89	0.51
1:A:3132:ASN:N	1:A:3419:ILE:HD11	2.25	0.51
2:C:913:MET:CE	2:C:959:THR:HG22	2.37	0.51
2:C:1864:ILE:HD11	2:C:1910:ILE:HG23	1.91	0.51
4:B:4545:CYS:SG	4:B:4579:ILE:HD13	2.50	0.51
8:F:26:PHE:CE2	8:F:52:VAL:HG11	2.46	0.51
1:A:2490:LEU:HD11	1:A:2611:MET:HG2	1.93	0.51
1:A:2935:LEU:HD12	1:A:2938:ILE:HD11	1.91	0.51
2:C:4138:PHE:CE1	2:C:4141:THR:HA	2.46	0.51
4:B:1605:SER:O	4:B:1687:LEU:HD22	2.11	0.51
4:B:3694:LEU:HD22	4:B:3715:ASN:HD22	1.76	0.51
12:D:509:ASN:HD21	12:D:512:HIS:HB3	1.74	0.51
1:A:1634:ILE:HD11	1:A:1637:VAL:HG22	1.93	0.51
4:B:1230:MET:HE1	4:B:1267:TYR:CA	2.41	0.51
4:B:1603:LYS:O	4:B:1607:PRO:N	2.43	0.51
4:B:1603:LYS:HA	4:B:1609:PHE:CD2	2.45	0.51
1:A:1108:LEU:O	1:A:1112:THR:N	2.42	0.51
4:B:1069:THR:HB	4:B:1070:PRO:HD2	1.92	0.51
4:B:1595:LEU:C	4:B:1618:LEU:HD21	2.36	0.51
12:D:603:LEU:HD22	12:D:611:VAL:HG12	1.91	0.51
1:A:1126:VAL:HG21	1:A:1135:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1868:GLY:O	1:A:1973:PHE:HA	2.11	0.51
4:B:1603:LYS:HG2	4:B:1609:PHE:C	2.36	0.51
1:A:935:VAL:HG22	1:A:1017:LEU:HD21	1.92	0.51
1:A:2564:MET:N	1:A:2565:PRO:HD2	2.26	0.51
2:C:834:VAL:CG2	2:C:881:ILE:HD11	2.40	0.51
4:B:1641:LEU:HD13	4:B:1662:MET:HB2	1.93	0.51
2:C:2177:ILE:CG2	2:C:2233:PRO:HA	2.39	0.50
4:B:804:ARG:NH1	4:B:898:PRO:O	2.44	0.50
4:B:3789:THR:HG22	4:B:3803:ASN:HD22	1.75	0.50
1:A:2432:TYR:CD1	1:A:2471:MET:HE1	2.46	0.50
1:A:4583:TYR:HB3	1:A:4584:PRO:HD2	1.94	0.50
4:B:1596:ASN:N	4:B:1618:LEU:HD21	2.26	0.50
4:B:1599:LEU:HD12	4:B:1618:LEU:HG	1.92	0.50
1:A:870:PRO:C	1:A:871:LEU:HD13	2.37	0.50
1:A:1482:ASN:HA	1:A:1487:VAL:HG11	1.92	0.50
2:C:2708:GLN:CD	2:C:2813:ILE:HD11	2.37	0.50
4:B:1490:GLN:OE1	4:B:3614:ILE:CB	2.57	0.50
4:B:2004:MET:HE2	4:B:2014:LEU:HD11	1.94	0.50
11:E:42:GLN:HE22	14:L:91:ASN:ND2	2.09	0.50
2:C:1132:LYS:HG2	2:C:1151:LEU:CG	2.40	0.50
4:B:1599:LEU:CB	4:B:1617:LEU:CD1	2.83	0.50
13:P:53:LEU:O	13:P:57:ILE:N	2.44	0.50
14:L:86:LEU:HD12	17:M:54:ASN:HB3	1.93	0.50
1:A:4562:ASN:CG	1:A:4562:ASN:O	2.54	0.50
4:B:1212:ILE:HB	4:B:1213:PRO:HD2	1.94	0.50
1:A:1209:LEU:CA	1:A:1273:PHE:HE1	2.23	0.50
2:C:3064:ILE:HG13	2:C:3115:ILE:HD12	1.94	0.50
4:B:1602:LYS:CB	4:B:1609:PHE:CE2	2.92	0.50
4:B:2621:ILE:HG23	4:B:2667:LEU:HD13	1.90	0.50
1:A:1276:GLN:OE1	12:D:153:HIS:CG	2.64	0.50
1:A:2117:GLU:HG2	1:A:2141:ILE:HD11	1.94	0.50
1:A:4240:VAL:HG11	1:A:4270:PRO:HG2	1.93	0.50
2:C:1296:ILE:HD11	2:C:1542:MET:SD	2.52	0.50
4:B:871:ILE:HG21	4:B:959:ILE:HD11	1.93	0.50
4:B:2005:ASN:N	4:B:2005:ASN:HD22	2.09	0.50
1:A:1915:VAL:HA	1:A:1970:VAL:HG21	1.94	0.50
2:C:2659:ALA:HB1	2:C:2858:VAL:HG13	1.94	0.50
2:C:1069:ARG:HH21	2:C:1155:ASN:ND2	2.10	0.50
4:B:898:PRO:N	4:B:1073:ILE:HG21	2.23	0.50
4:B:2704:GLN:O	4:B:2707:ALA:N	2.31	0.50
2:C:403:GLU:O	4:B:2999:ASN:OD1	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:972:LEU:HD13	2:C:1029:GLU:HG2	1.94	0.49
2:C:1017:MET:HE2	2:C:1030:VAL:HB	1.94	0.49
4:B:1238:LYS:HG2	4:B:1311:MET:CB	2.42	0.49
1:A:675:ILE:HG22	1:A:686:VAL:HA	1.94	0.49
1:A:3131:ILE:HD12	1:A:3422:LEU:HD11	1.93	0.49
4:B:2099:ASP:HB2	4:B:2100:PRO:HD3	1.94	0.49
12:D:519:ALA:HB1	12:D:545:VAL:HG12	1.94	0.49
1:A:1209:LEU:CB	1:A:1273:PHE:CE1	2.92	0.49
1:A:3322:ALA:HB2	1:A:3333:LEU:HD12	1.94	0.49
2:C:2770:ASN:O	2:C:2771:PHE:C	2.55	0.49
1:A:3223:LEU:HD11	1:A:3332:ILE:HD11	1.94	0.49
2:C:1069:ARG:HH21	2:C:1155:ASN:HD22	1.60	0.49
2:C:2705:ASP:O	2:C:2706:PHE:C	2.55	0.49
4:B:1527:ILE:HG23	4:B:1615:GLN:NE2	2.27	0.49
4:B:1602:LYS:HB3	4:B:1683:GLU:CB	2.24	0.49
11:E:133:PHE:HZ	12:D:360:ALA:HB3	1.77	0.49
12:D:545:VAL:HA	12:D:562:THR:HG22	1.94	0.49
2:C:1989:THR:HG23	2:C:2019:LEU:HD22	1.94	0.49
4:B:898:PRO:HG3	4:B:1077:ARG:HG3	1.94	0.49
4:B:2619:SER:N	4:B:2620:PRO:HD2	2.27	0.49
1:A:1862:MET:HE2	1:A:1973:PHE:HZ	1.76	0.49
2:C:1221:THR:O	2:C:1225:THR:HG23	2.12	0.49
2:C:2002:VAL:HG12	2:C:2002:VAL:O	2.13	0.49
2:C:2719:VAL:HG13	2:C:2720:PRO:HD3	1.94	0.49
11:E:41:VAL:HG22	11:E:42:GLN:HG3	1.95	0.49
1:A:1219:PHE:CE1	1:A:1263:TYR:C	2.90	0.49
1:A:1563:PRO:O	1:A:1567:ASN:N	2.44	0.49
2:C:2212:LEU:HD11	18:C:4203:ADP:H8	1.77	0.49
4:B:3446:SER:HB2	4:B:3489:THR:HG23	1.94	0.49
1:A:883:THR:HA	1:A:886:ILE:HD12	1.94	0.49
1:A:2840:VAL:HG22	18:A:4703:ADP:HN62	1.78	0.49
1:A:3533:PRO:CD	1:A:3648:THR:HG22	2.41	0.49
4:B:715:LEU:O	4:B:717:MET:N	2.45	0.49
4:B:898:PRO:HG2	4:B:1077:ARG:HD2	1.95	0.49
4:B:4359:LEU:HD22	4:B:4404:ALA:CB	2.43	0.49
4:B:4359:LEU:HD22	4:B:4404:ALA:HB2	1.94	0.49
1:A:1522:GLU:HG3	1:A:1523:PRO:HD3	1.95	0.49
1:A:2793:VAL:HG23	1:A:2804:ALA:HB2	1.95	0.49
1:A:3691:LEU:HB3	1:A:3719:THR:HG22	1.95	0.49
4:B:1603:LYS:CD	4:B:1617:LEU:HD22	2.43	0.49
4:B:1708:ALA:HA	4:B:1711:TRP:NE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2769:ARG:CD	4:B:2836:GLN:HE22	2.26	0.49
4:B:3676:LEU:HD21	4:B:3733:ALA:HB2	1.95	0.49
12:D:162:LEU:C	12:D:162:LEU:HD23	2.38	0.49
17:M:84:LEU:HD12	17:M:84:LEU:C	2.38	0.49
1:A:1230:TYR:CB	1:A:1290:ILE:N	2.76	0.48
1:A:2938:ILE:HD12	1:A:2999:LEU:HD21	1.95	0.48
4:B:1058:LYS:HG3	4:B:1166:GLU:O	2.12	0.48
4:B:1128:PRO:HG2	4:B:1131:HIS:CG	2.48	0.48
4:B:3809:TYR:CE2	4:B:3959:MET:HE2	2.48	0.48
1:A:1676:CYS:HG	1:A:1683:TRP:CD1	2.31	0.48
1:A:1889:LEU:HD12	1:A:1920:TRP:CZ2	2.48	0.48
2:C:1188:LEU:HD21	2:C:1218:VAL:HG22	1.95	0.48
2:C:2740:ILE:HG22	2:C:2741:ASP:H	1.78	0.48
4:B:938:PHE:HB3	4:B:956:LEU:HD13	1.95	0.48
4:B:2267:ILE:HG22	4:B:2271:TRP:HZ3	1.78	0.48
4:B:3850:LEU:O	4:B:3931:ARG:NH2	2.43	0.48
6:H:70:THR:HG23	11:E:68:THR:HB	1.95	0.48
1:A:2418:ILE:HG22	1:A:2419:PRO:CD	2.43	0.48
1:A:4461:LEU:HD21	1:A:4516:ILE:HG21	1.95	0.48
2:C:2803:MET:HE3	2:C:2810:ALA:CB	2.44	0.48
2:C:3938:LEU:HD12	2:C:3982:LYS:HD3	1.94	0.48
4:B:696:THR:HG22	4:B:697:THR:HG23	1.95	0.48
4:B:883:ASN:HA	4:B:886:ILE:HG22	1.95	0.48
7:G:136:MET:HE1	12:D:251:MET:C	2.38	0.48
9:N:76:THR:CG2	11:E:39:GLN:HE22	2.23	0.48
10:O:98:ALA:CB	12:D:105:MET:HE2	2.43	0.48
12:D:299:VAL:HG11	12:D:605:GLY:HA3	1.94	0.48
1:A:3303:ILE:HD11	1:A:3340:TYR:CE2	2.48	0.48
2:C:2709:ALA:HA	2:C:2758:MET:SD	2.53	0.48
4:B:1602:LYS:HB3	4:B:1609:PHE:CE2	2.40	0.48
9:N:89:GLN:HG2	9:N:94:ASP:HB2	1.94	0.48
1:A:1634:ILE:CD1	1:A:1656:ILE:HG23	2.44	0.48
1:A:3248:LEU:HB2	3:Q:104:TYR:CE1	2.48	0.48
1:A:3331:GLY:O	1:A:3335:TRP:N	2.45	0.48
2:C:29:VAL:CG1	2:C:116:THR:HG21	2.43	0.48
2:C:1047:LEU:HG	2:C:1111:LEU:HD11	1.94	0.48
2:C:1132:LYS:HG3	2:C:1151:LEU:HD21	1.89	0.48
2:C:2357:LEU:C	2:C:2357:LEU:HD13	2.38	0.48
4:B:558:VAL:HG11	4:B:599:ILE:HD11	1.94	0.48
2:C:1385:ILE:HA	2:C:1388:THR:HG22	1.96	0.48
4:B:669:ILE:CD1	4:B:752:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:898:PRO:N	4:B:1073:ILE:HG23	2.29	0.48
6:H:67:SER:O	11:E:72:GLY:HA2	2.14	0.48
2:C:913:MET:HE2	2:C:959:THR:HA	1.95	0.48
4:B:1599:LEU:CD1	4:B:1617:LEU:HB3	2.19	0.48
4:B:2758:GLN:HE22	4:B:2834:TYR:H	1.62	0.48
12:D:87:THR:HG22	12:D:98:THR:HA	1.95	0.48
1:A:2697:ARG:NH1	18:A:4701:ADP:O3B	2.36	0.48
2:C:1270:PHE:CG	2:C:1336:ALA:HB2	2.49	0.48
2:C:1856:TYR:CE2	2:C:1903:VAL:HG22	2.49	0.48
4:B:3223:ALA:HB1	4:B:3349:ILE:HD13	1.94	0.48
8:F:87:TYR:HB3	8:F:98:LEU:HD11	1.94	0.48
1:A:3748:ARG:HB3	1:A:3749:PRO:HD3	1.95	0.48
2:C:2734:PHE:CE2	2:C:2767:LYS:HG3	2.49	0.48
4:B:1535:SER:HB3	4:B:1623:ASN:OD1	2.14	0.48
11:E:423:GLY:N	11:E:501:GLU:OE1	2.47	0.48
2:C:968:MET:HB2	2:C:1026:PHE:CZ	2.48	0.48
4:B:447:THR:OG1	4:B:513:ASP:HB3	2.14	0.48
4:B:1819:SER:HA	4:B:1857:VAL:HG13	1.96	0.48
4:B:2308:LEU:HD23	4:B:2316:VAL:HG22	1.96	0.48
2:C:2826:VAL:O	2:C:2828:GLN:N	2.47	0.47
4:B:751:GLY:O	4:B:752:ILE:C	2.56	0.47
4:B:1114:LEU:HA	4:B:1117:ILE:HD12	1.96	0.47
4:B:1531:ILE:CG2	4:B:1622:SER:CB	2.85	0.47
4:B:2987:VAL:HG12	4:B:2987:VAL:O	2.14	0.47
4:B:3350:PHE:HA	4:B:3353:VAL:HG12	1.95	0.47
10:O:30:TYR:N	10:O:31:PRO:CD	2.78	0.47
1:A:1634:ILE:HD11	1:A:1637:VAL:CG2	2.44	0.47
2:C:10:LEU:HD11	2:C:67:CYS:HB3	1.96	0.47
2:C:306:LEU:HD11	2:C:317:LYS:HG2	1.95	0.47
2:C:1081:ILE:HD11	2:C:1117:GLN:HB2	1.96	0.47
2:C:1262:TRP:CE2	2:C:1321:SER:HB2	2.49	0.47
2:C:2717:ALA:C	2:C:2803:MET:HE1	2.39	0.47
4:B:898:PRO:CG	4:B:1073:ILE:CG2	2.85	0.47
4:B:1205:PHE:HE2	4:B:1286:LYS:CA	2.27	0.47
4:B:2210:TYR:HA	4:B:2260:TRP:O	2.14	0.47
4:B:3245:LEU:O	4:B:3247:SER:N	2.46	0.47
4:B:3863:LEU:N	4:B:3863:LEU:HD22	2.29	0.47
9:N:84:GLN:HB2	10:O:64:VAL:HG21	1.95	0.47
1:A:1539:LYS:HE2	4:B:3859:VAL:HG21	1.95	0.47
2:C:364:ILE:C	2:C:383:GLU:CB	2.87	0.47
2:C:2212:LEU:C	2:C:2212:LEU:HD13	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2659:ALA:HB1	2:C:2858:VAL:CG2	2.39	0.47
2:C:2800:PRO:HG3	2:C:2818:VAL:HG21	1.96	0.47
4:B:765:PHE:O	4:B:767:SER:N	2.43	0.47
4:B:1483:ASP:O	4:B:1487:MET:N	2.47	0.47
4:B:2769:ARG:HD2	4:B:2836:GLN:HE22	1.79	0.47
1:A:3577:THR:HG22	1:A:3622:LYS:HB2	1.95	0.47
2:C:214:LEU:O	2:C:231:ILE:HA	2.14	0.47
2:C:1047:LEU:O	2:C:1051:GLN:HG3	2.14	0.47
2:C:2687:ALA:HB1	2:C:2830:VAL:CG2	2.40	0.47
2:C:2795:MET:N	2:C:2796:PRO:CD	2.78	0.47
4:B:2804:ILE:O	4:B:2806:GLU:N	2.47	0.47
4:B:3657:PHE:O	4:B:3661:VAL:HG23	2.14	0.47
4:B:3931:ARG:HB2	4:B:3938:MET:HE3	1.96	0.47
8:F:33:LEU:HD11	11:E:99:ILE:HG21	1.96	0.47
2:C:4128:THR:HA	2:C:4163:MET:O	2.14	0.47
4:B:736:LEU:HD12	4:B:859:TYR:HB2	1.96	0.47
4:B:1075:TRP:CE3	4:B:1076:LEU:HB3	2.48	0.47
4:B:4348:VAL:HG21	4:B:4453:ALA:HB2	1.96	0.47
1:A:1118:LEU:HD12	1:A:1142:ILE:HG13	1.96	0.47
1:A:1162:LEU:C	1:A:1162:LEU:HD23	2.39	0.47
1:A:1760:HIS:O	1:A:1764:LEU:HG	2.15	0.47
1:A:2866:VAL:HG11	1:A:3026:TRP:CZ3	2.50	0.47
2:C:29:VAL:HG11	2:C:116:THR:HG21	1.97	0.47
2:C:2617:VAL:HG22	2:C:3183:ILE:HG21	1.96	0.47
2:C:2738:ILE:HD12	2:C:2740:ILE:O	2.14	0.47
4:B:591:TRP:HD1	11:E:411:TYR:OH	1.97	0.47
4:B:915:PRO:HA	4:B:925:THR:HA	1.95	0.47
4:B:2040:LEU:HD13	4:B:2083:LEU:HD22	1.96	0.47
4:B:2155:MET:HE1	4:B:2195:LYS:HB3	1.96	0.47
4:B:2936:ILE:HG22	4:B:3012:ILE:HD13	1.95	0.47
5:I:75:TRP:CE3	5:I:109:LYS:HB2	2.49	0.47
17:M:3:HIS:CE1	17:M:78:ASN:HD22	2.33	0.47
1:A:1149:ILE:HG21	1:A:1187:TRP:CZ2	2.50	0.47
1:A:2511:ASP:HB2	1:A:2514:LYS:HB2	1.96	0.47
1:A:3568:LEU:C	1:A:3568:LEU:HD23	2.40	0.47
4:B:1897:GLY:O	4:B:2001:PHE:HA	2.14	0.47
2:C:2082:LEU:HD11	2:C:2096:ILE:CD1	2.44	0.47
2:C:2730:LEU:HD23	2:C:2738:ILE:HD13	1.97	0.47
4:B:1666:ASP:HB2	4:B:1870:ASN:HD21	1.79	0.47
4:B:3236:LYS:N	4:B:3237:PRO:HD2	2.28	0.47
4:B:3878:ILE:CD1	4:B:3887:ALA:HB2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4422:ASP:HB2	1:A:4423:PRO:HD2	1.96	0.47
2:C:39:LEU:HD23	2:C:83:CYS:SG	2.55	0.47
2:C:2688:GLN:N	2:C:2689:PRO:CD	2.78	0.47
2:C:2734:PHE:HE2	2:C:2767:LYS:HG3	1.79	0.47
4:B:721:ASN:OD1	4:B:777:PHE:CD2	2.68	0.47
4:B:898:PRO:HG2	4:B:1077:ARG:CB	2.40	0.47
4:B:2115:VAL:HG12	4:B:2323:PHE:CE2	2.50	0.47
4:B:2200:SER:O	4:B:2204:SER:N	2.48	0.47
4:B:2531:ARG:C	4:B:2649:LEU:HD21	2.40	0.47
4:B:3887:ALA:O	4:B:3890:LEU:N	2.48	0.47
6:H:20:MET:O	6:H:24:VAL:HG23	2.15	0.47
1:A:61:GLU:CB	1:A:98:ILE:O	2.63	0.47
1:A:766:GLY:HA3	1:A:780:TYR:CE1	2.50	0.47
1:A:1136:MET:HA	1:A:1136:MET:HE2	1.95	0.47
1:A:1487:VAL:HG23	1:A:1490:PHE:CE1	2.50	0.47
1:A:3286:PHE:CE2	1:A:3290:LEU:HD11	2.50	0.47
1:A:3897:PRO:HA	1:A:3900:ILE:HG22	1.97	0.47
2:C:2740:ILE:HG13	2:C:2744:LYS:HB3	1.97	0.47
4:B:521:PHE:CE2	4:B:605:LYS:HB3	2.49	0.47
4:B:898:PRO:HB3	4:B:1077:ARG:CA	2.43	0.47
4:B:3826:THR:HG22	4:B:3942:LEU:HD22	1.97	0.47
11:E:75:HIS:CG	11:E:75:HIS:O	2.68	0.47
1:A:3242:VAL:HA	1:A:3248:LEU:HD11	1.95	0.46
2:C:1101:PHE:HB3	2:C:1107:MET:HE2	1.96	0.46
2:C:1128:PHE:CZ	2:C:1151:LEU:HB3	2.40	0.46
2:C:3483:LEU:HD12	2:C:3490:TRP:CD1	2.50	0.46
4:B:1599:LEU:N	4:B:1621:LEU:CD2	2.77	0.46
4:B:1944:SER:HA	4:B:1998:VAL:HG11	1.96	0.46
4:B:2971:ILE:HG23	4:B:2974:LEU:HB2	1.97	0.46
2:C:884:ARG:HA	2:C:889:ILE:HD11	1.97	0.46
4:B:459:ILE:HG23	4:B:499:LEU:HD11	1.97	0.46
4:B:1536:GLU:C	4:B:1625:GLN:NE2	2.73	0.46
4:B:3284:MET:SD	4:B:3290:PHE:CD1	3.08	0.46
5:I:97:MET:O	5:I:105:VAL:HB	2.15	0.46
1:A:3307:GLU:N	1:A:3308:PRO:HD2	2.30	0.46
2:C:169:TYR:HB3	4:B:865:VAL:HG21	1.97	0.46
2:C:1864:ILE:HD11	2:C:1910:ILE:CG2	2.44	0.46
2:C:3072:ILE:HD12	2:C:3102:LEU:HD11	1.97	0.46
3:Q:43:GLY:HA3	3:Q:67:SER:CB	2.45	0.46
4:B:885:GLN:O	4:B:1075:TRP:CD1	2.69	0.46
4:B:3255:THR:CB	4:B:3337:CYS:SG	3.02	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:95:LEU:HD23	5:I:107:ILE:HD11	1.97	0.46
7:G:145:LEU:HD22	12:D:248:MET:HG3	1.96	0.46
11:E:224:ASN:HD21	11:E:277:SER:CB	2.27	0.46
12:D:75:LEU:HD23	12:D:75:LEU:H	1.81	0.46
1:A:1667:ILE:HD12	1:A:1838:PHE:CD1	2.51	0.46
2:C:2698:LEU:HD21	2:C:2820:ILE:CA	2.46	0.46
2:C:2826:VAL:C	2:C:2828:GLN:N	2.73	0.46
2:C:4113:VAL:HG12	2:C:4114:PRO:HD2	1.96	0.46
1:A:1151:MET:HE2	14:L:49:LEU:HD11	1.98	0.46
2:C:3151:LYS:CE	2:C:3217:ILE:HD11	2.45	0.46
4:B:3290:PHE:O	4:B:3293:LYS:N	2.48	0.46
4:B:3481:ILE:HG21	4:B:3488:ILE:CD1	2.46	0.46
11:E:261:HIS:CE1	11:E:283:SER:HB3	2.51	0.46
16:J:68:MET:HB3	16:J:76:TRP:CD1	2.50	0.46
1:A:2515:MET:HA	1:A:2553:LYS:O	2.16	0.46
2:C:58:PHE:CD2	2:C:71:GLN:HB3	2.50	0.46
2:C:102:TYR:O	2:C:106:LEU:HB2	2.16	0.46
2:C:859:ILE:CB	2:C:864:MET:SD	3.04	0.46
2:C:2705:ASP:O	2:C:2708:GLN:N	2.49	0.46
4:B:1238:LYS:HE2	4:B:1308:LEU:N	2.26	0.46
4:B:2890:GLY:HA3	4:B:3048:PHE:HB2	1.97	0.46
8:F:74:ILE:HD12	8:F:77:ILE:HD11	1.98	0.46
1:A:3610:VAL:HB	1:A:3615:MET:HE3	1.97	0.46
2:C:3412:HIS:HA	2:C:3415:ILE:HD12	1.96	0.46
4:B:3154:GLN:CB	4:B:3419:ALA:HB1	2.46	0.46
11:E:566:ASN:HB2	11:E:567:PRO:HD2	1.98	0.46
1:A:2704:LYS:O	1:A:2708:THR:HG23	2.16	0.46
1:A:2723:ILE:HG21	1:A:2776:LYS:HE2	1.98	0.46
4:B:447:THR:HG21	4:B:513:ASP:C	2.41	0.46
4:B:744:MET:HE1	4:B:772:ILE:HG23	1.98	0.46
4:B:2771:TRP:O	4:B:2772:ALA:C	2.59	0.46
4:B:3343:ILE:O	4:B:3346:PHE:HB3	2.16	0.46
1:A:3268:PHE:CD1	3:Q:35:ILE:CB	2.99	0.46
1:A:4139:ILE:HD13	1:A:4223:TYR:OH	2.16	0.46
1:A:4477:MET:HG3	1:A:4524:VAL:HG23	1.98	0.46
2:C:2708:GLN:HE21	2:C:2809:ALA:HA	1.80	0.46
4:B:1109:THR:C	4:B:1113:LEU:HG	2.41	0.46
4:B:1602:LYS:HA	4:B:1683:GLU:CB	2.46	0.46
4:B:3258:VAL:HG11	4:B:3321:PHE:CZ	2.51	0.46
11:E:152:LEU:HD22	11:E:486:THR:HG22	1.97	0.46
12:D:367:LEU:HD12	12:D:368:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:THR:HB	1:A:1074:MET:SD	2.56	0.46
4:B:1620:ILE:HG23	4:B:1630:VAL:HG13	1.97	0.46
1:A:5:LYS:CB	1:A:48:GLU:HA	2.46	0.45
1:A:92:ALA:O	1:A:124:THR:CB	2.63	0.45
1:A:1113:GLU:O	1:A:1116:LYS:N	2.49	0.45
1:A:2116:VAL:HG23	1:A:2173:VAL:HG11	1.98	0.45
4:B:1127:ASN:CB	4:B:1128:PRO:CD	2.94	0.45
4:B:1538:ILE:HG21	4:B:1622:SER:OG	2.16	0.45
4:B:2904:THR:HG21	4:B:2911:ILE:HB	1.98	0.45
4:B:3268:THR:HG22	4:B:3269:LEU:HD12	1.97	0.45
5:I:12:ILE:HG21	7:G:119:PRO:HG2	1.98	0.45
2:C:106:LEU:N	2:C:106:LEU:HD12	2.31	0.45
2:C:257:MET:HE1	2:C:296:ILE:HD11	1.98	0.45
2:C:973:LYS:HA	2:C:976:ILE:HD12	1.98	0.45
2:C:2218:VAL:HG23	2:C:2247:THR:HG21	1.99	0.45
2:C:3611:ALA:O	2:C:3615:CYS:SG	2.71	0.45
4:B:447:THR:OG1	4:B:448:LYS:N	2.47	0.45
4:B:523:LEU:C	4:B:523:LEU:HD23	2.41	0.45
4:B:883:ASN:HD21	4:B:971:MET:HE2	1.81	0.45
4:B:1117:ILE:O	4:B:1120:THR:OG1	2.27	0.45
4:B:1606:PHE:CB	4:B:1687:LEU:HB2	2.41	0.45
7:G:103:ILE:N	7:G:104:PRO:HD2	2.31	0.45
12:D:66:LEU:HD21	12:D:73:LYS:HG2	1.98	0.45
12:D:372:VAL:HG13	12:D:414:PHE:CZ	2.51	0.45
2:C:1728:LEU:HD12	2:C:1728:LEU:O	2.17	0.45
2:C:1834:TRP:CG	2:C:1884:CYS:HG	2.34	0.45
4:B:2897:GLN:HA	4:B:2947:MET:CE	2.46	0.45
4:B:4017:LEU:HD12	4:B:4044:ILE:HD13	1.97	0.45
1:A:1522:GLU:N	1:A:1523:PRO:CD	2.80	0.45
1:A:1676:CYS:HG	1:A:1683:TRP:NE1	2.14	0.45
2:C:1142:VAL:HG21	2:C:1167:ILE:HD13	1.97	0.45
4:B:3264:ASN:HB2	4:B:3306:ILE:HD11	1.98	0.45
4:B:4475:ILE:HD13	4:B:4525:THR:HG23	1.98	0.45
1:A:1013:VAL:HG13	1:A:1076:LEU:CD1	2.45	0.45
1:A:2727:LEU:HD22	1:A:2772:GLU:HG2	1.99	0.45
1:A:3120:GLY:HA2	1:A:3696:LEU:HD13	1.98	0.45
1:A:4534:CYS:SG	1:A:4535:LYS:N	2.90	0.45
2:C:2792:TYR:O	2:C:2796:PRO:HG3	2.17	0.45
4:B:1599:LEU:HA	4:B:1617:LEU:HD11	1.99	0.45
4:B:2839:ILE:N	4:B:2840:PRO:HD2	2.32	0.45
4:B:3339:TRP:CZ2	4:B:3343:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3914:LEU:O	4:B:3914:LEU:HG	2.17	0.45
5:I:10:MET:HB3	5:I:15:LEU:HD21	1.98	0.45
1:A:1171:ILE:HD13	1:A:1171:ILE:H	1.82	0.45
1:A:2027:PHE:CE2	1:A:2051:ILE:HG23	2.50	0.45
1:A:2866:VAL:HG11	1:A:3026:TRP:CH2	2.52	0.45
2:C:798:GLU:CB	2:C:824:MET:HE2	2.46	0.45
2:C:1048:LEU:C	2:C:1048:LEU:HD13	2.42	0.45
2:C:1174:LEU:CD1	2:C:1191:ILE:HG22	2.47	0.45
2:C:3276:THR:HG23	2:C:3656:ASN:HA	1.98	0.45
4:B:3241:GLU:O	4:B:3244:ASN:N	2.49	0.45
4:B:4543:TYR:CE2	4:B:4545:CYS:HB3	2.52	0.45
11:E:153:PHE:HB3	11:E:200:TRP:CE2	2.52	0.45
12:D:364:ALA:HB1	12:D:414:PHE:CE1	2.52	0.45
1:A:2877:THR:HG21	1:A:2923:LEU:HD13	1.98	0.45
2:C:221:SER:O	2:C:282:ARG:NH1	2.49	0.45
2:C:1612:ILE:N	2:C:1613:PRO:HD2	2.32	0.45
2:C:1674:LEU:HD21	2:C:1797:LEU:HD11	1.98	0.45
2:C:2365:GLY:HA2	18:C:4206:ADP:O3'	2.16	0.45
2:C:2532:GLU:N	2:C:2533:PRO:HD2	2.31	0.45
2:C:2555:LEU:HD12	2:C:2555:LEU:C	2.42	0.45
4:B:24:ILE:O	4:B:25:GLN:CB	2.64	0.45
4:B:436:PHE:CZ	4:B:499:LEU:HD23	2.52	0.45
4:B:3481:ILE:HG21	4:B:3488:ILE:HD12	1.99	0.45
4:B:4322:GLU:HB3	4:B:4325:ASN:HB3	1.98	0.45
12:D:162:LEU:HD23	12:D:162:LEU:O	2.16	0.45
12:D:564:ASP:HA	12:D:590:LEU:HD13	1.98	0.45
1:A:1601:ARG:NE	1:A:1688:GLU:OE1	2.49	0.45
1:A:1825:ILE:HG21	1:A:1889:LEU:CD2	2.47	0.45
1:A:3252:GLN:HE22	3:Q:36:PRO:HA	1.82	0.45
1:A:4562:ASN:O	1:A:4562:ASN:ND2	2.50	0.45
2:C:537:GLU:O	2:C:698:GLU:O	2.34	0.45
2:C:1524:ARG:HH22	2:C:3759:ILE:HG21	1.81	0.45
1:A:1638:THR:HG21	1:A:1655:GLN:HE21	1.81	0.45
1:A:2340:GLN:NE2	1:A:2399:TYR:OH	2.50	0.45
4:B:3271:ASP:CG	4:B:3272:PRO:HD2	2.41	0.45
4:B:4510:LEU:HD22	4:B:4563:LEU:HD11	1.99	0.45
1:A:1790:HIS:CE1	1:A:1794:ILE:HD11	2.52	0.45
1:A:3564:LYS:CG	1:A:3615:MET:HE1	2.47	0.45
2:C:895:LEU:C	2:C:895:LEU:HD23	2.41	0.45
2:C:2332:LEU:HD13	18:C:4206:ADP:O2'	2.17	0.45
4:B:1700:ILE:CG2	4:B:1729:ILE:HD13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2889:VAL:HG11	4:B:3047:TRP:CZ3	2.52	0.45
4:B:3740:ILE:O	4:B:3744:ARG:N	2.48	0.45
4:B:4272:ILE:HG22	4:B:4518:MET:HE1	1.98	0.45
5:I:98:PHE:HB3	5:I:104:ALA:HA	1.99	0.45
1:A:1087:THR:O	1:A:1087:THR:HG22	2.17	0.44
1:A:2033:LEU:HD23	1:A:2097:LEU:HD22	1.99	0.44
1:A:4252:PRO:HG3	1:A:4265:TYR:CG	2.52	0.44
2:C:1382:THR:HA	2:C:1385:ILE:HG22	1.99	0.44
2:C:3244:VAL:HB	2:C:3878:VAL:HG22	2.00	0.44
2:C:4082:TRP:CZ2	2:C:4091:GLY:HA3	2.52	0.44
4:B:1209:ALA:HB2	4:B:1286:LYS:CB	2.47	0.44
11:E:164:VAL:HG22	11:E:181:TYR:CE1	2.52	0.44
12:D:397:ASP:CB	12:D:398:PRO:CD	2.96	0.44
12:D:517:ILE:HG12	12:D:550:TRP:CE2	2.51	0.44
1:A:3102:LEU:HD23	1:A:3451:THR:HG23	1.97	0.44
1:A:4347:LEU:CD1	1:A:4368:LEU:HD23	2.47	0.44
4:B:473:VAL:O	4:B:473:VAL:HG13	2.18	0.44
4:B:751:GLY:C	4:B:753:GLU:N	2.75	0.44
4:B:1237:ARG:CZ	4:B:1263:THR:H	2.28	0.44
4:B:1943:LEU:HD11	4:B:1950:GLY:HA3	1.98	0.44
4:B:2959:LEU:O	4:B:2959:LEU:HD13	2.17	0.44
1:A:753:LEU:N	1:A:754:PRO:HD2	2.32	0.44
1:A:1696:LYS:HA	1:A:1836:TYR:CE1	2.52	0.44
1:A:4143:ARG:NH1	1:A:4610:LEU:O	2.50	0.44
2:C:928:VAL:HA	2:C:951:TYR:CE1	2.52	0.44
2:C:4025:PRO:HG3	2:C:4165:MET:HE1	1.99	0.44
4:B:808:PRO:CD	4:B:1077:ARG:HH11	2.26	0.44
4:B:1602:LYS:HD2	4:B:1683:GLU:HG3	1.90	0.44
4:B:1606:PHE:CA	4:B:1687:LEU:HD13	2.38	0.44
4:B:1708:ALA:HA	4:B:1711:TRP:CD1	2.51	0.44
4:B:2897:GLN:HA	4:B:2947:MET:HE2	1.99	0.44
4:B:3020:LEU:C	4:B:3020:LEU:HD12	2.43	0.44
4:B:3450:ASP:CG	4:B:3451:SER:N	2.75	0.44
6:H:85:ALA:HB2	11:E:75:HIS:CD2	2.53	0.44
14:L:99:LEU:N	14:L:100:PRO:HD2	2.33	0.44
1:A:1790:HIS:NE2	1:A:1794:ILE:HD11	2.32	0.44
1:A:3877:ILE:HD11	1:A:3900:ILE:HD13	1.98	0.44
2:C:1132:LYS:CG	2:C:1151:LEU:CD1	2.79	0.44
2:C:1927:SER:CB	2:C:1946:ILE:HG21	2.47	0.44
4:B:3081:ASN:HD21	4:B:3484:LYS:CD	2.30	0.44
4:B:3252:VAL:HG22	4:B:3333:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:LEU:HD23	1:A:1190:LEU:C	2.43	0.44
1:A:3572:MET:HE1	1:A:3594:VAL:HG22	1.99	0.44
1:A:3709:ASP:CB	1:A:3712:LEU:HD12	2.47	0.44
2:C:870:LYS:HE2	2:C:2325:ASP:O	2.18	0.44
2:C:2096:ILE:HD13	2:C:2137:VAL:HG11	2.00	0.44
2:C:2621:GLU:HG3	2:C:2900:VAL:HG21	1.98	0.44
2:C:3054:SER:OG	2:C:3055:ALA:N	2.50	0.44
4:B:1189:GLN:HA	4:B:1192:ASN:ND2	2.32	0.44
4:B:1599:LEU:CA	4:B:1617:LEU:HD11	2.48	0.44
4:B:1603:LYS:CA	4:B:1609:PHE:HB2	2.47	0.44
11:E:49:ASP:HA	14:L:85:SER:HA	1.99	0.44
11:E:140:HIS:CE1	12:D:362:LEU:HD21	2.53	0.44
1:A:470:PHE:CB	1:A:485:THR:CB	2.95	0.44
1:A:1525:PHE:HB2	1:A:1541:PHE:CD2	2.51	0.44
1:A:2548:ALA:HB2	1:A:2603:LYS:HG2	1.99	0.44
1:A:2602:MET:SD	1:A:2602:MET:N	2.90	0.44
1:A:2840:VAL:HG11	1:A:3041:THR:HG21	2.00	0.44
1:A:3240:VAL:HG22	1:A:3335:TRP:CE3	2.52	0.44
2:C:870:LYS:CE	2:C:2325:ASP:O	2.65	0.44
4:B:1537:ASP:N	4:B:1625:GLN:HG3	2.31	0.44
4:B:1606:PHE:CG	4:B:1687:LEU:HD13	2.49	0.44
4:B:3264:ASN:CB	4:B:3306:ILE:HD11	2.47	0.44
1:A:3257:VAL:HG21	1:A:3266:VAL:HG13	1.98	0.44
1:A:3564:LYS:HG2	1:A:3615:MET:HE1	1.98	0.44
2:C:2357:LEU:HD12	2:C:2512:ILE:HG22	1.99	0.44
4:B:737:VAL:HG13	4:B:737:VAL:O	2.17	0.44
4:B:744:MET:CE	4:B:773:VAL:HG23	2.48	0.44
4:B:1596:ASN:OD1	4:B:1618:LEU:HD11	2.17	0.44
4:B:3223:ALA:HB1	4:B:3349:ILE:CD1	2.47	0.44
4:B:3326:MET:O	4:B:3327:ALA:O	2.34	0.44
16:J:40:ALA:CB	16:J:68:MET:HE1	2.48	0.44
1:A:3877:ILE:HG13	1:A:3946:LEU:HD21	1.99	0.44
4:B:1819:SER:HA	4:B:1857:VAL:CG1	2.48	0.44
4:B:3823:ILE:HG23	4:B:4286:LEU:HD12	1.99	0.44
4:B:4206:ARG:CZ	4:B:4573:ILE:HD13	2.46	0.44
12:D:183:ARG:HB2	15:K:72:TYR:HE2	1.83	0.44
1:A:1143:ARG:CZ	12:D:169:ASN:ND2	2.81	0.44
4:B:898:PRO:CG	4:B:1077:ARG:CG	2.96	0.44
4:B:1602:LYS:C	4:B:1609:PHE:CE2	2.96	0.44
14:L:69:ILE:HG22	14:L:69:ILE:O	2.18	0.44
1:A:1862:MET:HE2	1:A:1973:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3746:GLN:O	1:A:3799:VAL:HG21	2.18	0.43
2:C:336:ILE:HG22	2:C:349:LEU:HD11	1.99	0.43
2:C:830:ASP:O	2:C:834:VAL:HG23	2.18	0.43
2:C:1839:PHE:CE1	2:C:1891:LEU:HD11	2.53	0.43
1:A:1205:GLN:HA	1:A:1208:TYR:HB3	1.99	0.43
1:A:2656:TYR:CG	1:A:2711:LYS:HD2	2.53	0.43
1:A:3224:LYS:HA	1:A:3281:LEU:HD11	2.00	0.43
1:A:3298:ILE:HG22	1:A:3300:GLU:HG3	1.99	0.43
1:A:4287:THR:HG22	1:A:4549:ILE:CD1	2.47	0.43
2:C:2691:VAL:HG22	2:C:2827:ILE:HG13	2.00	0.43
2:C:2800:PRO:HA	2:C:2814:CYS:HB3	1.99	0.43
2:C:3381:SER:N	2:C:3382:PRO:HD2	2.33	0.43
4:B:1490:GLN:CD	4:B:3572:SER:HB3	2.35	0.43
4:B:3494:PRO:HA	4:B:3497:ILE:HG22	2.00	0.43
11:E:62:ASN:HB2	15:K:40:ASN:HB2	2.00	0.43
1:A:944:LEU:HD23	1:A:944:LEU:N	2.33	0.43
4:B:745:GLU:HA	4:B:748:VAL:HG12	1.99	0.43
4:B:1142:SER:O	4:B:1146:VAL:HG23	2.18	0.43
4:B:1490:GLN:HB2	4:B:3614:ILE:CG2	2.46	0.43
4:B:1599:LEU:HD11	4:B:1618:LEU:CB	2.47	0.43
1:A:1219:PHE:CE2	1:A:1263:TYR:CE2	3.05	0.43
2:C:1702:ASP:OD1	2:C:1703:LYS:N	2.51	0.43
2:C:2564:LEU:C	2:C:2564:LEU:HD13	2.43	0.43
4:B:951:MET:N	4:B:952:PRO:HD2	2.33	0.43
4:B:1602:LYS:CA	4:B:1683:GLU:CB	2.96	0.43
4:B:1728:GLN:HE21	4:B:1868:ILE:HD12	1.83	0.43
4:B:3330:SER:O	4:B:3331:TYR:C	2.61	0.43
4:B:3335:LYS:O	4:B:3336:LEU:C	2.61	0.43
12:D:509:ASN:HA	12:D:550:TRP:CD1	2.54	0.43
1:A:966:SER:HB3	1:A:989:ILE:HD12	1.99	0.43
2:C:3528:LEU:N	2:C:3529:PRO:CD	2.82	0.43
4:B:429:LEU:HD22	4:B:496:ILE:HD12	2.00	0.43
4:B:1238:LYS:HE3	4:B:1308:LEU:N	2.18	0.43
4:B:1490:GLN:HE22	4:B:3572:SER:HB3	1.69	0.43
4:B:1595:LEU:C	4:B:1618:LEU:CD2	2.92	0.43
12:D:174:GLN:HE22	14:L:49:LEU:HB3	1.82	0.43
12:D:304:TRP:CZ2	12:D:603:LEU:HD12	2.54	0.43
1:A:1596:ARG:HD3	1:A:1603:TYR:CD1	2.54	0.43
2:C:1040:VAL:HA	2:C:1102:CYS:SG	2.59	0.43
2:C:2708:GLN:CG	2:C:2809:ALA:HB1	2.49	0.43
2:C:2771:PHE:O	2:C:2774:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2829:ASP:C	2:C:2832:PRO:HD2	2.44	0.43
2:C:3438:HIS:ND1	2:C:3443:LYS:HB2	2.34	0.43
2:C:4084:ILE:HG22	2:C:4085:GLY:N	2.34	0.43
4:B:1936:MET:HG2	4:B:1966:VAL:HG22	2.01	0.43
4:B:3654:GLU:O	4:B:3658:ILE:HG13	2.18	0.43
1:A:3131:ILE:HG21	1:A:3418:LEU:HB3	2.00	0.43
1:A:3199:GLU:O	1:A:3203:PRO:HD2	2.19	0.43
1:A:3587:VAL:HG11	1:A:3638:LEU:HD13	2.00	0.43
1:A:4046:CYS:SG	1:A:4074:ILE:HG23	2.59	0.43
2:C:321:ARG:HA	2:C:342:ALA:HB2	2.01	0.43
2:C:2728:TYR:CG	2:C:2728:TYR:O	2.71	0.43
2:C:2755:LEU:C	2:C:2757:LEU:H	2.27	0.43
4:B:1527:ILE:CG2	4:B:1615:GLN:CD	2.87	0.43
4:B:1599:LEU:HD21	4:B:1618:LEU:N	2.34	0.43
12:D:92:TYR:CG	17:M:29:LYS:HB3	2.53	0.43
1:A:3223:LEU:HD21	1:A:3332:ILE:HD11	2.01	0.43
2:C:164:HIS:CE1	4:B:957:GLN:HG3	2.53	0.43
2:C:2242:HIS:HB2	2:C:2289:LEU:CD1	2.48	0.43
2:C:3010:LEU:HA	2:C:3102:LEU:HB2	2.00	0.43
4:B:1051:ASP:HB3	4:B:1162:THR:HG21	1.99	0.43
4:B:1602:LYS:CA	4:B:1683:GLU:HB3	2.48	0.43
12:D:624:GLY:N	12:D:625:PRO:CD	2.82	0.43
1:A:1653:ILE:HB	1:A:1674:VAL:HB	2.00	0.43
1:A:2821:CYS:HB3	1:A:2841:LEU:HD13	2.01	0.43
1:A:4172:TYR:CD2	1:A:4195:ARG:NH2	2.86	0.43
1:A:4541:LEU:HD21	1:A:4597:LEU:HD13	2.00	0.43
2:C:261:ILE:N	2:C:262:PRO:HD2	2.34	0.43
2:C:3460:ASN:N	2:C:3460:ASN:ND2	2.67	0.43
4:B:1212:ILE:HG22	4:B:1213:PRO:CD	2.49	0.43
4:B:3267:ILE:HD12	4:B:3279:LYS:HD3	2.00	0.43
4:B:4119:ILE:HD12	4:B:4130:LEU:HD13	2.01	0.43
4:B:669:ILE:HD13	4:B:752:ILE:HD11	2.01	0.43
4:B:724:HIS:O	4:B:724:HIS:CD2	2.72	0.43
4:B:1075:TRP:CZ3	4:B:1076:LEU:HD13	2.53	0.43
4:B:1602:LYS:HA	4:B:1683:GLU:CG	2.49	0.43
4:B:1602:LYS:HE2	4:B:1683:GLU:OE2	2.19	0.43
4:B:3269:LEU:O	4:B:3269:LEU:HD22	2.19	0.43
12:D:353:LEU:HG	12:D:363:LEU:HD21	2.01	0.43
1:A:994:GLU:O	1:A:998:VAL:HG23	2.19	0.42
2:C:2079:ILE:HG21	2:C:2082:LEU:HD13	2.00	0.42
2:C:2943:LYS:HB3	2:C:2994:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1096:ARG:O	4:B:1100:ASP:N	2.46	0.42
4:B:1858:ASP:O	4:B:1892:ASN:ND2	2.52	0.42
1:A:3251:ILE:HG22	1:A:3252:GLN:N	2.34	0.42
2:C:287:PHE:HB3	2:C:320:PRO:HB2	2.01	0.42
2:C:2093:GLN:HB2	2:C:2096:ILE:HG22	2.00	0.42
2:C:4072:ILE:HD12	2:C:4110:ALA:HB2	2.00	0.42
4:B:3223:ALA:O	4:B:3226:SER:OG	2.37	0.42
4:B:3327:ALA:O	4:B:3328:GLY:C	2.62	0.42
5:I:35:LEU:HD22	5:I:95:LEU:HD13	2.01	0.42
14:L:85:SER:C	14:L:86:LEU:HD13	2.44	0.42
1:A:2455:GLN:HB2	1:A:2458:GLN:HE21	1.85	0.42
1:A:3305:LEU:CD2	3:Q:81:ARG:CB	2.97	0.42
1:A:3816:ARG:HA	1:A:3973:TYR:CE1	2.54	0.42
2:C:259:PRO:HD2	2:C:328:TYR:CE2	2.53	0.42
2:C:1742:LEU:HD12	2:C:1780:LEU:HD22	1.99	0.42
2:C:2708:GLN:HG2	2:C:2809:ALA:HB1	2.00	0.42
2:C:2727:ILE:HD13	2:C:2745:LYS:HD3	2.01	0.42
2:C:4049:ILE:HD11	2:C:4110:ALA:HB1	2.01	0.42
4:B:439:LEU:HD21	4:B:456:ILE:HG23	2.01	0.42
4:B:1761:GLN:HE22	4:B:1798:ARG:HG3	1.84	0.42
4:B:2692:LEU:O	4:B:2695:HIS:N	2.52	0.42
5:I:12:ILE:HG23	7:G:120:THR:CG2	2.49	0.42
7:G:126:LEU:HD13	8:F:79:LEU:HD23	2.02	0.42
10:O:19:LEU:O	10:O:19:LEU:HD23	2.19	0.42
1:A:3131:ILE:HD12	1:A:3422:LEU:CD1	2.48	0.42
1:A:4123:HIS:NE2	1:A:4188:PRO:HD3	2.34	0.42
1:A:4448:GLN:HE21	1:A:4448:GLN:HB3	1.68	0.42
2:C:2687:ALA:CB	2:C:2830:VAL:HG22	2.44	0.42
2:C:2803:MET:HB3	2:C:2814:CYS:SG	2.60	0.42
2:C:3276:THR:OG1	2:C:3658:ARG:NH2	2.53	0.42
4:B:572:MET:HE2	4:B:584:PRO:CB	2.49	0.42
4:B:790:ILE:HG12	4:B:836:ILE:HG23	2.00	0.42
4:B:2609:MET:N	4:B:2610:PRO:HD2	2.35	0.42
6:H:11:ILE:HG22	6:H:79:LEU:HB3	2.01	0.42
12:D:314:VAL:HG21	12:D:611:VAL:HG21	2.01	0.42
2:C:2715:PRO:HG2	2:C:2719:VAL:HB	2.02	0.42
2:C:3711:LEU:HD21	2:C:3725:LEU:HD23	2.02	0.42
4:B:1886:THR:HA	4:B:4193:ILE:HG23	2.02	0.42
4:B:2040:LEU:HD12	4:B:2040:LEU:HA	1.90	0.42
4:B:2116:THR:HG23	4:B:2325:ASN:CG	2.44	0.42
11:E:121:TYR:HB3	12:D:266:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:367:LEU:N	11:E:388:ASP:OD2	2.53	0.42
1:A:1539:LYS:HE2	4:B:3859:VAL:HG22	2.00	0.42
1:A:1782:GLU:O	1:A:1786:THR:HG23	2.19	0.42
1:A:1926:PHE:CE2	1:A:1934:LEU:HD22	2.54	0.42
1:A:4126:TRP:CZ2	1:A:4130:ILE:HD11	2.55	0.42
2:C:2246:ARG:CD	2:C:2344:ARG:HG2	2.50	0.42
2:C:2719:VAL:CG1	2:C:2720:PRO:HD3	2.50	0.42
4:B:719:VAL:O	4:B:722:TYR:HB3	2.19	0.42
4:B:3122:LEU:HD11	4:B:3448:ILE:HG12	2.01	0.42
12:D:439:ILE:HD13	12:D:484:CYS:HB3	2.02	0.42
1:A:3884:THR:HA	1:A:3891:PRO:HA	2.01	0.42
2:C:1191:ILE:HG23	2:C:1201:PHE:CE2	2.54	0.42
2:C:2687:ALA:C	2:C:2689:PRO:HD2	2.45	0.42
2:C:4081:ALA:N	2:C:4094:ILE:O	2.51	0.42
4:B:58:SER:H	4:B:71:CYS:CB	2.32	0.42
4:B:898:PRO:HB3	4:B:1077:ARG:HA	2.01	0.42
4:B:1626:ASN:ND2	4:B:1655:THR:HG21	2.35	0.42
4:B:2267:ILE:HG22	4:B:2271:TRP:CZ3	2.53	0.42
4:B:2560:VAL:HG13	4:B:2601:ILE:HD13	2.02	0.42
4:B:2667:LEU:O	4:B:2670:ASN:N	2.53	0.42
4:B:3885:ASN:O	4:B:3889:GLN:HG2	2.19	0.42
11:E:384:LEU:C	11:E:384:LEU:HD12	2.44	0.42
1:A:1220:THR:HG22	1:A:1279:LYS:CA	2.50	0.42
2:C:2082:LEU:HG	2:C:2137:VAL:HG21	2.00	0.42
2:C:2792:TYR:O	2:C:2796:PRO:HD3	2.19	0.42
4:B:1192:ASN:OD1	4:B:1193:ALA:N	2.52	0.42
4:B:2716:PHE:CD2	4:B:2716:PHE:C	2.98	0.42
5:I:93:THR:HB	5:I:109:LYS:HB3	2.00	0.42
12:D:422:ARG:NH2	12:D:424:MET:SD	2.92	0.42
1:A:1143:ARG:NH1	12:D:169:ASN:ND2	2.67	0.42
1:A:1227:ARG:H	1:A:1286:THR:CB	2.33	0.42
2:C:908:LEU:CD1	2:C:948:LEU:HD13	2.50	0.42
2:C:1128:PHE:CZ	2:C:1151:LEU:HD13	2.54	0.42
4:B:1163:ARG:O	4:B:1167:MET:N	2.53	0.42
4:B:2776:LYS:NZ	4:B:2814:ILE:HG23	2.35	0.42
9:N:68:CYS:HA	10:O:101:CYS:HA	2.01	0.42
12:D:526:ARG:HB2	12:D:528:TRP:CH2	2.54	0.42
1:A:598:ARG:HD3	12:D:319:TYR:CE1	2.55	0.42
1:A:1027:CYS:O	1:A:1027:CYS:SG	2.78	0.42
1:A:2159:THR:HG22	1:A:2624:ARG:HD2	2.01	0.42
1:A:3638:LEU:HA	1:A:3641:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4113:ILE:HD11	1:A:4134:CYS:SG	2.59	0.42
2:C:997:LEU:HB2	2:C:1051:GLN:HE22	1.84	0.42
2:C:2082:LEU:HD11	2:C:2096:ILE:HD13	2.02	0.42
2:C:2711:SER:HB2	2:C:2755:LEU:HD23	2.02	0.42
2:C:3034:LEU:HB3	2:C:3041:ILE:HG22	2.02	0.42
5:I:19:MET:HB2	5:I:22:LYS:HG2	2.01	0.42
9:N:76:THR:HG21	11:E:39:GLN:NE2	2.26	0.42
9:N:86:THR:HG22	11:E:25:THR:HG22	2.01	0.42
1:A:4056:ILE:CD1	1:A:4072:LEU:HD21	2.47	0.41
2:C:868:ILE:O	2:C:872:ARG:N	2.46	0.41
4:B:2192:CYS:O	4:B:2196:THR:HG23	2.19	0.41
4:B:3582:ILE:HG23	4:B:3582:ILE:O	2.19	0.41
4:B:4110:ALA:HA	4:B:4159:MET:HE1	2.01	0.41
4:B:4227:PHE:CD1	4:B:4263:ALA:HA	2.55	0.41
4:B:4287:LEU:HD11	4:B:4393:LEU:HG	2.01	0.41
12:D:66:LEU:N	12:D:66:LEU:HD22	2.35	0.41
12:D:68:GLU:O	12:D:69:ASP:C	2.62	0.41
1:A:1918:GLY:HA3	1:A:1967:ILE:HG21	2.02	0.41
2:C:162:GLY:HA2	2:C:203:HIS:CE1	2.55	0.41
2:C:1236:ASN:HB3	2:C:1240:MET:HE2	2.01	0.41
2:C:2066:GLN:CA	2:C:2066:GLN:NE2	2.83	0.41
4:B:1068:LYS:CB	4:B:1084:LYS:HE2	2.50	0.41
4:B:1490:GLN:CG	4:B:3614:ILE:HG21	2.38	0.41
5:I:15:LEU:HD22	12:D:212:ILE:HD13	2.01	0.41
11:E:492:ASP:HA	11:E:495:TYR:CE2	2.54	0.41
11:E:517:LYS:O	11:E:521:THR:HG23	2.20	0.41
1:A:1620:PRO:HB2	1:A:1639:PHE:CE1	2.54	0.41
1:A:3308:PRO:HB3	3:Q:33:PHE:CB	2.50	0.41
1:A:3951:THR:OG1	1:A:4293:SER:HB2	2.21	0.41
2:C:115:LYS:O	2:C:119:TYR:N	2.53	0.41
2:C:3408:LEU:HD23	2:C:3413:LYS:HA	2.01	0.41
2:C:3927:VAL:HG21	2:C:4031:ALA:HB2	2.02	0.41
4:B:2026:ALA:HB1	4:B:4200:VAL:HG12	2.02	0.41
1:A:1151:MET:HE2	14:L:49:LEU:CD1	2.50	0.41
1:A:3758:TYR:CE2	1:A:3762:ILE:HD11	2.55	0.41
2:C:2812:GLY:O	2:C:2813:ILE:C	2.63	0.41
4:B:1933:LYS:HG3	4:B:1965:VAL:HG11	2.01	0.41
12:D:562:THR:O	12:D:563:MET:C	2.62	0.41
2:C:2742:LYS:HG3	2:C:2743:ASN:HD22	1.85	0.41
4:B:441:LYS:O	11:E:518:ASN:ND2	2.53	0.41
4:B:679:ARG:HB2	11:E:186:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:984:ASN:HA	4:B:987:ARG:HD3	2.03	0.41
4:B:1061:GLN:HG2	4:B:1091:VAL:CG1	2.50	0.41
4:B:3571:ILE:HD11	4:B:3593:LEU:HD22	2.03	0.41
4:B:3877:LEU:HD13	4:B:3928:LEU:CD1	2.51	0.41
6:H:68:PHE:HA	11:E:71:ARG:O	2.20	0.41
14:L:92:VAL:HG12	14:L:92:VAL:O	2.20	0.41
17:M:57:VAL:HG22	17:M:82:LEU:HG	2.01	0.41
1:A:8:LYS:CB	1:A:109:SER:HA	2.50	0.41
1:A:151:ILE:O	1:A:153:PHE:N	2.53	0.41
2:C:1702:ASP:OD1	2:C:1702:ASP:C	2.63	0.41
2:C:2005:PRO:HB2	2:C:2145:PHE:CD1	2.55	0.41
2:C:2007:LEU:HD13	2:C:2126:ALA:HB3	2.02	0.41
2:C:2770:ASN:O	2:C:2773:ASP:N	2.45	0.41
4:B:1237:ARG:HH21	4:B:1263:THR:CA	2.34	0.41
4:B:3268:THR:HG23	4:B:3309:GLN:OE1	2.20	0.41
4:B:3582:ILE:HG23	4:B:3626:THR:HG22	2.02	0.41
4:B:3594:LEU:HD22	4:B:3641:CYS:SG	2.61	0.41
1:A:1205:GLN:HG2	12:D:166:PHE:CD1	2.56	0.41
1:A:1638:THR:HB	1:A:1655:GLN:HG2	2.03	0.41
1:A:4301:MET:HE1	1:A:4412:ASP:HB2	2.02	0.41
2:C:10:LEU:HD13	2:C:10:LEU:C	2.45	0.41
2:C:531:GLU:HA	2:C:546:LYS:C	2.46	0.41
2:C:1328:LEU:HG	2:C:1333:VAL:HG21	2.02	0.41
2:C:1383:ASP:O	2:C:1387:VAL:HG23	2.20	0.41
2:C:2812:GLY:O	2:C:2815:SER:CB	2.68	0.41
4:B:459:ILE:HG23	4:B:499:LEU:CD1	2.50	0.41
4:B:2417:LEU:N	4:B:2418:PRO:HD2	2.35	0.41
9:N:88:TYR:N	10:O:81:ILE:O	2.54	0.41
1:A:1642:ALA:HB2	1:A:1652:GLN:HB3	2.03	0.41
1:A:3062:HIS:CE1	1:A:3477:MET:HE2	2.56	0.41
1:A:3132:ASN:CA	1:A:3419:ILE:HD11	2.51	0.41
2:C:2826:VAL:O	2:C:2827:ILE:C	2.64	0.41
2:C:3136:LEU:HD21	2:C:3221:SER:HB2	2.02	0.41
2:C:3588:VAL:HG11	2:C:3621:TRP:CD2	2.56	0.41
4:B:2157:LEU:HD21	4:B:2196:THR:CG2	2.51	0.41
4:B:2715:TYR:O	4:B:2718:PHE:N	2.54	0.41
4:B:3321:PHE:CE1	4:B:3337:CYS:SG	3.14	0.41
4:B:3907:PRO:HG3	4:B:3934:ARG:HD3	2.03	0.41
8:F:11:LEU:HB3	8:F:23:TYR:OH	2.21	0.41
2:C:841:ILE:HG13	2:C:891:ILE:HD13	2.02	0.41
2:C:2717:ALA:CB	2:C:2803:MET:SD	3.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3622:ILE:HD11	2:C:3624:LEU:HD21	2.03	0.41
4:B:722:TYR:O	4:B:723:ASN:C	2.64	0.41
4:B:1536:GLU:O	4:B:1625:GLN:NE2	2.54	0.41
4:B:1599:LEU:CD2	4:B:1621:LEU:HB2	2.51	0.41
4:B:1602:LYS:CB	4:B:1683:GLU:CB	2.87	0.41
4:B:1603:LYS:HA	4:B:1609:PHE:HB2	2.03	0.41
4:B:2609:MET:N	4:B:2610:PRO:CD	2.84	0.41
4:B:2900:CYS:SG	4:B:3019:VAL:HG11	2.60	0.41
4:B:3255:THR:HG23	4:B:3337:CYS:SG	2.61	0.41
4:B:4106:ASN:HD21	4:B:4141:ILE:HB	1.85	0.41
1:A:1698:ILE:HG21	1:A:1722:ILE:HD13	2.03	0.41
1:A:1967:ILE:O	1:A:1970:VAL:HG23	2.21	0.41
1:A:2963:ILE:HD13	1:A:2987:PHE:HB2	2.03	0.41
1:A:3131:ILE:HG21	1:A:3418:LEU:CB	2.51	0.41
2:C:3442:GLY:O	2:C:3443:LYS:C	2.63	0.41
4:B:766:ILE:O	4:B:769:SER:OG	2.38	0.41
4:B:898:PRO:HG2	4:B:1077:ARG:CG	2.51	0.41
4:B:915:PRO:C	4:B:917:ILE:H	2.27	0.41
4:B:1119:LYS:HB3	4:B:1138:LYS:HD3	2.02	0.41
4:B:2180:CYS:SG	4:B:2181:PHE:N	2.94	0.41
4:B:2695:HIS:O	4:B:2695:HIS:CD2	2.74	0.41
4:B:3826:THR:HG22	4:B:3942:LEU:CD2	2.51	0.41
2:C:22:SER:HB3	2:C:341:TRP:HB2	2.03	0.40
4:B:55:GLN:O	4:B:85:LYS:HA	2.22	0.40
4:B:137:LEU:O	4:B:138:ASN:CB	2.69	0.40
4:B:642:LEU:C	4:B:642:LEU:HD13	2.46	0.40
4:B:1480:HIS:O	4:B:1484:LEU:HG	2.21	0.40
4:B:1598:TYR:CD2	4:B:1621:LEU:CG	3.04	0.40
4:B:2537:ILE:HA	4:B:2654:LEU:O	2.21	0.40
4:B:3767:MET:HG3	4:B:3768:ASP:N	2.35	0.40
4:B:4040:MET:HG2	4:B:4075:PHE:HB2	2.03	0.40
4:B:4220:LEU:O	4:B:4220:LEU:HD23	2.21	0.40
4:B:4480:ILE:O	4:B:4480:ILE:HG22	2.21	0.40
6:H:24:VAL:HG22	6:H:49:PHE:HZ	1.86	0.40
13:P:27:ASN:HA	13:P:95:GLU:HA	2.03	0.40
1:A:1698:ILE:CG2	1:A:1722:ILE:HD13	2.51	0.40
1:A:3322:ALA:CB	1:A:3333:LEU:HD12	2.51	0.40
1:A:4347:LEU:HD11	1:A:4368:LEU:HD23	2.02	0.40
2:C:225:GLN:OE1	2:C:225:GLN:N	2.54	0.40
2:C:1328:LEU:HG	2:C:1333:VAL:HG11	2.02	0.40
4:B:911:ILE:HD11	4:B:991:ASP:CG	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:937:PHE:CD1	4:B:937:PHE:N	2.88	0.40
4:B:1071:GLU:HG2	4:B:1079:ASN:HD22	1.86	0.40
1:A:1161:SER:O	1:A:1164:ASP:N	2.54	0.40
1:A:1631:PHE:HB2	1:A:1634:ILE:HG21	2.01	0.40
2:C:1305:LYS:N	2:C:1306:PRO:CD	2.84	0.40
4:B:722:TYR:O	4:B:723:ASN:O	2.39	0.40
4:B:4187:ILE:O	4:B:4212:LEU:HD21	2.21	0.40
16:J:44:THR:HG22	16:J:64:LEU:HD22	2.03	0.40
1:A:1562:ILE:HB	1:A:1563:PRO:HD3	2.04	0.40
1:A:1857:THR:HG21	1:A:1997:VAL:HG22	2.04	0.40
1:A:2576:LEU:HD13	1:A:2621:ILE:HG13	2.04	0.40
1:A:2789:LEU:HD21	1:A:2811:ILE:HD13	2.03	0.40
2:C:1559:LEU:CD2	2:C:1607:LEU:HD21	2.50	0.40
2:C:2775:VAL:HG22	2:C:2824:TYR:CE1	2.56	0.40
2:C:3460:ASN:HB3	2:C:3466:ALA:HB1	2.03	0.40
4:B:808:PRO:CG	4:B:1077:ARG:HB2	2.52	0.40
4:B:1602:LYS:HD2	4:B:1683:GLU:CB	2.48	0.40
4:B:1627:ALA:HB3	4:B:1628:PRO:HD3	2.03	0.40
4:B:2055:PHE:CE1	4:B:2106:LEU:HD21	2.56	0.40
4:B:3080:LEU:HD12	4:B:3484:LYS:HE2	2.03	0.40
4:B:4548:TYR:CD2	4:B:4553:ARG:HD2	2.57	0.40
11:E:37:ILE:HG23	11:E:39:GLN:HG3	2.04	0.40
1:A:1118:LEU:HD13	1:A:1118:LEU:HA	1.99	0.40
1:A:1541:PHE:HA	1:A:1544:ILE:HB	2.03	0.40
1:A:1787:ILE:HD13	1:A:1847:ILE:HD11	2.04	0.40
2:C:1839:PHE:HE1	2:C:1891:LEU:HD11	1.86	0.40
2:C:2007:LEU:HD21	2:C:2128:MET:HE3	2.04	0.40
2:C:3151:LYS:HE3	2:C:3217:ILE:HD11	2.03	0.40
4:B:801:ILE:HG22	4:B:802:ILE:N	2.36	0.40
4:B:1538:ILE:HD13	4:B:1622:SER:HG	1.83	0.40
4:B:2146:ILE:O	4:B:2150:THR:HG23	2.22	0.40
4:B:2150:THR:CG2	4:B:2203:ASN:HD22	2.35	0.40
4:B:4129:ILE:HG23	4:B:4169:MET:SD	2.61	0.40
8:F:11:LEU:HD22	8:F:23:TYR:CE1	2.56	0.40
8:F:97:MET:HG3	8:F:98:LEU:N	2.35	0.40
16:J:21:PHE:CD1	16:J:21:PHE:C	2.99	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	4381/4620 (95%)	4081 (93%)	258 (6%)	42 (1%)	12	49
2	C	3914/4168 (94%)	3582 (92%)	283 (7%)	49 (1%)	9	42
3	Q	190/202 (94%)	163 (86%)	24 (13%)	3 (2%)	7	38
4	B	4488/4595 (98%)	4017 (90%)	383 (8%)	88 (2%)	6	31
5	I	104/110 (94%)	95 (91%)	8 (8%)	1 (1%)	12	49
6	H	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
7	G	92/159 (58%)	87 (95%)	5 (5%)	0	100	100
8	F	108/133 (81%)	96 (89%)	11 (10%)	1 (1%)	14	51
9	N	112/117 (96%)	92 (82%)	17 (15%)	3 (3%)	4	25
10	O	118/132 (89%)	103 (87%)	10 (8%)	5 (4%)	2	17
11	E	551/670 (82%)	496 (90%)	51 (9%)	4 (1%)	18	56
12	D	569/667 (85%)	510 (90%)	51 (9%)	8 (1%)	9	40
13	P	103/122 (84%)	86 (84%)	11 (11%)	6 (6%)	1	14
14	L	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	12	49
15	K	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
16	J	93/111 (84%)	84 (90%)	8 (9%)	1 (1%)	11	46
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	4	27
All	All	15181/16189 (94%)	13817 (91%)	1150 (8%)	214 (1%)	11	40

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	ILE

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Mol	Chain	Res	Type
1	A	4235	PHE
2	C	435	MET
2	C	529	GLU
2	C	2733	TYR
2	C	2744	LYS
2	C	3054	SER
2	C	3443	LYS
3	Q	19	PRO
3	Q	39	GLU
4	B	6	GLN
4	B	37	GLN
4	B	533	ARG
4	B	692	LEU
4	B	750	PRO
4	B	765	PHE
4	B	1127	ASN
4	B	1607	PRO
4	B	2249	GLU
4	B	2741	PHE
4	B	2760	SER
4	B	3248	PRO
4	B	3267	ILE
4	B	3329	GLN
4	B	3331	TYR
4	B	3333	ALA
9	N	7	GLU
10	O	29	PHE
11	E	37	ILE
12	D	397	ASP
13	P	37	PRO
13	P	107	ILE
13	P	119	PRO
17	M	51	TYR
1	A	27	ILE
1	A	28	VAL
1	A	158	GLU
1	A	282	ARG
1	A	720	GLU
1	A	1670	THR
1	A	4430	TRP
1	A	4563	LYS
2	C	140	ILE

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Mol	Chain	Res	Type
2	C	155	GLU
2	C	322	GLU
2	C	400	GLY
2	C	861	SER
2	C	1170	ALA
2	C	1901	LEU
2	C	2718	GLY
2	C	2759	LYS
2	C	2771	PHE
2	C	3619	GLY
2	C	4106	PRO
3	Q	49	LEU
4	B	18	LEU
4	B	19	SER
4	B	24	ILE
4	B	27	GLU
4	B	74	TYR
4	B	136	PRO
4	B	138	ASN
4	B	307	PRO
4	B	720	ASP
4	B	723	ASN
4	B	751	GLY
4	B	752	ILE
4	B	799	VAL
4	B	801	ILE
4	B	1124	ILE
4	B	1947	GLY
4	B	1990	GLY
4	B	2353	MET
4	B	3323	GLU
4	B	3327	ALA
4	B	3328	GLY
4	B	3332	ALA
4	B	4152	ASN
4	B	4228	PRO
4	B	4484	GLU
4	B	4489	GLU
4	B	4527	CYS
5	I	51	ALA
10	O	31	PRO
11	E	19	ASN

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Mol	Chain	Res	Type
11	E	350	LYS
12	D	168	TYR
12	D	563	MET
13	P	36	TYR
17	M	50	GLY
1	A	18	CYS
1	A	103	ASP
1	A	149	GLU
1	A	283	PRO
1	A	818	LEU
1	A	970	TYR
1	A	1172	THR
1	A	1347	TRP
1	A	1396	PRO
2	C	223	THR
2	C	237	ASP
2	C	390	THR
2	C	1214	TYR
2	C	2362	GLY
2	C	2716	PRO
2	C	2732	GLY
2	C	2735	ASN
2	C	2746	PRO
2	C	2750	SER
2	C	2770	ASN
2	C	2805	SER
2	C	4092	TYR
4	B	361	LYS
4	B	764	GLN
4	B	774	ASP
4	B	806	ASN
4	B	898	PRO
4	B	2252	TYR
4	B	2969	GLY
4	B	3246	GLY
4	B	4225	GLU
9	N	25	PHE
11	E	275	THR
12	D	236	MET
16	J	101	GLU
1	A	26	MET
1	A	127	THR

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Mol	Chain	Res	Type
1	A	152	GLN
1	A	591	LYS
1	A	1030	SER
1	A	1897	ASN
1	A	3585	ASN
1	A	4562	ASN
1	A	4599	CYS
2	C	84	TYR
2	C	1897	ASN
2	C	2247	THR
2	C	2756	LYS
2	C	3983	ALA
4	B	169	LYS
4	B	334	TYR
4	B	1333	ILE
4	B	1489	SER
4	B	1856	ILE
4	B	2469	ALA
4	B	2491	TRP
4	B	2571	THR
4	B	3223	ALA
4	B	3237	PRO
4	B	3268	THR
4	B	3273	ASP
12	D	231	LYS
12	D	523	TRP
13	P	68	LEU
13	P	71	GLN
14	L	71	ASP
1	A	101	PRO
1	A	106	LYS
1	A	3972	SER
2	C	392	ASN
2	C	881	ILE
2	C	1082	ASP
2	C	2066	GLN
2	C	4090	ASP
4	B	89	ILE
4	B	99	LEU
4	B	306	GLN
4	B	719	VAL
4	B	1626	ASN

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Mol	Chain	Res	Type
4	B	1641	LEU
4	B	2207	ASP
4	B	3302	ILE
4	B	3306	ILE
4	B	3466	ALA
4	B	4144	ARG
4	B	4182	PRO
10	O	77	PRO
12	D	321	PHE
12	D	398	PRO
1	A	772	TRP
1	A	878	VAL
1	A	1745	ASN
2	C	438	GLY
4	B	407	LEU
4	B	2702	LYS
4	B	3221	LEU
8	F	29	SER
1	A	817	VAL
1	A	1171	ILE
1	A	1401	ILE
4	B	2	GLY
9	N	80	GLY
10	O	53	PRO
1	A	3535	GLY
2	C	442	ILE
2	C	2813	ILE
4	B	1212	ILE
4	B	1213	PRO
4	B	4150	GLY
2	C	99	GLY
2	C	1401	PRO
4	B	3258	VAL
2	C	2826	VAL
4	B	88	GLY
4	B	2186	PRO
4	B	3261	ILE
4	B	4147	GLY
10	O	25	ILE
2	C	1717	VAL
2	C	2715	PRO

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	3420/4197 (82%)	3332 (97%)	88 (3%)	40	62
2	C	3149/3691 (85%)	3090 (98%)	59 (2%)	50	67
3	Q	10/186 (5%)	10 (100%)	0	100	100
4	B	3497/4145 (84%)	3398 (97%)	99 (3%)	38	60
5	I	91/95 (96%)	87 (96%)	4 (4%)	25	47
6	H	82/83 (99%)	80 (98%)	2 (2%)	43	64
7	G	86/149 (58%)	86 (100%)	0	100	100
8	F	93/109 (85%)	85 (91%)	8 (9%)	10	29
9	N	85/104 (82%)	83 (98%)	2 (2%)	43	64
10	O	106/119 (89%)	98 (92%)	8 (8%)	12	33
11	E	484/597 (81%)	468 (97%)	16 (3%)	33	55
12	D	507/609 (83%)	486 (96%)	21 (4%)	27	49
14	L	87/99 (88%)	84 (97%)	3 (3%)	32	54
15	K	80/82 (98%)	79 (99%)	1 (1%)	61	74
16	J	81/97 (84%)	77 (95%)	4 (5%)	22	43
17	M	78/78 (100%)	74 (95%)	4 (5%)	21	42
All	All	11936/14440 (83%)	11617 (97%)	319 (3%)	40	61

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	ASP
1	A	582	THR
1	A	613	LEU
1	A	616	LYS
1	A	674	LEU
1	A	751	LEU
1	A	758	ASP
1	A	763	LEU

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Mol	Chain	Res	Type
1	A	810	LEU
1	A	818	LEU
1	A	871	LEU
1	A	1016	PHE
1	A	1020	PHE
1	A	1023	PHE
1	A	1069	TYR
1	A	1086	SER
1	A	1132	LEU
1	A	1135	VAL
1	A	1136	MET
1	A	1171	ILE
1	A	1205	GLN
1	A	1559	LYS
1	A	1566	GLN
1	A	1567	ASN
1	A	1573	PHE
1	A	1581	LEU
1	A	1605	VAL
1	A	1609	THR
1	A	1631	PHE
1	A	1634	ILE
1	A	1644	ASP
1	A	1711	LEU
1	A	1758	LYS
1	A	1780	LYS
1	A	1792	LYS
1	A	1922	CYS
1	A	2011	LYS
1	A	2026	LYS
1	A	2098	LEU
1	A	2124	ILE
1	A	2131	ILE
1	A	2228	THR
1	A	2231	THR
1	A	2254	LEU
1	A	2320	SER
1	A	2340	GLN
1	A	2418	ILE
1	A	2426	GLU
1	A	2434	SER
1	A	2470	GLU

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Mol	Chain	Res	Type
1	A	2471	MET
1	A	2487	ASN
1	A	2686	THR
1	A	2729	LEU
1	A	2844	ASP
1	A	2991	VAL
1	A	3122	ASN
1	A	3203	PRO
1	A	3255	GLU
1	A	3283	ASP
1	A	3306	LEU
1	A	3315	ASP
1	A	3345	LYS
1	A	3419	ILE
1	A	3449	LEU
1	A	3495	ILE
1	A	3578	LEU
1	A	3637	GLU
1	A	3681	VAL
1	A	3881	SER
1	A	3951	THR
1	A	3952	LEU
1	A	3973	TYR
1	A	4046	CYS
1	A	4108	THR
1	A	4130	ILE
1	A	4143	ARG
1	A	4201	VAL
1	A	4287	THR
1	A	4448	GLN
1	A	4465	THR
1	A	4497	SER
1	A	4498	LEU
1	A	4504	SER
1	A	4506	THR
1	A	4524	VAL
1	A	4542	ASP
1	A	4562	ASN
2	C	36	PHE
2	C	39	LEU
2	C	62	LEU
2	C	110	ASP

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Mol	Chain	Res	Type
2	C	111	THR
2	C	214	LEU
2	C	239	TRP
2	C	346	LEU
2	C	352	LEU
2	C	1249	ASP
2	C	1281	MET
2	C	1324	VAL
2	C	1358	ILE
2	C	1453	CYS
2	C	1499	CYS
2	C	1503	ILE
2	C	1526	ILE
2	C	1572	HIS
2	C	1650	ASP
2	C	1660	ASP
2	C	1722	ASP
2	C	1728	LEU
2	C	1868	CYS
2	C	1953	GLN
2	C	2043	ASN
2	C	2066	GLN
2	C	2122	THR
2	C	2177	ILE
2	C	2223	LEU
2	C	2224	LEU
2	C	2225	SER
2	C	2245	GLU
2	C	2265	ILE
2	C	2292	CYS
2	C	2295	ILE
2	C	2432	ASN
2	C	2488	ILE
2	C	2576	LYS
2	C	2696	SER
2	C	2711	SER
2	C	2712	PHE
2	C	2757	LEU
2	C	2771	PHE
2	C	2776	ASP
2	C	3022	ILE
2	C	3059	ASN

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Mol	Chain	Res	Type
2	C	3062	GLU
2	C	3405	ARG
2	C	3460	ASN
2	C	3602	GLN
2	C	3793	THR
2	C	3800	THR
2	C	3844	LYS
2	C	3877	GLU
2	C	3883	SER
2	C	3918	VAL
2	C	4050	GLN
2	C	4113	VAL
2	C	4146	MET
4	B	440	GLU
4	B	480	ILE
4	B	536	ILE
4	B	580	LEU
4	B	581	ASN
4	B	609	LEU
4	B	641	ILE
4	B	693	GLU
4	B	725	ILE
4	B	766	ILE
4	B	769	SER
4	B	773	VAL
4	B	801	ILE
4	B	802	ILE
4	B	804	ARG
4	B	937	PHE
4	B	1067	ILE
4	B	1153	VAL
4	B	1176	VAL
4	B	1183	THR
4	B	1186	PRO
4	B	1208	LYS
4	B	1213	PRO
4	B	1734	THR
4	B	1758	LYS
4	B	1929	ASP
4	B	2005	ASN
4	B	2040	LEU
4	B	2080	LYS

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Mol	Chain	Res	Type
4	B	2090	LYS
4	B	2117	ASP
4	B	2139	GLN
4	B	2176	VAL
4	B	2177	ARG
4	B	2206	GLU
4	B	2258	HIS
4	B	2346	ILE
4	B	2396	MET
4	B	2419	LYS
4	B	2441	LEU
4	B	2576	LEU
4	B	2610	PRO
4	B	2619	SER
4	B	2653	CYS
4	B	2752	CYS
4	B	2758	GLN
4	B	2776	LYS
4	B	2846	LEU
4	B	2849	LYS
4	B	2873	SER
4	B	2874	ARG
4	B	2887	LEU
4	B	2888	LEU
4	B	2931	GLU
4	B	2949	THR
4	B	2959	LEU
4	B	2963	ASN
4	B	2971	ILE
4	B	2982	SER
4	B	3004	LEU
4	B	3080	LEU
4	B	3119	LYS
4	B	3222	PRO
4	B	3231	VAL
4	B	3240	THR
4	B	3258	VAL
4	B	3269	LEU
4	B	3288	GLN
4	B	3330	SER
4	B	3343	ILE
4	B	3349	ILE

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Mol	Chain	Res	Type
4	B	3350	PHE
4	B	3355	PRO
4	B	3450	ASP
4	B	3488	ILE
4	B	3489	THR
4	B	3614	ILE
4	B	3694	LEU
4	B	3756	MET
4	B	3757	LEU
4	B	3800	LEU
4	B	3850	LEU
4	B	3942	LEU
4	B	3976	ASP
4	B	4012	PHE
4	B	4104	LYS
4	B	4182	PRO
4	B	4255	SER
4	B	4279	CYS
4	B	4334	LYS
4	B	4352	GLU
4	B	4369	GLU
4	B	4441	ILE
4	B	4443	ARG
4	B	4476	THR
4	B	4482	GLU
4	B	4520	SER
4	B	4547	VAL
4	B	4553	ARG
5	I	19	MET
5	I	60	CYS
5	I	81	GLU
5	I	97	MET
6	H	8	GLN
6	H	12	LYS
8	F	9	ASP
8	F	13	GLN
8	F	41	SER
8	F	51	LEU
8	F	62	VAL
8	F	81	THR
8	F	96	THR
8	F	97	MET

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Mol	Chain	Res	Type
9	N	18	ASP
9	N	43	VAL
10	O	22	LEU
10	O	32	SER
10	O	46	LEU
10	O	57	ASN
10	O	77	PRO
10	O	99	SER
10	O	103	TRP
10	O	122	CYS
11	E	37	ILE
11	E	44	ASN
11	E	47	PHE
11	E	49	ASP
11	E	193	MET
11	E	266	THR
11	E	281	THR
11	E	353	VAL
11	E	361	LEU
11	E	385	SER
11	E	402	ILE
11	E	422	SER
11	E	515	LYS
11	E	519	LEU
11	E	560	HIS
11	E	567	PRO
12	D	62	THR
12	D	75	LEU
12	D	90	ASP
12	D	104	GLN
12	D	106	ILE
12	D	169	ASN
12	D	172	GLU
12	D	177	ASN
12	D	196	CYS
12	D	266	TYR
12	D	371	THR
12	D	372	VAL
12	D	392	ASN
12	D	395	HIS
12	D	399	VAL
12	D	414	PHE

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Mol	Chain	Res	Type
12	D	477	GLU
12	D	488	TYR
12	D	527	ILE
12	D	584	ILE
12	D	595	PHE
14	L	50	GLU
14	L	51	LYS
14	L	86	LEU
15	K	18	MET
16	J	21	PHE
16	J	86	CYS
16	J	91	ASN
16	J	100	ILE
17	M	10	THR
17	M	60	ASN
17	M	64	HIS
17	M	73	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	642	ASN
1	A	719	GLN
1	A	793	GLN
1	A	797	ASN
1	A	837	GLN
1	A	852	ASN
1	A	1041	ASN
1	A	1205	GLN
1	A	1515	GLN
1	A	1566	GLN
1	A	1567	ASN
1	A	1666	ASN
1	A	1690	ASN
1	A	1718	GLN
1	A	1728	GLN
1	A	1897	ASN
1	A	1902	HIS
1	A	1940	GLN
1	A	1977	ASN
1	A	2028	ASN

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Mol	Chain	Res	Type
1	A	2221	ASN
1	A	2251	ASN
1	A	2267	ASN
1	A	2279	ASN
1	A	2340	GLN
1	A	2455	GLN
1	A	2458	GLN
1	A	2508	ASN
1	A	2573	GLN
1	A	2581	GLN
1	A	2606	GLN
1	A	2619	ASN
1	A	2628	GLN
1	A	2715	ASN
1	A	2735	HIS
1	A	2795	ASN
1	A	2874	GLN
1	A	2889	GLN
1	A	3084	GLN
1	A	3122	ASN
1	A	3252	GLN
1	A	3311	ASN
1	A	3343	HIS
1	A	3466	ASN
1	A	3506	GLN
1	A	3523	ASN
1	A	3539	ASN
1	A	3582	ASN
1	A	3606	GLN
1	A	3694	ASN
1	A	4079	HIS
1	A	4088	GLN
1	A	4125	ASN
1	A	4330	ASN
1	A	4417	ASN
1	A	4479	GLN
1	A	4574	ASN
1	A	4607	HIS
2	C	17	GLN
2	C	45	ASN
2	C	168	ASN
2	C	170	GLN

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Mol	Chain	Res	Type
2	C	203	HIS
2	C	246	HIS
2	C	281	ASN
2	C	305	ASN
2	C	964	GLN
2	C	1077	GLN
2	C	1155	ASN
2	C	1173	ASN
2	C	1238	GLN
2	C	1300	GLN
2	C	1394	HIS
2	C	1570	GLN
2	C	1727	ASN
2	C	1863	HIS
2	C	1867	HIS
2	C	1888	GLN
2	C	1981	ASN
2	C	2052	GLN
2	C	2066	GLN
2	C	2074	GLN
2	C	2121	ASN
2	C	2123	GLN
2	C	2207	HIS
2	C	2211	ASN
2	C	2217	ASN
2	C	2367	GLN
2	C	2401	GLN
2	C	2421	GLN
2	C	2483	ASN
2	C	2566	GLN
2	C	2778	ASN
2	C	2784	ASN
2	C	2819	ASN
2	C	2947	ASN
2	C	2953	ASN
2	C	3051	ASN
2	C	3103	HIS
2	C	3158	GLN
2	C	3460	ASN
2	C	3547	GLN
2	C	3631	GLN
2	C	3654	HIS

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Mol	Chain	Res	Type
2	C	3674	GLN
2	C	3693	GLN
2	C	3751	ASN
2	C	3766	ASN
2	C	3791	HIS
2	C	3801	ASN
2	C	3819	ASN
2	C	3870	GLN
2	C	4040	GLN
2	C	4050	GLN
2	C	4068	ASN
2	C	4109	ASN
2	C	4143	ASN
4	B	435	GLN
4	B	672	ASN
4	B	721	ASN
4	B	723	ASN
4	B	724	HIS
4	B	764	GLN
4	B	775	GLN
4	B	832	ASN
4	B	837	GLN
4	B	883	ASN
4	B	923	GLN
4	B	957	GLN
4	B	975	ASN
4	B	984	ASN
4	B	1061	GLN
4	B	1079	ASN
4	B	1081	GLN
4	B	1127	ASN
4	B	1135	HIS
4	B	1196	ASN
4	B	1522	GLN
4	B	1626	ASN
4	B	1698	GLN
4	B	1728	GLN
4	B	1761	GLN
4	B	1770	ASN
4	B	1807	GLN
4	B	1820	GLN
4	B	1837	GLN

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Mol	Chain	Res	Type
4	B	1870	ASN
4	B	1956	ASN
4	B	1969	GLN
4	B	2005	ASN
4	B	2038	ASN
4	B	2069	GLN
4	B	2085	GLN
4	B	2148	GLN
4	B	2169	GLN
4	B	2203	ASN
4	B	2392	HIS
4	B	2462	ASN
4	B	2476	GLN
4	B	2489	ASN
4	B	2579	ASN
4	B	2591	ASN
4	B	2608	ASN
4	B	2646	GLN
4	B	2656	GLN
4	B	2695	HIS
4	B	2828	GLN
4	B	2833	GLN
4	B	2836	GLN
4	B	2897	GLN
4	B	3042	ASN
4	B	3049	HIS
4	B	3076	GLN
4	B	3081	ASN
4	B	3104	ASN
4	B	3288	GLN
4	B	3394	GLN
4	B	3407	GLN
4	B	3521	ASN
4	B	3540	GLN
4	B	3584	GLN
4	B	3640	GLN
4	B	3656	GLN
4	B	3663	ASN
4	B	3715	ASN
4	B	3743	GLN
4	B	3769	HIS
4	B	3772	GLN

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Mol	Chain	Res	Type
4	B	3803	ASN
4	B	3875	GLN
4	B	3879	ASN
4	B	4021	GLN
4	B	4042	GLN
4	B	4097	ASN
4	B	4152	ASN
4	B	4158	ASN
4	B	4176	ASN
4	B	4177	GLN
4	B	4214	ASN
4	B	4294	GLN
4	B	4346	GLN
4	B	4448	GLN
5	I	100	ASN
6	H	36	ASN
7	G	101	ASN
7	G	129	GLN
7	G	149	GLN
8	F	27	ASN
8	F	64	GLN
9	N	75	GLN
9	N	89	GLN
9	N	99	GLN
10	O	27	ASN
11	E	31	GLN
11	E	39	GLN
11	E	42	GLN
11	E	52	ASN
11	E	75	HIS
11	E	87	ASN
11	E	188	GLN
11	E	196	GLN
11	E	220	ASN
11	E	224	ASN
11	E	237	ASN
11	E	259	ASN
11	E	305	ASN
11	E	377	ASN
11	E	379	ASN
11	E	481	GLN
12	D	64	GLN

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Mol	Chain	Res	Type
12	D	126	GLN
12	D	153	HIS
12	D	169	ASN
12	D	216	HIS
12	D	294	GLN
12	D	298	ASN
12	D	324	GLN
12	D	405	ASN
12	D	425	ASN
12	D	431	ASN
12	D	465	ASN
12	D	509	ASN
12	D	572	ASN
12	D	592	ASN
14	L	28	GLN
15	K	8	GLN
15	K	67	ASN
17	M	2	ASN
17	M	36	GLN
17	M	60	ASN
17	M	78	ASN

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](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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
18	ADP	C	4203	20	28,29,29	0.50	0	43,45,45	0.83	1 (2%)
19	ATP	A	4702	20	32,33,33	0.51	0	48,52,52	0.59	0
19	ATP	C	4201	20	32,33,33	0.47	0	48,52,52	0.59	0
18	ADP	A	4703	-	28,29,29	0.50	0	43,45,45	0.58	0
19	ATP	B	4701	20	32,33,33	0.50	0	48,52,52	0.62	0
18	ADP	C	4206	20	28,29,29	0.46	0	43,45,45	0.60	0
18	ADP	B	4706	20	28,29,29	0.48	0	43,45,45	0.44	0
18	ADP	B	4705	20	28,29,29	0.54	0	43,45,45	0.51	0
18	ADP	A	4701	20	28,29,29	0.47	0	43,45,45	0.52	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
18	ADP	C	4203	20	-	7/16/32/32	0/3/3/3
19	ATP	A	4702	20	-	5/22/38/38	0/3/3/3
19	ATP	C	4201	20	-	6/22/38/38	0/3/3/3
18	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/22/38/38	0/3/3/3
18	ADP	C	4206	20	-	4/16/32/32	0/3/3/3
18	ADP	B	4706	20	-	2/16/32/32	0/3/3/3
18	ADP	B	4705	20	-	5/16/32/32	0/3/3/3
18	ADP	A	4701	20	-	5/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4203	ADP	C4-N9-C1'	2.03	131.39	126.63

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4203	ADP	C5'-O5'-PA-O1A
18	C	4203	ADP	C5'-O5'-PA-O2A
18	C	4203	ADP	C5'-O5'-PA-O3A
18	C	4206	ADP	O4'-C4'-C5'-O5'
18	B	4705	ADP	PB-O3A-PA-O5'
18	B	4705	ADP	C5'-O5'-PA-O1A
18	B	4705	ADP	C5'-O5'-PA-O3A
19	C	4201	ATP	C5'-O5'-PA-O1A
19	C	4201	ATP	C5'-O5'-PA-O3A
18	C	4203	ADP	C3'-C4'-C5'-O5'
18	C	4203	ADP	O4'-C4'-C5'-O5'
19	C	4201	ATP	O4'-C1'-N9-C4
18	C	4206	ADP	C3'-C4'-C5'-O5'
19	A	4702	ATP	O4'-C4'-C5'-O5'
18	B	4706	ADP	PA-O3A-PB-O2B
18	C	4203	ADP	C2'-C1'-N9-C4
19	C	4201	ATP	O4'-C1'-N9-C8
19	A	4702	ATP	PB-O3A-PA-O2A
19	A	4702	ATP	C3'-C4'-C5'-O5'
18	C	4203	ADP	C2'-C1'-N9-C8
18	B	4705	ADP	C5'-O5'-PA-O2A
18	B	4705	ADP	C4'-C5'-O5'-PA
18	A	4701	ADP	O4'-C4'-C5'-O5'
18	B	4706	ADP	C4'-C5'-O5'-PA
18	C	4206	ADP	PB-O3A-PA-O1A
18	A	4703	ADP	C4'-C5'-O5'-PA
18	A	4701	ADP	PA-O3A-PB-O1B
18	A	4701	ADP	PA-O3A-PB-O2B
19	A	4702	ATP	PB-O3B-PG-O2G
19	A	4702	ATP	PB-O3A-PA-O1A
19	C	4201	ATP	PG-O3B-PB-O2B
19	C	4201	ATP	O4'-C4'-C5'-O5'
18	A	4701	ADP	C4'-C5'-O5'-PA
18	C	4206	ADP	PB-O3A-PA-O2A

There are no ring outliers.

5 monomers are involved in 6 short contacts:

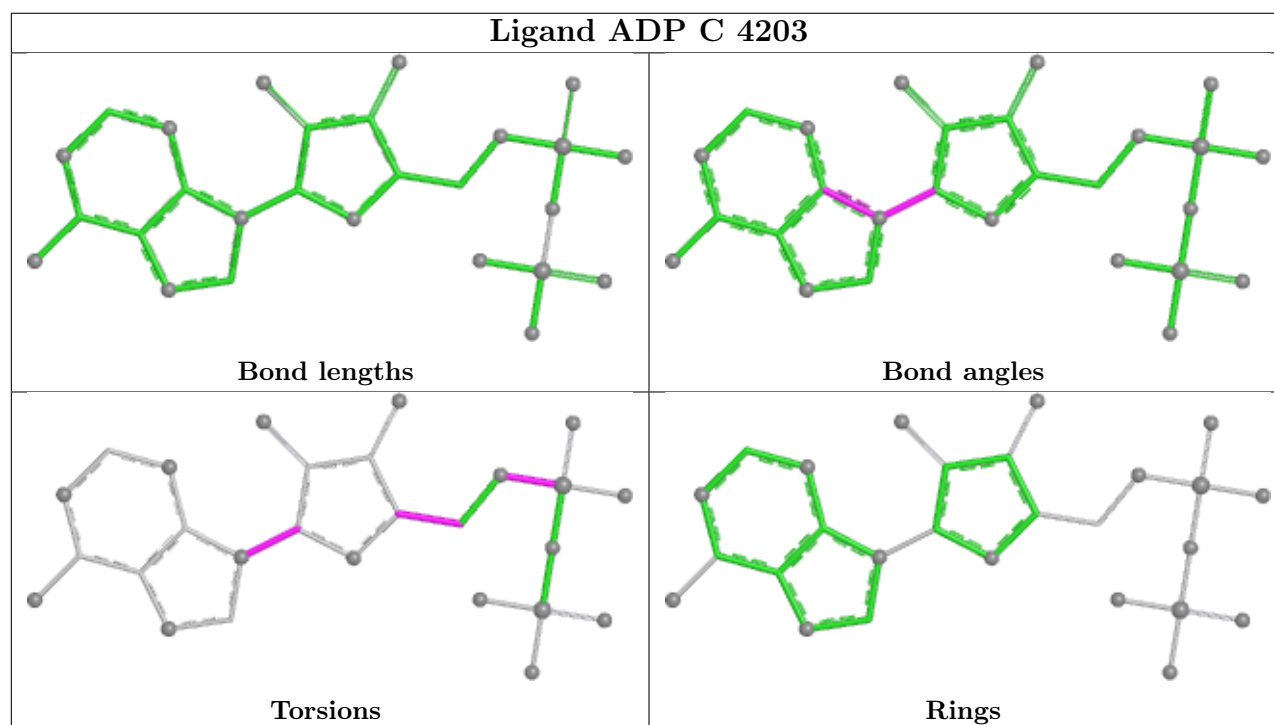
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4203	ADP	1	0
18	A	4703	ADP	1	0
19	B	4701	ATP	1	0

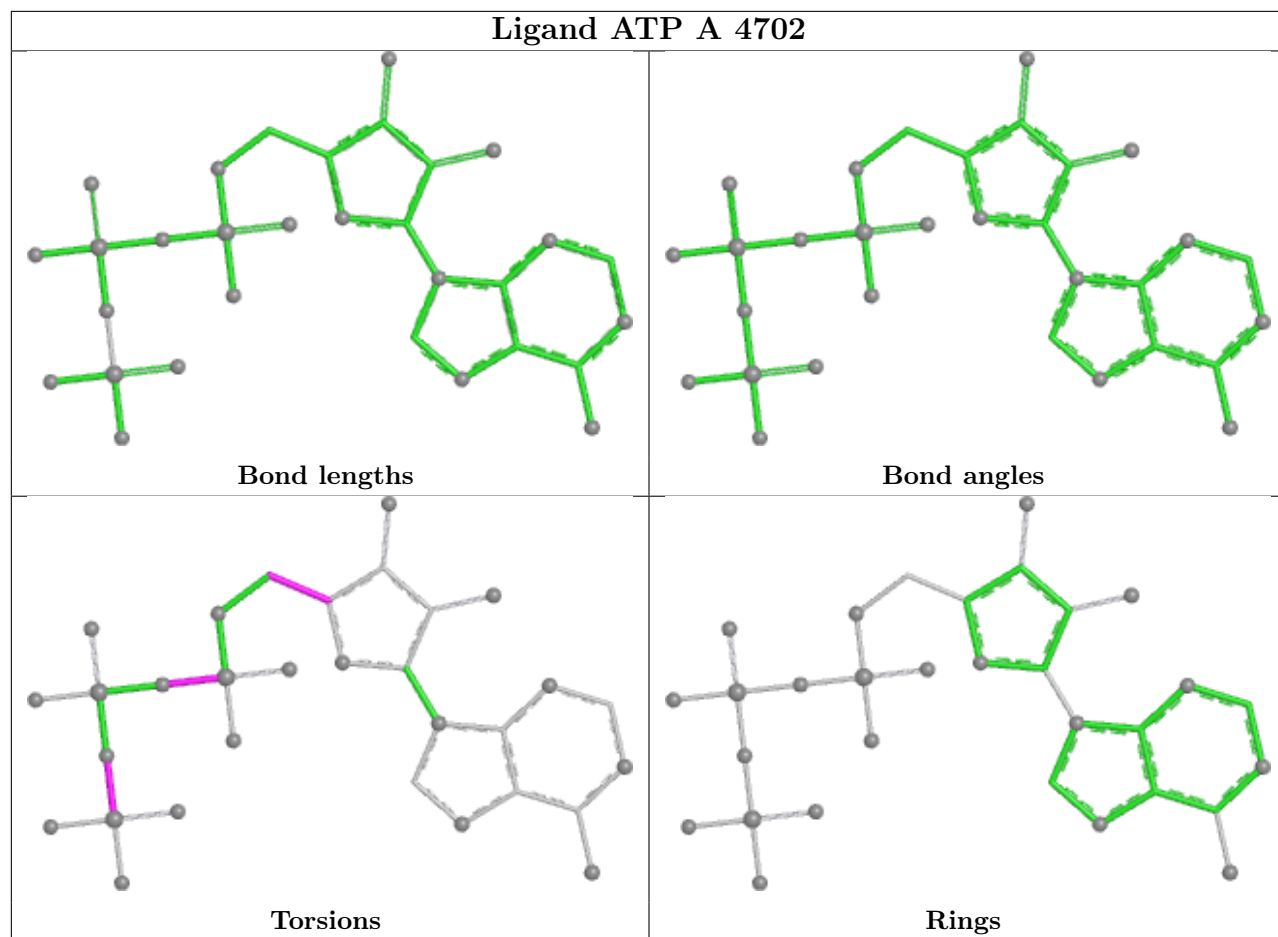
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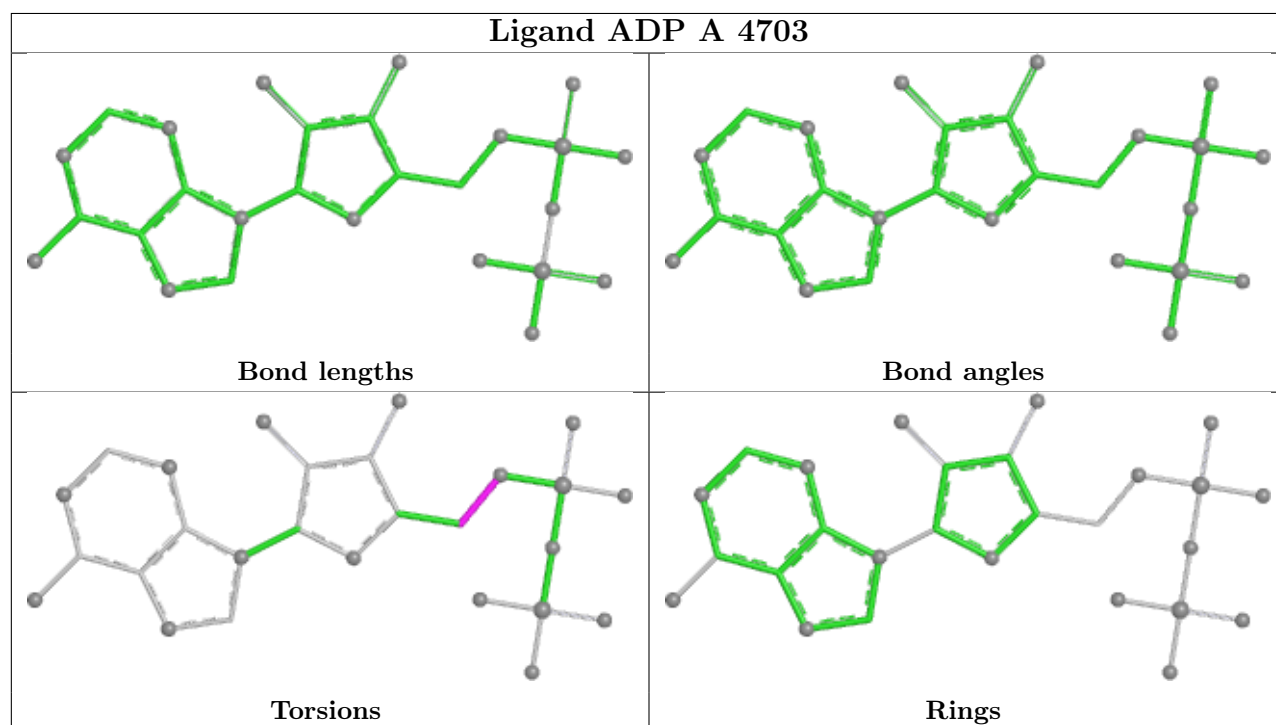
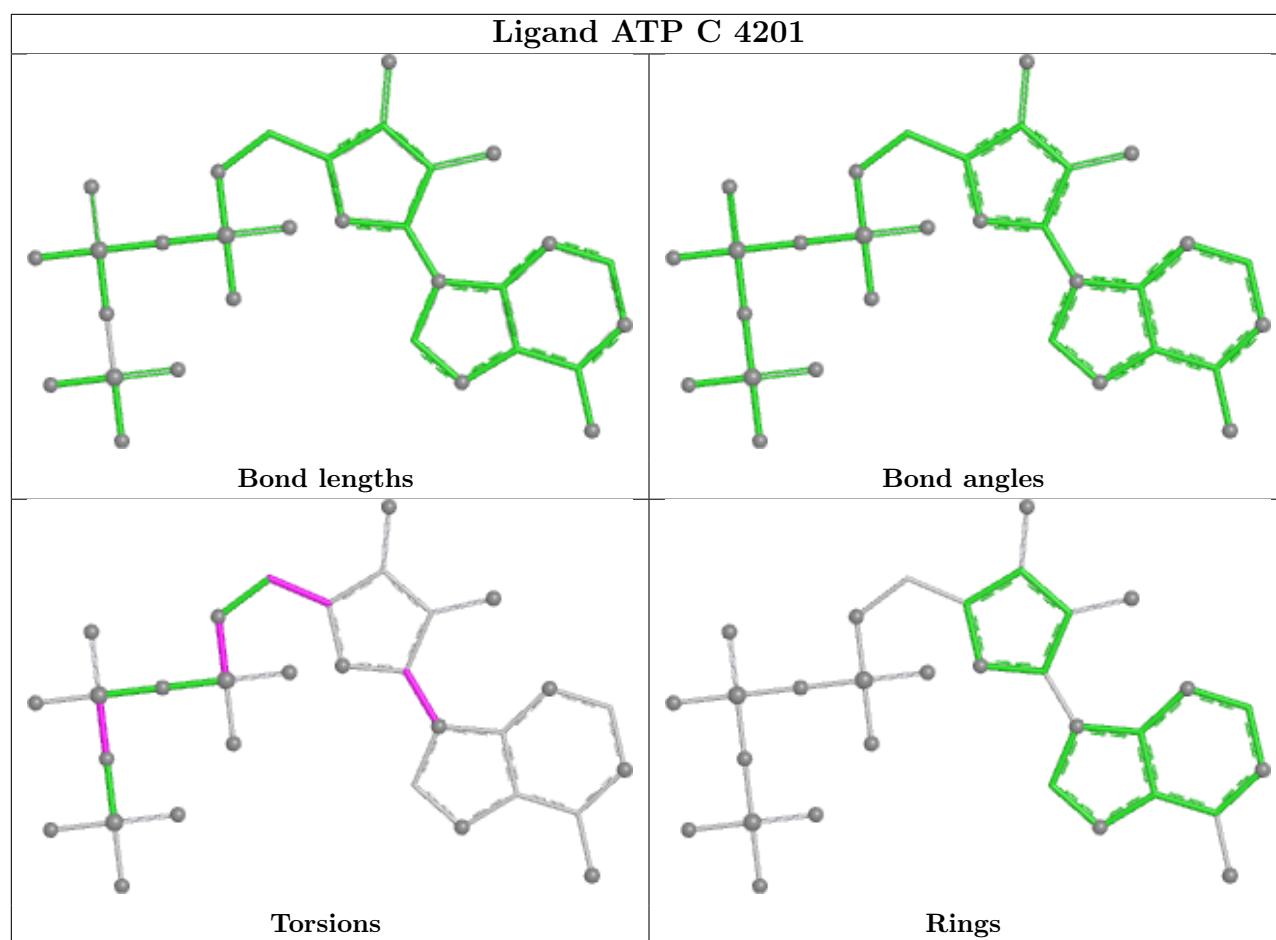
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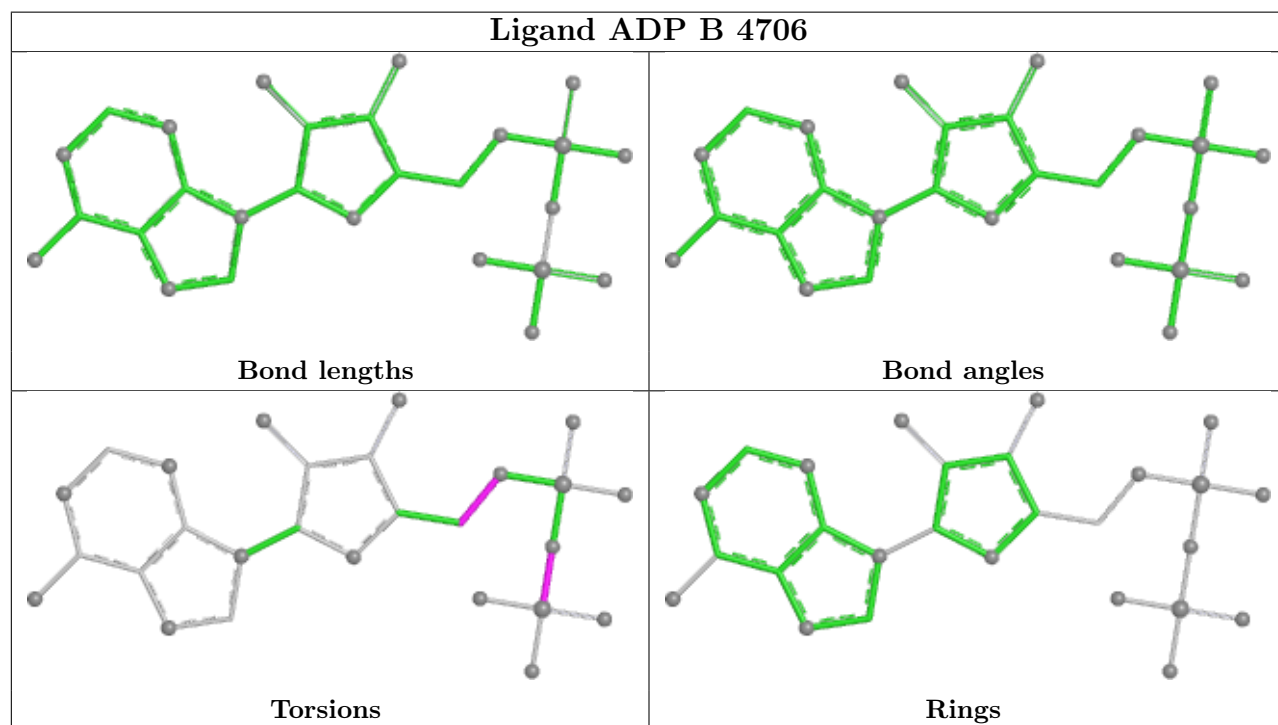
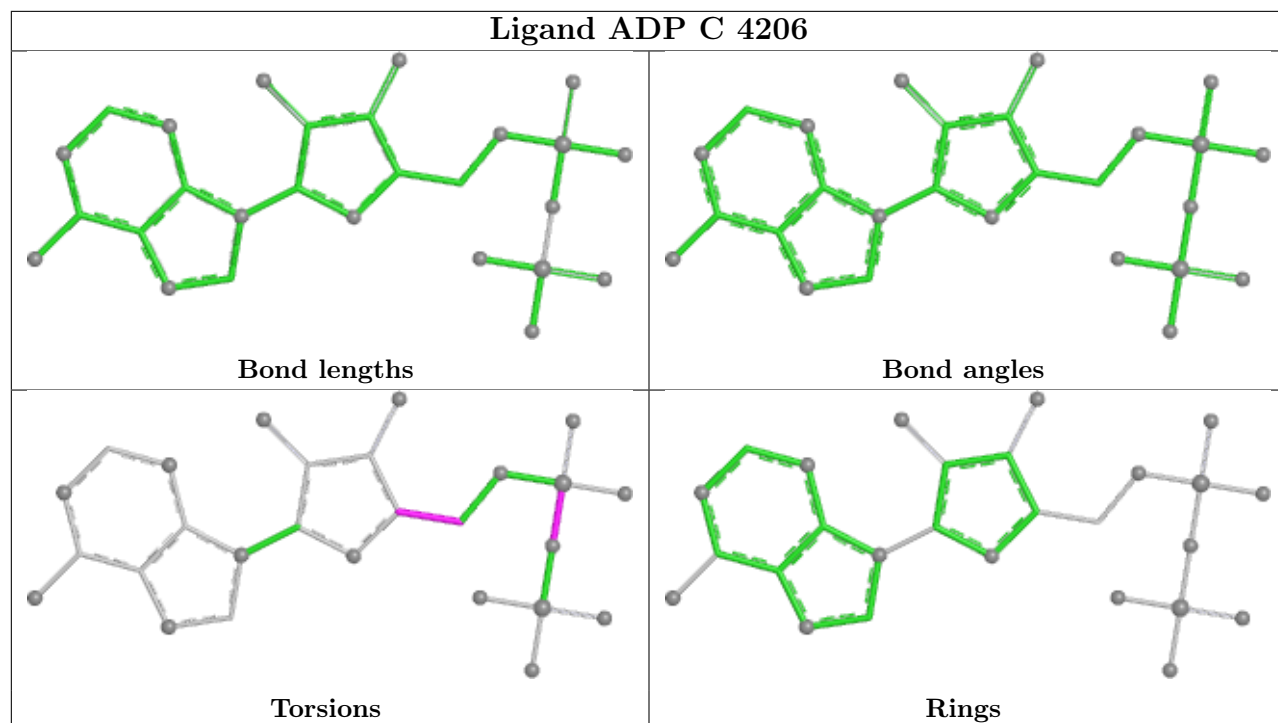
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4206	ADP	2	0
18	A	4701	ADP	1	0

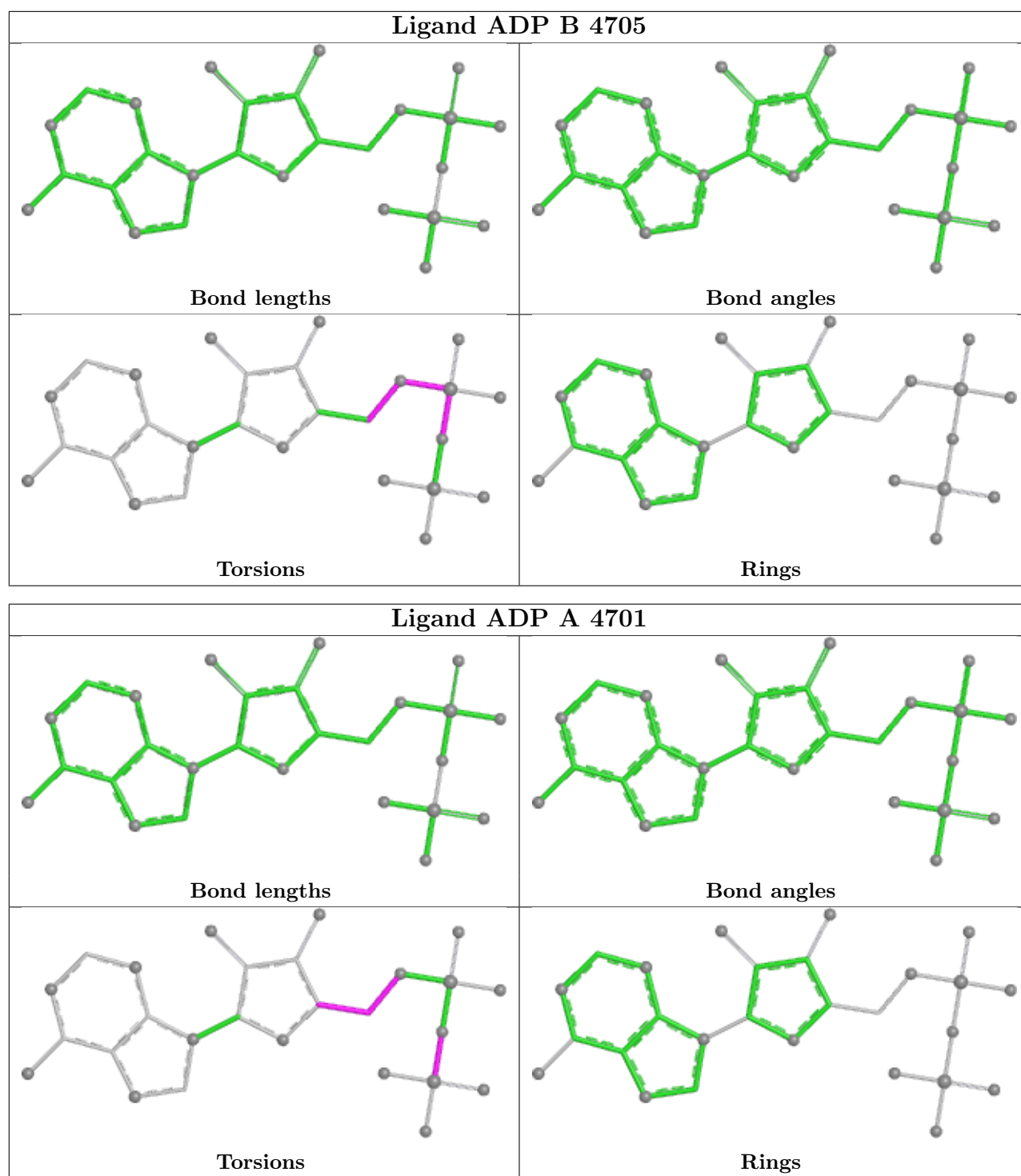
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











5.7 Other polymers ⓘ

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	4
2	C	3
4	B	3
12	D	2
13	P	1
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	364:ILE	C	365:PHE	N	4.18
1	B	25:GLN	C	26:LYS	N	3.78
1	D	216:HIS	C	217:GLN	N	3.67
1	A	53:ILE	C	54:PHE	N	3.57
1	A	115:ASP	C	116:ASN	N	3.46
1	A	40:LEU	C	41:LEU	N	3.38
1	A	24:LYS	C	25:ASP	N	3.36
1	P	15:SER	C	16:GLU	N	3.31
1	C	305:ASN	C	306:LEU	N	3.20
1	G	58:SER	C	59:GLU	N	3.19
1	D	238:SER	C	239:THR	N	3.15
1	B	994:SER	C	995:TYR	N	2.89
1	B	1606:PHE	C	1607:PRO	N	1.73
1	C	1136:PHE	C	1137:PRO	N	1.65

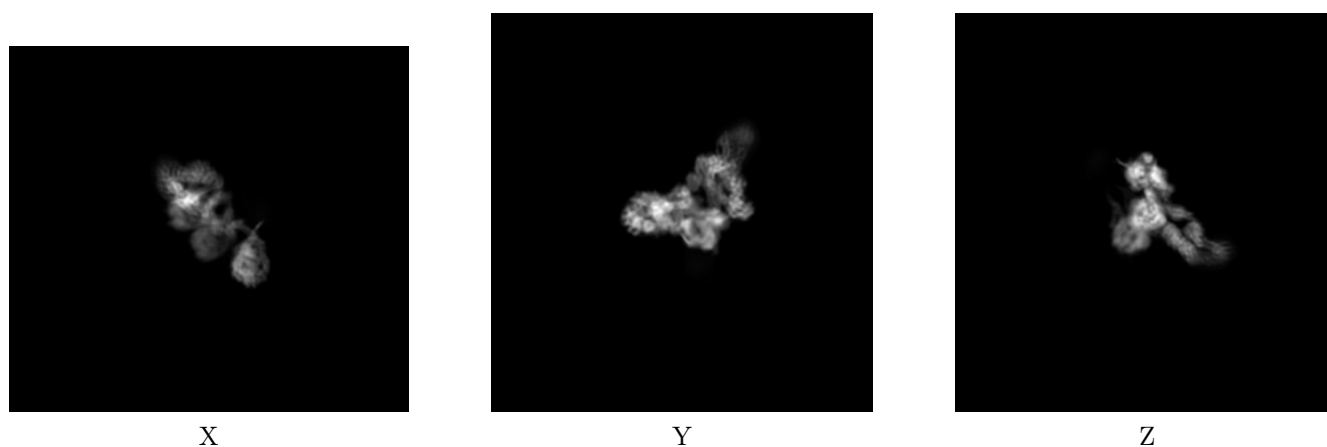
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22840. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

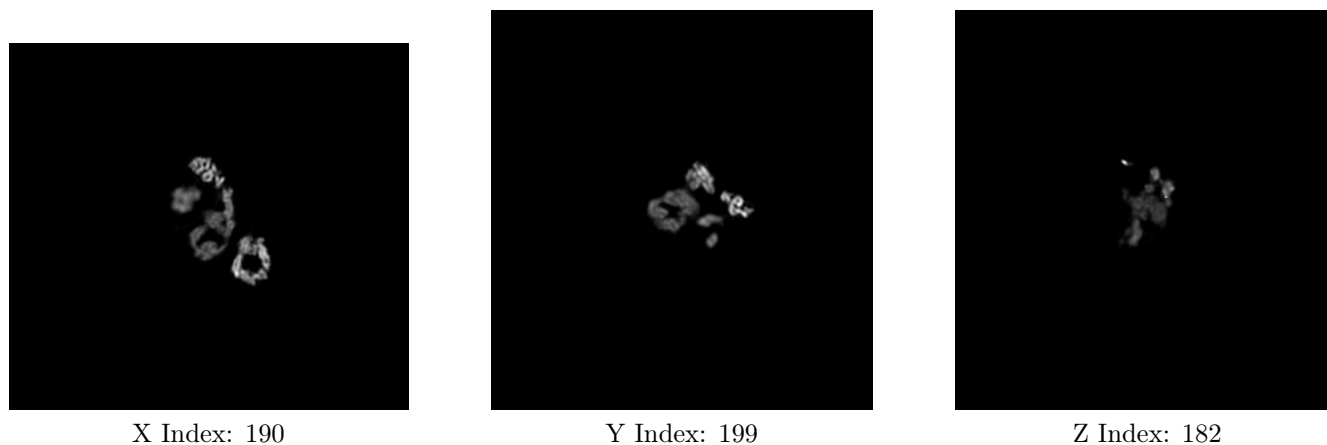
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



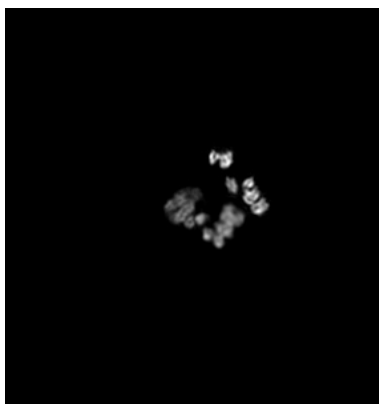
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 186

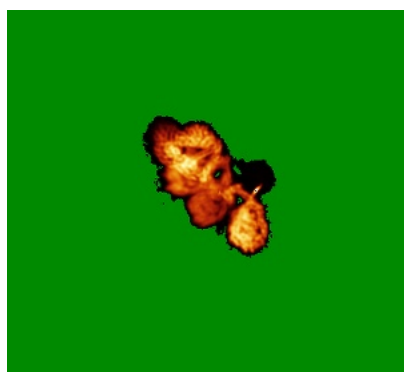


Z Index: 209

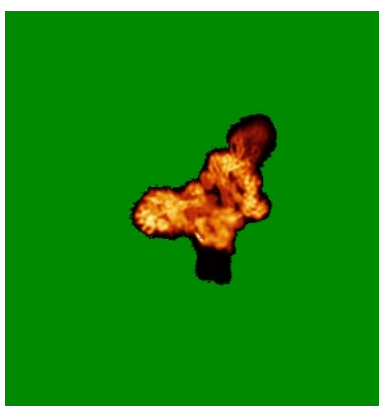
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

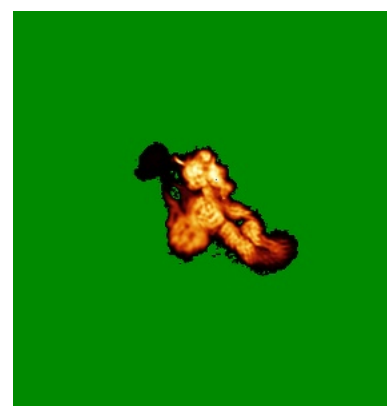
6.4.1 Primary map



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

This section was not generated.

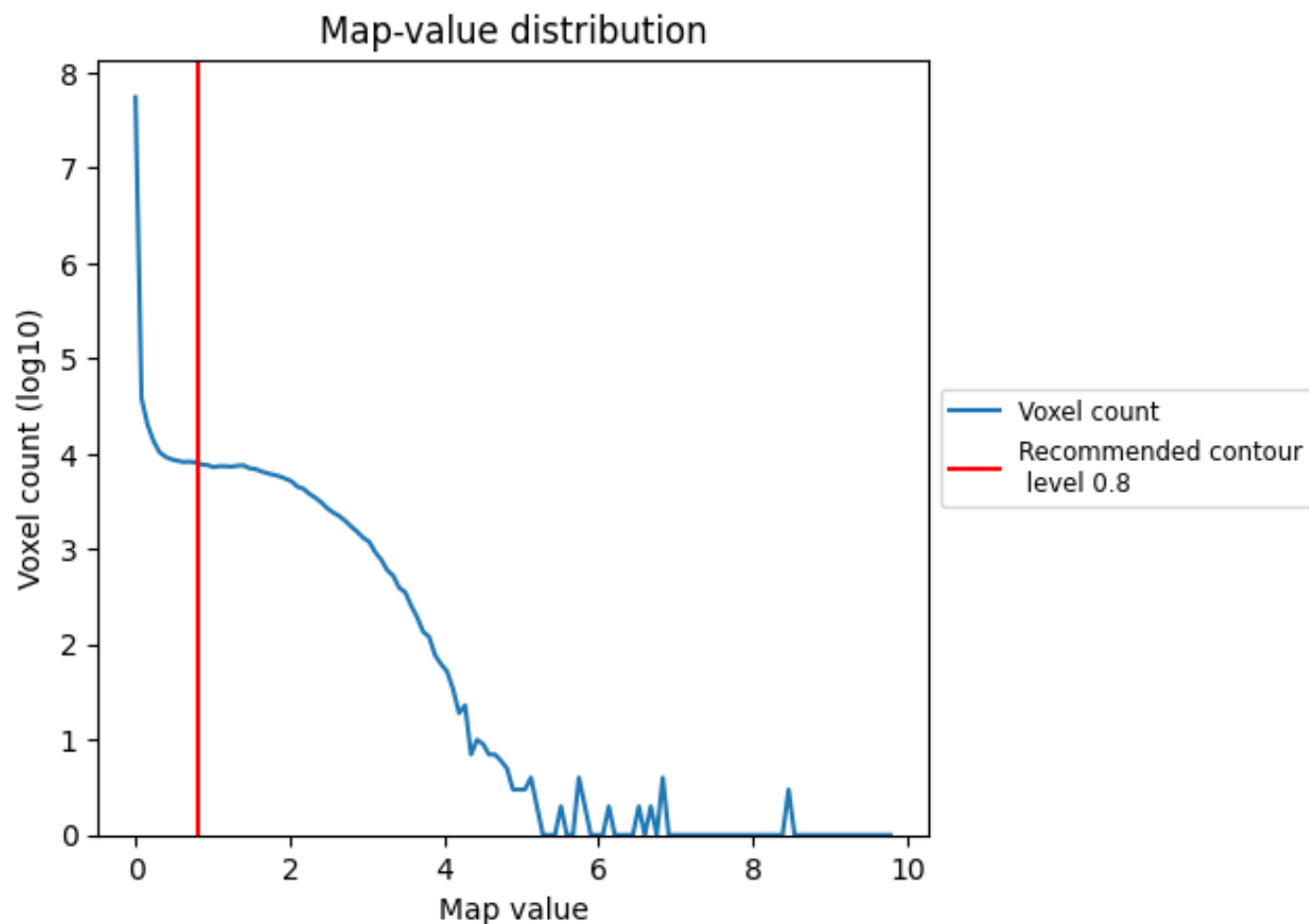
6.6 Mask visualisation

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

7 Map analysis [i](#)

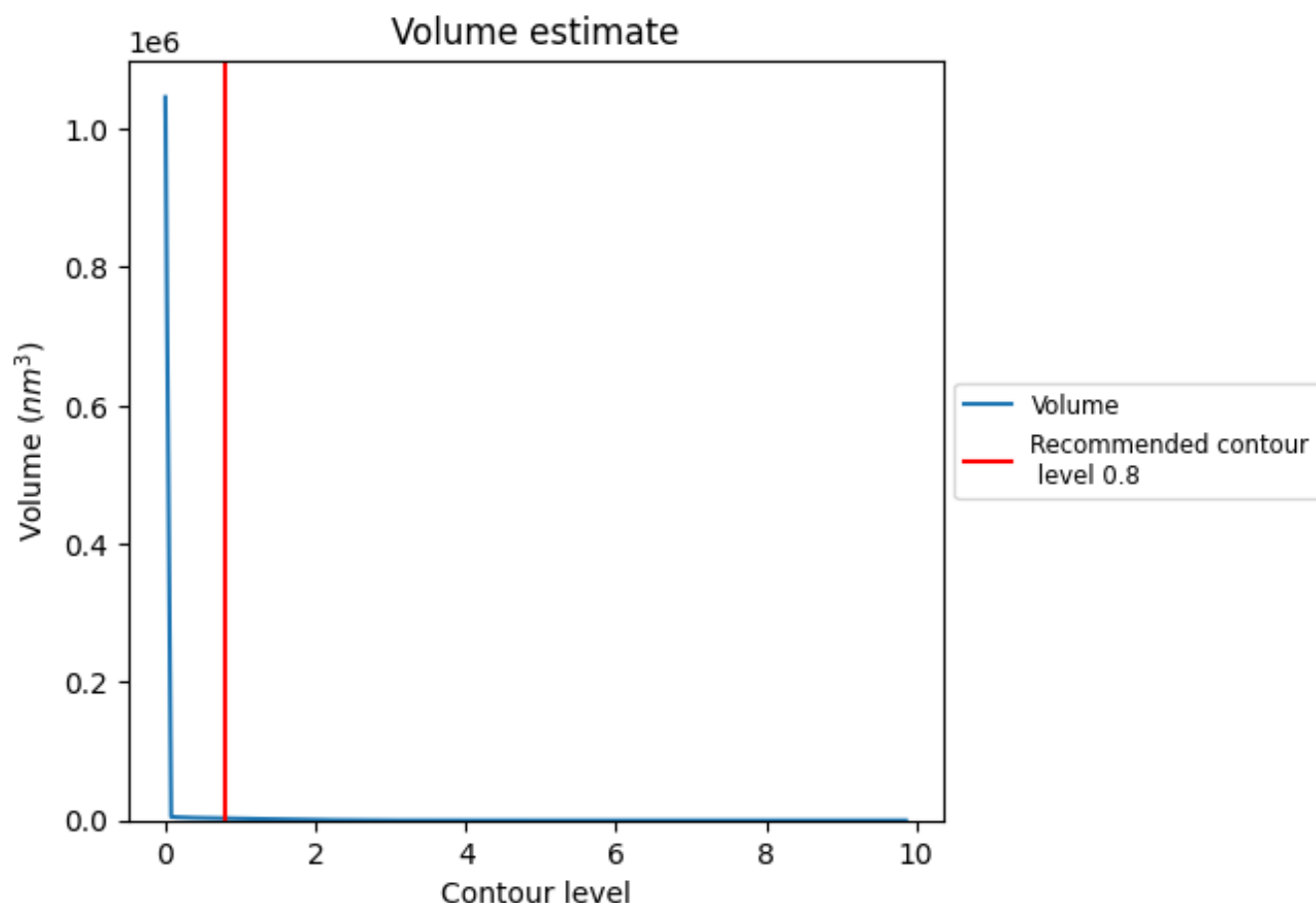
This section contains the results of statistical analysis of the map.

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 2909 nm³; this corresponds to an approximate mass of 2628 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

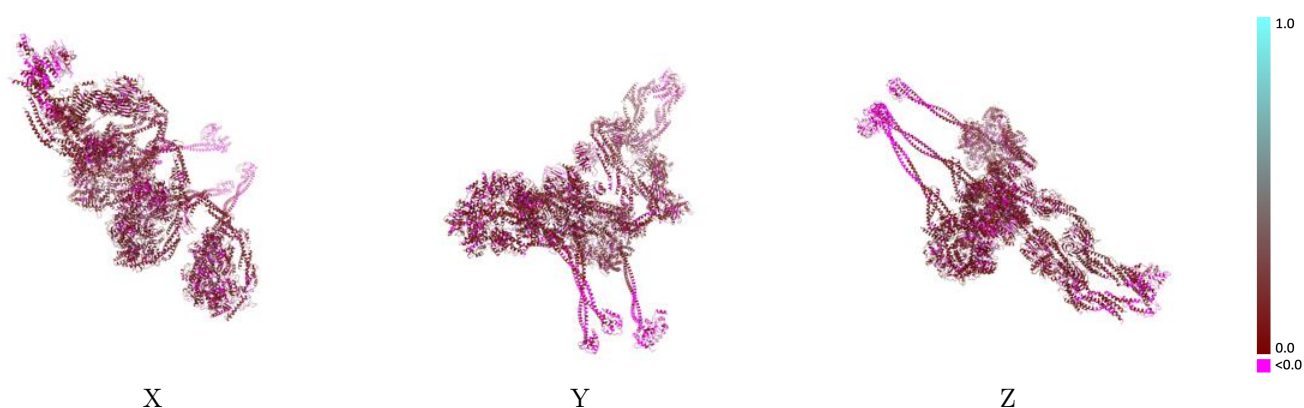
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22840 and PDB model 7KEK. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

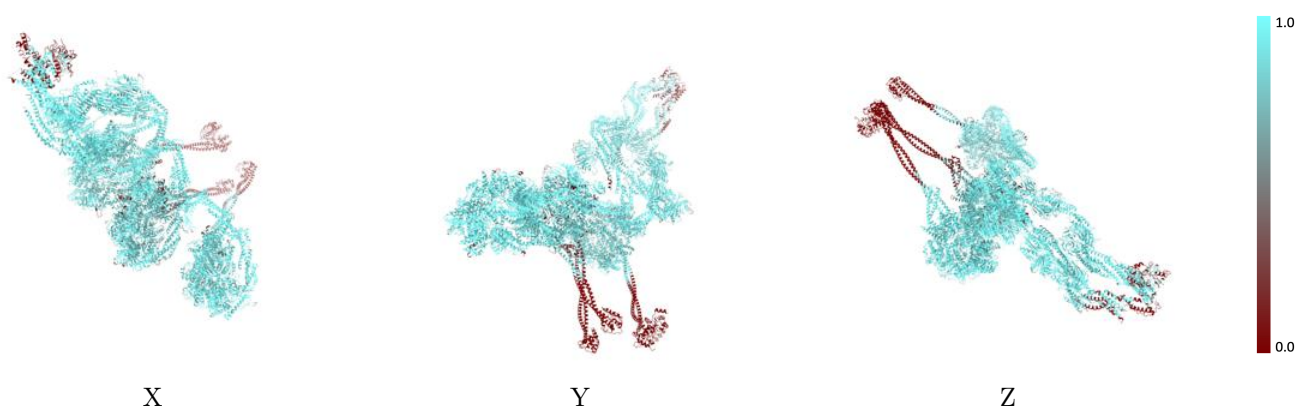
This section was not generated.

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



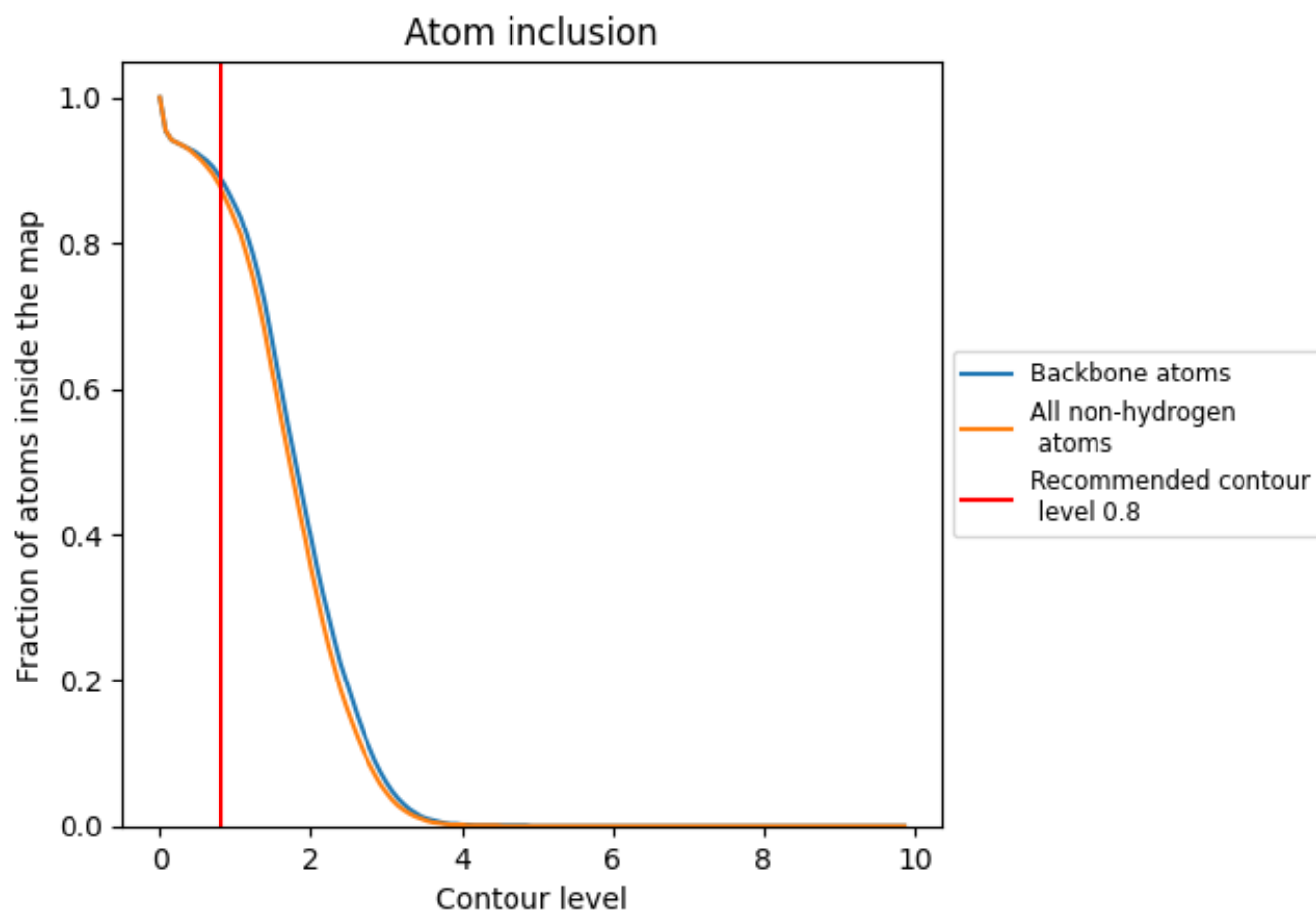
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.0820
A	 0.8690	 0.0750
B	 0.8440	 0.0940
C	 0.9000	 0.0720
D	 0.9770	 0.0930
E	 0.9660	 0.0980
F	 0.9940	 0.1150
G	 0.9730	 0.1140
H	 0.9880	 0.1000
I	 0.9670	 0.1140
J	 0.9860	 0.0810
K	 0.9850	 0.0970
L	 0.9870	 0.1020
M	 0.9720	 0.0830
N	 0.9110	 0.0660
O	 0.9670	 0.0780
P	 0.9760	 0.1150
Q	 0.0000	 -0.0530

