



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:22 AM EDT

PDB ID : 7KEK
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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

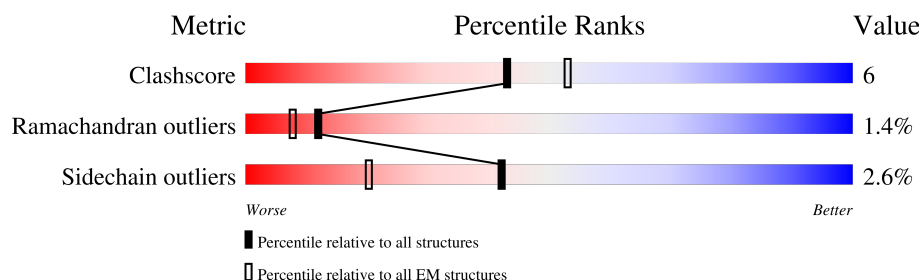
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>12%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
2	C	4168	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>
3	Q	202	<div> <div>95%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
4	B	4595	<div> <div>13%</div> <div>84%</div> <div>13%</div> <div>• •</div> </div>
5	I	110	<div> <div>76%</div> <div>17%</div> <div>• •</div> </div>
6	H	92	<div> <div>88%</div> <div>10%</div> <div>• •</div> </div>
7	G	159	<div> <div>52%</div> <div>8%</div> <div>40%</div> </div>
8	F	133	<div> <div>68%</div> <div>14%</div> <div>•</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
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		

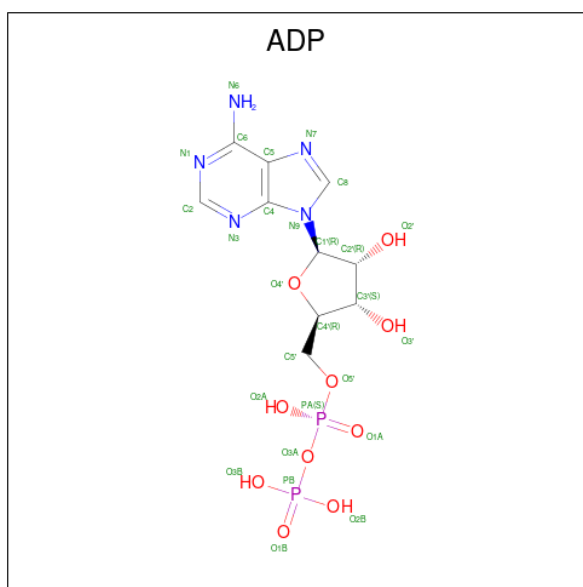
- Molecule 16 is a protein called Dynein light chain LC8_2b.

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

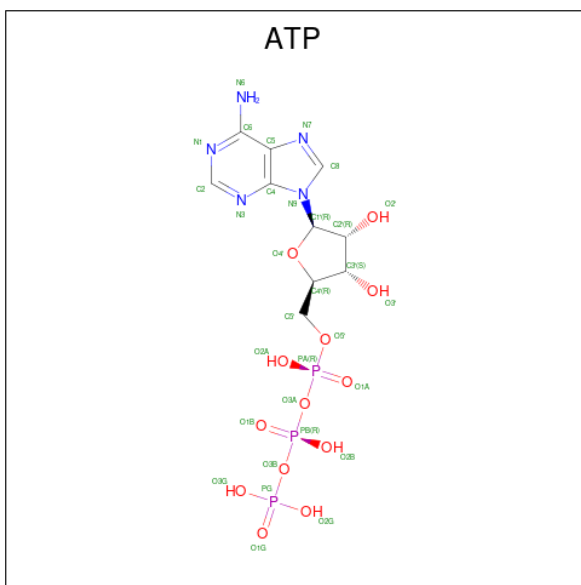
- Molecule 17 is a protein called Dynein light chain LC8_3a.

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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

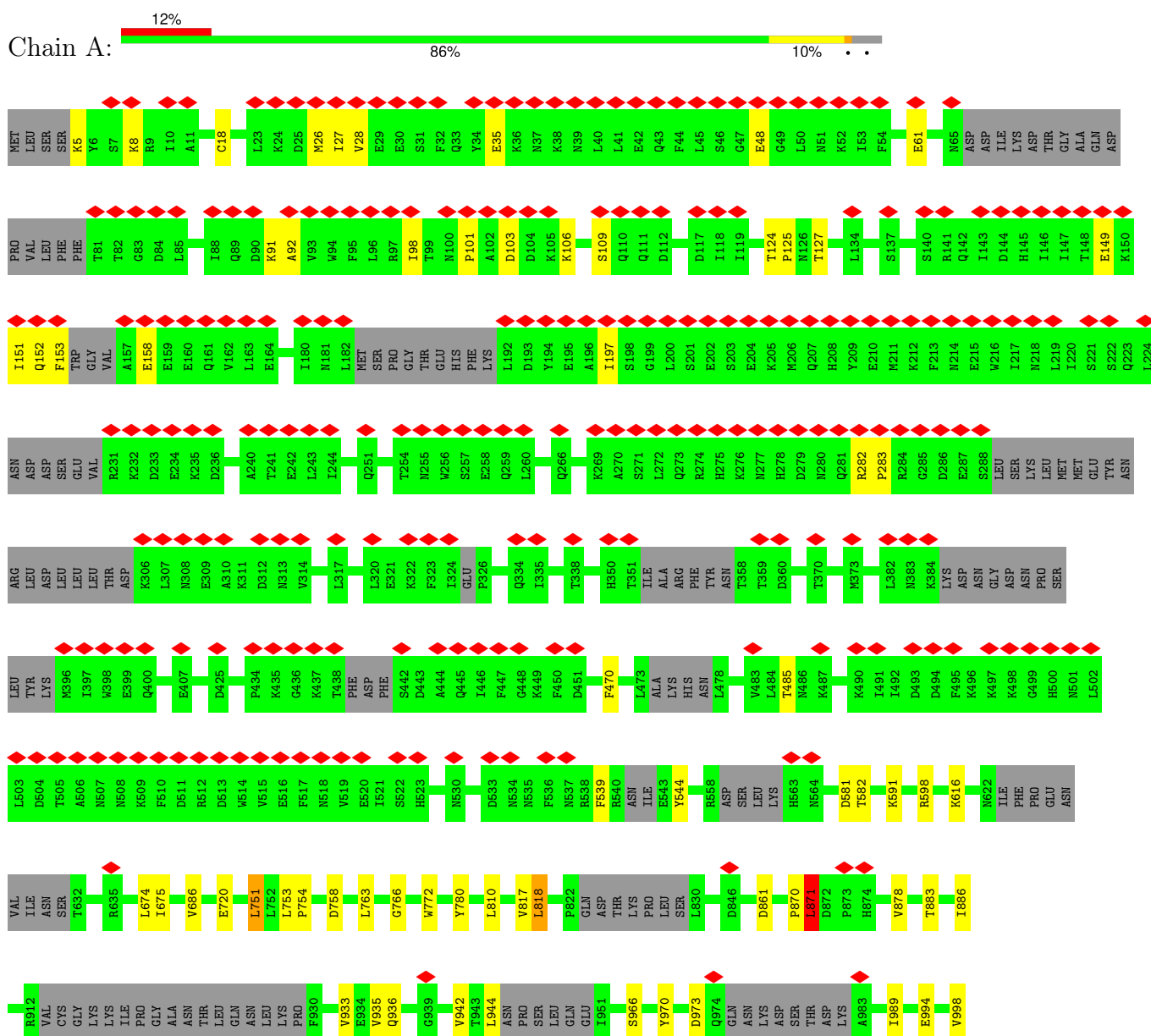
- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

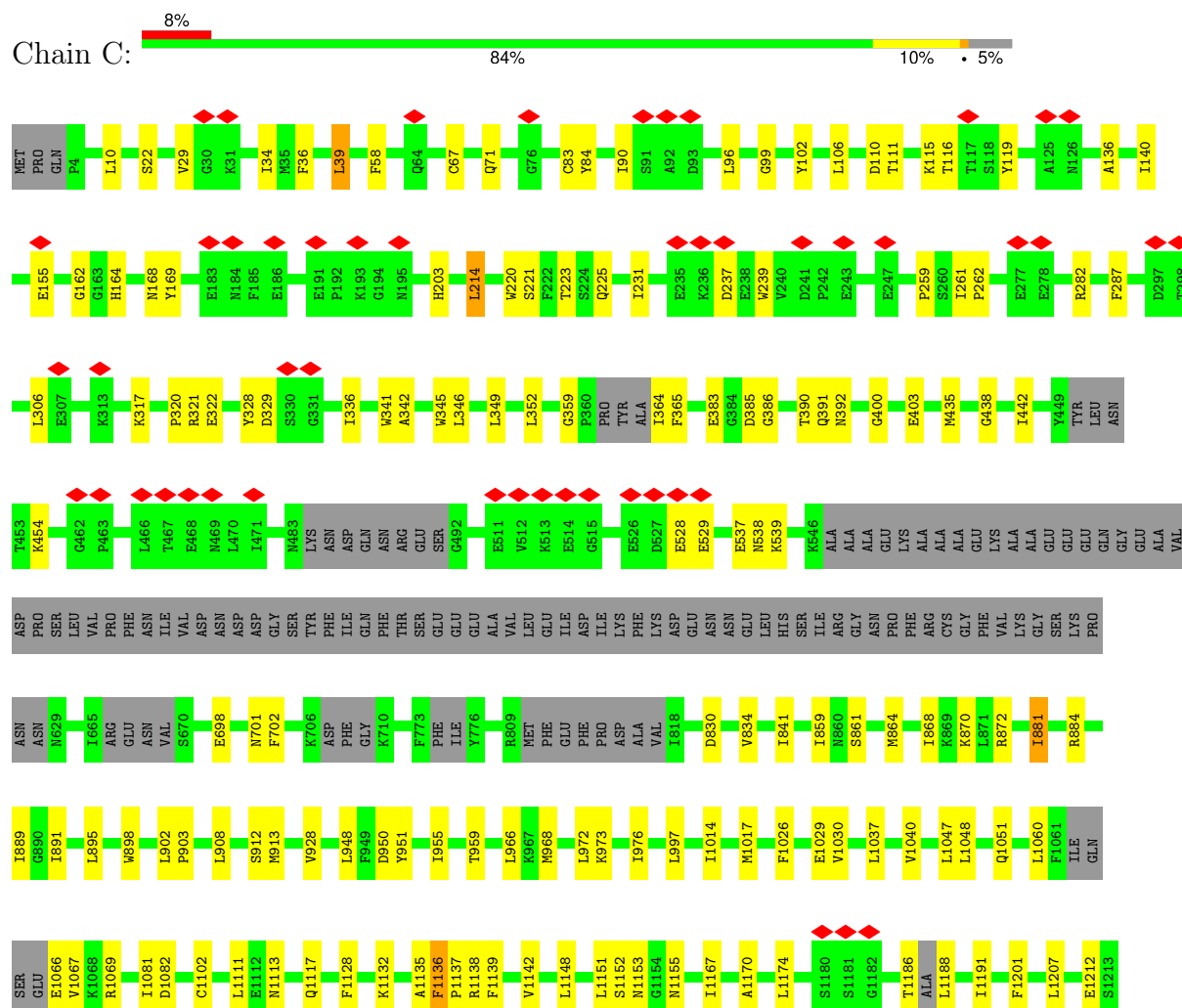
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





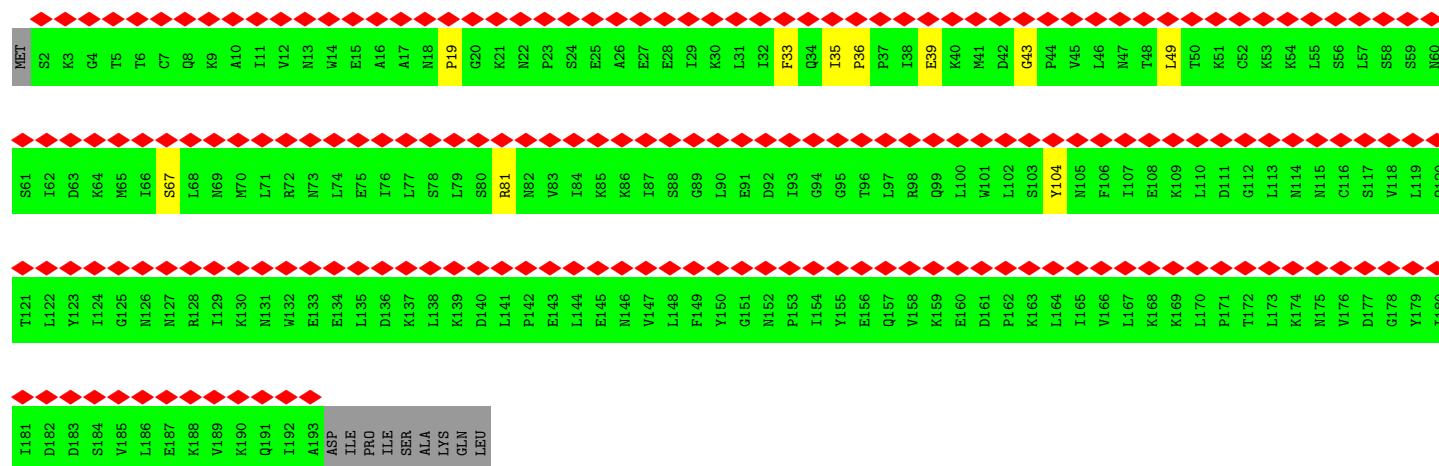
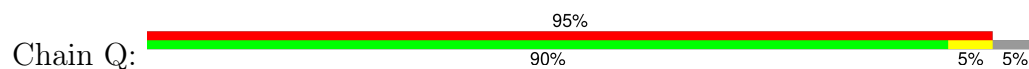
- Molecule 2: Dynein gamma heavy chain



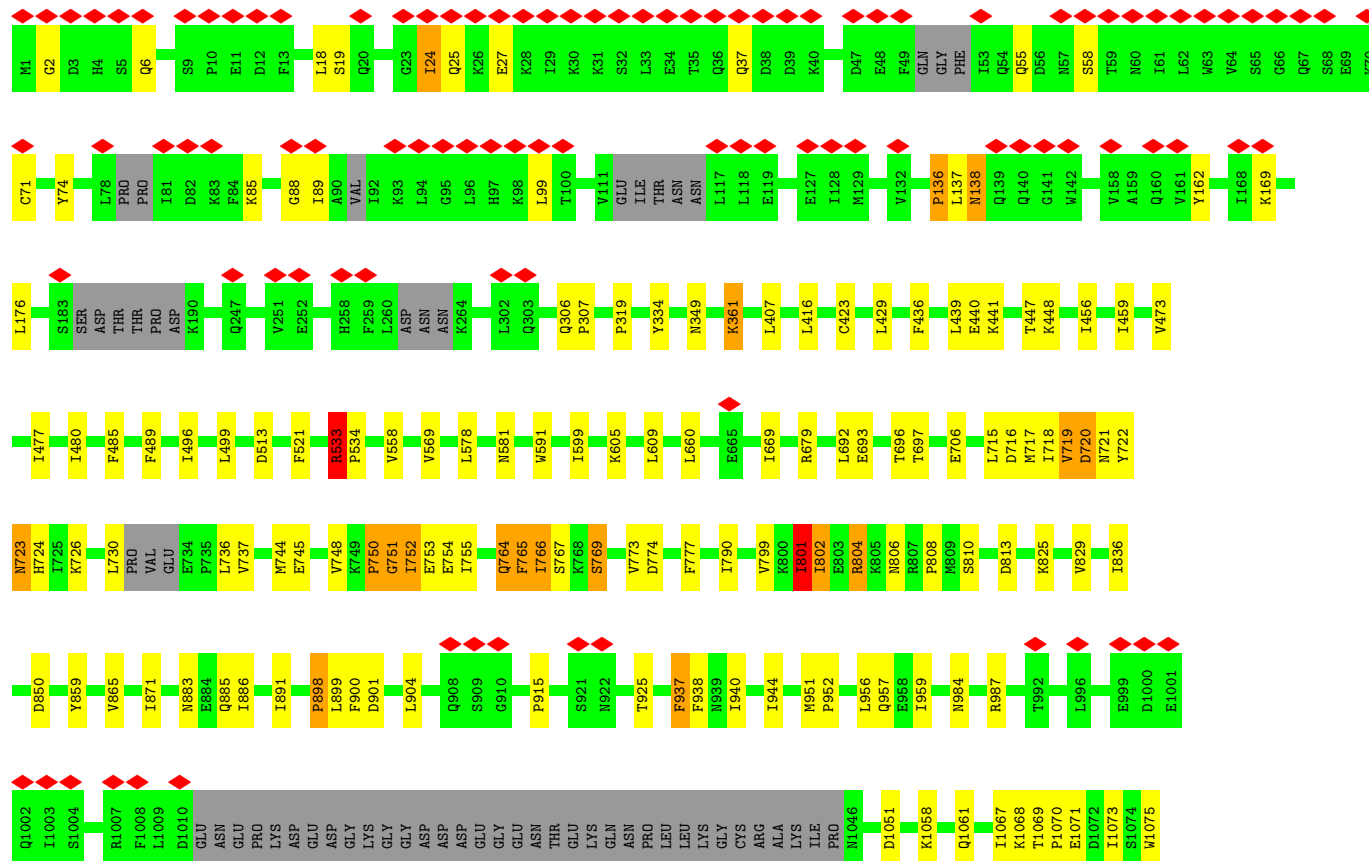
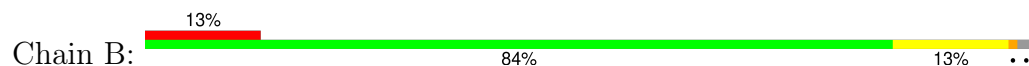




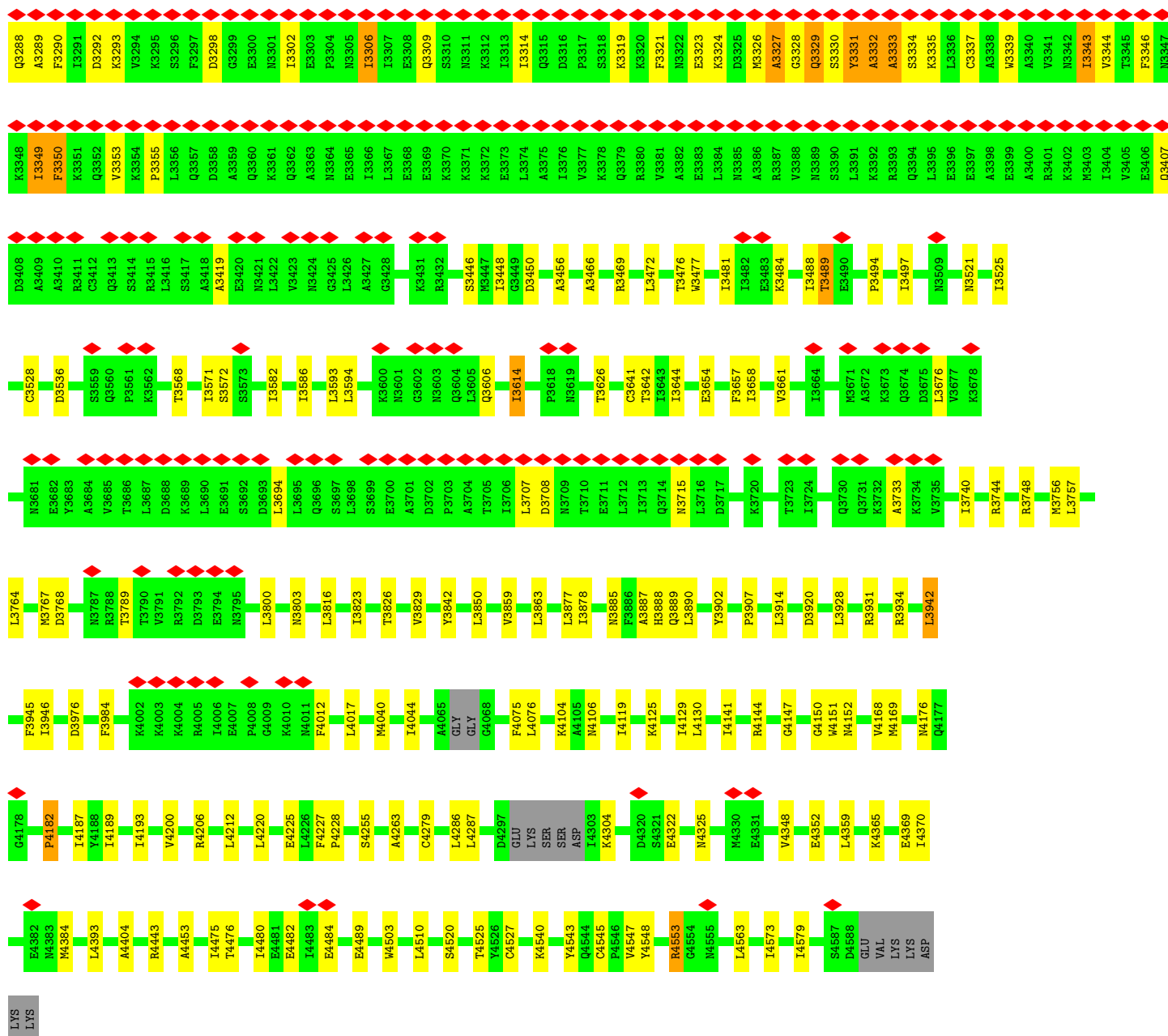
• Molecule 3: Dynein light chain 1



• Molecule 4: Dynein beta heavy chain



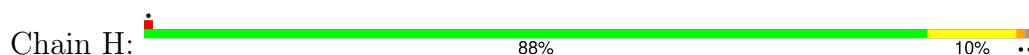
E3228	L1076	A1193	D1483	E1647	A1903	I2146	L2308	K2614	D2763	Q2897	N2999	R3168	E3228
A3229	R1077	F1205	L1484	P1648	G1904	T2150	V2316	S2619	Q2764	C2900	N3000	E3169	A3229
A3230	N1079	K1208	M1487	P1649	D1929	L2157	F2323	P2620	G2765	T2904	L3001	E3170	A3230
V3231	M1083	A1209	S1488	A1650	K1933	L2174	W2353	L2621	K2766	G2908	L3004	T3171	V3231
D3232	K1084	I1212	S1489	N1651	M1936	C2180	D2363	R2625	R2769	I2911	I3012	D3172	D3232
C3233	V1091	P1213	Q1490	P1652	A1937	F2181	D2364	Q2638	W2770	G2908	V3019	L3173	C3233
L3234	R1096	Q1220	K1492	E1654	L1943	P2186	V2365	D2647	A2772	I2923	L3020	L3174	L3234
K3235	D1100	K1223	L1508	T1655	S1944	C2192	L2417	L2648	K2776	R2926	C3021	I3175	K3235
P3237	F1101	D1227	W1518	M1662	G1947	T2196	P2418	L2649	T2797	E2931	R3032	K3177	P3237
H3238	L1102	M1230	I1527	D1666	G1950	S2200	K2419	L2654	E2798	E2931	W3047	V3178	H3238
V3239	Q1105	E1234	I1531	E1683	V1965	N2203	L2420	N2655	S2801	K2934	F3048	G3179	V3239
T3240	F1106	T1109	L1534	L1687	V1966	S2204	K2421	L2667	K2802	K2935	V3059	K3180	T3240
E3241	Q1110	Q1113	S1535	L1687	Q1969	G2205	Q2422	L2667	K2803	I2936	E3066	E3181	E3241
M3242	L1113	L1114	E1536	E1690	Q1969	E2206	M2423	N2670	I2804	K2937	T3071	S3182	M3242
K3243	D1537	K1243	D1537	E1690	Q1969	D2207	K2424	N2670	G2805	K2938	E3072	A3183	K3243
N3244	L1138	LEU	I1538	I1700	G1990	Y2210	E2425	L2692	E2806	I2942	T3072	L3184	N3244
L3245	L1117	PRO	M1559	A1708	V1998	S2220	E2426	W2693	P2807	L2947	E3073	A3185	L3245
G3246	E1118	ASP	L1595	W1711	F2001	D2221	D2427	A2694	P2808	M2947	E3073	E3186	G3246
S3247	K1119	THR	M1596	D1712	N2005	K2229	E2428	H2695	E2809	T2947	L3080	E3187	S3247
P3248	I1124	GIU	D1597	S1713	N2005	T2230	D2428	L2696	T2810	T2949	N3081	E3188	P3248
R3249	R1127	S1251	Y1598	G1714	A2026	E2232	D2429	S2697	E2811	L2959	V3085	Q3189	R3249
A3250	P1128	T1263	L1599	D1715	L2040	K2231	W2491	T2699	E2812	N2963	L3122	T3190	A3250
G3251	H1131	Y1267	K1602	Q1728	L2040	E2232	E2488	D2700	P2813	G2969	E3137	I3191	G3251
V3252	K1138	K1606	K1604	I1729	F2055	K2248	E2488	D2701	L2814	W2970	M3138	A3192	V3252
L3253	S1142	R1607	S1605	T1734	K2069	E2249	W2491	K2702	A2826	I2971	L3137	A3194	L3253
G3256	V1146	E1284	F1609	G1751	L2083	K2253	D2498	K2705	G2829	L2974	N3141	E3195	G3256
I3267	D1149	E1285	Q1615	G1752	L2083	A2254	Y2499	M2706	L2830	F2975	I3142	E3196	I3267
T3268	V1153	K1286	S1616	Q1761	D2099	T2255	L2500	A2707	L2831	P2976	E3145	E3197	T3268
L3269	T1162	M1294	L1617	Q1761	P2100	K2258	R2531	V2711	L2832	E2978	N3146	K3198	L3269
N3270	R1163	L1308	L1618	R1798	W2103	K2259	R2531	T2714	Q2833	E2978	K3149	T3199	N3270
D3271	E1166	M1167	T1619	S1819	W2103	A2264	L2637	T2715	Y2834	F2978	V3150	L3262	D3271
P3272	M1183	T1333	I1620	I1856	V2115	T2264	V2560	Y2718	T2835	E2978	Q3151	A3202	P3272
E3274	Q1189	P1186	S1622	V1857	T2116	D2264	T2571	K2740	Q2836	S2982	G3152	A3203	E3274
K3275	D1190	A1336	Q1625	D1858	D2117	L2267	T2571	F2741	L2839	V2984	L3153	A3204	K3275
V3276	N1192	H1480	N1626	S1864	F2122	E2287	N2588	R2742	P2840	S2985	Q3154	A3205	V3276
W3277			A1627	I1868	T2126	E2270	G2589	C2752	L2846	S2985	E3155	A3206	W3277
K3278			P1628	G1869	I2126	W2271	G2589	G2757	L2846	S2987	E3156	A3207	K3278
K3279			K1629	N1870	K2132	E2272	T2586	T2759	K2857	R2988	E3156	A3208	K3279
A3280			V1630	T1886	Q2139	E2273	T2586	G2761	A2858	R2988	V3159	K3209	A3280
V3281			L1641	N1892		E2273	T2586	G2762	V2863	R2989	K3160	S3210	V3281
T3282				G1897		E2273	T2586	G2762	V2863	R2989	M3161	K3211	T3282
F3283						E2273	T2586	G2762	V2863	R2989	K3161	K3211	F3283
M3284						E2273	T2586	G2762	V2863	R2989	K3161	K3211	M3284
N3285						E2273	T2586	G2762	V2863	R2989	K3161	K3211	N3285
N3286						E2273	T2586	G2762	V2863	R2989	K3161	K3211	N3286
P3287						E2273	T2586	G2762	V2863	R2989	K3161	K3211	P3287



• Molecule 5: Dynein light chain LC8_1a (LC10)



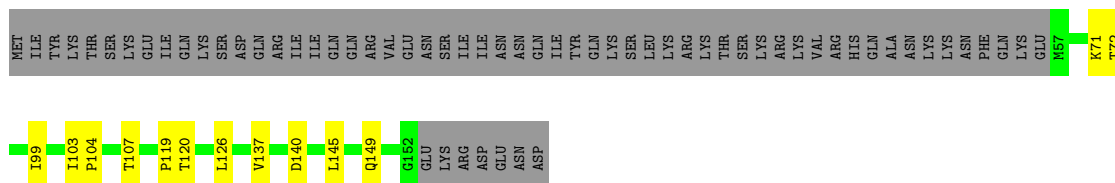
• Molecule 6: Dynein light chain LC8_1b (DLC82)





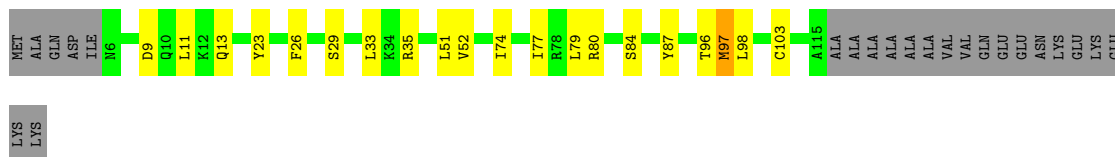
• Molecule 7: Dynein light chain roadblock LC7B

Chain G: 52% 8% 40%



• Molecule 8: Dynein light chain roadblock LC7A

Chain F: 68% 14% 17%



• Molecule 9: Dynein light chain Tctex_b

Chain N: 8% 85% 13%



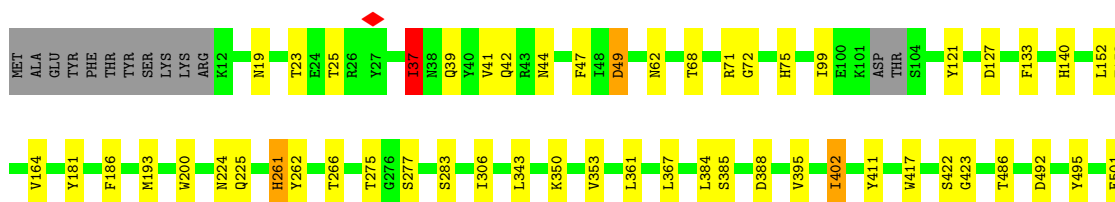
• Molecule 10: Dynein light chain Tctex_a (LC2A)

Chain O: 75% 14% 9%

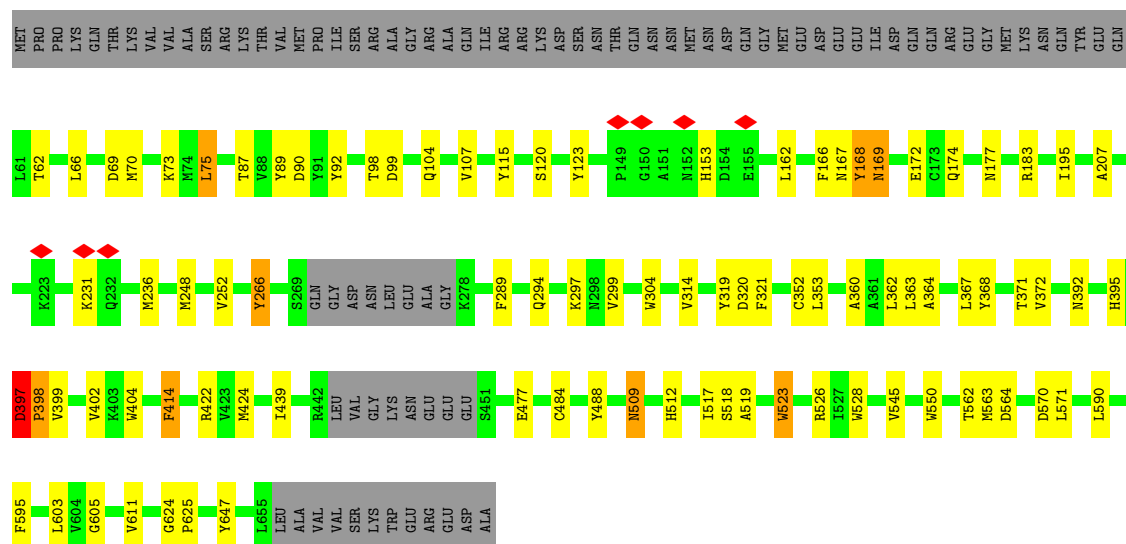


• Molecule 11: Dynein intermediate chain DIC3

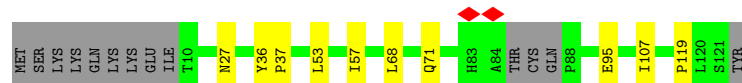
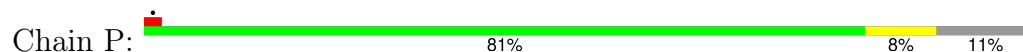
Chain E: 73% 9% 17%



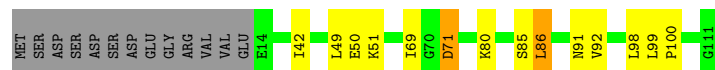
- Molecule 12: Dynein intermediate chain DIC2



- Molecule 13: Thioredoxin LC3BL



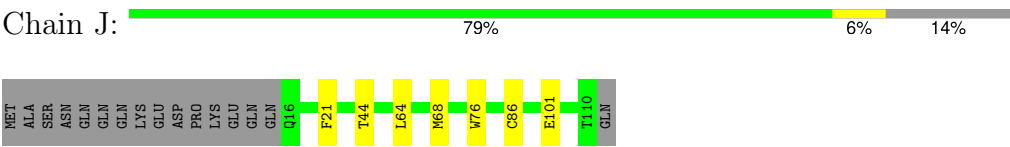
- Molecule 14: Dynein light chain LC8 3b



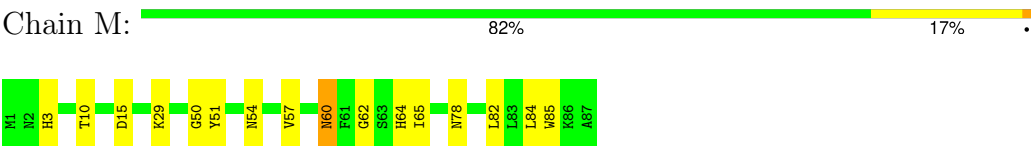
- Molecule 15: Dynein light chain LC8 2a (LC8E)



● Molecule 16: Dynein light chain LC8_2b



● Molecule 17: Dynein light chain LC8_3a



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 (\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 (\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: MG, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/34464	0.78	1/46623 (0.0%)
2	C	0.69	1/31037 (0.0%)	0.80	5/42000 (0.0%)
3	Q	0.86	0/1005	0.84	0/1388
4	B	0.70	2/35205 (0.0%)	0.81	7/47647 (0.0%)
5	I	0.68	0/838	0.77	0/1131
6	H	0.67	0/767	0.77	0/1031
7	G	0.69	0/755	0.77	0/1018
8	F	0.68	0/875	0.77	0/1178
9	N	0.69	0/867	0.78	0/1179
10	O	0.67	0/1004	0.80	0/1349
11	E	0.67	0/4522	0.78	0/6114
12	D	0.66	0/4772	0.78	1/6458 (0.0%)
13	P	0.87	0/538	0.86	0/746
14	L	0.66	0/800	0.76	0/1076
15	K	0.66	0/776	0.73	0/1038
16	J	0.63	0/831	0.74	0/1118
17	M	0.65	0/752	0.76	0/1006
All	All	0.69	3/119808 (0.0%)	0.79	14/162100 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1606	PHE	C-N	20.47	1.73	1.34
2	C	1136	PHE	C-N	16.22	1.65	1.34
4	B	730	LEU	C-O	5.28	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1136	PHE	O-C-N	26.30	171.08	121.10
2	C	1136	PHE	C-N-CD	23.12	176.95	128.40
4	B	1606	PHE	O-C-N	-20.88	81.42	121.10
4	B	1606	PHE	C-N-CD	-20.37	75.80	120.60
2	C	1136	PHE	CA-C-N	-18.02	66.65	117.10
2	C	1136	PHE	C-N-CA	-13.06	67.16	122.00
4	B	1606	PHE	CA-C-N	10.97	147.81	117.10
4	B	1606	PHE	C-N-CA	10.59	166.47	122.00
4	B	3248	PRO	N-CA-CB	-6.34	95.62	102.60
4	B	533	ARG	CB-CA-C	6.17	122.75	110.40
4	B	1127	ASN	CB-CA-C	5.70	121.79	110.40
12	D	397	ASP	CB-CA-C	5.15	120.71	110.40
2	C	2824	TYR	CB-CA-C	-5.14	100.11	110.40
1	A	1016	PHE	CB-CA-C	5.10	120.61	110.40

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
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	319	0
2	C	30436	0	29388	319	0
3	Q	1002	0	498	6	0
4	B	34604	0	33084	703	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	13	0
10	O	986	0	1002	11	0
11	E	4423	0	4291	40	0
12	D	4664	0	4484	65	0
13	P	541	0	220	2	0
14	L	783	0	811	9	0
15	K	754	0	716	3	0
16	J	806	0	769	2	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	1466	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 6.

All (1466) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1223:VAL:HG11	1:A:1282:GLU:C	1.17	1.47
4:B:1599:LEU:CG	4:B:1617:LEU:HG	1.41	1.45
4:B:1606:PHE:CE1	4:B:1687:LEU:HA	1.50	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
4:B:1602:LYS:HD2	4:B:1683:GLU:CD	1.40	1.40
4:B:1606:PHE:C	4:B:1607:PRO:N	1.73	1.38
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: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:1490:GLN:CD	4:B:3614:ILE:HG21	1.48	1.33
4:B:1606:PHE:C	4:B:1607:PRO:CD	1.97	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.26
2:C:1136:PHE:CD2	2:C:1139:PHE:N	2.05	1.24
4:B:1603:LYS:HE2	4:B:1609:PHE:C	1.56	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
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
1:A:1223:VAL:CG1	1:A:1282:GLU:C	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD	4:B:1683:GLU:CD	2.22	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
4:B:1531:ILE:HG23	4:B:1622:SER:OG	1.49	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: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
4:B:1606:PHE:CD1	4:B:1687:LEU:CB	2.42	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
1:A:1230:TYR:CB	1:A:1289:GLU:C	2.29	1.01
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:808:PRO:CG	4:B:1077:ARG:CD	2.36	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: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:1535:SER:HB2	4:B:1622:SER:C	1.81	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:1606:PHE:C	4:B:1607:PRO:HD3	1.80	0.98
1:A:1219:PHE:CE2	1:A:1263:TYR:CD2	2.50	0.98
2:C:1136:PHE:CD2	2:C:1138:ARG:C	2.37	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:1531:ILE:CG2	4:B:1622:SER:HG	1.78	0.97
4:B:1599:LEU:HA	4:B:1621:LEU:CD2	1.94	0.96
4:B:1599:LEU:CD2	4:B:1617:LEU:C	2.34	0.96
4:B:1238:LYS:HE2	4:B:1308:LEU:HA	1.47	0.96
4:B:765:PHE:O	4:B:766:ILE:C	2.00	0.95
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
2:C:1136:PHE:CD2	2:C:1138:ARG:N	2.36	0.94
4:B:1490:GLN:CD	4:B:3614:ILE:CG2	2.32	0.93
4:B:891:ILE:HD13	4:B:1075:TRP:HA	1.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1599:LEU:HB2	4:B:1617:LEU:CD2	1.99	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:750:PRO:O	4:B:751:GLY:C	2.09	0.88
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
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
4:B:1490:GLN:CD	4:B:3568:THR:O	2.14	0.86
1:A:1219:PHE:CZ	1:A:1263:TYR:CG	2.58	0.85
4:B:716:ASP:O	4:B:717:MET:C	2.11	0.85
4:B:1598:TYR:CD2	4:B:1621:LEU:HD23	2.11	0.85
4:B:1599:LEU:HD22	4:B:1617:LEU:C	1.95	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:1531:ILE:HG23	4:B:1622:SER:HG	1.35	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:B:901:ASP:HA	4:B:1077:ARG:O	1.80	0.80
4:B:900:PHE:HB2	4:B:1076:LEU:HD12	1.64	0.80
4:B:349:ASN:HA	4:B:416:LEU:HD21	1.64	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
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:1599:LEU:C	4:B:1617:LEU:HD21	2.02	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1066:GLU:N	2:C:1152:SER:HG	1.82	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:1599:LEU:CA	4:B:1621:LEU:CD2	2.63	0.76
2:C:1066:GLU:N	2:C:1153:ASN:CG	2.38	0.75
4:B:1537:ASP:HB3	4:B:1624:GLY:CA	2.14	0.75
1:A:1223:VAL:HG13	1:A:1283:LEU:C	1.95	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:715:LEU:O	4:B:716:ASP:C	2.22	0.75
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
4:B:3253:ILE:O	4:B:3253:ILE:HG22	1.88	0.74
1:A:1016:PHE:CZ	1:A:1069:TYR:HB2	2.22	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:1234:GLU:CD	4:B:1304:ASP:CB	2.43	0.73
1:A:933:VAL:HG11	1:A:944:LEU:HD12	1.68	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1602:LYS:CE	4:B:1683:GLU:CD	2.56	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
2:C:1067:VAL:N	2:C:1152:SER:CB	2.50	0.70
4:B:719:VAL:O	4:B:720:ASP:C	2.29	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
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: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:1599:LEU:HD21	4:B:1617:LEU:C	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1599:LEU:CD1	4:B:1617:LEU:C	2.62	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:1067:VAL:N	2:C:1152:SER:C	2.42	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
1:A:1276:GLN:CD	12:D:153:HIS:CE1	2.67	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
2:C:359:GLY:O	2:C:386:GLY: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1069:ARG:HG2	2:C:1155:ASN:CG	2.17	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: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: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
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
4:B:764:GLN:O	4:B:765:PHE:O	2.17	0.63
1:A:3128:THR:HG22	1:A:3422:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1880:VAL:HA	2:C:1883:ILE:HD12	1.79	0.63
4:B:898:PRO:HB3	4:B:1076:LEU:C	2.18	0.63
1:A:3212:VAL:HG13	1:A:3335:TRP:CD1	2.34	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
2:C:1135:ALA:HB1	2:C:1212:GLU:CD	2.20	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
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
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:764:GLN:C	4:B:766:ILE:N	2.51	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:1230:MET:HE1	4:B:1267:TYR:HA	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3326:MET:O	4:B:3327:ALA:C	2.40	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
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
4:B:898:PRO:CB	4:B:1076:LEU:C	2.71	0.59
1:A:1632:ASP:HB2	1:A:1892:PHE:CD1	2.37	0.59
2:C:1132:LYS:HE3	2:C:1151:LEU:HD21	1.60	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
4:B:1603:LYS:CE	4:B:1609:PHE:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:3223:LEU:HD11	1:A:3332:ILE:CD1	2.34	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
1:A:4599:CYS:O	1:A:4599:CYS:SG	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1535:SER:HB3	4:B:1623:ASN:CG	2.25	0.56
4:B:3984:PHE:CE2	4:B:4076:LEU:HD11	2.40	0.56
1:A:1544:ILE:HG12	1:A:1580:LYS:HG2	1.88	0.56
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
2:C:1541:LEU:HD13	2:C:1584:LEU:HD22	1.88	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
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
2:C:913:MET:CE	2:C:959:THR:HG22	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1535:SER:CB	4:B:1622:SER:C	2.65	0.55
4:B:2040:LEU:CD1	4:B:2083:LEU:HD22	2.35	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
2:C:2128:MET:HE1	2:C:2137:VAL:HG21	1.88	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
4:B:1490:GLN:OE1	4:B:3568:THR:O	2.24	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
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
14:L:42:ILE:HD12	14:L:98:LEU:HD12	1.89	0.54
4:B:898:PRO:CB	4:B:1077:ARG:CB	2.84	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:744:MET:HE1	4:B:773:VAL:HG23	1.90	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
2:C:214:LEU:C	2:C:214:LEU:HD22	2.29	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
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
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
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
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:1136:PHE:CE2	2:C:1138:ARG:C	2.53	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
4:B:3257:ARG:O	4:B:3258:VAL:C	2.45	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:2711:VAL:HA	4:B:2714:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:2128:MET:HE1	2:C:2137:VAL:CG2	2.39	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
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
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:765:PHE:O	4:B:767:SER:N	2.43	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
4:B:3331:TYR:O	4:B:3332:ALA:C	2.47	0.52
4:B:3332:ALA:O	4:B:3333:ALA:C	2.48	0.52
1:A:2676:TRP:CD2	1:A:2699:LEU:HD21	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1017:MET:HE2	2:C:1030:VAL:HB	1.91	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
4:B:825:LYS:O	4:B:829:VAL:HG23	2.10	0.52
4:B:898:PRO:CG	4:B:1073:ILE:CG1	2.77	0.52
4:B:1599:LEU:HD13	4:B:1617:LEU:C	2.30	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:1276:GLN:CD	12:D:153:HIS:ND1	2.63	0.51
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1868:GLY:O	1:A:1973:PHE:HA	2.11	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
2:C:2007:LEU:HD11	2:C:2128:MET:HE2	1.93	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: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:1482:ASN:HA	1:A:1487:VAL:HG11	1.92	0.50
4:B:1490:GLN:OE1	4:B:3614:ILE:CB	2.57	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
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
1:A:1183:LEU:C	1:A:1183:LEU:HD23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:972:LEU:HD13	2:C:1029:GLU:HG2	1.94	0.49
4:B:1238:LYS:HG2	4:B:1311:MET:CB	2.42	0.49
4:B:1527:ILE:HG23	4:B:1615:GLN:CD	2.32	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
4:B:1602:LYS:C	4:B:1609:PHE:CD2	2.86	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
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
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
9:N:90:ASP:O	9:N:93:THR:OG1	2.25	0.49
11:E:41:VAL:HG22	11:E:42:GLN:HG3	1.95	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
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
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: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
9:N:76:THR:CG2	11:E:39:GLN:HE22	2.23	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:913:MET:HE1	2:C:959:THR:HG22	1.96	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
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
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
4:B:720:ASP:O	4:B:721:ASN:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:2758:MET:O	2:C:2759:LYS:C	2.52	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
1:A:1687:LEU:C	1:A:1687:LEU:HD23	2.35	0.47
2:C:2826:VAL:O	2:C:2828:GLN:N	2.47	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
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: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:1483:ASP:O	4:B:1487:MET:N	2.47	0.47
4:B:1490:GLN:CG	4:B:3614:ILE:HG21	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
4:B:447:THR:OG1	4:B:448:LYS:N	2.47	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:4562:ASN:CG	1:A:4562:ASN:O	2.54	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: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
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:4113:VAL:HG12	2:C:4114:PRO:HD2	1.96	0.46
2:C:3151:LYS:CE	2:C:3217:ILE:HD11	2.45	0.46
4:B:1595:LEU:C	4:B:1618:LEU:HD21	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1603:LYS:HG2	4:B:1609:PHE:C	2.36	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
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: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: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
1:A:870:PRO:C	1:A:871:LEU:HD13	2.37	0.46
1:A:1009:THR:HB	1:A:1074:MET:SD	2.56	0.46
2:C:2708:GLN:CD	2:C:2813:ILE:HD11	2.37	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:4534:CYS:SG	1:A:4535:LYS:N	2.90	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
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
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: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
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:O	12:D:162:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:972:LEU:HD21	2:C:1017:MET:HE1	1.96	0.45
2:C:2770:ASN:O	2:C:2771:PHE:C	2.55	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
2:C:972:LEU:HD11	2:C:1017:MET:HE3	1.98	0.45
2:C:2332:LEU:HD13	18:C:4206:ADP:O2'	2.17	0.45
2:C:2705:ASP:O	2:C:2706:PHE:C	2.55	0.45
4:B:1700:ILE:CG2	4:B:1729:ILE:HD13	2.47	0.45
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
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
4:B:1230:MET:HE2	4:B:1267:TYR:HA	1.98	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: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
4:B:808:PRO:CD	4:B:1077:ARG:HH11	2.26	0.44
4:B:1230:MET:HE1	4:B:1267:TYR:CA	2.47	0.44
4:B:1602:LYS:HD2	4:B:1683:GLU:HG3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
12:D:162:LEU:HD23	12:D:162:LEU:C	2.38	0.44
17:M:84:LEU:HD12	17:M:84:LEU:C	2.38	0.44
1:A:3257:VAL:HG21	1:A:3266:VAL:HG13	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
1:A:3877:ILE:HG13	1:A:3946:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:L:69:ILE:HG22	14:L:69:ILE:O	2.18	0.44
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
4:B:2299:MET:HE3	4:B:2300:ARG:O	2.17	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:2357:LEU:C	2:C:2357:LEU:HD13	2.38	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: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
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
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
1:A:1162:LEU:C	1:A:1162:LEU:HD23	2.39	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
12:D:174:GLN:HE22	14:L:49:LEU:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:364:ILE:C	2:C:383:GLU:CB	2.87	0.43
2:C:2728:TYR:CG	2:C:2728:TYR:O	2.71	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:751:GLY:O	4:B:752:ILE:C	2.56	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
2:C:2212:LEU:C	2:C:2212:LEU:HD13	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:I:35:LEU:HD22	5:I:95:LEU:HD13	2.01	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: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
1:A:3568:LEU:C	1:A:3568:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2040:LEU:HD12	4:B:2040:LEU:HA	1.90	0.42
11:E:121:TYR:HB3	12:D:266:TYR:OH	2.19	0.42
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: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:2531:ARG:C	4:B:2649:LEU:HD21	2.40	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
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
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
4:B:1536:GLU:C	4:B:1625:GLN:NE2	2.73	0.42
4:B:3767:MET:HG3	4:B:3768:ASP:N	2.35	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: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
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:2066:GLN:CA	2:C:2066:GLN:NE2	2.83	0.41
2:C:2826:VAL:C	2:C:2828:GLN:N	2.73	0.41
4:B:1068:LYS:CB	4:B:1084:LYS:HE2	2.50	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:3758:TYR:CE2	1:A:3762:ILE:HD11	2.55	0.41
4:B:1933:LYS:HG3	4:B:1965:VAL:HG11	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:447:THR:HG21	4:B:513:ASP:C	2.41	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
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
4:B:2771:TRP:O	4:B:2772:ALA:C	2.59	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:3132:ASN:CA	1:A:3419:ILE:HD11	2.51	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:1109:THR:C	4:B:1113:LEU:HG	2.41	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:895:LEU:C	2:C:895:LEU:HD23	2.41	0.41
2:C:2717:ALA:CB	2:C:2803:MET:SD	3.06	0.41
2:C:3622:ILE:HD11	2:C:3624:LEU:HD21	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:898:PRO:HG2	4:B:1077:ARG:CG	2.51	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:3271:ASP:CG	4:B:3272:PRO:HD2	2.41	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1048:LEU:HD13	2:C:1048:LEU:C	2.42	0.40
2:C:1559:LEU:CD2	2:C:1607:LEU:HD21	2.50	0.40
2:C:2555:LEU:HD12	2:C:2555:LEU:C	2.42	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: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: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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	13 49
2	C	3914/4168 (94%)	3582 (92%)	283 (7%)	49 (1%)	10 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	190/202 (94%)	163 (86%)	24 (13%)	3 (2%)	8	38
4	B	4488/4595 (98%)	4017 (90%)	383 (8%)	88 (2%)	6	32
5	I	104/110 (94%)	95 (91%)	8 (8%)	1 (1%)	13	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	52
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%)	19	57
12	D	569/667 (85%)	510 (90%)	51 (9%)	8 (1%)	9	41
13	P	103/122 (84%)	86 (84%)	11 (11%)	6 (6%)	1	14
14	L	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	13	49
15	K	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
16	J	93/111 (84%)	84 (90%)	8 (9%)	1 (1%)	12	47
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	5	27
All	All	15181/16189 (94%)	13817 (91%)	1150 (8%)	214 (1%)	12	41

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	3338 (98%)	82 (2%)	44 62
2	C	3149/3691 (85%)	3095 (98%)	54 (2%)	56 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	10/186 (5%)	10 (100%)	0	100	100
4	B	3497/4145 (84%)	3399 (97%)	98 (3%)	38	57
5	I	91/95 (96%)	87 (96%)	4 (4%)	24	45
6	H	82/83 (99%)	80 (98%)	2 (2%)	44	62
7	G	86/149 (58%)	85 (99%)	1 (1%)	67	78
8	F	93/109 (85%)	86 (92%)	7 (8%)	11	31
9	N	85/104 (82%)	84 (99%)	1 (1%)	67	78
10	O	106/119 (89%)	99 (93%)	7 (7%)	14	34
11	E	484/597 (81%)	467 (96%)	17 (4%)	31	51
12	D	507/609 (83%)	482 (95%)	25 (5%)	21	42
14	L	87/99 (88%)	83 (95%)	4 (5%)	23	44
15	K	80/82 (98%)	79 (99%)	1 (1%)	65	77
16	J	81/97 (84%)	79 (98%)	2 (2%)	42	61
17	M	78/78 (100%)	74 (95%)	4 (5%)	20	41
All	All	11936/14440 (83%)	11627 (97%)	309 (3%)	42	59

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	ASP
1	A	582	THR
1	A	616	LYS
1	A	674	LEU
1	A	751	LEU
1	A	758	ASP
1	A	763	LEU
1	A	810	LEU
1	A	818	LEU
1	A	861	ASP
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	1136	MET

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Mol	Chain	Res	Type
1	A	1153	PHE
1	A	1171	ILE
1	A	1201	TYR
1	A	1205	GLN
1	A	1559	LYS
1	A	1567	ASN
1	A	1573	PHE
1	A	1581	LEU
1	A	1609	THR
1	A	1631	PHE
1	A	1634	ILE
1	A	1644	ASP
1	A	1711	LEU
1	A	1778	ARG
1	A	1922	CYS
1	A	2034	CYS
1	A	2075	MET
1	A	2098	LEU
1	A	2228	THR
1	A	2267	ASN
1	A	2320	SER
1	A	2418	ILE
1	A	2426	GLU
1	A	2434	SER
1	A	2443	CYS
1	A	2470	GLU
1	A	2471	MET
1	A	2487	ASN
1	A	2729	LEU
1	A	2844	ASP
1	A	2901	ASP
1	A	3046	PHE
1	A	3122	ASN
1	A	3125	GLN
1	A	3203	PRO
1	A	3283	ASP
1	A	3308	PRO
1	A	3315	ASP
1	A	3345	LYS
1	A	3449	LEU
1	A	3578	LEU
1	A	3588	ASP

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Mol	Chain	Res	Type
1	A	3647	PHE
1	A	3881	SER
1	A	3951	THR
1	A	3952	LEU
1	A	3973	TYR
1	A	4046	CYS
1	A	4130	ILE
1	A	4143	ARG
1	A	4155	TYR
1	A	4216	PHE
1	A	4287	THR
1	A	4288	PHE
1	A	4448	GLN
1	A	4465	THR
1	A	4497	SER
1	A	4504	SER
1	A	4506	THR
1	A	4542	ASP
1	A	4562	ASN
1	A	4578	CYS
1	A	4588	ASP
1	A	4593	PHE
2	C	36	PHE
2	C	39	LEU
2	C	110	ASP
2	C	111	THR
2	C	214	LEU
2	C	220	TRP
2	C	239	TRP
2	C	329	ASP
2	C	346	LEU
2	C	352	LEU
2	C	950	ASP
2	C	1113	ASN
2	C	1249	ASP
2	C	1453	CYS
2	C	1499	CYS
2	C	1650	ASP
2	C	1660	ASP
2	C	1702	ASP
2	C	1722	ASP
2	C	1868	CYS

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Mol	Chain	Res	Type
2	C	1884	CYS
2	C	1953	GLN
2	C	2043	ASN
2	C	2066	GLN
2	C	2121	ASN
2	C	2122	THR
2	C	2224	LEU
2	C	2225	SER
2	C	2292	CYS
2	C	2432	ASN
2	C	2483	ASN
2	C	2488	ILE
2	C	2696	SER
2	C	2711	SER
2	C	2712	PHE
2	C	2728	TYR
2	C	2748	ASP
2	C	2757	LEU
2	C	2771	PHE
2	C	2776	ASP
2	C	3059	ASN
2	C	3460	ASN
2	C	3602	GLN
2	C	3704	ASN
2	C	3793	THR
2	C	3824	PHE
2	C	3877	GLU
2	C	3883	SER
2	C	3908	ASP
2	C	3918	VAL
2	C	4050	GLN
2	C	4092	TYR
2	C	4113	VAL
2	C	4146	MET
4	B	423	CYS
4	B	440	GLU
4	B	480	ILE
4	B	485	PHE
4	B	489	PHE
4	B	581	ASN
4	B	609	LEU
4	B	693	GLU

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Mol	Chain	Res	Type
4	B	706	GLU
4	B	766	ILE
4	B	769	SER
4	B	801	ILE
4	B	802	ILE
4	B	804	ARG
4	B	810	SER
4	B	813	ASP
4	B	850	ASP
4	B	937	PHE
4	B	1067	ILE
4	B	1183	THR
4	B	1186	PRO
4	B	1208	LYS
4	B	1213	PRO
4	B	1518	TRP
4	B	1537	ASP
4	B	1559	MET
4	B	1607	PRO
4	B	1734	THR
4	B	1929	ASP
4	B	2103	MET
4	B	2139	GLN
4	B	2206	GLU
4	B	2258	HIS
4	B	2419	LYS
4	B	2425	GLU
4	B	2454	ASP
4	B	2607	PHE
4	B	2610	PRO
4	B	2647	ASP
4	B	2653	CYS
4	B	2752	CYS
4	B	2846	LEU
4	B	2873	SER
4	B	2874	ARG
4	B	2931	GLU
4	B	2949	THR
4	B	2959	LEU
4	B	2963	ASN
4	B	2971	ILE
4	B	2982	SER

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Mol	Chain	Res	Type
4	B	3004	LEU
4	B	3032	ARG
4	B	3080	LEU
4	B	3222	PRO
4	B	3231	VAL
4	B	3269	LEU
4	B	3288	GLN
4	B	3298	ASP
4	B	3330	SER
4	B	3343	ILE
4	B	3349	ILE
4	B	3350	PHE
4	B	3355	PRO
4	B	3407	GLN
4	B	3450	ASP
4	B	3469	ARG
4	B	3489	THR
4	B	3521	ASN
4	B	3614	ILE
4	B	3708	ASP
4	B	3756	MET
4	B	3757	LEU
4	B	3800	LEU
4	B	3842	TYR
4	B	3920	ASP
4	B	3942	LEU
4	B	3945	PHE
4	B	3976	ASP
4	B	4012	PHE
4	B	4104	LYS
4	B	4125	LYS
4	B	4151	TRP
4	B	4176	ASN
4	B	4182	PRO
4	B	4255	SER
4	B	4279	CYS
4	B	4304	LYS
4	B	4352	GLU
4	B	4365	LYS
4	B	4369	GLU
4	B	4443	ARG
4	B	4476	THR

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Mol	Chain	Res	Type
4	B	4482	GLU
4	B	4503	TRP
4	B	4520	SER
4	B	4540	LYS
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	68	PHE
7	G	140	ASP
8	F	9	ASP
8	F	13	GLN
8	F	35	ARG
8	F	51	LEU
8	F	84	SER
8	F	96	THR
8	F	97	MET
9	N	18	ASP
10	O	22	LEU
10	O	32	SER
10	O	77	PRO
10	O	99	SER
10	O	103	TRP
10	O	104	ASP
10	O	122	CYS
11	E	37	ILE
11	E	44	ASN
11	E	47	PHE
11	E	49	ASP
11	E	127	ASP
11	E	193	MET
11	E	225	GLN
11	E	261	HIS
11	E	262	TYR
11	E	266	THR
11	E	353	VAL
11	E	361	LEU
11	E	385	SER
11	E	402	ILE

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Mol	Chain	Res	Type
11	E	422	SER
11	E	515	LYS
11	E	560	HIS
12	D	62	THR
12	D	69	ASP
12	D	75	LEU
12	D	90	ASP
12	D	99	ASP
12	D	104	GLN
12	D	115	TYR
12	D	169	ASN
12	D	172	GLU
12	D	177	ASN
12	D	266	TYR
12	D	289	PHE
12	D	320	ASP
12	D	371	THR
12	D	392	ASN
12	D	395	HIS
12	D	399	VAL
12	D	414	PHE
12	D	477	GLU
12	D	488	TYR
12	D	509	ASN
12	D	518	SER
12	D	523	TRP
12	D	570	ASP
12	D	595	PHE
14	L	50	GLU
14	L	51	LYS
14	L	71	ASP
14	L	86	LEU
15	K	18	MET
16	J	21	PHE
16	J	86	CYS
17	M	10	THR
17	M	15	ASP
17	M	60	ASN
17	M	64	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	687	ASN
1	A	804	ASN
1	A	837	GLN
1	A	1114	GLN
1	A	1205	GLN
1	A	1566	GLN
1	A	1567	ASN
1	A	1585	GLN
1	A	1624	GLN
1	A	1666	ASN
1	A	1690	ASN
1	A	1718	GLN
1	A	1728	GLN
1	A	1940	GLN
1	A	2095	ASN
1	A	2251	ASN
1	A	2279	ASN
1	A	2340	GLN
1	A	2369	GLN
1	A	2373	GLN
1	A	2458	GLN
1	A	2479	GLN
1	A	2487	ASN
1	A	2508	ASN
1	A	2628	GLN
1	A	2889	GLN
1	A	3113	GLN
1	A	3122	ASN
1	A	3252	GLN
1	A	3311	ASN
1	A	3343	HIS
1	A	3606	GLN
1	A	3746	GLN
1	A	3888	GLN
1	A	4088	GLN
1	A	4137	HIS
1	A	4330	ASN
1	A	4479	GLN
1	A	4574	ASN
2	C	17	GLN
2	C	168	ASN
2	C	1051	GLN

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Mol	Chain	Res	Type
2	C	1113	ASN
2	C	1155	ASN
2	C	1238	GLN
2	C	1300	GLN
2	C	1428	ASN
2	C	1888	GLN
2	C	1981	ASN
2	C	2066	GLN
2	C	2142	GLN
2	C	2207	HIS
2	C	2217	ASN
2	C	2483	ASN
2	C	2778	ASN
2	C	2784	ASN
2	C	2819	ASN
2	C	2951	ASN
2	C	2953	ASN
2	C	3004	ASN
2	C	3460	ASN
2	C	3654	HIS
2	C	3674	GLN
2	C	3791	HIS
2	C	3870	GLN
2	C	3958	ASN
2	C	4050	GLN
2	C	4068	ASN
2	C	4143	ASN
4	B	672	ASN
4	B	721	ASN
4	B	724	HIS
4	B	764	GLN
4	B	775	GLN
4	B	832	ASN
4	B	883	ASN
4	B	923	GLN
4	B	957	GLN
4	B	975	ASN
4	B	1079	ASN
4	B	1081	GLN
4	B	1625	GLN
4	B	1728	GLN
4	B	1761	GLN

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Mol	Chain	Res	Type
4	B	1807	GLN
4	B	1870	ASN
4	B	1956	ASN
4	B	1969	GLN
4	B	2005	ASN
4	B	2038	ASN
4	B	2148	GLN
4	B	2203	ASN
4	B	2325	ASN
4	B	2462	ASN
4	B	2476	GLN
4	B	2591	ASN
4	B	2608	ASN
4	B	2656	GLN
4	B	2836	GLN
4	B	2897	GLN
4	B	2940	ASN
4	B	3042	ASN
4	B	3081	ASN
4	B	3093	ASN
4	B	3288	GLN
4	B	3407	GLN
4	B	3521	ASN
4	B	3715	ASN
4	B	3772	GLN
4	B	3803	ASN
4	B	3879	ASN
4	B	4097	ASN
4	B	4106	ASN
4	B	4176	ASN
4	B	4177	GLN
5	I	100	ASN
6	H	36	ASN
7	G	129	GLN
7	G	149	GLN
9	N	75	GLN
11	E	31	GLN
11	E	39	GLN
11	E	42	GLN
11	E	52	ASN
11	E	122	GLN
11	E	144	ASN

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Mol	Chain	Res	Type
11	E	224	ASN
11	E	237	ASN
11	E	379	ASN
11	E	481	GLN
12	D	64	GLN
12	D	153	HIS
12	D	167	ASN
12	D	177	ASN
12	D	294	GLN
12	D	298	ASN
12	D	324	GLN
12	D	413	ASN
12	D	431	ASN
14	L	28	GLN
14	L	64	GLN
16	J	87	GLN
17	M	3	HIS
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	$\# Z > 2$
19	ATP	A	4702	20	28,33,33	0.71	0	34,52,52	0.79	1 (2%)
18	ADP	B	4705	20	24,29,29	0.79	0	29,45,45	0.75	1 (3%)
18	ADP	B	4706	20	24,29,29	0.75	0	29,45,45	0.70	1 (3%)
18	ADP	A	4701	20	24,29,29	0.75	0	29,45,45	0.79	1 (3%)
18	ADP	C	4206	20	24,29,29	0.73	0	29,45,45	1.03	2 (6%)
18	ADP	C	4203	20	24,29,29	0.76	1 (4%)	29,45,45	1.25	2 (6%)
19	ATP	B	4701	20	28,33,33	0.71	0	34,52,52	0.84	1 (2%)
19	ATP	C	4201	20	28,33,33	0.69	0	34,52,52	0.78	1 (2%)
18	ADP	A	4703	-	24,29,29	0.75	0	29,45,45	1.05	2 (6%)

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
19	ATP	A	4702	20	-	5/18/38/38	0/3/3/3
18	ADP	B	4705	20	-	5/12/32/32	0/3/3/3
18	ADP	B	4706	20	-	2/12/32/32	0/3/3/3
18	ADP	A	4701	20	-	5/12/32/32	0/3/3/3
18	ADP	C	4206	20	-	4/12/32/32	0/3/3/3
18	ADP	C	4203	20	-	5/12/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/18/38/38	0/3/3/3
19	ATP	C	4201	20	-	4/18/38/38	0/3/3/3
18	ADP	A	4703	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4203	ADP	C8-N7	-2.02	1.31	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4203	ADP	C4'-O4'-C1'	-4.29	106.00	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4703	ADP	C4'-O4'-C1'	-3.95	106.31	109.92
18	C	4206	ADP	C4'-O4'-C1'	-3.56	106.67	109.92
18	C	4203	ADP	C1'-N9-C4	2.70	131.39	126.64
19	B	4701	ATP	C5-C6-N6	2.40	123.97	120.31
18	C	4206	ADP	C5-C6-N6	2.25	123.74	120.31
19	A	4702	ATP	C5-C6-N6	2.21	123.67	120.31
18	B	4706	ADP	C5-C6-N6	2.19	123.64	120.31
19	C	4201	ATP	C5-C6-N6	2.17	123.61	120.31
18	B	4705	ADP	C5-C6-N6	2.08	123.48	120.31
18	A	4701	ADP	C5-C6-N6	2.06	123.45	120.31
18	A	4703	ADP	C5-C6-N6	2.05	123.43	120.31

There are no chirality outliers.

All (31) 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'
18	C	4206	ADP	C3'-C4'-C5'-O5'
19	A	4702	ATP	O4'-C4'-C5'-O5'
18	B	4706	ADP	PA-O3A-PB-O2B
19	A	4702	ATP	PB-O3A-PA-O2A
19	A	4702	ATP	C3'-C4'-C5'-O5'
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

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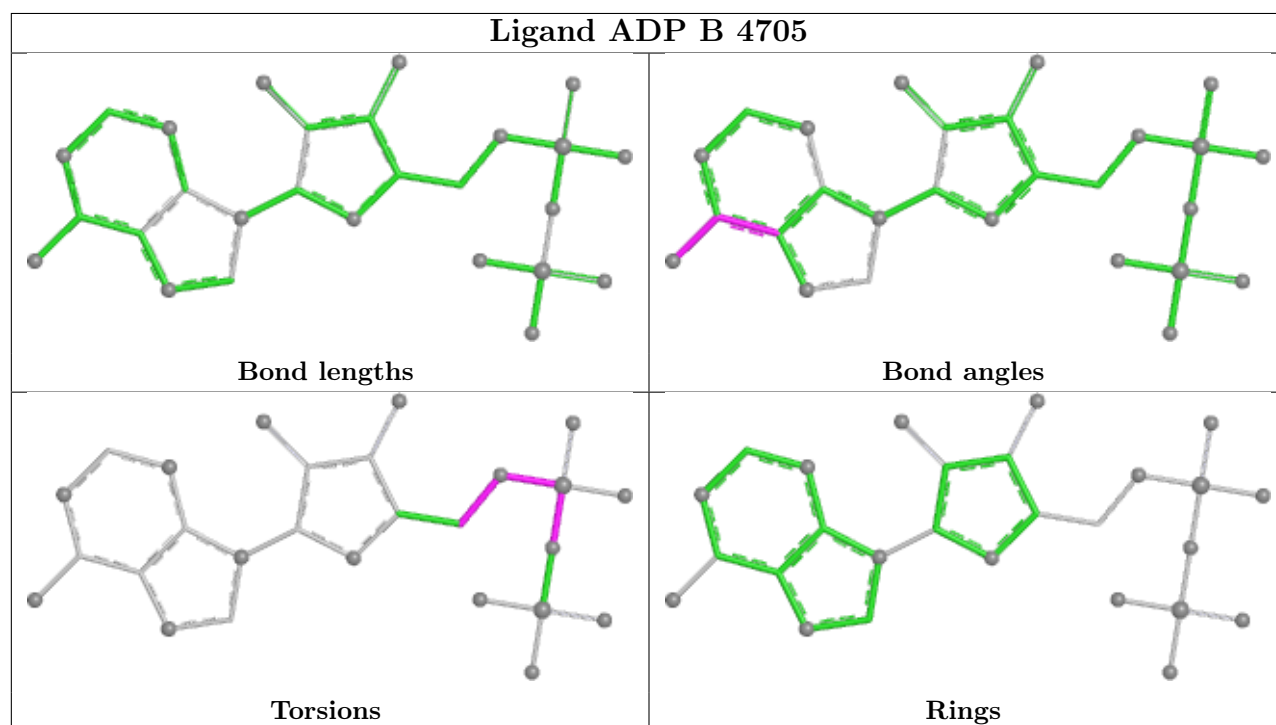
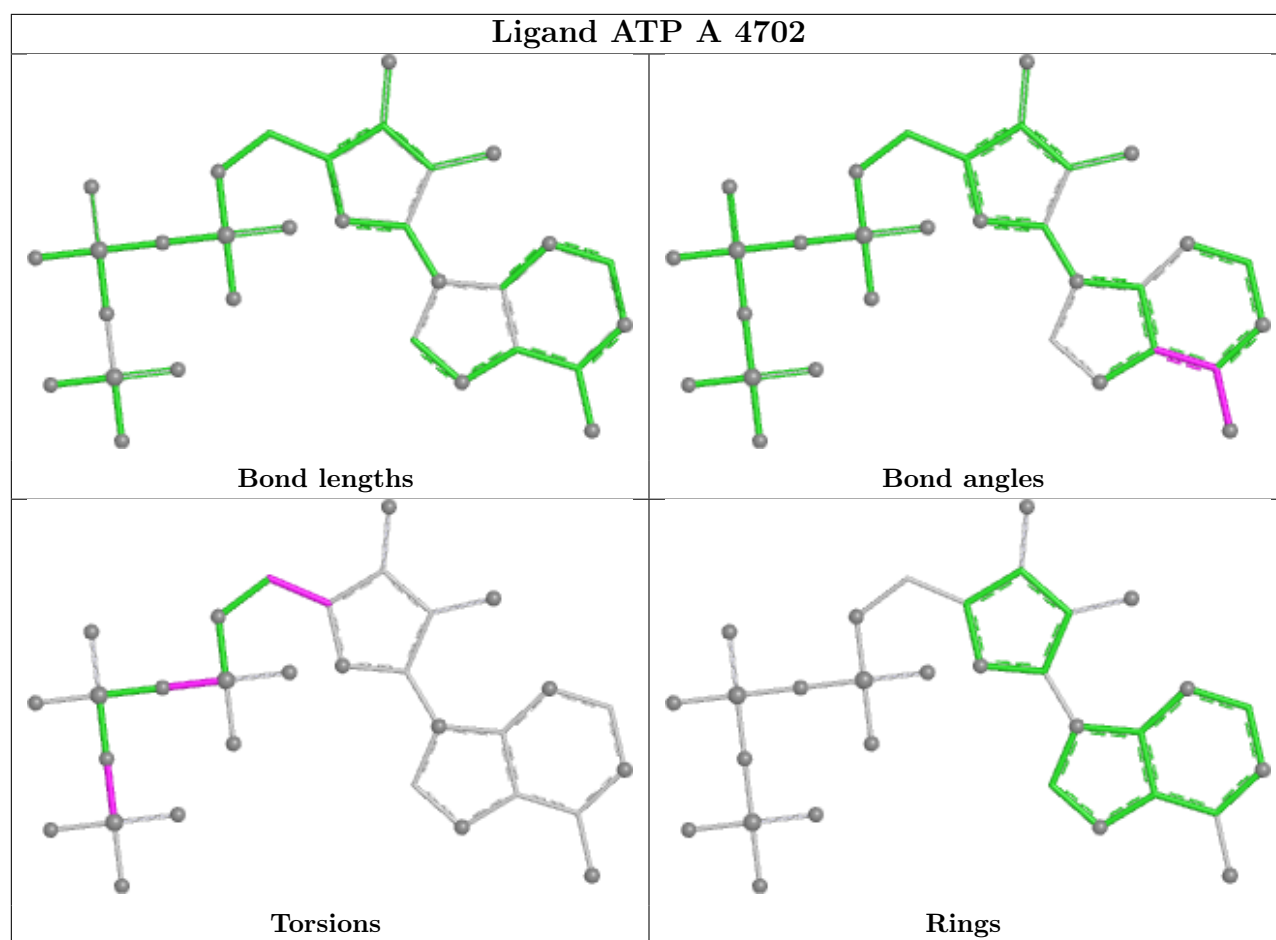
Mol	Chain	Res	Type	Atoms
19	A	4702	ATP	PB-O3A-PA-O1A
19	C	4201	ATP	PG-O3B-PB-O2B
19	C	4201	ATP	O4'-C4'-C5'-O5'
18	A	4701	ADP	C4'-C5'-O5'-PA
18	C	4206	ADP	PB-O3A-PA-O2A

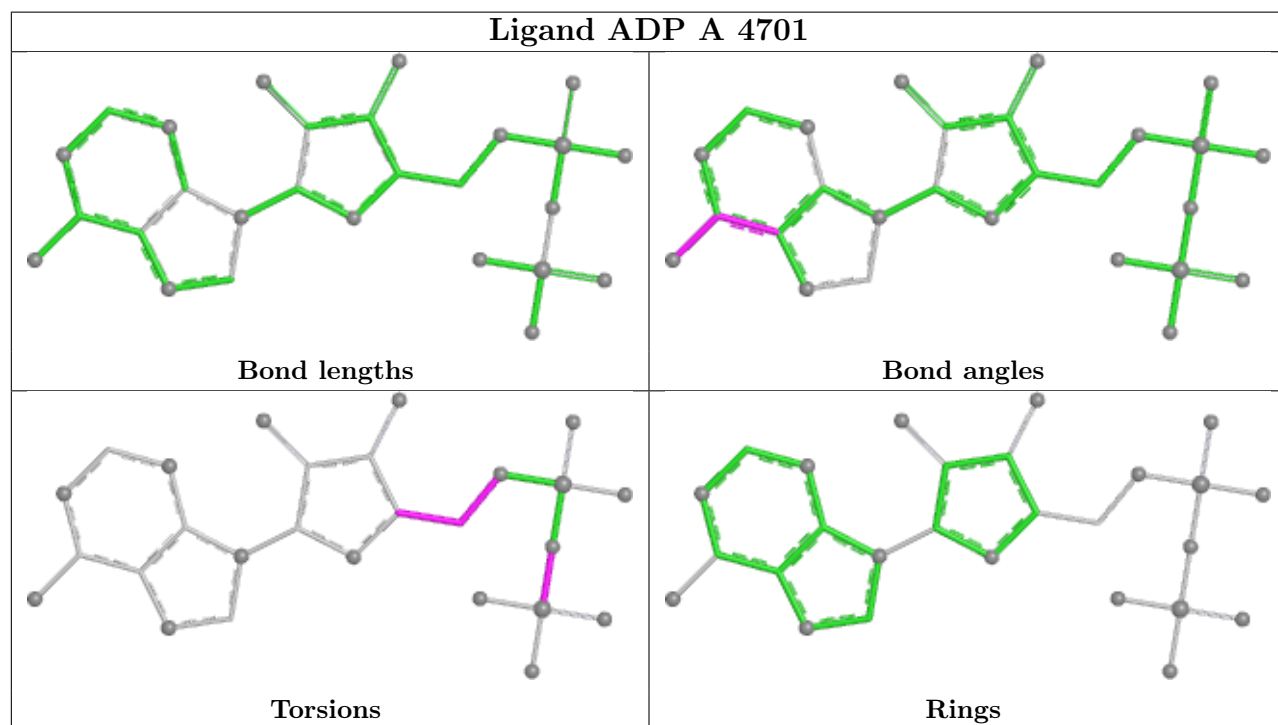
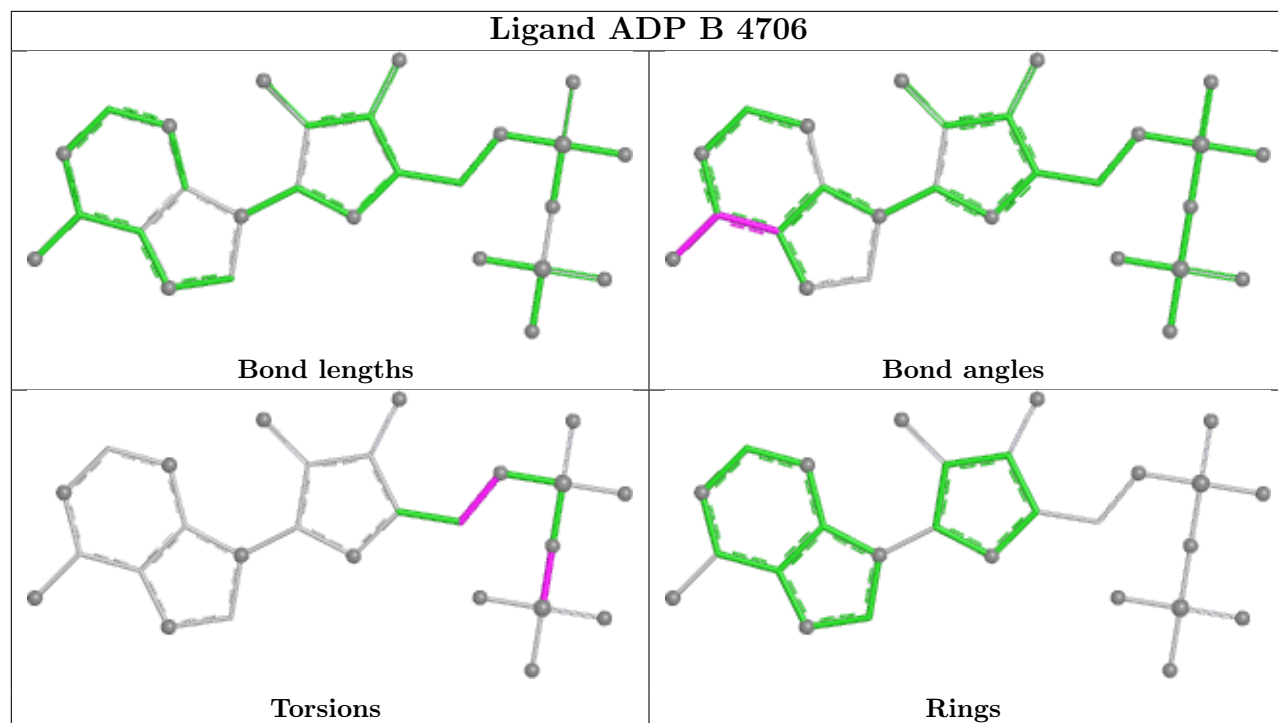
There are no ring outliers.

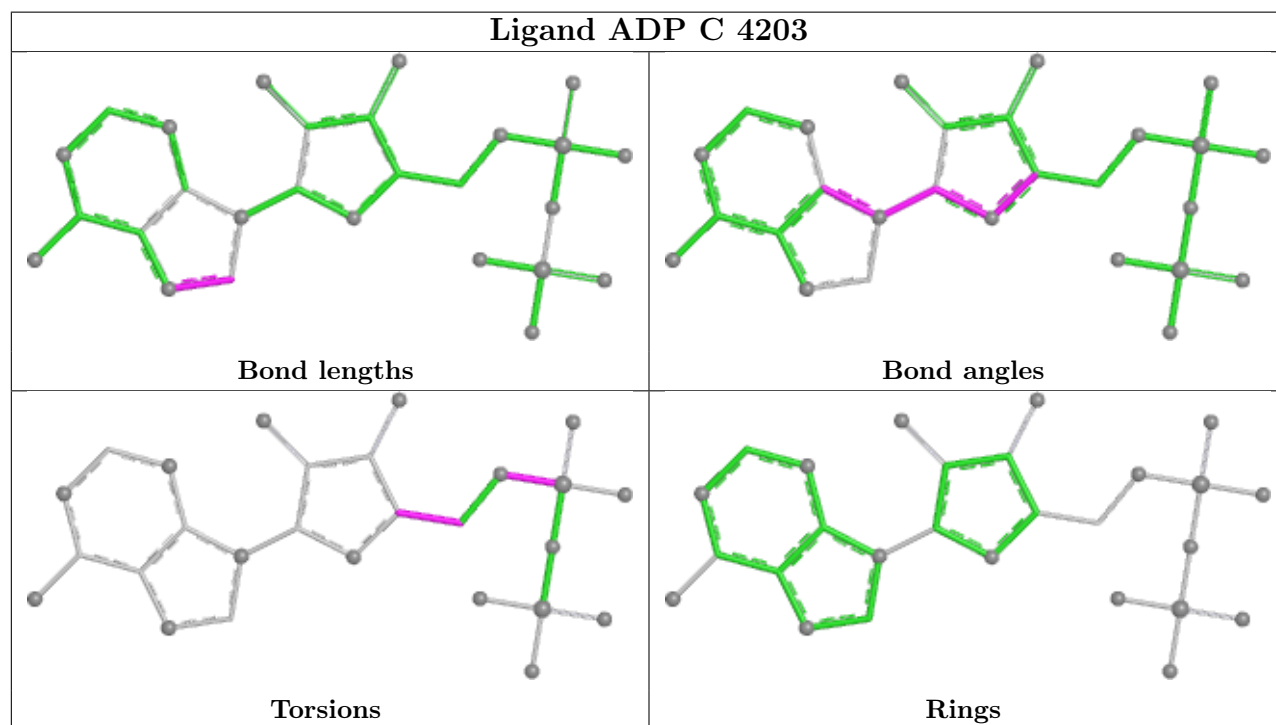
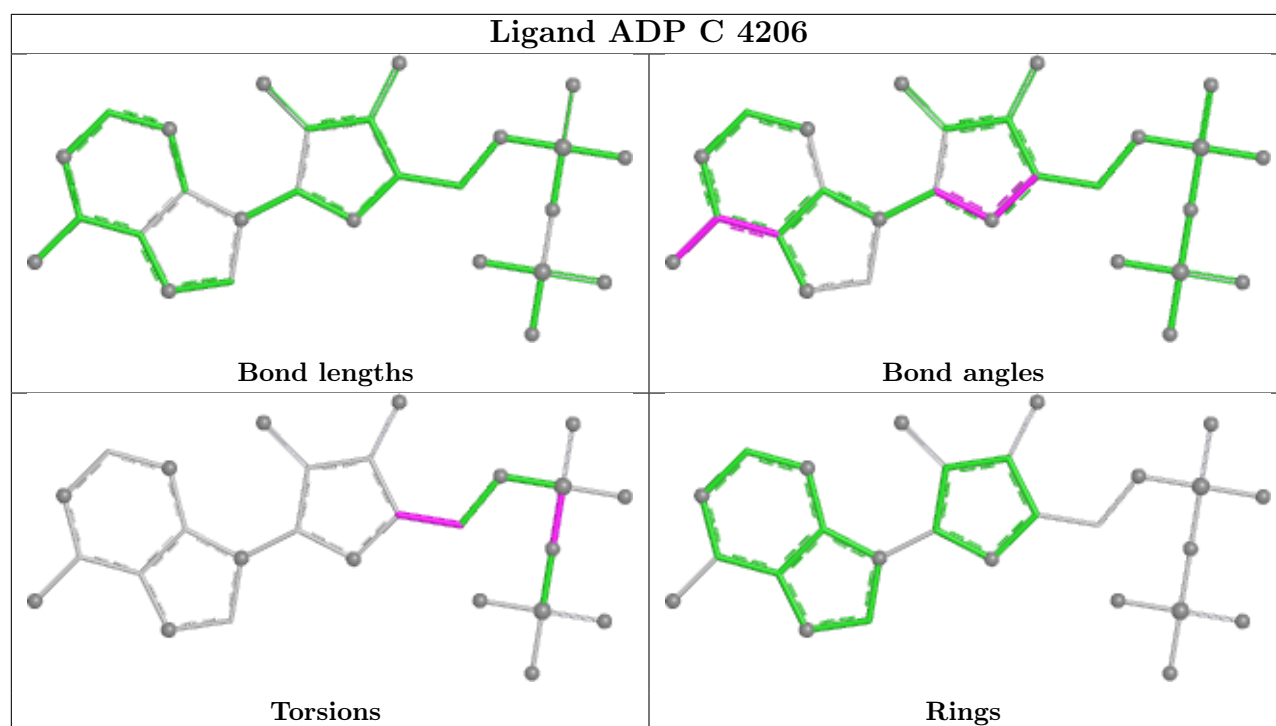
5 monomers are involved in 6 short contacts:

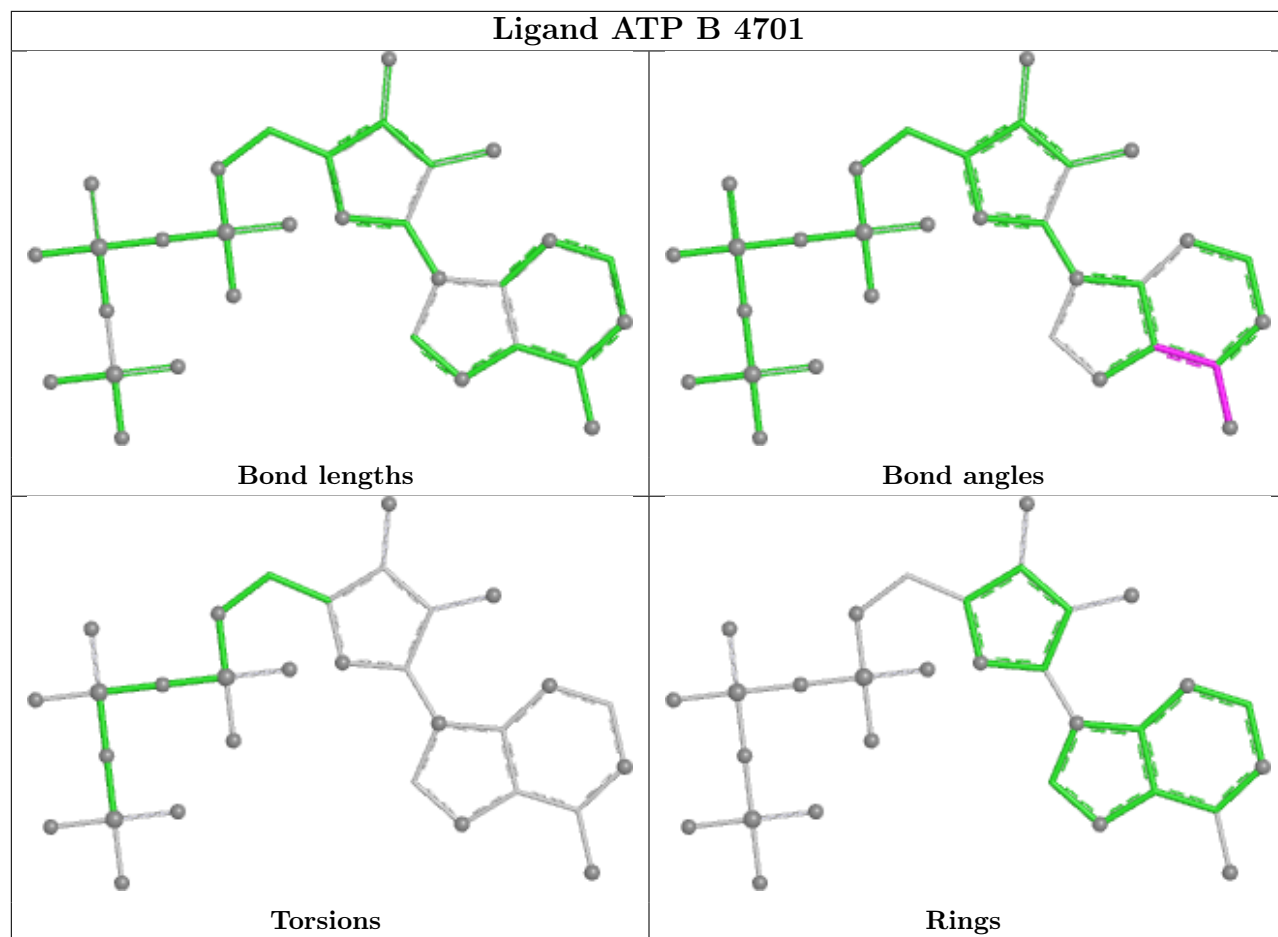
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	4701	ADP	1	0
18	C	4206	ADP	2	0
18	C	4203	ADP	1	0
19	B	4701	ATP	1	0
18	A	4703	ADP	1	0

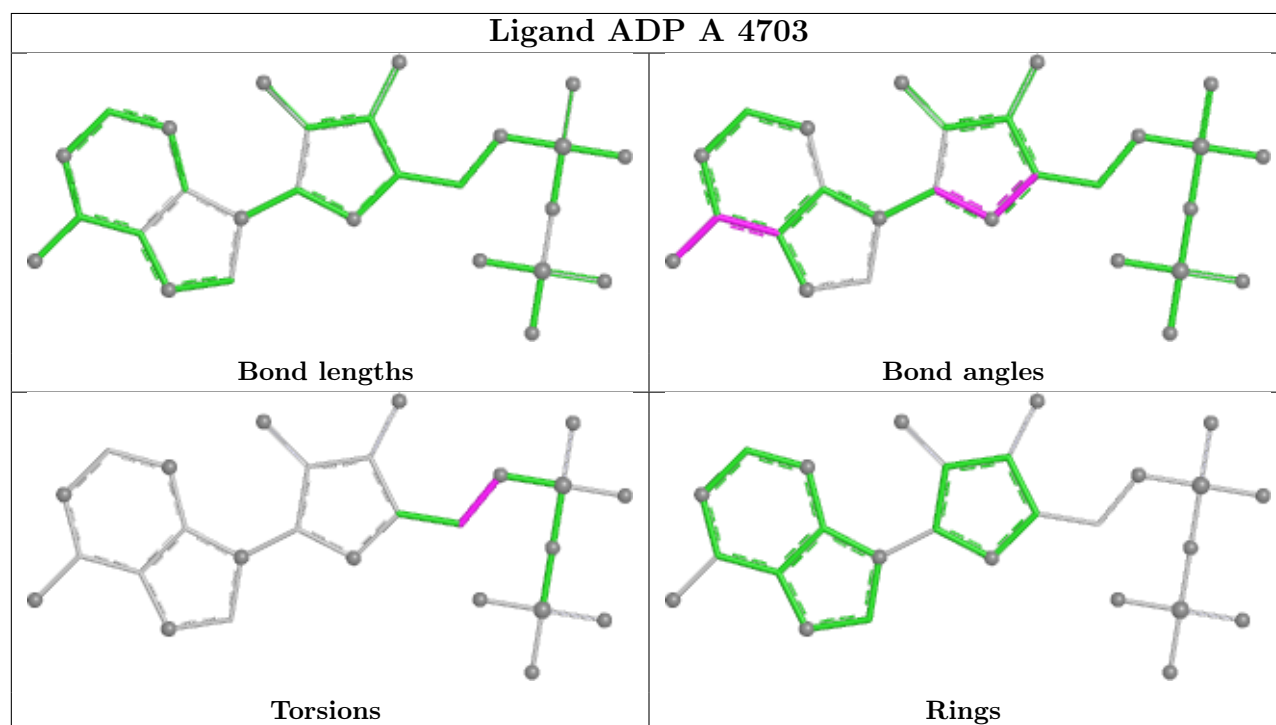
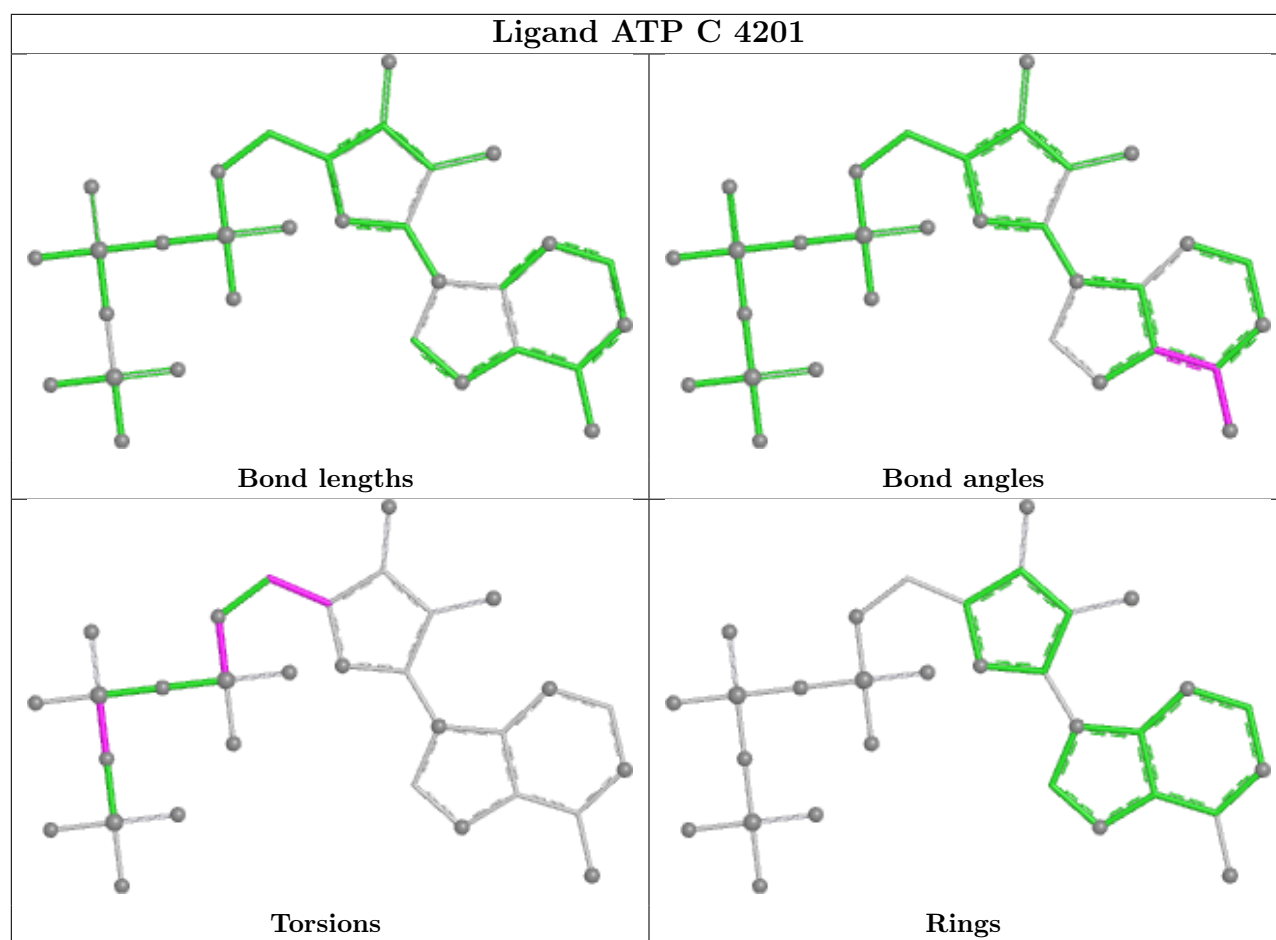
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

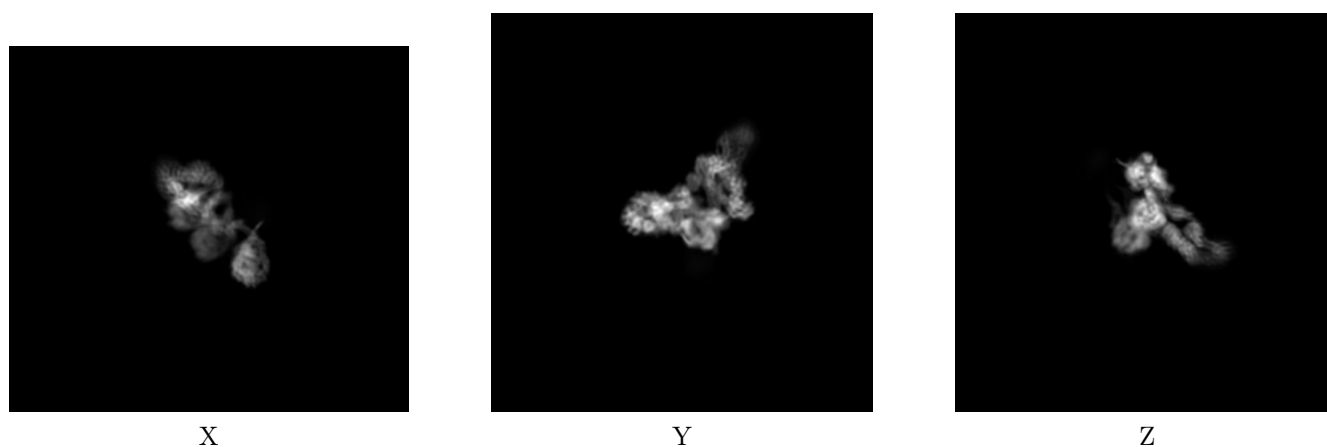
6 Map visualisation [i](#)

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](#)

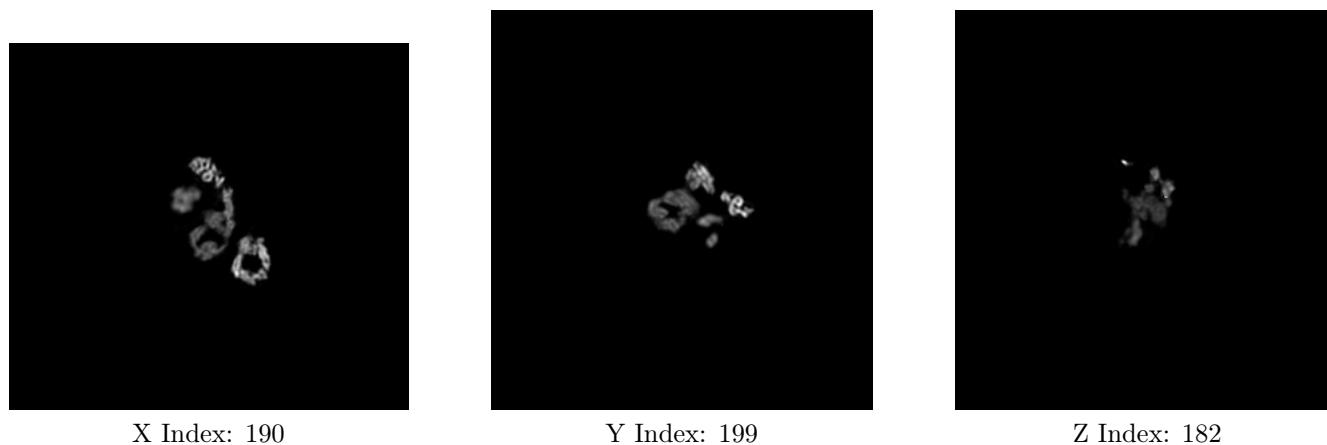
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



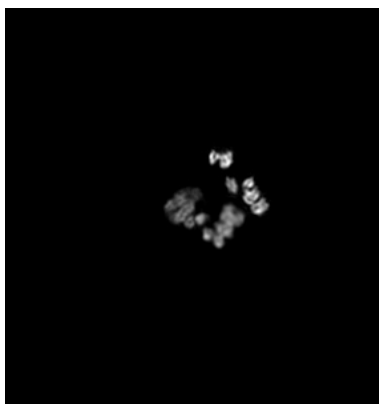
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 186

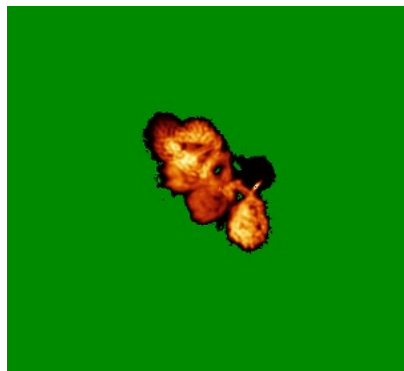


Z Index: 209

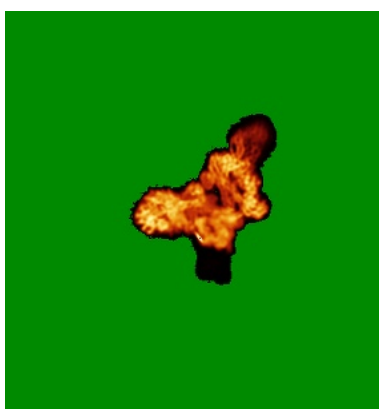
The images above show the largest variance slices of the map in three orthogonal directions.

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

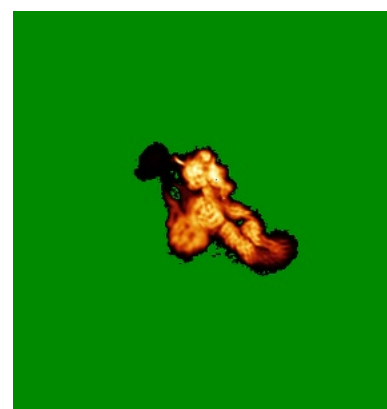
6.4.1 Primary map



X



Y

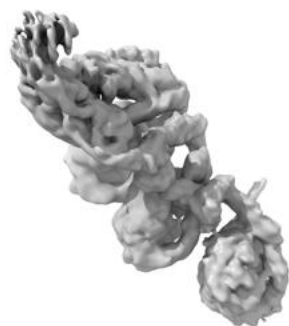


Z

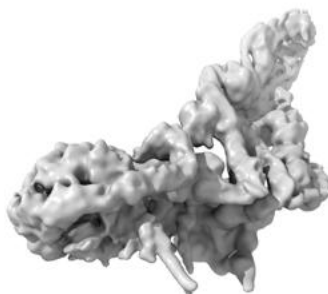
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

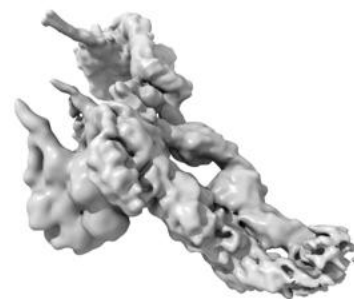
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

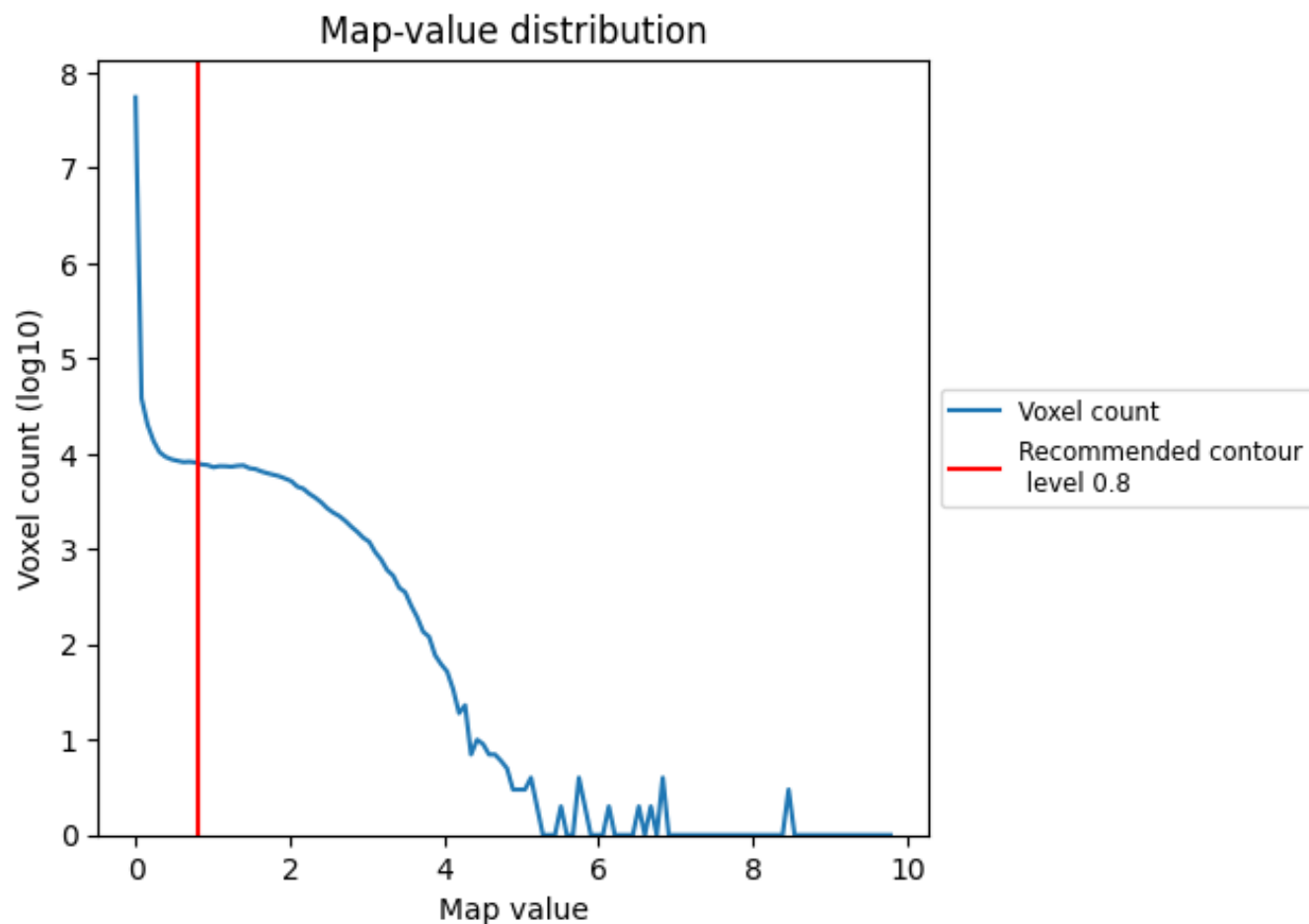
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

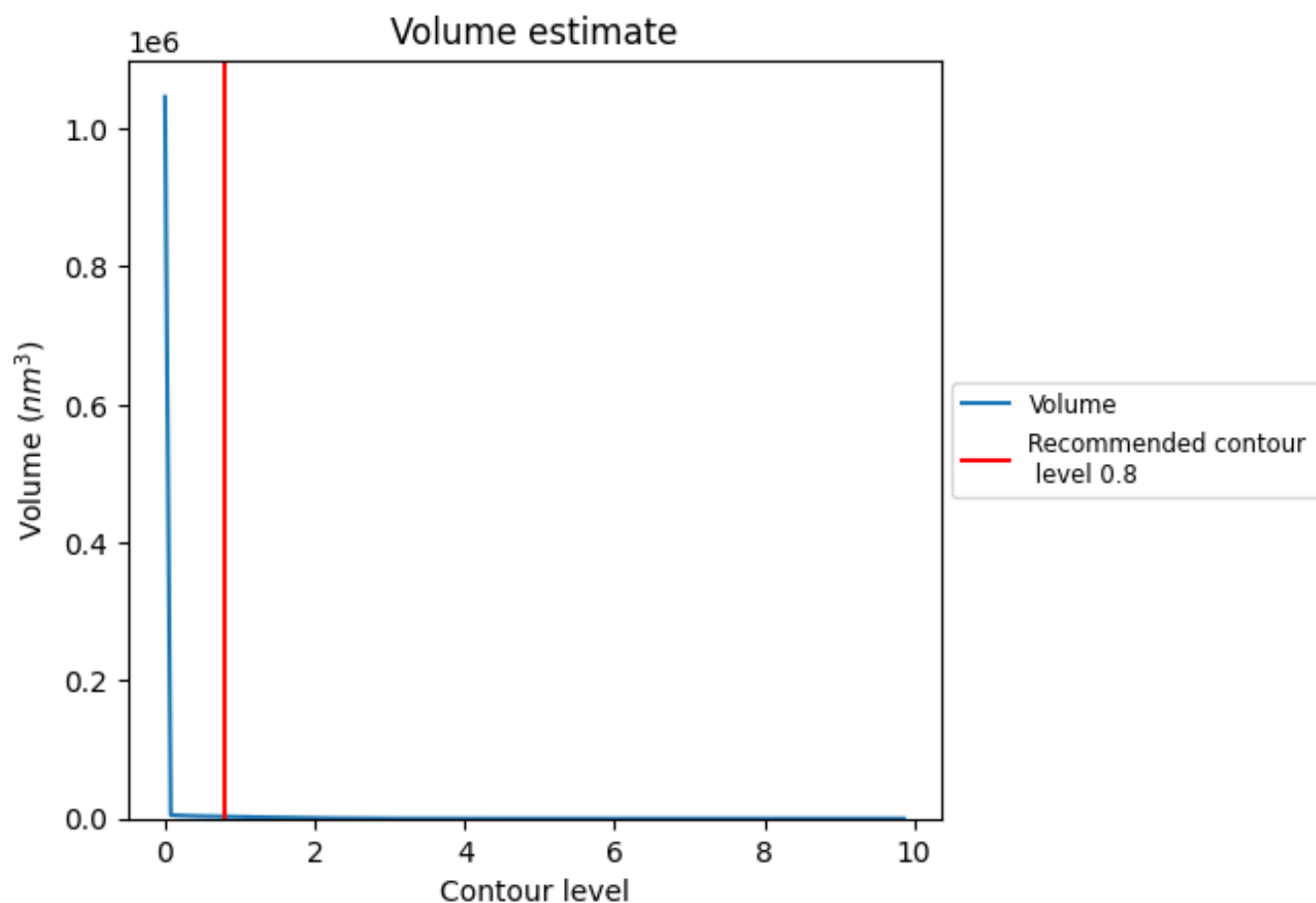
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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.

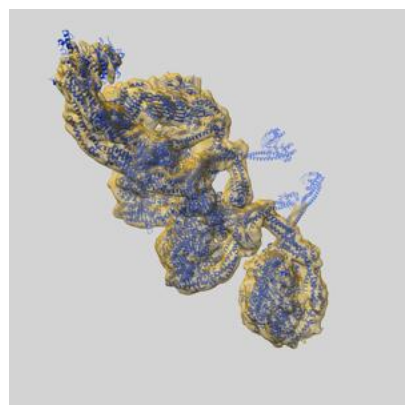
8 Fourier-Shell correlation ⓘ

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

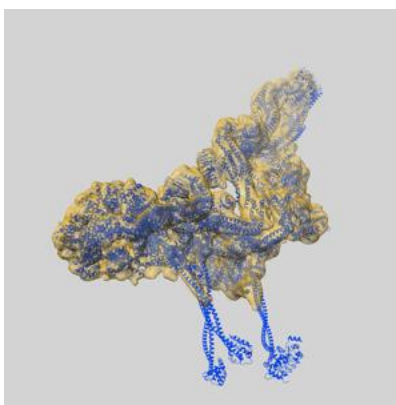
9 Map-model fit [i](#)

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](#).

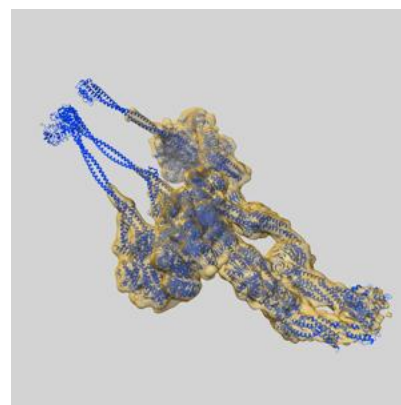
9.1 Map-model overlay [i](#)



X



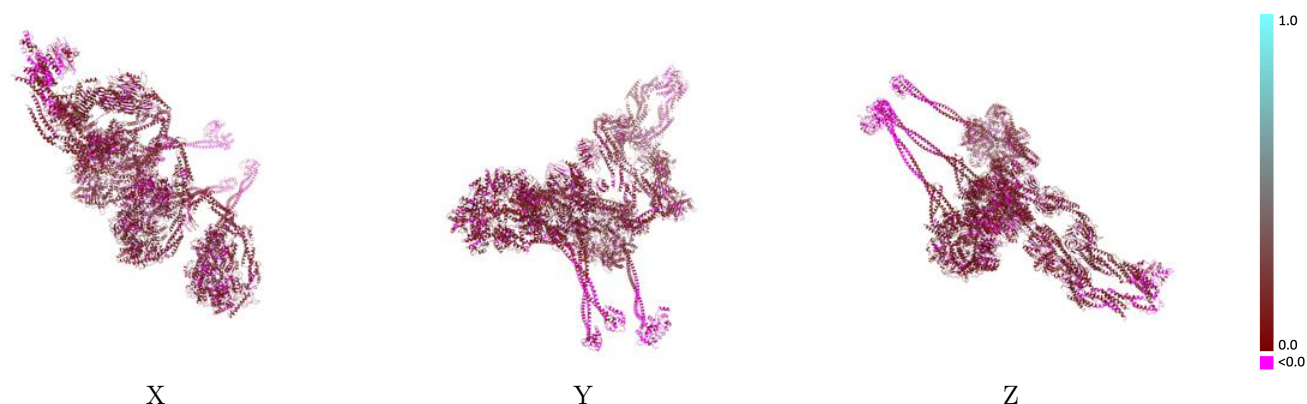
Y



Z

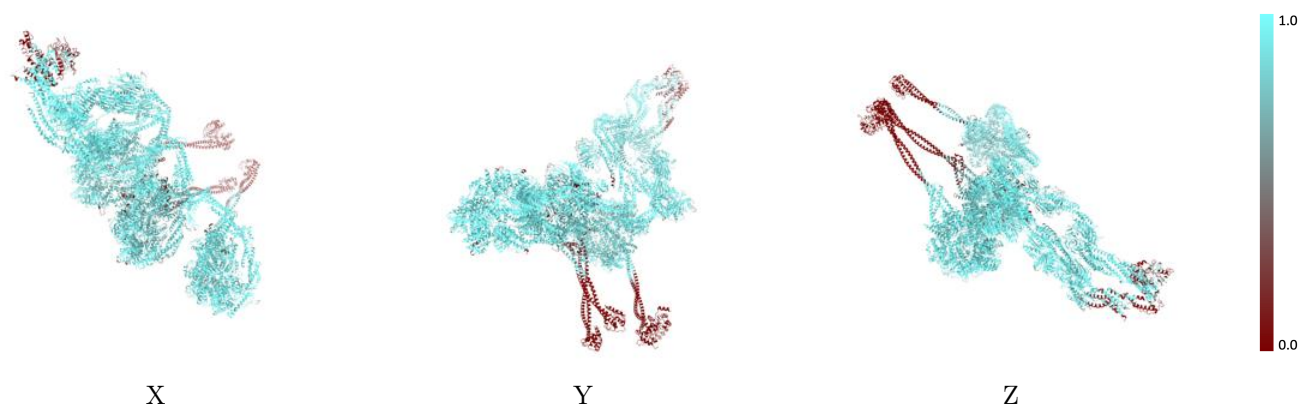
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



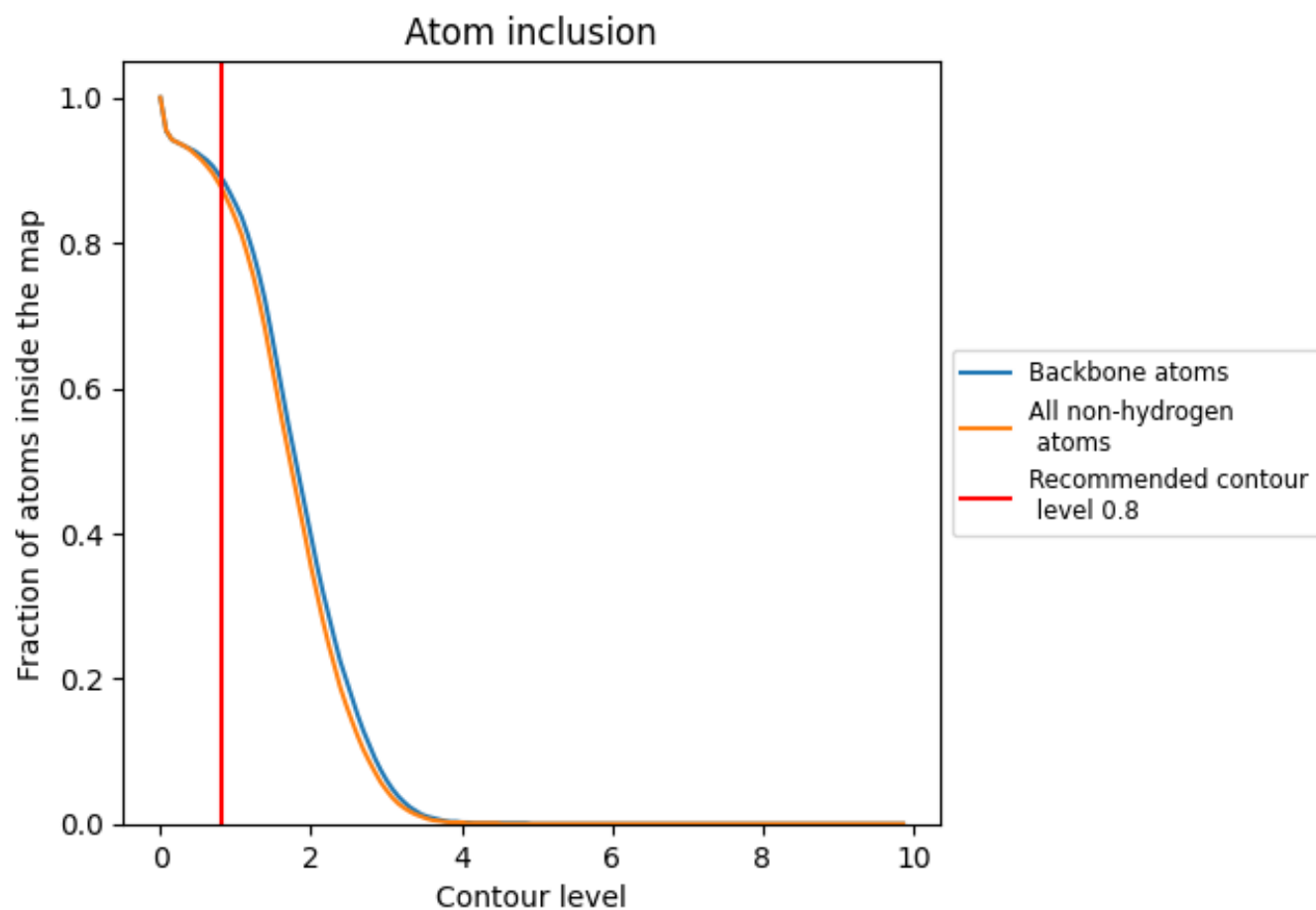
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.1140
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	 -0.0550

