



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:39 PM UTC

PDB ID : 9E17 / pdb_00009e17
EMDB ID : EMD-26205
Title : Structure of RyR1 in the primed state in the presence of caffeine (reprocessed /reanalyzed from EMPIAR-10997, 7TZC, EMD-26205)
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.45 Å(reported)
Based on initial model : 7TZC

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

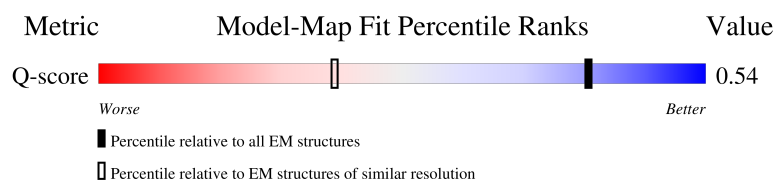
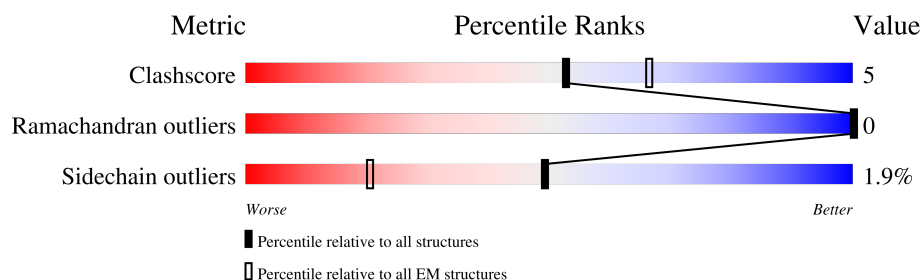
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.45 Å.

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



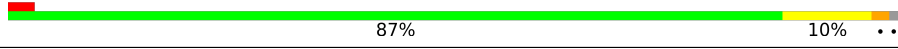
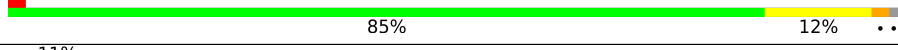
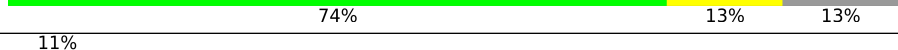
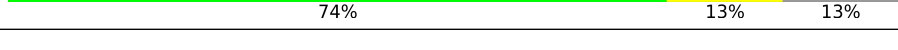
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5931 (1.96 - 2.95)

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	C	150	33% 76% 23% ..
1	D	150	30% 79% 20% ..
1	E	150	33% 78% 21% .
1	K	150	33% 79% 19% ..

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Mol	Chain	Length	Quality of chain
2	F	108	
2	H	108	
2	J	108	
2	O	108	
3	A	5037	
3	B	5037	
3	G	5037	
3	I	5037	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 149476 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	D	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	E	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	C	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	J	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	O	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	G	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	I	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total	Ca	0
			4	4	
4	D	4	Total	Ca	0
			4	4	
4	E	4	Total	Ca	0
			4	4	
4	C	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	
4	I	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

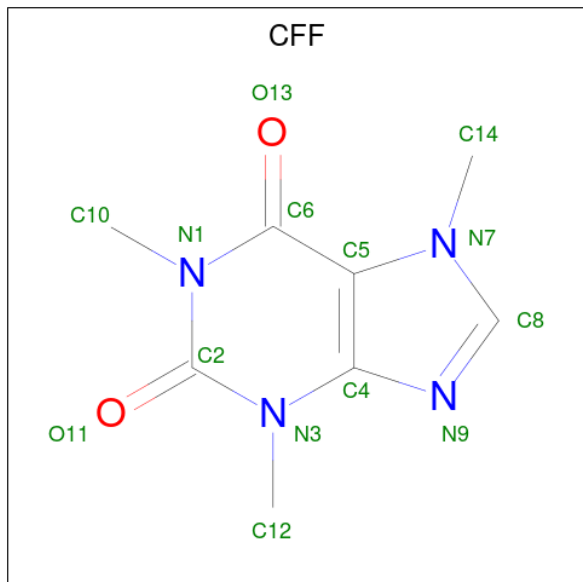


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

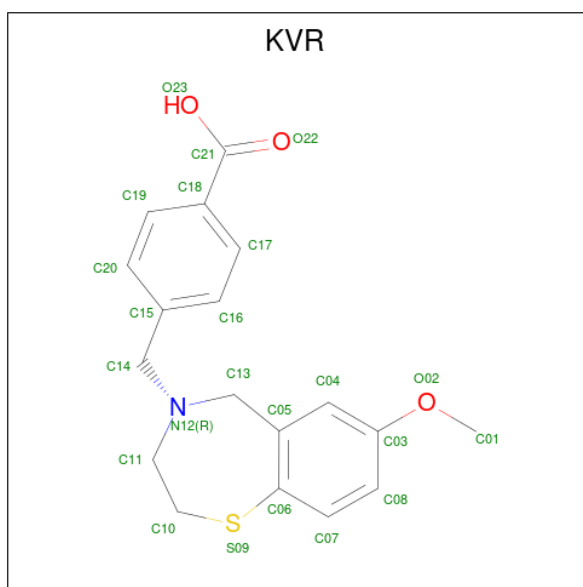
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Zn 1 1	0
6	B	1	Total Zn 1 1	0
6	G	1	Total Zn 1 1	0
6	I	1	Total Zn 1 1	0

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



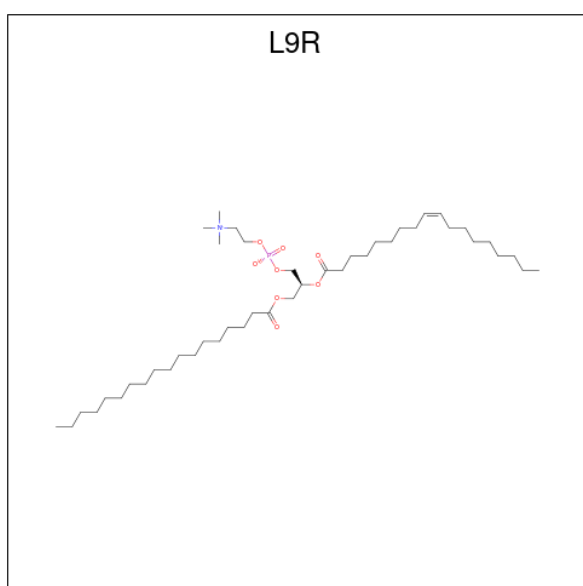
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	G	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	I	1	Total	C	N	O	S	0
			23	18	1	3	1	

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: L9R) (formula: C₄₄H₈₆NO₈P).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1	

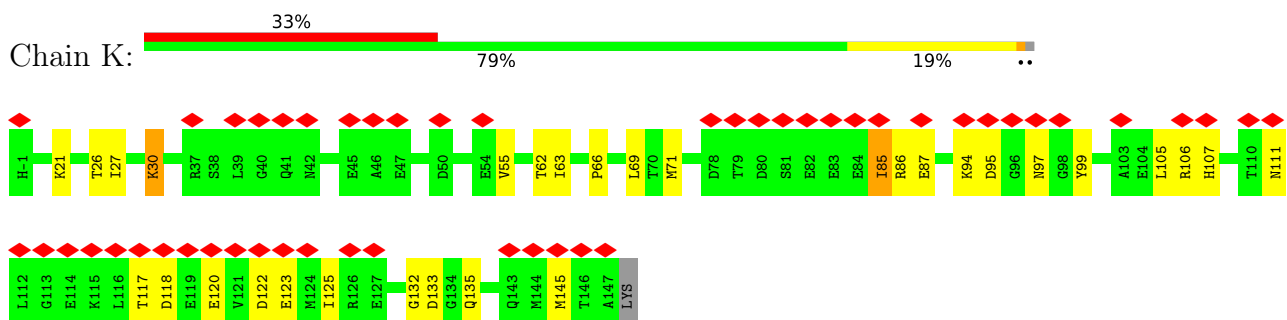
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	O	0
			1	1	
10	B	1	Total	O	0
			1	1	
10	G	1	Total	O	0
			1	1	
10	I	1	Total	O	0
			1	1	

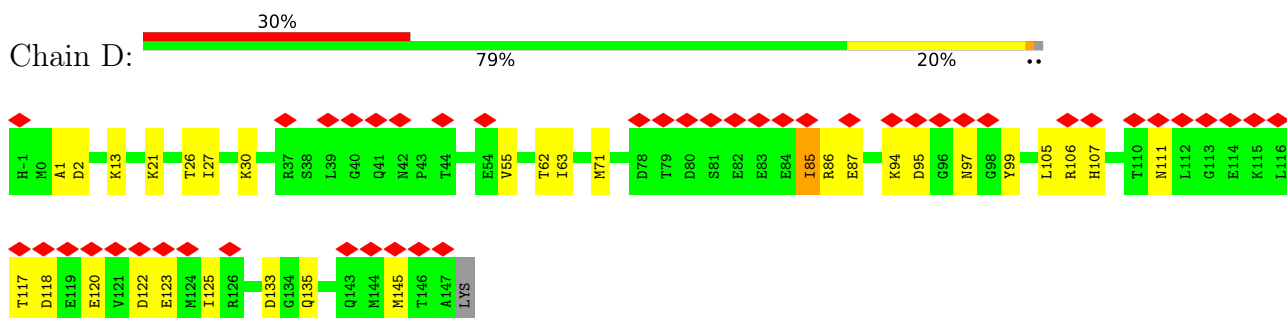
3 Residue-property plots

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.

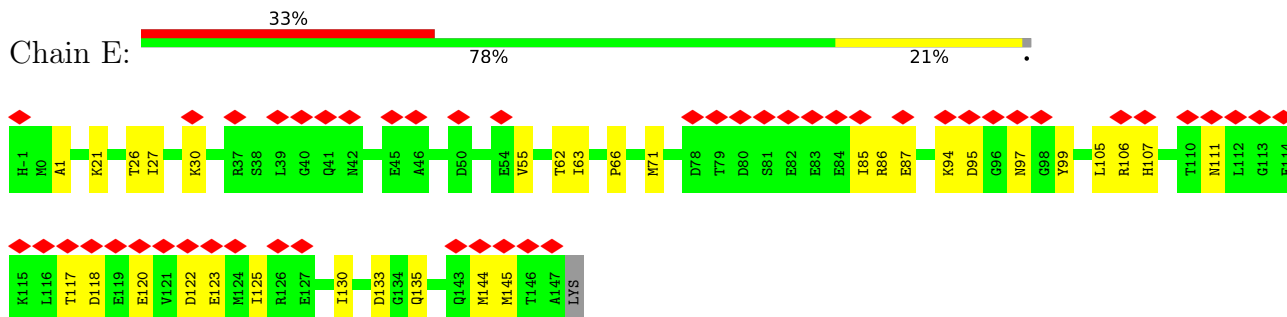
• Molecule 1: Calmodulin-1



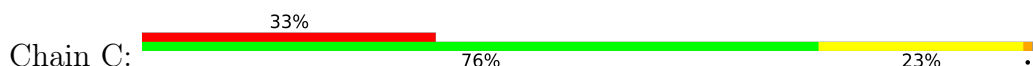
• Molecule 1: Calmodulin-1

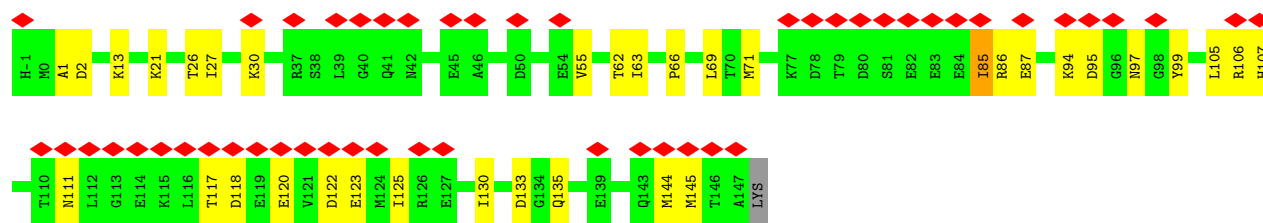


• Molecule 1: Calmodulin-1

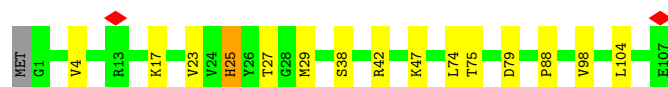
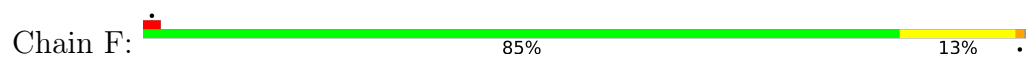


• Molecule 1: Calmodulin-1

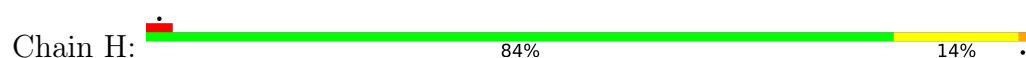




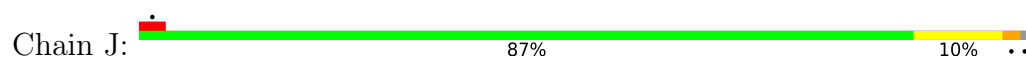
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



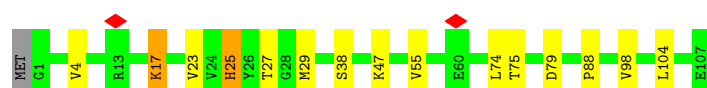
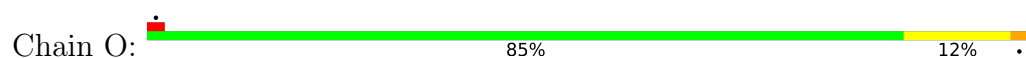
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



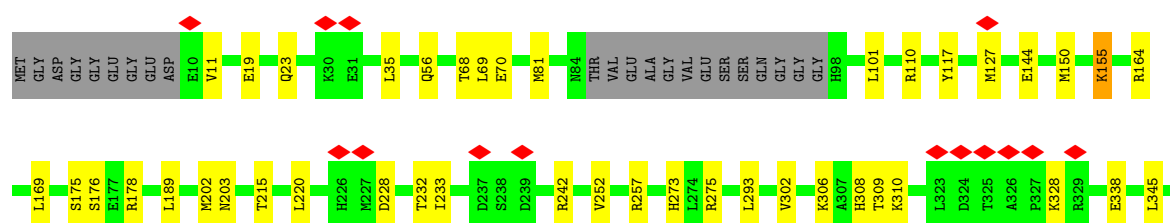
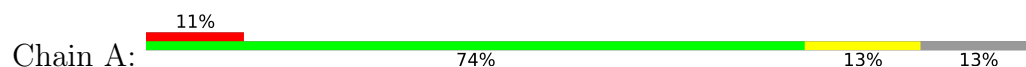
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 3: Ryanodine receptor 1

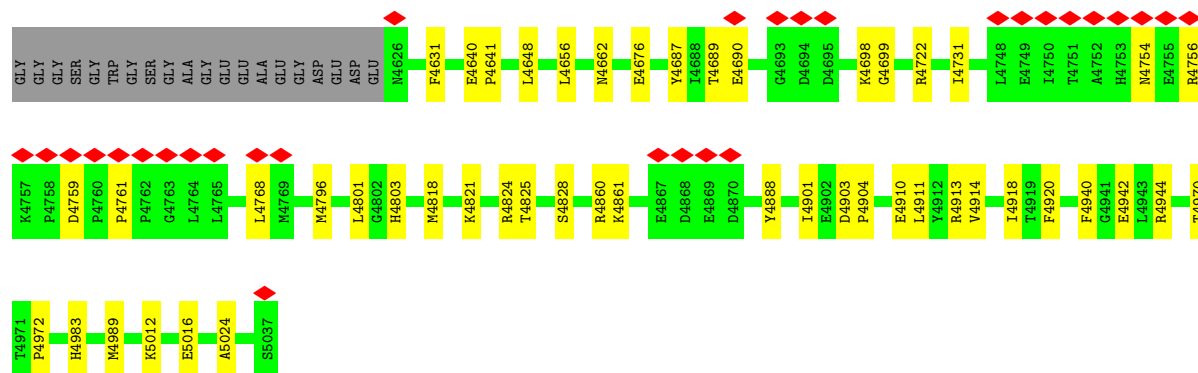




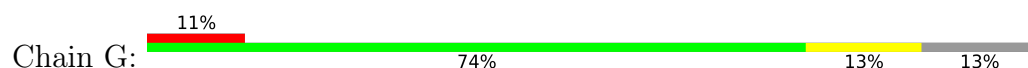


I2804	Y2805	R2806	Y2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	K2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	L2743															
N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	L2752	S2753	F2754	I2755	K2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	G2766	V2766	K2677	L2678	K2689	S2720	S2721	K2722	N2774	W2775	S2776	Y2777	G2778	N2779	E2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	F2788	P2789	K2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803
M2578	V2579	D2580	Y2587	S2590	I2614	M2618	H2621	L2626	L2633	P2640	L2644	R2650	C2651	W2661	F2664	G2665	V2666	K2677	L2678	K2689	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	E2738	P2739	V2740	E2741	T2742	L2743															
S2309	D2320	I2321	R2355	E2382	R2385	P2390	R2392	V2397	ARG	ASP	ARG	ARG	ARG	HIS	PHE	GLY	GLU	P2410	F2411	E2412	E2413	N2414	R2415	E2449	R2452	K2461	D2482	G2483	V2495	H2498	E2513	N2514	G2515	D2516	L2519	T2538	F2541	R2575																					
LYS	PRO	GLU	GLU	LEU	PRO	ALA	E2088	K2089	K2090	E2108	R2126	Q2127	M2153	L2159	I2167	E2175	N2176	M2178	I2182	M2186	N2187	L2201	G2202	M2203	V2212	G2216	G2217	G2218	E2219	T2220	K2221	E2222	I2223	M2228	F2235	R2244	Y2256	G2264	Q2308																				
R1993	R1994	T1995	R1996	E1997	F1998	R1999	S2000	P2001	Q2005	A2016	D2017	E2018	E2019	D2020	C2021	R2028	Q2029	D2033	D2037	Q2045	L2046	GLU	GLY	GLU	GLU	GLU	GLU	GLU	PRO	GLY	GLY	LYS	LYS	ASP	L1922	E1923	M1929	G1947	D1948	L1980	F1984	T1985	M1986	S1987	A1988	A1989	E1990	T1991	A1992										
L1676	R1680	D1690	Q1693	L1694	L1715	I1716	E1721	E1733	G1751	R1752	K1753	G1754	G1755	M1756	A1757	R1758	L1771	A1784	A1788	A1789	G1790	V1791	A1792	E1793	A1794	E1805	K1810	M1814	V1819	R1820	Q1824	D1828	T1872	E1873	E1874	GLU	GLU	GLU	GLU	GLU																			
G1451	T1454	P1455	D1456	D1465	K1468	V1469	E1479	Q1480	G1481	K1488	C1489	C1492	M1493	M1494	P1503	G1504	Q1505	Q1506	G1507	R1508	V1520	M1527	V1554	L1555	I1562	Q1569	T1572	L1575	M1579	R1619	E1622	L1634	T1635	M1636	L1639	L1653	Q1660																						
ALA	GLY	THR	PRO	LEU	ALA	PRO	PRO	GLY	LEU	ASN	GLN	PRO	PRO	ALA	GLU	ASP	GLU	GLU	LYS	ASN	ARG	ALA	ALA	ARG	ARG	ALA	GLY	LYS	GLY	PRO	THR	PRO	LEU	ARG	LEU	PRO	THR	VAL	ALA	D1419	N1420	R1421	C1447	V1448															
A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	R987	L988	A989	E990	N991	D999	R1000	W1005	S1008	R1017	L1021	V1022	P1023	Y1024	K1032	T1044	L1045	L1046	L1047	G1048	Y1049	G1050	V1051	N1052	T1053	E1054	D1057	Q1058	E1059	P1060	S1061	Q1062	V1063	E1064									





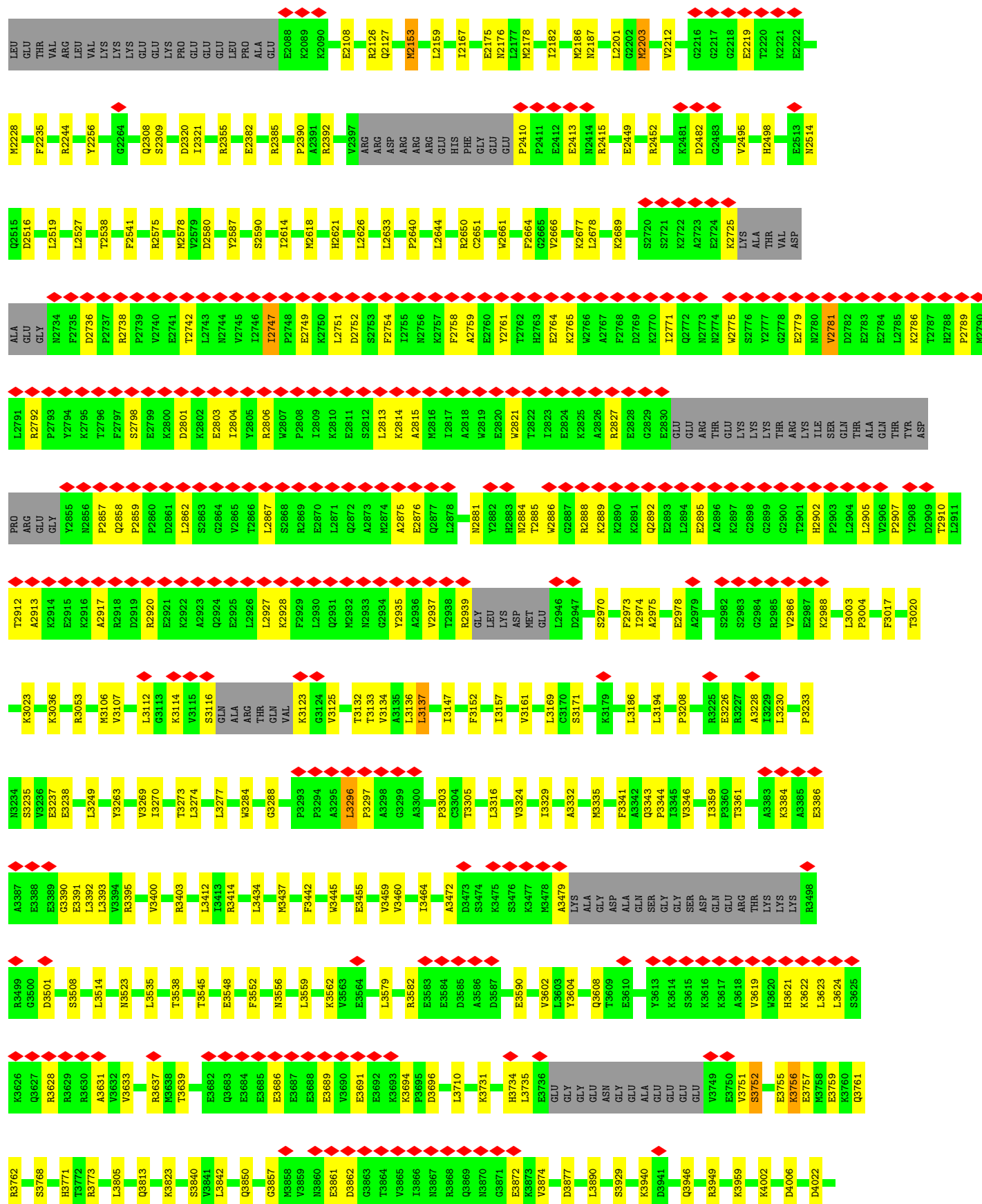
• Molecule 3: Ryanodine receptor 1

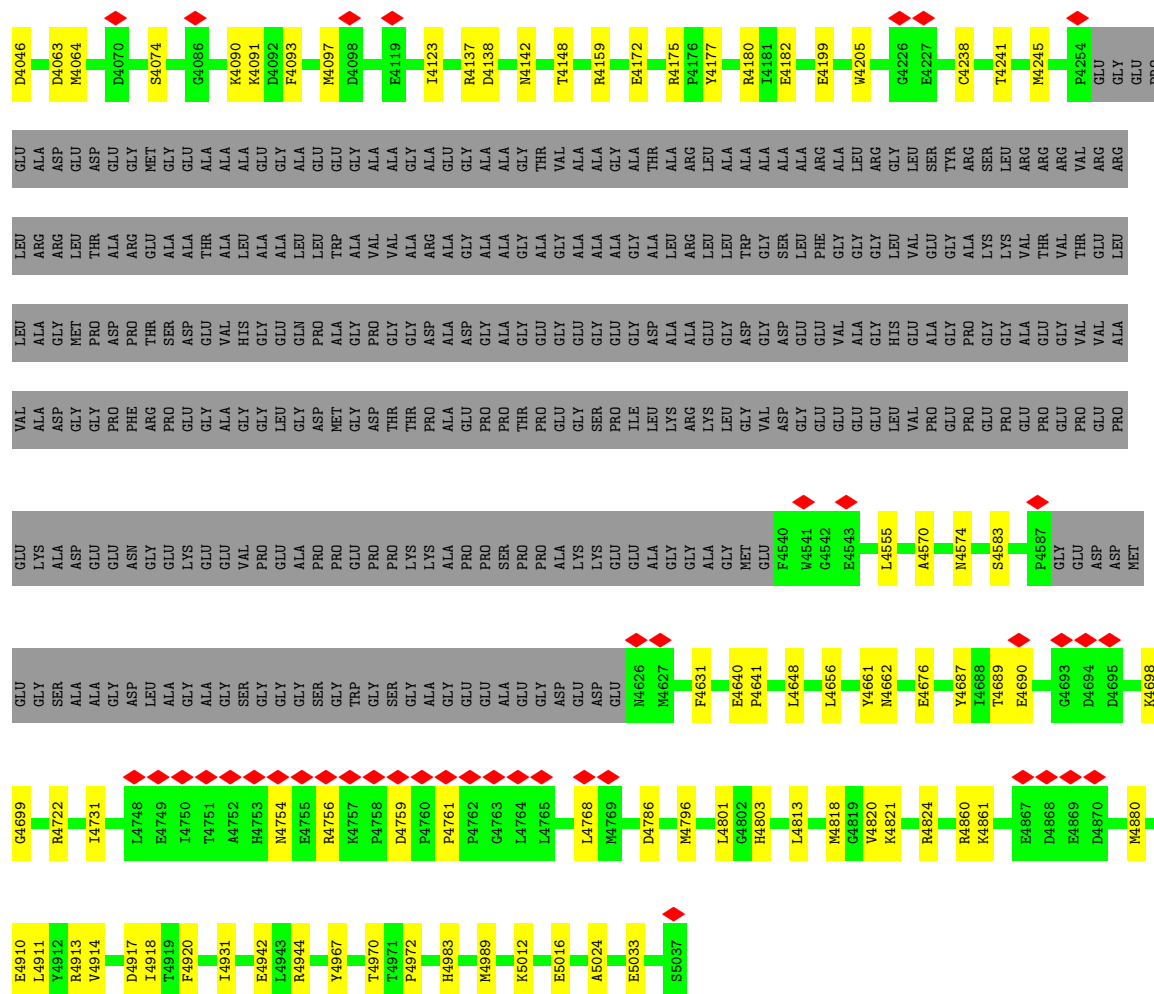












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	333010	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.887	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, CFF, KVR, CA, L9R

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	C	0.10	0/1187	0.24	0/1594
1	D	0.09	0/1187	0.24	0/1594
1	E	0.09	0/1187	0.24	0/1594
1	K	0.09	0/1187	0.24	0/1594
2	F	0.33	0/850	0.49	0/1146
2	H	0.33	0/850	0.49	0/1146
2	J	0.33	0/850	0.49	0/1146
2	O	0.33	0/850	0.49	0/1146
3	A	0.15	0/35977	0.30	3/48726 (0.0%)
3	B	0.15	0/35977	0.30	3/48726 (0.0%)
3	G	0.15	0/35977	0.30	3/48726 (0.0%)
3	I	0.15	0/35977	0.30	3/48726 (0.0%)
All	All	0.15	0/152056	0.30	12/205864 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4920	PHE	N-CA-C	-5.60	105.17	112.23
3	I	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	A	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	B	4920	PHE	N-CA-C	-5.56	105.23	112.23
3	B	4970	THR	CA-C-N	5.08	130.59	120.94
3	B	4970	THR	C-N-CA	5.08	130.59	120.94
3	G	4970	THR	CA-C-N	5.07	130.58	120.94
3	G	4970	THR	C-N-CA	5.07	130.58	120.94
3	I	4970	THR	CA-C-N	5.07	130.57	120.94
3	I	4970	THR	C-N-CA	5.07	130.57	120.94
3	A	4970	THR	CA-C-N	5.07	130.56	120.94
3	A	4970	THR	C-N-CA	5.07	130.56	120.94

There are no chirality outliers.

There are no planarity outliers.

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	C	1174	0	1099	22	0
1	D	1174	0	1099	18	0
1	E	1174	0	1099	18	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	374	0
3	B	35150	0	34797	371	0
3	G	35150	0	34797	370	0
3	I	35150	0	34797	377	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0
9	B	108	0	172	5	0
9	G	108	0	172	8	0
9	I	108	0	172	7	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0
10	I	1	0	0	0	0
All	All	149476	0	147732	1560	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 5.

All (1560) 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)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78
3:G:2779:GLU:HG3	3:G:2792:ARG:HG2	1.66	0.78
3:I:2779:GLU:HG3	3:I:2792:ARG:HG2	1.66	0.77
3:B:2779:GLU:HG3	3:B:2792:ARG:HG2	1.66	0.77
3:A:1505:GLN:HG3	3:G:2771:ILE:HG12	1.67	0.77
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.68	0.76
3:I:2175:GLU:HG3	3:I:2228:MET:HB2	1.68	0.76
1:C:106:ARG:HH22	1:C:118:ASP:HA	1.50	0.76
3:A:2175:GLU:HG3	3:A:2228:MET:HB2	1.68	0.76
3:G:2175:GLU:HG3	3:G:2228:MET:HB2	1.68	0.76
1:D:106:ARG:HH22	1:D:118:ASP:HA	1.50	0.75
1:K:106:ARG:HH22	1:K:118:ASP:HA	1.50	0.75
1:E:106:ARG:HH22	1:E:118:ASP:HA	1.50	0.75
3:G:2765:LYS:NZ	3:G:2859:PRO:O	2.22	0.73
3:I:2765:LYS:NZ	3:I:2859:PRO:O	2.22	0.72
1:K:111:ASN:O	3:A:1996:ARG:NH2	2.20	0.72
3:B:2765:LYS:NZ	3:B:2859:PRO:O	2.22	0.72
3:A:2765:LYS:NZ	3:A:2859:PRO:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2771:ILE:HG12	3:I:1505:GLN:HG3	1.74	0.70
3:G:3114:LYS:HD3	3:G:3116:SER:H	1.58	0.69
3:B:3114:LYS:HD3	3:B:3116:SER:H	1.58	0.68
3:I:3114:LYS:HD3	3:I:3116:SER:H	1.58	0.68
3:A:1280:GLN:O	3:A:1281:ASN:ND2	2.27	0.68
3:B:876:GLU:HG2	3:B:918:ARG:HD3	1.76	0.68
3:I:858:THR:HB	3:I:930:LYS:HD2	1.76	0.68
3:A:368:ARG:HE	3:A:2308:GLN:HG3	1.59	0.68
3:A:3114:LYS:HD3	3:A:3116:SER:H	1.58	0.68
3:I:1280:GLN:O	3:I:1281:ASN:ND2	2.27	0.68
3:G:876:GLU:HG2	3:G:918:ARG:HD3	1.76	0.67
3:B:368:ARG:HE	3:B:2308:GLN:HG3	1.59	0.67
3:B:1280:GLN:O	3:B:1281:ASN:ND2	2.27	0.67
3:G:858:THR:HB	3:G:930:LYS:HD2	1.76	0.67
3:A:2771:ILE:HG12	3:B:1505:GLN:HG3	1.77	0.67
3:G:1280:GLN:O	3:G:1281:ASN:ND2	2.27	0.67
3:A:858:THR:HB	3:A:930:LYS:HD2	1.76	0.67
3:G:368:ARG:HE	3:G:2308:GLN:HG3	1.59	0.67
3:I:876:GLU:HG2	3:I:918:ARG:HD3	1.75	0.67
3:A:2781:VAL:HA	3:A:2789:PRO:HB2	1.78	0.66
3:I:368:ARG:HE	3:I:2308:GLN:HG3	1.59	0.66
3:A:1520:VAL:HG12	3:A:1527:MET:HG2	1.78	0.66
3:G:2781:VAL:HA	3:G:2789:PRO:HB2	1.78	0.66
3:A:876:GLU:HG2	3:A:918:ARG:HD3	1.75	0.66
3:I:2781:VAL:HA	3:I:2789:PRO:HB2	1.78	0.66
3:A:3020:THR:HG23	3:A:3023:LYS:H	1.60	0.66
3:B:858:THR:HB	3:B:930:LYS:HD2	1.76	0.66
3:B:2781:VAL:HA	3:B:2789:PRO:HB2	1.78	0.66
3:B:3020:THR:HG23	3:B:3023:LYS:H	1.60	0.66
3:I:3020:THR:HG23	3:I:3023:LYS:H	1.60	0.66
1:K:133:ASP:HA	3:A:3460:VAL:HG11	1.77	0.66
3:B:2792:ARG:NH2	3:B:2798:SER:OG	2.29	0.66
3:I:961:MET:SD	3:I:961:MET:N	2.69	0.65
1:D:133:ASP:HA	3:I:3460:VAL:HG11	1.77	0.65
3:G:1520:VAL:HG12	3:G:1527:MET:HG2	1.78	0.65
3:I:2792:ARG:NH2	3:I:2798:SER:OG	2.29	0.65
3:B:1520:VAL:HG12	3:B:1527:MET:HG2	1.78	0.65
3:I:1520:VAL:HG12	3:I:1527:MET:HG2	1.78	0.65
3:A:2792:ARG:NH2	3:A:2798:SER:OG	2.29	0.65
3:B:972:LEU:HD22	3:B:1044:ARG:HB3	1.79	0.65
3:G:2792:ARG:NH2	3:G:2798:SER:OG	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3020:THR:HG23	3:G:3023:LYS:H	1.60	0.65
3:A:972:LEU:HD22	3:A:1044:ARG:HB3	1.79	0.64
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.79	0.64
3:G:972:LEU:HD22	3:G:1044:ARG:HB3	1.79	0.64
3:B:101:LEU:HB3	3:B:150:MET:HE1	1.80	0.64
3:I:399:GLN:HG2	3:I:403:MET:HE2	1.80	0.64
1:D:1:ALA:HB3	3:I:3861:GLU:HG2	1.79	0.64
3:A:101:LEU:HB3	3:A:150:MET:HE1	1.80	0.64
3:B:399:GLN:HG2	3:B:403:MET:HE2	1.80	0.64
3:A:545:ASP:OD1	3:A:582:HIS:NE2	2.28	0.64
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.79	0.64
3:G:2978:GLU:OE2	3:G:3053:ARG:NH1	2.31	0.64
3:I:2978:GLU:OE2	3:I:3053:ARG:NH1	2.31	0.64
3:G:399:GLN:HG2	3:G:403:MET:HE2	1.80	0.63
3:A:399:GLN:HG2	3:A:403:MET:HE2	1.80	0.63
3:I:972:LEU:HD22	3:I:1044:ARG:HB3	1.79	0.63
3:B:2978:GLU:OE2	3:B:3053:ARG:NH1	2.31	0.63
3:G:638:ILE:HD11	3:G:1636:MET:HE2	1.81	0.63
3:G:961:MET:SD	3:G:961:MET:N	2.69	0.63
3:I:2018:GLU:OE1	3:I:2028:ARG:NH1	2.32	0.63
3:A:638:ILE:HD11	3:A:1636:MET:HE2	1.81	0.63
3:A:961:MET:SD	3:A:961:MET:N	2.69	0.62
3:A:2018:GLU:OE1	3:A:2028:ARG:NH1	2.32	0.62
3:G:3329:ILE:HD11	3:G:3332:ALA:HB2	1.79	0.62
3:I:101:LEU:HB3	3:I:150:MET:HE1	1.80	0.62
3:G:101:LEU:HB3	3:G:150:MET:HE1	1.80	0.62
3:G:2018:GLU:OE1	3:G:2028:ARG:NH1	2.32	0.62
3:A:2309:SER:OG	3:A:2321:ILE:O	2.15	0.62
3:A:3017:PHE:O	3:A:3036:LYS:NZ	2.33	0.62
3:I:3329:ILE:HD11	3:I:3332:ALA:HB2	1.79	0.62
3:I:3959:LYS:NZ	3:I:4022:ASP:OD2	2.32	0.62
3:A:2978:GLU:OE2	3:A:3053:ARG:NH1	2.31	0.62
3:G:3017:PHE:O	3:G:3036:LYS:NZ	2.33	0.62
3:B:3445:TRP:NE1	3:B:3455:GLU:OE1	2.33	0.62
3:G:2614:ILE:HG23	3:G:2618:MET:HE3	1.82	0.62
3:I:3579:LEU:HB2	3:I:3582:ARG:HG2	1.81	0.62
3:G:1116:GLY:HA3	3:G:1132:TRP:HB3	1.81	0.62
3:G:3445:TRP:NE1	3:G:3455:GLU:OE1	2.32	0.62
3:I:2902:HIS:HB3	3:I:2905:LEU:HG	1.82	0.62
3:B:2018:GLU:OE1	3:B:2028:ARG:NH1	2.32	0.62
3:B:2614:ILE:HG23	3:B:2618:MET:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3579:LEU:HB2	3:G:3582:ARG:HG2	1.81	0.62
3:I:2614:ILE:HG23	3:I:2618:MET:HE3	1.82	0.62
3:I:3017:PHE:O	3:I:3036:LYS:NZ	2.33	0.62
3:B:2410:PRO:HB3	3:B:2415:ARG:HB3	1.82	0.61
3:B:2902:HIS:HB3	3:B:2905:LEU:HG	1.82	0.61
3:B:3959:LYS:NZ	3:B:4022:ASP:OD2	2.32	0.61
3:A:2614:ILE:HG23	3:A:2618:MET:HE3	1.82	0.61
3:A:3445:TRP:NE1	3:A:3455:GLU:OE1	2.32	0.61
3:B:1066:GLN:HB2	3:B:1071:ARG:HE	1.65	0.61
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.81	0.61
3:B:3579:LEU:HB2	3:B:3582:ARG:HG2	1.81	0.61
3:I:638:ILE:HD11	3:I:1636:MET:HE2	1.81	0.61
3:I:1116:GLY:HA3	3:I:1132:TRP:HB3	1.81	0.61
3:I:2410:PRO:HB3	3:I:2415:ARG:HB3	1.82	0.61
3:I:3445:TRP:NE1	3:I:3455:GLU:OE1	2.32	0.61
3:B:961:MET:SD	3:B:961:MET:N	2.69	0.61
3:B:3017:PHE:O	3:B:3036:LYS:NZ	2.33	0.61
3:B:622:THR:HG23	3:B:626:LEU:HD12	1.83	0.61
3:G:1066:GLN:HB2	3:G:1071:ARG:HE	1.65	0.61
3:A:2902:HIS:HB3	3:A:2905:LEU:HG	1.82	0.61
3:A:2382:GLU:OE1	3:A:2385:ARG:NH1	2.31	0.61
3:B:638:ILE:HD11	3:B:1636:MET:HE2	1.81	0.61
3:A:622:THR:HG23	3:A:626:LEU:HD12	1.83	0.61
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.81	0.61
3:G:4583:SER:HB3	3:G:4631:PHE:HE2	1.66	0.61
3:G:545:ASP:OD1	3:G:582:HIS:NE2	2.28	0.60
3:A:1066:GLN:HB2	3:A:1071:ARG:HE	1.65	0.60
3:A:2410:PRO:HB3	3:A:2415:ARG:HB3	1.82	0.60
3:G:2902:HIS:HB3	3:G:2905:LEU:HG	1.82	0.60
3:A:228:ASP:OD2	3:B:155:LYS:NZ	2.30	0.60
3:A:3579:LEU:HB2	3:A:3582:ARG:HG2	1.81	0.60
3:G:2410:PRO:HB3	3:G:2415:ARG:HB3	1.82	0.60
3:I:622:THR:HG23	3:I:626:LEU:HD12	1.83	0.60
3:I:2309:SER:OG	3:I:2321:ILE:O	2.15	0.60
3:B:2309:SER:OG	3:B:2321:ILE:O	2.15	0.60
3:G:622:THR:HG23	3:G:626:LEU:HD12	1.83	0.60
3:G:897:ARG:NH2	3:G:899:ASP:OD1	2.35	0.60
3:G:1089:TYR:HD2	3:G:1152:MET:HG2	1.67	0.60
3:I:1066:GLN:HB2	3:I:1071:ARG:HE	1.65	0.60
1:E:99:TYR:HB3	1:E:135:GLN:HB3	1.84	0.60
3:A:4583:SER:HB3	3:A:4631:PHE:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:545:ASP:OD1	3:I:582:HIS:NE2	2.28	0.60
1:C:99:TYR:HB3	1:C:135:GLN:HB3	1.84	0.60
1:K:99:TYR:HB3	1:K:135:GLN:HB3	1.84	0.59
3:A:1089:TYR:HD2	3:A:1152:MET:HG2	1.67	0.59
3:B:633:LEU:HD13	3:B:1639:LEU:HD21	1.84	0.59
3:G:2309:SER:OG	3:G:2321:ILE:O	2.16	0.59
3:G:2382:GLU:OE1	3:G:2385:ARG:NH1	2.31	0.59
3:B:4583:SER:HB3	3:B:4631:PHE:HE2	1.66	0.59
3:G:492:ASP:OD1	3:G:546:TRP:NE1	2.33	0.59
3:I:984:LEU:HD12	3:I:987:ARG:HH12	1.68	0.59
3:A:3959:LYS:NZ	3:A:4022:ASP:OD2	2.32	0.59
3:B:545:ASP:OD1	3:B:582:HIS:NE2	2.28	0.59
3:B:830:ARG:NH2	3:B:832:GLU:OE2	2.36	0.59
3:I:830:ARG:NH2	3:I:832:GLU:OE2	2.36	0.59
3:I:4583:SER:HB3	3:I:4631:PHE:HE2	1.66	0.59
3:A:1448:VAL:HG22	3:A:1554:VAL:HG23	1.85	0.59
3:B:2382:GLU:OE1	3:B:2385:ARG:NH1	2.31	0.59
3:G:633:LEU:HD13	3:G:1639:LEU:HD21	1.84	0.59
3:G:3751:VAL:O	3:G:3756:LYS:NZ	2.35	0.59
1:K:55:VAL:HG21	1:K:71:MET:HB2	1.85	0.59
3:A:894:GLY:HA3	3:A:903:LEU:HB3	1.85	0.59
3:A:897:ARG:NH2	3:A:899:ASP:OD1	2.35	0.59
3:B:894:GLY:HA3	3:B:903:LEU:HB3	1.85	0.59
3:G:830:ARG:NH2	3:G:832:GLU:OE2	2.36	0.59
3:G:3959:LYS:NZ	3:G:4022:ASP:OD2	2.32	0.59
3:A:3751:VAL:O	3:A:3756:LYS:NZ	2.35	0.59
3:G:984:LEU:HD12	3:G:987:ARG:HH12	1.68	0.59
3:B:1089:TYR:HD2	3:B:1152:MET:HG2	1.67	0.59
3:G:155:LYS:NZ	3:I:228:ASP:OD2	2.34	0.59
3:G:1505:GLN:HG3	3:I:2771:ILE:HG12	1.84	0.59
3:B:897:ARG:NH2	3:B:899:ASP:OD1	2.35	0.59
3:B:984:LEU:HD12	3:B:987:ARG:HH12	1.68	0.59
3:I:19:GLU:HG2	3:I:68:THR:HG22	1.85	0.59
3:I:2382:GLU:OE1	3:I:2385:ARG:NH1	2.31	0.59
3:G:516:LYS:O	3:G:520:ASN:ND2	2.31	0.59
3:I:1089:TYR:HD2	3:I:1152:MET:HG2	1.67	0.59
3:B:3751:VAL:O	3:B:3756:LYS:NZ	2.35	0.58
3:B:4138:ASP:O	3:B:4142:ASN:ND2	2.34	0.58
3:I:3751:VAL:O	3:I:3756:LYS:NZ	2.35	0.58
3:B:4570:ALA:O	3:B:4574:ASN:ND2	2.33	0.58
3:G:19:GLU:HG2	3:G:68:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:897:ARG:NH2	3:I:899:ASP:OD1	2.35	0.58
3:I:1619:ARG:NH2	3:I:1622:GLU:OE1	2.37	0.58
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.86	0.58
3:B:19:GLU:HG2	3:B:68:THR:HG22	1.85	0.58
3:B:3132:THR:HG23	3:B:3136:LEU:HD23	1.85	0.58
3:G:894:GLY:HA3	3:G:903:LEU:HB3	1.85	0.58
3:G:1448:VAL:HG22	3:G:1554:VAL:HG23	1.85	0.58
1:D:99:TYR:HB3	1:D:135:GLN:HB3	1.84	0.58
3:B:1448:VAL:HG22	3:B:1554:VAL:HG23	1.85	0.58
3:I:894:GLY:HA3	3:I:903:LEU:HB3	1.85	0.58
1:C:55:VAL:HG21	1:C:71:MET:HB2	1.85	0.58
2:O:23:VAL:HG22	2:O:47:LYS:HG2	1.86	0.58
3:I:1448:VAL:HG22	3:I:1554:VAL:HG23	1.85	0.58
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.86	0.58
1:E:55:VAL:HG21	1:E:71:MET:HB2	1.85	0.58
3:A:3579:LEU:HD12	3:A:3582:ARG:HE	1.69	0.58
3:A:633:LEU:HD13	3:A:1639:LEU:HD21	1.84	0.58
3:A:830:ARG:NH2	3:A:832:GLU:OE2	2.36	0.58
3:A:955:LEU:O	3:A:966:LYS:NZ	2.31	0.58
3:A:2650:ARG:NH1	3:A:2651:CYS:SG	2.77	0.58
3:B:516:LYS:O	3:B:520:ASN:ND2	2.31	0.58
3:B:2650:ARG:NH1	3:B:2651:CYS:SG	2.77	0.58
3:G:1619:ARG:NH2	3:G:1622:GLU:OE1	2.36	0.58
3:A:19:GLU:HG2	3:A:68:THR:HG22	1.85	0.58
3:B:1619:ARG:NH2	3:B:1622:GLU:OE1	2.37	0.58
3:G:2650:ARG:NH1	3:G:2651:CYS:SG	2.77	0.58
3:G:3132:THR:HG23	3:G:3136:LEU:HD23	1.85	0.57
3:I:633:LEU:HD13	3:I:1639:LEU:HD21	1.84	0.57
3:I:2650:ARG:NH1	3:I:2651:CYS:SG	2.77	0.57
3:I:56:GLN:O	3:I:309:THR:OG1	2.19	0.57
3:I:70:GLU:OE2	3:I:110:ARG:NE	2.34	0.57
3:I:492:ASP:OD1	3:I:546:TRP:NE1	2.33	0.57
1:D:55:VAL:HG21	1:D:71:MET:HB2	1.85	0.57
3:A:984:LEU:HD12	3:A:987:ARG:HH12	1.68	0.57
3:A:3132:THR:HG23	3:A:3136:LEU:HD23	1.85	0.57
3:I:3579:LEU:HD12	3:I:3582:ARG:HE	1.69	0.57
3:A:1619:ARG:NH2	3:A:1622:GLU:OE1	2.36	0.57
2:J:23:VAL:HG22	2:J:47:LYS:HG2	1.86	0.57
3:I:516:LYS:O	3:I:520:ASN:ND2	2.31	0.57
3:B:1987:SER:HB2	3:B:1994:ARG:HH22	1.70	0.57
3:G:110:ARG:NH2	3:G:117:TYR:OH	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4689:THR:OG1	3:A:4690:GLU:OE1	2.23	0.57
3:G:3579:LEU:HD12	3:G:3582:ARG:HE	1.69	0.57
3:I:3132:THR:HG23	3:I:3136:LEU:HD23	1.85	0.57
3:B:127:MET:SD	3:B:127:MET:N	2.78	0.57
3:B:492:ASP:OD1	3:B:546:TRP:NE1	2.33	0.57
3:G:1987:SER:HB2	3:G:1994:ARG:HH22	1.70	0.57
3:A:1792:ALA:O	3:A:2176:ASN:ND2	2.38	0.57
3:G:3759:GLU:OE2	3:G:3762:ARG:NH2	2.38	0.57
3:B:426:ARG:NH2	3:B:509:GLU:OE2	2.38	0.56
3:G:1131:ARG:NH1	3:G:1178:ALA:O	2.38	0.56
3:I:3759:GLU:OE2	3:I:3762:ARG:NH2	2.38	0.56
3:G:384:MET:SD	3:G:384:MET:N	2.77	0.56
3:I:426:ARG:NH2	3:I:509:GLU:OE2	2.38	0.56
3:A:110:ARG:NH2	3:A:117:TYR:OH	2.38	0.56
3:B:1792:ALA:O	3:B:2176:ASN:ND2	2.38	0.56
3:B:2514:ASN:ND2	3:B:2516:ASP:OD1	2.38	0.56
3:B:3324:VAL:HG11	3:B:3361:THR:HG22	1.88	0.56
3:B:3579:LEU:HD12	3:B:3582:ARG:HE	1.69	0.56
3:G:3324:VAL:HG11	3:G:3361:THR:HG22	1.88	0.56
3:I:1131:ARG:NH1	3:I:1178:ALA:O	2.38	0.56
3:I:1454:THR:OG1	3:I:1456:ASP:OD1	2.20	0.56
3:B:3270:ILE:HA	3:B:3274:LEU:HD12	1.88	0.56
3:G:426:ARG:NH2	3:G:509:GLU:OE2	2.38	0.56
3:G:2514:ASN:ND2	3:G:2516:ASP:OD1	2.39	0.56
3:I:110:ARG:NH2	3:I:117:TYR:OH	2.38	0.56
3:I:1792:ALA:O	3:I:2176:ASN:ND2	2.38	0.56
3:I:3324:VAL:HG11	3:I:3361:THR:HG22	1.88	0.56
3:A:127:MET:SD	3:A:127:MET:N	2.78	0.56
3:A:384:MET:SD	3:A:384:MET:N	2.77	0.56
3:A:3455:GLU:OE2	3:A:3508:SER:OG	2.24	0.56
3:B:1131:ARG:NH1	3:B:1178:ALA:O	2.38	0.56
3:B:3759:GLU:OE2	3:B:3762:ARG:NH2	2.38	0.56
3:B:4689:THR:OG1	3:B:4690:GLU:OE1	2.23	0.56
3:G:3270:ILE:HA	3:G:3274:LEU:HD12	1.88	0.56
3:A:3523:ASN:O	3:A:3582:ARG:NH2	2.39	0.56
3:I:1987:SER:HB2	3:I:1994:ARG:HH22	1.70	0.56
3:I:2514:ASN:ND2	3:I:2516:ASP:OD1	2.39	0.56
3:A:3759:GLU:OE2	3:A:3762:ARG:NH2	2.38	0.56
3:B:110:ARG:NH2	3:B:117:TYR:OH	2.38	0.56
3:B:302:VAL:HB	3:B:306:LYS:HE3	1.88	0.56
3:I:127:MET:SD	3:I:127:MET:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3523:ASN:O	3:I:3582:ARG:NH2	2.39	0.56
3:A:904:HIS:HD1	3:A:905:PRO:HD2	1.71	0.56
3:G:1792:ALA:O	3:G:2176:ASN:ND2	2.38	0.56
3:G:2644:LEU:HD13	3:G:2678:LEU:HD21	1.88	0.56
3:B:667:MET:SD	3:B:790:ARG:NH2	2.80	0.56
3:G:1676:LEU:HD22	3:G:2167:ILE:HD12	1.88	0.56
3:G:4942:GLU:OE1	3:I:4944:ARG:NH1	2.39	0.56
3:I:4570:ALA:O	3:I:4574:ASN:ND2	2.33	0.56
3:A:1141:ARG:HB3	3:G:3479:ALA:HA	1.88	0.55
3:A:2514:ASN:ND2	3:A:2516:ASP:OD1	2.39	0.55
3:A:3270:ILE:HA	3:A:3274:LEU:HD12	1.88	0.55
3:A:3324:VAL:HG11	3:A:3361:THR:HG22	1.88	0.55
3:B:3400:VAL:HG23	3:B:3403:ARG:HH21	1.71	0.55
3:G:127:MET:SD	3:G:127:MET:N	2.78	0.55
3:I:904:HIS:HD1	3:I:905:PRO:HD2	1.71	0.55
3:A:302:VAL:HB	3:A:306:LYS:HE3	1.88	0.55
3:A:426:ARG:NH2	3:A:509:GLU:OE2	2.38	0.55
3:G:904:HIS:HD1	3:G:905:PRO:HD2	1.71	0.55
1:K:145:MET:SD	1:K:145:MET:N	2.80	0.55
3:A:1131:ARG:NH1	3:A:1178:ALA:O	2.38	0.55
3:G:3400:VAL:HG23	3:G:3403:ARG:HH21	1.71	0.55
3:G:3455:GLU:OE2	3:G:3508:SER:OG	2.24	0.55
3:I:1676:LEU:HD22	3:I:2167:ILE:HD12	1.88	0.55
3:I:3270:ILE:HA	3:I:3274:LEU:HD12	1.88	0.55
1:D:145:MET:SD	1:D:145:MET:N	2.80	0.55
3:A:1676:LEU:HD22	3:A:2167:ILE:HD12	1.88	0.55
2:J:75:THR:HG23	2:J:98:VAL:HG22	1.89	0.55
3:B:904:HIS:HD1	3:B:905:PRO:HD2	1.71	0.55
3:B:2159:LEU:HD13	3:B:2203:MET:HG3	1.88	0.55
3:B:3169:LEU:HD12	3:B:3194:LEU:HD11	1.89	0.55
3:G:817:PRO:O	3:G:820:ARG:NH2	2.40	0.55
3:I:667:MET:SD	3:I:790:ARG:NH2	2.80	0.55
3:I:2827:ARG:NH2	3:I:2935:TYR:OH	2.40	0.55
1:C:145:MET:SD	1:C:145:MET:N	2.80	0.55
2:O:75:THR:HG23	2:O:98:VAL:HG22	1.89	0.55
3:B:2827:ARG:NH2	3:B:2935:TYR:OH	2.40	0.55
3:G:1057:ASP:OD1	3:G:1057:ASP:N	2.31	0.55
3:I:2159:LEU:HD13	3:I:2203:MET:HG3	1.88	0.55
3:I:2644:LEU:HD13	3:I:2678:LEU:HD21	1.88	0.55
3:A:667:MET:SD	3:A:790:ARG:NH2	2.80	0.55
3:A:3169:LEU:HD12	3:A:3194:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4944:ARG:NH1	3:B:4942:GLU:OE1	2.39	0.55
3:G:4689:THR:OG1	3:G:4690:GLU:OE1	2.23	0.55
3:I:4901:ILE:HG13	3:I:4913:ARG:NH2	2.21	0.55
2:F:75:THR:HG23	2:F:98:VAL:HG22	1.89	0.55
3:A:1987:SER:HB2	3:A:1994:ARG:HH22	1.70	0.55
3:B:3523:ASN:O	3:B:3582:ARG:NH2	2.39	0.55
3:B:3696:ASP:OD2	3:B:3773:ARG:NE	2.38	0.55
3:I:3940:LYS:O	3:I:4002:LYS:NZ	2.39	0.55
3:I:4689:THR:OG1	3:I:4690:GLU:OE1	2.23	0.55
1:E:145:MET:N	1:E:145:MET:SD	2.80	0.55
3:A:817:PRO:O	3:A:820:ARG:NH2	2.40	0.55
3:A:2827:ARG:NH2	3:A:2935:TYR:OH	2.40	0.55
3:G:302:VAL:HB	3:G:306:LYS:HE3	1.88	0.55
3:G:2827:ARG:NH2	3:G:2935:TYR:OH	2.40	0.55
3:G:3696:ASP:OD2	3:G:3773:ARG:NE	2.38	0.55
3:G:4901:ILE:HG13	3:G:4913:ARG:NH2	2.21	0.55
3:I:3169:LEU:HD12	3:I:3194:LEU:HD11	1.89	0.55
3:I:4238:CYS:HA	3:I:4989:MET:HE1	1.89	0.55
3:A:2159:LEU:HD13	3:A:2203:MET:HG3	1.88	0.55
3:B:4137:ARG:NH2	3:B:4199:GLU:OE2	2.40	0.55
3:G:3523:ASN:O	3:G:3582:ARG:NH2	2.39	0.55
3:G:4137:ARG:NH2	3:G:4199:GLU:OE2	2.40	0.55
3:G:4238:CYS:HA	3:G:4989:MET:HE1	1.89	0.55
3:I:384:MET:SD	3:I:384:MET:N	2.77	0.55
3:I:4676:GLU:OE2	3:I:4698:LYS:NZ	2.40	0.55
2:H:75:THR:HG23	2:H:98:VAL:HG22	1.89	0.55
3:B:4944:ARG:NH1	3:I:4942:GLU:OE1	2.41	0.55
3:G:2159:LEU:HD13	3:G:2203:MET:HG3	1.88	0.55
3:G:2519:LEU:HD13	3:G:2575:ARG:HG3	1.89	0.55
3:I:302:VAL:HB	3:I:306:LYS:HE3	1.88	0.55
3:A:1062:GLN:NE2	3:A:1064:GLU:OE1	2.37	0.54
3:A:3400:VAL:HG23	3:A:3403:ARG:HH21	1.71	0.54
3:A:3940:LYS:O	3:A:4002:LYS:NZ	2.39	0.54
3:G:667:MET:SD	3:G:790:ARG:NH2	2.80	0.54
3:G:3169:LEU:HD12	3:G:3194:LEU:HD11	1.89	0.54
3:I:2892:GLN:NE2	3:I:2895:GLU:OE2	2.40	0.54
3:I:3400:VAL:HG23	3:I:3403:ARG:HH21	1.71	0.54
3:A:2892:GLN:NE2	3:A:2895:GLU:OE2	2.40	0.54
3:A:4570:ALA:O	3:A:4574:ASN:ND2	2.33	0.54
3:A:4676:GLU:OE2	3:A:4698:LYS:NZ	2.40	0.54
3:I:924:MET:HG3	5:I:5305:ATP:HN61	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.88	0.54
2:O:88:PRO:HB2	3:B:1680:ARG:HH12	1.73	0.54
3:B:1676:LEU:HD22	3:B:2167:ILE:HD12	1.88	0.54
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.88	0.54
3:B:3455:GLU:OE2	3:B:3508:SER:OG	2.24	0.54
3:G:2892:GLN:NE2	3:G:2895:GLU:OE2	2.40	0.54
1:E:95:ASP:OD2	1:E:97:ASN:ND2	2.41	0.54
3:A:70:GLU:OE2	3:A:110:ARG:NE	2.34	0.54
3:A:155:LYS:NZ	3:G:228:ASP:OD2	2.31	0.54
3:A:530:ILE:HG22	3:A:536:ASN:HB3	1.90	0.54
3:A:4137:ARG:NH2	3:A:4199:GLU:OE2	2.40	0.54
3:A:4901:ILE:HG13	3:A:4913:ARG:NH2	2.21	0.54
3:B:530:ILE:HG22	3:B:536:ASN:HB3	1.90	0.54
3:B:4676:GLU:OE2	3:B:4698:LYS:NZ	2.40	0.54
3:B:4901:ILE:HG13	3:B:4913:ARG:NH2	2.21	0.54
3:G:1062:GLN:NE2	3:G:1064:GLU:OE1	2.37	0.54
3:G:1252:HIS:O	3:G:1275:ARG:NH1	2.41	0.54
3:I:23:GLN:NE2	3:I:203:ASN:OD1	2.41	0.54
3:I:1252:HIS:O	3:I:1275:ARG:NH1	2.41	0.54
3:I:2519:LEU:HD13	3:I:2575:ARG:HG3	1.89	0.54
3:B:23:GLN:NE2	3:B:203:ASN:OD1	2.41	0.54
3:B:1252:HIS:O	3:B:1275:ARG:NH1	2.41	0.54
3:A:492:ASP:OD1	3:A:546:TRP:NE1	2.33	0.54
3:B:2892:GLN:NE2	3:B:2895:GLU:OE2	2.40	0.54
3:G:23:GLN:NE2	3:G:203:ASN:OD1	2.40	0.54
3:I:3233:PRO:HB2	3:I:3238:GLU:HB2	1.90	0.54
3:B:3335:MET:SD	3:B:3403:ARG:NH1	2.81	0.54
3:G:56:GLN:O	3:G:309:THR:OG1	2.19	0.54
3:G:70:GLU:OE2	3:G:110:ARG:NE	2.34	0.54
3:G:530:ILE:HG22	3:G:536:ASN:HB3	1.90	0.54
3:G:3335:MET:SD	3:G:3403:ARG:NH1	2.81	0.54
3:G:4570:ALA:O	3:G:4574:ASN:ND2	2.33	0.54
3:I:817:PRO:O	3:I:820:ARG:NH2	2.40	0.54
3:I:3335:MET:SD	3:I:3403:ARG:NH1	2.81	0.54
3:I:4137:ARG:NH2	3:I:4199:GLU:OE2	2.40	0.54
3:G:924:MET:HG3	5:G:5305:ATP:HN61	1.72	0.54
3:G:2178:MET:HE3	3:G:2182:ILE:HD11	1.90	0.54
3:I:530:ILE:HG22	3:I:536:ASN:HB3	1.90	0.54
3:B:817:PRO:O	3:B:820:ARG:NH2	2.40	0.54
3:B:913:LEU:HD12	3:B:914:PRO:HD2	1.89	0.54
3:G:1454:THR:OG1	3:G:1456:ASP:OD1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ASP:OD2	1:C:97:ASN:ND2	2.41	0.54
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.89	0.54
3:A:4942:GLU:OE1	3:G:4944:ARG:NH1	2.41	0.54
3:B:924:MET:HG3	5:B:5305:ATP:HN61	1.72	0.54
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.89	0.54
3:B:3233:PRO:HB2	3:B:3238:GLU:HB2	1.90	0.54
3:G:293:LEU:HD13	3:G:378:LEU:HD12	1.90	0.54
3:G:4676:GLU:OE2	3:G:4698:LYS:NZ	2.40	0.54
3:I:2970:SER:HA	3:I:2973:PHE:CE2	2.43	0.54
3:I:3455:GLU:OE2	3:I:3508:SER:OG	2.24	0.54
3:A:23:GLN:NE2	3:A:203:ASN:OD1	2.40	0.53
3:G:2970:SER:HA	3:G:2973:PHE:CE2	2.44	0.53
3:A:293:LEU:HD13	3:A:378:LEU:HD12	1.90	0.53
3:B:1454:THR:OG1	3:B:1456:ASP:OD1	2.20	0.53
3:B:3940:LYS:O	3:B:4002:LYS:NZ	2.39	0.53
3:A:1252:HIS:O	3:A:1275:ARG:NH1	2.41	0.53
3:B:4238:CYS:HA	3:B:4989:MET:HE1	1.89	0.53
3:I:293:LEU:HD13	3:I:378:LEU:HD12	1.90	0.53
1:K:95:ASP:OD2	1:K:97:ASN:ND2	2.41	0.53
3:A:3335:MET:SD	3:A:3403:ARG:NH1	2.81	0.53
3:I:913:LEU:HD12	3:I:914:PRO:HD2	1.89	0.53
1:K:27:ILE:HB	1:K:63:ILE:HB	1.91	0.53
1:D:95:ASP:OD2	1:D:97:ASN:ND2	2.41	0.53
3:A:924:MET:HG3	5:A:5305:ATP:HN61	1.72	0.53
3:A:2178:MET:HE3	3:A:2182:ILE:HD11	1.90	0.53
3:G:745:SER:HB2	3:G:758:ARG:HB2	1.91	0.53
3:I:1062:GLN:NE2	3:I:1064:GLU:OE1	2.37	0.53
3:I:2178:MET:HE3	3:I:2182:ILE:HD11	1.90	0.53
3:A:3157:ILE:HA	3:A:3161:VAL:HB	1.91	0.53
3:A:4238:CYS:HA	3:A:4989:MET:HE1	1.89	0.53
3:G:3233:PRO:HB2	3:G:3238:GLU:HB2	1.90	0.53
3:A:913:LEU:HD12	3:A:914:PRO:HD2	1.89	0.53
3:G:3850:GLN:NE2	3:G:3872:GLU:OE1	2.36	0.53
3:G:3940:LYS:O	3:G:4002:LYS:NZ	2.39	0.53
1:D:27:ILE:HB	1:D:63:ILE:HB	1.90	0.53
3:A:3628:ARG:NH1	3:A:3857:GLY:O	2.42	0.53
3:G:400:ALA:HA	3:G:403:MET:HE3	1.91	0.53
3:G:913:LEU:HD12	3:G:914:PRO:HD2	1.89	0.53
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.43	0.53
3:B:228:ASP:OD2	3:I:155:LYS:NZ	2.34	0.53
3:G:975:VAL:HG12	3:G:1044:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4138:ASP:O	3:G:4142:ASN:ND2	2.34	0.53
3:I:215:THR:HG22	3:I:273:HIS:HA	1.90	0.53
3:I:975:VAL:HG12	3:I:1044:ARG:HH11	1.74	0.53
3:B:1062:GLN:NE2	3:B:1064:GLU:OE1	2.37	0.53
3:B:2178:MET:HE3	3:B:2182:ILE:HD11	1.90	0.53
3:B:3850:GLN:NE2	3:B:3872:GLU:OE1	2.36	0.53
3:G:3157:ILE:HA	3:G:3161:VAL:HB	1.91	0.53
3:B:2754:PHE:HE2	3:B:2813:LEU:HD11	1.74	0.52
3:A:215:THR:HG22	3:A:273:HIS:HA	1.90	0.52
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.43	0.52
3:B:3628:ARG:NH1	3:B:3857:GLY:O	2.42	0.52
3:G:1093:GLU:HB3	3:G:1201:HIS:HB3	1.92	0.52
3:G:3296:LEU:HG	3:G:3297:PRO:HD3	1.92	0.52
3:I:745:SER:HB2	3:I:758:ARG:HB2	1.91	0.52
3:I:4759:ASP:O	3:I:4761:PRO:HD3	2.09	0.52
1:C:1:ALA:HB3	3:B:3861:GLU:HG2	1.90	0.52
3:A:4759:ASP:O	3:A:4761:PRO:HD3	2.09	0.52
3:B:3157:ILE:HA	3:B:3161:VAL:HB	1.91	0.52
3:G:2754:PHE:HE2	3:G:2813:LEU:HD11	1.74	0.52
3:I:400:ALA:HA	3:I:403:MET:HE3	1.91	0.52
1:E:27:ILE:HB	1:E:63:ILE:HB	1.90	0.52
3:A:3296:LEU:HG	3:A:3297:PRO:HD3	1.92	0.52
3:B:70:GLU:OE2	3:B:110:ARG:NE	2.34	0.52
3:B:215:THR:HG22	3:B:273:HIS:HA	1.90	0.52
3:B:293:LEU:HD13	3:B:378:LEU:HD12	1.90	0.52
3:B:499:THR:HG23	3:B:502:HIS:H	1.74	0.52
3:A:3233:PRO:HB2	3:A:3238:GLU:HB2	1.90	0.52
3:I:1093:GLU:HB3	3:I:1201:HIS:HB3	1.92	0.52
3:I:3628:ARG:NH1	3:I:3857:GLY:O	2.42	0.52
1:C:27:ILE:HB	1:C:63:ILE:HB	1.90	0.52
3:A:499:THR:HG23	3:A:502:HIS:H	1.74	0.52
3:I:3813:GLN:NE2	3:I:3890:LEU:O	2.43	0.52
3:A:745:SER:HB2	3:A:758:ARG:HB2	1.91	0.52
3:A:1093:GLU:HB3	3:A:1201:HIS:HB3	1.92	0.52
3:B:2986:VAL:HG22	3:B:2988:LYS:H	1.75	0.52
3:B:3296:LEU:HG	3:B:3297:PRO:HD3	1.92	0.52
3:B:919:ASN:HA	3:B:922:LEU:HB2	1.92	0.52
3:G:215:THR:HG22	3:G:273:HIS:HA	1.90	0.52
3:G:499:THR:HG23	3:G:502:HIS:H	1.74	0.52
3:I:2986:VAL:HG22	3:I:2988:LYS:H	1.75	0.52
3:I:3157:ILE:HA	3:I:3161:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:975:VAL:HG12	3:B:1044:ARG:HH11	1.74	0.52
3:B:1156:THR:OG1	3:B:1157:GLU:OE1	2.28	0.52
3:B:3288:GLY:HA2	3:B:3303:PRO:HB3	1.91	0.52
3:G:3288:GLY:HA2	3:G:3303:PRO:HB3	1.91	0.52
3:B:56:GLN:O	3:B:309:THR:OG1	2.19	0.51
3:B:3446:SER:O	3:B:3452:LYS:NZ	2.42	0.51
3:G:919:ASN:HA	3:G:922:LEU:HB2	1.92	0.51
3:I:3296:LEU:HG	3:I:3297:PRO:HD3	1.92	0.51
3:A:975:VAL:HG12	3:A:1044:ARG:HH11	1.74	0.51
3:A:3696:ASP:OD2	3:A:3773:ARG:NE	2.38	0.51
3:B:1093:GLU:HB3	3:B:1201:HIS:HB3	1.92	0.51
3:I:919:ASN:HA	3:I:922:LEU:HB2	1.92	0.51
3:B:955:LEU:O	3:B:966:LYS:NZ	2.31	0.51
3:G:3813:GLN:NE2	3:G:3890:LEU:O	2.43	0.51
3:G:4759:ASP:O	3:G:4761:PRO:HD3	2.09	0.51
3:A:400:ALA:HA	3:A:403:MET:HE3	1.91	0.51
3:B:400:ALA:HA	3:B:403:MET:HE3	1.91	0.51
3:B:4759:ASP:O	3:B:4761:PRO:HD3	2.09	0.51
3:G:408:ALA:HB2	3:G:483:MET:HE1	1.92	0.51
3:G:891:TRP:HA	3:G:902:ARG:HB3	1.93	0.51
3:I:3414:ARG:HE	3:I:3472:ALA:HB3	1.75	0.51
3:I:3850:GLN:NE2	3:I:3872:GLU:OE1	2.36	0.51
3:A:3288:GLY:HA2	3:A:3303:PRO:HB3	1.91	0.51
3:B:745:SER:HB2	3:B:758:ARG:HB2	1.91	0.51
3:B:3414:ARG:HE	3:B:3472:ALA:HB3	1.75	0.51
3:I:891:TRP:HA	3:I:902:ARG:HB3	1.93	0.51
3:I:3696:ASP:OD2	3:I:3773:ARG:NE	2.38	0.51
3:A:56:GLN:O	3:A:309:THR:OG1	2.19	0.51
3:A:891:TRP:HA	3:A:902:ARG:HB3	1.93	0.51
3:A:3850:GLN:NE2	3:A:3872:GLU:OE1	2.36	0.51
3:B:35:LEU:HD11	3:B:189:LEU:HD13	1.93	0.51
3:G:176:SER:OG	3:G:178:ARG:NH1	2.38	0.51
3:I:2754:PHE:HE2	3:I:2813:LEU:HD11	1.74	0.51
3:A:408:ALA:HB2	3:A:483:MET:HE1	1.92	0.51
3:A:1454:THR:OG1	3:A:1456:ASP:OD1	2.20	0.51
3:A:2754:PHE:HE2	3:A:2813:LEU:HD11	1.74	0.51
3:B:384:MET:SD	3:B:384:MET:N	2.77	0.51
3:I:499:THR:HG23	3:I:502:HIS:H	1.74	0.51
3:A:3414:ARG:HE	3:A:3472:ALA:HB3	1.75	0.51
3:I:3132:THR:HA	3:I:3136:LEU:HB3	1.93	0.51
3:B:3479:ALA:HA	3:I:1141:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3552:PHE:O	3:G:3556:ASN:ND2	2.35	0.51
3:I:1992:ALA:HA	3:I:1995:THR:HG22	1.93	0.51
3:A:35:LEU:HD11	3:A:189:LEU:HD13	1.93	0.51
3:A:1272:LEU:HD22	3:A:1289:LEU:HD11	1.93	0.51
3:B:3208:PRO:HB2	3:B:3237:GLU:HG3	1.93	0.51
3:I:228:ASP:OD1	3:I:228:ASP:N	2.44	0.51
3:I:955:LEU:O	3:I:966:LYS:NZ	2.31	0.51
1:C:130:ILE:O	3:B:3499:ARG:NH1	2.43	0.50
3:A:1057:ASP:OD1	3:A:1057:ASP:N	2.31	0.50
3:B:3813:GLN:NE2	3:B:3890:LEU:O	2.43	0.50
3:G:1272:LEU:HD22	3:G:1289:LEU:HD11	1.93	0.50
3:I:35:LEU:HD11	3:I:189:LEU:HD13	1.93	0.50
3:I:2736:ASP:OD1	3:I:2736:ASP:N	2.44	0.50
3:I:3288:GLY:HA2	3:I:3303:PRO:HB3	1.91	0.50
3:B:408:ALA:HB2	3:B:483:MET:HE1	1.92	0.50
3:G:3414:ARG:HE	3:G:3472:ALA:HB3	1.75	0.50
1:C:86:ARG:NH2	1:C:87:GLU:OE2	2.45	0.50
3:A:919:ASN:HA	3:A:922:LEU:HB2	1.92	0.50
3:B:891:TRP:HA	3:B:902:ARG:HB3	1.93	0.50
3:G:1289:LEU:HD12	3:G:1562:ILE:HD11	1.93	0.50
3:I:4138:ASP:O	3:I:4142:ASN:ND2	2.34	0.50
3:B:1272:LEU:HD22	3:B:1289:LEU:HD11	1.93	0.50
3:G:35:LEU:HD11	3:G:189:LEU:HD13	1.93	0.50
3:G:2986:VAL:HG22	3:G:2988:LYS:H	1.75	0.50
3:G:3132:THR:HA	3:G:3136:LEU:HB3	1.93	0.50
3:I:408:ALA:HB2	3:I:483:MET:HE1	1.92	0.50
3:I:1272:LEU:HD22	3:I:1289:LEU:HD11	1.93	0.50
2:F:88:PRO:HB2	3:A:1680:ARG:HH12	1.76	0.50
3:A:835:ARG:NH2	3:A:1210:SER:O	2.38	0.50
3:I:892:THR:HA	3:I:961:MET:HB3	1.94	0.50
3:A:892:THR:HA	3:A:961:MET:HB3	1.94	0.50
1:D:86:ARG:NH2	1:D:87:GLU:OE2	2.45	0.50
3:A:2986:VAL:HG22	3:A:2988:LYS:H	1.75	0.50
3:G:3628:ARG:NH1	3:G:3857:GLY:O	2.42	0.50
3:A:4138:ASP:O	3:A:4142:ASN:ND2	2.34	0.50
3:B:4801:LEU:HD22	9:B:5308:L9R:H13A	1.93	0.50
3:G:4172:GLU:OE1	3:G:4175:ARG:NH1	2.45	0.50
3:A:1992:ALA:HA	3:A:1995:THR:HG22	1.93	0.50
3:G:955:LEU:O	3:G:966:LYS:NZ	2.31	0.50
3:B:1733:GLU:HG2	3:B:2201:LEU:HD23	1.94	0.49
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4172:GLU:OE1	3:B:4175:ARG:NH1	2.45	0.49
3:G:892:THR:HA	3:G:961:MET:HB3	1.94	0.49
3:G:1992:ALA:HA	3:G:1995:THR:HG22	1.93	0.49
3:G:3208:PRO:HB2	3:G:3237:GLU:HG3	1.93	0.49
3:I:2867:LEU:HB2	3:I:2928:LYS:HZ3	1.77	0.49
3:A:1232:ARG:NH2	3:A:1828:ASP:O	2.45	0.49
3:A:4172:GLU:OE1	3:A:4175:ARG:NH1	2.45	0.49
1:K:86:ARG:NH2	1:K:87:GLU:OE2	2.45	0.49
1:E:111:ASN:O	3:G:1996:ARG:NH2	2.34	0.49
3:A:1289:LEU:HD12	3:A:1562:ILE:HD11	1.93	0.49
3:A:1733:GLU:HG2	3:A:2201:LEU:HD23	1.94	0.49
3:G:4801:LEU:HD22	9:G:5308:L9R:H13A	1.93	0.49
1:E:66:PRO:HG3	3:G:2186:MET:HB3	1.94	0.49
3:A:1469:VAL:HG13	3:A:1492:CYS:HB3	1.95	0.49
3:B:892:THR:HA	3:B:961:MET:HB3	1.94	0.49
3:G:889:GLN:HB3	3:G:902:ARG:HH21	1.78	0.49
3:G:3133:THR:HG23	3:G:3134:VAL:HG23	1.94	0.49
3:I:1980:LEU:HD11	3:I:1994:ARG:HB3	1.94	0.49
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.93	0.49
3:A:4972:PRO:HB3	3:B:5024:ALA:HB3	1.94	0.49
3:B:228:ASP:OD1	3:B:228:ASP:N	2.44	0.49
3:B:1289:LEU:HD12	3:B:1562:ILE:HD11	1.93	0.49
3:G:4182:GLU:OE1	3:G:4983:HIS:NE2	2.46	0.49
3:I:3133:THR:HG23	3:I:3134:VAL:HG23	1.94	0.49
3:I:4172:GLU:OE1	3:I:4175:ARG:NH1	2.45	0.49
3:I:4182:GLU:OE1	3:I:4983:HIS:NE2	2.46	0.49
1:E:86:ARG:NH2	1:E:87:GLU:OE2	2.45	0.49
3:B:1992:ALA:HA	3:B:1995:THR:HG22	1.93	0.49
3:G:1232:ARG:NH2	3:G:1828:ASP:O	2.45	0.49
3:G:2867:LEU:HB2	3:G:2928:LYS:HZ3	1.77	0.49
3:I:1289:LEU:HD12	3:I:1562:ILE:HD11	1.93	0.49
3:I:3208:PRO:HB2	3:I:3237:GLU:HG3	1.93	0.49
3:A:2867:LEU:HB2	3:A:2928:LYS:HZ3	1.78	0.49
3:A:3208:PRO:HB2	3:A:3237:GLU:HG3	1.93	0.49
3:B:2884:ASN:OD1	3:B:2885:THR:N	2.46	0.49
3:B:3633:VAL:HG12	3:B:3637:ARG:HE	1.78	0.49
3:A:4182:GLU:OE1	3:A:4983:HIS:NE2	2.46	0.49
3:A:4801:LEU:HD22	9:A:5308:L9R:H13A	1.93	0.49
3:B:1980:LEU:HD11	3:B:1994:ARG:HB3	1.94	0.49
3:I:1733:GLU:HG2	3:I:2201:LEU:HD23	1.95	0.49
3:I:3459:VAL:HG13	3:I:3464:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3132:THR:HG22	3:A:3137:LEU:HD13	1.95	0.49
3:A:3133:THR:HG23	3:A:3134:VAL:HG23	1.94	0.49
3:A:5012:LYS:NZ	3:A:5016:GLU:OE2	2.41	0.49
3:B:2867:LEU:HB2	3:B:2928:LYS:HZ3	1.77	0.49
3:B:4182:GLU:OE1	3:B:4983:HIS:NE2	2.46	0.49
3:I:2884:ASN:OD1	3:I:2885:THR:N	2.46	0.49
3:A:3633:VAL:HG12	3:A:3637:ARG:HE	1.78	0.49
2:O:55:VAL:HA	3:B:1784:ALA:HA	1.95	0.49
3:G:3633:VAL:HG12	3:G:3637:ARG:HE	1.78	0.49
3:I:3132:THR:HG22	3:I:3137:LEU:HD13	1.95	0.49
3:I:4801:LEU:HD22	9:I:5308:L9R:H13A	1.93	0.49
3:A:1447:CYS:HB3	3:A:1555:LEU:HB3	1.95	0.48
3:B:3459:VAL:HG13	3:B:3464:ILE:HB	1.95	0.48
3:G:228:ASP:OD1	3:G:228:ASP:N	2.44	0.48
3:G:1980:LEU:HD11	3:G:1994:ARG:HB3	1.94	0.48
3:G:2884:ASN:OD1	3:G:2885:THR:N	2.46	0.48
3:A:3459:VAL:HG13	3:A:3464:ILE:HB	1.95	0.48
2:J:88:PRO:HB2	3:I:1680:ARG:HH12	1.77	0.48
3:B:889:GLN:HB3	3:B:902:ARG:HH21	1.78	0.48
3:B:990:GLU:HG3	3:B:1024:TYR:HB3	1.94	0.48
3:G:1733:GLU:HG2	3:G:2201:LEU:HD23	1.95	0.48
3:G:3514:LEU:HD21	3:G:3602:VAL:HG13	1.95	0.48
3:I:4983:HIS:O	5:I:5301:ATP:N6	2.46	0.48
1:C:117:THR:OG1	1:C:120:GLU:OE1	2.31	0.48
3:A:4983:HIS:O	5:A:5301:ATP:N6	2.46	0.48
3:B:1232:ARG:NH2	3:B:1828:ASP:O	2.45	0.48
3:B:3514:LEU:HD21	3:B:3602:VAL:HG13	1.95	0.48
3:G:919:ASN:HA	3:G:922:LEU:HD23	1.96	0.48
3:G:990:GLU:HG3	3:G:1024:TYR:HB3	1.94	0.48
3:G:3459:VAL:HG13	3:G:3464:ILE:HB	1.95	0.48
3:G:4731:ILE:O	3:I:4074:SER:OG	2.31	0.48
3:I:2725:LYS:HE2	3:I:2738:ARG:HH22	1.79	0.48
3:A:889:GLN:HB3	3:A:902:ARG:HH21	1.78	0.48
3:B:1575:LEU:HD13	3:B:1579:MET:HE3	1.95	0.48
3:G:3545:THR:HG22	3:G:3548:GLU:HG3	1.95	0.48
3:G:3757:GLU:OE2	3:G:3761:GLN:NE2	2.46	0.48
3:I:919:ASN:HA	3:I:922:LEU:HD23	1.96	0.48
3:I:3633:VAL:HG12	3:I:3637:ARG:HE	1.78	0.48
3:A:228:ASP:OD1	3:A:228:ASP:N	2.44	0.48
3:A:516:LYS:O	3:A:520:ASN:ND2	2.31	0.48
3:A:1575:LEU:HD13	3:A:1579:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1447:CYS:HB3	3:B:1555:LEU:HB3	1.95	0.48
3:B:1469:VAL:HG13	3:B:1492:CYS:HB3	1.95	0.48
3:B:2725:LYS:HE2	3:B:2738:ARG:HH22	1.78	0.48
3:B:3133:THR:HG23	3:B:3134:VAL:HG23	1.94	0.48
3:G:2736:ASP:O	3:G:2738:ARG:NH1	2.47	0.48
3:I:990:GLU:HG3	3:I:1024:TYR:HB3	1.94	0.48
3:I:1447:CYS:HB3	3:I:1555:LEU:HB3	1.95	0.48
3:I:3552:PHE:O	3:I:3556:ASN:ND2	2.35	0.48
9:I:5307:L9R:H6A	9:I:5307:L9R:H4A	1.47	0.48
3:A:1101:ARG:NH1	3:A:1115:LEU:O	2.46	0.48
3:A:3504:SER:HG	3:A:3507:THR:HG1	1.54	0.48
2:H:42:ARG:HD3	3:G:1780:PRO:HG2	1.96	0.48
3:B:1101:ARG:NH1	3:B:1115:LEU:O	2.46	0.48
3:G:684:VAL:HG22	3:G:781:VAL:HG12	1.96	0.48
3:G:2736:ASP:OD1	3:G:2736:ASP:N	2.44	0.48
3:G:3132:THR:HG22	3:G:3137:LEU:HD13	1.94	0.48
3:G:3316:LEU:HD21	3:G:3346:VAL:HG23	1.96	0.48
3:I:1469:VAL:HG13	3:I:1492:CYS:HB3	1.95	0.48
1:D:2:ASP:OD2	3:I:2244:ARG:NH1	2.46	0.48
3:A:919:ASN:HA	3:A:922:LEU:HD23	1.96	0.48
3:A:2884:ASN:OD1	3:A:2885:THR:N	2.46	0.48
3:A:4074:SER:OG	3:B:4731:ILE:O	2.31	0.48
3:B:925:SER:O	3:B:928:THR:OG1	2.32	0.48
3:G:1469:VAL:HG13	3:G:1492:CYS:HB3	1.95	0.48
3:I:728:ARG:NH2	3:I:1489:CYS:SG	2.87	0.48
3:A:3316:LEU:HD21	3:A:3346:VAL:HG23	1.96	0.48
3:A:4731:ILE:O	3:G:4074:SER:OG	2.31	0.48
3:B:3132:THR:HG22	3:B:3137:LEU:HD13	1.95	0.48
3:B:4983:HIS:O	5:B:5301:ATP:N6	2.46	0.48
3:G:2725:LYS:HE2	3:G:2738:ARG:HH22	1.79	0.48
3:I:1575:LEU:HD13	3:I:1579:MET:HE3	1.95	0.48
3:I:3757:GLU:OE2	3:I:3761:GLN:NE2	2.46	0.48
1:E:133:ASP:HA	3:G:3460:VAL:HG11	1.95	0.48
3:A:990:GLU:HG3	3:A:1024:TYR:HB3	1.94	0.48
3:A:2587:TYR:O	3:A:2590:SER:OG	2.31	0.48
3:A:3545:THR:HG22	3:A:3548:GLU:HG3	1.95	0.48
3:B:4555:LEU:HD21	3:B:4656:LEU:HD22	1.96	0.48
3:G:1447:CYS:HB3	3:G:1555:LEU:HB3	1.95	0.48
3:I:3545:THR:HG22	3:I:3548:GLU:HG3	1.95	0.48
3:I:4555:LEU:HD21	3:I:4656:LEU:HD22	1.96	0.48
3:A:793:LEU:HD12	3:A:821:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3757:GLU:OE2	3:A:3761:GLN:NE2	2.46	0.48
3:B:728:ARG:NH2	3:B:1489:CYS:SG	2.87	0.48
3:B:793:LEU:HD12	3:B:821:LEU:HD21	1.96	0.48
3:B:3768:SER:HA	3:B:3771:HIS:CD2	2.49	0.48
3:G:3768:SER:HA	3:G:3771:HIS:CD2	2.49	0.48
3:I:1078:GLU:OE2	3:I:1654:SER:OG	2.26	0.48
3:A:1503:PRO:HA	3:A:1508:ARG:HH22	1.79	0.47
3:A:1980:LEU:HD11	3:A:1994:ARG:HB3	1.94	0.47
3:A:2725:LYS:HE2	3:A:2738:ARG:HH22	1.79	0.47
3:A:2736:ASP:O	3:A:2738:ARG:NH1	2.47	0.47
3:B:919:ASN:HA	3:B:922:LEU:HD23	1.96	0.47
3:B:2736:ASP:O	3:B:2738:ARG:NH1	2.47	0.47
3:B:3545:THR:HG22	3:B:3548:GLU:HG3	1.95	0.47
3:B:3757:GLU:OE2	3:B:3761:GLN:NE2	2.46	0.47
3:G:728:ARG:NH2	3:G:1489:CYS:SG	2.87	0.47
3:G:3946:GLN:OE1	3:G:3949:ARG:NH2	2.39	0.47
3:A:728:ARG:NH2	3:A:1489:CYS:SG	2.87	0.47
3:A:3263:TYR:HD1	3:A:3270:ILE:HD12	1.79	0.47
3:A:3768:SER:HA	3:A:3771:HIS:CD2	2.49	0.47
3:A:3813:GLN:NE2	3:A:3890:LEU:O	2.43	0.47
3:B:1503:PRO:HA	3:B:1508:ARG:HH22	1.79	0.47
3:B:3263:TYR:HD1	3:B:3270:ILE:HD12	1.79	0.47
3:G:4983:HIS:O	5:G:5301:ATP:N6	2.46	0.47
3:I:1503:PRO:HA	3:I:1508:ARG:HH22	1.79	0.47
3:I:3514:LEU:HD21	3:I:3602:VAL:HG13	1.95	0.47
1:D:13:LYS:NZ	3:I:2187:ASN:O	2.43	0.47
3:A:176:SER:OG	3:A:178:ARG:NH1	2.38	0.47
3:A:935:LEU:HD23	3:A:987:ARG:HH11	1.80	0.47
3:I:889:GLN:HB3	3:I:902:ARG:HH21	1.78	0.47
3:I:2029:GLN:NE2	3:I:2033:ASP:OD1	2.48	0.47
3:I:2736:ASP:O	3:I:2738:ARG:NH1	2.47	0.47
3:I:3768:SER:HA	3:I:3771:HIS:CD2	2.49	0.47
1:C:13:LYS:NZ	3:B:2187:ASN:O	2.45	0.47
3:B:3552:PHE:O	3:B:3556:ASN:ND2	2.35	0.47
3:B:4006:ASP:OD1	3:B:4006:ASP:N	2.46	0.47
3:G:1575:LEU:HD13	3:G:1579:MET:HE3	1.95	0.47
3:I:2203:MET:HE3	3:I:2235:PHE:HZ	1.80	0.47
3:A:1569:GLN:HB2	3:A:1572:ILE:HD12	1.97	0.47
9:A:5308:L9R:H44	9:A:5308:L9R:H47A	1.52	0.47
3:I:793:LEU:HD12	3:I:821:LEU:HD21	1.96	0.47
3:I:925:SER:O	3:I:928:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4972:PRO:HB3	3:I:5024:ALA:HB3	1.96	0.47
3:G:793:LEU:HD12	3:G:821:LEU:HD21	1.96	0.47
3:G:3535:LEU:O	3:G:3538:THR:OG1	2.31	0.47
3:G:4006:ASP:OD1	3:G:4006:ASP:N	2.46	0.47
3:A:144:GLU:OE1	3:G:2452:ARG:NH1	2.47	0.47
3:A:2815:ALA:HB1	3:A:2881:ASN:HD22	1.80	0.47
3:A:3479:ALA:HA	3:B:1141:ARG:HB3	1.96	0.47
3:A:3514:LEU:HD21	3:A:3602:VAL:HG13	1.95	0.47
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.95	0.47
3:B:935:LEU:HD23	3:B:987:ARG:HH11	1.80	0.47
3:B:2020:ASP:OD1	3:B:2020:ASP:N	2.47	0.47
3:B:2029:GLN:NE2	3:B:2033:ASP:OD1	2.47	0.47
3:B:2815:ALA:HB1	3:B:2881:ASN:HD22	1.80	0.47
3:G:835:ARG:NH2	3:G:1210:SER:O	2.38	0.47
3:G:943:ASP:HB2	3:G:1050:GLY:HA3	1.97	0.47
3:G:1569:GLN:HB2	3:G:1572:ILE:HD12	1.97	0.47
3:G:2029:GLN:NE2	3:G:2033:ASP:OD1	2.47	0.47
3:G:4148:THR:HG21	3:G:4180:ARG:HH21	1.80	0.47
3:I:684:VAL:HG22	3:I:781:VAL:HG12	1.96	0.47
3:I:1101:ARG:NH1	3:I:1115:LEU:O	2.46	0.47
3:I:3343:GLN:O	3:I:3346:VAL:HG12	2.15	0.47
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.96	0.47
3:A:2029:GLN:NE2	3:A:2033:ASP:OD1	2.48	0.47
3:A:4006:ASP:N	3:A:4006:ASP:OD1	2.46	0.47
3:B:2626:LEU:HD22	3:B:2640:PRO:HB3	1.97	0.47
3:G:935:LEU:HD23	3:G:987:ARG:HH11	1.80	0.47
3:I:1232:ARG:NH2	3:I:1828:ASP:O	2.45	0.47
3:I:3316:LEU:HD21	3:I:3346:VAL:HG23	1.96	0.47
9:I:5308:L9R:H4A	9:I:5308:L9R:H7B	1.45	0.47
3:A:2538:THR:HG23	3:A:2541:PHE:H	1.80	0.47
3:A:3343:GLN:O	3:A:3346:VAL:HG12	2.15	0.47
9:A:5308:L9R:H7B	9:A:5308:L9R:H4A	1.45	0.47
3:B:872:GLU:HA	3:B:922:LEU:HD11	1.97	0.47
3:B:3343:GLN:O	3:B:3346:VAL:HG12	2.15	0.47
3:B:3862:ASP:OD1	3:B:3862:ASP:N	2.48	0.47
3:G:144:GLU:HG3	3:G:175:SER:HB3	1.96	0.47
3:G:815:VAL:O	3:G:1007:TYR:OH	2.27	0.47
3:G:1653:LEU:O	3:G:1660:GLN:NE2	2.48	0.47
3:G:2626:LEU:HD22	3:G:2640:PRO:HB3	1.97	0.47
9:G:5307:L9R:H33A	9:I:5308:L9R:H3A	1.97	0.47
3:I:2626:LEU:HD22	3:I:2640:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2815:ALA:HB1	3:I:2881:ASN:HD22	1.80	0.47
3:I:3263:TYR:HD1	3:I:3270:ILE:HD12	1.79	0.47
1:E:94:LYS:HE3	1:E:107:HIS:HB3	1.97	0.47
3:A:872:GLU:HA	3:A:922:LEU:HD11	1.97	0.47
3:A:2626:LEU:HD22	3:A:2640:PRO:HB3	1.97	0.47
3:A:3862:ASP:OD1	3:A:3862:ASP:N	2.48	0.47
3:B:176:SER:OG	3:B:178:ARG:NH1	2.38	0.47
3:B:1819:VAL:HG13	3:B:1929:MET:HE1	1.97	0.47
3:I:835:ARG:NH2	3:I:1210:SER:O	2.38	0.47
3:I:935:LEU:HD23	3:I:987:ARG:HH11	1.80	0.47
3:I:943:ASP:HB2	3:I:1050:GLY:HA3	1.97	0.47
3:I:1569:GLN:HB2	3:I:1572:ILE:HD12	1.97	0.47
3:A:2452:ARG:NH1	3:B:144:GLU:OE1	2.49	0.46
3:B:835:ARG:NH2	3:B:1210:SER:O	2.38	0.46
3:B:2203:MET:HE3	3:B:2235:PHE:HZ	1.80	0.46
3:G:2538:THR:HG23	3:G:2541:PHE:H	1.80	0.46
3:G:3343:GLN:O	3:G:3346:VAL:HG12	2.15	0.46
1:D:94:LYS:HE3	1:D:107:HIS:HB3	1.97	0.46
1:C:94:LYS:HE3	1:C:107:HIS:HB3	1.97	0.46
3:A:943:ASP:HB2	3:A:1050:GLY:HA3	1.97	0.46
3:B:1569:GLN:HB2	3:B:1572:ILE:HD12	1.97	0.46
3:B:3944:GLU:OE1	3:B:3946:GLN:N	2.47	0.46
3:G:1503:PRO:HA	3:G:1508:ARG:HH22	1.79	0.46
3:G:1771:LEU:HB3	3:G:2153:MET:HE3	1.98	0.46
3:G:1819:VAL:HG13	3:G:1929:MET:HE1	1.97	0.46
3:G:3263:TYR:HD1	3:G:3270:ILE:HD12	1.79	0.46
3:G:3412:LEU:HD11	3:G:3434:LEU:HD21	1.98	0.46
3:G:5024:ALA:HB3	3:I:4972:PRO:HB3	1.96	0.46
3:I:1819:VAL:HG13	3:I:1929:MET:HE1	1.97	0.46
3:I:2182:ILE:HG22	3:I:2186:MET:HE2	1.97	0.46
3:I:2538:THR:HG23	3:I:2541:PHE:H	1.80	0.46
3:A:1771:LEU:HB3	3:A:2153:MET:HE3	1.98	0.46
3:A:2182:ILE:HG22	3:A:2186:MET:HE2	1.97	0.46
3:A:2203:MET:HE3	3:A:2235:PHE:HZ	1.80	0.46
3:A:3412:LEU:HD11	3:A:3434:LEU:HD21	1.98	0.46
3:B:4074:SER:OG	3:I:4731:ILE:O	2.33	0.46
3:G:1101:ARG:NH1	3:G:1115:LEU:O	2.46	0.46
3:G:2182:ILE:HG22	3:G:2186:MET:HE2	1.97	0.46
3:G:2203:MET:HE3	3:G:2235:PHE:HZ	1.80	0.46
3:G:4555:LEU:HD21	3:G:4656:LEU:HD22	1.96	0.46
3:I:2587:TYR:O	3:I:2590:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1819:VAL:HG13	3:A:1929:MET:HE1	1.97	0.46
3:B:3316:LEU:HD21	3:B:3346:VAL:HG23	1.96	0.46
3:I:144:GLU:HG3	3:I:175:SER:HB3	1.96	0.46
3:I:4687:TYR:OH	3:I:4699:GLY:O	2.26	0.46
3:A:144:GLU:HG3	3:A:175:SER:HB3	1.96	0.46
3:A:1465:ASP:OD1	3:A:1468:LYS:HG2	2.16	0.46
3:B:1653:LEU:O	3:B:1660:GLN:NE2	2.48	0.46
3:G:1996:ARG:HH21	3:G:1999:ARG:HE	1.64	0.46
3:G:2815:ALA:HB1	3:G:2881:ASN:HD22	1.80	0.46
3:G:3604:TYR:O	3:G:3608:GLN:HG2	2.16	0.46
3:I:2020:ASP:OD1	3:I:2020:ASP:N	2.47	0.46
3:I:3946:GLN:OE1	3:I:3949:ARG:NH2	2.39	0.46
3:I:4006:ASP:OD1	3:I:4006:ASP:N	2.46	0.46
3:I:4148:THR:HG21	3:I:4180:ARG:HH21	1.80	0.46
1:K:94:LYS:HE3	1:K:107:HIS:HB3	1.97	0.46
3:A:3552:PHE:O	3:A:3556:ASN:ND2	2.35	0.46
3:G:943:ASP:OD2	3:G:945:LYS:NZ	2.47	0.46
3:A:4148:THR:HG21	3:A:4180:ARG:HH21	1.80	0.46
3:A:4555:LEU:HD21	3:A:4656:LEU:HD22	1.96	0.46
3:B:3412:LEU:HD11	3:B:3434:LEU:HD21	1.98	0.46
3:G:275:ARG:NH1	3:G:338:GLU:OE2	2.49	0.46
3:I:1465:ASP:OD1	3:I:1468:LYS:HG2	2.16	0.46
3:A:1810:LYS:HG2	3:A:1814:MET:HE2	1.98	0.46
3:B:2587:TYR:O	3:B:2590:SER:OG	2.31	0.46
3:B:2736:ASP:OD1	3:B:2736:ASP:N	2.44	0.46
3:G:886:ARG:HB3	3:G:891:TRP:CG	2.51	0.46
3:G:3842:LEU:HB2	3:G:3929:SER:HB2	1.98	0.46
3:I:663:TYR:CD2	3:I:804:PRO:HB3	2.51	0.46
3:I:1653:LEU:O	3:I:1660:GLN:NE2	2.48	0.46
1:K:117:THR:OG1	1:K:120:GLU:OE1	2.31	0.46
3:A:803:LEU:HD12	3:A:804:PRO:HD2	1.98	0.46
3:A:2309:SER:OG	3:A:2320:ASP:OD1	2.34	0.46
3:B:943:ASP:HB2	3:B:1050:GLY:HA3	1.97	0.46
3:B:2538:THR:HG23	3:B:2541:PHE:H	1.80	0.46
3:B:3840:SER:OG	3:B:3877:ASP:OD1	2.29	0.46
3:I:815:VAL:O	3:I:1007:TYR:OH	2.27	0.46
9:I:5307:L9R:H32A	9:I:5307:L9R:H35A	1.75	0.46
3:A:886:ARG:HB3	3:A:891:TRP:CG	2.51	0.46
3:I:2917:ALA:HA	3:I:2920:ARG:HB3	1.98	0.46
1:K:122:ASP:HA	1:K:125:ILE:HG22	1.99	0.45
1:E:117:THR:OG1	1:E:120:GLU:OE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1024:TYR:CZ	3:B:1032:LYS:HG3	2.51	0.45
3:B:1771:LEU:HB3	3:B:2153:MET:HE3	1.98	0.45
3:B:2309:SER:OG	3:B:2320:ASP:OD1	2.34	0.45
3:B:2355:ARG:NH2	3:B:2449:GLU:OE2	2.49	0.45
3:B:3604:TYR:O	3:B:3608:GLN:HG2	2.16	0.45
3:B:4754:ASN:HB3	3:B:4756:ARG:HH21	1.81	0.45
3:I:1771:LEU:HB3	3:I:2153:MET:HE3	1.98	0.45
1:K:132:GLY:O	3:A:3456:GLN:NE2	2.43	0.45
3:A:1996:ARG:HH21	3:A:1999:ARG:HE	1.64	0.45
3:A:2917:ALA:HA	3:A:2920:ARG:HB3	1.98	0.45
3:A:3604:TYR:O	3:A:3608:GLN:HG2	2.16	0.45
3:B:144:GLU:HG3	3:B:175:SER:HB3	1.96	0.45
3:B:950:LEU:HD13	3:B:970:LEU:HG	1.99	0.45
3:G:663:TYR:CD2	3:G:804:PRO:HB3	2.51	0.45
9:G:5307:L9R:H6A	9:G:5307:L9R:H4A	1.46	0.45
3:I:943:ASP:OD2	3:I:945:LYS:NZ	2.47	0.45
1:C:2:ASP:OD2	3:B:2244:ARG:NH1	2.49	0.45
3:A:4000:MET:SD	3:A:4020:GLN:NE2	2.73	0.45
3:G:336:PRO:HA	3:G:337:PRO:HD3	1.88	0.45
3:G:803:LEU:HD12	3:G:804:PRO:HD2	1.98	0.45
3:I:872:GLU:HA	3:I:922:LEU:HD11	1.97	0.45
3:I:3412:LEU:HD11	3:I:3434:LEU:HD21	1.97	0.45
3:I:5012:LYS:NZ	3:I:5016:GLU:OE2	2.41	0.45
3:A:233:ILE:O	3:A:257:ARG:NH1	2.49	0.45
3:B:2182:ILE:HG22	3:B:2186:MET:HE2	1.97	0.45
3:B:4148:THR:HG21	3:B:4180:ARG:HH21	1.80	0.45
3:B:5012:LYS:NZ	3:B:5016:GLU:OE2	2.41	0.45
9:B:5307:L9R:H6A	9:B:5307:L9R:H4A	1.46	0.45
3:G:1024:TYR:CZ	3:G:1032:LYS:HG3	2.51	0.45
3:I:886:ARG:HB3	3:I:891:TRP:CG	2.51	0.45
3:A:663:TYR:CD2	3:A:804:PRO:HB3	2.51	0.45
3:B:758:ARG:HG2	3:B:763:PRO:HA	1.99	0.45
3:B:2917:ALA:HA	3:B:2920:ARG:HB3	1.99	0.45
3:G:1810:LYS:HG2	3:G:1814:MET:HE2	1.98	0.45
3:G:2309:SER:OG	3:G:2320:ASP:OD1	2.34	0.45
3:G:3862:ASP:OD1	3:G:3862:ASP:N	2.48	0.45
3:I:665:GLU:HB2	3:I:792:LEU:HB2	1.98	0.45
3:I:2309:SER:OG	3:I:2320:ASP:OD1	2.34	0.45
3:I:2881:ASN:HA	3:I:2884:ASN:ND2	2.32	0.45
3:I:3604:TYR:O	3:I:3608:GLN:HG2	2.16	0.45
3:A:2974:ILE:HG13	3:A:2975:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4754:ASN:HB3	3:A:4756:ARG:HH21	1.81	0.45
9:A:5307:L9R:H32A	9:A:5307:L9R:H35A	1.75	0.45
3:B:2974:ILE:HG13	3:B:2975:ALA:N	2.32	0.45
3:G:872:GLU:HA	3:G:922:LEU:HD11	1.97	0.45
3:G:2917:ALA:HA	3:G:2920:ARG:HB3	1.99	0.45
9:G:5308:L9R:H4A	9:G:5308:L9R:H7B	1.45	0.45
3:I:1810:LYS:HG2	3:I:1814:MET:HE2	1.98	0.45
3:I:2907:PRO:O	3:I:2910:THR:OG1	2.35	0.45
3:I:4754:ASN:HB3	3:I:4756:ARG:HH21	1.81	0.45
3:A:665:GLU:HB2	3:A:792:LEU:HB2	1.98	0.45
3:A:950:LEU:HD13	3:A:970:LEU:HG	1.99	0.45
3:A:1008:SER:HB3	3:A:1017:ARG:HB3	1.99	0.45
3:B:665:GLU:HB2	3:B:792:LEU:HB2	1.98	0.45
3:B:803:LEU:HD12	3:B:804:PRO:HD2	1.98	0.45
3:B:1099:GLU:OE2	3:B:1125:ASN:ND2	2.50	0.45
3:B:3842:LEU:HB2	3:B:3929:SER:HB2	1.98	0.45
3:G:1465:ASP:OD1	3:G:1468:LYS:HG2	2.16	0.45
3:I:1996:ARG:HH21	3:I:1999:ARG:HE	1.64	0.45
3:I:2677:LYS:HE2	3:I:2677:LYS:HB3	1.81	0.45
3:I:3840:SER:OG	3:I:3877:ASP:OD1	2.29	0.45
3:A:758:ARG:HG2	3:A:763:PRO:HA	1.99	0.45
3:A:2736:ASP:OD1	3:A:2736:ASP:N	2.44	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:HE1	1.82	0.45
3:B:1008:SER:HB3	3:B:1017:ARG:HB3	1.99	0.45
3:G:2881:ASN:HA	3:G:2884:ASN:ND2	2.32	0.45
3:G:3226:GLU:C	3:G:3228:ALA:H	2.25	0.45
3:G:3731:LYS:HA	3:G:3734:HIS:CE1	2.52	0.45
3:I:803:LEU:HD12	3:I:804:PRO:HD2	1.98	0.45
3:I:3226:GLU:C	3:I:3228:ALA:H	2.25	0.45
3:I:3731:LYS:HA	3:I:3734:HIS:CE1	2.52	0.45
3:I:3842:LEU:HB2	3:I:3929:SER:HB2	1.98	0.45
1:E:122:ASP:HA	1:E:125:ILE:HG22	1.99	0.45
3:A:648:ILE:HG23	3:A:814:ALA:HB3	1.99	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:CE1	2.52	0.45
3:B:663:TYR:CD2	3:B:804:PRO:HB3	2.51	0.45
3:B:2912:THR:OG1	3:B:2913:ALA:N	2.50	0.45
3:G:4648:LEU:HD12	3:G:4803:HIS:HE1	1.82	0.45
3:I:856:VAL:H	3:I:991:ASN:ND2	2.15	0.45
3:I:2355:ARG:NH2	3:I:2449:GLU:OE2	2.50	0.45
3:I:2974:ILE:HG13	3:I:2975:ALA:N	2.32	0.45
3:A:856:VAL:H	3:A:991:ASN:ND2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3842:LEU:HB2	3:A:3929:SER:HB2	1.98	0.45
3:A:4152:GLU:OE1	3:A:4194:TYR:OH	2.28	0.45
9:A:5308:L9R:H3A	9:B:5307:L9R:H33A	1.99	0.45
2:O:4:VAL:HG22	2:O:74:LEU:HD22	1.99	0.45
3:B:648:ILE:HG23	3:B:814:ALA:HB3	1.99	0.45
3:B:1465:ASP:OD1	3:B:1468:LYS:HG2	2.16	0.45
3:B:1810:LYS:HG2	3:B:1814:MET:HE2	1.98	0.45
3:B:2452:ARG:NH1	3:I:144:GLU:OE1	2.50	0.45
3:G:2912:THR:OG1	3:G:2913:ALA:N	2.50	0.45
3:G:2974:ILE:HG13	3:G:2975:ALA:N	2.32	0.45
3:I:1024:TYR:CZ	3:I:1032:LYS:HG3	2.51	0.45
3:I:4661:TYR:OH	3:I:4786:ASP:OD2	2.33	0.45
3:A:275:ARG:NH1	3:A:338:GLU:OE2	2.49	0.44
3:A:4687:TYR:OH	3:A:4699:GLY:O	2.26	0.44
2:J:4:VAL:HG22	2:J:74:LEU:HD22	2.00	0.44
3:B:275:ARG:NH1	3:B:338:GLU:OE2	2.49	0.44
3:G:613:ALA:HB2	3:G:1676:LEU:HD12	1.99	0.44
3:G:3731:LYS:HA	3:G:3734:HIS:HE1	1.82	0.44
3:I:3872:GLU:HG3	3:I:3874:VAL:H	1.83	0.44
3:A:1024:TYR:CZ	3:A:1032:LYS:HG3	2.51	0.44
3:A:3332:ALA:HB3	3:A:3403:ARG:NH1	2.32	0.44
3:A:4640:GLU:HB3	3:A:4641:PRO:HD3	2.00	0.44
3:B:886:ARG:HB3	3:B:891:TRP:CG	2.51	0.44
3:B:1996:ARG:HH21	3:B:1999:ARG:HE	1.64	0.44
3:B:3731:LYS:HA	3:B:3734:HIS:HE1	1.82	0.44
3:I:275:ARG:NH1	3:I:338:GLU:OE2	2.49	0.44
3:I:3106:MET:HE2	3:I:3186:LEU:HD13	2.00	0.44
3:A:2020:ASP:OD1	3:A:2020:ASP:N	2.47	0.44
3:A:2821:TRP:HD1	3:A:2939:ARG:HA	1.82	0.44
3:A:3106:MET:HE2	3:A:3186:LEU:HD13	2.00	0.44
3:A:3805:LEU:HB3	3:A:3890:LEU:HB3	1.99	0.44
2:H:88:PRO:HB2	3:G:1680:ARG:HH12	1.82	0.44
3:B:943:ASP:OD2	3:B:945:LYS:NZ	2.47	0.44
3:B:2821:TRP:HD1	3:B:2939:ARG:HA	1.82	0.44
3:G:2355:ARG:NH2	3:G:2449:GLU:OE2	2.49	0.44
3:G:2875:ALA:HB2	3:G:2927:LEU:HD22	2.00	0.44
3:G:3872:GLU:HG3	3:G:3874:VAL:H	1.82	0.44
3:I:2912:THR:OG1	3:I:2913:ALA:N	2.50	0.44
1:D:122:ASP:HA	1:D:125:ILE:HG22	1.99	0.44
3:A:2881:ASN:HA	3:A:2884:ASN:ND2	2.32	0.44
3:A:2912:THR:OG1	3:A:2913:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2633:LEU:O	3:B:2689:LYS:NZ	2.51	0.44
3:B:3106:MET:HE2	3:B:3186:LEU:HD13	2.00	0.44
3:G:952:LYS:HD3	3:G:970:LEU:HA	2.00	0.44
3:G:1008:SER:HB3	3:G:1017:ARG:HB3	1.99	0.44
3:G:3171:SER:O	3:G:3174:SER:OG	2.30	0.44
3:G:3332:ALA:HB3	3:G:3403:ARG:NH1	2.32	0.44
3:I:176:SER:OG	3:I:178:ARG:NH1	2.38	0.44
3:I:758:ARG:HG2	3:I:763:PRO:HA	1.99	0.44
3:I:952:LYS:HD3	3:I:970:LEU:HA	2.00	0.44
3:A:923:GLN:O	3:A:927:GLU:HG2	2.18	0.44
3:A:2355:ARG:NH2	3:A:2449:GLU:OE2	2.50	0.44
3:A:3946:GLN:OE1	3:A:3949:ARG:NH2	2.39	0.44
3:B:856:VAL:H	3:B:991:ASN:ND2	2.15	0.44
3:B:4000:MET:SD	3:B:4020:GLN:NE2	2.73	0.44
3:B:4640:GLU:HB3	3:B:4641:PRO:HD3	2.00	0.44
3:G:3106:MET:HE2	3:G:3186:LEU:HD13	2.00	0.44
3:G:4177:TYR:CE1	3:G:4199:GLU:HG3	2.53	0.44
3:I:2821:TRP:HD1	3:I:2939:ARG:HA	1.83	0.44
3:I:3442:PHE:CG	3:I:3514:LEU:HD22	2.53	0.44
3:I:3805:LEU:HB3	3:I:3890:LEU:HB3	1.99	0.44
3:I:4640:GLU:HB3	3:I:4641:PRO:HD3	2.00	0.44
3:I:4648:LEU:HD12	3:I:4803:HIS:HE1	1.82	0.44
1:K:85:ILE:H	1:K:85:ILE:HG13	1.57	0.44
3:A:613:ALA:HB2	3:A:1676:LEU:HD12	2.00	0.44
3:A:783:PHE:HB2	3:A:787:VAL:HG21	1.99	0.44
3:A:1694:LEU:HB3	3:A:1715:LEU:HD12	2.00	0.44
3:A:3872:GLU:HG3	3:A:3874:VAL:H	1.82	0.44
3:B:69:LEU:HD13	3:B:101:LEU:HD11	1.99	0.44
3:B:932:LEU:HD21	3:B:988:LEU:HD11	2.00	0.44
3:B:3332:ALA:HB3	3:B:3403:ARG:NH1	2.32	0.44
3:B:4177:TYR:CE1	3:B:4199:GLU:HG3	2.53	0.44
3:G:69:LEU:HD13	3:G:101:LEU:HD11	1.99	0.44
3:G:758:ARG:HG2	3:G:763:PRO:HA	1.99	0.44
3:G:2108:GLU:O	3:G:3694:LYS:NZ	2.51	0.44
3:G:2633:LEU:O	3:G:2689:LYS:NZ	2.51	0.44
3:G:4648:LEU:HD12	3:G:4803:HIS:CE1	2.53	0.44
3:I:1008:SER:HB3	3:I:1017:ARG:HB3	1.99	0.44
3:I:3731:LYS:HA	3:I:3734:HIS:HE1	1.82	0.44
3:I:4177:TYR:CE1	3:I:4199:GLU:HG3	2.53	0.44
1:C:111:ASN:O	3:B:1996:ARG:NH2	2.36	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:VAL:HG22	2:H:74:LEU:HD22	2.00	0.44
3:B:783:PHE:HB2	3:B:787:VAL:HG21	1.99	0.44
3:B:1820:ARG:O	3:B:1824:GLN:HG2	2.18	0.44
3:B:3731:LYS:HA	3:B:3734:HIS:CE1	2.52	0.44
3:G:4000:MET:SD	3:G:4020:GLN:NE2	2.73	0.44
3:G:4754:ASN:HB3	3:G:4756:ARG:HH21	1.81	0.44
3:G:4818:MET:HA	3:G:4824:ARG:HH11	1.83	0.44
9:G:5308:L9R:H20	9:G:5308:L9R:H23	1.32	0.44
3:I:950:LEU:HD13	3:I:970:LEU:HG	1.99	0.44
3:B:923:GLN:O	3:B:927:GLU:HG2	2.18	0.44
3:B:3872:GLU:HG3	3:B:3874:VAL:H	1.82	0.44
3:G:648:ILE:HG23	3:G:814:ALA:HB3	1.99	0.44
3:G:856:VAL:H	3:G:991:ASN:ND2	2.15	0.44
3:G:950:LEU:HD13	3:G:970:LEU:HG	1.99	0.44
3:G:3752:SER:OG	3:G:3755:GLU:OE1	2.34	0.44
3:I:2633:LEU:O	3:I:2689:LYS:NZ	2.51	0.44
3:I:2875:ALA:HB2	3:I:2927:LEU:HD22	2.00	0.44
1:C:122:ASP:HA	1:C:125:ILE:HG22	1.98	0.44
3:A:664:PHE:HB3	3:A:811:CYS:SG	2.58	0.44
3:A:943:ASP:OD2	3:A:945:LYS:NZ	2.47	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:HE1	1.82	0.44
3:A:4818:MET:HA	3:A:4824:ARG:HH11	1.83	0.44
3:A:5024:ALA:HB3	3:G:4972:PRO:HB3	1.98	0.44
3:B:1716:ILE:O	3:B:1721:GLU:N	2.51	0.44
3:B:2765:LYS:HA	3:B:2765:LYS:HD3	1.78	0.44
3:B:3226:GLU:C	3:B:3228:ALA:H	2.25	0.44
3:B:4648:LEU:HD12	3:B:4803:HIS:HE1	1.82	0.44
3:G:979:PRO:O	3:G:982:THR:OG1	2.33	0.44
3:G:2821:TRP:HD1	3:G:2939:ARG:HA	1.82	0.44
3:G:4640:GLU:HB3	3:G:4641:PRO:HD3	2.00	0.44
3:I:664:PHE:HB3	3:I:811:CYS:SG	2.58	0.44
3:I:783:PHE:HB2	3:I:787:VAL:HG21	1.99	0.44
3:I:3230:LEU:H	3:I:3230:LEU:HD23	1.83	0.44
1:C:85:ILE:H	1:C:85:ILE:HG13	1.57	0.43
3:A:932:LEU:HD21	3:A:988:LEU:HD11	2.00	0.43
3:A:1653:LEU:O	3:A:1660:GLN:NE2	2.48	0.43
3:A:2633:LEU:O	3:A:2689:LYS:NZ	2.51	0.43
3:A:2875:ALA:HB2	3:A:2927:LEU:HD22	2.00	0.43
3:A:3446:SER:O	3:A:3452:LYS:NZ	2.42	0.43
3:A:3752:SER:OG	3:A:3755:GLU:OE1	2.34	0.43
3:A:4177:TYR:CE1	3:A:4199:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4205:TRP:HZ3	3:A:4989:MET:HE3	1.83	0.43
3:G:923:GLN:O	3:G:927:GLU:HG2	2.18	0.43
3:G:1141:ARG:HB3	3:I:3479:ALA:HA	2.00	0.43
3:I:2765:LYS:HD3	3:I:2765:LYS:HA	1.78	0.43
3:I:3621:HIS:ND1	3:I:3623:LEU:HD23	2.33	0.43
3:I:3862:ASP:OD1	3:I:3862:ASP:N	2.48	0.43
3:A:815:VAL:O	3:A:1007:TYR:OH	2.27	0.43
3:A:1820:ARG:O	3:A:1824:GLN:HG2	2.18	0.43
3:A:3442:PHE:CG	3:A:3514:LEU:HD22	2.53	0.43
3:A:3556:ASN:HB3	3:A:3559:LEU:HD13	2.00	0.43
2:J:42:ARG:HD3	3:I:1780:PRO:HG2	1.99	0.43
3:B:952:LYS:HD3	3:B:970:LEU:HA	2.00	0.43
3:B:3805:LEU:HB3	3:B:3890:LEU:HB3	1.99	0.43
3:G:664:PHE:HB3	3:G:811:CYS:SG	2.58	0.43
3:G:2580:ASP:OD1	3:G:2621:HIS:HB2	2.19	0.43
3:I:451:TYR:CZ	3:I:474:ARG:HD2	2.53	0.43
2:F:4:VAL:HG22	2:F:74:LEU:HD22	2.00	0.43
3:A:3123:LYS:HG3	3:A:3125:VAL:H	1.83	0.43
3:A:3621:HIS:C	3:A:3622:LYS:HG3	2.43	0.43
3:B:233:ILE:O	3:B:257:ARG:NH1	2.49	0.43
3:B:451:TYR:CZ	3:B:474:ARG:HD2	2.53	0.43
3:B:664:PHE:HB3	3:B:811:CYS:SG	2.58	0.43
3:B:2764:GLU:HG3	3:B:2857:PRO:HB3	2.01	0.43
3:B:2881:ASN:HA	3:B:2884:ASN:ND2	2.32	0.43
3:B:3852:LYS:HE3	3:B:3852:LYS:HB3	1.89	0.43
3:G:3123:LYS:HG3	3:G:3125:VAL:H	1.83	0.43
3:G:4205:TRP:HZ3	3:G:4989:MET:HE3	1.84	0.43
3:G:4861:LYS:H	3:G:4861:LYS:HG3	1.53	0.43
3:I:1694:LEU:HB3	3:I:1715:LEU:HD12	2.00	0.43
3:I:3332:ALA:HB3	3:I:3403:ARG:NH1	2.32	0.43
3:I:3535:LEU:O	3:I:3538:THR:OG1	2.31	0.43
3:B:1022:VAL:HG22	3:B:1023:PRO:HD2	2.01	0.43
3:B:1694:LEU:HB3	3:B:1715:LEU:HD12	2.00	0.43
3:B:3621:HIS:C	3:B:3622:LYS:HG3	2.43	0.43
3:G:1099:GLU:OE2	3:G:1125:ASN:ND2	2.50	0.43
3:G:3689:GLU:C	3:G:3691:GLU:H	2.26	0.43
3:G:3805:LEU:HB3	3:G:3890:LEU:HB3	1.99	0.43
3:I:1168:VAL:HG11	3:I:1176:GLU:HG2	2.00	0.43
3:I:2888:ARG:O	3:I:2892:GLN:HG2	2.18	0.43
3:I:3752:SER:OG	3:I:3755:GLU:OE1	2.35	0.43
3:I:4205:TRP:HZ3	3:I:4989:MET:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5308:L9R:H44	9:I:5308:L9R:H47A	1.52	0.43
3:A:2108:GLU:O	3:A:3694:LYS:NZ	2.51	0.43
3:A:2580:ASP:OD1	3:A:2621:HIS:HB2	2.19	0.43
3:A:2764:GLU:HG3	3:A:2857:PRO:HB3	2.01	0.43
3:A:3159:ASP:OD1	3:A:3159:ASP:N	2.52	0.43
3:A:3226:GLU:C	3:A:3228:ALA:H	2.25	0.43
3:A:3621:HIS:ND1	3:A:3623:LEU:HD23	2.33	0.43
3:A:3852:LYS:HE3	3:A:3852:LYS:HB3	1.89	0.43
3:A:4967:TYR:OH	3:A:5033:GLU:OE2	2.29	0.43
2:J:25:HIS:CD2	2:J:104:LEU:HD11	2.54	0.43
3:B:1168:VAL:HG11	3:B:1176:GLU:HG2	2.00	0.43
3:B:2677:LYS:HB3	3:B:2677:LYS:HE2	1.81	0.43
3:G:665:GLU:HB2	3:G:792:LEU:HB2	1.98	0.43
3:G:3621:HIS:C	3:G:3622:LYS:HG3	2.43	0.43
3:I:328:LYS:HE3	3:I:328:LYS:HB3	1.80	0.43
3:I:2580:ASP:OD1	3:I:2621:HIS:HB2	2.19	0.43
2:F:42:ARG:HD3	3:A:1780:PRO:HG2	2.01	0.43
1:D:117:THR:OG1	1:D:120:GLU:OE1	2.31	0.43
3:A:365:LYS:HB3	3:A:365:LYS:HE3	1.80	0.43
3:A:1099:GLU:OE2	3:A:1125:ASN:ND2	2.50	0.43
3:A:3230:LEU:HD23	3:A:3230:LEU:H	1.83	0.43
2:O:25:HIS:CD2	2:O:104:LEU:HD11	2.54	0.43
3:B:11:VAL:HG11	3:B:164:ARG:HD3	2.01	0.43
3:G:783:PHE:HB2	3:G:787:VAL:HG21	1.99	0.43
3:I:169:LEU:HD22	3:I:202:MET:HG3	2.00	0.43
3:I:613:ALA:HB2	3:I:1676:LEU:HD12	1.99	0.43
3:I:923:GLN:O	3:I:927:GLU:HG2	2.18	0.43
3:I:1022:VAL:HG22	3:I:1023:PRO:HD2	2.01	0.43
3:I:1206:GLN:HA	3:I:1227:ALA:O	2.18	0.43
3:I:1773:PRO:HA	3:I:1774:PRO:HD3	1.90	0.43
3:I:4818:MET:HA	3:I:4824:ARG:HH11	1.83	0.43
3:A:69:LEU:HD13	3:A:101:LEU:HD11	1.99	0.43
3:A:451:TYR:CZ	3:A:474:ARG:HD2	2.53	0.43
3:A:2888:ARG:O	3:A:2892:GLN:HG2	2.18	0.43
3:B:613:ALA:HB2	3:B:1676:LEU:HD12	1.99	0.43
3:B:2580:ASP:OD1	3:B:2621:HIS:HB2	2.19	0.43
3:B:3442:PHE:CG	3:B:3514:LEU:HD22	2.53	0.43
3:B:3556:ASN:HB3	3:B:3559:LEU:HD13	2.00	0.43
3:B:4205:TRP:CZ3	3:B:4989:MET:HE3	2.54	0.43
3:G:11:VAL:HG11	3:G:164:ARG:HD3	2.01	0.43
3:I:69:LEU:HD13	3:I:101:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:648:ILE:HG23	3:I:814:ALA:HB3	1.99	0.43
3:I:932:LEU:HD21	3:I:988:LEU:HD11	2.00	0.43
3:I:1057:ASP:OD1	3:I:1057:ASP:N	2.31	0.43
3:I:1753:LYS:HB3	3:I:1758:ARG:HA	2.01	0.43
3:I:2108:GLU:O	3:I:3694:LYS:NZ	2.51	0.43
3:I:3621:HIS:C	3:I:3622:LYS:HG3	2.44	0.43
3:I:4648:LEU:HD12	3:I:4803:HIS:CE1	2.53	0.43
3:A:11:VAL:HG11	3:A:164:ARG:HD3	2.01	0.43
3:A:1022:VAL:HG22	3:A:1023:PRO:HD2	2.01	0.43
3:A:1168:VAL:HG11	3:A:1176:GLU:HG2	2.00	0.43
3:A:4661:TYR:OH	3:A:4786:ASP:OD2	2.33	0.43
3:B:169:LEU:HD22	3:B:202:MET:HG3	2.00	0.43
3:B:2875:ALA:HB2	3:B:2927:LEU:HD22	2.00	0.43
3:B:3621:HIS:ND1	3:B:3623:LEU:HD23	2.33	0.43
3:G:3442:PHE:CG	3:G:3514:LEU:HD22	2.53	0.43
3:I:11:VAL:HG11	3:I:164:ARG:HD3	2.01	0.43
3:I:232:THR:HG21	3:I:252:VAL:HG21	2.01	0.43
3:A:952:LYS:HD3	3:A:970:LEU:HA	2.00	0.43
3:A:1206:GLN:HA	3:A:1227:ALA:O	2.18	0.43
3:A:3391:GLU:HG3	3:A:3395:ARG:HE	1.84	0.43
3:A:3392:LEU:HD13	3:A:3395:ARG:HD2	2.01	0.43
3:A:3944:GLU:OE1	3:A:3946:GLN:N	2.47	0.43
3:A:4205:TRP:CZ3	3:A:4989:MET:HE3	2.54	0.43
9:A:5307:L9R:H6A	9:A:5307:L9R:H4A	1.46	0.43
2:O:17:LYS:HE3	2:O:17:LYS:HB3	1.84	0.43
3:B:2108:GLU:O	3:B:3694:LYS:NZ	2.51	0.43
3:B:3123:LYS:HG3	3:B:3125:VAL:H	1.83	0.43
3:B:4648:LEU:HD12	3:B:4803:HIS:CE1	2.53	0.43
3:G:2888:ARG:O	3:G:2892:GLN:HG2	2.18	0.43
3:G:3556:ASN:HB3	3:G:3559:LEU:HD13	1.99	0.43
3:I:233:ILE:O	3:I:257:ARG:NH1	2.49	0.43
3:I:2801:ASP:HA	3:I:2804:ILE:HG12	2.01	0.43
3:A:925:SER:O	3:A:928:THR:OG1	2.32	0.43
3:B:2021:CYS:O	3:B:2028:ARG:NH2	2.52	0.43
3:G:451:TYR:CZ	3:G:474:ARG:HD2	2.53	0.43
3:G:1022:VAL:HG22	3:G:1023:PRO:HD2	2.01	0.43
3:G:3230:LEU:H	3:G:3230:LEU:HD23	1.82	0.43
3:G:3269:VAL:HA	3:G:3273:THR:HB	2.01	0.43
3:G:3391:GLU:HG3	3:G:3395:ARG:HE	1.84	0.43
3:G:3621:HIS:ND1	3:G:3623:LEU:HD23	2.33	0.43
3:I:3689:GLU:C	3:I:3691:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASP:HA	3:B:3460:VAL:HG11	2.01	0.42
3:A:3628:ARG:HG3	3:A:3631:ALA:HB3	2.01	0.42
3:B:3171:SER:O	3:B:3174:SER:OG	2.30	0.42
3:B:3384:LYS:HD2	3:B:3386:GLU:HB3	2.01	0.42
3:B:3392:LEU:HD13	3:B:3395:ARG:HD2	2.01	0.42
3:B:4818:MET:HA	3:B:4824:ARG:HH11	1.83	0.42
3:G:1168:VAL:HG11	3:G:1176:GLU:HG2	2.00	0.42
3:I:1154:ASP:OD1	3:I:1156:THR:OG1	2.37	0.42
3:I:1948:ASP:OD1	3:I:2126:ARG:NH2	2.48	0.42
3:I:4205:TRP:CZ3	3:I:4989:MET:HE3	2.54	0.42
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.54	0.42
3:A:1716:ILE:O	3:A:1721:GLU:N	2.51	0.42
3:A:2661:TRP:HB3	3:A:2664:PHE:HB2	2.01	0.42
3:B:3230:LEU:H	3:B:3230:LEU:HD23	1.83	0.42
3:B:4910:GLU:O	3:B:4914:VAL:HG13	2.19	0.42
3:G:365:LYS:HE3	3:G:365:LYS:HB3	1.81	0.42
3:G:932:LEU:HD21	3:G:988:LEU:HD11	2.00	0.42
3:G:3392:LEU:HD13	3:G:3395:ARG:HD2	2.01	0.42
3:G:4205:TRP:CZ3	3:G:4989:MET:HE3	2.54	0.42
9:G:5307:L9R:H32A	9:G:5307:L9R:H35A	1.75	0.42
3:I:233:ILE:HD12	3:I:242:ARG:HB3	2.01	0.42
3:I:1716:ILE:O	3:I:1721:GLU:N	2.51	0.42
3:I:3384:LYS:HD2	3:I:3386:GLU:HB3	2.01	0.42
3:I:3556:ASN:HB3	3:I:3559:LEU:HD13	1.99	0.42
3:A:169:LEU:HD22	3:A:202:MET:HG3	2.00	0.42
3:A:1753:LYS:HB3	3:A:1758:ARG:HA	2.01	0.42
3:A:2801:ASP:HA	3:A:2804:ILE:HG12	2.01	0.42
3:A:3414:ARG:HH21	3:A:3472:ALA:H	1.67	0.42
2:H:7:ILE:HA	3:G:719:LEU:HD11	2.01	0.42
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.54	0.42
3:B:233:ILE:HD12	3:B:242:ARG:HB3	2.01	0.42
3:B:892:THR:HB	3:B:962:SER:H	1.84	0.42
3:G:4152:GLU:OE1	3:G:4194:TYR:OH	2.28	0.42
3:I:1820:ARG:O	3:I:1824:GLN:HG2	2.18	0.42
3:I:2764:GLU:HG3	3:I:2857:PRO:HB3	2.01	0.42
1:K:30:LYS:HE3	1:K:30:LYS:HB3	1.94	0.42
1:E:1:ALA:HB3	3:G:3861:GLU:HG2	2.01	0.42
1:E:26:THR:HB	1:E:62:THR:HB	2.02	0.42
3:A:1690:ASP:OD2	3:A:1693:GLN:NE2	2.52	0.42
3:A:3689:GLU:C	3:A:3691:GLU:H	2.26	0.42
3:B:1000:ARG:HB3	3:B:1005:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3689:GLU:C	3:B:3691:GLU:H	2.26	0.42
3:G:2661:TRP:HB3	3:G:2664:PHE:HB2	2.01	0.42
3:G:2751:LEU:HD23	3:G:2751:LEU:H	1.84	0.42
3:I:3123:LYS:HG3	3:I:3125:VAL:H	1.83	0.42
1:C:66:PRO:HG3	3:B:2186:MET:HB3	2.02	0.42
1:C:120:GLU:HA	1:C:123:GLU:HG3	2.02	0.42
3:A:2514:ASN:OD1	3:A:2514:ASN:N	2.53	0.42
3:A:4910:GLU:O	3:A:4914:VAL:HG13	2.19	0.42
3:B:938:HIS:HB3	3:B:1054:GLU:HB3	2.01	0.42
3:B:1947:CYS:SG	3:B:2127:GLN:NE2	2.92	0.42
3:B:2888:ARG:O	3:B:2892:GLN:HG2	2.18	0.42
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	2.02	0.42
3:G:1154:ASP:OD1	3:G:1156:THR:OG1	2.37	0.42
3:G:2716:ASP:OD1	3:G:2716:ASP:N	2.53	0.42
3:G:2764:GLU:HG3	3:G:2857:PRO:HB3	2.01	0.42
3:I:707:VAL:HG23	3:I:782:SER:HB3	2.02	0.42
3:I:788:LYS:HE3	3:I:788:LYS:HB2	1.84	0.42
3:I:3414:ARG:HH21	3:I:3472:ALA:H	1.67	0.42
1:D:111:ASN:O	3:I:1996:ARG:NH2	2.40	0.42
3:A:3235:SER:OG	3:A:3237:GLU:OE1	2.37	0.42
3:A:3269:VAL:HA	3:A:3273:THR:HB	2.01	0.42
3:B:1753:LYS:HB3	3:B:1758:ARG:HA	2.01	0.42
3:B:2751:LEU:HD23	3:B:2751:LEU:H	1.84	0.42
3:B:3284:TRP:HB3	3:B:3305:THR:HG21	2.02	0.42
3:G:169:LEU:HD22	3:G:202:MET:HG3	2.00	0.42
3:G:707:VAL:HG23	3:G:782:SER:HB3	2.02	0.42
3:G:1820:ARG:O	3:G:1824:GLN:HG2	2.18	0.42
3:G:2021:CYS:O	3:G:2028:ARG:NH2	2.52	0.42
3:G:3235:SER:OG	3:G:3237:GLU:OE1	2.37	0.42
3:G:3414:ARG:HH21	3:G:3472:ALA:H	1.67	0.42
3:A:2677:LYS:HE2	3:A:2677:LYS:HB3	1.81	0.42
3:G:1000:ARG:HB3	3:G:1005:TRP:HB2	2.01	0.42
3:G:1206:GLN:HA	3:G:1227:ALA:O	2.18	0.42
3:G:1690:ASP:OD2	3:G:1693:GLN:NE2	2.52	0.42
3:G:1716:ILE:O	3:G:1721:GLU:N	2.51	0.42
3:I:1099:GLU:OE2	3:I:1125:ASN:ND2	2.50	0.42
3:I:2661:TRP:HB3	3:I:2664:PHE:HB2	2.02	0.42
3:I:3003:LEU:HB2	3:I:3004:PRO:HD3	2.02	0.42
3:I:4967:TYR:OH	3:I:5033:GLU:OE2	2.29	0.42
1:C:26:THR:HB	1:C:62:THR:HB	2.02	0.42
3:A:892:THR:HB	3:A:962:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2021:CYS:O	3:A:2028:ARG:NH2	2.52	0.42
3:A:2390:PRO:C	3:A:2392:ARG:H	2.28	0.42
3:A:3284:TRP:HB3	3:A:3305:THR:HG21	2.02	0.42
3:A:3384:LYS:HD2	3:A:3386:GLU:HB3	2.01	0.42
3:B:232:THR:HG21	3:B:252:VAL:HG21	2.01	0.42
3:B:863:LEU:HD11	3:B:930:LYS:NZ	2.35	0.42
3:B:901:LYS:HG3	3:B:903:LEU:HG	2.02	0.42
3:B:4205:TRP:HZ3	3:B:4989:MET:HE3	1.83	0.42
3:G:233:ILE:HD12	3:G:242:ARG:HB3	2.01	0.42
3:G:901:LYS:HD2	3:G:901:LYS:HA	1.84	0.42
3:G:925:SER:O	3:G:928:THR:OG1	2.32	0.42
3:G:1753:LYS:HB3	3:G:1758:ARG:HA	2.01	0.42
3:G:3628:ARG:HG3	3:G:3631:ALA:HB3	2.01	0.42
3:G:3944:GLU:OE1	3:G:3946:GLN:N	2.47	0.42
3:G:4091:LYS:HE2	3:G:4091:LYS:HB2	1.89	0.42
3:I:2021:CYS:O	3:I:2028:ARG:NH2	2.52	0.42
3:I:4910:GLU:O	3:I:4914:VAL:HG13	2.19	0.42
1:K:120:GLU:HA	1:K:123:GLU:HG3	2.02	0.42
3:A:863:LEU:HD11	3:A:930:LYS:NZ	2.35	0.42
3:B:1948:ASP:OD1	3:B:2126:ARG:NH2	2.48	0.42
3:B:3235:SER:OG	3:B:3237:GLU:OE1	2.37	0.42
3:B:3269:VAL:HA	3:B:3273:THR:HB	2.01	0.42
3:B:3628:ARG:HG3	3:B:3631:ALA:HB3	2.01	0.42
3:B:3946:GLN:OE1	3:B:3949:ARG:NH2	2.39	0.42
3:B:4888:TYR:HE1	3:I:4917:ASP:HB2	1.84	0.42
9:B:5308:L9R:H23	9:B:5308:L9R:H20	1.32	0.42
3:G:4910:GLU:O	3:G:4914:VAL:HG13	2.19	0.42
3:I:892:THR:HB	3:I:962:SER:H	1.84	0.42
3:I:979:PRO:O	3:I:982:THR:OG1	2.33	0.42
3:I:1947:CYS:SG	3:I:2127:GLN:NE2	2.92	0.42
3:I:2514:ASN:OD1	3:I:2514:ASN:N	2.53	0.42
3:I:3390:GLY:HA2	3:I:3393:LEU:HD23	2.02	0.42
1:D:26:THR:HB	1:D:62:THR:HB	2.02	0.42
3:A:2212:VAL:HG11	3:A:2256:TYR:CE2	2.55	0.42
3:A:2263:ILE:HD12	3:A:2263:ILE:HA	1.95	0.42
3:A:2751:LEU:H	3:A:2751:LEU:HD23	1.84	0.42
3:B:1206:GLN:HA	3:B:1227:ALA:O	2.18	0.42
3:B:3390:GLY:HA2	3:B:3393:LEU:HD23	2.02	0.42
3:B:3535:LEU:O	3:B:3538:THR:OG1	2.31	0.42
3:G:870:ILE:HD12	3:G:870:ILE:HA	1.96	0.42
3:G:2519:LEU:HD22	3:G:2578:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2907:PRO:O	3:G:2910:THR:OG1	2.35	0.42
3:I:2858:GLN:HB2	3:I:2859:PRO:HD3	2.02	0.42
3:I:3392:LEU:HD13	3:I:3395:ARG:HD2	2.01	0.42
1:D:120:GLU:HA	1:D:123:GLU:HG3	2.02	0.41
1:E:120:GLU:HA	1:E:123:GLU:HG3	2.02	0.41
1:E:144:MET:HE3	1:E:144:MET:HB3	1.94	0.41
3:B:336:PRO:HA	3:B:337:PRO:HD3	1.88	0.41
3:B:707:VAL:HG23	3:B:782:SER:HB3	2.02	0.41
3:B:872:GLU:HG2	3:B:922:LEU:HD21	2.02	0.41
3:B:1057:ASP:OD1	3:B:1057:ASP:N	2.31	0.41
3:B:2661:TRP:HB3	3:B:2664:PHE:HB2	2.01	0.41
3:G:232:THR:HG21	3:G:252:VAL:HG21	2.01	0.41
3:G:345:LEU:HB3	3:G:387:ALA:HB1	2.02	0.41
3:G:938:HIS:HB3	3:G:1054:GLU:HB3	2.01	0.41
3:G:1694:LEU:HB3	3:G:1715:LEU:HD12	2.00	0.41
3:G:2212:VAL:HG11	3:G:2256:TYR:CE2	2.55	0.41
3:G:4093:PHE:O	3:G:4097:MET:HG2	2.20	0.41
3:I:1690:ASP:OD2	3:I:1693:GLN:NE2	2.52	0.41
3:I:3269:VAL:HA	3:I:3273:THR:HB	2.01	0.41
3:A:901:LYS:HG3	3:A:903:LEU:HG	2.02	0.41
3:B:881:LEU:HD13	3:B:881:LEU:HA	1.92	0.41
3:G:892:THR:HB	3:G:962:SER:H	1.84	0.41
3:I:3235:SER:OG	3:I:3237:GLU:OE1	2.37	0.41
3:I:4046:ASP:OD1	3:I:4159:ARG:NH2	2.48	0.41
1:K:66:PRO:HG3	3:A:2192:TYR:OH	2.21	0.41
1:C:144:MET:HE3	1:C:144:MET:HB3	1.94	0.41
3:A:232:THR:HG21	3:A:252:VAL:HG21	2.01	0.41
3:A:233:ILE:HD12	3:A:242:ARG:HB3	2.01	0.41
3:A:4861:LYS:H	3:A:4861:LYS:HG3	1.53	0.41
3:B:2514:ASN:OD1	3:B:2514:ASN:N	2.53	0.41
3:B:2519:LEU:HD22	3:B:2578:MET:HE1	2.02	0.41
3:G:954:LYS:HB3	3:G:966:LYS:HE3	2.03	0.41
3:I:2751:LEU:H	3:I:2751:LEU:HD23	1.84	0.41
3:A:707:VAL:HG23	3:A:782:SER:HB3	2.02	0.41
3:A:1823:GLY:O	3:A:1825:HIS:ND1	2.52	0.41
3:B:1805:GLU:CD	3:B:1805:GLU:H	2.29	0.41
3:G:233:ILE:O	3:G:257:ARG:NH1	2.49	0.41
3:G:3384:LYS:HD2	3:G:3386:GLU:HB3	2.01	0.41
3:G:3852:LYS:HE3	3:G:3852:LYS:HB3	1.89	0.41
3:I:901:LYS:HG3	3:I:903:LEU:HG	2.02	0.41
3:I:3107:VAL:HG21	3:I:3171:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3391:GLU:HG3	3:I:3395:ARG:HE	1.84	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.91	0.41
3:A:797:HIS:CG	3:A:821:LEU:HD23	2.56	0.41
3:A:901:LYS:HD2	3:A:901:LYS:HA	1.84	0.41
3:A:938:HIS:HB3	3:A:1054:GLU:HB3	2.01	0.41
3:A:2716:ASP:OD1	3:A:2716:ASP:N	2.53	0.41
3:A:3147:ILE:HG23	3:A:3152:PHE:HB2	2.02	0.41
3:A:4825:THR:O	3:A:4828:SER:OG	2.32	0.41
3:A:4917:ASP:HB2	3:G:4888:TYR:HE1	1.84	0.41
3:B:2749:GLU:HG3	3:B:2752:ASP:HB2	2.03	0.41
3:B:3391:GLU:HG3	3:B:3395:ARG:HE	1.84	0.41
3:B:4093:PHE:O	3:B:4097:MET:HG2	2.20	0.41
9:B:5308:L9R:H44	9:B:5308:L9R:H47A	1.52	0.41
3:G:462:GLU:HG3	3:G:3710:LEU:HD13	2.02	0.41
3:G:2514:ASN:OD1	3:G:2514:ASN:N	2.53	0.41
3:G:4060:LYS:HD2	3:G:4060:LYS:HA	1.91	0.41
3:I:938:HIS:HB3	3:I:1054:GLU:HB3	2.02	0.41
3:I:954:LYS:HB3	3:I:966:LYS:HE3	2.03	0.41
3:I:2390:PRO:C	3:I:2392:ARG:H	2.28	0.41
3:I:2775:TRP:CD2	3:I:2786:LYS:HE3	2.56	0.41
3:I:3628:ARG:HG3	3:I:3631:ALA:HB3	2.01	0.41
3:A:1154:ASP:OD1	3:A:1156:THR:OG1	2.37	0.41
3:A:2749:GLU:HG3	3:A:2752:ASP:HB2	2.03	0.41
3:A:2858:GLN:HB2	3:A:2859:PRO:HD3	2.02	0.41
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	2.02	0.41
3:B:330:ASP:OD1	3:B:330:ASP:N	2.53	0.41
3:B:2858:GLN:HB2	3:B:2859:PRO:HD3	2.02	0.41
3:B:4063:ASP:OD1	3:B:4064:MET:N	2.54	0.41
3:B:4241:THR:HG22	3:B:4245:MET:HE3	2.03	0.41
3:G:144:GLU:OE1	3:I:2452:ARG:NH1	2.53	0.41
3:G:308:HIS:CE1	3:G:310:LYS:HB3	2.56	0.41
3:G:881:LEU:HD13	3:G:881:LEU:HA	1.92	0.41
3:G:1805:GLU:CD	3:G:1805:GLU:H	2.29	0.41
3:G:2801:ASP:HA	3:G:2804:ILE:HG12	2.01	0.41
3:G:2858:GLN:HB2	3:G:2859:PRO:HD3	2.02	0.41
3:G:3390:GLY:HA2	3:G:3393:LEU:HD23	2.02	0.41
3:G:5012:LYS:NZ	3:G:5016:GLU:OE2	2.41	0.41
3:I:4063:ASP:OD1	3:I:4064:MET:N	2.54	0.41
2:F:27:THR:HG23	2:F:38:SER:HB2	2.03	0.41
3:A:872:GLU:HG2	3:A:922:LEU:HD21	2.03	0.41
3:A:1000:ARG:HB3	3:A:1005:TRP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2495:VAL:HG22	3:A:2498:HIS:CE1	2.56	0.41
3:A:3249:LEU:HD23	3:A:3277:LEU:HD21	2.03	0.41
9:A:5308:L9R:H39	9:A:5308:L9R:H42A	1.76	0.41
3:B:2747:ILE:HD13	3:B:2814:LYS:HG2	2.02	0.41
3:B:3107:VAL:HG21	3:B:3171:SER:HB2	2.03	0.41
3:G:797:HIS:CG	3:G:821:LEU:HD23	2.56	0.41
3:G:1078:GLU:OE2	3:G:1654:SER:OG	2.26	0.41
3:G:3159:ASP:OD1	3:G:3159:ASP:N	2.52	0.41
3:G:3501:ASP:OD1	3:G:3501:ASP:N	2.54	0.41
3:G:4839:MET:HE2	3:I:4820:VAL:HG11	2.03	0.41
3:I:1000:ARG:HB3	3:I:1005:TRP:HB2	2.01	0.41
3:I:1805:GLU:CD	3:I:1805:GLU:H	2.29	0.41
3:I:2519:LEU:HD22	3:I:2578:MET:HE1	2.02	0.41
3:I:2886:TRP:HA	3:I:2889:LYS:NZ	2.36	0.41
3:I:3284:TRP:HB3	3:I:3305:THR:HG21	2.02	0.41
3:A:880:GLU:CD	3:A:910:PHE:HB3	2.46	0.41
3:A:2519:LEU:HD22	3:A:2578:MET:HE1	2.02	0.41
3:A:2782:ASP:OD1	3:A:2782:ASP:N	2.54	0.41
3:A:3390:GLY:HA2	3:A:3393:LEU:HD23	2.02	0.41
3:A:3680:ALA:HB1	3:A:3683:GLN:NE2	2.36	0.41
3:B:462:GLU:HG3	3:B:3710:LEU:HD13	2.02	0.41
3:B:2886:TRP:HA	3:B:2889:LYS:NZ	2.36	0.41
3:B:2907:PRO:O	3:B:2910:THR:OG1	2.35	0.41
3:B:3590:GLU:CD	3:B:3590:GLU:H	2.29	0.41
3:G:2785:LEU:C	3:G:2786:LYS:HG3	2.46	0.41
3:G:3147:ILE:HG23	3:G:3152:PHE:HB2	2.02	0.41
3:G:3590:GLU:H	3:G:3590:GLU:CD	2.29	0.41
3:G:3680:ALA:HB1	3:G:3683:GLN:NE2	2.36	0.41
3:G:3688:GLU:C	3:G:3690:VAL:H	2.29	0.41
3:I:330:ASP:OD1	3:I:330:ASP:N	2.53	0.41
3:I:653:ALA:HB3	3:I:656:SER:HB2	2.03	0.41
3:I:863:LEU:HD11	3:I:930:LYS:NZ	2.35	0.41
3:I:872:GLU:HG2	3:I:922:LEU:HD21	2.03	0.41
3:I:1804:LEU:HD13	3:I:1853:ILE:HD12	2.03	0.41
3:I:2747:ILE:HD13	3:I:2814:LYS:HG2	2.02	0.41
3:I:3359:ILE:HG23	3:I:3437:MET:HE1	2.02	0.41
3:I:4091:LYS:HB2	3:I:4091:LYS:HE2	1.89	0.41
3:A:1575:LEU:HD23	3:A:1575:LEU:HA	1.90	0.41
3:A:1805:GLU:CD	3:A:1805:GLU:H	2.29	0.41
3:A:1997:GLU:O	3:A:2000:SER:OG	2.37	0.41
3:A:2785:LEU:C	3:A:2786:LYS:HG3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3590:GLU:H	3:A:3590:GLU:CD	2.29	0.41
3:B:275:ARG:HH21	3:B:328:LYS:HG3	1.86	0.41
3:B:954:LYS:HB3	3:B:966:LYS:HE3	2.03	0.41
3:B:2212:VAL:HG11	3:B:2256:TYR:CE2	2.55	0.41
3:B:2495:VAL:HG22	3:B:2498:HIS:CE1	2.56	0.41
3:B:2801:ASP:HA	3:B:2804:ILE:HG12	2.01	0.41
3:B:3688:GLU:C	3:B:3690:VAL:H	2.29	0.41
3:B:4060:LYS:HD2	3:B:4060:LYS:HA	1.91	0.41
3:B:4687:TYR:OH	3:B:4699:GLY:O	2.26	0.41
3:G:901:LYS:HG3	3:G:903:LEU:HG	2.02	0.41
3:G:1997:GLU:O	3:G:2000:SER:OG	2.37	0.41
3:G:2749:GLU:HG3	3:G:2752:ASP:HB2	2.03	0.41
3:G:3107:VAL:HG21	3:G:3171:SER:HB2	2.03	0.41
3:G:3284:TRP:HB3	3:G:3305:THR:HG21	2.02	0.41
3:G:3734:HIS:CG	3:G:3735:LEU:N	2.89	0.41
3:G:4661:TYR:OH	3:G:4786:ASP:OD2	2.33	0.41
3:I:275:ARG:HH21	3:I:328:LYS:HG3	1.86	0.41
3:I:308:HIS:CE1	3:I:310:LYS:HB3	2.56	0.41
3:I:797:HIS:CG	3:I:821:LEU:HD23	2.56	0.41
3:I:870:ILE:HG12	3:I:1051:TYR:HE2	1.86	0.41
3:I:2212:VAL:HG11	3:I:2256:TYR:CE2	2.55	0.41
3:I:3590:GLU:H	3:I:3590:GLU:CD	2.29	0.41
3:I:4093:PHE:O	3:I:4097:MET:HG2	2.20	0.41
3:I:4880:MET:HE3	3:I:4880:MET:HB2	1.97	0.41
9:I:5308:L9R:H23	9:I:5308:L9R:H20	1.32	0.41
1:K:26:THR:HB	1:K:62:THR:HB	2.02	0.41
3:A:345:LEU:HB3	3:A:387:ALA:HB1	2.02	0.41
3:A:2751:LEU:O	3:A:2755:ILE:HG12	2.21	0.41
3:A:3157:ILE:HG23	3:A:3161:VAL:HG12	2.03	0.41
3:A:4063:ASP:OD1	3:A:4064:MET:N	2.54	0.41
9:A:5308:L9R:H23	9:A:5308:L9R:H20	1.32	0.41
2:H:27:THR:HG23	2:H:38:SER:HB2	2.03	0.41
3:B:653:ALA:HB3	3:B:656:SER:HB2	2.03	0.41
3:B:871:ARG:CZ	3:B:922:LEU:HD12	2.51	0.41
3:B:2390:PRO:C	3:B:2392:ARG:H	2.28	0.41
3:B:3147:ILE:HG23	3:B:3152:PHE:HB2	2.02	0.41
3:B:3359:ILE:HG23	3:B:3437:MET:HE1	2.02	0.41
3:B:3414:ARG:HH21	3:B:3472:ALA:H	1.67	0.41
3:B:3734:HIS:CG	3:B:3735:LEU:N	2.89	0.41
3:B:4152:GLU:OE1	3:B:4194:TYR:OH	2.28	0.41
3:G:2390:PRO:C	3:G:2392:ARG:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2495:VAL:HG22	3:G:2498:HIS:CE1	2.56	0.41
3:G:3003:LEU:HB2	3:G:3004:PRO:HD3	2.02	0.41
3:I:462:GLU:HG3	3:I:3710:LEU:HD13	2.02	0.41
3:I:3501:ASP:N	3:I:3501:ASP:OD1	2.54	0.41
1:D:85:ILE:H	1:D:85:ILE:HG13	1.57	0.40
3:A:308:HIS:CE1	3:A:310:LYS:HB3	2.56	0.40
3:A:2282:ASP:HA	3:A:2341:VAL:HG13	2.03	0.40
3:A:2413:GLU:OE2	3:A:2414:ASN:ND2	2.54	0.40
3:A:3359:ILE:HG23	3:A:3437:MET:HE1	2.02	0.40
3:A:3501:ASP:OD1	3:A:3501:ASP:N	2.54	0.40
3:A:4241:THR:HG22	3:A:4245:MET:HE3	2.03	0.40
3:B:979:PRO:O	3:B:982:THR:OG1	2.33	0.40
3:B:1997:GLU:O	3:B:2000:SER:OG	2.37	0.40
3:G:871:ARG:CZ	3:G:922:LEU:HD12	2.51	0.40
3:G:4063:ASP:OD1	3:G:4064:MET:N	2.54	0.40
3:G:4754:ASN:OD1	3:G:4755:GLU:N	2.47	0.40
3:I:336:PRO:HA	3:I:337:PRO:HD3	1.88	0.40
3:I:2495:VAL:HG22	3:I:2498:HIS:CE1	2.56	0.40
3:I:2749:GLU:HG3	3:I:2752:ASP:HB2	2.03	0.40
3:I:3823:LYS:HA	3:I:3823:LYS:HD3	1.87	0.40
1:K:69:LEU:HD23	1:K:69:LEU:HA	1.91	0.40
3:A:462:GLU:HG3	3:A:3710:LEU:HD13	2.02	0.40
3:A:871:ARG:CZ	3:A:922:LEU:HD12	2.51	0.40
3:A:954:LYS:HB3	3:A:966:LYS:HE3	2.03	0.40
3:A:2886:TRP:HA	3:A:2889:LYS:NZ	2.36	0.40
3:A:3341:PHE:O	3:A:3344:PRO:HD2	2.21	0.40
3:A:3535:LEU:O	3:A:3538:THR:OG1	2.31	0.40
3:A:4093:PHE:O	3:A:4097:MET:HG2	2.20	0.40
3:A:4154:VAL:HG12	3:A:4157:ASP:HB2	2.03	0.40
2:O:27:THR:HG23	2:O:38:SER:HB2	2.03	0.40
3:B:1634:LEU:HD23	3:B:1634:LEU:HA	1.92	0.40
3:B:1690:ASP:OD2	3:B:1693:GLN:NE2	2.52	0.40
3:B:2751:LEU:O	3:B:2755:ILE:HG12	2.21	0.40
3:B:4940:PHE:HZ	3:I:4931:ILE:HG23	1.87	0.40
3:G:863:LEU:HD11	3:G:930:LYS:NZ	2.35	0.40
3:G:2775:TRP:CD2	3:G:2786:LYS:HE3	2.56	0.40
3:G:2881:ASN:HA	3:G:2884:ASN:HD21	1.87	0.40
3:G:3249:LEU:HD23	3:G:3277:LEU:HD21	2.03	0.40
3:G:3341:PHE:O	3:G:3344:PRO:HD2	2.21	0.40
3:I:871:ARG:HB2	3:I:929:LEU:HD12	2.04	0.40
3:I:880:GLU:CD	3:I:910:PHE:HB3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2758:PHE:HA	3:I:2761:TYR:HB2	2.04	0.40
3:I:3341:PHE:O	3:I:3344:PRO:HD2	2.21	0.40
3:I:3562:LYS:HE2	3:I:3562:LYS:HB2	1.91	0.40
3:A:672:VAL:O	3:A:680:THR:OG1	2.35	0.40
3:A:870:ILE:HG12	3:A:1051:TYR:HE2	1.86	0.40
3:A:1079:LYS:HA	3:A:1189:LEU:HD11	2.04	0.40
3:A:2740:VAL:HG21	3:A:2819:TRP:HE1	1.87	0.40
3:A:2747:ILE:HD13	3:A:2814:LYS:HG2	2.02	0.40
3:A:3971:GLY:N	3:A:3972:PRO:HA	2.37	0.40
9:A:5307:L9R:H33A	9:G:5308:L9R:H3A	2.03	0.40
3:B:308:HIS:CE1	3:B:310:LYS:HB3	2.56	0.40
3:B:797:HIS:CG	3:B:821:LEU:HD23	2.56	0.40
3:B:2413:GLU:OE2	3:B:2414:ASN:ND2	2.54	0.40
3:B:4825:THR:O	3:B:4828:SER:OG	2.32	0.40
3:G:571:SER:OG	3:G:573:GLU:OE1	2.34	0.40
3:G:880:GLU:CD	3:G:910:PHE:HB3	2.46	0.40
3:G:2001:PRO:O	3:G:2005:GLN:HG3	2.21	0.40
3:G:2282:ASP:HA	3:G:2341:VAL:HG13	2.03	0.40
3:G:2413:GLU:OE2	3:G:2414:ASN:ND2	2.54	0.40
3:G:2759:ALA:HB1	3:G:2806:ARG:HB2	2.04	0.40
3:G:3359:ILE:HG23	3:G:3437:MET:HE1	2.02	0.40
9:G:5308:L9R:H42A	9:G:5308:L9R:H39	1.76	0.40
3:I:345:LEU:HB3	3:I:387:ALA:HB1	2.02	0.40
3:I:871:ARG:CZ	3:I:922:LEU:HD12	2.51	0.40
3:I:2001:PRO:O	3:I:2005:GLN:HG3	2.21	0.40
3:I:2527:LEU:HD12	3:I:2527:LEU:HA	1.92	0.40
3:I:2759:ALA:HB1	3:I:2806:ARG:HB2	2.04	0.40
3:I:3734:HIS:CG	3:I:3735:LEU:N	2.89	0.40
3:I:4241:THR:HG22	3:I:4245:MET:HE3	2.03	0.40
3:A:275:ARG:HE	3:A:328:LYS:HE2	1.87	0.40
3:A:3107:VAL:HG21	3:A:3171:SER:HB2	2.03	0.40
2:J:17:LYS:HE3	2:J:17:LYS:HB3	1.84	0.40
3:B:683:ARG:HG2	3:B:717:ASP:HB3	2.04	0.40
3:B:1488:LYS:HE3	3:B:1488:LYS:HB2	1.86	0.40
3:B:2001:PRO:O	3:B:2005:GLN:HG3	2.22	0.40
3:B:2740:VAL:HG21	3:B:2819:TRP:HE1	1.86	0.40
3:B:2758:PHE:HA	3:B:2761:TYR:HB2	2.04	0.40
3:B:2775:TRP:CD2	3:B:2786:LYS:HE3	2.56	0.40
3:B:3157:ILE:HG23	3:B:3161:VAL:HG12	2.03	0.40
3:G:653:ALA:HB3	3:G:656:SER:HB2	2.03	0.40
3:G:1948:ASP:OD1	3:G:2126:ARG:NH2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4090:LYS:HG2	3:G:4123:ILE:HD11	2.03	0.40
3:G:4967:TYR:OH	3:G:5033:GLU:OE2	2.29	0.40
3:I:1079:LYS:HA	3:I:1189:LEU:HD11	2.04	0.40
3:I:4090:LYS:HG2	3:I:4123:ILE:HD11	2.04	0.40
3:I:4813:LEU:HD23	3:I:4813:LEU:HA	1.87	0.40
1:E:130:ILE:H	1:E:130:ILE:HG13	1.72	0.40
3:A:1947:CYS:SG	3:A:2127:GLN:NE2	2.92	0.40
3:A:3717:ASP:OD1	3:A:3717:ASP:N	2.55	0.40
3:A:4090:LYS:HG2	3:A:4123:ILE:HD11	2.03	0.40
3:B:1451:GLY:HA3	3:B:1494:MET:HA	2.04	0.40
3:B:3159:ASP:OD1	3:B:3159:ASP:N	2.52	0.40
3:B:3501:ASP:OD1	3:B:3501:ASP:N	2.54	0.40
3:G:1079:LYS:HA	3:G:1189:LEU:HD11	2.04	0.40
3:I:1488:LYS:HB2	3:I:1488:LYS:HE3	1.86	0.40
3:I:1823:GLY:O	3:I:1825:HIS:ND1	2.52	0.40
3:I:3147:ILE:HG23	3:I:3152:PHE:HB2	2.02	0.40
3:I:3249:LEU:HD23	3:I:3277:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	J	105/108 (97%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21180 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	D	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	E	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	K	127/128 (99%)	123 (97%)	4 (3%)	35	50
2	F	89/90 (99%)	85 (96%)	4 (4%)	24	37
2	H	89/90 (99%)	85 (96%)	4 (4%)	24	37
2	J	89/90 (99%)	85 (96%)	4 (4%)	24	37
2	O	89/90 (99%)	85 (96%)	4 (4%)	24	37
3	A	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	B	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	G	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	I	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
All	All	16208/17976 (90%)	15904 (98%)	304 (2%)	49	64

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	21	LYS
1	K	30	LYS
1	K	85	ILE
1	K	105	LEU
2	F	17	LYS
2	F	25	HIS
2	F	29	MET
2	F	79	ASP
1	D	21	LYS
1	D	30	LYS
1	D	85	ILE
1	D	105	LEU
1	E	21	LYS
1	E	30	LYS
1	E	85	ILE
1	E	105	LEU
1	C	21	LYS
1	C	30	LYS
1	C	85	ILE
1	C	105	LEU
3	A	81	MET
3	A	155	LYS
3	A	220	LEU
3	A	860	GLN
3	A	862	VAL
3	A	869	ARG
3	A	873	LYS
3	A	881	LEU
3	A	882	TRP
3	A	887	ILE
3	A	898	ASP
3	A	907	LEU
3	A	908	VAL
3	A	911	HIS
3	A	913	LEU
3	A	922	LEU
3	A	945	LYS
3	A	950	LEU
3	A	951	LYS
3	A	957	LYS
3	A	958	THR
3	A	959	TYR
3	A	961	MET

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Mol	Chain	Res	Type
3	A	962	SER
3	A	972	LEU
3	A	976	ARG
3	A	984	LEU
3	A	999	ASP
3	A	1021	LEU
3	A	1022	VAL
3	A	1057	ASP
3	A	1506	GLN
3	A	1872	THR
3	A	1923	GLU
3	A	1990	GLU
3	A	2037	ASP
3	A	2153	MET
3	A	2203	MET
3	A	2219	GLU
3	A	2413	GLU
3	A	2482	ASP
3	A	2666	VAL
3	A	2742	THR
3	A	2747	ILE
3	A	2781	VAL
3	A	2803	GLU
3	A	2862	LEU
3	A	2876	GLU
3	A	2937	VAL
3	A	3112	LEU
3	A	3137	LEU
3	A	3296	LEU
3	A	3619	VAL
3	A	3624	LEU
3	A	3639	THR
3	A	3686	GLU
3	A	3752	SER
3	A	3756	LYS
3	A	4662	ASN
3	A	4722	ARG
3	A	4768	LEU
3	A	4796	MET
3	A	4821	LYS
3	A	4860	ARG
3	A	4861	LYS

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Mol	Chain	Res	Type
3	A	4903	ASP
3	A	4911	LEU
3	A	4918	ILE
2	H	17	LYS
2	H	25	HIS
2	H	29	MET
2	H	79	ASP
2	J	17	LYS
2	J	25	HIS
2	J	29	MET
2	J	79	ASP
2	O	17	LYS
2	O	25	HIS
2	O	29	MET
2	O	79	ASP
3	B	81	MET
3	B	155	LYS
3	B	220	LEU
3	B	860	GLN
3	B	862	VAL
3	B	869	ARG
3	B	873	LYS
3	B	881	LEU
3	B	882	TRP
3	B	887	ILE
3	B	898	ASP
3	B	907	LEU
3	B	908	VAL
3	B	911	HIS
3	B	913	LEU
3	B	922	LEU
3	B	945	LYS
3	B	950	LEU
3	B	951	LYS
3	B	957	LYS
3	B	958	THR
3	B	959	TYR
3	B	961	MET
3	B	962	SER
3	B	972	LEU
3	B	976	ARG
3	B	984	LEU

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Mol	Chain	Res	Type
3	B	999	ASP
3	B	1021	LEU
3	B	1022	VAL
3	B	1057	ASP
3	B	1506	GLN
3	B	1872	THR
3	B	1923	GLU
3	B	1990	GLU
3	B	2037	ASP
3	B	2153	MET
3	B	2203	MET
3	B	2219	GLU
3	B	2413	GLU
3	B	2482	ASP
3	B	2666	VAL
3	B	2742	THR
3	B	2747	ILE
3	B	2781	VAL
3	B	2803	GLU
3	B	2862	LEU
3	B	2876	GLU
3	B	2937	VAL
3	B	3112	LEU
3	B	3137	LEU
3	B	3296	LEU
3	B	3619	VAL
3	B	3624	LEU
3	B	3639	THR
3	B	3686	GLU
3	B	3752	SER
3	B	3756	LYS
3	B	4662	ASN
3	B	4722	ARG
3	B	4768	LEU
3	B	4796	MET
3	B	4821	LYS
3	B	4860	ARG
3	B	4861	LYS
3	B	4903	ASP
3	B	4911	LEU
3	B	4918	ILE
3	G	81	MET

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Mol	Chain	Res	Type
3	G	155	LYS
3	G	220	LEU
3	G	860	GLN
3	G	862	VAL
3	G	869	ARG
3	G	873	LYS
3	G	881	LEU
3	G	882	TRP
3	G	887	ILE
3	G	898	ASP
3	G	907	LEU
3	G	908	VAL
3	G	911	HIS
3	G	913	LEU
3	G	922	LEU
3	G	945	LYS
3	G	950	LEU
3	G	951	LYS
3	G	957	LYS
3	G	958	THR
3	G	959	TYR
3	G	961	MET
3	G	962	SER
3	G	972	LEU
3	G	976	ARG
3	G	984	LEU
3	G	999	ASP
3	G	1021	LEU
3	G	1022	VAL
3	G	1057	ASP
3	G	1506	GLN
3	G	1872	THR
3	G	1923	GLU
3	G	1990	GLU
3	G	2037	ASP
3	G	2153	MET
3	G	2203	MET
3	G	2219	GLU
3	G	2413	GLU
3	G	2482	ASP
3	G	2666	VAL
3	G	2742	THR

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Mol	Chain	Res	Type
3	G	2747	ILE
3	G	2781	VAL
3	G	2803	GLU
3	G	2862	LEU
3	G	2876	GLU
3	G	2937	VAL
3	G	3112	LEU
3	G	3137	LEU
3	G	3296	LEU
3	G	3619	VAL
3	G	3624	LEU
3	G	3639	THR
3	G	3686	GLU
3	G	3752	SER
3	G	3756	LYS
3	G	4662	ASN
3	G	4722	ARG
3	G	4768	LEU
3	G	4796	MET
3	G	4821	LYS
3	G	4860	ARG
3	G	4861	LYS
3	G	4903	ASP
3	G	4911	LEU
3	G	4918	ILE
3	I	81	MET
3	I	155	LYS
3	I	220	LEU
3	I	860	GLN
3	I	862	VAL
3	I	869	ARG
3	I	873	LYS
3	I	881	LEU
3	I	882	TRP
3	I	887	ILE
3	I	898	ASP
3	I	907	LEU
3	I	908	VAL
3	I	911	HIS
3	I	913	LEU
3	I	922	LEU
3	I	945	LYS

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Mol	Chain	Res	Type
3	I	950	LEU
3	I	951	LYS
3	I	957	LYS
3	I	958	THR
3	I	959	TYR
3	I	961	MET
3	I	962	SER
3	I	972	LEU
3	I	976	ARG
3	I	984	LEU
3	I	999	ASP
3	I	1021	LEU
3	I	1022	VAL
3	I	1057	ASP
3	I	1506	GLN
3	I	1872	THR
3	I	1923	GLU
3	I	1990	GLU
3	I	2037	ASP
3	I	2153	MET
3	I	2203	MET
3	I	2219	GLU
3	I	2413	GLU
3	I	2482	ASP
3	I	2666	VAL
3	I	2742	THR
3	I	2747	ILE
3	I	2781	VAL
3	I	2803	GLU
3	I	2862	LEU
3	I	2876	GLU
3	I	2937	VAL
3	I	3112	LEU
3	I	3137	LEU
3	I	3296	LEU
3	I	3619	VAL
3	I	3624	LEU
3	I	3639	THR
3	I	3686	GLU
3	I	3752	SER
3	I	3756	LYS
3	I	4662	ASN

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Mol	Chain	Res	Type
3	I	4722	ARG
3	I	4768	LEU
3	I	4796	MET
3	I	4821	LYS
3	I	4860	ARG
3	I	4861	LYS
3	I	4903	ASP
3	I	4911	LEU
3	I	4918	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	53	ASN
1	K	107	HIS
1	K	135	GLN
2	F	20	GLN
1	D	53	ASN
1	D	107	HIS
1	D	135	GLN
1	E	-1	HIS
1	E	53	ASN
1	E	135	GLN
1	C	53	ASN
1	C	107	HIS
1	C	135	GLN
3	A	224	HIS
3	A	495	ASN
3	A	838	HIS
3	A	938	HIS
3	A	963	ASN
3	A	991	ASN
3	A	1035	ASN
3	A	1640	HIS
3	A	1660	GLN
3	A	2003	GLN
3	A	2092	GLN
3	A	2180	GLN
3	A	2260	ASN
3	A	2420	HIS
3	A	2441	HIS
3	A	2515	GLN

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Mol	Chain	Res	Type
3	A	2673	HIS
3	A	2772	GLN
3	A	2883	HIS
3	A	2892	GLN
3	A	2933	ASN
3	A	3030	HIS
3	A	3180	ASN
3	A	3449	HIS
3	A	3667	HIS
3	A	3734	HIS
3	A	3761	GLN
3	A	3766	GLN
3	A	4109	GLN
3	A	4547	GLN
3	A	4558	ASN
3	A	4626	ASN
2	H	20	GLN
2	J	20	GLN
2	O	20	GLN
3	B	224	HIS
3	B	495	ASN
3	B	938	HIS
3	B	963	ASN
3	B	991	ASN
3	B	1035	ASN
3	B	1640	HIS
3	B	1660	GLN
3	B	2003	GLN
3	B	2180	GLN
3	B	2260	ASN
3	B	2420	HIS
3	B	2441	HIS
3	B	2515	GLN
3	B	2772	GLN
3	B	2892	GLN
3	B	2933	ASN
3	B	3030	HIS
3	B	3180	ASN
3	B	3449	HIS
3	B	3667	HIS
3	B	3761	GLN
3	B	3766	GLN

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Mol	Chain	Res	Type
3	B	4109	GLN
3	B	4558	ASN
3	B	4626	ASN
3	G	224	HIS
3	G	495	ASN
3	G	838	HIS
3	G	938	HIS
3	G	963	ASN
3	G	991	ASN
3	G	1035	ASN
3	G	1206	GLN
3	G	1420	ASN
3	G	1640	HIS
3	G	1660	GLN
3	G	2003	GLN
3	G	2092	GLN
3	G	2260	ASN
3	G	2441	HIS
3	G	2515	GLN
3	G	2673	HIS
3	G	2892	GLN
3	G	2933	ASN
3	G	3180	ASN
3	G	3667	HIS
3	G	3761	GLN
3	G	3766	GLN
3	G	4109	GLN
3	G	4558	ASN
3	G	4626	ASN
3	I	224	HIS
3	I	495	ASN
3	I	838	HIS
3	I	938	HIS
3	I	963	ASN
3	I	991	ASN
3	I	1035	ASN
3	I	1420	ASN
3	I	1640	HIS
3	I	1660	GLN
3	I	2003	GLN
3	I	2092	GLN
3	I	2180	GLN

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Mol	Chain	Res	Type
3	I	2260	ASN
3	I	2441	HIS
3	I	2515	GLN
3	I	2772	GLN
3	I	2892	GLN
3	I	2933	ASN
3	I	3030	HIS
3	I	3180	ASN
3	I	3449	HIS
3	I	3667	HIS
3	I	3734	HIS
3	I	3761	GLN
3	I	3766	GLN
3	I	4109	GLN
3	I	4558	ASN
3	I	4626	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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
8	KVR	A	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
5	ATP	G	5305	-	32,33,33	0.25	0	48,52,52	0.29	0
5	ATP	I	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
9	L9R	A	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	I	5304	-	15,15,15	0.37	0	23,23,23	0.45	0
9	L9R	B	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
9	L9R	B	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	I	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	G	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	G	5304	-	15,15,15	0.36	0	23,23,23	0.44	0
8	KVR	G	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.56	4 (12%)
5	ATP	A	5305	-	32,33,33	0.25	0	48,52,52	0.29	0
9	L9R	I	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
8	KVR	I	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	G	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	G	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
5	ATP	I	5305	-	32,33,33	0.26	0	48,52,52	0.29	0
7	CFF	A	5304	-	15,15,15	0.36	0	23,23,23	0.45	0
7	CFF	B	5304	-	15,15,15	0.37	0	23,23,23	0.45	0
9	L9R	A	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	B	5305	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
5	ATP	B	5301	-	32,33,33	0.29	0	48,52,52	0.39	0
8	KVR	B	5306	-	24,25,25	1.42	3 (12%)	31,34,34	1.55	4 (12%)

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
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
5	ATP	G	5305	-	-	8/22/38/38	0/3/3/3
5	ATP	I	5301	-	-	8/22/38/38	0/3/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
7	CFF	I	5304	-	-	-	0/2/2/2
9	L9R	B	5308	-	-	34/57/57/57	-
9	L9R	B	5307	-	-	30/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	L9R	I	5307	-	-	30/57/57/57	-
9	L9R	G	5308	-	-	34/57/57/57	-
7	CFF	G	5304	-	-	-	0/2/2/2
8	KVR	G	5306	-	-	2/10/20/20	0/2/3/3
5	ATP	A	5305	-	-	8/22/38/38	0/3/3/3
9	L9R	I	5308	-	-	34/57/57/57	-
8	KVR	I	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	G	5307	-	-	30/57/57/57	-
5	ATP	G	5301	-	-	8/22/38/38	0/3/3/3
5	ATP	I	5305	-	-	8/22/38/38	0/3/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
7	CFF	A	5304	-	-	-	0/2/2/2
9	L9R	A	5307	-	-	30/57/57/57	-
5	ATP	B	5305	-	-	8/22/38/38	0/3/3/3
5	ATP	A	5301	-	-	8/22/38/38	0/3/3/3
5	ATP	B	5301	-	-	8/22/38/38	0/3/3/3
7	CFF	B	5304	-	-	-	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.92	1.82	1.77
8	I	5306	KVR	C06-S09	4.91	1.82	1.77
8	A	5306	KVR	C06-S09	4.88	1.82	1.77
8	G	5306	KVR	C06-S09	4.86	1.82	1.77
9	A	5307	L9R	O2-C31	3.60	1.44	1.34
9	B	5307	L9R	O2-C31	3.60	1.44	1.34
9	G	5307	L9R	O2-C31	3.60	1.44	1.34
9	I	5307	L9R	O2-C31	3.60	1.44	1.34
9	A	5308	L9R	O2-C31	3.55	1.44	1.34
9	B	5308	L9R	O2-C31	3.55	1.44	1.34
9	I	5308	L9R	O2-C31	3.55	1.44	1.34
9	G	5308	L9R	O2-C31	3.53	1.44	1.34
9	G	5307	L9R	O3-C11	3.16	1.42	1.33
9	A	5307	L9R	O3-C11	3.14	1.42	1.33
9	I	5307	L9R	O3-C11	3.14	1.42	1.33
9	B	5307	L9R	O3-C11	3.14	1.42	1.33
9	A	5308	L9R	O3-C11	3.03	1.42	1.33
9	B	5308	L9R	O3-C11	3.03	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	5308	L9R	O3-C11	3.03	1.42	1.33
9	I	5308	L9R	O3-C11	3.02	1.42	1.33
8	G	5306	KVR	C13-C05	2.63	1.55	1.51
8	A	5306	KVR	C13-C05	2.61	1.55	1.51
8	B	5306	KVR	C13-C05	2.58	1.55	1.51
8	I	5306	KVR	C13-C05	2.58	1.55	1.51
9	A	5307	L9R	C32-C31	2.54	1.58	1.50
9	I	5307	L9R	C32-C31	2.54	1.58	1.50
9	B	5307	L9R	C32-C31	2.53	1.58	1.50
9	G	5307	L9R	C32-C31	2.53	1.58	1.50
9	B	5308	L9R	C32-C31	2.34	1.57	1.50
9	G	5308	L9R	C32-C31	2.34	1.57	1.50
9	A	5308	L9R	C32-C31	2.34	1.57	1.50
9	I	5308	L9R	C32-C31	2.34	1.57	1.50
8	A	5306	KVR	C13-N12	-2.30	1.45	1.47
8	I	5306	KVR	C13-N12	-2.30	1.45	1.47
8	B	5306	KVR	C13-N12	-2.30	1.45	1.47
8	G	5306	KVR	C13-N12	-2.29	1.45	1.47
9	I	5308	L9R	O2-C2	-2.24	1.41	1.46
9	A	5308	L9R	O2-C2	-2.24	1.41	1.46
9	B	5308	L9R	O2-C2	-2.23	1.41	1.46
9	G	5308	L9R	O2-C2	-2.23	1.41	1.46
9	A	5307	L9R	O2-C2	-2.14	1.41	1.46
9	B	5307	L9R	O2-C2	-2.13	1.41	1.46
9	G	5307	L9R	O2-C2	-2.13	1.41	1.46
9	I	5307	L9R	O2-C2	-2.10	1.41	1.46
9	I	5307	L9R	P-O3P	2.08	1.67	1.59
9	A	5307	L9R	P-O3P	2.08	1.67	1.59
9	G	5307	L9R	P-O3P	2.08	1.67	1.59
9	B	5307	L9R	P-O3P	2.07	1.67	1.59

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	5306	KVR	C10-S09-C06	5.26	110.17	102.71
8	A	5306	KVR	C10-S09-C06	5.26	110.16	102.71
8	B	5306	KVR	C10-S09-C06	5.24	110.14	102.71
8	I	5306	KVR	C10-S09-C06	5.24	110.13	102.71
9	G	5308	L9R	O2-C31-C32	4.04	120.22	111.48
9	A	5308	L9R	O2-C31-C32	4.03	120.20	111.48
9	I	5308	L9R	O2-C31-C32	4.03	120.20	111.48
9	B	5308	L9R	O2-C31-C32	4.01	120.16	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	5307	L9R	O2-C31-C32	3.92	119.96	111.48
9	A	5307	L9R	O2-C31-C32	3.92	119.95	111.48
9	I	5307	L9R	O2-C31-C32	3.92	119.95	111.48
9	G	5307	L9R	O2-C31-C32	3.89	119.90	111.48
8	G	5306	KVR	C11-C10-S09	-3.52	110.15	114.26
8	A	5306	KVR	C11-C10-S09	-3.50	110.16	114.26
8	B	5306	KVR	C11-C10-S09	-3.48	110.18	114.26
8	I	5306	KVR	C11-C10-S09	-3.48	110.19	114.26
9	I	5307	L9R	O3-C11-C12	2.86	120.56	111.83
9	B	5307	L9R	O3-C11-C12	2.86	120.56	111.83
9	A	5307	L9R	O3-C11-C12	2.85	120.53	111.83
9	G	5307	L9R	O3-C11-C12	2.83	120.48	111.83
8	I	5306	KVR	C14-N12-C11	-2.79	106.56	111.09
8	G	5306	KVR	C14-N12-C11	-2.78	106.57	111.09
8	A	5306	KVR	C14-N12-C11	-2.76	106.60	111.09
9	A	5308	L9R	O3-C11-C12	2.76	120.24	111.83
9	I	5308	L9R	O3-C11-C12	2.76	120.24	111.83
9	B	5308	L9R	O3-C11-C12	2.75	120.23	111.83
9	G	5308	L9R	O3-C11-C12	2.75	120.23	111.83
8	B	5306	KVR	C14-N12-C11	-2.73	106.66	111.09
9	I	5307	L9R	C4-C5-N	-2.32	108.36	115.82
9	B	5307	L9R	C4-C5-N	-2.32	108.36	115.82
9	G	5307	L9R	C4-C5-N	-2.31	108.39	115.82
9	A	5307	L9R	C4-C5-N	-2.31	108.40	115.82
8	A	5306	KVR	O23-C21-C18	2.26	120.64	114.84
8	I	5306	KVR	O23-C21-C18	2.26	120.64	114.84
8	B	5306	KVR	O23-C21-C18	2.26	120.63	114.84
8	G	5306	KVR	O23-C21-C18	2.24	120.57	114.84

There are no chirality outliers.

All (328) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5301	ATP	C5'-O5'-PA-O3A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A
5	B	5301	ATP	C5'-O5'-PA-O1A
5	B	5301	ATP	C5'-O5'-PA-O2A
5	B	5301	ATP	C5'-O5'-PA-O3A
5	B	5305	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	B	5305	ATP	C5'-O5'-PA-O3A
5	G	5301	ATP	C5'-O5'-PA-O1A
5	G	5301	ATP	C5'-O5'-PA-O2A
5	G	5301	ATP	C5'-O5'-PA-O3A
5	G	5305	ATP	C5'-O5'-PA-O2A
5	G	5305	ATP	C5'-O5'-PA-O3A
5	I	5301	ATP	C5'-O5'-PA-O1A
5	I	5301	ATP	C5'-O5'-PA-O2A
5	I	5301	ATP	C5'-O5'-PA-O3A
5	I	5305	ATP	C5'-O5'-PA-O2A
5	I	5305	ATP	C5'-O5'-PA-O3A
8	A	5306	KVR	C15-C14-N12-C11
8	A	5306	KVR	C15-C14-N12-C13
8	B	5306	KVR	C15-C14-N12-C11
8	B	5306	KVR	C15-C14-N12-C13
8	G	5306	KVR	C15-C14-N12-C11
8	G	5306	KVR	C15-C14-N12-C13
8	I	5306	KVR	C15-C14-N12-C11
8	I	5306	KVR	C15-C14-N12-C13
9	A	5308	L9R	C1-O3P-P-O1P
9	A	5308	L9R	C1-O3P-P-O4P
9	A	5308	L9R	C4-O4P-P-O1P
9	A	5308	L9R	C4-O4P-P-O2P
9	A	5308	L9R	C4-O4P-P-O3P
9	A	5308	L9R	O4P-C4-C5-N
9	B	5308	L9R	C1-O3P-P-O1P
9	B	5308	L9R	C1-O3P-P-O4P
9	B	5308	L9R	C4-O4P-P-O1P
9	B	5308	L9R	C4-O4P-P-O2P
9	B	5308	L9R	C4-O4P-P-O3P
9	B	5308	L9R	O4P-C4-C5-N
9	G	5308	L9R	C1-O3P-P-O1P
9	G	5308	L9R	C1-O3P-P-O4P
9	G	5308	L9R	C4-O4P-P-O1P
9	G	5308	L9R	C4-O4P-P-O2P
9	G	5308	L9R	C4-O4P-P-O3P
9	G	5308	L9R	O4P-C4-C5-N
9	I	5308	L9R	C1-O3P-P-O1P
9	I	5308	L9R	C1-O3P-P-O4P
9	I	5308	L9R	C4-O4P-P-O1P
9	I	5308	L9R	C4-O4P-P-O2P
9	I	5308	L9R	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
9	I	5308	L9R	O4P-C4-C5-N
9	A	5307	L9R	C32-C31-O2-C2
9	B	5307	L9R	C32-C31-O2-C2
9	G	5307	L9R	C32-C31-O2-C2
9	I	5307	L9R	C32-C31-O2-C2
9	A	5308	L9R	C20-C21-C22-C23
9	B	5308	L9R	C20-C21-C22-C23
9	G	5308	L9R	C20-C21-C22-C23
9	I	5308	L9R	C20-C21-C22-C23
9	A	5308	L9R	C13-C14-C15-C16
9	B	5308	L9R	C13-C14-C15-C16
9	G	5308	L9R	C13-C14-C15-C16
9	A	5307	L9R	C12-C11-O3-C3
9	B	5307	L9R	C12-C11-O3-C3
9	G	5307	L9R	C12-C11-O3-C3
9	I	5307	L9R	C12-C11-O3-C3
9	I	5308	L9R	C13-C14-C15-C16
9	A	5307	L9R	O11-C11-O3-C3
9	B	5307	L9R	O11-C11-O3-C3
9	G	5307	L9R	O11-C11-O3-C3
9	I	5307	L9R	O11-C11-O3-C3
9	A	5307	L9R	O31-C31-O2-C2
9	B	5307	L9R	O31-C31-O2-C2
9	G	5307	L9R	O31-C31-O2-C2
9	I	5307	L9R	O31-C31-O2-C2
9	A	5308	L9R	C11-C12-C13-C14
9	B	5308	L9R	C11-C12-C13-C14
9	G	5308	L9R	C11-C12-C13-C14
9	I	5308	L9R	C11-C12-C13-C14
9	G	5307	L9R	C32-C33-C34-C35
9	I	5307	L9R	C32-C33-C34-C35
9	A	5307	L9R	C32-C33-C34-C35
9	B	5307	L9R	C32-C33-C34-C35
9	A	5308	L9R	C35-C36-C37-C38
9	B	5308	L9R	C35-C36-C37-C38
9	G	5308	L9R	C35-C36-C37-C38
9	I	5308	L9R	C35-C36-C37-C38
9	A	5307	L9R	C33-C34-C35-C36
9	B	5307	L9R	C33-C34-C35-C36
9	G	5307	L9R	C33-C34-C35-C36
9	I	5307	L9R	C33-C34-C35-C36
9	A	5307	L9R	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	A	5308	L9R	C22-C23-C24-C25
9	B	5307	L9R	C16-C17-C18-C19
9	B	5308	L9R	C22-C23-C24-C25
9	G	5307	L9R	C16-C17-C18-C19
9	G	5308	L9R	C22-C23-C24-C25
9	I	5307	L9R	C16-C17-C18-C19
9	I	5308	L9R	C22-C23-C24-C25
9	A	5308	L9R	C15-C16-C17-C18
9	B	5308	L9R	C15-C16-C17-C18
9	G	5308	L9R	C15-C16-C17-C18
9	I	5308	L9R	C15-C16-C17-C18
9	A	5307	L9R	C20-C21-C22-C23
9	B	5307	L9R	C20-C21-C22-C23
9	G	5307	L9R	C20-C21-C22-C23
9	I	5307	L9R	C20-C21-C22-C23
9	A	5308	L9R	C16-C17-C18-C19
9	B	5308	L9R	C16-C17-C18-C19
9	G	5308	L9R	C16-C17-C18-C19
9	I	5308	L9R	C16-C17-C18-C19
9	A	5308	L9R	C42-C43-C44-C45
9	G	5308	L9R	C42-C43-C44-C45
9	I	5308	L9R	C42-C43-C44-C45
9	B	5308	L9R	C42-C43-C44-C45
9	A	5307	L9R	C44-C45-C46-C47
9	B	5307	L9R	C44-C45-C46-C47
9	G	5307	L9R	C44-C45-C46-C47
9	I	5307	L9R	C44-C45-C46-C47
9	A	5307	L9R	C21-C22-C23-C24
9	B	5307	L9R	C21-C22-C23-C24
9	G	5307	L9R	C21-C22-C23-C24
9	I	5307	L9R	C21-C22-C23-C24
5	A	5301	ATP	O4'-C4'-C5'-O5'
5	B	5301	ATP	O4'-C4'-C5'-O5'
5	G	5301	ATP	O4'-C4'-C5'-O5'
5	I	5301	ATP	O4'-C4'-C5'-O5'
9	A	5307	L9R	C4-C5-N-C6
9	B	5307	L9R	C4-C5-N-C6
9	G	5307	L9R	C4-C5-N-C6
9	I	5307	L9R	C4-C5-N-C6
9	A	5308	L9R	C12-C13-C14-C15
9	B	5308	L9R	C12-C13-C14-C15
9	G	5308	L9R	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	I	5308	L9R	C12-C13-C14-C15
9	A	5307	L9R	O3P-C1-C2-O2
9	B	5307	L9R	O3P-C1-C2-O2
9	G	5307	L9R	O3P-C1-C2-O2
9	I	5307	L9R	O3P-C1-C2-O2
9	G	5308	L9R	C24-C25-C26-C27
9	I	5308	L9R	C24-C25-C26-C27
9	A	5308	L9R	C24-C25-C26-C27
9	B	5308	L9R	C24-C25-C26-C27
9	A	5307	L9R	C4-C5-N-C8
9	B	5307	L9R	C4-C5-N-C8
9	G	5307	L9R	C4-C5-N-C8
9	I	5307	L9R	C4-C5-N-C8
9	A	5308	L9R	C41-C42-C43-C44
9	G	5308	L9R	C41-C42-C43-C44
9	I	5308	L9R	C41-C42-C43-C44
9	B	5308	L9R	C41-C42-C43-C44
9	A	5308	L9R	C33-C34-C35-C36
9	B	5308	L9R	C33-C34-C35-C36
9	G	5308	L9R	C33-C34-C35-C36
9	I	5308	L9R	C33-C34-C35-C36
9	B	5307	L9R	C4-C5-N-C7
9	A	5308	L9R	C32-C33-C34-C35
9	B	5308	L9R	C32-C33-C34-C35
9	G	5308	L9R	C32-C33-C34-C35
9	I	5308	L9R	C32-C33-C34-C35
9	A	5307	L9R	C41-C42-C43-C44
9	B	5307	L9R	C41-C42-C43-C44
9	G	5307	L9R	C41-C42-C43-C44
9	I	5307	L9R	C41-C42-C43-C44
9	A	5308	L9R	C40-C41-C42-C43
9	B	5308	L9R	C40-C41-C42-C43
9	G	5308	L9R	C40-C41-C42-C43
9	I	5308	L9R	C40-C41-C42-C43
5	A	5301	ATP	C3'-C4'-C5'-O5'
5	B	5301	ATP	C3'-C4'-C5'-O5'
5	G	5301	ATP	C3'-C4'-C5'-O5'
5	I	5301	ATP	C3'-C4'-C5'-O5'
9	I	5308	L9R	C17-C18-C19-C20
9	A	5308	L9R	C17-C18-C19-C20
9	B	5308	L9R	C17-C18-C19-C20
9	G	5308	L9R	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
9	A	5308	L9R	C12-C11-O3-C3
9	B	5308	L9R	C12-C11-O3-C3
9	G	5308	L9R	C12-C11-O3-C3
9	I	5308	L9R	C12-C11-O3-C3
9	A	5307	L9R	C4-C5-N-C7
9	G	5307	L9R	C4-C5-N-C7
9	I	5307	L9R	C4-C5-N-C7
9	A	5307	L9R	C37-C38-C39-C40
9	B	5307	L9R	C37-C38-C39-C40
9	G	5307	L9R	C37-C38-C39-C40
9	I	5307	L9R	C37-C38-C39-C40
9	A	5307	L9R	C35-C36-C37-C38
9	B	5307	L9R	C35-C36-C37-C38
9	G	5307	L9R	C35-C36-C37-C38
9	I	5307	L9R	C35-C36-C37-C38
9	A	5308	L9R	C19-C20-C21-C22
9	B	5308	L9R	C19-C20-C21-C22
9	G	5308	L9R	C19-C20-C21-C22
9	I	5308	L9R	C19-C20-C21-C22
9	A	5308	L9R	C14-C15-C16-C17
9	B	5308	L9R	C14-C15-C16-C17
9	I	5308	L9R	C14-C15-C16-C17
9	G	5308	L9R	C14-C15-C16-C17
9	B	5308	L9R	C44-C45-C46-C47
9	A	5308	L9R	C44-C45-C46-C47
9	G	5308	L9R	C44-C45-C46-C47
9	I	5308	L9R	C44-C45-C46-C47
9	A	5308	L9R	C18-C19-C20-C21
9	B	5308	L9R	C18-C19-C20-C21
9	I	5308	L9R	C18-C19-C20-C21
9	G	5308	L9R	C18-C19-C20-C21
9	I	5307	L9R	C24-C25-C26-C27
9	A	5307	L9R	C24-C25-C26-C27
9	B	5307	L9R	C24-C25-C26-C27
9	G	5307	L9R	C24-C25-C26-C27
9	I	5308	L9R	O11-C11-O3-C3
9	A	5307	L9R	O3P-C1-C2-C3
9	B	5307	L9R	O3P-C1-C2-C3
9	G	5307	L9R	O3P-C1-C2-C3
9	I	5307	L9R	O3P-C1-C2-C3
9	A	5307	L9R	C45-C46-C47-C48
9	B	5307	L9R	C45-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
9	G	5307	L9R	C45-C46-C47-C48
9	I	5307	L9R	C45-C46-C47-C48
9	A	5308	L9R	O11-C11-O3-C3
9	B	5308	L9R	O11-C11-O3-C3
9	G	5308	L9R	O11-C11-O3-C3
5	A	5305	ATP	O4'-C1'-N9-C4
5	G	5305	ATP	O4'-C1'-N9-C4
9	A	5307	L9R	C1-C2-C3-O3
9	B	5307	L9R	C1-C2-C3-O3
9	G	5307	L9R	C1-C2-C3-O3
9	I	5307	L9R	C1-C2-C3-O3
9	A	5307	L9R	O2-C2-C3-O3
9	B	5307	L9R	O2-C2-C3-O3
9	G	5307	L9R	O2-C2-C3-O3
9	I	5307	L9R	O2-C2-C3-O3
9	A	5307	L9R	C13-C14-C15-C16
9	A	5307	L9R	C15-C16-C17-C18
9	B	5307	L9R	C13-C14-C15-C16
9	G	5307	L9R	C13-C14-C15-C16
9	G	5307	L9R	C15-C16-C17-C18
9	I	5307	L9R	C13-C14-C15-C16
9	B	5307	L9R	C15-C16-C17-C18
9	I	5307	L9R	C15-C16-C17-C18
5	A	5305	ATP	O4'-C1'-N9-C8
5	B	5305	ATP	O4'-C1'-N9-C8
5	G	5305	ATP	O4'-C1'-N9-C8
5	I	5305	ATP	O4'-C1'-N9-C8
5	B	5305	ATP	O4'-C1'-N9-C4
5	I	5305	ATP	O4'-C1'-N9-C4
9	A	5308	L9R	C39-C40-C41-C42
9	B	5308	L9R	C39-C40-C41-C42
9	G	5308	L9R	C39-C40-C41-C42
9	I	5308	L9R	C39-C40-C41-C42
9	A	5307	L9R	C4-O4P-P-O1P
9	A	5308	L9R	C4-C5-N-C7
9	B	5307	L9R	C4-O4P-P-O1P
9	B	5308	L9R	C4-C5-N-C7
9	G	5307	L9R	C4-O4P-P-O1P
9	G	5308	L9R	C4-C5-N-C7
9	I	5307	L9R	C4-O4P-P-O1P
9	I	5308	L9R	C4-C5-N-C7
5	A	5305	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	B	5305	ATP	C3'-C4'-C5'-O5'
5	G	5305	ATP	C3'-C4'-C5'-O5'
5	I	5305	ATP	C3'-C4'-C5'-O5'
9	A	5308	L9R	C4-C5-N-C6
9	B	5308	L9R	C4-C5-N-C6
9	G	5308	L9R	C4-C5-N-C6
9	I	5308	L9R	C4-C5-N-C6
9	A	5308	L9R	C23-C24-C25-C26
9	B	5308	L9R	C23-C24-C25-C26
9	I	5308	L9R	C23-C24-C25-C26
9	G	5308	L9R	C23-C24-C25-C26
5	A	5305	ATP	O4'-C4'-C5'-O5'
5	B	5305	ATP	O4'-C4'-C5'-O5'
5	G	5305	ATP	O4'-C4'-C5'-O5'
5	I	5305	ATP	O4'-C4'-C5'-O5'
5	A	5301	ATP	PG-O3B-PB-O3A
5	G	5301	ATP	PG-O3B-PB-O3A
9	A	5308	L9R	C4-C5-N-C8
9	B	5308	L9R	C4-C5-N-C8
9	G	5308	L9R	C4-C5-N-C8
9	I	5308	L9R	C4-C5-N-C8
9	A	5307	L9R	C40-C41-C42-C43
9	B	5307	L9R	C40-C41-C42-C43
9	G	5307	L9R	C40-C41-C42-C43
9	I	5307	L9R	C40-C41-C42-C43
9	B	5308	L9R	C25-C26-C27-C28
9	G	5308	L9R	C25-C26-C27-C28
9	I	5308	L9R	C25-C26-C27-C28
9	A	5308	L9R	C25-C26-C27-C28
5	B	5301	ATP	PG-O3B-PB-O3A
5	I	5301	ATP	PG-O3B-PB-O3A
5	A	5301	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O2B
5	B	5301	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O2B
5	G	5301	ATP	PG-O3B-PB-O1B
5	G	5305	ATP	PG-O3B-PB-O1B
5	G	5305	ATP	PG-O3B-PB-O2B
5	I	5301	ATP	PG-O3B-PB-O1B
5	I	5305	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	I	5305	ATP	PG-O3B-PB-O2B
9	I	5307	L9R	C12-C13-C14-C15
9	G	5307	L9R	C12-C13-C14-C15
9	A	5307	L9R	C12-C13-C14-C15
9	B	5307	L9R	C12-C13-C14-C15
9	A	5307	L9R	O2-C31-C32-C33
9	B	5307	L9R	O2-C31-C32-C33
9	G	5307	L9R	O2-C31-C32-C33
9	I	5307	L9R	O2-C31-C32-C33
9	B	5307	L9R	C43-C44-C45-C46
9	A	5307	L9R	C43-C44-C45-C46
9	G	5307	L9R	C43-C44-C45-C46
9	I	5307	L9R	C43-C44-C45-C46
5	A	5301	ATP	C4'-C5'-O5'-PA
5	B	5301	ATP	C4'-C5'-O5'-PA
5	G	5301	ATP	C4'-C5'-O5'-PA
5	I	5301	ATP	C4'-C5'-O5'-PA
9	I	5308	L9R	C45-C46-C47-C48
9	A	5308	L9R	C45-C46-C47-C48
9	B	5308	L9R	C45-C46-C47-C48
9	G	5308	L9R	C45-C46-C47-C48
9	B	5307	L9R	O31-C31-C32-C33
9	I	5307	L9R	O31-C31-C32-C33
9	A	5307	L9R	O31-C31-C32-C33
9	G	5307	L9R	O31-C31-C32-C33

There are no ring outliers.

16 monomers are involved in 34 short contacts:

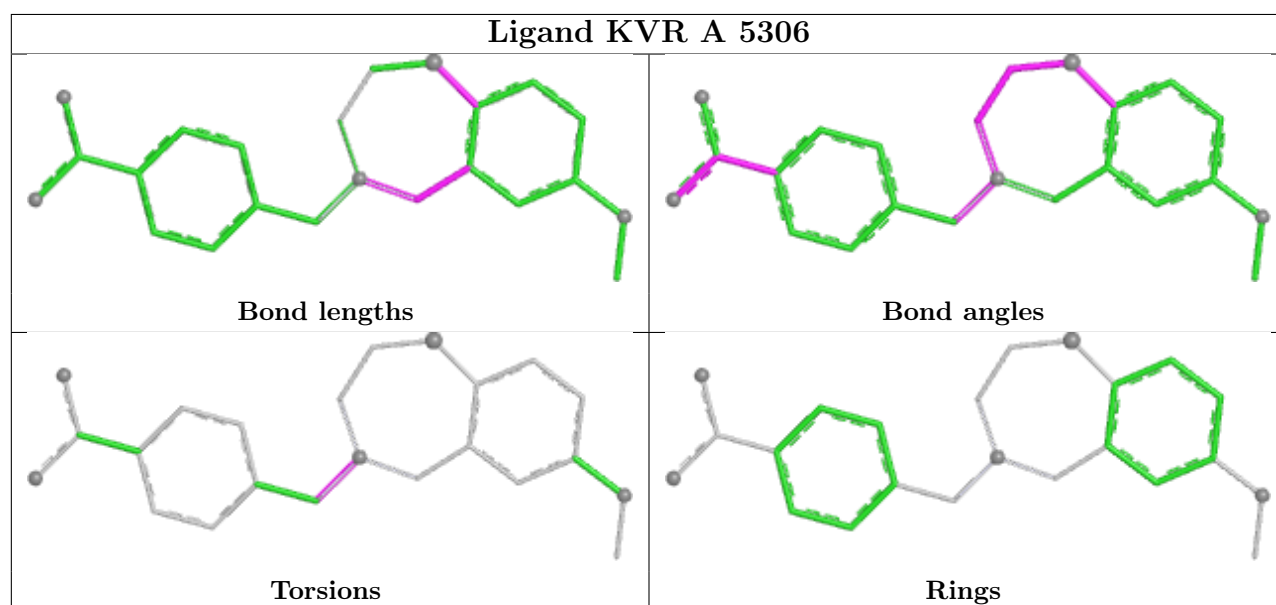
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	5305	ATP	1	0
5	I	5301	ATP	1	0
9	A	5308	L9R	6	0
9	B	5308	L9R	3	0
9	B	5307	L9R	2	0
9	I	5307	L9R	2	0
9	G	5308	L9R	5	0
5	A	5305	ATP	1	0
9	I	5308	L9R	5	0
9	G	5307	L9R	3	0
5	G	5301	ATP	1	0
5	I	5305	ATP	1	0

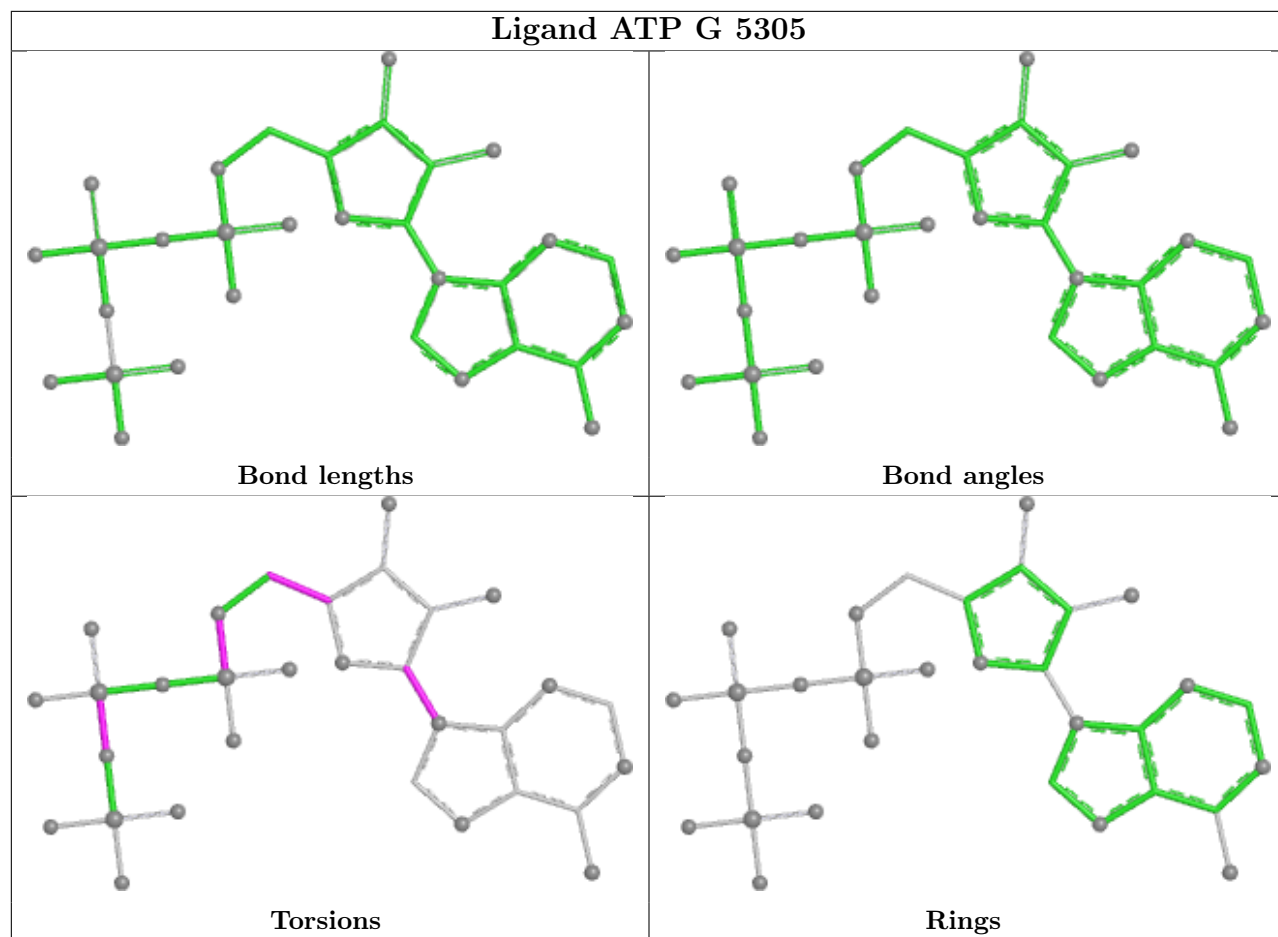
Continued on next page...

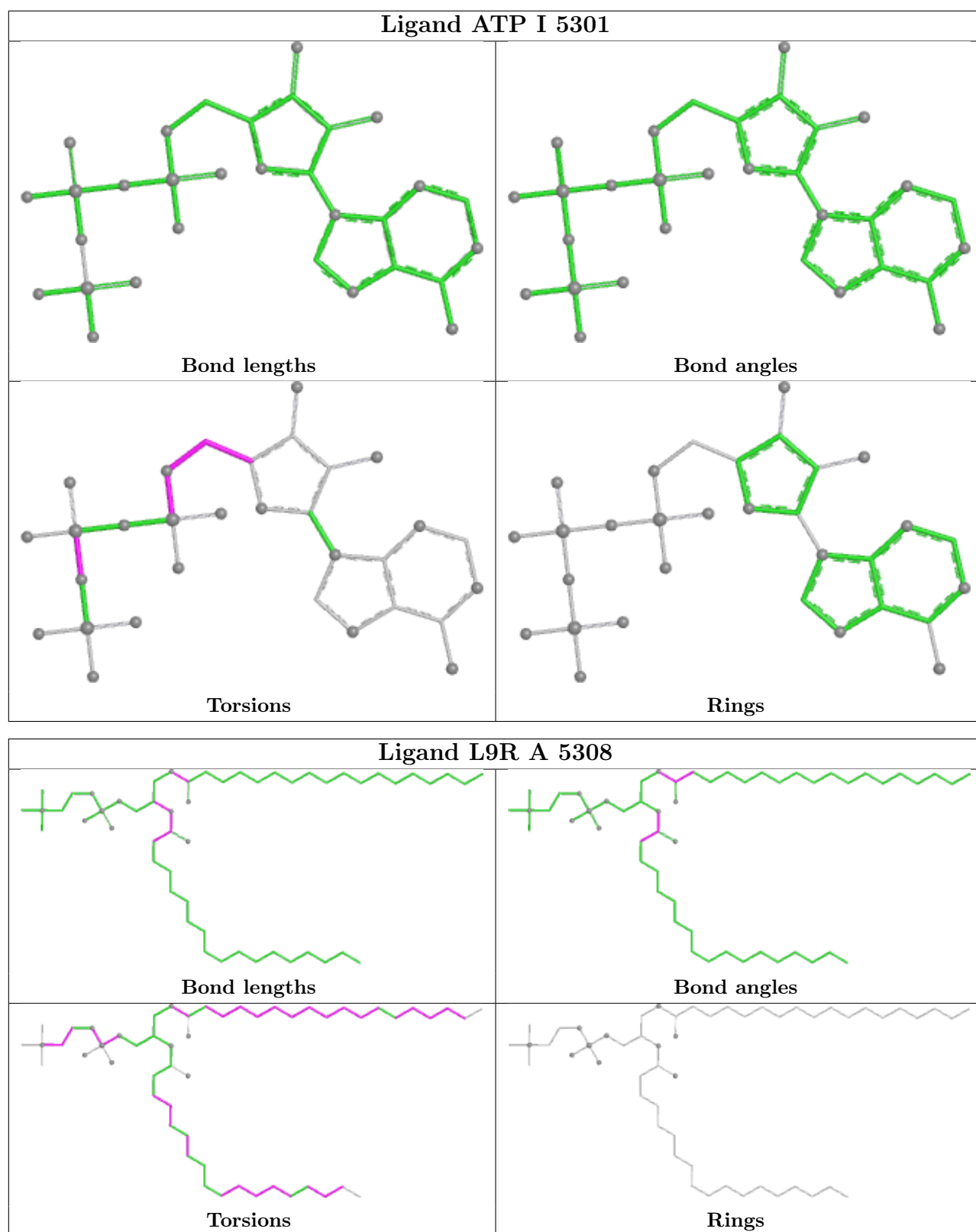
Continued from previous page...

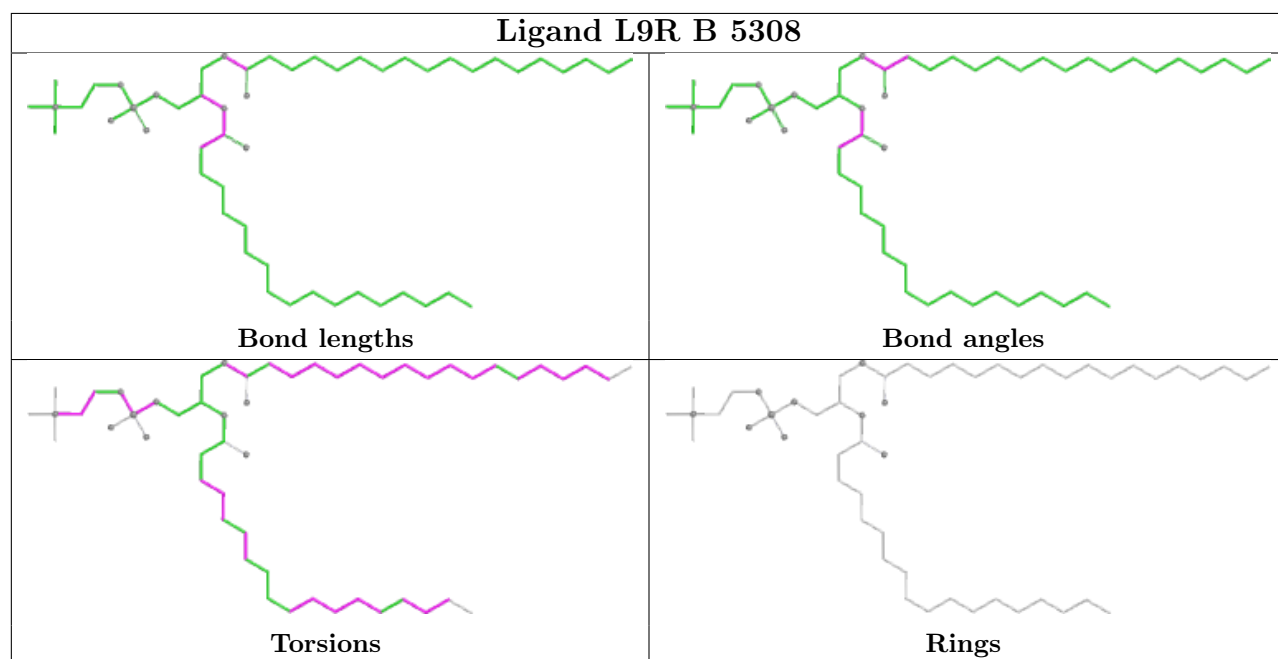
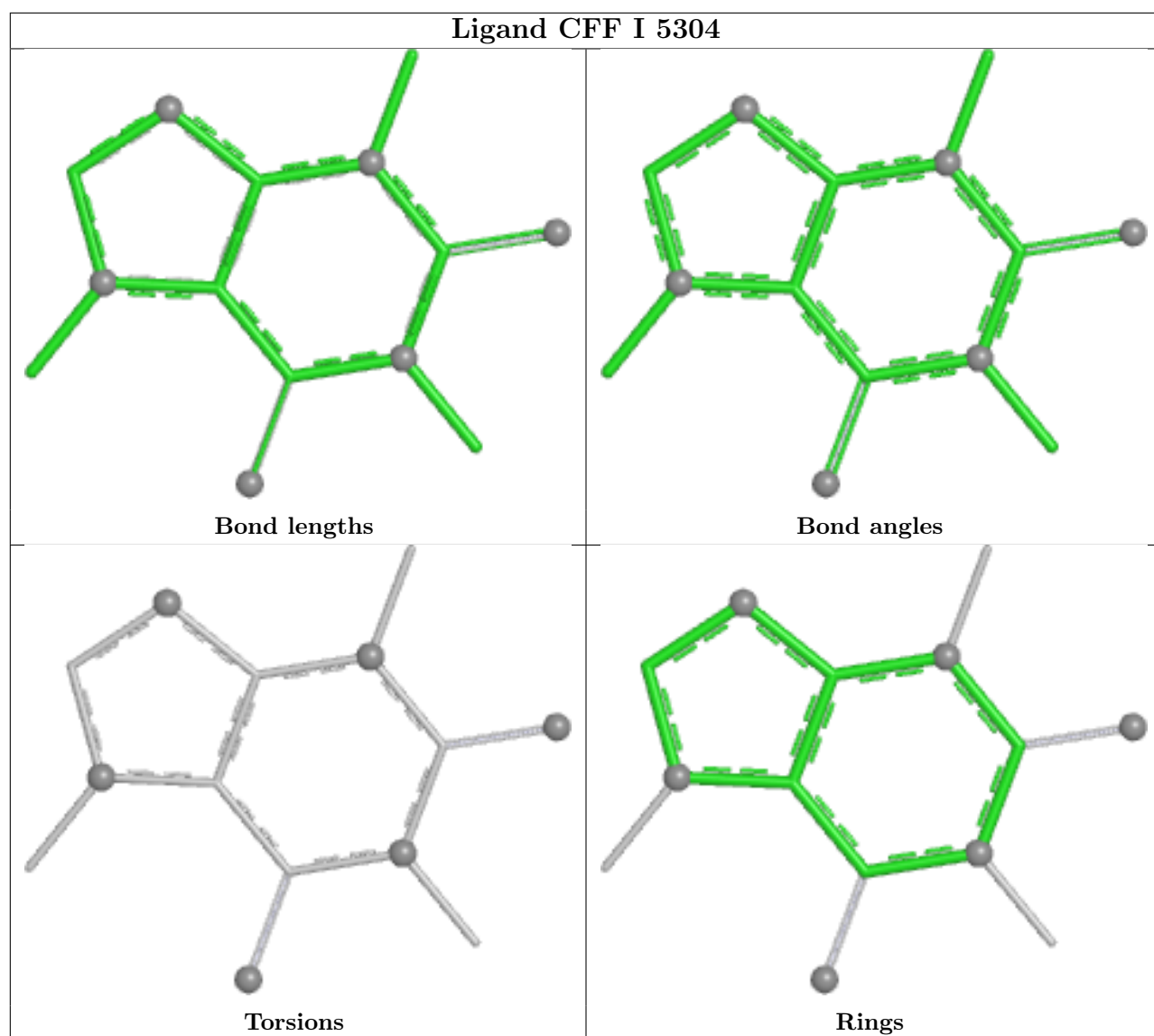
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	5307	L9R	3	0
5	B	5305	ATP	1	0
5	A	5301	ATP	1	0
5	B	5301	ATP	1	0

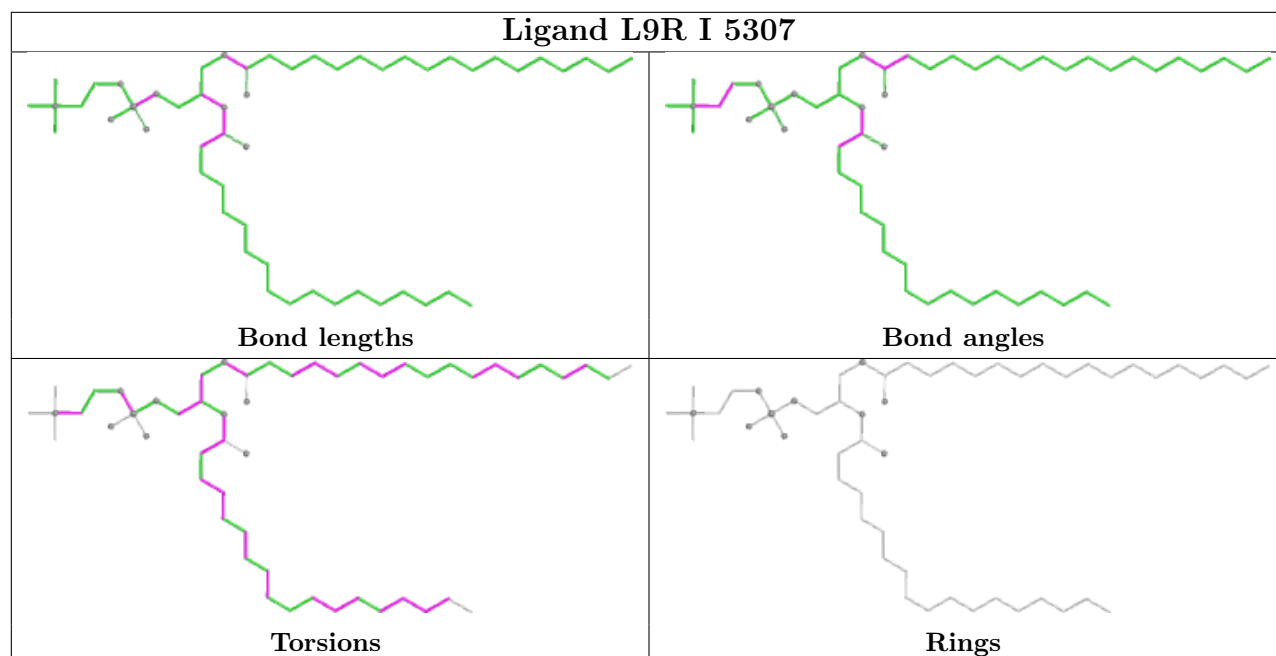
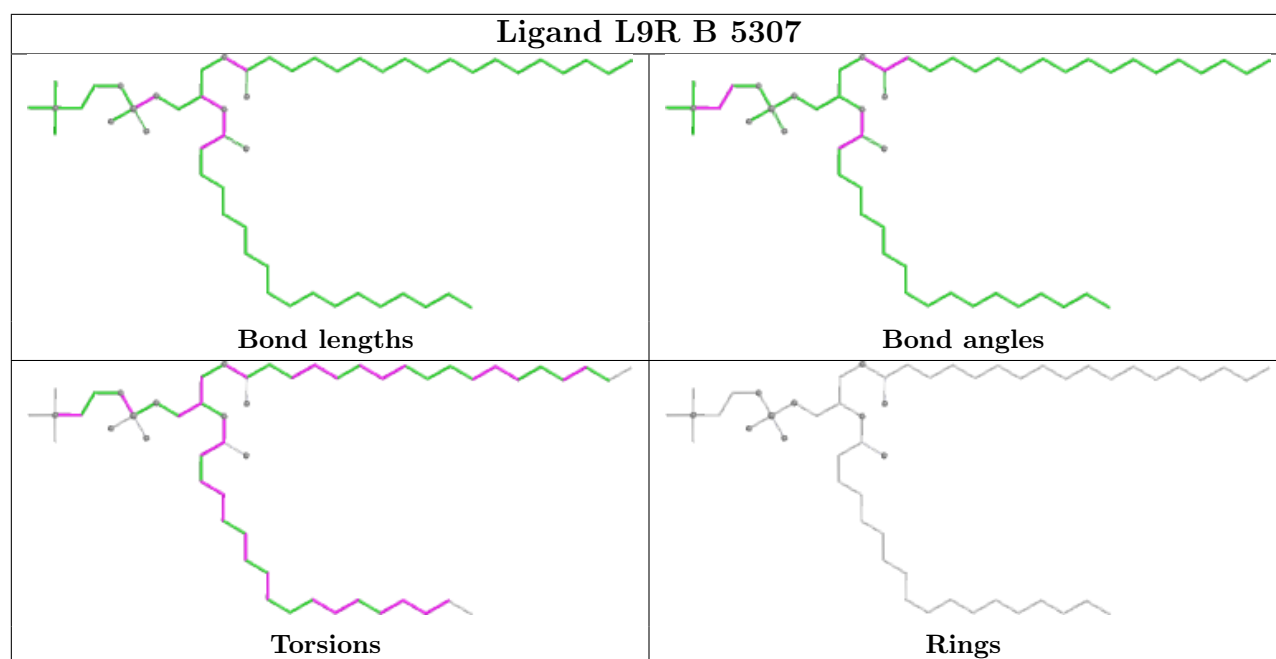
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

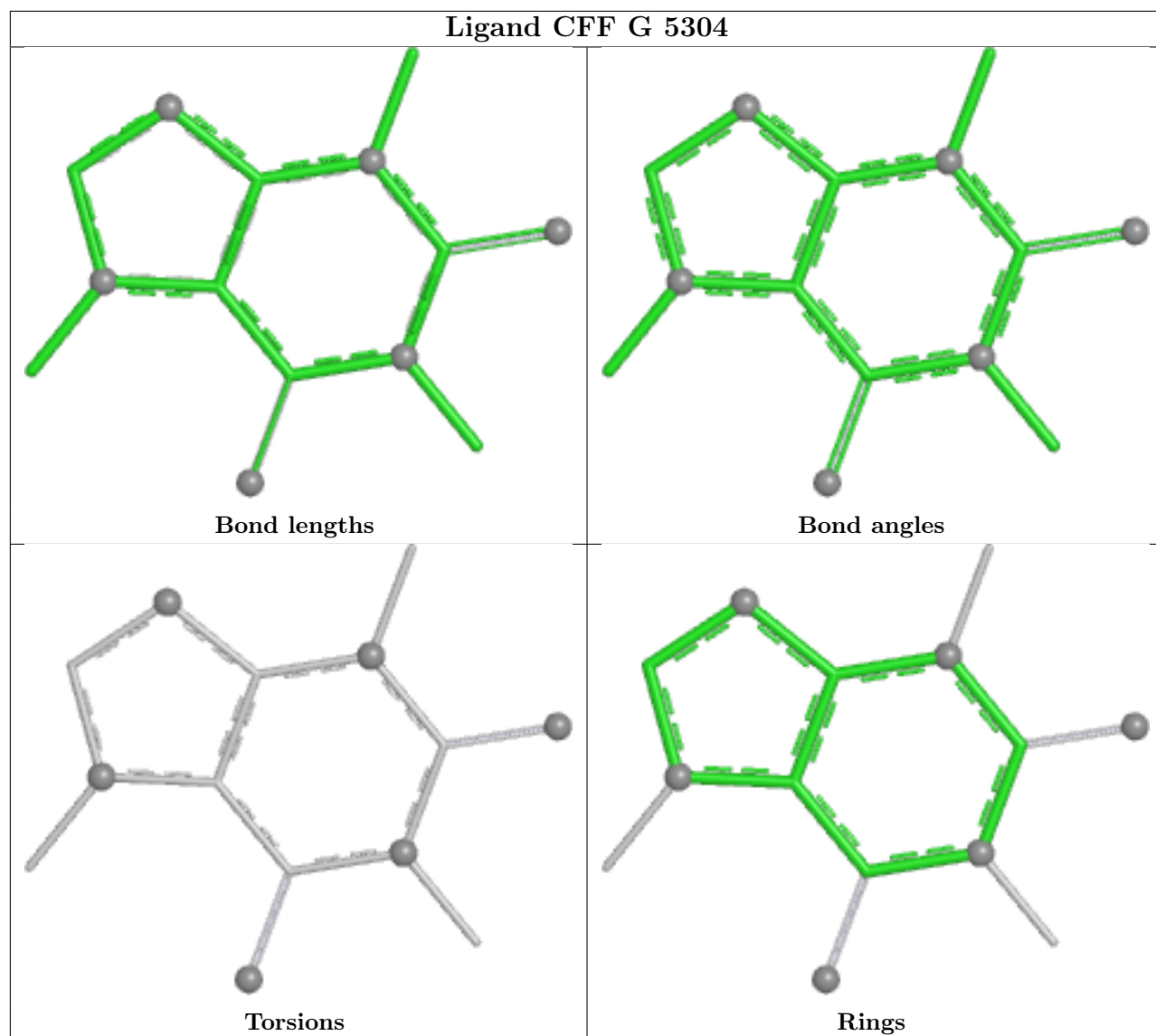
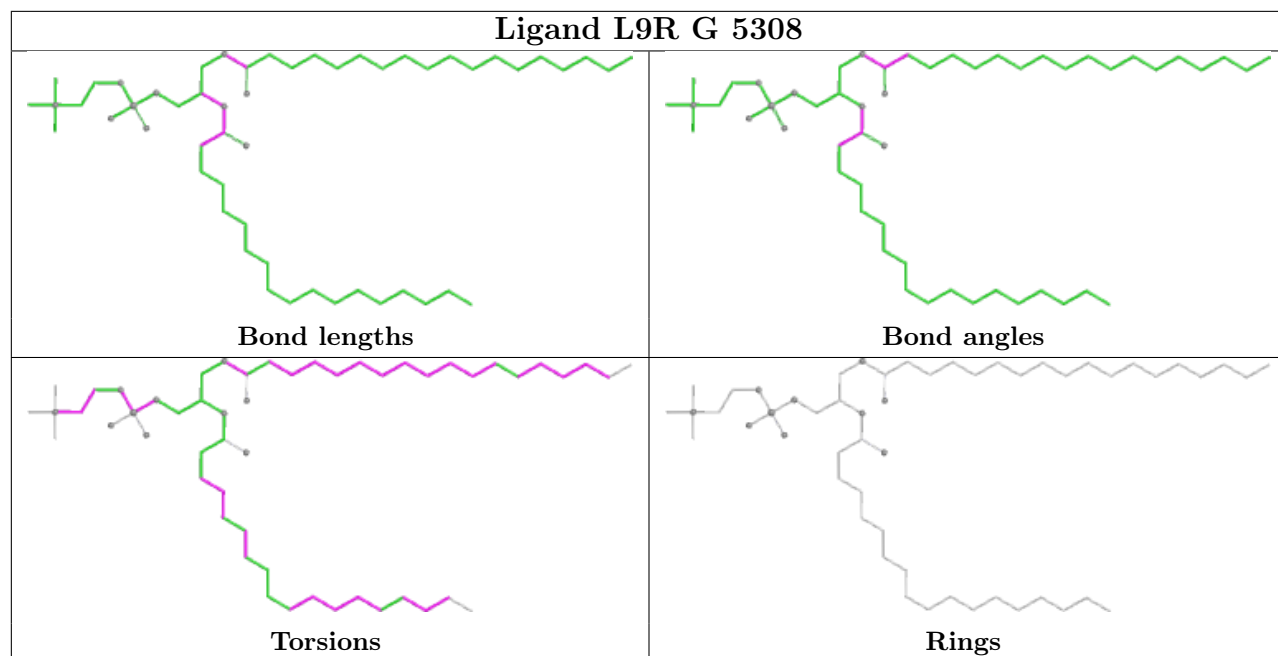




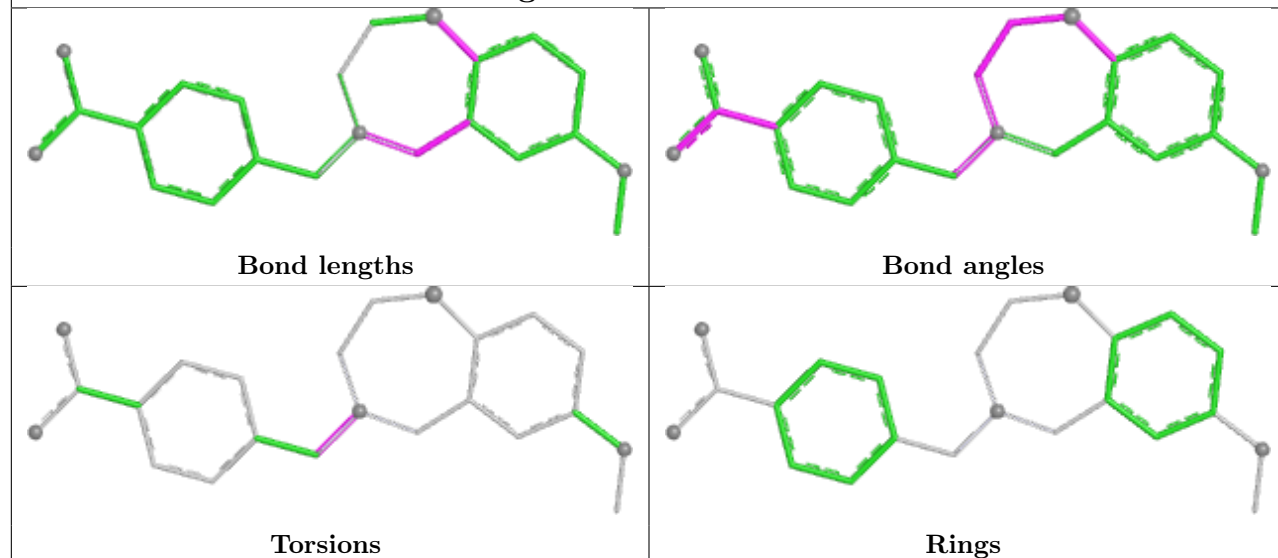




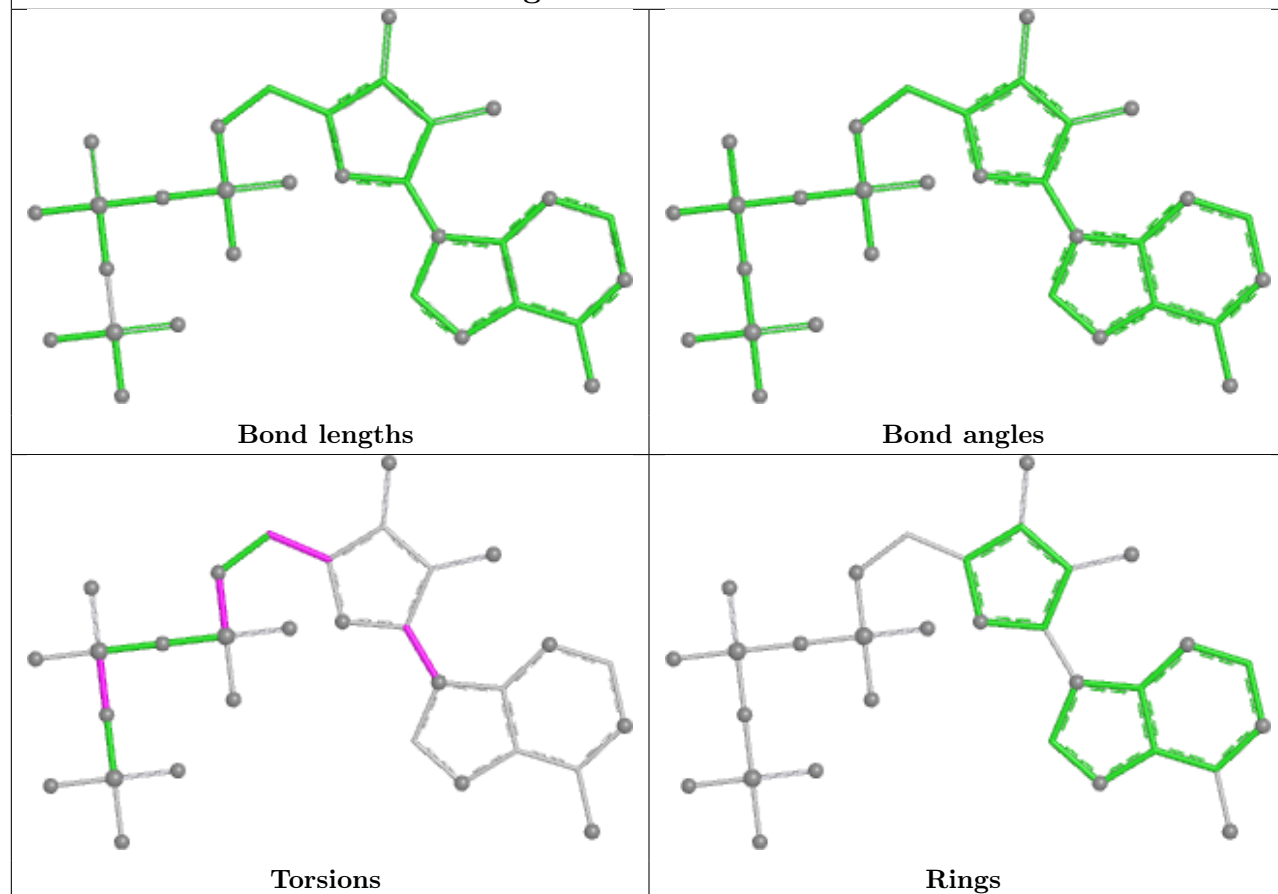


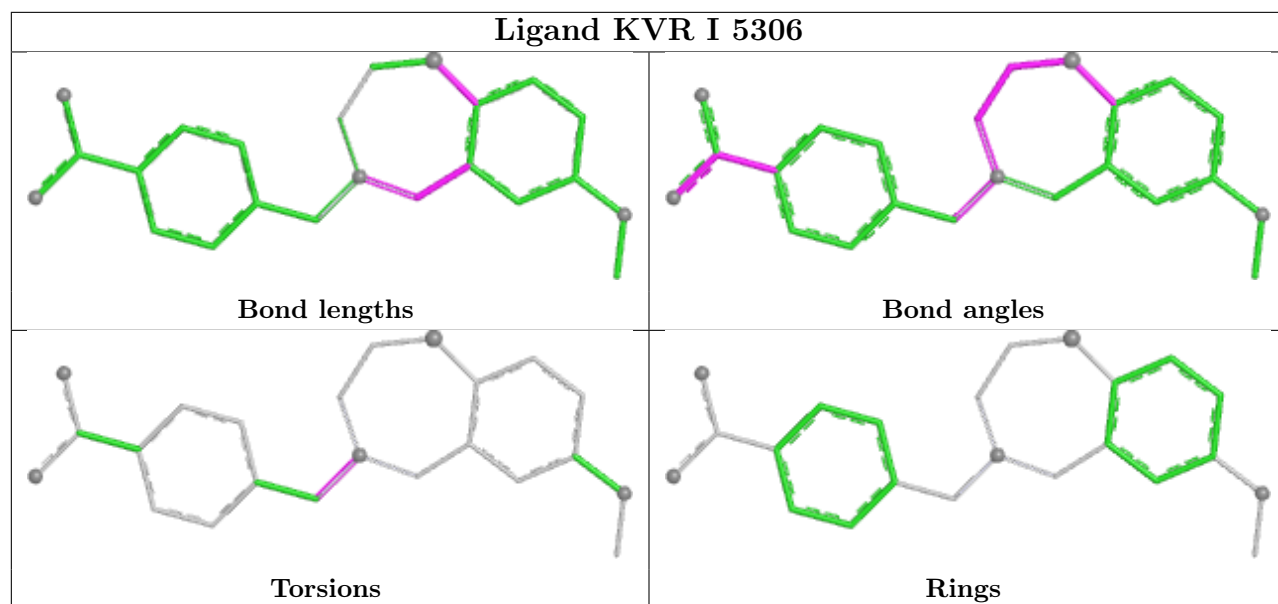
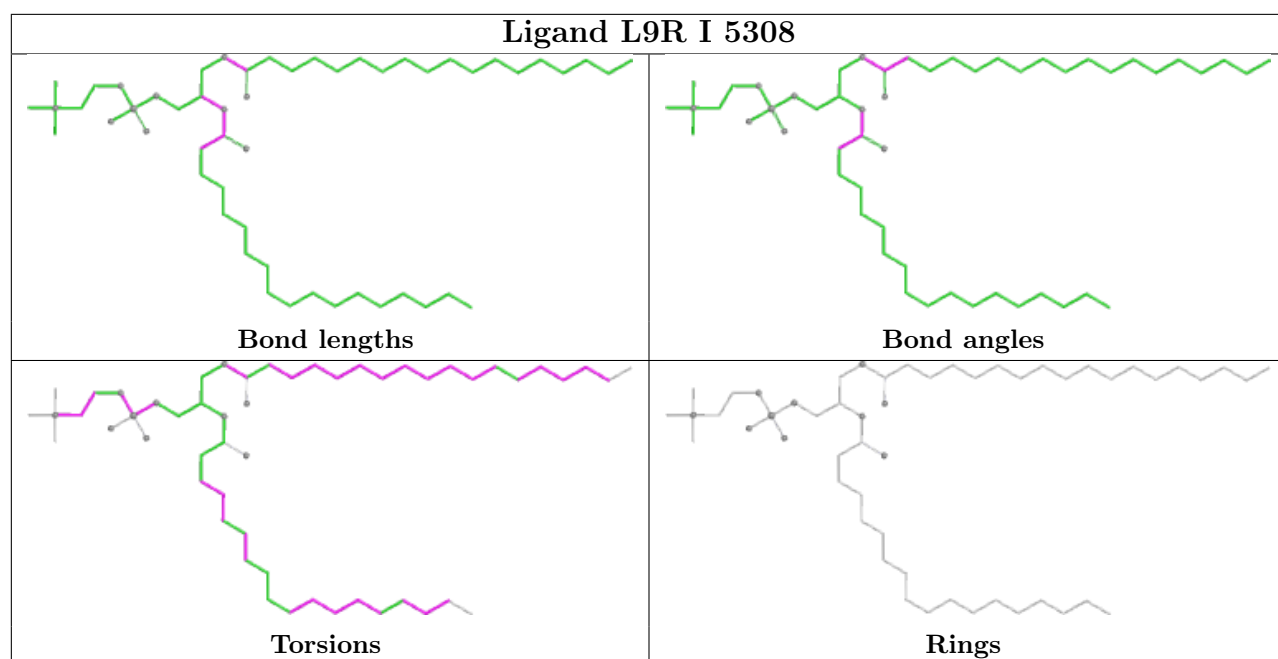


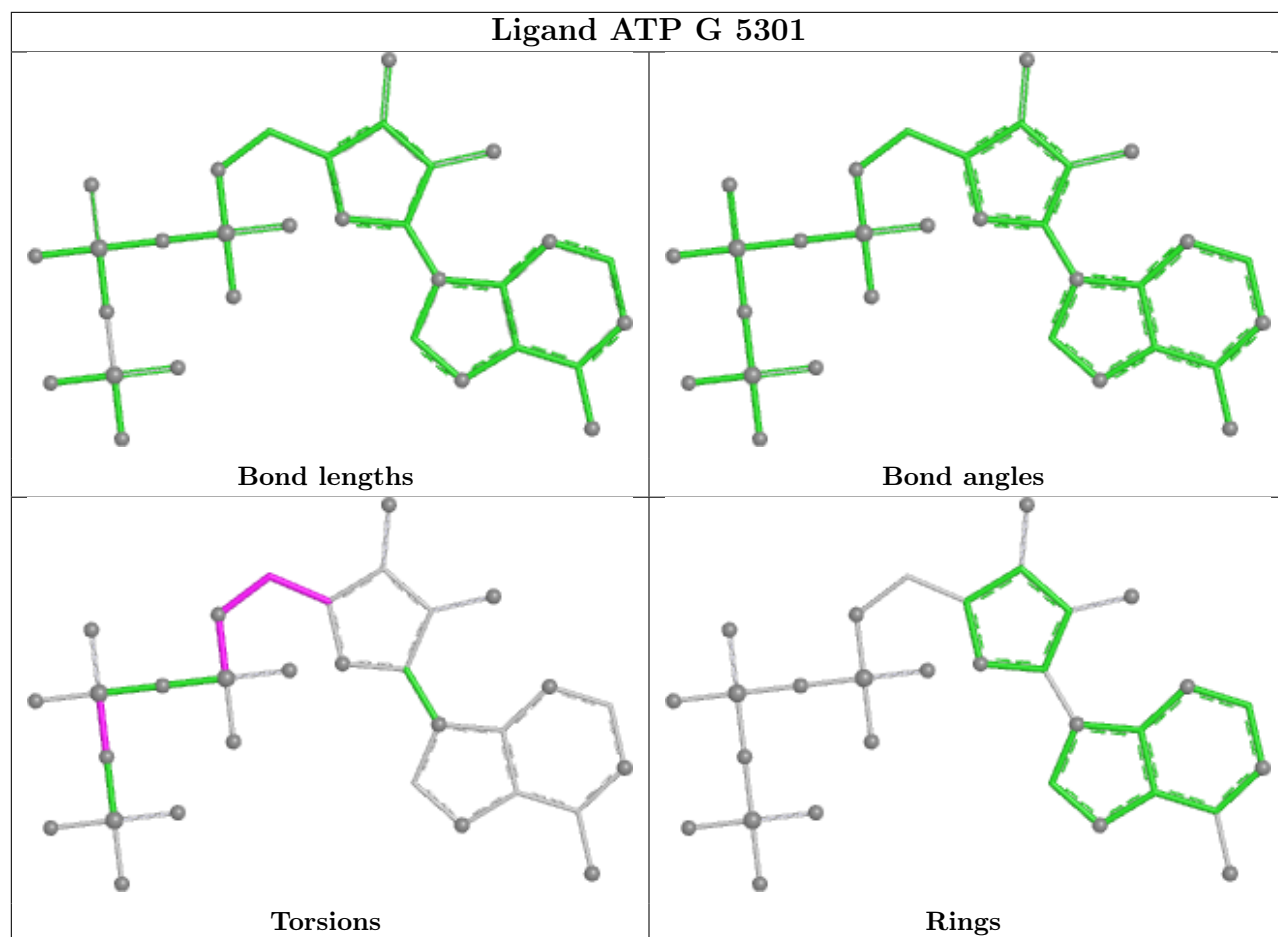
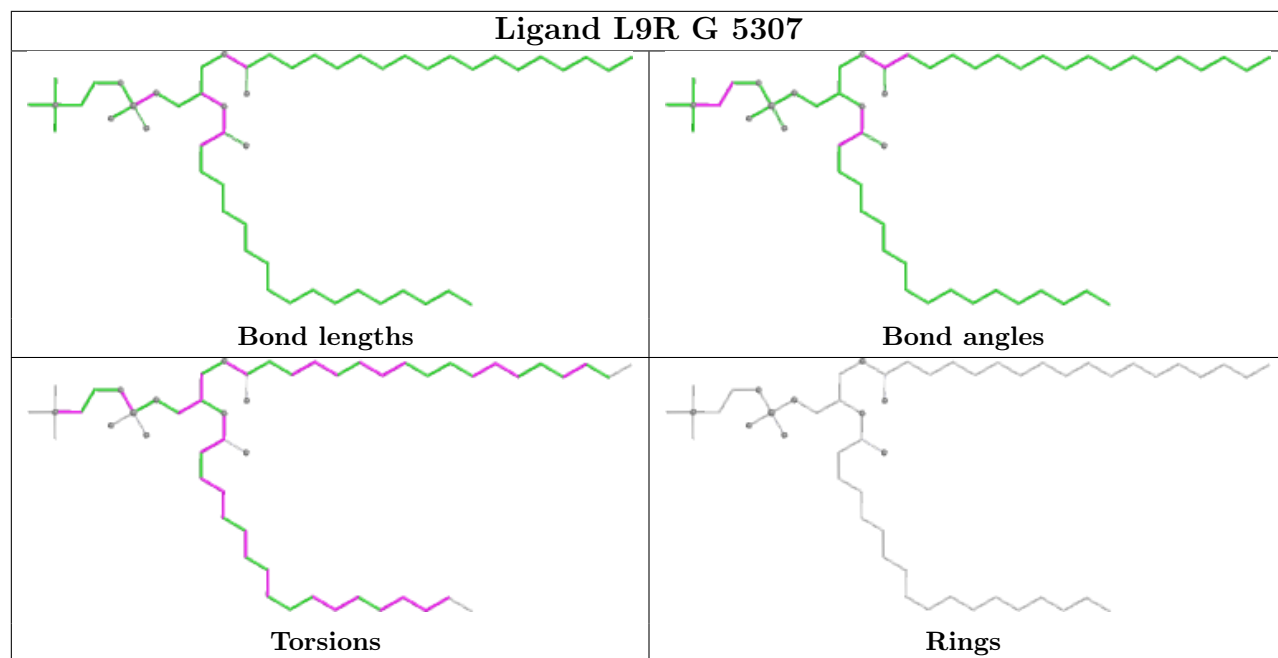
Ligand KVR G 5306

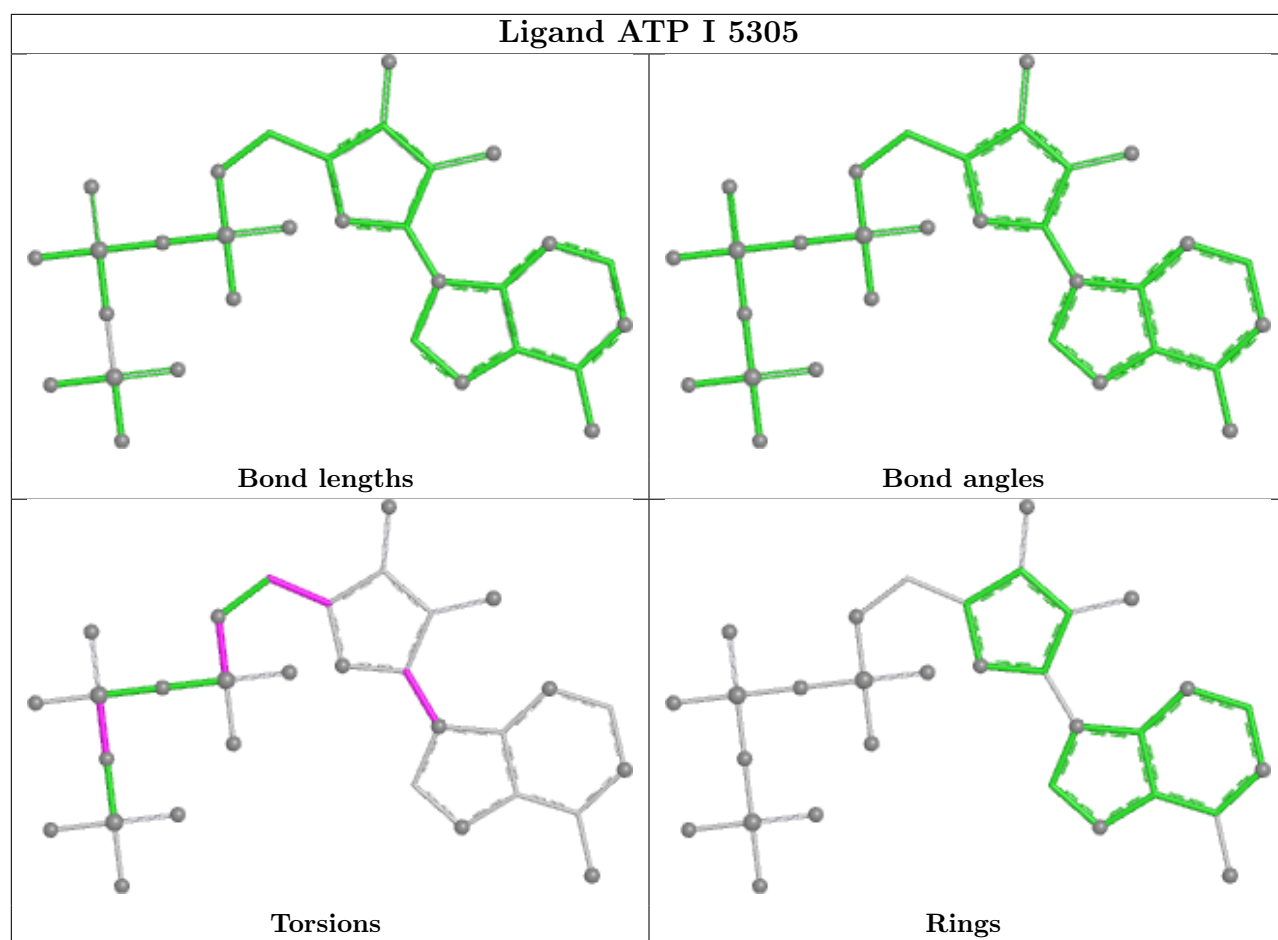


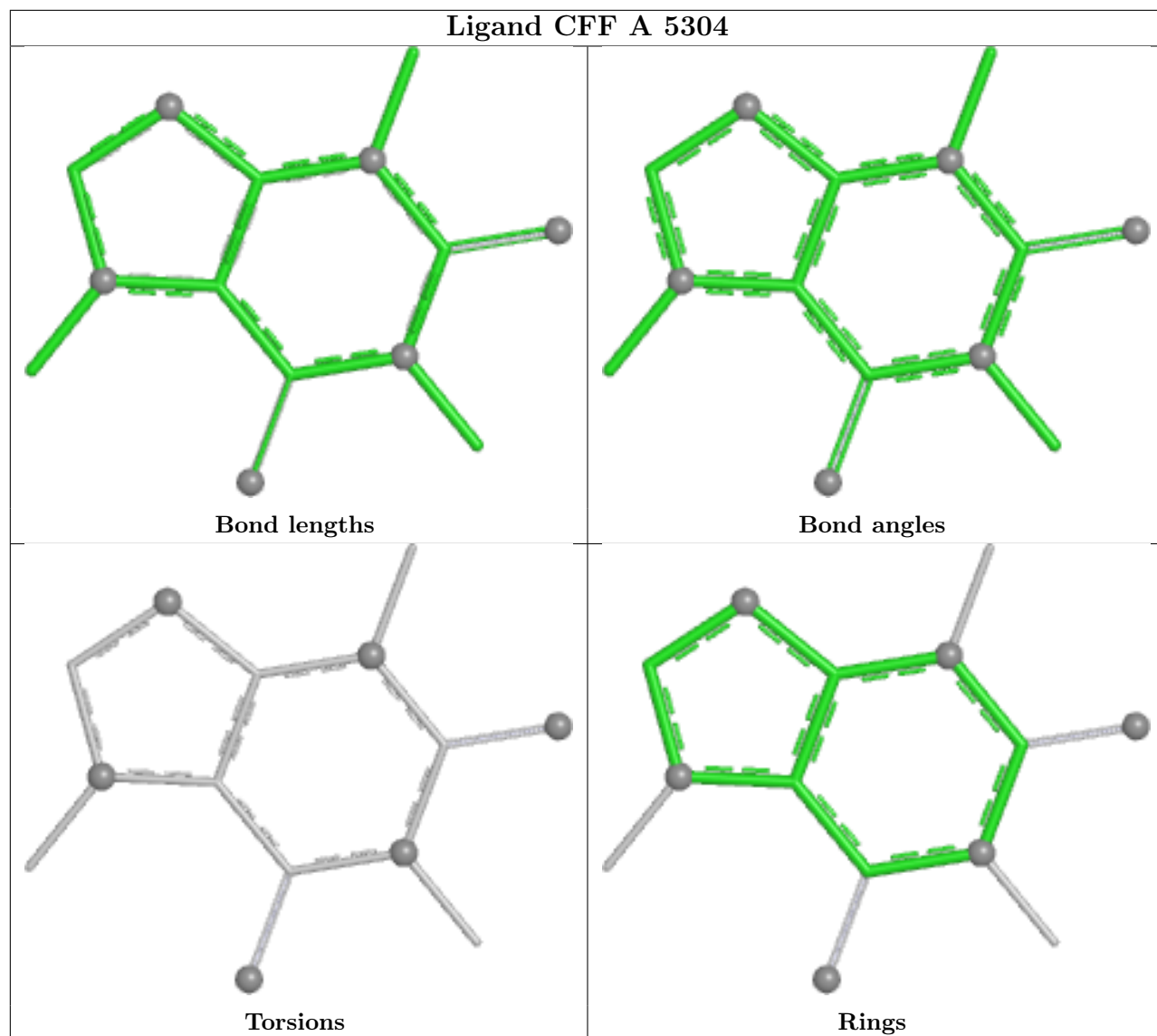
Ligand ATP A 5305

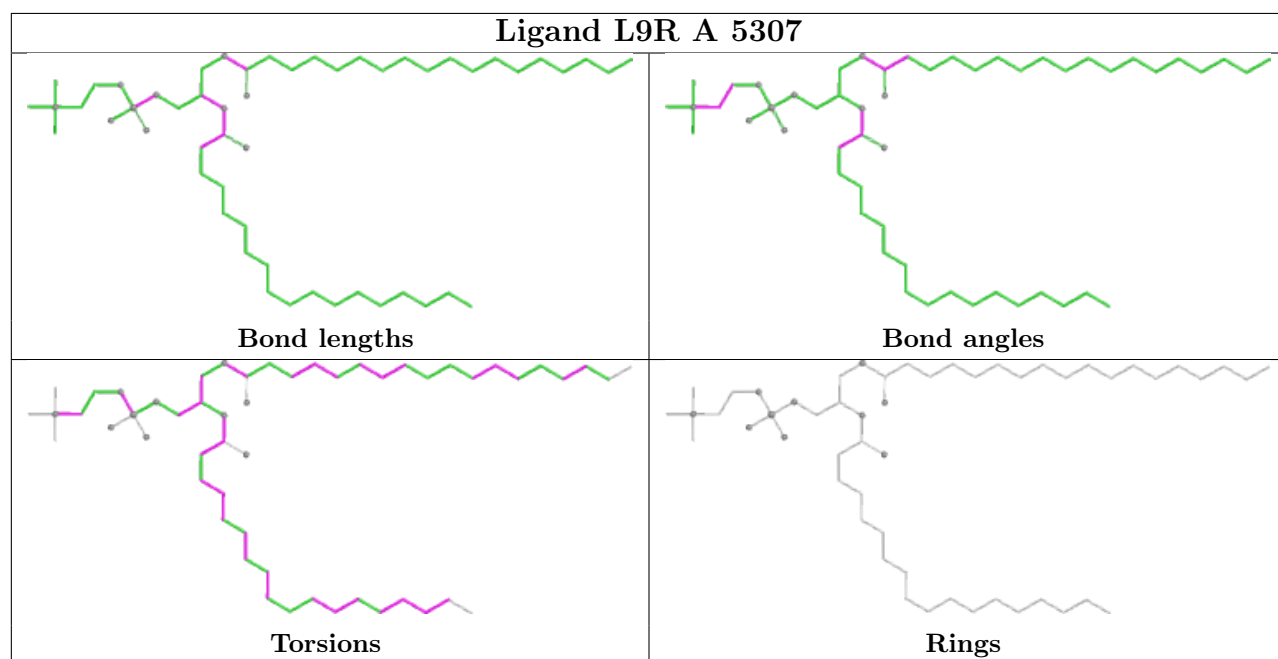
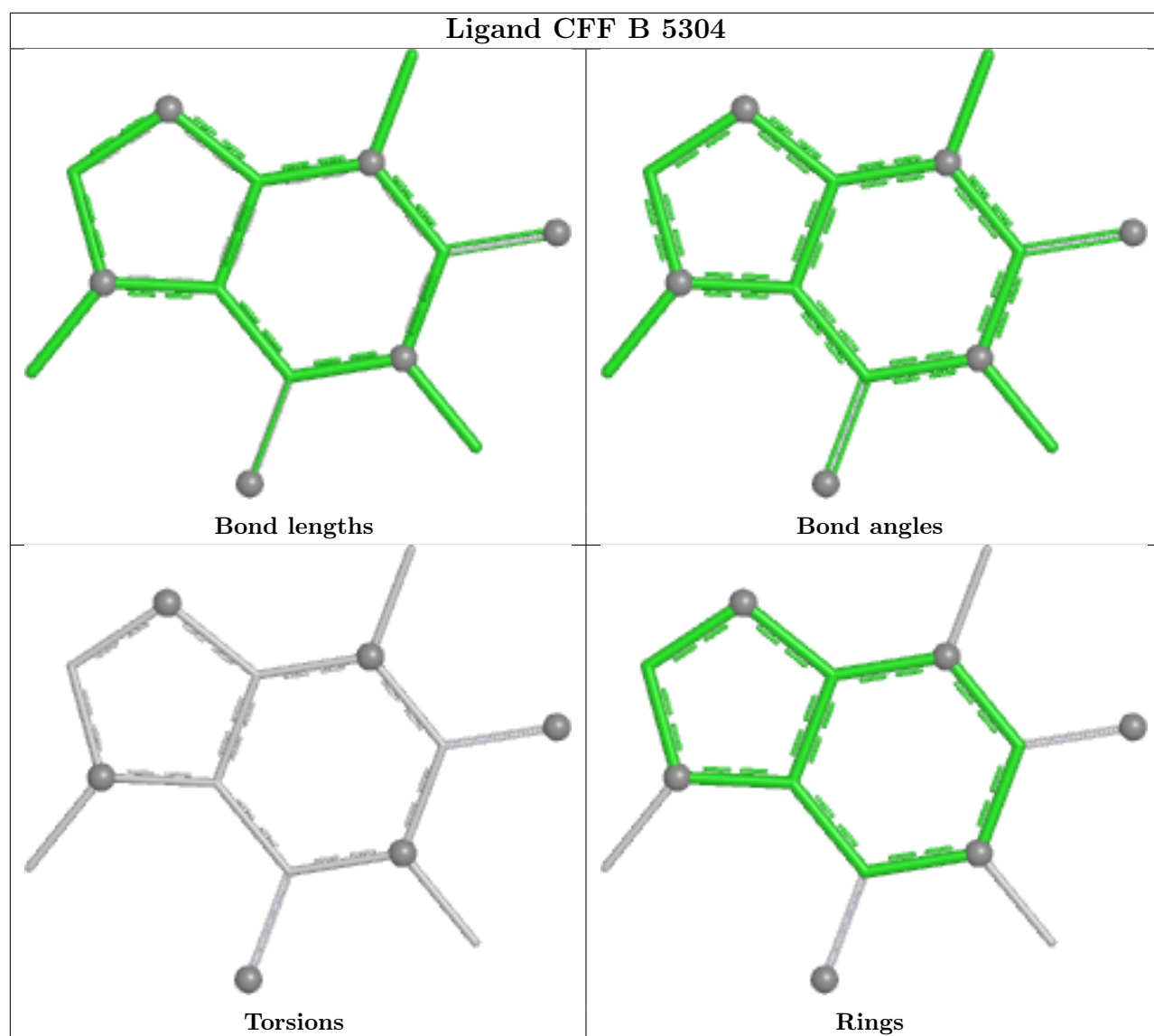


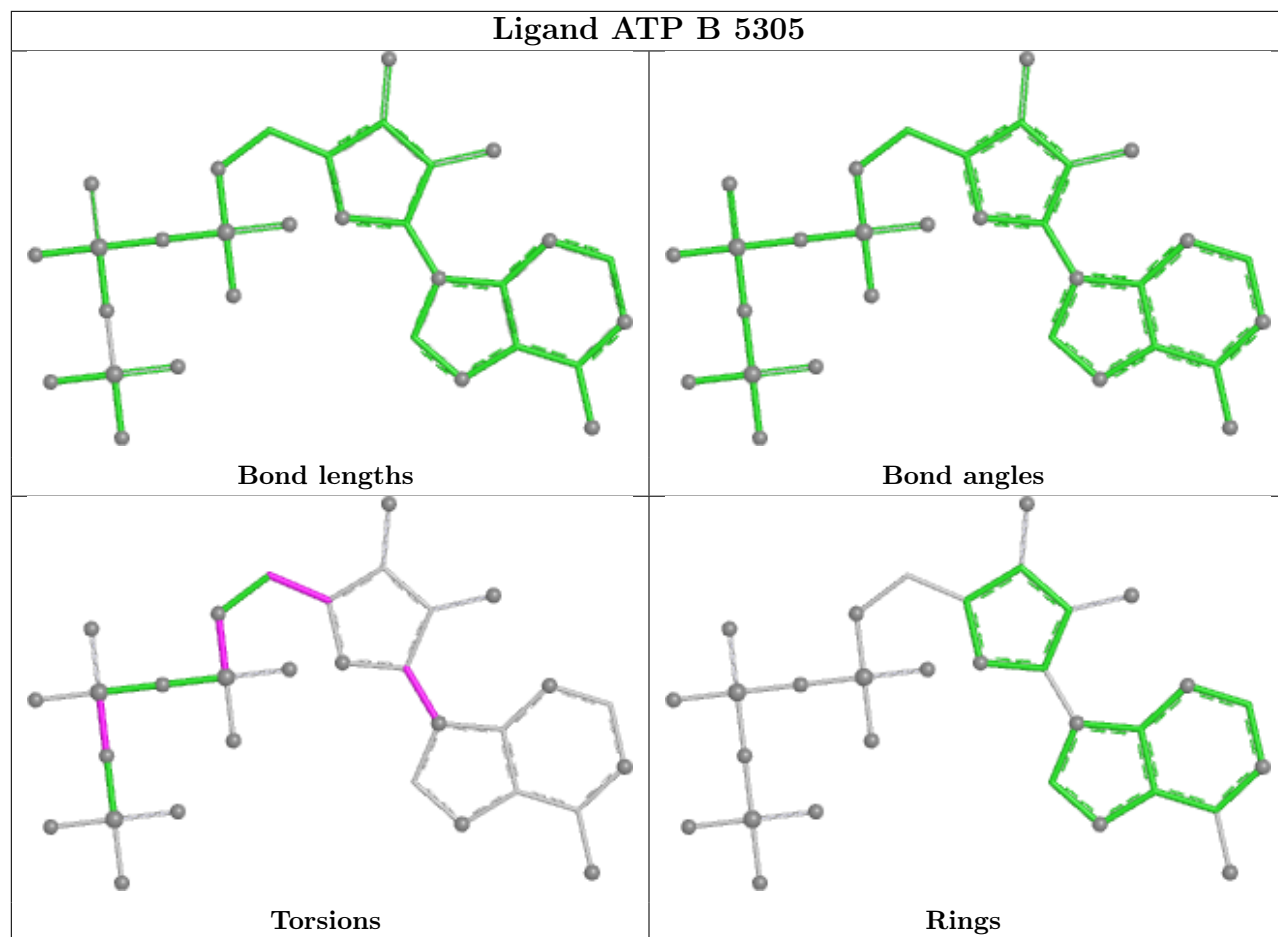


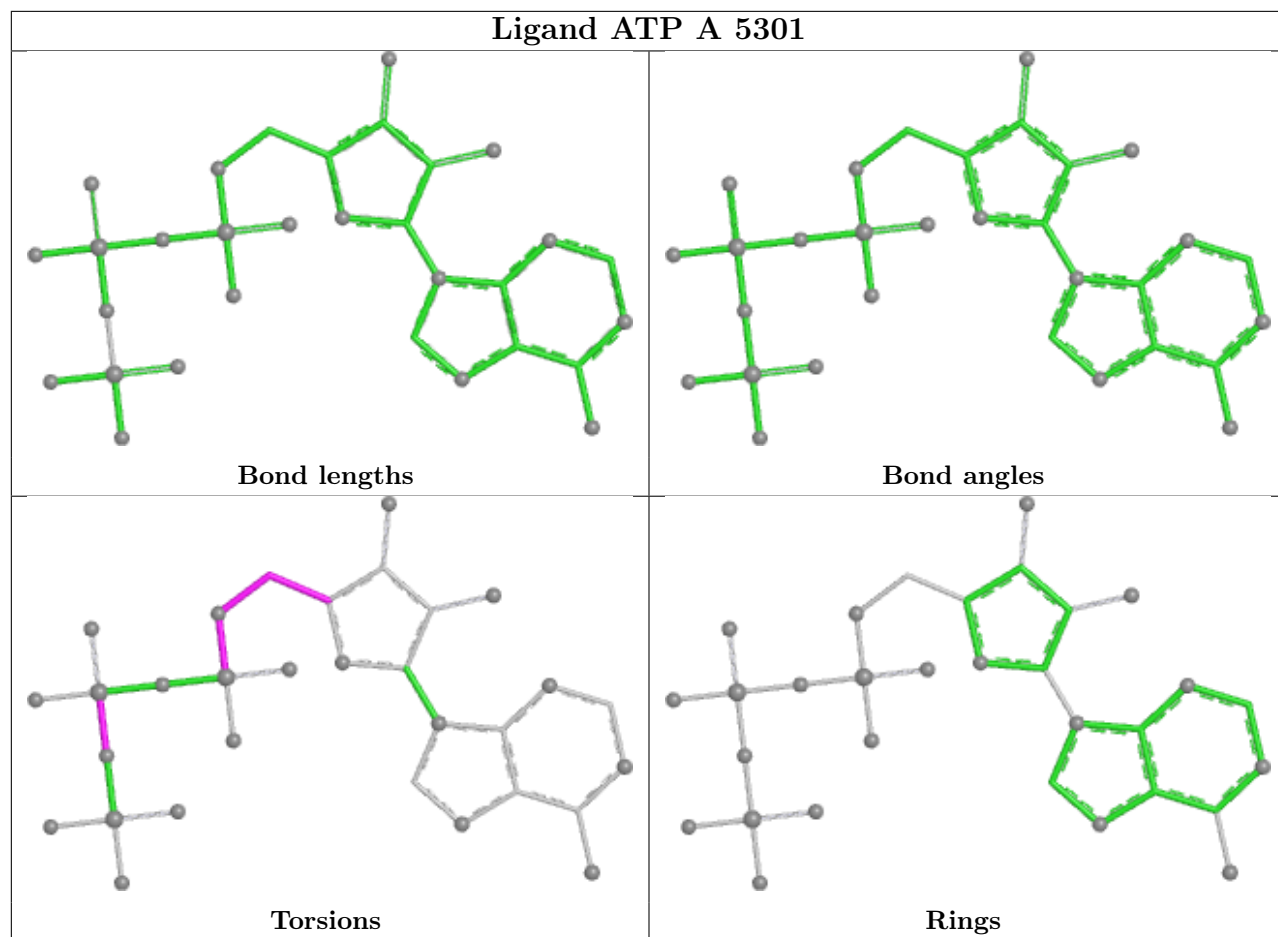


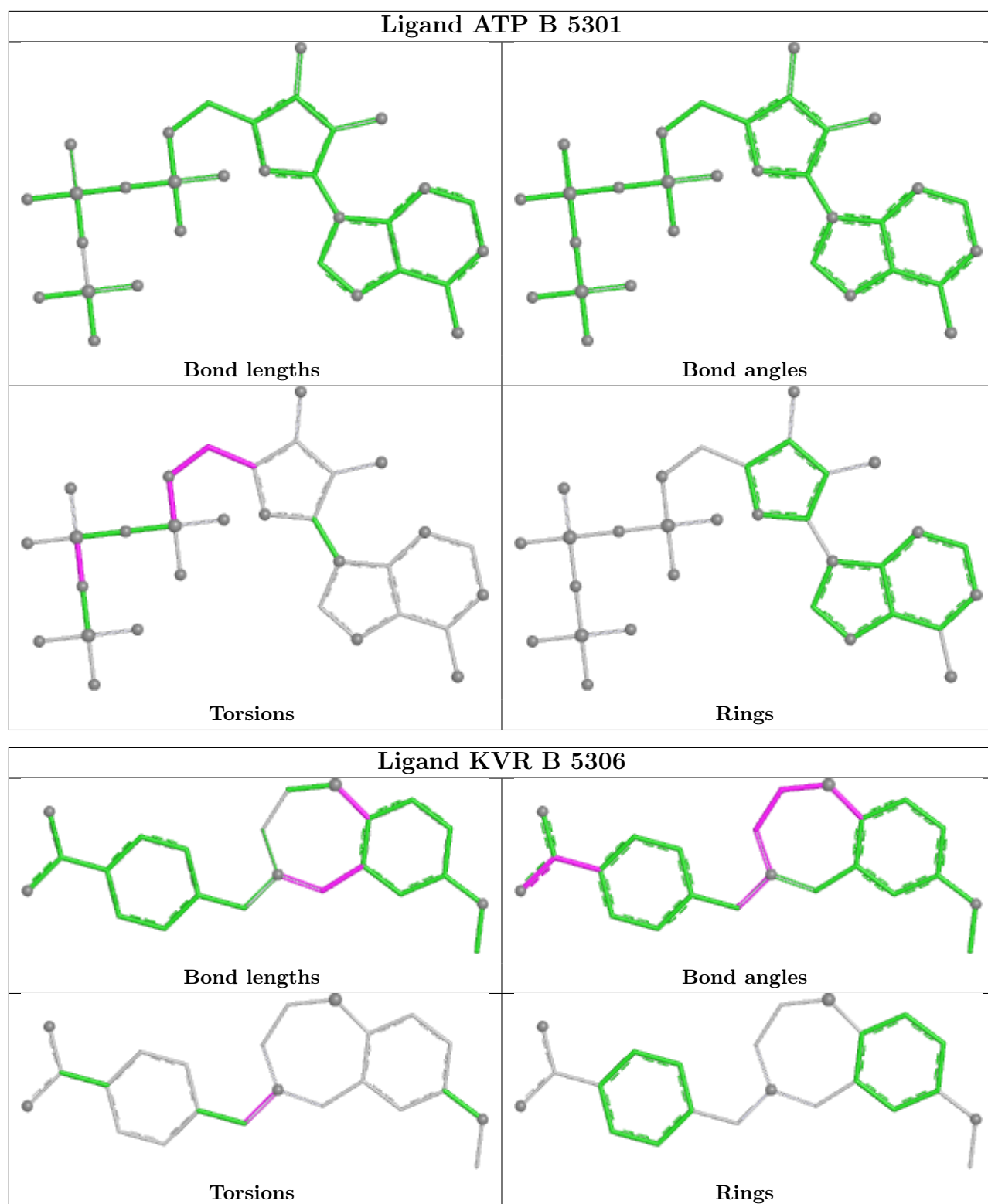












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

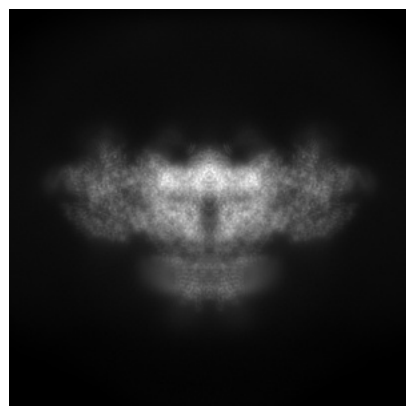
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26205. These allow visual inspection of the internal detail of the map and identification of artifacts.

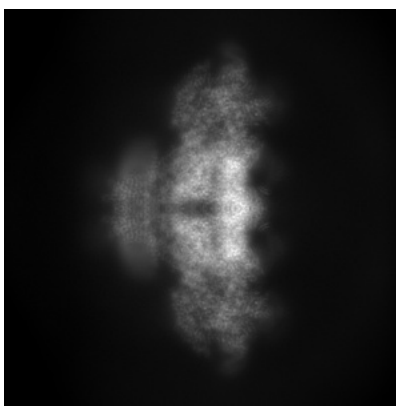
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

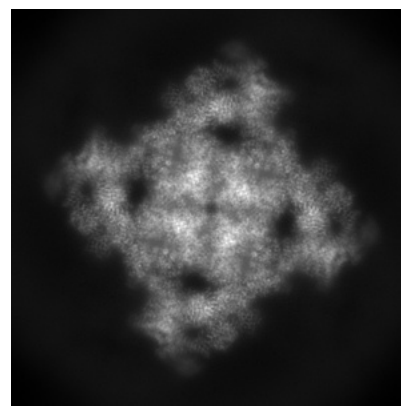
6.1.1 Primary map



X

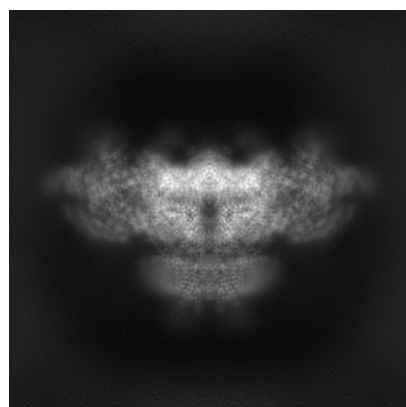


Y

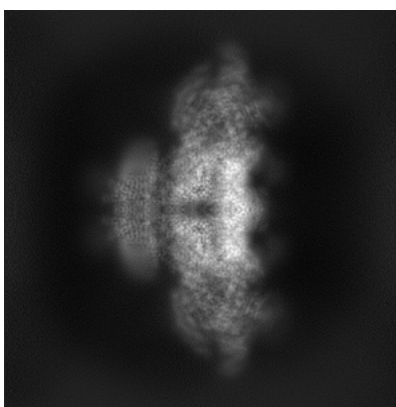


Z

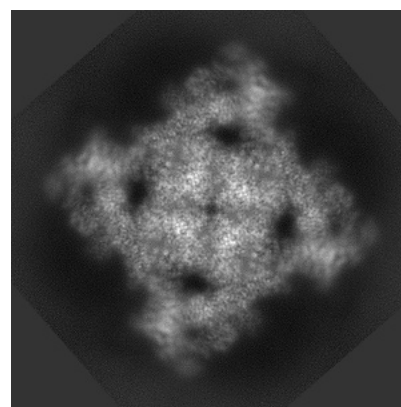
6.1.2 Raw map



X



Y



Z

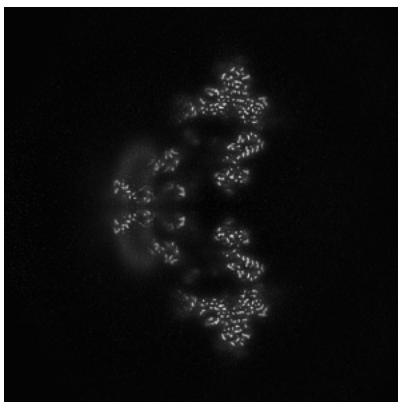
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

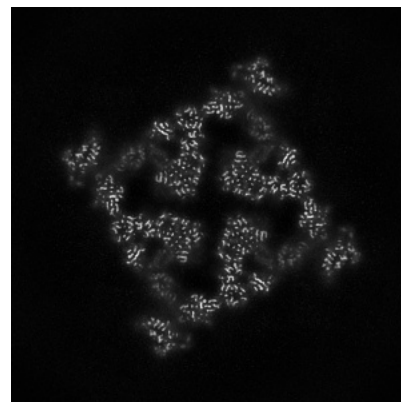
6.2.1 Primary map



X Index: 256

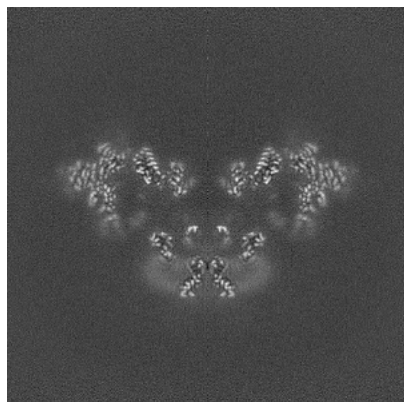


Y Index: 256

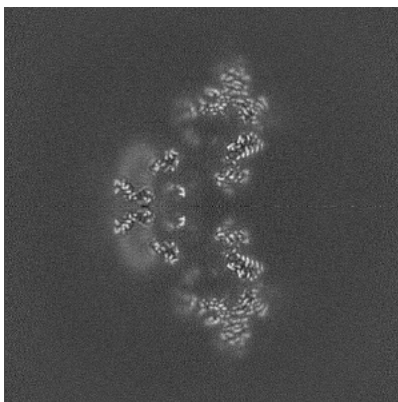


Z Index: 256

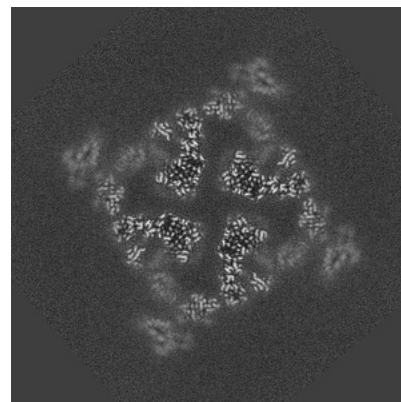
6.2.2 Raw map



X Index: 256



Y Index: 256

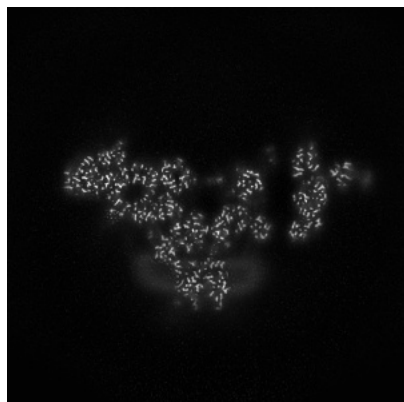


Z Index: 256

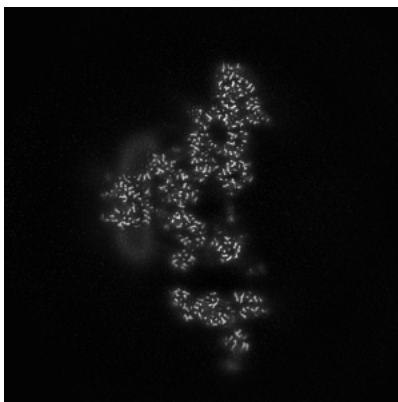
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

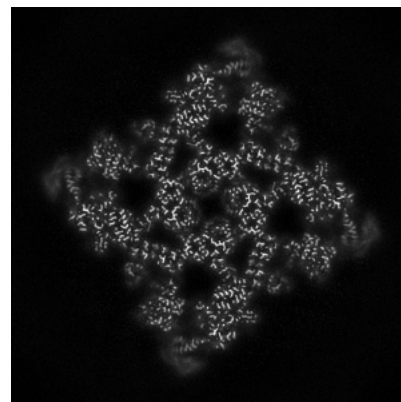
6.3.1 Primary map



X Index: 272

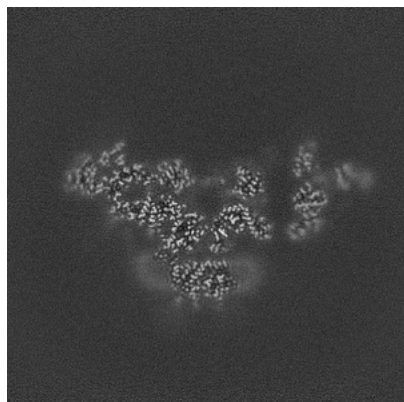


Y Index: 272

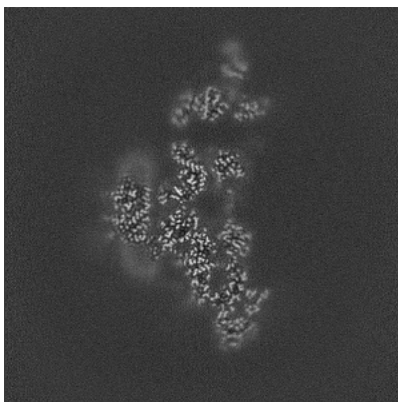


Z Index: 286

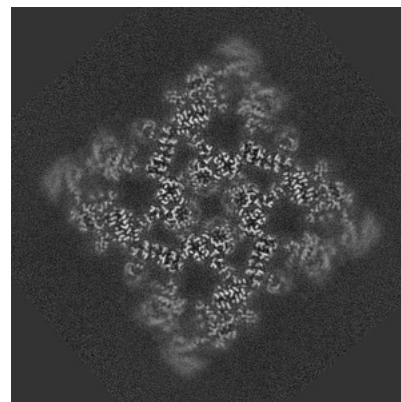
6.3.2 Raw map



X Index: 275



Y Index: 237

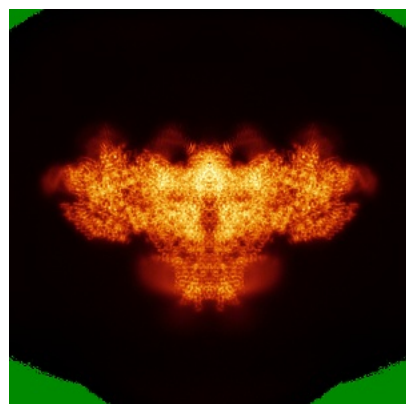


Z Index: 286

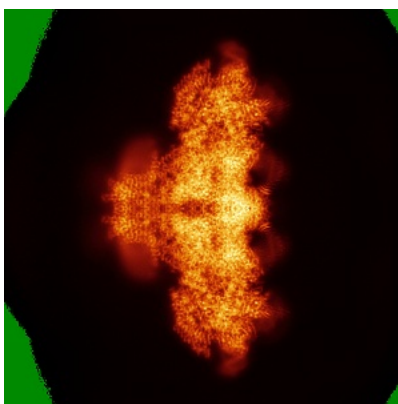
The images above show the largest variance slices of the map in three orthogonal directions.

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

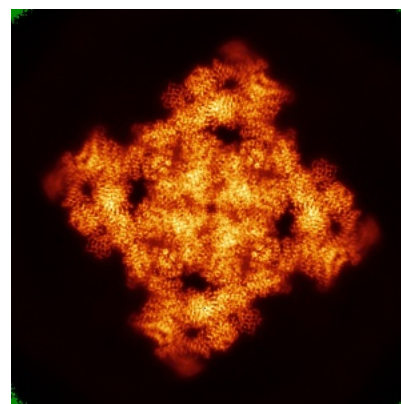
6.4.1 Primary map



X



Y

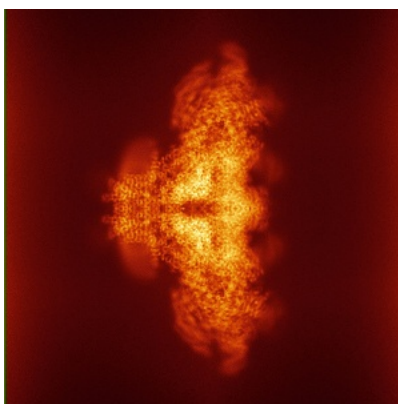


Z

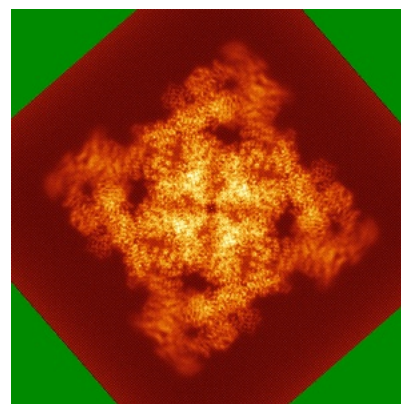
6.4.2 Raw map



X



Y

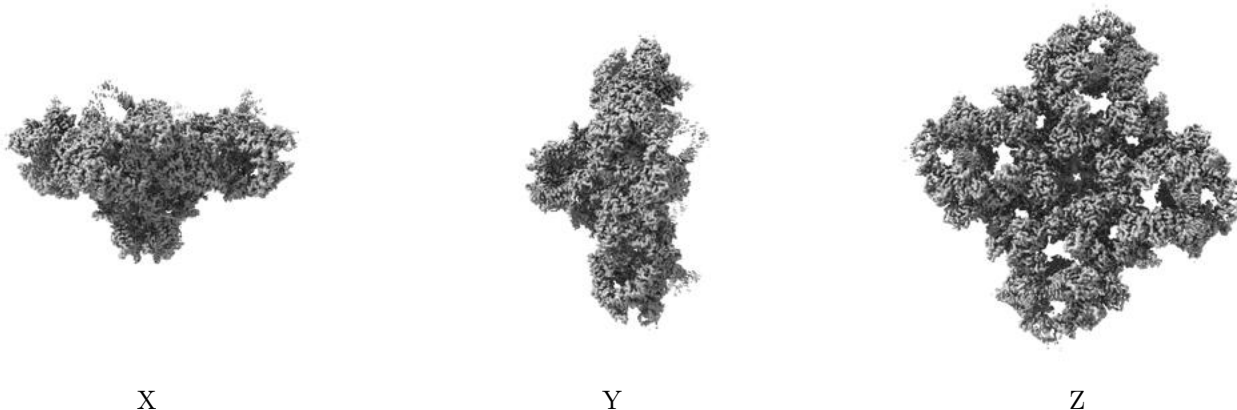


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

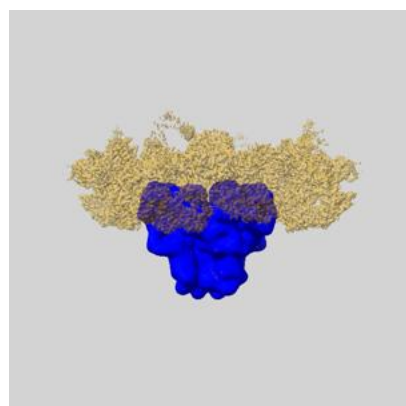
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

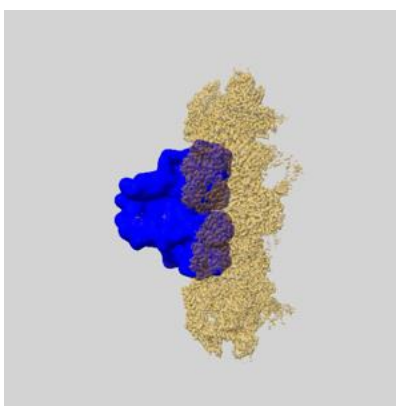
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

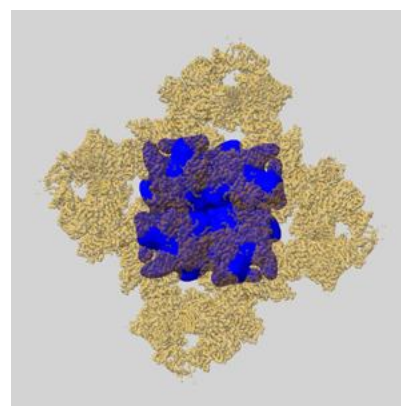
6.6.1 emd_26205_msk_1.map [i](#)



X

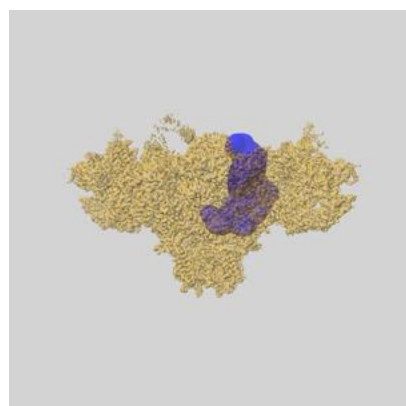


Y

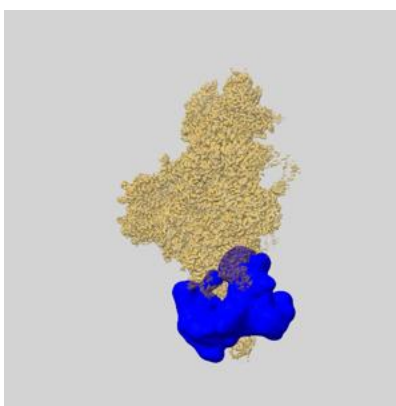


Z

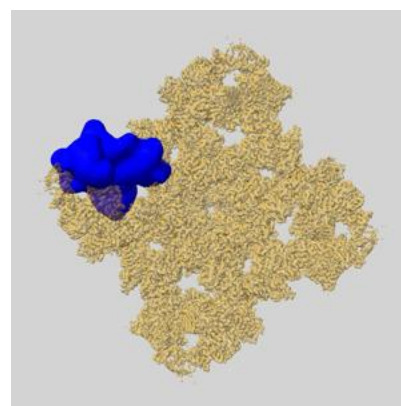
6.6.2 emd_26205_msk_2.map [i](#)



X

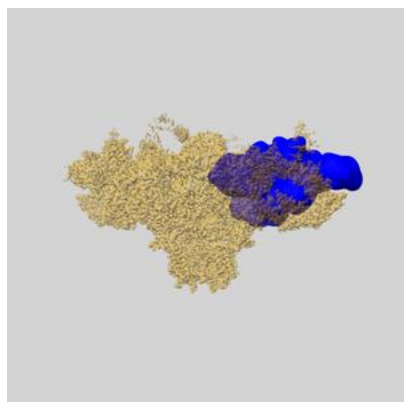


Y

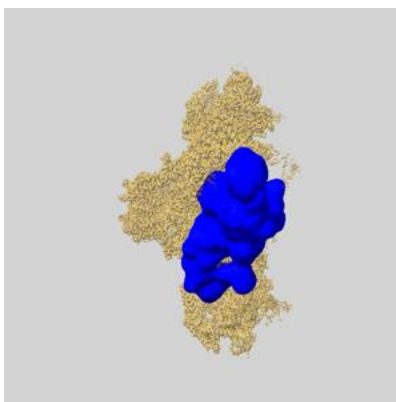


Z

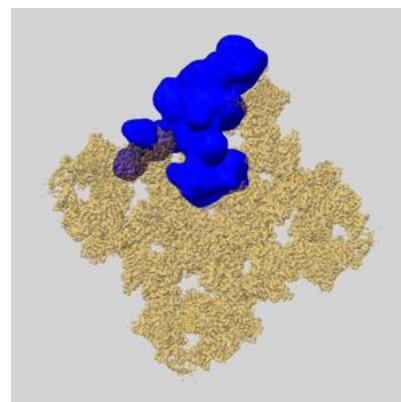
6.6.3 emd_26205_msk_3.map [i](#)



X



Y

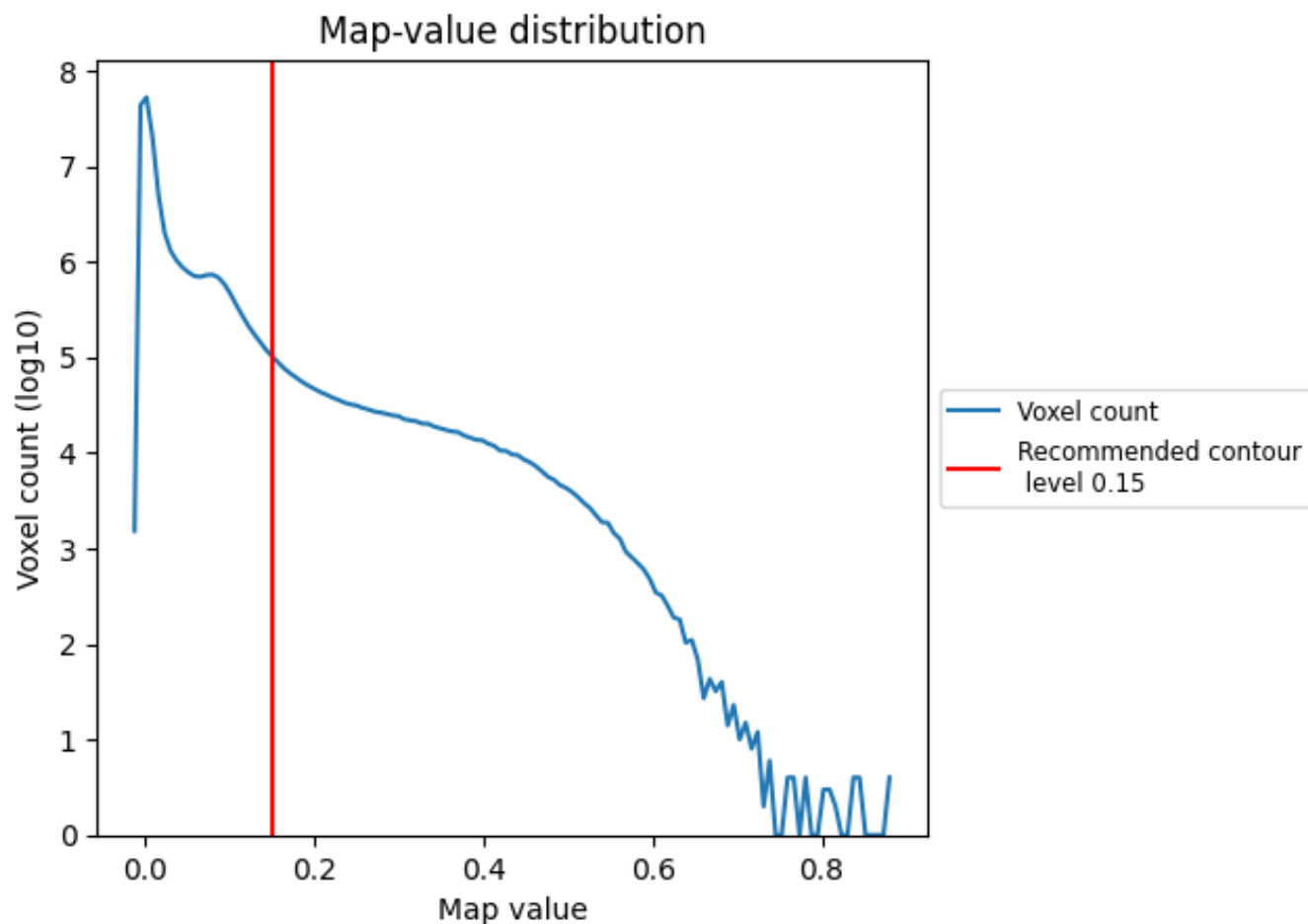


Z

7 Map analysis [i](#)

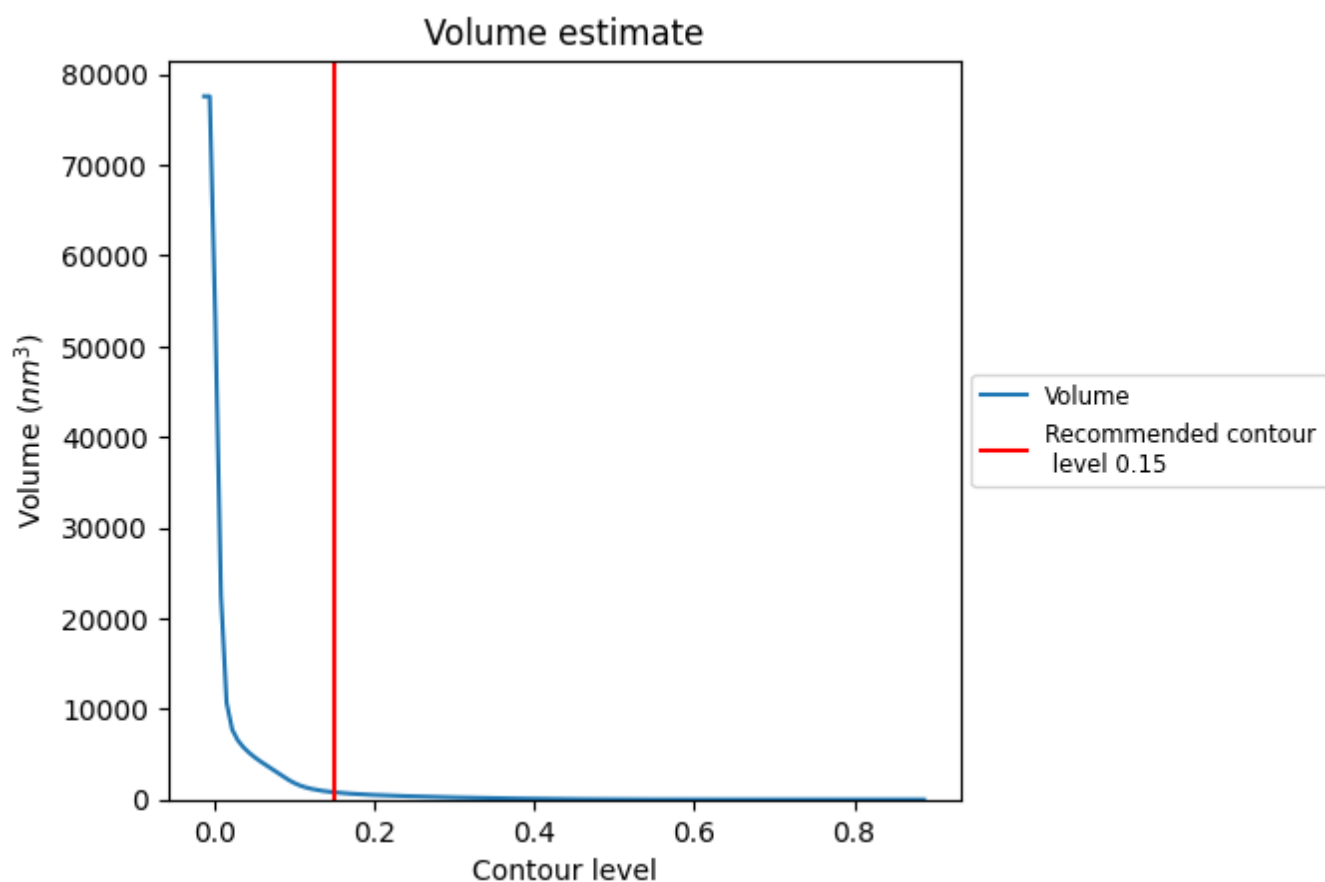
This section contains the results of statistical analysis of the map.

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.

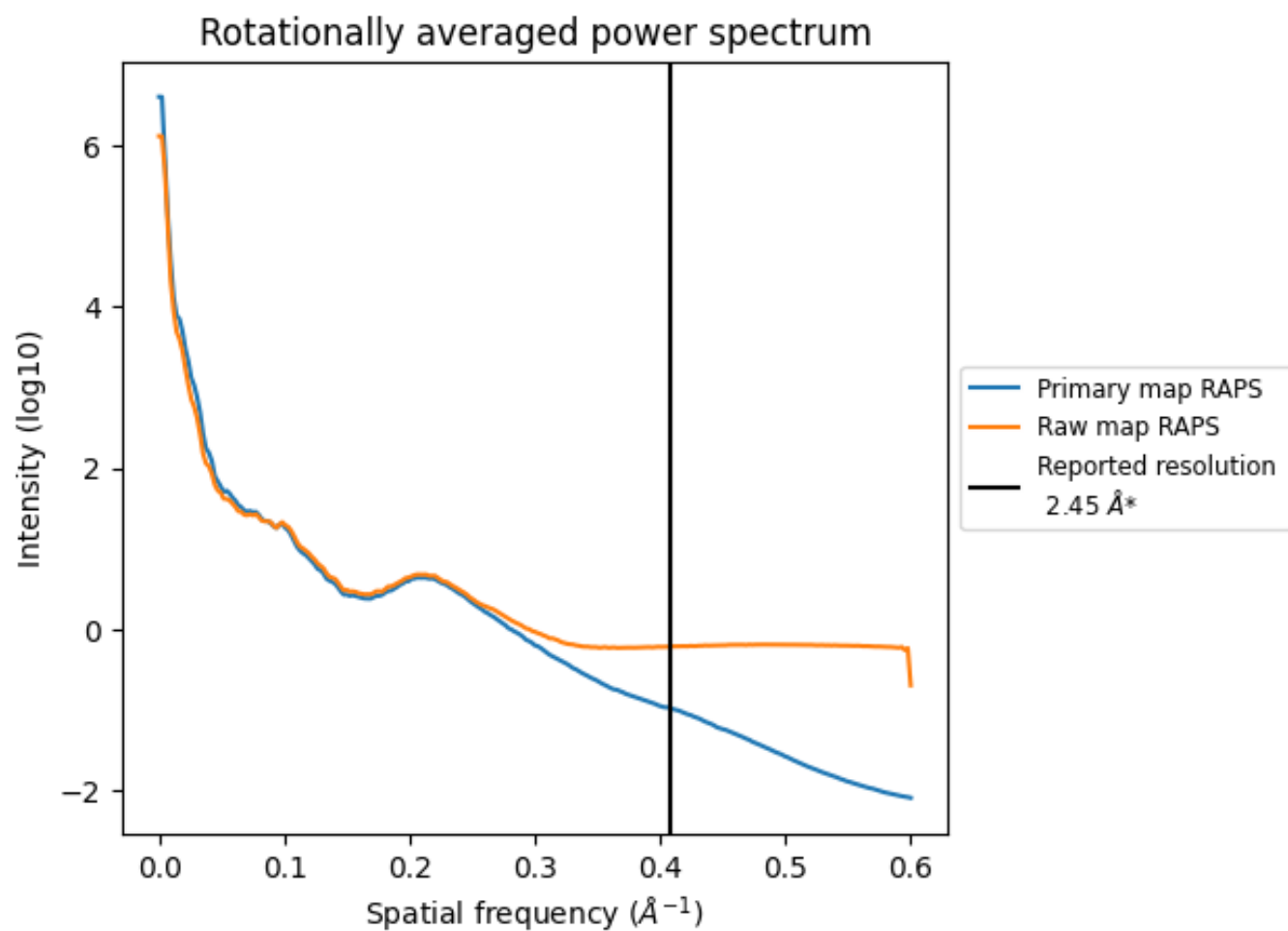
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 800 nm³; this corresponds to an approximate mass of 723 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

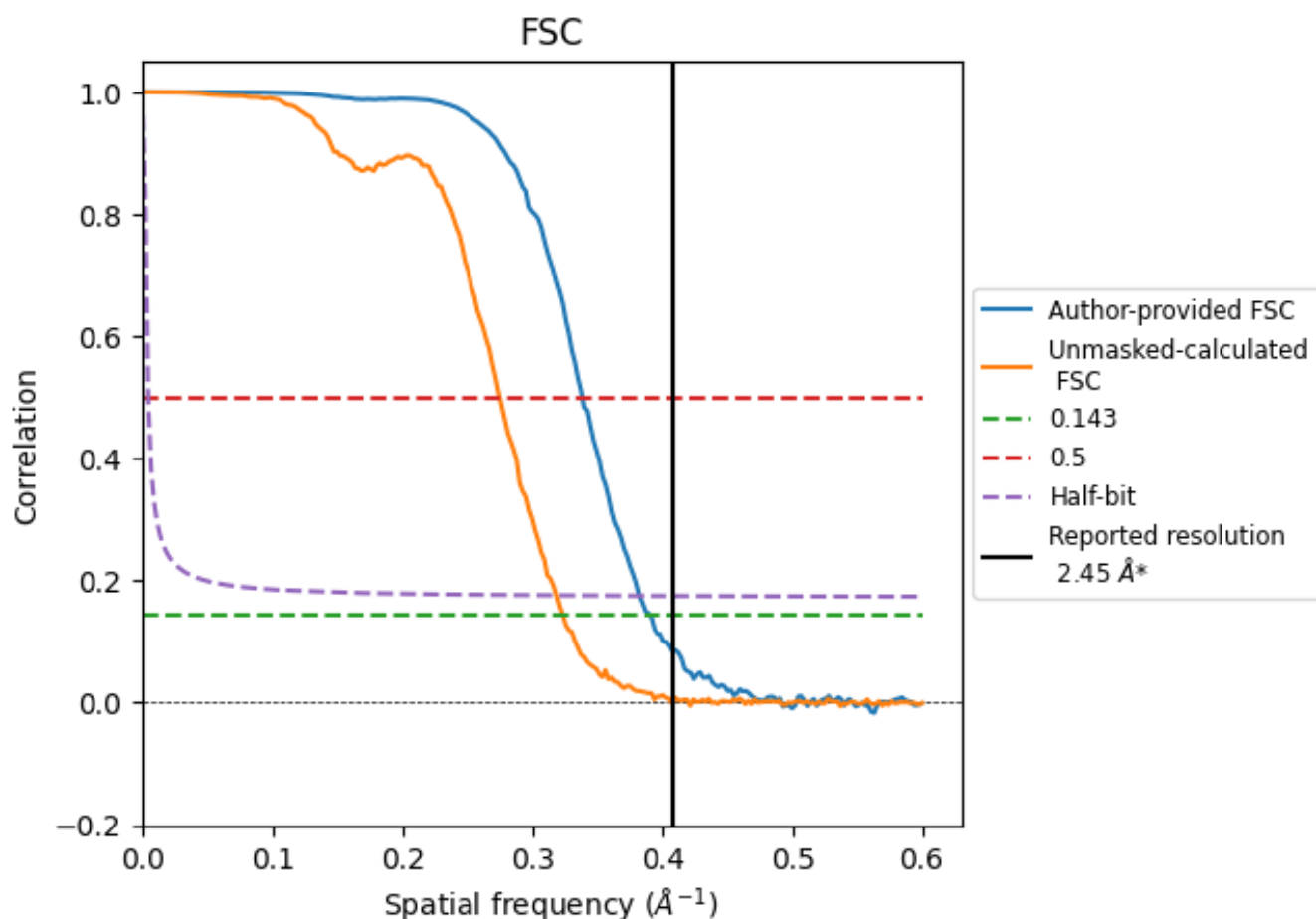


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.408 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

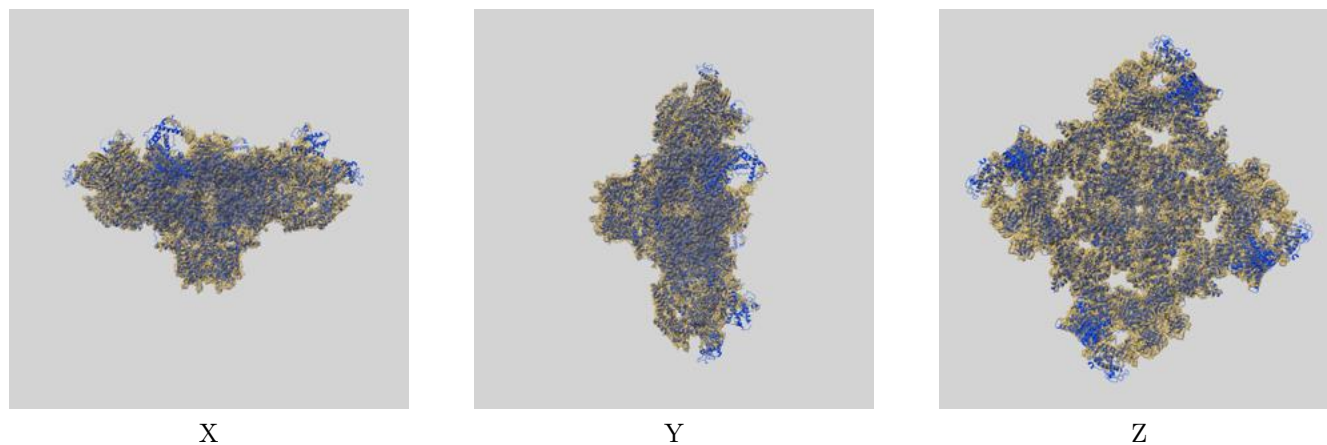
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.56	2.95	2.62
Unmasked-calculated*	3.09	3.63	3.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.45 by more than 10 %

9 Map-model fit [i](#)

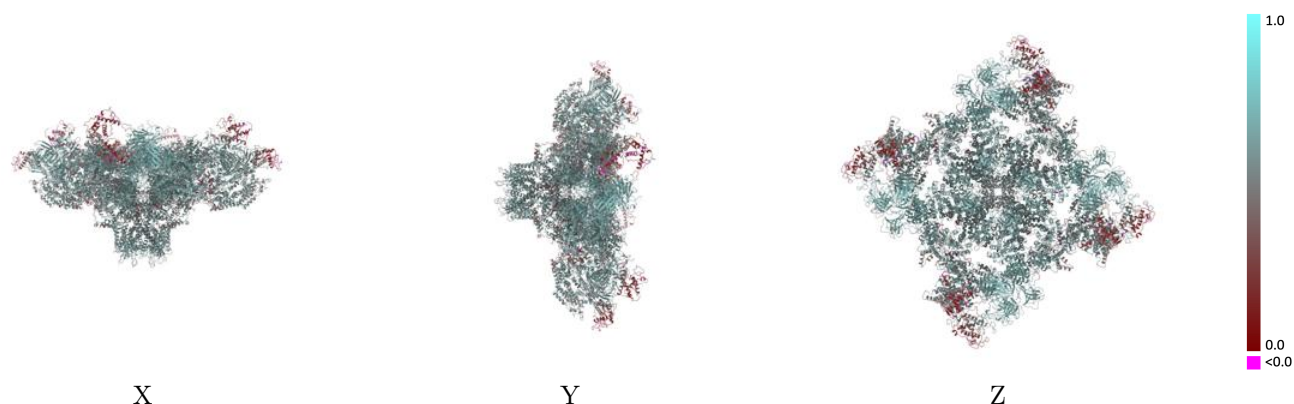
This section contains information regarding the fit between EMDB map EMD-26205 and PDB model 9E17. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



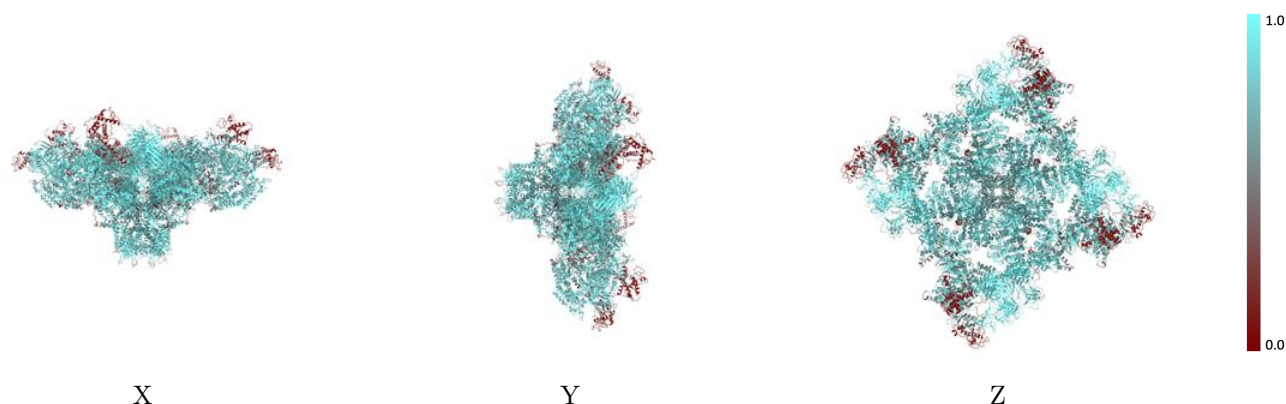
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



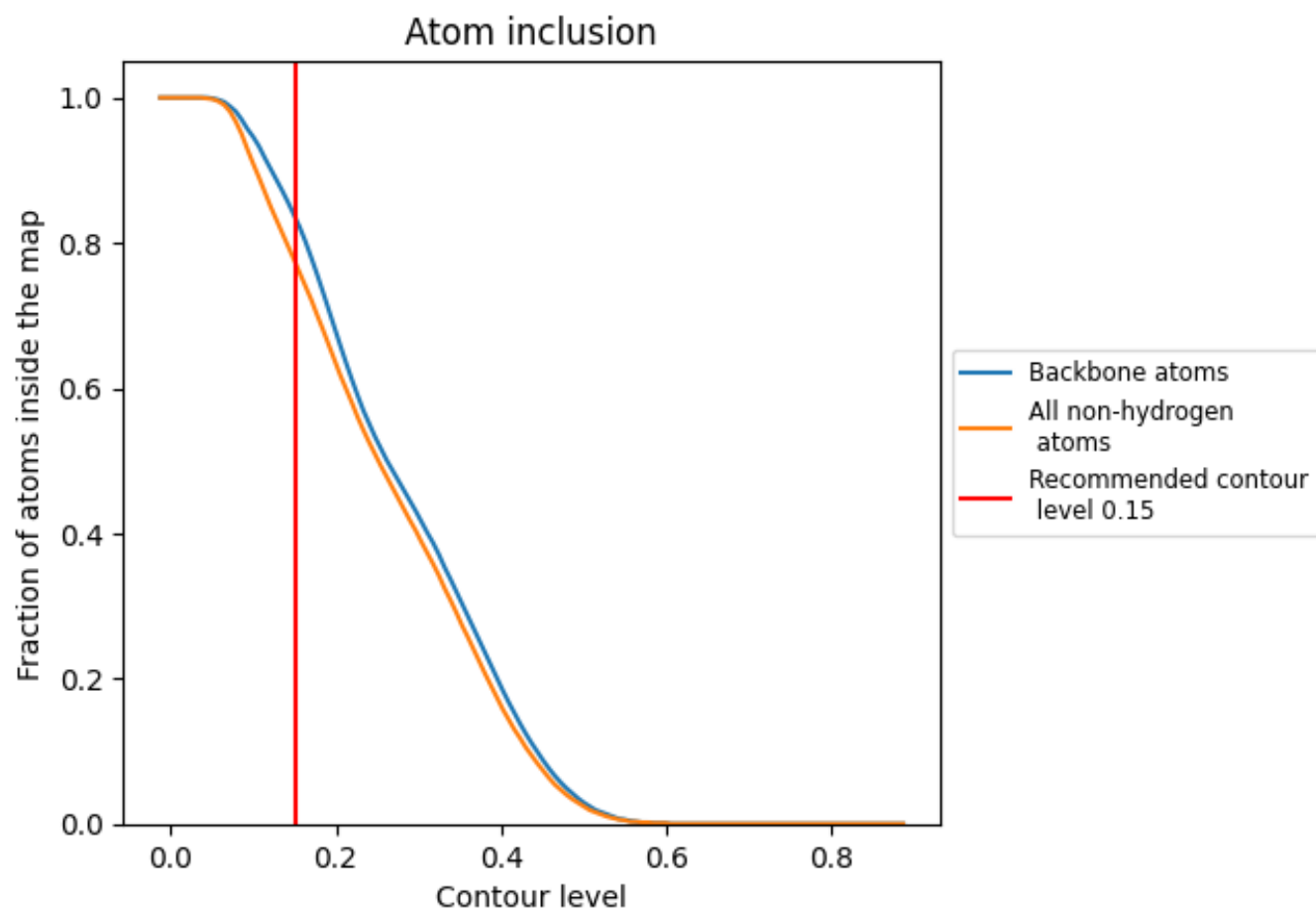
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.5400
A	0.7900	0.5430
B	0.7890	0.5400
C	0.5240	0.4370
D	0.5310	0.4320
E	0.5310	0.4390
F	0.8040	0.6020
G	0.7890	0.5410
H	0.7930	0.6020
I	0.7890	0.5420
J	0.7890	0.6020
K	0.5280	0.4400
O	0.8020	0.6030

