



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 06:02 pm BST

PDB ID : 9S5Z / pdb_00009s5z
EMDB ID : EMD-54617
Title : Primed-state RyR1 with activating ligand mixture (Calcium/ACP/Caffeine)
in the native membrane solved by StA
Authors : Mikirtumov, V.
Deposited on : 2025-07-30
Resolution : 4.43 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:

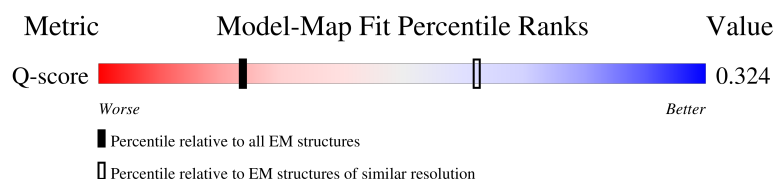
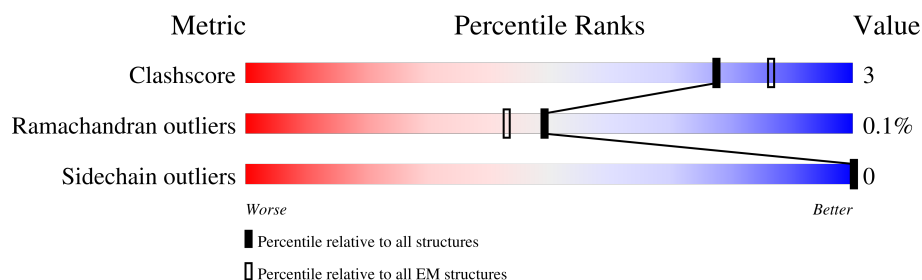
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 4.43 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.



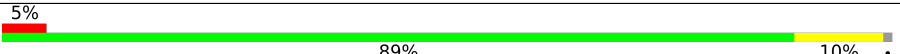
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3083 (3.93 - 4.93)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	11% 81% 6% 13%
1	B	5037	11% 81% 6% 13%
1	C	5037	11% 81% 6% 13%
1	D	5037	11% 81% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	 5%89%10%
2	F	108	 5%90%9%
2	G	108	 5%90%9%
2	H	108	 5%89%10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 286236 atoms, of which 142368 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69827	22323	34739	6046	6482	237		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	F	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	G	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1661	527	829	146	155	4		

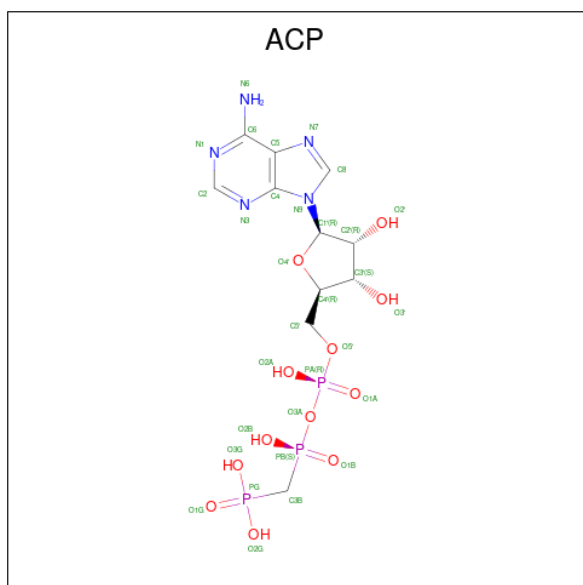
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

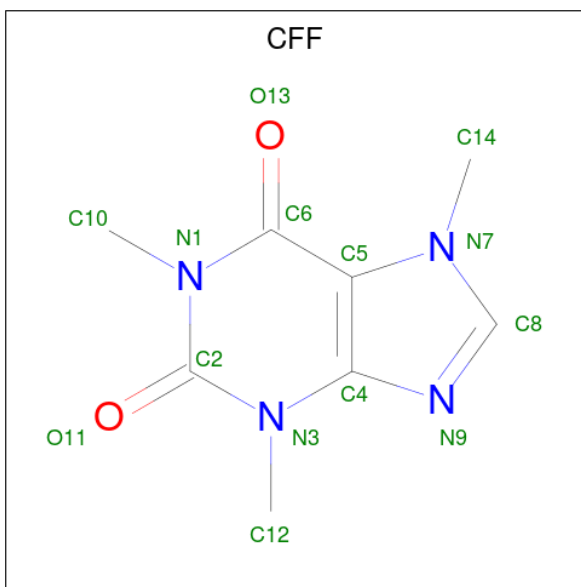
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



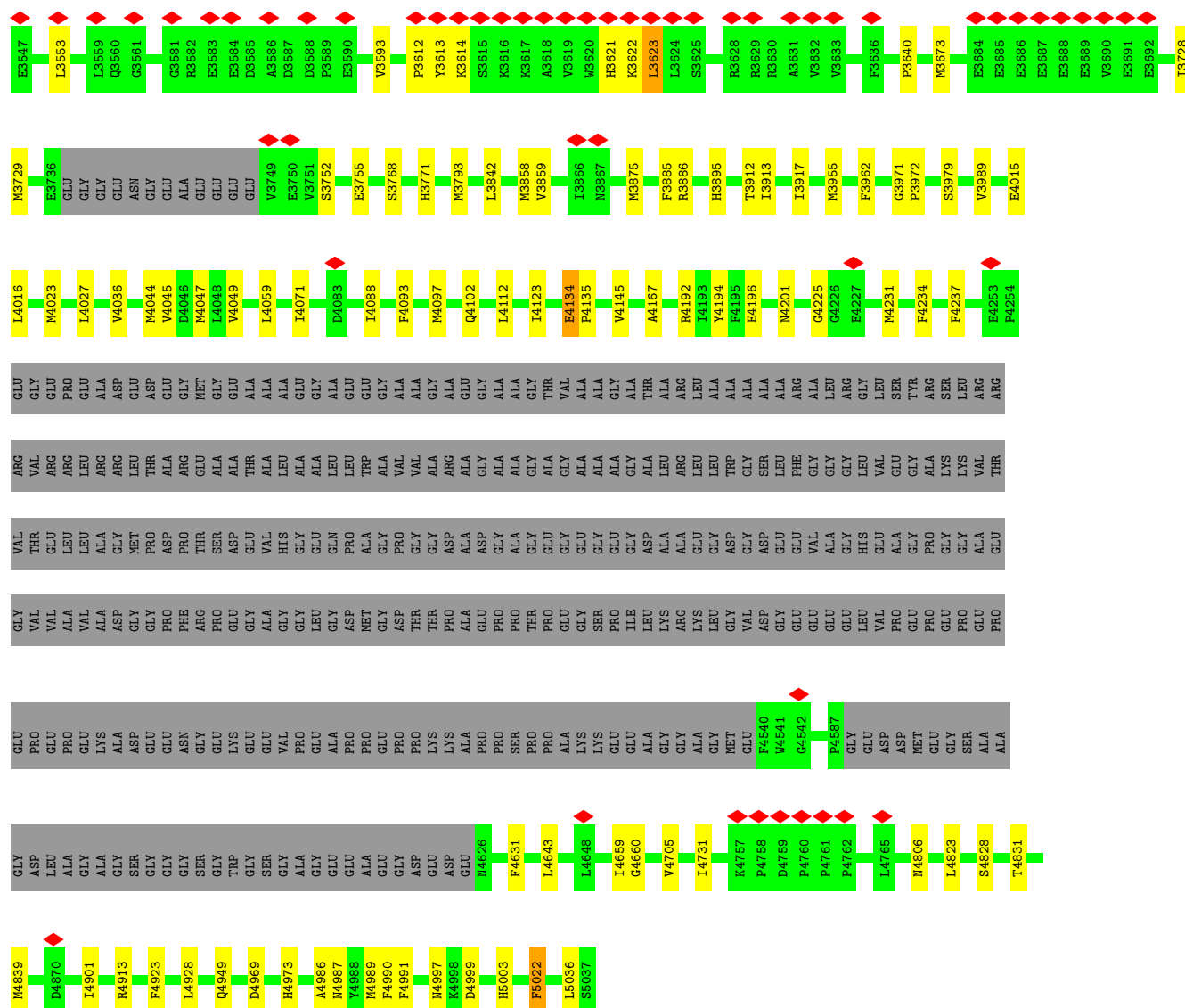
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
5	B	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
5	C	1	Total 45	C 11	H 14	N 5	O 12	P 3	0
5	D	1	Total 45	C 11	H 14	N 5	O 12	P 3	0

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).

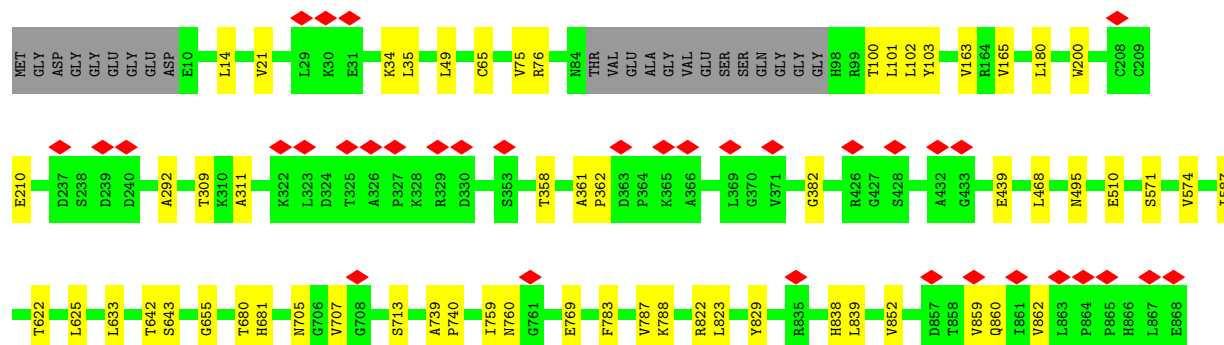
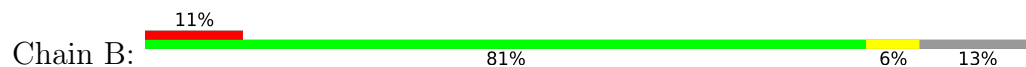


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
6	D	1	Total	C	H	N	O	0
			24	8	10	4	2	



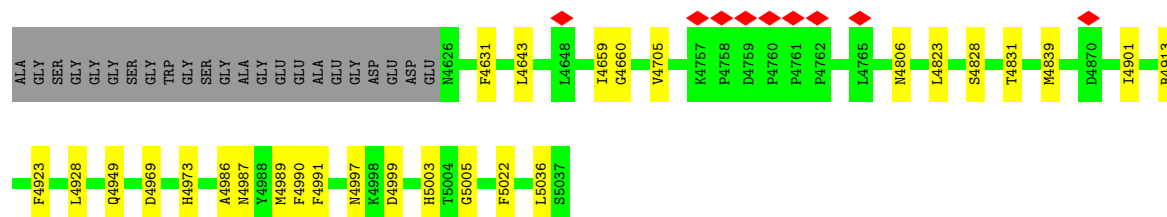


• Molecule 1: Ryanodine receptor 1

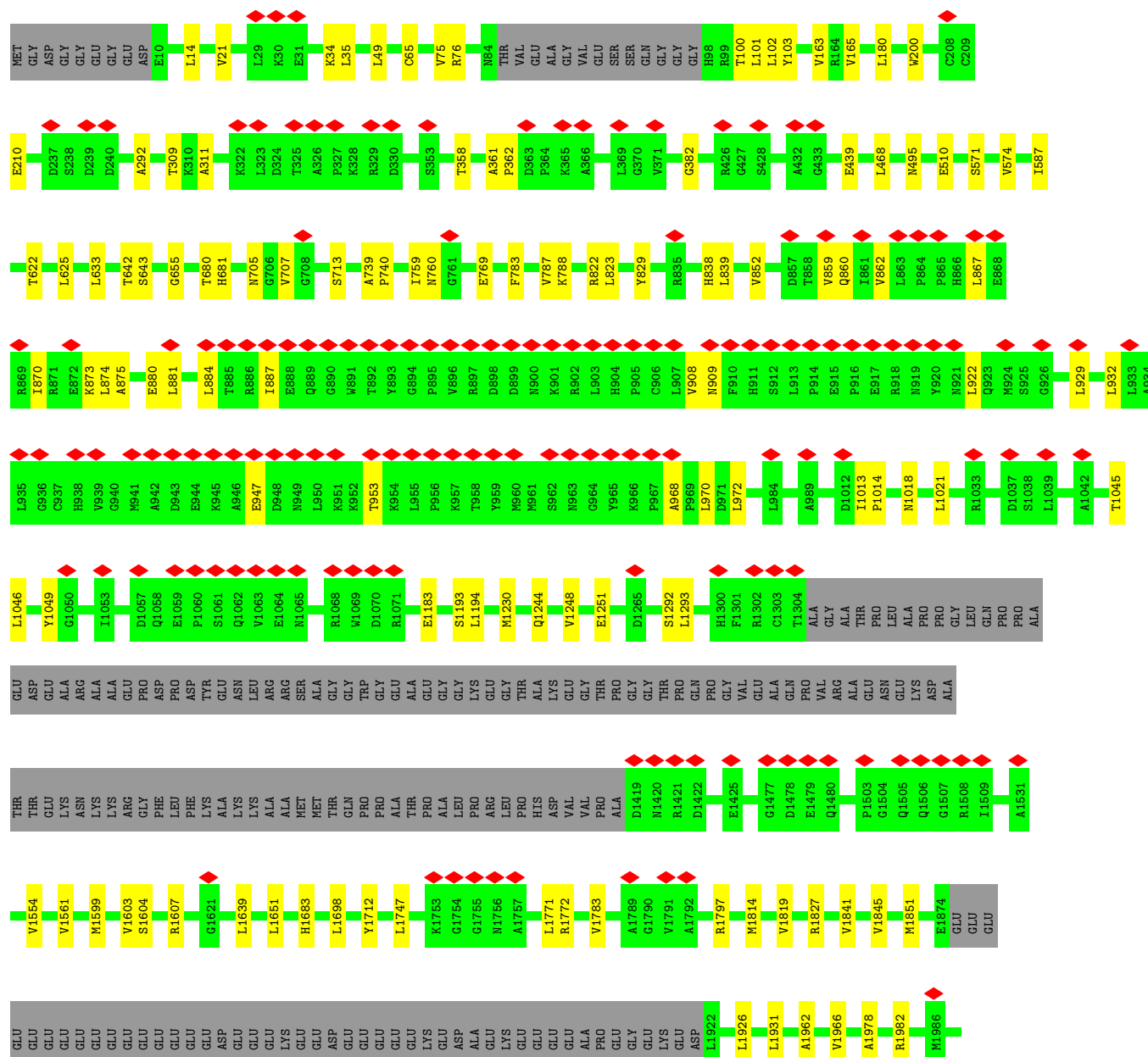
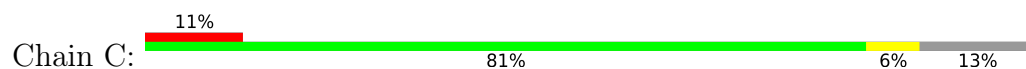


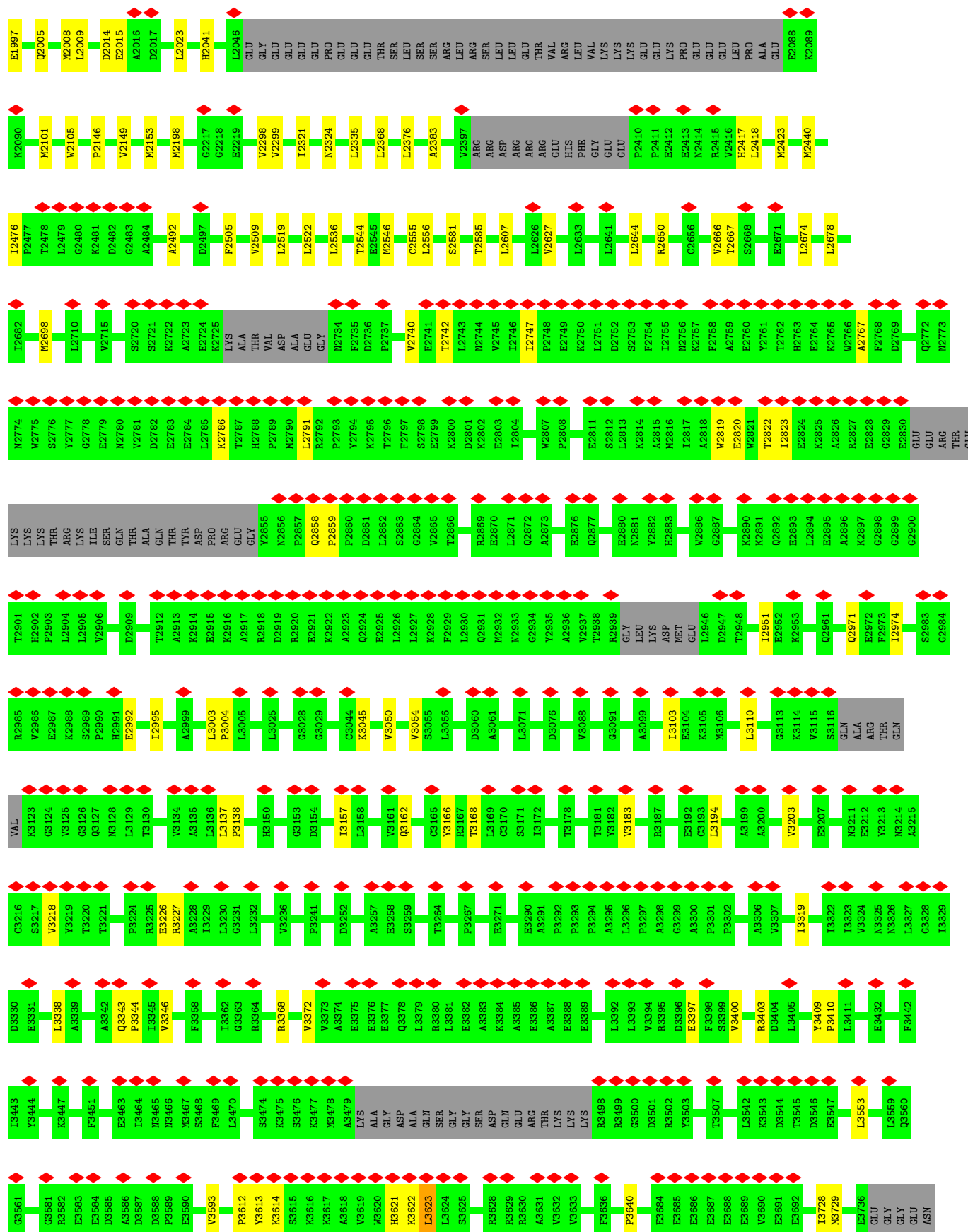


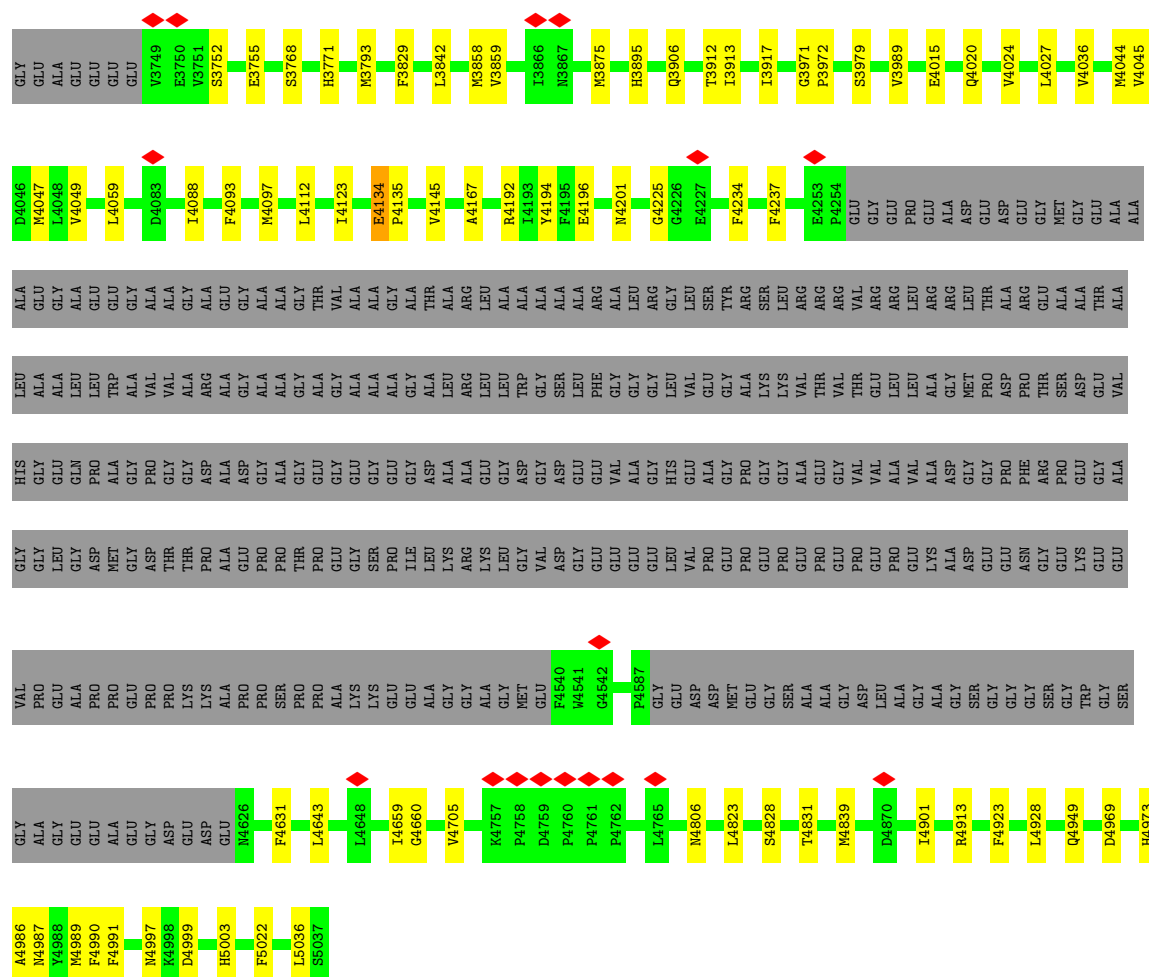




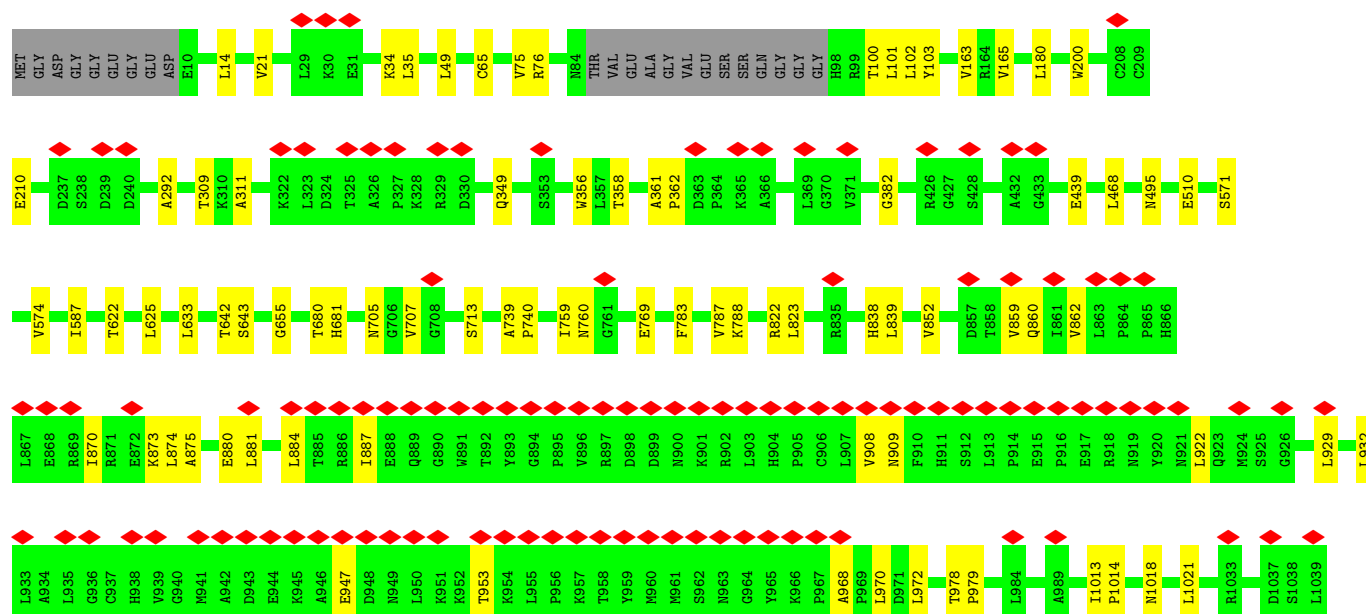
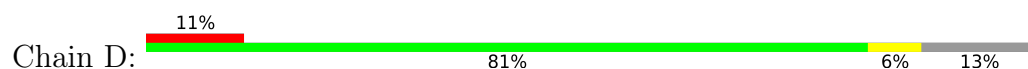
• Molecule 1: Ryanodine receptor 1



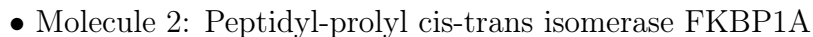


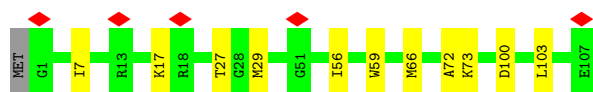
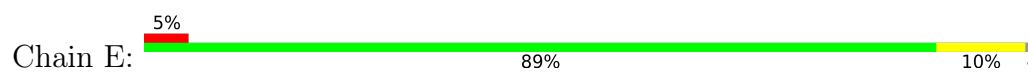


● Molecule 1: Ryanodine receptor 1

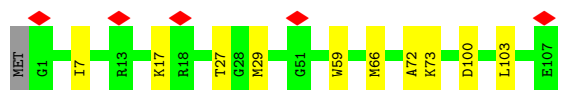
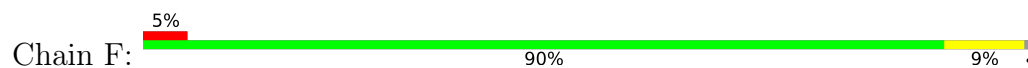




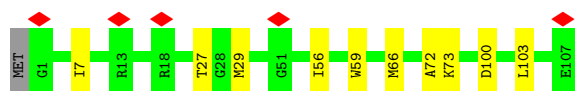
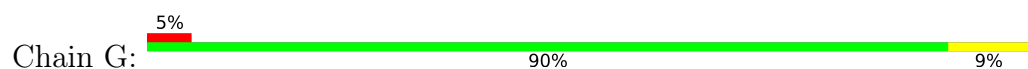




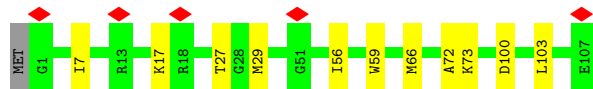
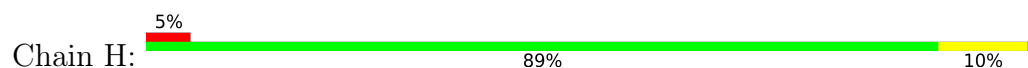
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	13358	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 ($e^-/\text{\AA}^2$)	117	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.633	Depositor
Minimum map value	0.000	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.207	Depositor
Recommended contour level	0.567	Depositor
Map size (Å)	409.80002, 409.80002, 409.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366, 1.366, 1.366	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	9/35885 (0.0%)	0.60	18/48603 (0.0%)
1	B	0.50	10/35885 (0.0%)	0.60	18/48603 (0.0%)
1	C	0.49	7/35885 (0.0%)	0.60	16/48603 (0.0%)
1	D	0.48	6/35885 (0.0%)	0.59	12/48603 (0.0%)
2	E	0.18	0/851	0.40	0/1146
2	F	0.18	0/851	0.40	0/1146
2	G	0.18	0/851	0.40	0/1146
2	H	0.18	0/851	0.40	0/1146
All	All	0.49	32/146944 (0.0%)	0.59	64/198996 (0.0%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5003	HIS	CE1-NE2	-8.28	1.24	1.32
1	B	5003	HIS	CE1-NE2	-8.19	1.24	1.32
1	A	3895	HIS	ND1-CE1	-8.14	1.24	1.32
1	D	5003	HIS	CE1-NE2	-8.06	1.24	1.32
1	B	3895	HIS	ND1-CE1	-8.02	1.24	1.32
1	D	3895	HIS	ND1-CE1	-7.94	1.24	1.32
1	C	5003	HIS	CE1-NE2	-7.93	1.24	1.32
1	C	3895	HIS	ND1-CE1	-7.89	1.24	1.32
1	A	5003	HIS	CD2-NE2	-7.56	1.29	1.37
1	B	5003	HIS	CD2-NE2	-7.51	1.29	1.37
1	D	5003	HIS	CD2-NE2	-7.41	1.29	1.37
1	C	5003	HIS	CD2-NE2	-7.32	1.29	1.37
1	C	4973	HIS	CE1-NE2	-6.26	1.26	1.32
1	B	4973	HIS	CE1-NE2	-6.21	1.26	1.32
1	A	4973	HIS	CE1-NE2	-6.11	1.26	1.32
1	B	4973	HIS	CD2-NE2	-5.74	1.31	1.37
1	C	4973	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	4973	HIS	CD2-NE2	-5.72	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4986	ALA	CA-CB	-5.42	1.45	1.53
1	A	3886	ARG	CZ-NH2	-5.40	1.26	1.33
1	B	3886	ARG	CZ-NH2	-5.40	1.26	1.33
1	B	4986	ALA	CA-CB	-5.40	1.45	1.53
1	A	4986	ALA	CA-CB	-5.38	1.45	1.53
1	A	4225	GLY	N-CA	-5.27	1.40	1.44
1	B	4225	GLY	N-CA	-5.27	1.40	1.44
1	D	4225	GLY	N-CA	-5.23	1.40	1.44
1	B	4192	ARG	CZ-NH2	-5.17	1.26	1.33
1	C	4192	ARG	CZ-NH2	-5.17	1.26	1.33
1	D	3886	ARG	CZ-NH2	-5.16	1.26	1.33
1	A	4192	ARG	CZ-NH2	-5.11	1.26	1.33
1	D	4973	HIS	CE1-NE2	-5.08	1.27	1.32
1	B	5005	GLY	N-CA	-5.01	1.38	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5003	HIS	CA-CB-CG	6.74	120.54	113.80
1	B	5003	HIS	CA-CB-CG	6.74	120.54	113.80
1	D	5003	HIS	CA-CB-CG	6.60	120.40	113.80
1	C	5003	HIS	CA-CB-CG	6.55	120.35	113.80
1	B	4225	GLY	CA-C-N	6.47	127.06	122.33
1	B	4225	GLY	C-N-CA	6.47	127.06	122.33
1	A	4225	GLY	CA-C-N	6.47	127.05	122.33
1	A	4225	GLY	C-N-CA	6.47	127.05	122.33
1	D	4225	GLY	CA-C-N	6.46	127.05	122.33
1	D	4225	GLY	C-N-CA	6.46	127.05	122.33
1	B	5022	PHE	CA-CB-CG	6.09	119.89	113.80
1	C	5022	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	4997	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	4997	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	5022	PHE	CA-CB-CG	6.02	119.82	113.80
1	C	4969	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	4997	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	4969	ASP	CA-CB-CG	5.89	118.49	112.60
1	C	4987	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	4987	ASN	CA-CB-CG	5.85	118.45	112.60
1	C	4997	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	4987	ASN	CA-CB-CG	5.81	118.41	112.60
1	B	4201	ASN	CA-CB-CG	5.76	118.36	112.60
1	B	4999	ASP	CA-CB-CG	5.75	118.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4201	ASN	CA-CB-CG	5.72	118.32	112.60
1	B	4234	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	4999	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	4201	ASN	CA-CB-CG	5.71	118.31	112.60
1	C	4234	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	4234	PHE	CA-CB-CG	5.65	119.45	113.80
1	D	4999	ASP	CA-CB-CG	5.65	118.25	112.60
1	D	5022	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	4969	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	4969	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	4999	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	4991	PHE	CA-CB-CG	5.49	119.29	113.80
1	C	4991	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	4991	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	3895	HIS	CA-CB-CG	5.45	119.25	113.80
1	D	4987	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	3895	HIS	CA-CB-CG	5.42	119.22	113.80
1	C	4225	GLY	CA-C-N	5.36	126.24	122.33
1	C	4225	GLY	C-N-CA	5.36	126.24	122.33
1	D	4201	ASN	CA-CB-CG	5.33	117.93	112.60
1	D	3895	HIS	CA-CB-CG	5.32	119.12	113.80
1	A	3962	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	4234	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	4990	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	3962	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	4990	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	3895	HIS	CA-CB-CG	5.21	119.02	113.80
1	A	4990	PHE	CA-CB-CG	5.19	118.99	113.80
1	D	4991	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	4196	GLU	CA-C-N	5.09	130.21	122.98
1	C	4196	GLU	C-N-CA	5.09	130.21	122.98
1	A	4237	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	4237	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	3885	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	3885	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	4196	GLU	CA-C-N	5.06	130.17	122.98
1	B	4196	GLU	C-N-CA	5.06	130.17	122.98
1	C	4237	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	4196	GLU	CA-C-N	5.02	130.11	122.98
1	A	4196	GLU	C-N-CA	5.02	130.11	122.98

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	A	35088	34739	34715	207	0
1	B	35088	34739	34715	202	0
1	C	35088	34739	34715	203	0
1	D	35088	34739	34715	203	0
2	E	832	829	831	9	0
2	F	832	829	831	8	0
2	G	832	829	831	8	0
2	H	832	829	831	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	14	14	0	0
5	B	31	14	14	0	0
5	C	31	14	14	0	0
5	D	31	14	14	0	0
6	A	14	10	10	0	0
6	B	14	10	10	0	0
6	C	14	10	10	0	0
6	D	14	10	10	0	0
All	All	143868	142368	142280	837	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 3.

All (837) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:GLN:OE1	1:A:862:VAL:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:860:GLN:OE1	1:C:862:VAL:HG13	1.85	0.76
1:D:1018:ASN:HB3	1:D:1021:LEU:HD23	1.67	0.76
1:D:860:GLN:OE1	1:D:862:VAL:HG13	1.85	0.76
1:A:1018:ASN:HB3	1:A:1021:LEU:HD23	1.67	0.76
1:B:860:GLN:OE1	1:B:862:VAL:HG13	1.85	0.76
1:C:1018:ASN:HB3	1:C:1021:LEU:HD23	1.67	0.75
1:B:1018:ASN:HB3	1:B:1021:LEU:HD23	1.67	0.74
1:B:929:LEU:HD21	1:B:1046:LEU:HD13	1.74	0.70
1:D:34:LYS:C	1:D:35:LEU:HD12	2.17	0.70
1:A:929:LEU:HD21	1:A:1046:LEU:HD13	1.74	0.70
1:C:929:LEU:HD21	1:C:1046:LEU:HD13	1.73	0.70
1:B:34:LYS:C	1:B:35:LEU:HD12	2.17	0.70
1:D:929:LEU:HD21	1:D:1046:LEU:HD13	1.74	0.69
1:A:34:LYS:C	1:A:35:LEU:HD12	2.17	0.69
1:C:34:LYS:C	1:C:35:LEU:HD12	2.17	0.69
1:C:2298:VAL:HG11	1:C:2335:LEU:HD21	1.77	0.66
1:B:2298:VAL:HG11	1:B:2335:LEU:HD21	1.77	0.66
1:A:2298:VAL:HG11	1:A:2335:LEU:HD21	1.77	0.66
1:D:2298:VAL:HG11	1:D:2335:LEU:HD21	1.77	0.65
1:B:1783:VAL:HG11	2:F:59:TRP:CH2	2.32	0.65
1:A:2536:LEU:HD13	1:A:2546:MET:HE1	1.80	0.64
1:D:1783:VAL:HG11	2:H:59:TRP:CH2	2.33	0.63
1:D:2536:LEU:HD13	1:D:2546:MET:HE1	1.80	0.63
1:A:1783:VAL:HG11	2:E:59:TRP:CH2	2.34	0.63
1:C:1230:MET:HE2	1:C:1827:ARG:HB3	1.81	0.63
1:B:2536:LEU:HD13	1:B:2546:MET:HE1	1.80	0.63
1:B:1230:MET:HE2	1:B:1827:ARG:HB3	1.81	0.63
1:C:4989:MET:HE3	1:C:4989:MET:HA	1.81	0.63
1:A:3989:VAL:HG11	1:A:4047:MET:HE2	1.81	0.62
1:B:4989:MET:HE3	1:B:4989:MET:HA	1.81	0.62
1:A:1230:MET:HE2	1:A:1827:ARG:HB3	1.81	0.62
1:B:3989:VAL:HG11	1:B:4047:MET:HE2	1.81	0.62
1:C:2536:LEU:HD13	1:C:2546:MET:HE1	1.80	0.61
1:C:3162:GLN:OE1	1:C:3218:VAL:HG13	2.00	0.61
1:D:3989:VAL:HG11	1:D:4047:MET:HE2	1.81	0.61
1:B:3162:GLN:OE1	1:B:3218:VAL:HG13	2.00	0.61
1:D:4989:MET:HE3	1:D:4989:MET:HA	1.82	0.61
1:C:870:ILE:HD11	1:C:1049:TYR:CE2	2.36	0.61
1:D:1230:MET:HE2	1:D:1827:ARG:HB3	1.81	0.61
1:A:2740:VAL:HG21	1:A:2819:TRP:CZ2	2.36	0.61
1:B:870:ILE:HD11	1:B:1049:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4989:MET:HE3	1:A:4989:MET:HA	1.81	0.61
1:C:2740:VAL:HG21	1:C:2819:TRP:CZ2	2.36	0.61
1:C:3989:VAL:HG11	1:C:4047:MET:HE2	1.81	0.61
1:A:3162:GLN:OE1	1:A:3218:VAL:HG13	2.00	0.60
1:D:2740:VAL:HG21	1:D:2819:TRP:CZ2	2.36	0.60
1:B:2740:VAL:HG21	1:B:2819:TRP:CZ2	2.36	0.60
1:D:3162:GLN:OE1	1:D:3218:VAL:HG13	2.00	0.60
1:C:1783:VAL:HG11	2:G:59:TRP:CH2	2.36	0.60
1:D:870:ILE:HD11	1:D:1049:TYR:CE2	2.36	0.60
1:A:2440:MET:N	1:A:2440:MET:HE2	2.17	0.60
1:A:870:ILE:HD11	1:A:1049:TYR:CE2	2.36	0.59
1:C:2440:MET:N	1:C:2440:MET:HE2	2.17	0.59
1:D:2440:MET:N	1:D:2440:MET:HE2	2.17	0.59
1:B:2440:MET:N	1:B:2440:MET:HE2	2.17	0.59
1:C:2368:LEU:HD21	1:C:2376:LEU:CD2	2.33	0.59
1:C:3368:ARG:O	1:C:3372:VAL:HG23	2.03	0.58
1:D:2368:LEU:HD21	1:D:2376:LEU:CD2	2.33	0.58
1:B:3368:ARG:O	1:B:3372:VAL:HG23	2.03	0.58
1:A:2368:LEU:HD21	1:A:2376:LEU:CD2	2.33	0.58
1:B:2368:LEU:HD21	1:B:2376:LEU:CD2	2.33	0.58
1:B:4145:VAL:HG13	1:B:4194:TYR:CB	2.34	0.58
1:D:3553:LEU:HB3	1:D:3593:VAL:HG12	1.86	0.58
1:C:2767:ALA:HA	1:C:2791:LEU:HD21	1.86	0.58
1:A:3368:ARG:O	1:A:3372:VAL:HG23	2.03	0.58
1:A:3553:LEU:HB3	1:A:3593:VAL:HG12	1.86	0.58
1:A:4145:VAL:HG13	1:A:4194:TYR:CB	2.34	0.58
1:C:4145:VAL:HG13	1:C:4194:TYR:CB	2.34	0.58
1:B:3553:LEU:HB3	1:B:3593:VAL:HG12	1.86	0.57
1:D:4145:VAL:HG13	1:D:4194:TYR:CB	2.34	0.57
1:C:2368:LEU:HD11	1:C:2376:LEU:HD21	1.86	0.57
1:B:2767:ALA:HA	1:B:2791:LEU:HD21	1.85	0.57
1:D:3368:ARG:O	1:D:3372:VAL:HG23	2.03	0.57
1:C:3553:LEU:HB3	1:C:3593:VAL:HG12	1.86	0.57
1:D:2767:ALA:HA	1:D:2791:LEU:HD21	1.86	0.57
1:A:2368:LEU:HD11	1:A:2376:LEU:HD21	1.86	0.57
1:A:587:ILE:HD11	1:A:625:LEU:HD13	1.87	0.56
1:B:1772:ARG:N	1:B:2153:MET:HE1	2.21	0.56
1:A:2555:CYS:C	1:A:2556:LEU:HD22	2.31	0.56
1:B:587:ILE:HD11	1:B:625:LEU:HD13	1.87	0.56
1:B:2555:CYS:C	1:B:2556:LEU:HD22	2.31	0.56
1:D:2555:CYS:C	1:D:2556:LEU:HD22	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2767:ALA:HA	1:A:2791:LEU:HD21	1.86	0.56
1:B:2368:LEU:HD11	1:B:2376:LEU:HD21	1.86	0.56
1:C:2555:CYS:C	1:C:2556:LEU:HD22	2.31	0.56
1:C:1772:ARG:N	1:C:2153:MET:HE1	2.21	0.56
1:D:3989:VAL:HG11	1:D:4047:MET:CE	2.36	0.56
1:D:3110:LEU:HD23	1:D:3183:VAL:HG22	1.88	0.56
1:D:1772:ARG:N	1:D:2153:MET:HE1	2.20	0.55
1:D:2368:LEU:HD11	1:D:2376:LEU:HD21	1.86	0.55
1:A:1772:ARG:N	1:A:2153:MET:HE1	2.21	0.55
1:B:2324:ASN:OD1	1:B:2324:ASN:O	2.25	0.55
1:B:2146:PRO:HA	1:B:2149:VAL:HG23	1.88	0.55
1:C:587:ILE:HD11	1:C:625:LEU:HD13	1.87	0.55
1:C:2146:PRO:HA	1:C:2149:VAL:HG23	1.88	0.55
1:C:3110:LEU:HD23	1:C:3183:VAL:HG22	1.88	0.55
1:A:2368:LEU:HD21	1:A:2376:LEU:HD21	1.88	0.55
1:A:3989:VAL:HG11	1:A:4047:MET:CE	2.36	0.55
1:D:2146:PRO:HA	1:D:2149:VAL:HG23	1.88	0.55
1:C:2324:ASN:OD1	1:C:2324:ASN:O	2.25	0.55
1:C:3989:VAL:HG11	1:C:4047:MET:CE	2.36	0.55
1:D:2368:LEU:HD21	1:D:2376:LEU:HD21	1.89	0.55
1:B:2198:MET:HE2	1:B:2198:MET:N	2.22	0.55
1:C:1244:GLN:OE1	1:C:1244:GLN:HA	2.07	0.55
1:A:3110:LEU:HD23	1:A:3183:VAL:HG22	1.88	0.54
1:C:2368:LEU:HD21	1:C:2376:LEU:HD21	1.88	0.54
1:B:2368:LEU:HD21	1:B:2376:LEU:HD21	1.88	0.54
1:D:103:TYR:CZ	1:D:163:VAL:HG22	2.42	0.54
1:D:587:ILE:HD11	1:D:625:LEU:HD13	1.87	0.54
1:D:2198:MET:HE2	1:D:2198:MET:N	2.22	0.54
1:A:1244:GLN:OE1	1:A:1244:GLN:HA	2.07	0.54
1:B:1244:GLN:HA	1:B:1244:GLN:OE1	2.07	0.54
1:D:2324:ASN:OD1	1:D:2324:ASN:O	2.25	0.54
1:A:2324:ASN:OD1	1:A:2324:ASN:O	2.25	0.54
1:B:3110:LEU:HD23	1:B:3183:VAL:HG22	1.88	0.54
1:B:3989:VAL:HG11	1:B:4047:MET:CE	2.36	0.54
1:D:1244:GLN:OE1	1:D:1244:GLN:HA	2.07	0.54
1:D:1251:GLU:N	1:D:1251:GLU:OE1	2.41	0.54
1:A:1251:GLU:N	1:A:1251:GLU:OE1	2.41	0.54
1:B:929:LEU:HD23	1:B:932:LEU:HD12	1.90	0.54
1:A:103:TYR:CZ	1:A:163:VAL:HG22	2.43	0.54
1:A:929:LEU:HD23	1:A:932:LEU:HD12	1.90	0.54
1:A:4839:MET:SD	1:B:4823:LEU:HD21	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2198:MET:N	1:C:2198:MET:HE2	2.22	0.54
1:D:3793:MET:HE2	1:D:3793:MET:N	2.23	0.54
1:A:2146:PRO:HA	1:A:2149:VAL:HG23	1.88	0.54
1:B:859:VAL:HG12	1:B:859:VAL:O	2.08	0.54
1:D:929:LEU:HD23	1:D:932:LEU:HD12	1.90	0.54
1:A:3793:MET:N	1:A:3793:MET:HE2	2.23	0.54
1:D:859:VAL:HG12	1:D:859:VAL:O	2.08	0.54
1:C:103:TYR:CZ	1:C:163:VAL:HG22	2.43	0.54
1:C:859:VAL:HG12	1:C:859:VAL:O	2.08	0.54
1:D:2740:VAL:HG21	1:D:2819:TRP:HZ2	1.73	0.54
1:A:633:LEU:HB3	1:A:1639:LEU:HD11	1.90	0.53
1:A:2740:VAL:HG21	1:A:2819:TRP:HZ2	1.73	0.53
1:C:1251:GLU:N	1:C:1251:GLU:OE1	2.41	0.53
1:A:2198:MET:N	1:A:2198:MET:HE2	2.22	0.53
1:B:103:TYR:CZ	1:B:163:VAL:HG22	2.42	0.53
1:B:1251:GLU:OE1	1:B:1251:GLU:N	2.41	0.53
1:C:1962:ALA:O	1:C:1966:VAL:HG23	2.08	0.53
1:C:2740:VAL:HG21	1:C:2819:TRP:HZ2	1.73	0.53
1:B:3793:MET:HE2	1:B:3793:MET:N	2.23	0.53
1:C:3793:MET:N	1:C:3793:MET:HE2	2.23	0.53
1:A:859:VAL:O	1:A:859:VAL:HG12	2.08	0.53
1:B:2740:VAL:HG21	1:B:2819:TRP:HZ2	1.73	0.53
1:A:1248:VAL:HG22	1:A:1599:MET:HE2	1.91	0.53
1:C:929:LEU:HD23	1:C:932:LEU:HD12	1.90	0.53
1:D:1248:VAL:HG22	1:D:1599:MET:HE2	1.91	0.53
1:A:571:SER:OG	1:A:574:VAL:HG23	2.09	0.53
1:A:3194:LEU:HD23	1:A:3194:LEU:O	2.10	0.52
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	1.91	0.52
1:D:1962:ALA:O	1:D:1966:VAL:HG23	2.08	0.52
1:B:1248:VAL:HG22	1:B:1599:MET:HE2	1.91	0.52
1:B:1962:ALA:O	1:B:1966:VAL:HG23	2.08	0.52
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	1.91	0.52
1:B:633:LEU:HB3	1:B:1639:LEU:HD11	1.90	0.52
1:C:870:ILE:HD12	1:C:873:LYS:HD2	1.92	0.52
1:D:571:SER:OG	1:D:574:VAL:HG23	2.09	0.52
1:B:571:SER:OG	1:B:574:VAL:HG23	2.09	0.52
1:C:1248:VAL:HG22	1:C:1599:MET:HE2	1.91	0.52
1:D:3194:LEU:HD23	1:D:3194:LEU:O	2.09	0.52
1:A:1962:ALA:O	1:A:1966:VAL:HG23	2.08	0.52
1:B:870:ILE:HD12	1:B:873:LYS:HD2	1.92	0.52
1:C:3194:LEU:HD23	1:C:3194:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:LEU:HB3	1:D:1639:LEU:HD11	1.90	0.52
1:D:769:GLU:N	1:D:769:GLU:OE1	2.43	0.52
1:D:870:ILE:HD12	1:D:873:LYS:HD2	1.92	0.52
1:C:3612:PRO:O	1:C:3613:TYR:CG	2.63	0.52
1:C:4036:VAL:HG21	1:C:5036:LEU:HG	1.92	0.52
1:B:3194:LEU:O	1:B:3194:LEU:HD23	2.09	0.51
1:C:571:SER:OG	1:C:574:VAL:HG23	2.09	0.51
1:A:870:ILE:HD12	1:A:873:LYS:HD2	1.92	0.51
1:A:2505:PHE:CE1	1:A:2509:VAL:HG21	2.46	0.51
1:B:4036:VAL:HG21	1:B:5036:LEU:HG	1.92	0.51
1:D:3612:PRO:O	1:D:3613:TYR:CG	2.64	0.51
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	1.91	0.51
1:A:4036:VAL:HG21	1:A:5036:LEU:HG	1.92	0.51
1:D:4036:VAL:HG21	1:D:5036:LEU:HG	1.92	0.51
1:D:2767:ALA:CA	1:D:2791:LEU:HD21	2.41	0.51
1:A:2767:ALA:CA	1:A:2791:LEU:HD21	2.41	0.51
1:C:633:LEU:HB3	1:C:1639:LEU:HD11	1.90	0.51
1:C:2505:PHE:CE1	1:C:2509:VAL:HG21	2.46	0.51
1:A:972:LEU:HD23	1:A:972:LEU:H	1.76	0.51
1:A:769:GLU:N	1:A:769:GLU:OE1	2.43	0.51
1:A:908:VAL:HG13	1:A:909:ASN:N	2.26	0.51
1:B:972:LEU:H	1:B:972:LEU:HD23	1.76	0.51
1:B:4839:MET:SD	1:C:4823:LEU:HD21	2.51	0.51
1:C:972:LEU:HD23	1:C:972:LEU:H	1.76	0.51
1:D:2505:PHE:CE1	1:D:2509:VAL:HG21	2.46	0.51
2:H:7:ILE:HD11	2:H:73:LYS:HG3	1.93	0.51
1:B:2505:PHE:CE1	1:B:2509:VAL:HG21	2.46	0.51
1:C:769:GLU:N	1:C:769:GLU:OE1	2.43	0.51
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	1.91	0.51
1:B:769:GLU:OE1	1:B:769:GLU:N	2.43	0.51
1:B:908:VAL:HG13	1:B:909:ASN:N	2.26	0.51
1:B:2767:ALA:CA	1:B:2791:LEU:HD21	2.41	0.51
1:D:1018:ASN:CB	1:D:1021:LEU:HD23	2.40	0.51
1:B:3612:PRO:O	1:B:3613:TYR:CG	2.64	0.51
1:C:14:LEU:HD21	1:C:165:VAL:HG22	1.93	0.51
1:A:3612:PRO:O	1:A:3613:TYR:CG	2.63	0.50
1:D:358:THR:HG21	1:D:382:GLY:HA2	1.93	0.50
1:A:14:LEU:HD21	1:A:165:VAL:HG22	1.93	0.50
1:A:4823:LEU:HD21	1:D:4839:MET:SD	2.51	0.50
1:D:908:VAL:HG13	1:D:909:ASN:N	2.26	0.50
1:A:707:VAL:HG13	1:A:713:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:VAL:HG13	1:C:713:SER:OG	2.12	0.50
1:C:908:VAL:HG13	1:C:909:ASN:N	2.26	0.50
1:A:358:THR:HG21	1:A:382:GLY:HA2	1.94	0.50
1:A:1771:LEU:HB3	1:A:2153:MET:HE2	1.94	0.50
1:B:707:VAL:HG13	1:B:713:SER:OG	2.12	0.50
1:B:1771:LEU:HB3	1:B:2153:MET:HE2	1.94	0.50
1:D:972:LEU:HD23	1:D:972:LEU:H	1.76	0.50
1:B:358:THR:HG21	1:B:382:GLY:HA2	1.93	0.50
1:C:2767:ALA:CA	1:C:2791:LEU:HD21	2.41	0.50
1:D:14:LEU:HD21	1:D:165:VAL:HG22	1.94	0.50
1:D:4045:VAL:O	1:D:4049:VAL:HG23	2.12	0.50
2:G:7:ILE:HD11	2:G:73:LYS:HG3	1.93	0.50
1:C:358:THR:HG21	1:C:382:GLY:HA2	1.93	0.50
1:C:4839:MET:SD	1:D:4823:LEU:HD21	2.52	0.50
1:D:1771:LEU:HB3	1:D:2153:MET:HE2	1.94	0.50
1:D:3157:ILE:HG22	1:D:3162:GLN:HG3	1.94	0.50
1:A:4045:VAL:O	1:A:4049:VAL:HG23	2.12	0.50
1:B:14:LEU:HD21	1:B:165:VAL:HG22	1.94	0.50
1:B:4045:VAL:O	1:B:4049:VAL:HG23	2.12	0.50
1:D:707:VAL:HG13	1:D:713:SER:OG	2.12	0.50
1:D:1248:VAL:HG22	1:D:1599:MET:CE	2.42	0.50
1:C:1018:ASN:CB	1:C:1021:LEU:HD23	2.40	0.49
2:F:7:ILE:HD11	2:F:73:LYS:HG3	1.93	0.49
1:B:2383:ALA:HB3	1:B:2423:MET:HE3	1.94	0.49
1:C:1248:VAL:HG22	1:C:1599:MET:CE	2.42	0.49
1:C:1771:LEU:HB3	1:C:2153:MET:HE2	1.94	0.49
1:A:705:ASN:OD1	1:A:705:ASN:C	2.55	0.49
1:A:100:THR:HG22	1:A:101:LEU:N	2.28	0.49
1:B:1248:VAL:HG22	1:B:1599:MET:CE	2.42	0.49
1:A:1248:VAL:HG22	1:A:1599:MET:CE	2.42	0.49
1:A:3157:ILE:HG22	1:A:3162:GLN:HG3	1.94	0.49
1:C:705:ASN:OD1	1:C:705:ASN:C	2.55	0.49
1:C:783:PHE:HB2	1:C:787:VAL:HG11	1.95	0.49
1:D:783:PHE:HB2	1:D:787:VAL:HG11	1.95	0.49
1:D:4828:SER:HA	1:D:4831:THR:HG22	1.95	0.49
1:A:4828:SER:HA	1:A:4831:THR:HG22	1.95	0.49
1:B:705:ASN:C	1:B:705:ASN:OD1	2.55	0.49
1:D:2383:ALA:HB3	1:D:2423:MET:HE3	1.94	0.49
2:E:7:ILE:HD11	2:E:73:LYS:HG3	1.93	0.49
1:A:4145:VAL:HG13	1:A:4194:TYR:HB2	1.95	0.49
1:D:3050:VAL:HG22	1:D:3054:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ALA:HB1	1:A:740:PRO:CD	2.43	0.49
1:C:739:ALA:HB1	1:C:740:PRO:CD	2.43	0.49
1:C:3157:ILE:HG22	1:C:3162:GLN:HG3	1.94	0.49
1:D:705:ASN:C	1:D:705:ASN:OD1	2.55	0.49
1:A:2519:LEU:HA	1:A:2522:LEU:HD12	1.95	0.49
1:B:100:THR:HG22	1:B:101:LEU:N	2.28	0.49
1:B:4145:VAL:HG13	1:B:4194:TYR:HB2	1.95	0.49
1:D:4145:VAL:HG13	1:D:4194:TYR:HB2	1.95	0.49
1:A:970:LEU:HD13	1:A:1045:THR:HG23	1.95	0.49
1:C:358:THR:HG21	1:C:382:GLY:CA	2.43	0.49
1:D:100:THR:HG22	1:D:101:LEU:N	2.28	0.49
1:A:2383:ALA:HB3	1:A:2423:MET:HE3	1.95	0.48
1:C:2383:ALA:HB3	1:C:2423:MET:HE3	1.94	0.48
1:C:4015:GLU:N	1:C:4015:GLU:OE1	2.47	0.48
1:C:4045:VAL:O	1:C:4049:VAL:HG23	2.12	0.48
1:C:4145:VAL:HG13	1:C:4194:TYR:HB2	1.95	0.48
1:A:3050:VAL:HG22	1:A:3054:VAL:HG12	1.95	0.48
1:B:358:THR:HG21	1:B:382:GLY:CA	2.43	0.48
1:B:4828:SER:HA	1:B:4831:THR:HG22	1.95	0.48
1:D:4015:GLU:N	1:D:4015:GLU:OE1	2.47	0.48
1:A:783:PHE:HB2	1:A:787:VAL:HG11	1.95	0.48
1:C:2417:HIS:CE1	1:C:2492:ALA:HB2	2.49	0.48
1:A:633:LEU:N	1:A:633:LEU:HD12	2.28	0.48
1:B:880:GLU:O	1:B:884:LEU:HD13	2.14	0.48
1:B:2519:LEU:HA	1:B:2522:LEU:HD12	1.95	0.48
1:C:4828:SER:HA	1:C:4831:THR:HG22	1.95	0.48
1:A:1018:ASN:CB	1:A:1021:LEU:HD23	2.40	0.48
1:B:633:LEU:HD12	1:B:633:LEU:N	2.28	0.48
1:B:3157:ILE:HG22	1:B:3162:GLN:HG3	1.94	0.48
1:D:358:THR:HG21	1:D:382:GLY:CA	2.43	0.48
1:D:633:LEU:HD12	1:D:633:LEU:N	2.28	0.48
1:D:2519:LEU:HA	1:D:2522:LEU:HD12	1.95	0.48
1:A:1183:GLU:OE1	1:A:1183:GLU:C	2.57	0.48
1:A:1783:VAL:O	2:E:56:ILE:HG23	2.13	0.48
1:A:3912:THR:HG22	1:A:3913:ILE:N	2.29	0.48
1:D:970:LEU:HD13	1:D:1045:THR:HG23	1.94	0.48
1:A:75:VAL:HG23	1:A:76:ARG:N	2.29	0.48
1:B:783:PHE:HB2	1:B:787:VAL:HG11	1.95	0.48
1:C:100:THR:HG22	1:C:101:LEU:N	2.28	0.48
1:D:739:ALA:HB1	1:D:740:PRO:CD	2.43	0.48
1:D:822:ARG:C	1:D:823:LEU:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:880:GLU:O	1:D:884:LEU:HD13	2.14	0.48
1:D:3397:GLU:HA	1:D:3400:VAL:HG12	1.96	0.48
1:B:739:ALA:HB1	1:B:740:PRO:CD	2.43	0.48
1:B:1018:ASN:CB	1:B:1021:LEU:HD23	2.40	0.48
1:C:2536:LEU:HD13	1:C:2546:MET:CE	2.44	0.48
1:D:75:VAL:HG23	1:D:76:ARG:N	2.29	0.48
1:D:1183:GLU:C	1:D:1183:GLU:OE1	2.57	0.48
1:D:2417:HIS:CE1	1:D:2492:ALA:HB2	2.49	0.48
1:A:2627:VAL:HG21	1:A:2674:LEU:HD12	1.96	0.48
1:A:3343:GLN:N	1:A:3344:PRO:CD	2.77	0.48
1:B:970:LEU:HD13	1:B:1045:THR:HG23	1.95	0.48
1:B:3050:VAL:HG22	1:B:3054:VAL:HG12	1.95	0.48
1:B:3103:ILE:HD13	1:B:3168:THR:HG23	1.95	0.48
1:C:633:LEU:N	1:C:633:LEU:HD12	2.28	0.48
1:C:3343:GLN:N	1:C:3344:PRO:CD	2.77	0.48
1:D:3103:ILE:HD13	1:D:3168:THR:HG23	1.95	0.48
1:A:4015:GLU:N	1:A:4015:GLU:OE1	2.47	0.48
1:B:822:ARG:C	1:B:823:LEU:HD12	2.39	0.48
1:B:4015:GLU:OE1	1:B:4015:GLU:N	2.47	0.48
1:D:4088:ILE:HG23	1:D:4088:ILE:O	2.14	0.48
1:A:880:GLU:O	1:A:884:LEU:HD13	2.14	0.47
1:A:2417:HIS:CE1	1:A:2492:ALA:HB2	2.49	0.47
1:A:3621:HIS:O	1:A:3622:LYS:HG3	2.14	0.47
1:A:4088:ILE:HG23	1:A:4088:ILE:O	2.14	0.47
1:B:75:VAL:HG23	1:B:76:ARG:N	2.29	0.47
1:B:3912:THR:HG22	1:B:3913:ILE:N	2.29	0.47
1:D:3343:GLN:N	1:D:3344:PRO:CD	2.77	0.47
1:C:75:VAL:HG23	1:C:76:ARG:N	2.29	0.47
1:C:3103:ILE:HD13	1:C:3168:THR:HG23	1.95	0.47
1:D:1193:SER:C	1:D:1194:LEU:HD12	2.39	0.47
1:A:1978:ALA:HB1	1:A:1982:ARG:HH11	1.80	0.47
1:B:2627:VAL:HG21	1:B:2674:LEU:HD12	1.96	0.47
1:B:3343:GLN:N	1:B:3344:PRO:CD	2.77	0.47
1:C:3912:THR:HG22	1:C:3913:ILE:N	2.29	0.47
1:C:4088:ILE:HG23	1:C:4088:ILE:O	2.14	0.47
1:A:358:THR:HG21	1:A:382:GLY:CA	2.44	0.47
1:A:3103:ILE:HD13	1:A:3168:THR:HG23	1.95	0.47
1:B:1193:SER:C	1:B:1194:LEU:HD12	2.39	0.47
1:C:880:GLU:O	1:C:884:LEU:HD13	2.14	0.47
1:C:970:LEU:HD13	1:C:1045:THR:HG23	1.95	0.47
1:C:1193:SER:C	1:C:1194:LEU:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3137:LEU:HB3	1:D:3138:PRO:HD3	1.96	0.47
1:A:3397:GLU:HA	1:A:3400:VAL:HG12	1.96	0.47
1:B:1183:GLU:C	1:B:1183:GLU:OE1	2.57	0.47
1:B:1997:GLU:HA	1:B:2008:MET:HE1	1.96	0.47
1:B:2101:MET:HE3	1:B:2105:TRP:CZ3	2.50	0.47
1:B:2417:HIS:CE1	1:B:2492:ALA:HB2	2.49	0.47
1:C:1183:GLU:C	1:C:1183:GLU:OE1	2.57	0.47
1:D:739:ALA:HB1	1:D:740:PRO:HD2	1.97	0.47
1:A:739:ALA:HB1	1:A:740:PRO:HD2	1.97	0.47
1:A:822:ARG:C	1:A:823:LEU:HD12	2.39	0.47
1:A:1554:VAL:HG21	1:A:1561:VAL:CG1	2.45	0.47
1:A:2440:MET:HE2	1:A:2440:MET:CA	2.45	0.47
1:B:3137:LEU:HB3	1:B:3138:PRO:HD3	1.96	0.47
1:C:2101:MET:HE3	1:C:2105:TRP:CZ3	2.50	0.47
1:C:2519:LEU:HA	1:C:2522:LEU:HD12	1.95	0.47
1:D:1978:ALA:HB1	1:D:1982:ARG:HH11	1.80	0.47
1:D:3621:HIS:O	1:D:3622:LYS:HG3	2.14	0.47
1:A:1814:MET:HE2	1:A:1814:MET:HA	1.97	0.47
1:A:2650:ARG:HA	1:A:2650:ARG:NE	2.30	0.47
1:B:739:ALA:HB1	1:B:740:PRO:HD2	1.97	0.47
1:B:1554:VAL:HG21	1:B:1561:VAL:CG1	2.45	0.47
1:B:1814:MET:HE2	1:B:1814:MET:HA	1.97	0.47
1:B:3372:VAL:HG22	1:B:3397:GLU:OE1	2.15	0.47
1:C:822:ARG:C	1:C:823:LEU:HD12	2.39	0.47
1:D:2101:MET:HE3	1:D:2105:TRP:CZ3	2.50	0.47
1:D:2858:GLN:N	1:D:2859:PRO:CD	2.78	0.47
1:B:2440:MET:HE2	1:B:2440:MET:CA	2.45	0.47
1:B:2536:LEU:HD13	1:B:2546:MET:CE	2.44	0.47
1:B:2858:GLN:N	1:B:2859:PRO:CD	2.78	0.47
1:B:3621:HIS:O	1:B:3622:LYS:HG3	2.14	0.47
1:C:739:ALA:HB1	1:C:740:PRO:HD2	1.97	0.47
1:C:1997:GLU:HA	1:C:2008:MET:HE1	1.96	0.47
1:D:1997:GLU:HA	1:D:2008:MET:HE1	1.96	0.47
1:D:2440:MET:HE2	1:D:2440:MET:CA	2.45	0.47
1:D:2627:VAL:HG21	1:D:2674:LEU:HD12	1.96	0.47
1:D:3912:THR:HG22	1:D:3913:ILE:N	2.29	0.47
1:A:3372:VAL:HG22	1:A:3397:GLU:OE1	2.15	0.47
1:B:908:VAL:HG13	1:B:909:ASN:H	1.80	0.47
1:B:1978:ALA:HB1	1:B:1982:ARG:HH11	1.79	0.47
1:D:1554:VAL:HG21	1:D:1561:VAL:CG1	2.45	0.47
1:A:1193:SER:C	1:A:1194:LEU:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2546:MET:SD	1:A:2546:MET:C	2.98	0.47
1:A:3137:LEU:HB3	1:A:3138:PRO:HD3	1.96	0.47
1:B:2005:GLN:O	1:B:2009:LEU:HD23	2.15	0.47
1:C:1814:MET:HE2	1:C:1814:MET:HA	1.97	0.47
1:C:3050:VAL:HG22	1:C:3054:VAL:HG12	1.95	0.47
1:B:2546:MET:C	1:B:2546:MET:SD	2.98	0.46
1:B:4088:ILE:O	1:B:4088:ILE:HG23	2.14	0.46
1:D:1814:MET:HA	1:D:1814:MET:HE2	1.97	0.46
1:D:2546:MET:SD	1:D:2546:MET:C	2.98	0.46
1:B:4705:VAL:HG22	1:B:4705:VAL:O	2.16	0.46
1:D:2650:ARG:HA	1:D:2650:ARG:NE	2.30	0.46
1:D:3403:ARG:HD3	1:D:3403:ARG:O	2.16	0.46
1:A:1997:GLU:HA	1:A:2008:MET:HE1	1.96	0.46
1:A:2101:MET:HE3	1:A:2105:TRP:CZ3	2.50	0.46
1:B:3397:GLU:HA	1:B:3400:VAL:HG12	1.96	0.46
1:C:2440:MET:HE2	1:C:2440:MET:CA	2.45	0.46
1:C:2546:MET:SD	1:C:2546:MET:C	2.98	0.46
1:C:4643:LEU:HD21	1:C:4806:ASN:CG	2.40	0.46
1:C:4705:VAL:O	1:C:4705:VAL:HG22	2.16	0.46
1:D:4134:GLU:HB3	1:D:4135:PRO:HD3	1.98	0.46
1:A:4134:GLU:HB3	1:A:4135:PRO:HD3	1.98	0.46
1:B:3917:ILE:HD11	1:B:3979:SER:OG	2.15	0.46
1:C:1554:VAL:HG21	1:C:1561:VAL:CG1	2.45	0.46
1:C:2627:VAL:HG21	1:C:2674:LEU:HD12	1.96	0.46
1:C:3166:TYR:OH	1:C:3203:VAL:HG21	2.16	0.46
1:C:3621:HIS:O	1:C:3622:LYS:HG3	2.14	0.46
1:D:3166:TYR:OH	1:D:3203:VAL:HG21	2.16	0.46
1:A:4643:LEU:HD21	1:A:4806:ASN:CG	2.40	0.46
1:C:1978:ALA:HB1	1:C:1982:ARG:HH11	1.79	0.46
1:C:2858:GLN:N	1:C:2859:PRO:CD	2.78	0.46
1:C:3917:ILE:HD11	1:C:3979:SER:OG	2.15	0.46
1:C:4134:GLU:HB3	1:C:4135:PRO:HD3	1.98	0.46
1:D:1783:VAL:O	2:H:56:ILE:HG23	2.16	0.46
1:D:2005:GLN:O	1:D:2009:LEU:HD23	2.15	0.46
1:A:2101:MET:HE3	1:A:2105:TRP:CE3	2.51	0.46
1:B:2650:ARG:HA	1:B:2650:ARG:NE	2.30	0.46
1:B:4134:GLU:HB3	1:B:4135:PRO:HD3	1.98	0.46
1:C:2005:GLN:O	1:C:2009:LEU:HD23	2.15	0.46
1:C:3397:GLU:HA	1:C:3400:VAL:HG12	1.96	0.46
1:C:3403:ARG:O	1:C:3403:ARG:HD3	2.16	0.46
1:D:4643:LEU:HD21	1:D:4806:ASN:CG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2536:LEU:HD13	1:A:2546:MET:CE	2.44	0.46
1:A:2858:GLN:N	1:A:2859:PRO:CD	2.78	0.46
1:C:2101:MET:HE3	1:C:2105:TRP:CE3	2.51	0.46
1:C:3137:LEU:HB3	1:C:3138:PRO:HD3	1.96	0.46
1:D:3917:ILE:HD11	1:D:3979:SER:OG	2.15	0.46
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.98	0.46
1:C:2650:ARG:HA	1:C:2650:ARG:NE	2.30	0.46
1:A:2005:GLN:O	1:A:2009:LEU:HD23	2.15	0.46
1:A:1013:ILE:N	1:A:1014:PRO:HD2	2.31	0.46
1:A:3403:ARG:O	1:A:3403:ARG:HD3	2.16	0.46
1:B:4027:LEU:HD21	1:B:4044:MET:SD	2.56	0.46
1:C:3614:LYS:HD2	1:C:3614:LYS:O	2.16	0.46
1:D:2536:LEU:HD13	1:D:2546:MET:CE	2.44	0.46
1:D:3372:VAL:HG22	1:D:3397:GLU:OE1	2.15	0.46
1:A:3166:TYR:OH	1:A:3203:VAL:HG21	2.16	0.45
1:B:4643:LEU:HD21	1:B:4806:ASN:CG	2.40	0.45
1:D:2101:MET:HE3	1:D:2105:TRP:CE3	2.51	0.45
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	1.98	0.45
1:D:4705:VAL:HG22	1:D:4705:VAL:O	2.16	0.45
1:A:3614:LYS:HD2	1:A:3614:LYS:O	2.16	0.45
1:B:2101:MET:HE3	1:B:2105:TRP:CE3	2.51	0.45
1:C:102:LEU:HD12	1:C:102:LEU:N	2.31	0.45
1:D:102:LEU:N	1:D:102:LEU:HD12	2.31	0.45
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.99	0.45
1:A:4027:LEU:HD21	1:A:4044:MET:SD	2.56	0.45
1:B:3166:TYR:OH	1:B:3203:VAL:HG21	2.15	0.45
1:B:3614:LYS:HD2	1:B:3614:LYS:O	2.16	0.45
1:C:908:VAL:HG13	1:C:909:ASN:H	1.81	0.45
1:C:1013:ILE:N	1:C:1014:PRO:HD2	2.31	0.45
1:C:3372:VAL:HG22	1:C:3397:GLU:OE1	2.15	0.45
1:D:1013:ILE:N	1:D:1014:PRO:HD2	2.31	0.45
1:D:3614:LYS:HD2	1:D:3614:LYS:O	2.16	0.45
1:A:3319:ILE:HG23	1:A:3338:LEU:HD21	1.99	0.45
1:B:3319:ILE:HG23	1:B:3338:LEU:HD21	1.99	0.45
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.98	0.45
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	1.98	0.45
1:C:1783:VAL:O	2:G:56:ILE:HG23	2.16	0.45
1:D:908:VAL:HG13	1:D:909:ASN:H	1.80	0.45
1:A:468:LEU:C	1:A:468:LEU:HD23	2.41	0.45
1:A:908:VAL:HG13	1:A:909:ASN:H	1.80	0.45
1:A:4705:VAL:O	1:A:4705:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3403:ARG:O	1:B:3403:ARG:HD3	2.16	0.45
1:C:870:ILE:HD13	1:C:947:GLU:CD	2.41	0.45
1:D:3319:ILE:HG23	1:D:3338:LEU:HD21	1.99	0.45
1:A:2819:TRP:O	1:A:2820:GLU:HG3	2.17	0.45
1:B:102:LEU:N	1:B:102:LEU:HD12	2.31	0.45
1:B:210:GLU:N	1:B:210:GLU:OE1	2.50	0.45
1:B:2819:TRP:O	1:B:2820:GLU:HG3	2.17	0.45
1:D:680:THR:HG22	1:D:681:HIS:N	2.32	0.45
1:D:3622:LYS:O	1:D:3623:LEU:C	2.60	0.45
1:A:870:ILE:HD13	1:A:947:GLU:CD	2.41	0.45
1:B:870:ILE:HD13	1:B:947:GLU:CD	2.41	0.45
1:C:680:THR:HG22	1:C:681:HIS:N	2.32	0.45
1:D:870:ILE:HD13	1:D:947:GLU:CD	2.41	0.45
1:A:3622:LYS:O	1:A:3623:LEU:C	2.60	0.45
1:A:3917:ILE:HD11	1:A:3979:SER:OG	2.15	0.45
1:B:439:GLU:N	1:B:439:GLU:OE1	2.50	0.45
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.31	0.45
1:D:468:LEU:C	1:D:468:LEU:HD23	2.41	0.45
1:A:102:LEU:HD12	1:A:102:LEU:N	2.31	0.45
1:A:439:GLU:OE1	1:A:439:GLU:N	2.50	0.45
1:A:4923:PHE:O	1:A:4928:LEU:HD23	2.17	0.45
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.99	0.45
1:C:3622:LYS:O	1:C:3623:LEU:C	2.60	0.45
1:A:680:THR:HG22	1:A:681:HIS:N	2.32	0.44
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	1.98	0.44
1:B:1013:ILE:N	1:B:1014:PRO:HD2	2.31	0.44
1:B:2742:THR:O	1:B:2742:THR:HG22	2.18	0.44
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.32	0.44
1:C:2819:TRP:O	1:C:2820:GLU:HG3	2.17	0.44
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	1.98	0.44
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.32	0.44
1:A:210:GLU:OE1	1:A:210:GLU:N	2.50	0.44
1:A:1637:MET:HE2	1:A:1637:MET:HB3	1.94	0.44
1:B:468:LEU:HD23	1:B:468:LEU:C	2.41	0.44
1:C:468:LEU:C	1:C:468:LEU:HD23	2.42	0.44
1:B:4112:LEU:CD2	1:B:4123:ILE:HD11	2.48	0.44
1:C:875:ALA:HB2	1:C:922:LEU:HD12	2.00	0.44
1:C:2198:MET:HE2	1:C:2198:MET:CA	2.48	0.44
1:C:3319:ILE:HG23	1:C:3338:LEU:HD21	1.99	0.44
1:D:210:GLU:OE1	1:D:210:GLU:N	2.50	0.44
1:D:838:HIS:C	1:D:839:LEU:HD12	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2198:MET:HE2	1:D:2198:MET:CA	2.48	0.44
1:A:2786:LYS:HD2	1:A:2786:LYS:O	2.18	0.44
1:A:2666:VAL:HG12	1:A:2667:THR:N	2.33	0.44
1:B:680:THR:HG22	1:B:681:HIS:N	2.32	0.44
1:B:1292:SER:C	1:B:1293:LEU:HD22	2.43	0.44
1:B:2198:MET:HE2	1:B:2198:MET:CA	2.48	0.44
1:C:2786:LYS:HD2	1:C:2786:LYS:O	2.18	0.44
1:C:4923:PHE:O	1:C:4928:LEU:HD23	2.17	0.44
1:D:1292:SER:C	1:D:1293:LEU:HD22	2.43	0.44
1:D:2819:TRP:O	1:D:2820:GLU:HG3	2.17	0.44
1:D:4949:GLN:HA	1:D:4949:GLN:OE1	2.18	0.44
1:A:2742:THR:HG22	1:A:2742:THR:O	2.18	0.44
1:B:2014:ASP:O	1:B:2015:GLU:HB3	2.18	0.44
1:D:881:LEU:HA	1:D:884:LEU:HB2	2.00	0.44
1:D:2666:VAL:HG12	1:D:2667:THR:N	2.33	0.44
1:D:4112:LEU:CD2	1:D:4123:ILE:HD11	2.48	0.44
1:A:2198:MET:HE2	1:A:2198:MET:CA	2.48	0.44
1:B:4923:PHE:O	1:B:4928:LEU:HD23	2.17	0.44
1:C:210:GLU:N	1:C:210:GLU:OE1	2.50	0.44
1:A:838:HIS:C	1:A:839:LEU:HD12	2.43	0.44
1:B:884:LEU:HA	1:B:887:ILE:HG22	2.00	0.44
1:B:4093:PHE:CE1	1:B:4097:MET:HG3	2.53	0.44
1:C:838:HIS:C	1:C:839:LEU:HD12	2.43	0.44
1:D:439:GLU:N	1:D:439:GLU:OE1	2.50	0.44
1:D:1230:MET:HE2	1:D:1827:ARG:CB	2.48	0.44
1:D:2014:ASP:O	1:D:2015:GLU:HB3	2.18	0.44
1:A:2698:MET:HE3	1:A:2698:MET:O	2.18	0.43
1:C:1292:SER:C	1:C:1293:LEU:HD22	2.43	0.43
1:C:2666:VAL:HG12	1:C:2667:THR:N	2.33	0.43
1:C:4949:GLN:OE1	1:C:4949:GLN:HA	2.18	0.43
1:D:884:LEU:HA	1:D:887:ILE:HG22	2.00	0.43
1:D:4923:PHE:O	1:D:4928:LEU:HD23	2.17	0.43
1:B:881:LEU:HA	1:B:884:LEU:HB2	2.00	0.43
1:B:2822:THR:O	1:B:2822:THR:HG23	2.18	0.43
1:C:439:GLU:N	1:C:439:GLU:OE1	2.50	0.43
1:D:2698:MET:HE3	1:D:2698:MET:O	2.18	0.43
1:D:2786:LYS:HD2	1:D:2786:LYS:O	2.18	0.43
1:A:884:LEU:HA	1:A:887:ILE:HG22	1.99	0.43
1:A:1292:SER:C	1:A:1293:LEU:HD22	2.43	0.43
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.32	0.43
1:B:2786:LYS:HD2	1:B:2786:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4631:PHE:CD1	1:B:4631:PHE:C	2.97	0.43
1:B:4949:GLN:OE1	1:B:4949:GLN:HA	2.18	0.43
1:A:953:THR:O	1:A:968:ALA:HA	2.19	0.43
1:A:2822:THR:O	1:A:2822:THR:HG23	2.18	0.43
1:B:787:VAL:HG22	1:B:788:LYS:N	2.34	0.43
1:B:4901:ILE:HD11	1:B:4913:ARG:CZ	2.49	0.43
1:C:2698:MET:HE3	1:C:2698:MET:O	2.18	0.43
1:C:2992:GLU:HA	1:C:2995:ILE:HG22	2.00	0.43
1:A:4112:LEU:CD2	1:A:4123:ILE:HD11	2.48	0.43
1:B:642:THR:HG22	1:B:643:SER:N	2.34	0.43
1:B:838:HIS:C	1:B:839:LEU:HD12	2.43	0.43
1:B:2005:GLN:OE1	1:B:3640:PRO:HA	2.19	0.43
1:B:2666:VAL:HG12	1:B:2667:THR:N	2.33	0.43
1:C:3409:TYR:N	1:C:3410:PRO:HD2	2.34	0.43
1:C:4093:PHE:CE1	1:C:4097:MET:HG3	2.53	0.43
1:C:4901:ILE:HD11	1:C:4913:ARG:CZ	2.49	0.43
1:D:4901:ILE:HD11	1:D:4913:ARG:CZ	2.49	0.43
1:A:875:ALA:HB2	1:A:922:LEU:HD12	2.00	0.43
1:A:1230:MET:HE2	1:A:1827:ARG:CB	2.48	0.43
1:A:4901:ILE:HD11	1:A:4913:ARG:CZ	2.49	0.43
1:A:4949:GLN:HA	1:A:4949:GLN:OE1	2.18	0.43
1:B:3622:LYS:O	1:B:3623:LEU:C	2.60	0.43
1:C:1230:MET:HE2	1:C:1827:ARG:CB	2.48	0.43
1:D:787:VAL:HG22	1:D:788:LYS:N	2.34	0.43
1:D:953:THR:O	1:D:968:ALA:HA	2.19	0.43
1:D:4093:PHE:CE1	1:D:4097:MET:HG3	2.53	0.43
1:A:3226:GLU:O	1:A:3227:ARG:HB2	2.19	0.43
1:A:3613:TYR:O	1:A:3614:LYS:C	2.62	0.43
1:A:4093:PHE:CE1	1:A:4097:MET:HG3	2.53	0.43
1:C:2822:THR:O	1:C:2822:THR:HG23	2.18	0.43
1:D:3409:TYR:N	1:D:3410:PRO:HD2	2.34	0.43
2:G:27:THR:HG22	2:G:29:MET:HE3	2.01	0.43
1:A:1747:LEU:HD21	1:A:2041:HIS:CD2	2.54	0.43
1:A:2951:ILE:HD12	1:A:2951:ILE:H	1.84	0.43
1:B:3226:GLU:O	1:B:3227:ARG:HB2	2.19	0.43
1:D:642:THR:HG22	1:D:643:SER:N	2.34	0.43
1:D:875:ALA:HB2	1:D:922:LEU:HD12	2.00	0.43
1:D:2544:THR:HG22	1:D:2546:MET:H	1.84	0.43
1:D:2742:THR:HG22	1:D:2742:THR:O	2.18	0.43
1:D:3728:ILE:HG23	1:D:3729:MET:N	2.34	0.43
2:H:27:THR:HG22	2:H:29:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:LEU:HD23	2:H:103:LEU:C	2.44	0.43
1:A:881:LEU:HA	1:A:884:LEU:HB2	2.00	0.43
1:A:1841:VAL:O	1:A:1845:VAL:HG23	2.19	0.43
1:A:2005:GLN:OE1	1:A:3640:PRO:HA	2.19	0.43
1:A:2440:MET:HE2	1:A:2440:MET:HA	2.01	0.43
1:A:3403:ARG:HD3	1:A:3403:ARG:C	2.43	0.43
1:A:3728:ILE:HG23	1:A:3729:MET:N	2.34	0.43
1:C:884:LEU:HA	1:C:887:ILE:HG22	2.00	0.43
1:D:1637:MET:HE2	1:D:1637:MET:HB3	1.93	0.43
1:D:2822:THR:O	1:D:2822:THR:HG23	2.18	0.43
1:A:2544:THR:HG22	1:A:2546:MET:H	1.84	0.43
1:B:35:LEU:HD23	1:B:49:LEU:HB3	2.00	0.43
1:B:495:ASN:OD1	1:B:495:ASN:O	2.37	0.43
1:B:2544:THR:HG22	1:B:2546:MET:H	1.84	0.43
1:B:3989:VAL:HG13	1:B:4023:MET:HE3	2.01	0.43
1:C:2742:THR:HG22	1:C:2742:THR:O	2.18	0.43
1:C:4112:LEU:CD2	1:C:4123:ILE:HD11	2.48	0.43
1:C:4631:PHE:CD1	1:C:4631:PHE:C	2.97	0.43
1:D:1747:LEU:HD21	1:D:2041:HIS:CD2	2.54	0.43
1:B:2992:GLU:HA	1:B:2995:ILE:HG22	2.00	0.42
1:C:2014:ASP:O	1:C:2015:GLU:HB3	2.18	0.42
1:C:3613:TYR:O	1:C:3614:LYS:C	2.62	0.42
1:C:4027:LEU:HD21	1:C:4044:MET:SD	2.58	0.42
1:D:361:ALA:O	1:D:362:PRO:C	2.62	0.42
1:D:929:LEU:HD23	1:D:932:LEU:CD1	2.49	0.42
1:D:3858:MET:O	1:D:3859:VAL:HG13	2.19	0.42
2:G:103:LEU:C	2:G:103:LEU:HD23	2.44	0.42
1:B:953:THR:O	1:B:968:ALA:HA	2.19	0.42
1:B:3403:ARG:HD3	1:B:3403:ARG:C	2.44	0.42
1:C:510:GLU:OE1	1:C:510:GLU:N	2.52	0.42
1:C:881:LEU:HA	1:C:884:LEU:HB2	2.00	0.42
1:C:953:THR:O	1:C:968:ALA:HA	2.19	0.42
1:C:2440:MET:HE2	1:C:2440:MET:HA	2.01	0.42
1:C:3226:GLU:O	1:C:3227:ARG:HB2	2.19	0.42
1:D:2992:GLU:HA	1:D:2995:ILE:HG22	2.00	0.42
1:D:4631:PHE:CD1	1:D:4631:PHE:C	2.97	0.42
2:E:103:LEU:C	2:E:103:LEU:HD23	2.44	0.42
2:F:27:THR:HG22	2:F:29:MET:HE3	2.01	0.42
1:A:3842:LEU:CD2	1:A:3875:MET:HE3	2.50	0.42
1:A:4631:PHE:C	1:A:4631:PHE:CD1	2.97	0.42
1:B:510:GLU:OE1	1:B:510:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:ALA:HB2	1:B:922:LEU:HD12	2.00	0.42
1:B:1747:LEU:HD21	1:B:2041:HIS:CD2	2.54	0.42
1:C:787:VAL:HG22	1:C:788:LYS:N	2.34	0.42
1:C:3403:ARG:HD3	1:C:3403:ARG:C	2.44	0.42
1:C:3728:ILE:HG23	1:C:3729:MET:N	2.34	0.42
1:D:2951:ILE:HD12	1:D:2951:ILE:H	1.84	0.42
1:A:2014:ASP:O	1:A:2015:GLU:HB3	2.18	0.42
1:A:2581:SER:O	1:A:2585:THR:HG23	2.20	0.42
1:A:2992:GLU:HA	1:A:2995:ILE:HG22	2.00	0.42
1:A:3989:VAL:HG13	1:A:4023:MET:HE3	2.01	0.42
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	2.00	0.42
1:B:1230:MET:HE2	1:B:1827:ARG:CB	2.48	0.42
1:B:3858:MET:O	1:B:3859:VAL:HG13	2.19	0.42
1:C:2951:ILE:HD12	1:C:2951:ILE:H	1.84	0.42
1:D:3403:ARG:HD3	1:D:3403:ARG:C	2.43	0.42
1:D:3613:TYR:O	1:D:3614:LYS:C	2.62	0.42
1:D:4027:LEU:HD21	1:D:4044:MET:SD	2.58	0.42
1:A:495:ASN:OD1	1:A:495:ASN:O	2.37	0.42
1:A:787:VAL:HG22	1:A:788:LYS:N	2.34	0.42
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.34	0.42
1:B:361:ALA:O	1:B:362:PRO:C	2.62	0.42
1:B:1931:LEU:N	1:B:1931:LEU:HD12	2.35	0.42
1:B:3728:ILE:HG23	1:B:3729:MET:N	2.34	0.42
1:B:4059:LEU:HD13	1:B:4167:ALA:HB2	2.00	0.42
1:C:1841:VAL:O	1:C:1845:VAL:HG23	2.19	0.42
1:D:1841:VAL:O	1:D:1845:VAL:HG23	2.19	0.42
1:D:3346:VAL:O	1:D:3346:VAL:HG22	2.20	0.42
1:A:35:LEU:HD23	1:A:49:LEU:HB3	2.01	0.42
1:B:929:LEU:HD23	1:B:932:LEU:CD1	2.49	0.42
1:B:3346:VAL:O	1:B:3346:VAL:HG22	2.20	0.42
1:C:1747:LEU:HD21	1:C:2041:HIS:CD2	2.54	0.42
1:C:3346:VAL:HG22	1:C:3346:VAL:O	2.20	0.42
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.37	0.42
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	2.00	0.42
1:D:495:ASN:OD1	1:D:495:ASN:O	2.37	0.42
1:D:3226:GLU:O	1:D:3227:ARG:HB2	2.19	0.42
2:F:103:LEU:C	2:F:103:LEU:HD23	2.44	0.42
1:A:642:THR:HG22	1:A:643:SER:N	2.34	0.42
1:A:929:LEU:HD23	1:A:932:LEU:CD1	2.49	0.42
1:B:21:VAL:HG12	1:B:65:CYS:O	2.20	0.42
1:B:2698:MET:HE3	1:B:2698:MET:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:THR:HG22	1:C:643:SER:N	2.34	0.42
1:C:1931:LEU:HD12	1:C:1931:LEU:N	2.35	0.42
1:A:510:GLU:OE1	1:A:510:GLU:N	2.52	0.42
1:B:2581:SER:O	1:B:2585:THR:HG23	2.20	0.42
1:B:3409:TYR:N	1:B:3410:PRO:HD2	2.34	0.42
1:B:3613:TYR:O	1:B:3614:LYS:C	2.62	0.42
1:C:35:LEU:HD23	1:C:49:LEU:HB3	2.01	0.42
1:C:495:ASN:OD1	1:C:495:ASN:O	2.37	0.42
1:C:2544:THR:HG22	1:C:2546:MET:H	1.84	0.42
1:D:2581:SER:O	1:D:2585:THR:HG23	2.20	0.42
2:E:27:THR:HG22	2:E:29:MET:HE3	2.01	0.42
1:A:655:GLY:C	1:A:852:VAL:HG22	2.45	0.42
1:B:874:LEU:HD12	1:B:1046:LEU:HG	2.02	0.42
1:B:2951:ILE:HD12	1:B:2951:ILE:H	1.84	0.42
1:C:3858:MET:O	1:C:3859:VAL:HG13	2.19	0.42
1:D:35:LEU:HD23	1:D:49:LEU:HB3	2.00	0.42
1:D:510:GLU:OE1	1:D:510:GLU:N	2.52	0.42
1:D:4659:ILE:HG23	1:D:4660:GLY:N	2.35	0.42
1:B:1841:VAL:O	1:B:1845:VAL:HG23	2.19	0.42
1:B:2440:MET:HE2	1:B:2440:MET:HA	2.01	0.42
1:C:21:VAL:HG12	1:C:65:CYS:O	2.20	0.42
1:C:361:ALA:O	1:C:362:PRO:C	2.62	0.42
1:C:929:LEU:HD23	1:C:932:LEU:CD1	2.49	0.42
1:D:2823:ILE:O	1:D:2823:ILE:HG23	2.20	0.42
1:D:3842:LEU:CD2	1:D:3875:MET:HE3	2.50	0.42
1:A:3346:VAL:O	1:A:3346:VAL:HG22	2.20	0.41
1:A:3858:MET:O	1:A:3859:VAL:HG13	2.19	0.41
1:B:655:GLY:C	1:B:852:VAL:HG22	2.45	0.41
1:B:3157:ILE:HG22	1:B:3162:GLN:CG	2.50	0.41
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.37	0.41
1:D:2005:GLN:OE1	1:D:3640:PRO:HA	2.19	0.41
1:D:2440:MET:HE2	1:D:2440:MET:HA	2.01	0.41
2:H:100:ASP:OD1	2:H:100:ASP:O	2.38	0.41
1:A:874:LEU:HD12	1:A:1046:LEU:HG	2.02	0.41
1:B:2009:LEU:HD12	1:B:2023:LEU:HD21	2.02	0.41
1:D:1931:LEU:HD12	1:D:1931:LEU:N	2.35	0.41
1:B:622:THR:O	1:B:622:THR:HG22	2.21	0.41
1:B:1603:VAL:HG12	1:B:1604:SER:N	2.36	0.41
1:B:4659:ILE:HG23	1:B:4660:GLY:N	2.35	0.41
1:C:180:LEU:HD23	1:C:200:TRP:CZ2	2.55	0.41
1:C:1603:VAL:HG12	1:C:1604:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2581:SER:O	1:C:2585:THR:HG23	2.20	0.41
1:D:180:LEU:HD23	1:D:200:TRP:CZ2	2.56	0.41
1:A:2009:LEU:HD12	1:A:2023:LEU:HD21	2.02	0.41
1:B:4112:LEU:HD23	1:B:4123:ILE:HD11	2.02	0.41
1:C:655:GLY:C	1:C:852:VAL:HG22	2.45	0.41
1:C:2005:GLN:OE1	1:C:3640:PRO:HA	2.19	0.41
1:C:2607:LEU:C	1:C:2607:LEU:HD23	2.46	0.41
2:E:100:ASP:OD1	2:E:100:ASP:O	2.39	0.41
2:F:66:MET:HE1	2:F:72:ALA:HB2	2.03	0.41
2:G:66:MET:HE1	2:G:72:ALA:HB2	2.03	0.41
1:A:622:THR:HG22	1:A:622:THR:O	2.21	0.41
1:A:1819:VAL:HG22	1:A:1926:LEU:HD21	2.02	0.41
1:A:1931:LEU:HD12	1:A:1931:LEU:N	2.35	0.41
1:B:1637:MET:HE2	1:B:1637:MET:HB3	1.94	0.41
1:B:3842:LEU:CD2	1:B:3875:MET:HE3	2.50	0.41
1:D:21:VAL:HG12	1:D:65:CYS:O	2.20	0.41
1:D:292:ALA:HB1	1:D:311:ALA:O	2.21	0.41
1:D:759:ILE:C	1:D:760:ASN:OD1	2.64	0.41
1:D:2321:ILE:HD11	1:D:2418:LEU:HD12	2.02	0.41
1:B:759:ILE:C	1:B:760:ASN:OD1	2.64	0.41
1:B:1927:LEU:HD22	1:B:2101:MET:SD	2.61	0.41
1:B:3768:SER:HA	1:B:3771:HIS:NE2	2.36	0.41
1:C:1698:LEU:HD22	1:C:1712:TYR:CZ	2.56	0.41
1:C:3842:LEU:CD2	1:C:3875:MET:HE3	2.50	0.41
1:D:622:THR:O	1:D:622:THR:HG22	2.21	0.41
1:D:655:GLY:C	1:D:852:VAL:HG22	2.45	0.41
1:D:3157:ILE:HG22	1:D:3162:GLN:CG	2.50	0.41
1:A:1698:LEU:HD22	1:A:1712:TYR:CZ	2.56	0.41
1:A:4659:ILE:HG23	1:A:4660:GLY:N	2.35	0.41
1:C:2368:LEU:HD21	1:C:2376:LEU:HD23	2.03	0.41
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	2.01	0.41
1:D:4112:LEU:HD23	1:D:4123:ILE:HD11	2.02	0.41
2:E:17:LYS:HE2	2:E:17:LYS:HA	2.03	0.41
1:A:21:VAL:HG12	1:A:65:CYS:O	2.20	0.41
1:A:1683:HIS:CG	1:A:1797:ARG:HH11	2.39	0.41
1:A:3768:SER:HA	1:A:3771:HIS:NE2	2.36	0.41
1:B:2607:LEU:HD23	1:B:2607:LEU:C	2.46	0.41
1:B:2823:ILE:O	1:B:2823:ILE:HG23	2.20	0.41
1:C:622:THR:O	1:C:622:THR:HG22	2.21	0.41
1:C:2321:ILE:HD11	1:C:2418:LEU:HD12	2.02	0.41
1:C:2971:GLN:NE2	1:C:3045:LYS:HE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4659:ILE:HG23	1:C:4660:GLY:N	2.35	0.41
1:D:1683:HIS:CG	1:D:1797:ARG:HH11	2.39	0.41
1:D:1819:VAL:HG22	1:D:1926:LEU:HD21	2.02	0.41
1:D:2368:LEU:HD21	1:D:2376:LEU:HD23	2.03	0.41
2:E:66:MET:HE1	2:E:72:ALA:HB2	2.03	0.41
1:A:1927:LEU:HD22	1:A:2101:MET:SD	2.61	0.41
1:A:2607:LEU:HD23	1:A:2607:LEU:C	2.46	0.41
1:A:2644:LEU:CD2	1:A:2678:LEU:HD21	2.51	0.41
1:A:2823:ILE:HG23	1:A:2823:ILE:O	2.20	0.41
1:A:3157:ILE:HG22	1:A:3162:GLN:CG	2.50	0.41
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.37	0.41
1:B:3050:VAL:HG22	1:B:3050:VAL:O	2.21	0.41
1:C:1683:HIS:CG	1:C:1797:ARG:HH11	2.38	0.41
1:C:1819:VAL:HG22	1:C:1926:LEU:HD21	2.02	0.41
1:C:1997:GLU:HG3	1:C:2008:MET:CE	2.51	0.41
1:C:2009:LEU:HD12	1:C:2023:LEU:HD21	2.02	0.41
1:C:3050:VAL:HG22	1:C:3050:VAL:O	2.21	0.41
1:C:3157:ILE:HG22	1:C:3162:GLN:CG	2.50	0.41
1:C:3768:SER:HA	1:C:3771:HIS:NE2	2.36	0.41
1:D:2009:LEU:HD12	1:D:2023:LEU:HD21	2.02	0.41
1:D:2146:PRO:O	1:D:2149:VAL:HG23	2.21	0.41
1:D:3768:SER:HA	1:D:3771:HIS:NE2	2.36	0.41
1:A:361:ALA:O	1:A:362:PRO:C	2.62	0.41
1:A:759:ILE:C	1:A:760:ASN:OD1	2.64	0.41
1:B:829:TYR:CD1	1:B:829:TYR:C	2.99	0.41
1:B:2128:TYR:HB2	1:B:3673:MET:HE1	2.03	0.41
1:B:4207:MET:HA	1:B:4207:MET:HE3	2.03	0.41
1:C:2644:LEU:CD2	1:C:2678:LEU:HD21	2.51	0.41
1:D:978:THR:HB	1:D:979:PRO:HD2	2.04	0.41
1:D:1698:LEU:HD22	1:D:1712:TYR:CZ	2.56	0.41
1:D:2607:LEU:C	1:D:2607:LEU:HD23	2.46	0.41
2:F:17:LYS:HE2	2:F:17:LYS:HA	2.03	0.41
2:H:17:LYS:HA	2:H:17:LYS:HE2	2.03	0.41
1:A:292:ALA:HB1	1:A:311:ALA:O	2.21	0.40
1:A:2368:LEU:HD21	1:A:2376:LEU:HD23	2.03	0.40
1:D:3050:VAL:HG22	1:D:3050:VAL:O	2.21	0.40
2:G:100:ASP:OD1	2:G:100:ASP:C	2.65	0.40
2:H:66:MET:HE1	2:H:72:ALA:HB2	2.02	0.40
1:A:180:LEU:HD23	1:A:200:TRP:CZ2	2.55	0.40
1:A:978:THR:HB	1:A:979:PRO:HD2	2.04	0.40
1:A:1603:VAL:HG12	1:A:1604:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2128:TYR:HB2	1:A:3673:MET:HE1	2.03	0.40
1:A:3050:VAL:HG22	1:A:3054:VAL:CG1	2.51	0.40
1:A:4071:ILE:HD11	1:A:4102:GLN:HG3	2.03	0.40
1:B:180:LEU:HD23	1:B:200:TRP:CZ2	2.55	0.40
1:B:1679:ASN:O	1:B:1682:ALA:HB3	2.22	0.40
1:B:1698:LEU:HD22	1:B:1712:TYR:CZ	2.56	0.40
1:C:2298:VAL:HG13	1:C:2299:VAL:N	2.36	0.40
1:D:3050:VAL:HG22	1:D:3054:VAL:CG1	2.51	0.40
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.37	0.40
1:D:4020:GLN:O	1:D:4024:VAL:HG23	2.21	0.40
1:A:2146:PRO:O	1:A:2149:VAL:HG23	2.21	0.40
1:A:2971:GLN:NE2	1:A:3045:LYS:HE2	2.36	0.40
1:A:3955:MET:HE1	1:A:4016:LEU:HA	2.04	0.40
1:A:4731:ILE:O	1:A:4731:ILE:HG22	2.21	0.40
1:B:1683:HIS:CG	1:B:1797:ARG:HH11	2.38	0.40
1:C:292:ALA:HB1	1:C:311:ALA:O	2.21	0.40
1:C:759:ILE:C	1:C:760:ASN:OD1	2.64	0.40
1:C:829:TYR:CD1	1:C:829:TYR:C	2.99	0.40
1:C:867:LEU:HA	1:C:870:ILE:HG22	2.04	0.40
1:C:1851:MET:HE3	1:C:1851:MET:HB3	1.96	0.40
1:C:3829:PHE:CZ	1:C:3906:GLN:NE2	2.90	0.40
1:C:4112:LEU:HD23	1:C:4123:ILE:HD11	2.02	0.40
1:D:874:LEU:HD12	1:D:1046:LEU:HG	2.02	0.40
2:F:100:ASP:OD1	2:F:100:ASP:C	2.65	0.40
2:G:100:ASP:OD1	2:G:100:ASP:O	2.39	0.40
1:A:1473:THR:HG23	1:A:1487:LEU:O	2.22	0.40
1:A:2747:ILE:O	1:A:2747:ILE:HG23	2.22	0.40
1:A:3160:ASP:O	1:A:3163:VAL:HG12	2.22	0.40
1:B:1473:THR:HG23	1:B:1487:LEU:O	2.21	0.40
1:B:2321:ILE:HD11	1:B:2418:LEU:HD12	2.02	0.40
1:B:2368:LEU:HD21	1:B:2376:LEU:HD23	2.03	0.40
1:B:2971:GLN:NE2	1:B:3045:LYS:HE2	2.36	0.40
1:B:3357:HIS:O	1:B:3361:THR:HG22	2.22	0.40
1:B:3829:PHE:CZ	1:B:3906:GLN:NE2	2.89	0.40
1:C:874:LEU:HD12	1:C:1046:LEU:HG	2.02	0.40
1:C:2146:PRO:O	1:C:2149:VAL:HG23	2.21	0.40
1:C:2747:ILE:O	1:C:2747:ILE:HG23	2.22	0.40
1:D:4207:MET:HE3	1:D:4207:MET:HA	2.03	0.40
2:E:100:ASP:OD1	2:E:100:ASP:C	2.65	0.40
2:F:100:ASP:OD1	2:F:100:ASP:O	2.39	0.40
1:A:2298:VAL:HG13	1:A:2299:VAL:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2321:ILE:HD11	1:A:2418:LEU:HD12	2.03	0.40
1:A:3050:VAL:HG22	1:A:3050:VAL:O	2.21	0.40
1:A:4231:MET:HE1	1:A:5022:PHE:CD2	2.57	0.40
1:B:292:ALA:HB1	1:B:311:ALA:O	2.21	0.40
1:B:1435:TYR:HB3	1:B:1575:LEU:HD13	2.04	0.40
1:B:1997:GLU:HG3	1:B:2008:MET:CE	2.51	0.40
1:C:1607:ARG:HH22	1:C:1651:LEU:HD12	1.87	0.40
1:C:2823:ILE:O	1:C:2823:ILE:HG23	2.20	0.40
1:C:4020:GLN:O	1:C:4024:VAL:HG23	2.21	0.40
1:D:349:GLN:NE2	1:D:356:TRP:CZ2	2.90	0.40
1:D:1603:VAL:HG12	1:D:1604:SER:N	2.36	0.40
1:D:1679:ASN:O	1:D:1682:ALA:HB3	2.22	0.40
1:D:1927:LEU:HD22	1:D:2101:MET:SD	2.61	0.40
1:D:2298:VAL:HG13	1:D:2299:VAL:N	2.36	0.40
1:D:3829:PHE:CZ	1:D:3906:GLN:NE2	2.89	0.40
1:D:4175:ARG:N	1:D:4176:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4376/5037 (87%)	4160 (95%)	213 (5%)	3 (0%)	48	83
1	B	4376/5037 (87%)	4157 (95%)	216 (5%)	3 (0%)	48	83
1	C	4376/5037 (87%)	4157 (95%)	216 (5%)	3 (0%)	48	83
1	D	4376/5037 (87%)	4158 (95%)	215 (5%)	3 (0%)	48	83
2	E	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	G	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
All	All	17924/20580 (87%)	17016 (95%)	896 (5%)	12 (0%)	49	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3623	LEU
1	A	4134	GLU
1	B	3623	LEU
1	B	4134	GLU
1	C	3623	LEU
1	C	4134	GLU
1	D	3623	LEU
1	D	4134	GLU
1	A	309	THR
1	B	309	THR
1	C	309	THR
1	D	309	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3827/4276 (90%)	3827 (100%)	0	100	100
1	B	3827/4276 (90%)	3827 (100%)	0	100	100
1	C	3827/4276 (90%)	3827 (100%)	0	100	100
1	D	3827/4276 (90%)	3827 (100%)	0	100	100
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15664/17464 (90%)	15664 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	113	HIS
1	A	399	GLN
1	A	678	GLN
1	A	681	HIS
1	A	812	HIS
1	A	879	HIS
1	A	921	ASN
1	A	963	ASN
1	A	1220	GLN
1	A	1299	GLN
1	A	1541	GLN
1	A	1545	ASN
1	A	1825	HIS
1	A	1970	GLN
1	A	2417	HIS
1	A	2441	HIS
1	A	3013	HIS
1	A	3150	HIS
1	A	3268	HIS
1	A	3611	HIS
1	A	3667	HIS
1	A	3895	HIS
1	A	3946	GLN
1	A	3960	GLN
1	A	4133	GLN
1	A	4812	HIS
1	A	5003	HIS
1	B	98	HIS
1	B	113	HIS
1	B	678	GLN
1	B	681	HIS
1	B	812	HIS
1	B	879	HIS
1	B	921	ASN
1	B	963	ASN
1	B	1220	GLN
1	B	1299	GLN
1	B	1458	HIS

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Mol	Chain	Res	Type
1	B	1541	GLN
1	B	1545	ASN
1	B	2417	HIS
1	B	2441	HIS
1	B	3013	HIS
1	B	3150	HIS
1	B	3268	HIS
1	B	3611	HIS
1	B	3667	HIS
1	B	3895	HIS
1	B	3960	GLN
1	B	3998	HIS
1	B	4133	GLN
1	B	4803	HIS
1	B	4812	HIS
1	B	5003	HIS
1	C	113	HIS
1	C	610	ASN
1	C	678	GLN
1	C	681	HIS
1	C	812	HIS
1	C	879	HIS
1	C	921	ASN
1	C	1220	GLN
1	C	1299	GLN
1	C	1458	HIS
1	C	1541	GLN
1	C	1545	ASN
1	C	1824	GLN
1	C	1825	HIS
1	C	2417	HIS
1	C	2441	HIS
1	C	2892	GLN
1	C	3013	HIS
1	C	3066	ASN
1	C	3149	GLN
1	C	3150	HIS
1	C	3268	HIS
1	C	3611	HIS
1	C	3667	HIS
1	C	3895	HIS
1	C	3960	GLN

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Mol	Chain	Res	Type
1	C	4133	GLN
1	C	4153	HIS
1	C	4812	HIS
1	C	5003	HIS
1	D	44	ASN
1	D	113	HIS
1	D	383	HIS
1	D	610	ASN
1	D	678	GLN
1	D	681	HIS
1	D	812	HIS
1	D	879	HIS
1	D	921	ASN
1	D	963	ASN
1	D	1220	GLN
1	D	1299	GLN
1	D	1458	HIS
1	D	1541	GLN
1	D	1545	ASN
1	D	1824	GLN
1	D	1825	HIS
1	D	1970	GLN
1	D	2417	HIS
1	D	2441	HIS
1	D	2892	GLN
1	D	3013	HIS
1	D	3150	HIS
1	D	3268	HIS
1	D	3611	HIS
1	D	3667	HIS
1	D	3895	HIS
1	D	3960	GLN
1	D	3998	HIS
1	D	4133	GLN
1	D	4812	HIS
1	D	5003	HIS

5.3.3 RNA ⓘ

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ACP	C	5102	-	30,33,33	1.32	4 (13%)	45,52,52	1.32	7 (15%)
5	ACP	B	5102	-	30,33,33	1.35	4 (13%)	45,52,52	1.31	7 (15%)
6	CFF	C	5104	-	15,15,15	0.80	0	23,23,23	0.87	0
6	CFF	D	5104	-	15,15,15	0.82	0	23,23,23	0.81	0
6	CFF	A	5104	-	15,15,15	0.79	0	23,23,23	0.83	0
5	ACP	A	5103	-	30,33,33	1.32	4 (13%)	45,52,52	1.36	8 (17%)
6	CFF	B	5104	-	15,15,15	0.80	0	23,23,23	0.83	0
5	ACP	D	5103	-	30,33,33	1.33	4 (13%)	45,52,52	1.34	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACP	C	5102	-	-	7/19/38/38	0/3/3/3
5	ACP	B	5102	-	-	6/19/38/38	0/3/3/3
6	CFF	C	5104	-	-	-	0/2/2/2
6	CFF	D	5104	-	-	-	0/2/2/2
6	CFF	A	5104	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACP	A	5103	-	-	6/19/38/38	0/3/3/3
6	CFF	B	5104	-	-	-	0/2/2/2
5	ACP	D	5103	-	-	6/19/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5102	ACP	PB-O2B	-3.28	1.48	1.56
5	C	5102	ACP	PB-O2B	-3.27	1.48	1.56
5	D	5103	ACP	PB-O2B	-3.25	1.48	1.56
5	A	5103	ACP	PB-O2B	-3.23	1.48	1.56
5	B	5102	ACP	PG-O3G	-3.13	1.47	1.54
5	C	5102	ACP	PG-O3G	-3.04	1.48	1.54
5	D	5103	ACP	PG-O2G	-3.01	1.48	1.54
5	A	5103	ACP	PG-O2G	-2.90	1.48	1.54
5	B	5102	ACP	PG-O2G	-2.90	1.48	1.54
5	D	5103	ACP	PG-O3G	-2.88	1.48	1.54
5	A	5103	ACP	PG-O3G	-2.86	1.48	1.54
5	C	5102	ACP	PG-O2G	-2.74	1.48	1.54
5	B	5102	ACP	C5-C4	-2.21	1.34	1.39
5	C	5102	ACP	C5-C4	-2.18	1.34	1.39
5	D	5103	ACP	C5-C4	-2.14	1.35	1.39
5	A	5103	ACP	C5-C4	-2.11	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5102	ACP	O3G-PG-C3B	3.41	114.68	106.40
5	B	5102	ACP	O3G-PG-C3B	3.21	114.20	106.40
5	B	5102	ACP	C5-C4-N3	-2.84	123.04	126.75
5	C	5102	ACP	C5-C4-N3	-2.82	123.07	126.75
5	D	5103	ACP	O3G-PG-C3B	2.81	113.21	106.40
5	A	5103	ACP	O3G-PG-C3B	2.81	113.21	106.40
5	A	5103	ACP	C5-C4-N3	-2.78	123.12	126.75
5	A	5103	ACP	C4-C5-N7	2.75	113.97	110.62
5	D	5103	ACP	C4-C5-N7	2.70	113.90	110.62
5	D	5103	ACP	C5-C4-N3	-2.68	123.25	126.75
5	C	5102	ACP	C4-C5-N7	2.63	113.82	110.62
5	B	5102	ACP	C4-C5-N7	2.58	113.76	110.62
5	B	5102	ACP	C5-C6-N1	2.46	122.67	117.39
5	A	5103	ACP	C5-C6-N1	2.45	122.65	117.39
5	C	5102	ACP	C5-C6-N1	2.43	122.60	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5103	ACP	C5-C6-N1	2.39	122.52	117.39
5	B	5102	ACP	PB-O3A-PA	-2.37	125.06	132.56
5	C	5102	ACP	PB-O3A-PA	-2.36	125.08	132.56
5	B	5102	ACP	C2-N1-C6	-2.26	114.88	118.77
5	A	5103	ACP	C2-N1-C6	-2.26	114.89	118.77
5	A	5103	ACP	PB-O3A-PA	-2.22	125.52	132.56
5	D	5103	ACP	PB-O3A-PA	-2.22	125.53	132.56
5	D	5103	ACP	C2-N1-C6	-2.21	114.97	118.77
5	C	5102	ACP	C2-N1-C6	-2.21	114.97	118.77
5	D	5103	ACP	O1G-PG-C3B	-2.20	106.50	111.24
5	C	5102	ACP	O2G-PG-O1G	-2.17	106.66	112.39
5	A	5103	ACP	O2G-PG-O1G	-2.14	106.74	112.39
5	A	5103	ACP	O1G-PG-C3B	-2.07	106.77	111.24
5	D	5103	ACP	O2G-PG-O1G	-2.06	106.94	112.39
5	B	5102	ACP	O2G-PG-O1G	-2.05	106.97	112.39

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5103	ACP	C4'-C5'-O5'-PA
5	B	5102	ACP	PB-C3B-PG-O1G
5	B	5102	ACP	C4'-C5'-O5'-PA
5	C	5102	ACP	PB-C3B-PG-O1G
5	C	5102	ACP	C4'-C5'-O5'-PA
5	D	5103	ACP	C4'-C5'-O5'-PA
5	C	5102	ACP	O4'-C4'-C5'-O5'
5	C	5102	ACP	C3'-C4'-C5'-O5'
5	A	5103	ACP	C3'-C4'-C5'-O5'
5	A	5103	ACP	O4'-C4'-C5'-O5'
5	D	5103	ACP	C3'-C4'-C5'-O5'
5	B	5102	ACP	C3'-C4'-C5'-O5'
5	D	5103	ACP	O4'-C4'-C5'-O5'
5	A	5103	ACP	C5'-O5'-PA-O3A
5	B	5102	ACP	C5'-O5'-PA-O3A
5	C	5102	ACP	C5'-O5'-PA-O3A
5	D	5103	ACP	C5'-O5'-PA-O3A
5	A	5103	ACP	C5'-O5'-PA-O1A
5	A	5103	ACP	C5'-O5'-PA-O2A
5	B	5102	ACP	C5'-O5'-PA-O2A
5	D	5103	ACP	C5'-O5'-PA-O1A
5	D	5103	ACP	C5'-O5'-PA-O2A

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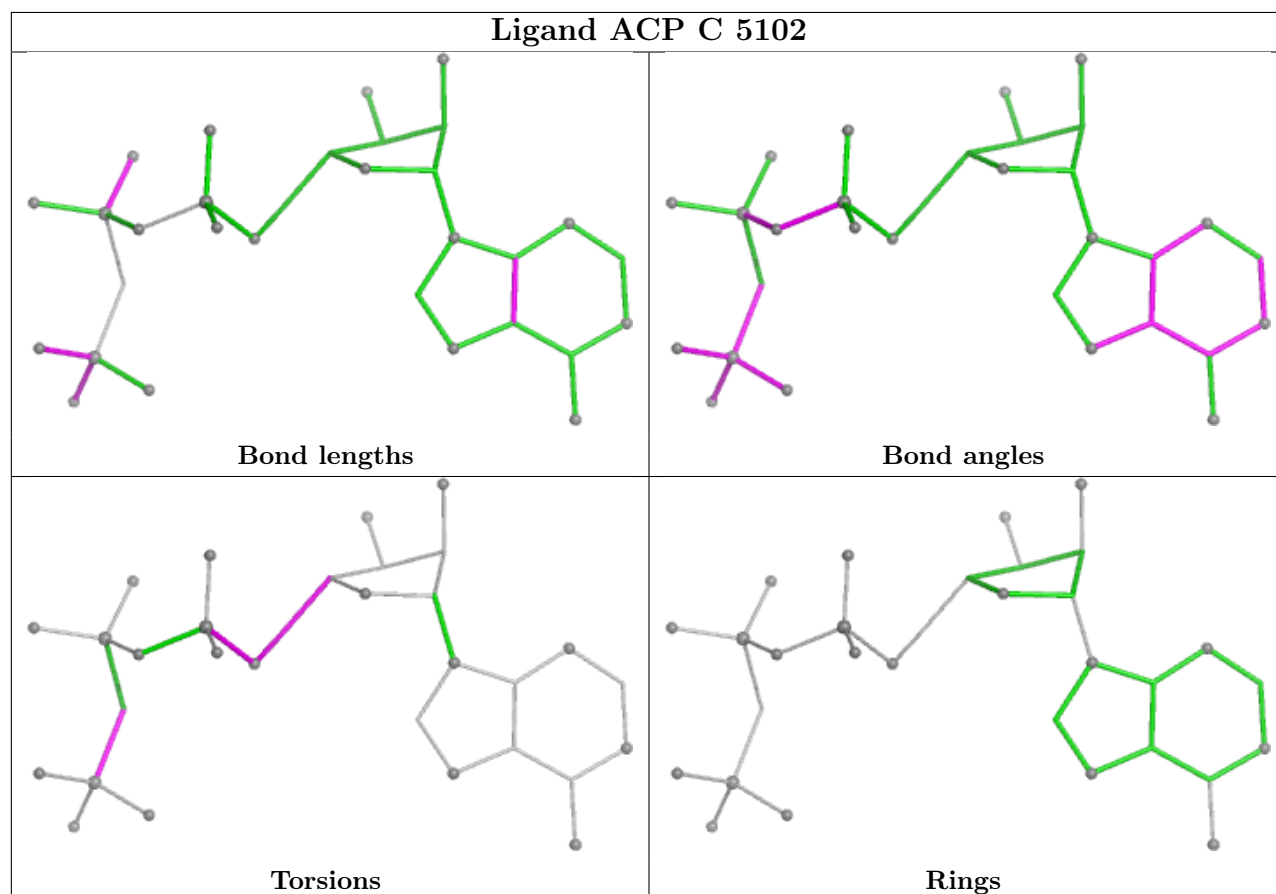
Continued from previous page...

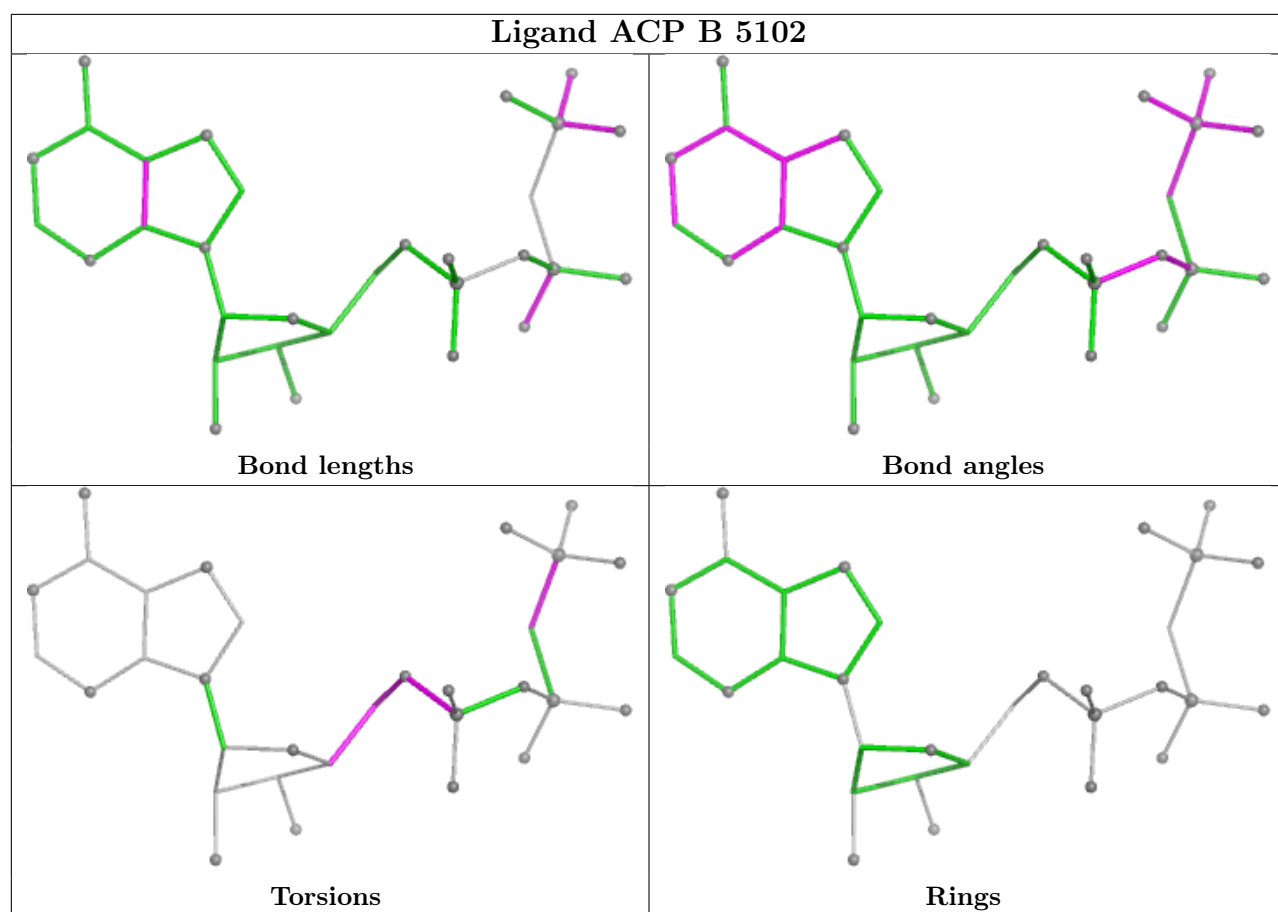
Mol	Chain	Res	Type	Atoms
5	C	5102	ACP	PB-C3B-PG-O2G
5	B	5102	ACP	O4'-C4'-C5'-O5'
5	C	5102	ACP	C5'-O5'-PA-O2A

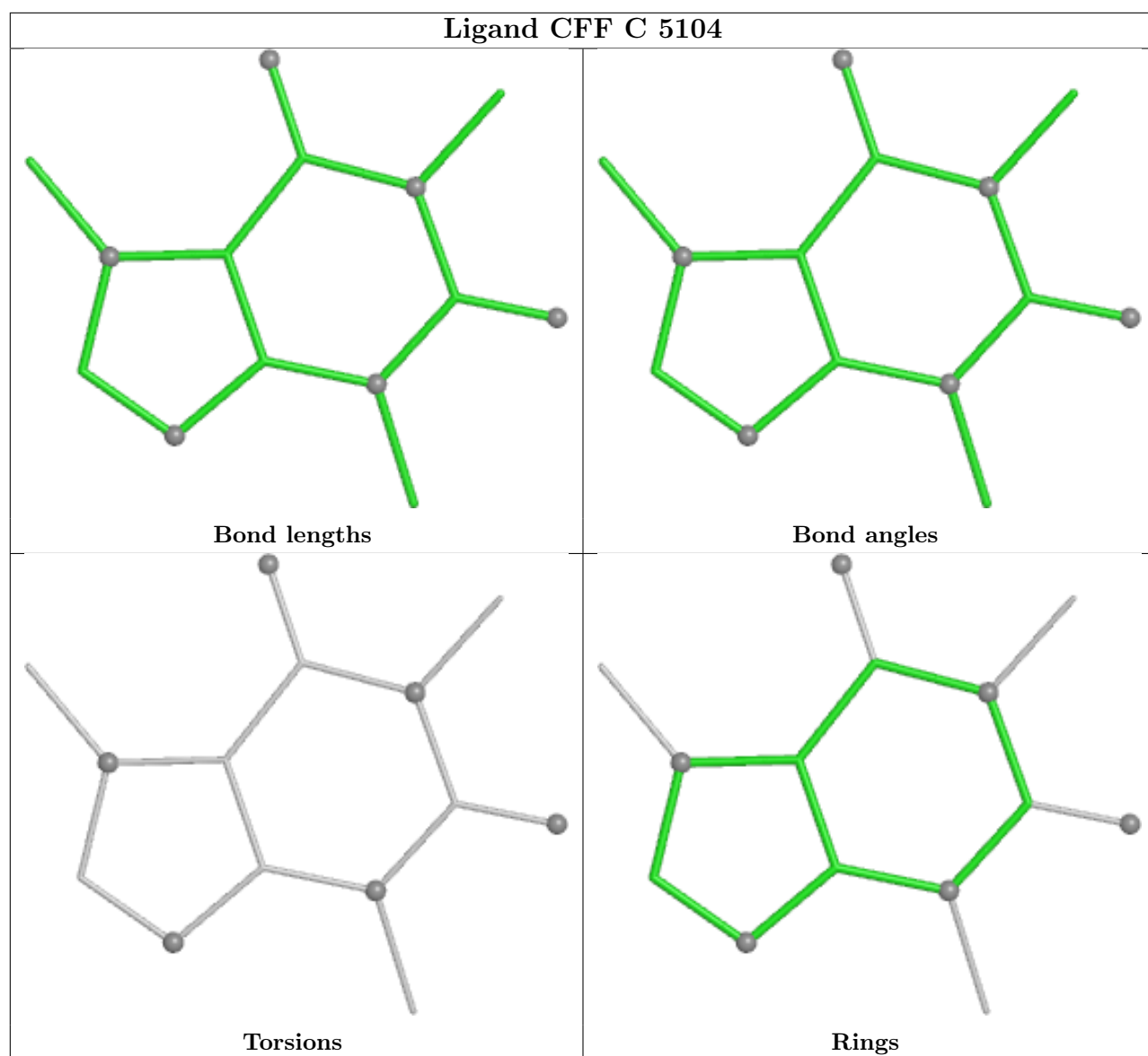
There are no ring outliers.

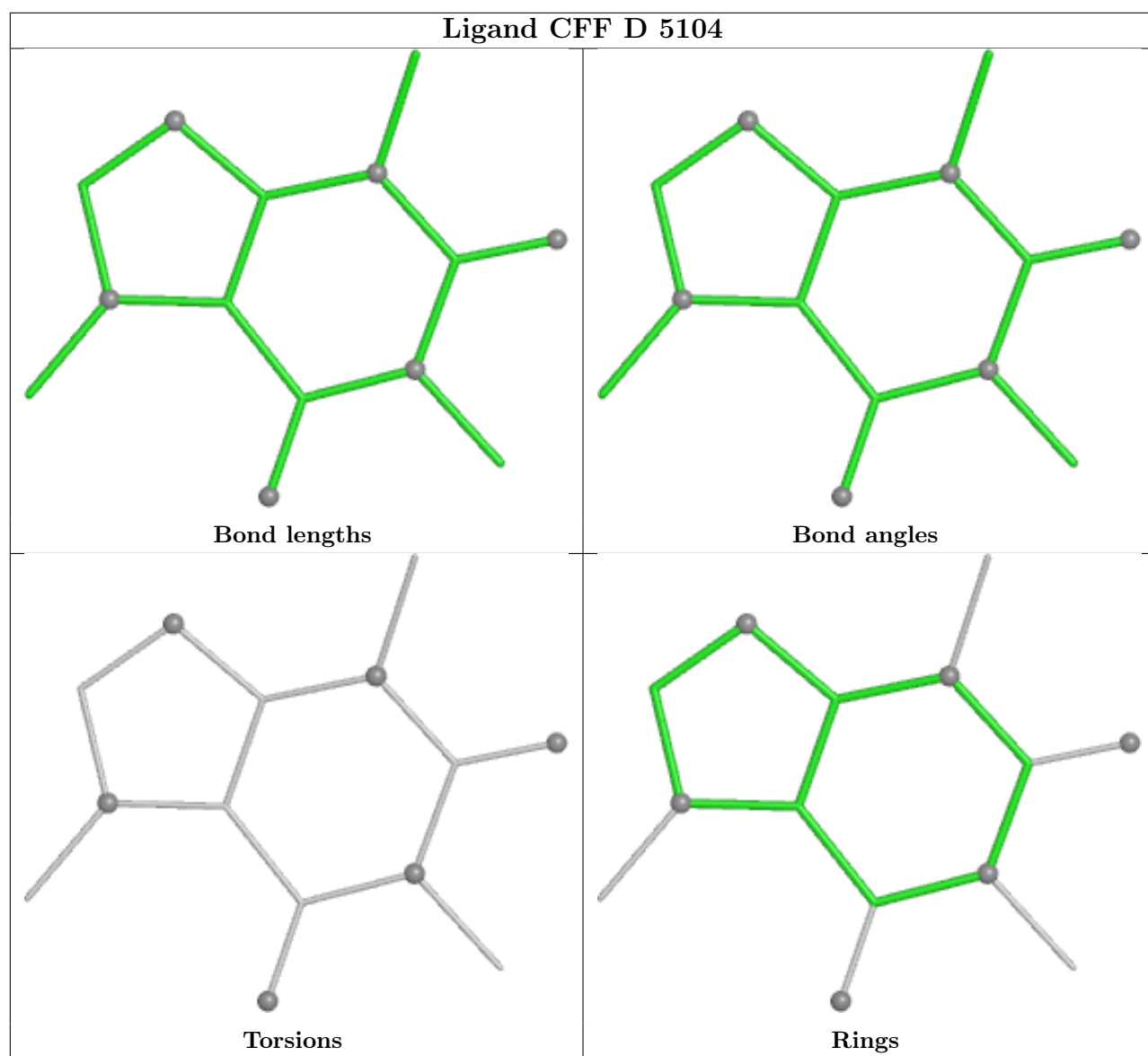
No monomer is involved in short contacts.

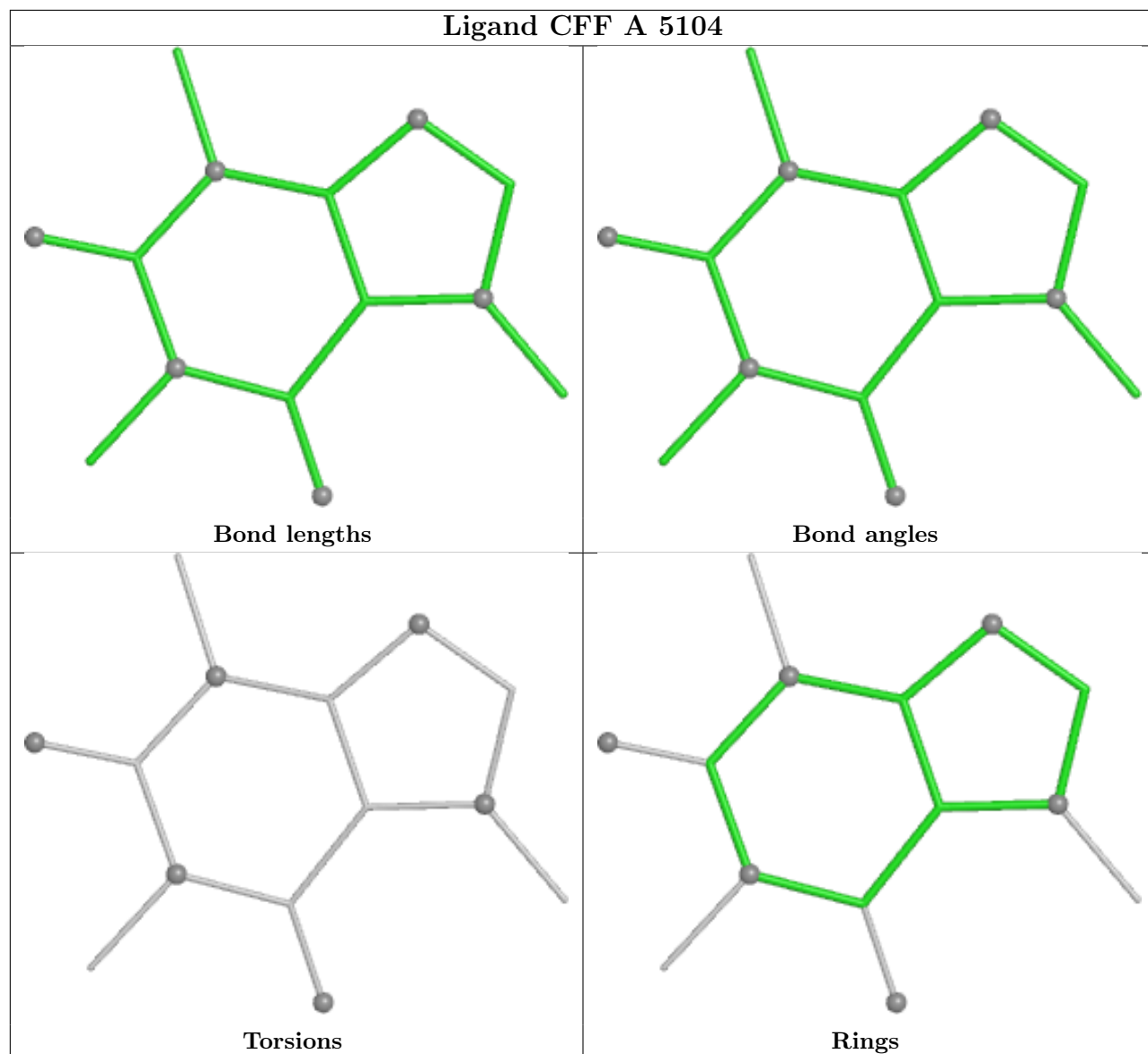
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

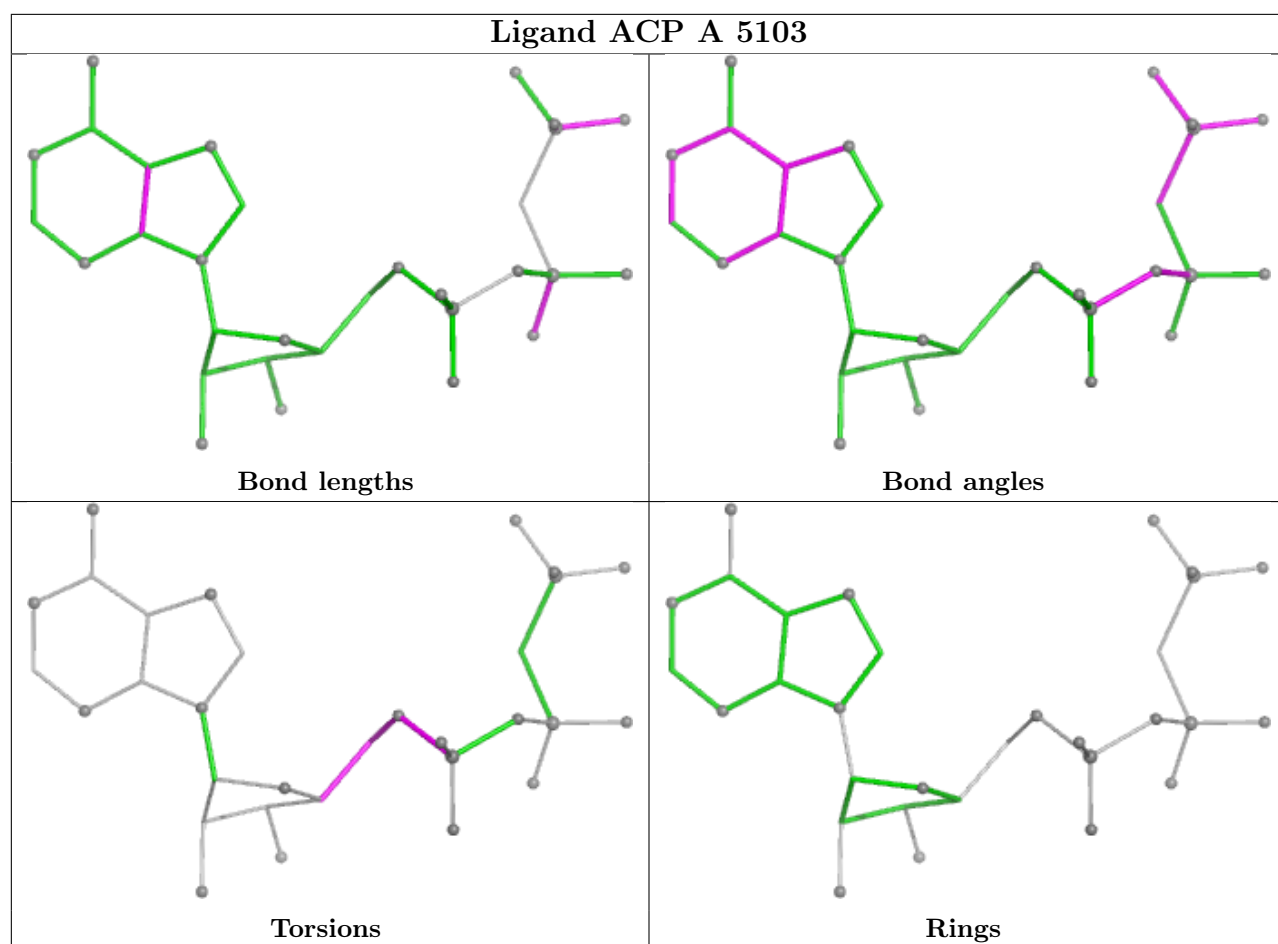


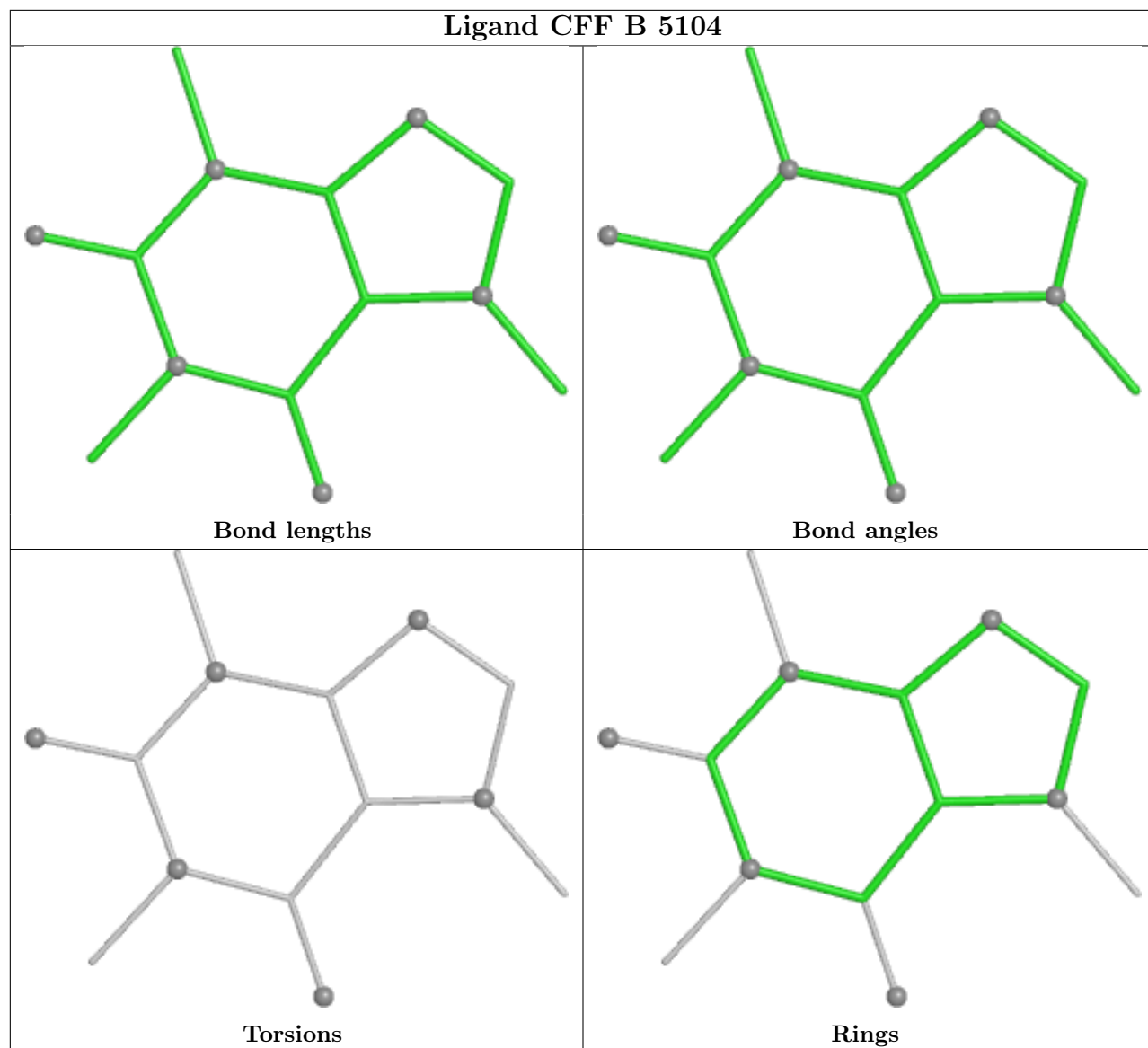


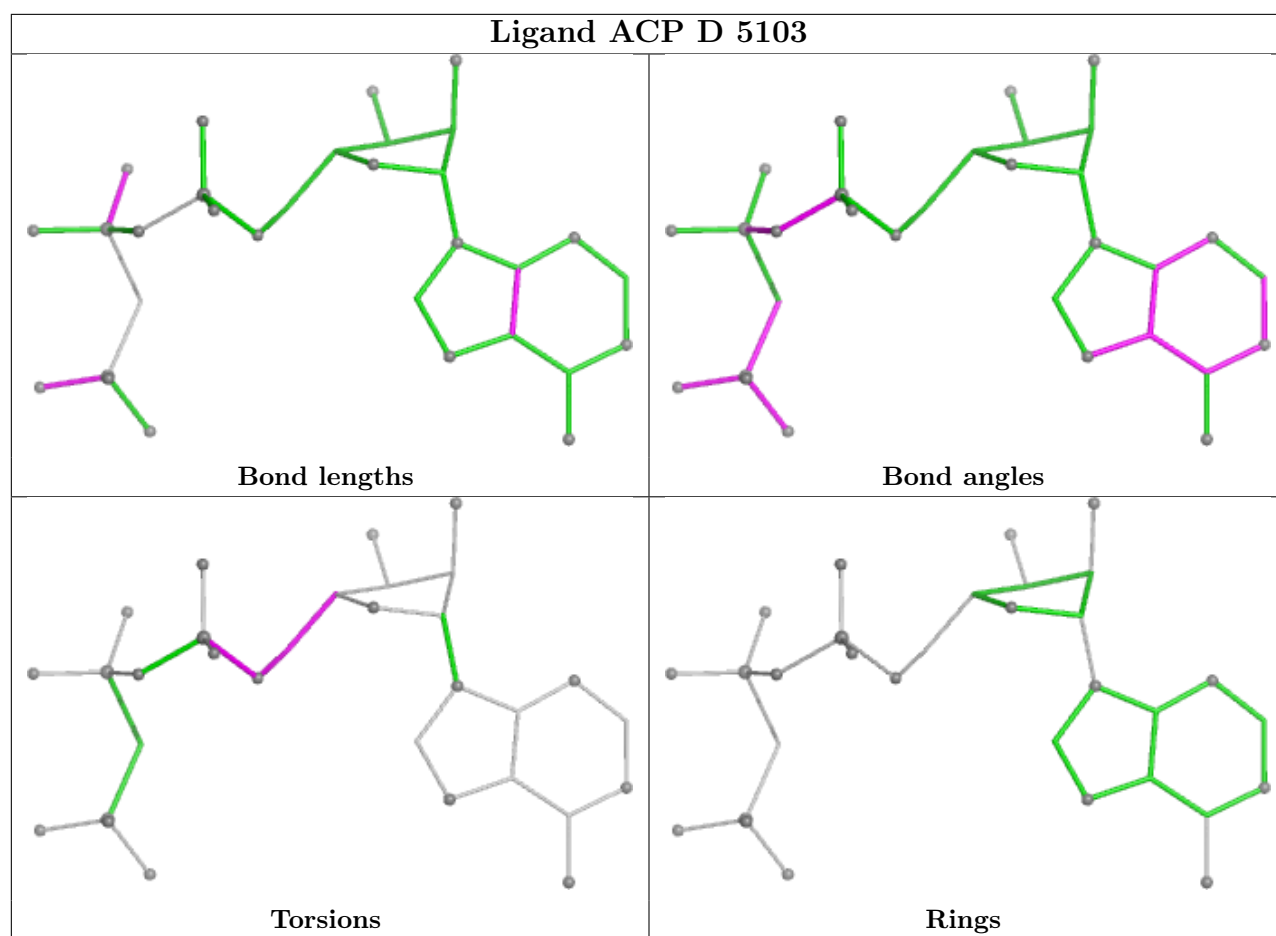












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

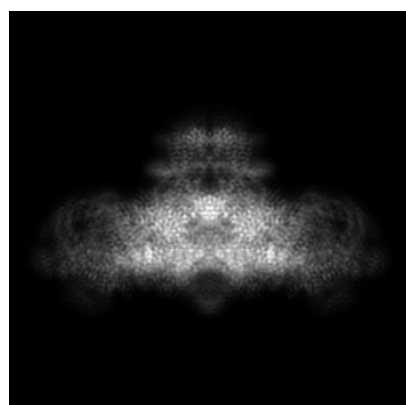
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54617. These allow visual inspection of the internal detail of the map and identification of artifacts.

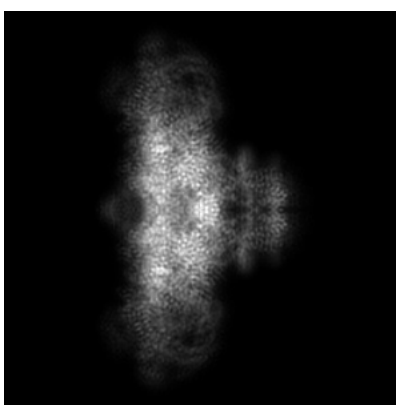
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

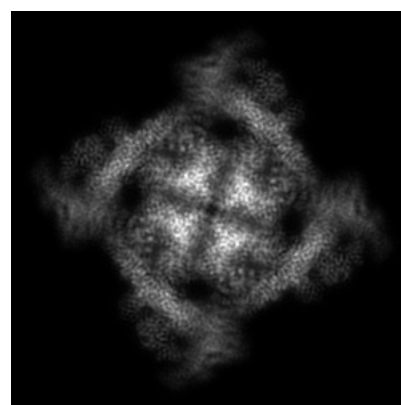
6.1.1 Primary map



X



Y

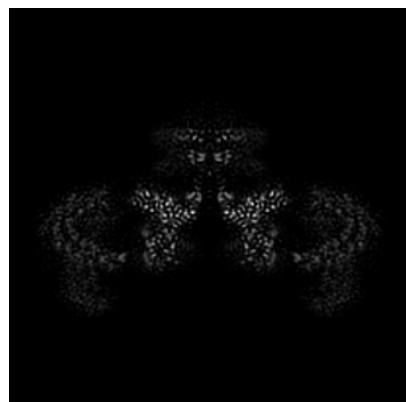


Z

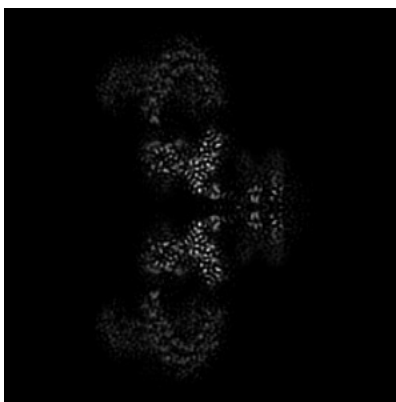
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

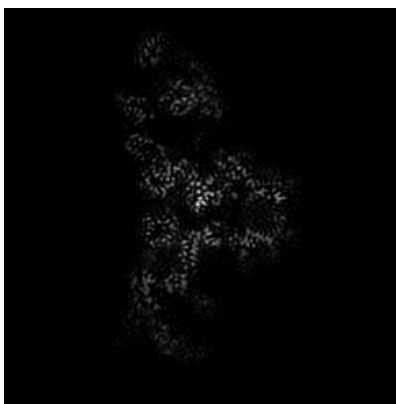
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 131



Y Index: 131

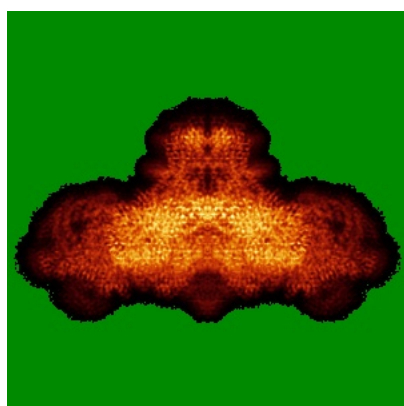


Z Index: 114

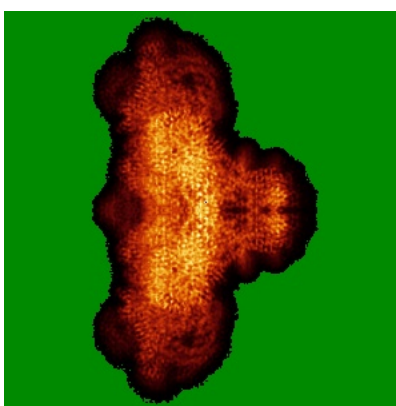
The images above show the largest variance slices of the map in three orthogonal directions.

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

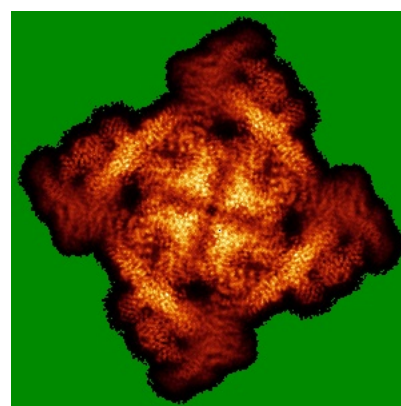
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.567. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

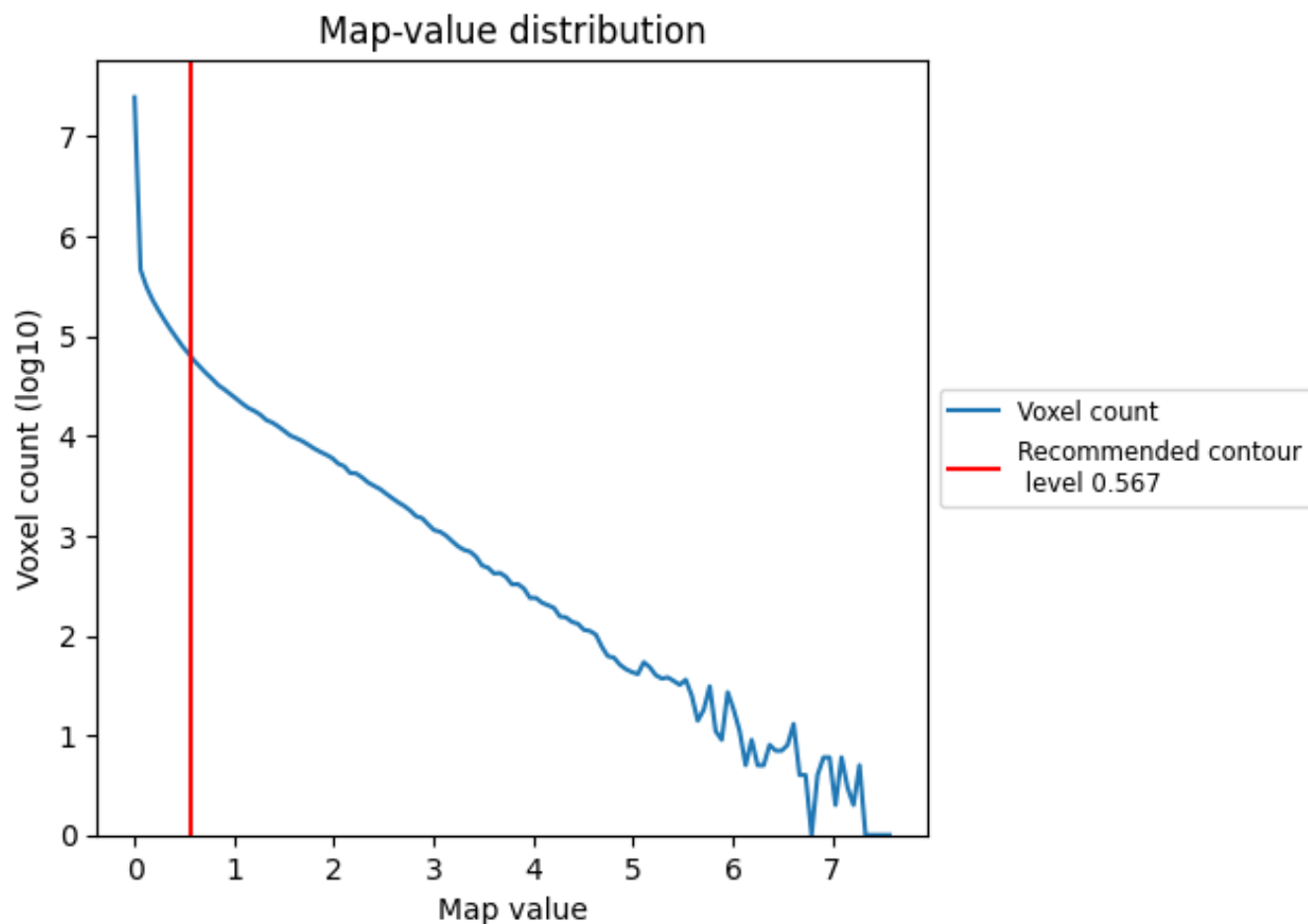
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

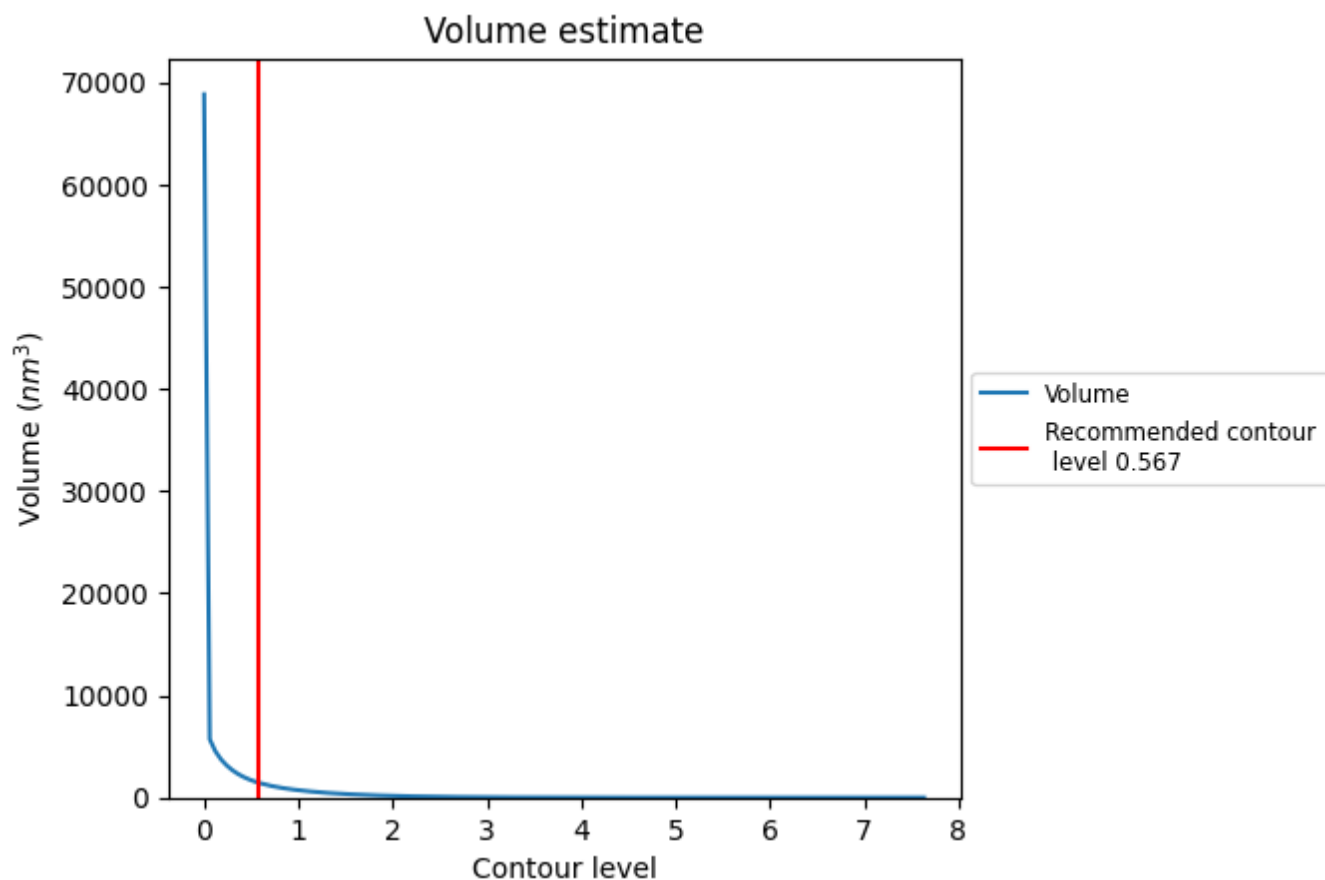
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

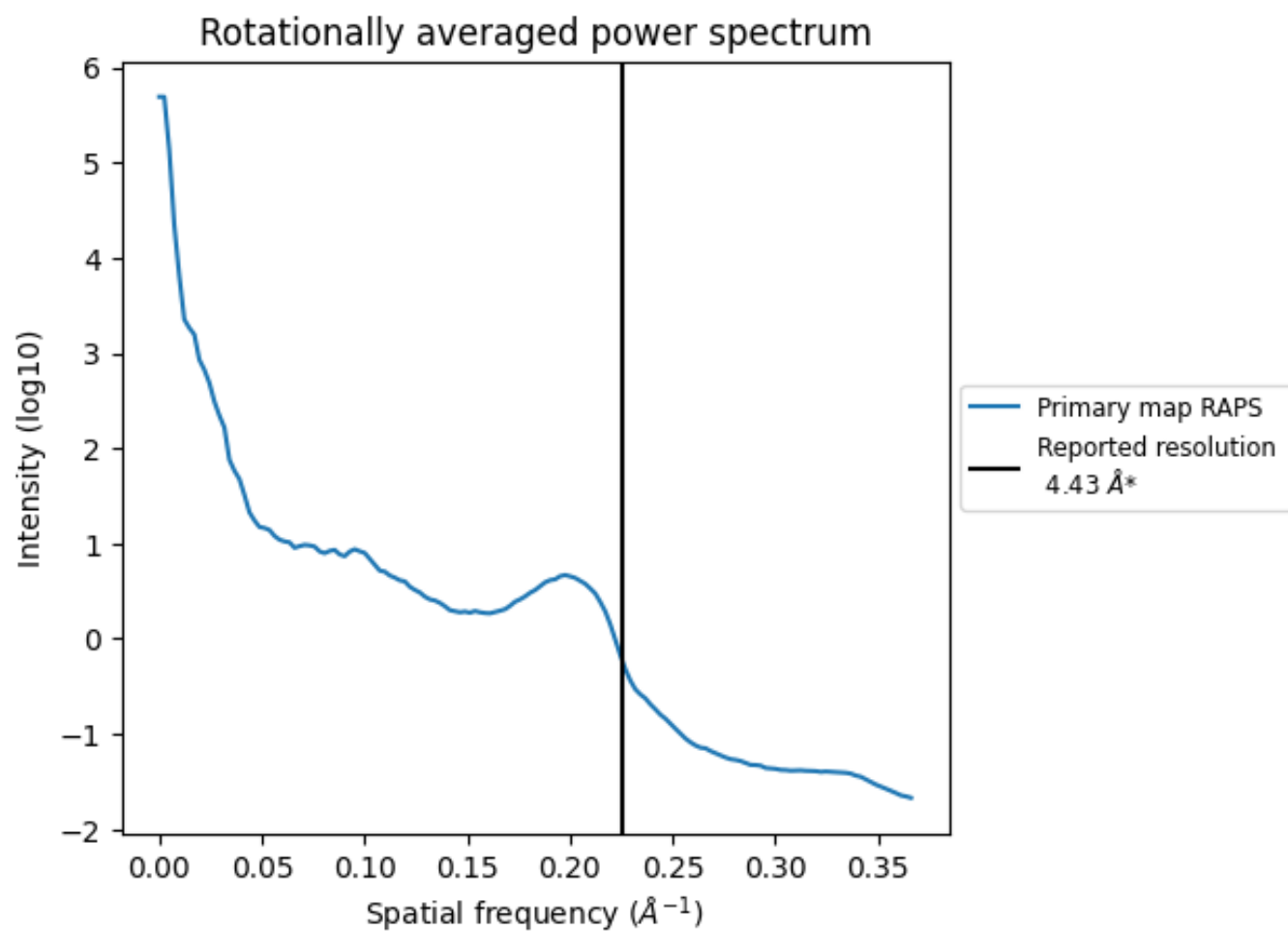
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1487 nm³; this corresponds to an approximate mass of 1343 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 0.226 Å⁻¹

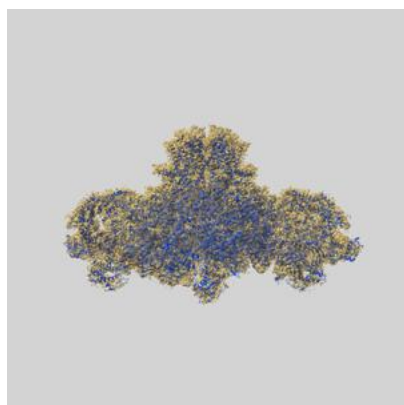
8 Fourier-Shell correlation

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

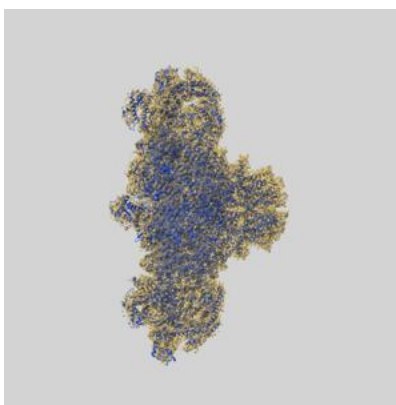
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54617 and PDB model 9S5Z. Per-residue inclusion information can be found in section 3 on page 7.

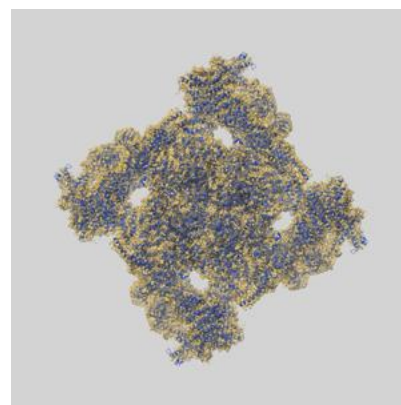
9.1 Map-model overlay [i](#)



X



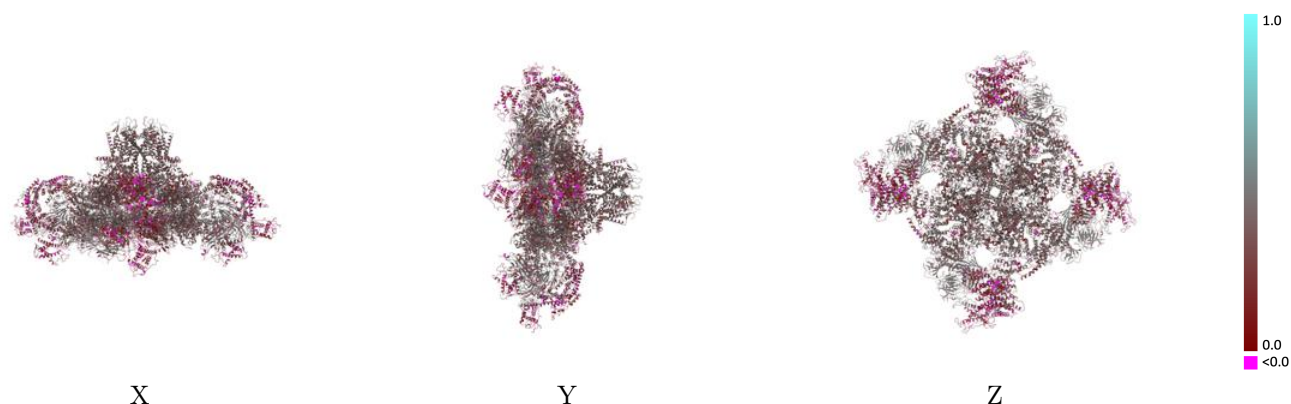
Y



Z

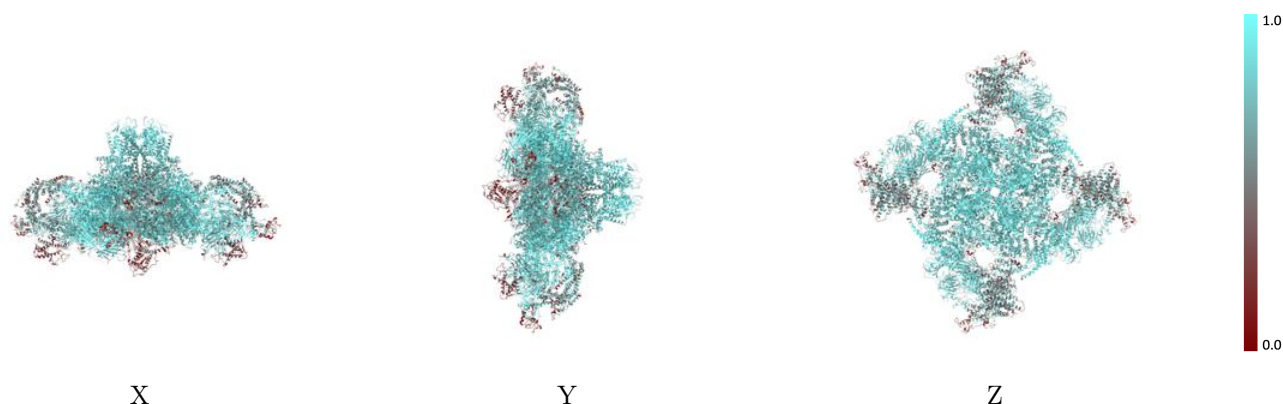
The images above show the 3D surface view of the map at the recommended contour level 0.567 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



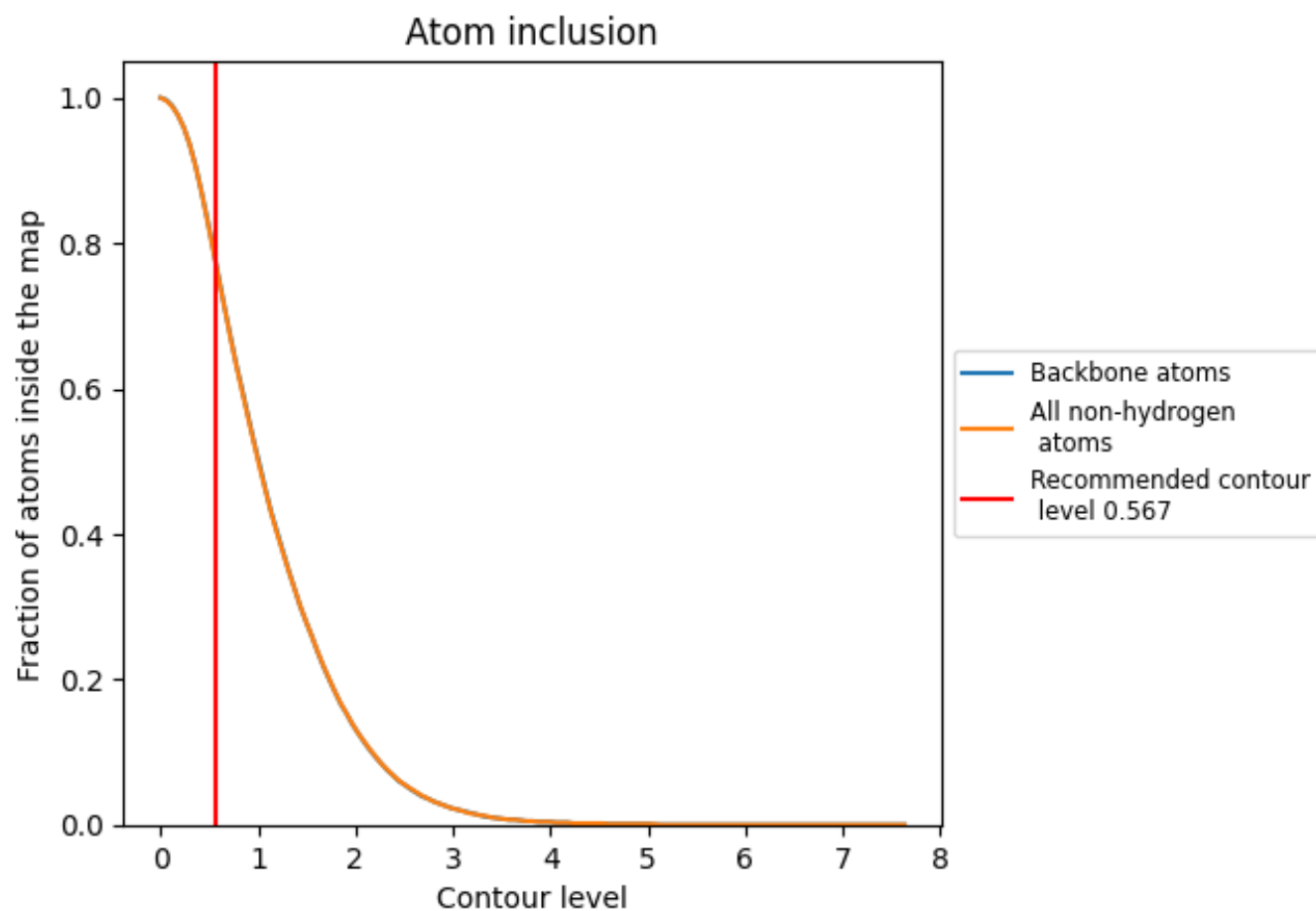
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.567).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (0.567) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.3240
A	0.7730	0.3230
B	0.7730	0.3230
C	0.7720	0.3230
D	0.7730	0.3230
E	0.8350	0.3720
F	0.8360	0.3740
G	0.8350	0.3760
H	0.8320	0.3720

1.0

0.0

<0.0