



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 03:20 pm BST

PDB ID : 9S2S / pdb_00009s2s
EMDB ID : EMD-54509
Title : Primed-state RyR1 with calcium in activating concentration in the native membrane
Authors : Mikirtumov, V.
Deposited on : 2025-07-22
Resolution : 3.80 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:

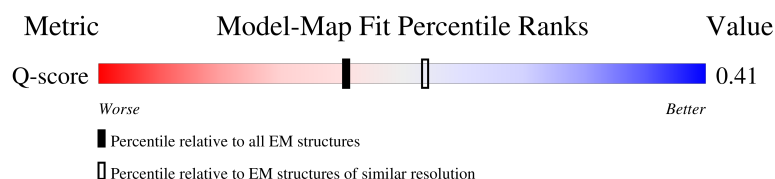
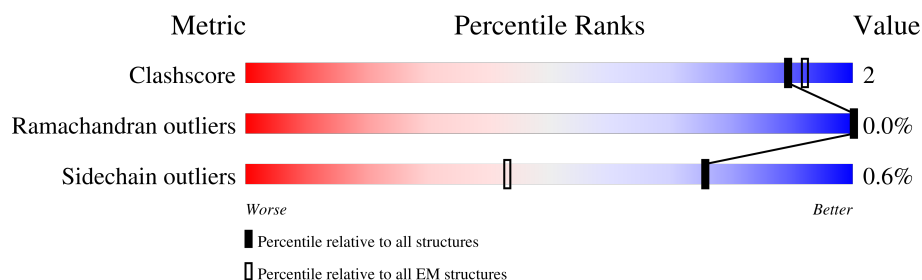
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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	10198 (3.30 - 4.30)

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	23% 82% 5% 13%
1	B	5037	22% 83% • 13%
1	C	5037	22% 83% 5% 13%
1	D	5037	22% 82% 6% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	6% 95% ...
2	F	108	• 95% ...
2	G	108	6% 95% ...
2	H	108	• 95% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 287012 atoms, of which 142908 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
			69822	22323	34734	6046	6482	237		
1	B	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	C	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	6046	6482	237		
1	D	4404	Total	C	H	N	O	S	0	0
			69822	22323	34734	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		

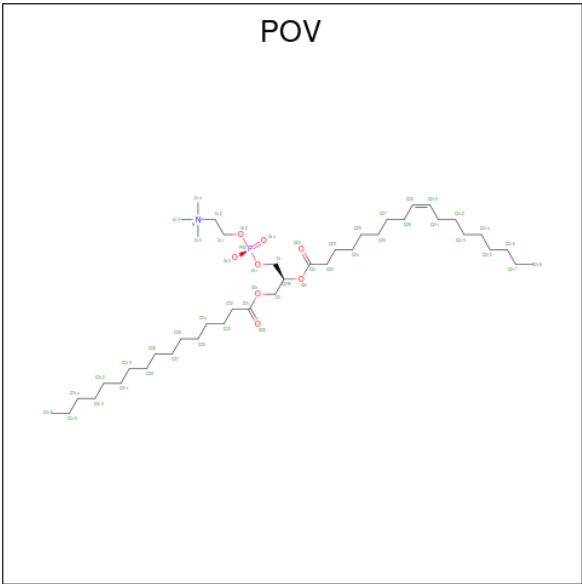
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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 (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
5	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
5	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
5	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
5	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

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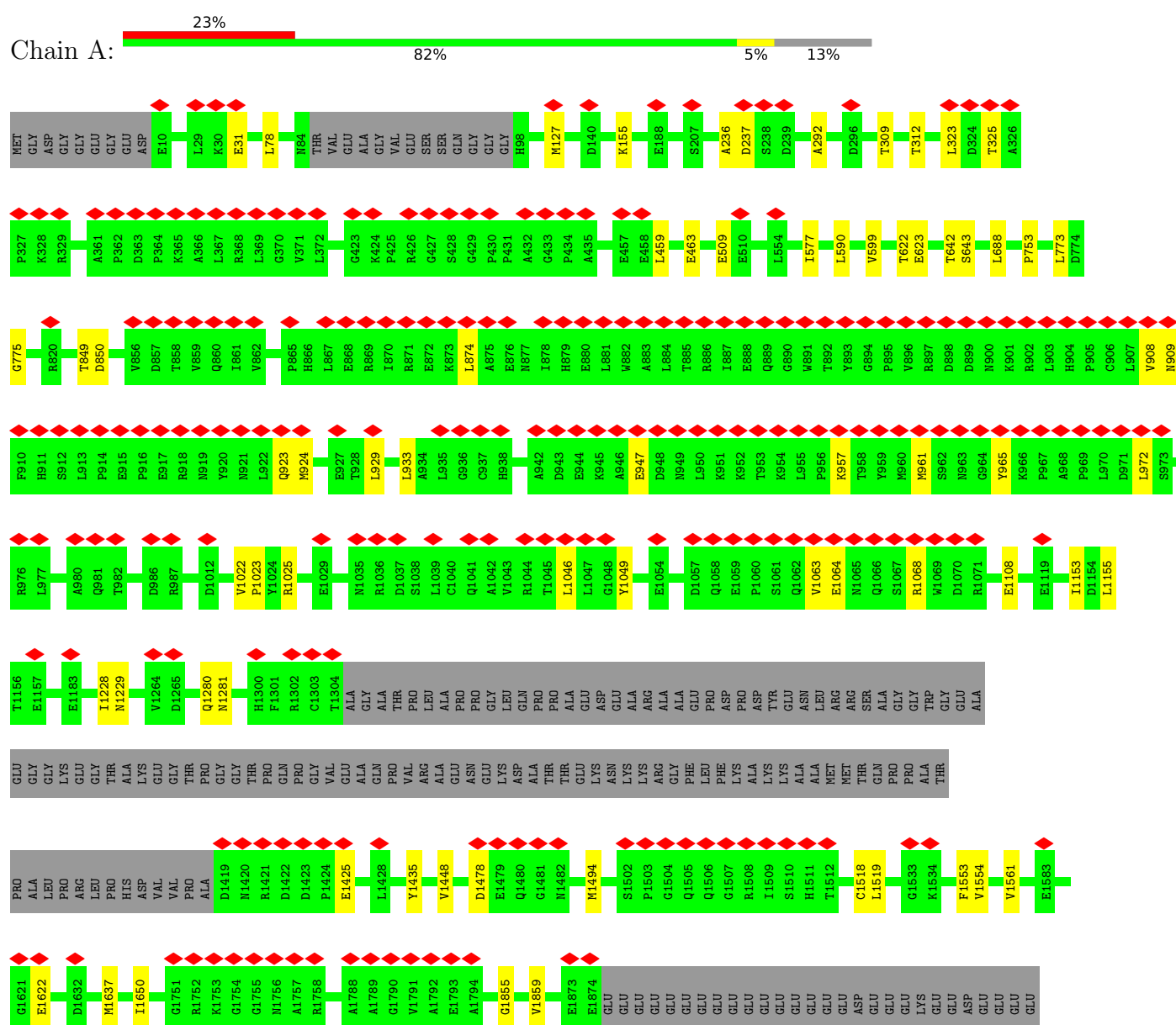
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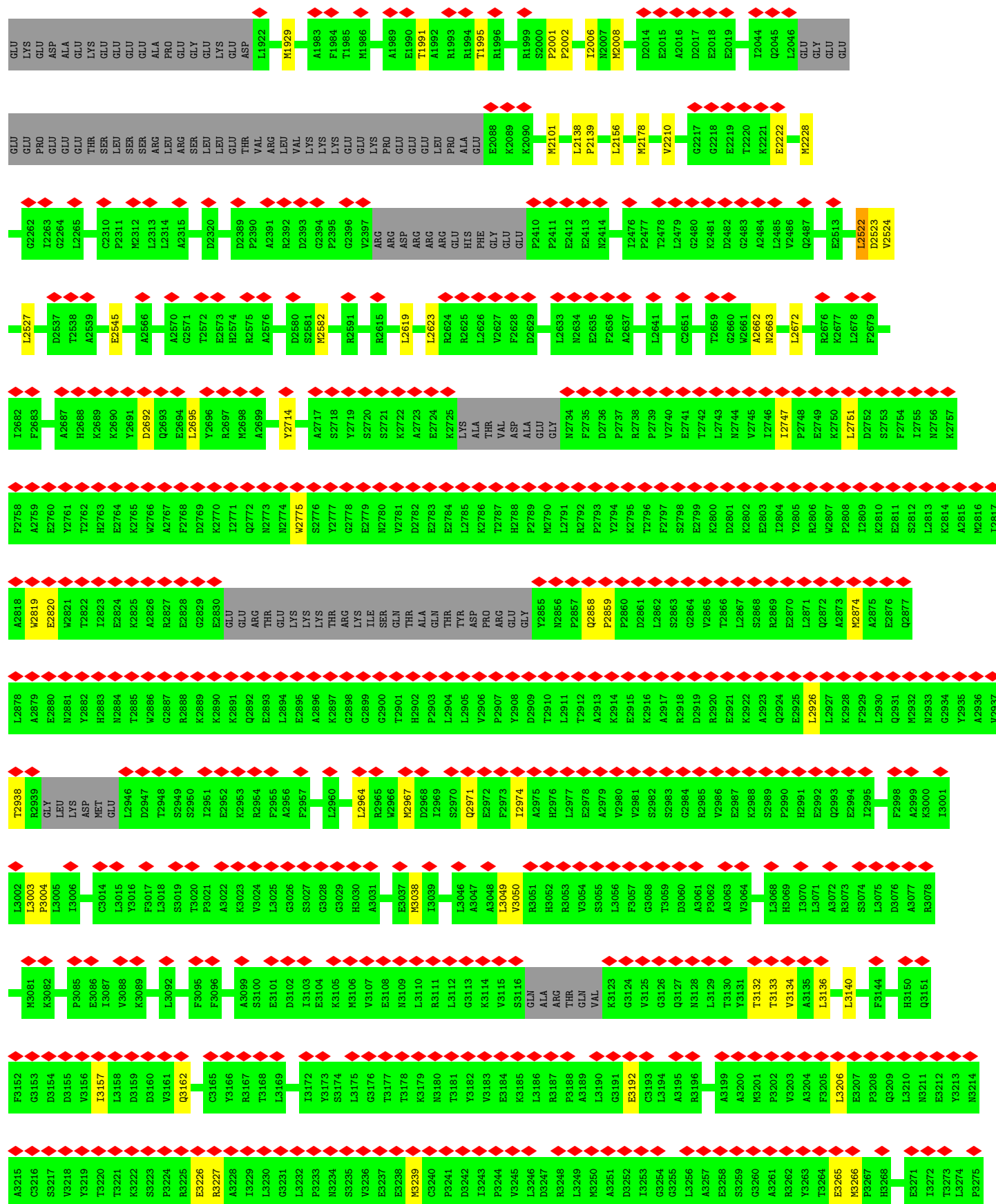
Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
5	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0
5	D	1	Total 134	C 42	H 82	N 1	O 8	P 1	0

3 Residue-property plots [i](#)

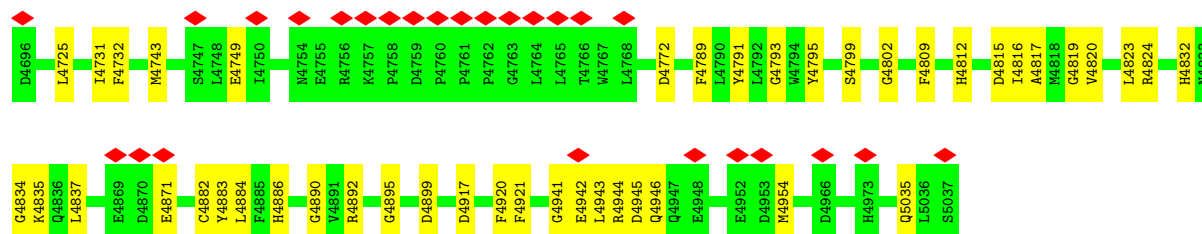
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 1

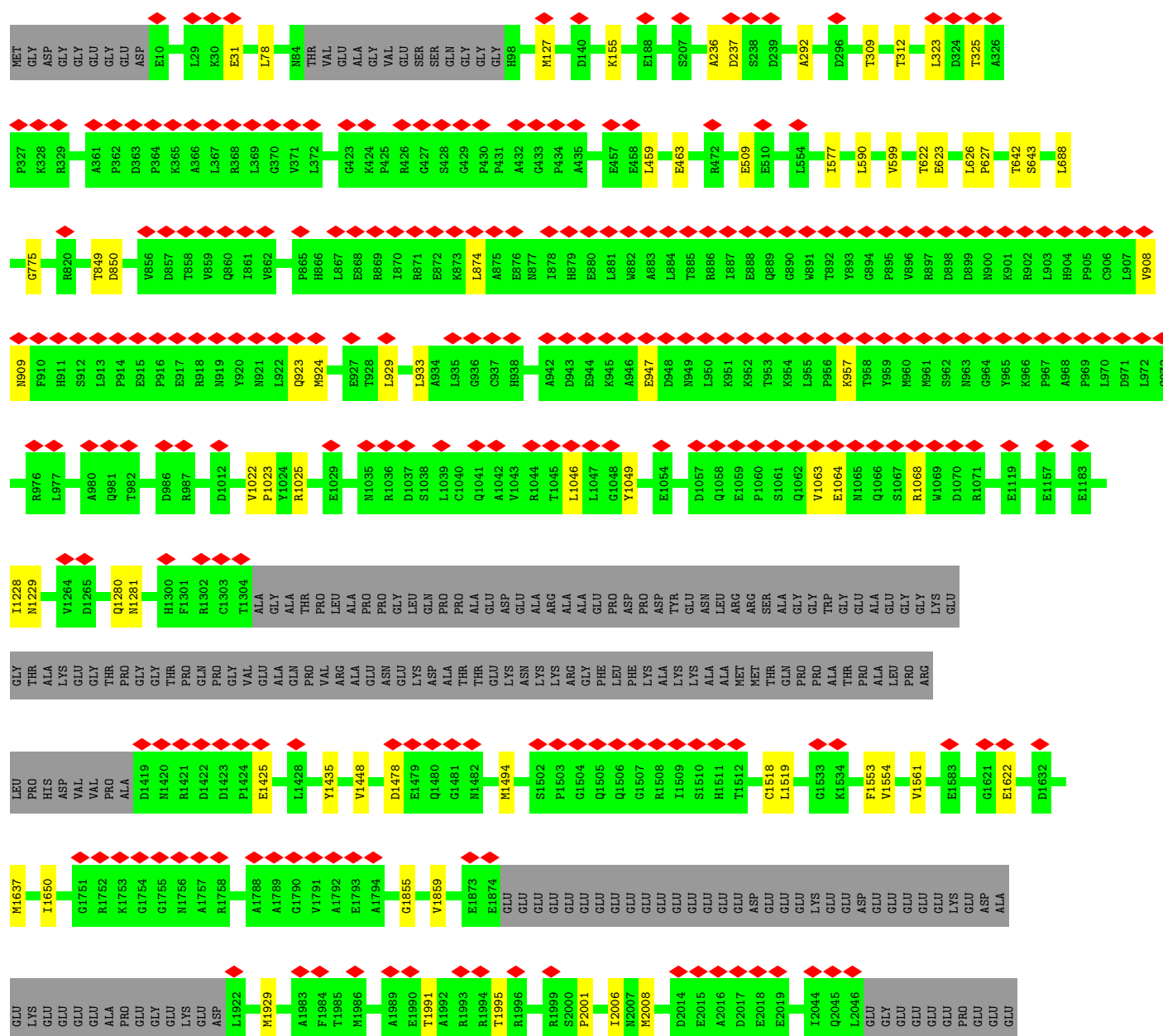
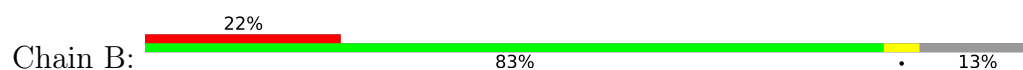






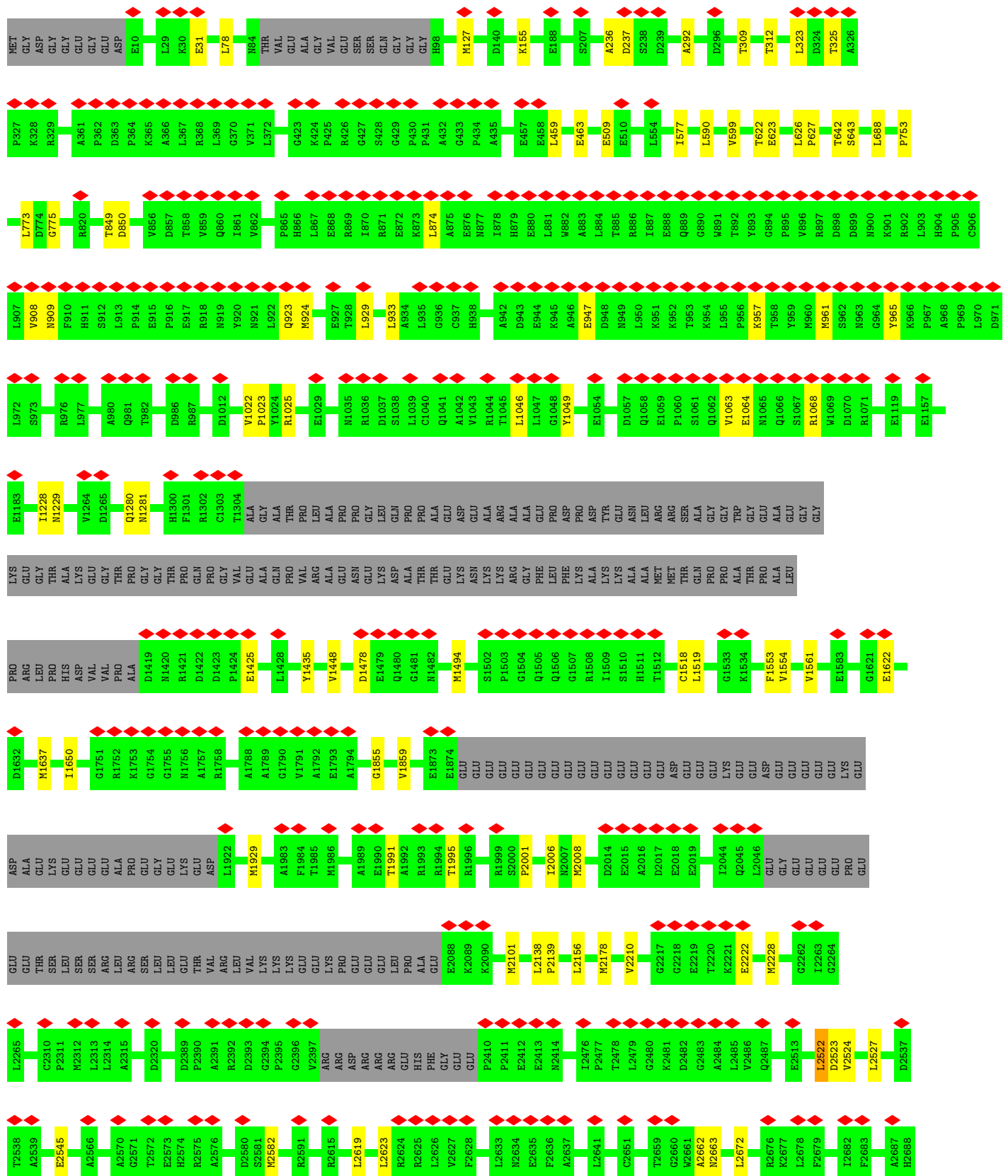
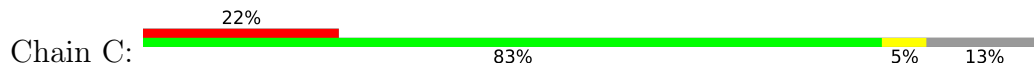


• Molecule 1: Ryanodine receptor 1

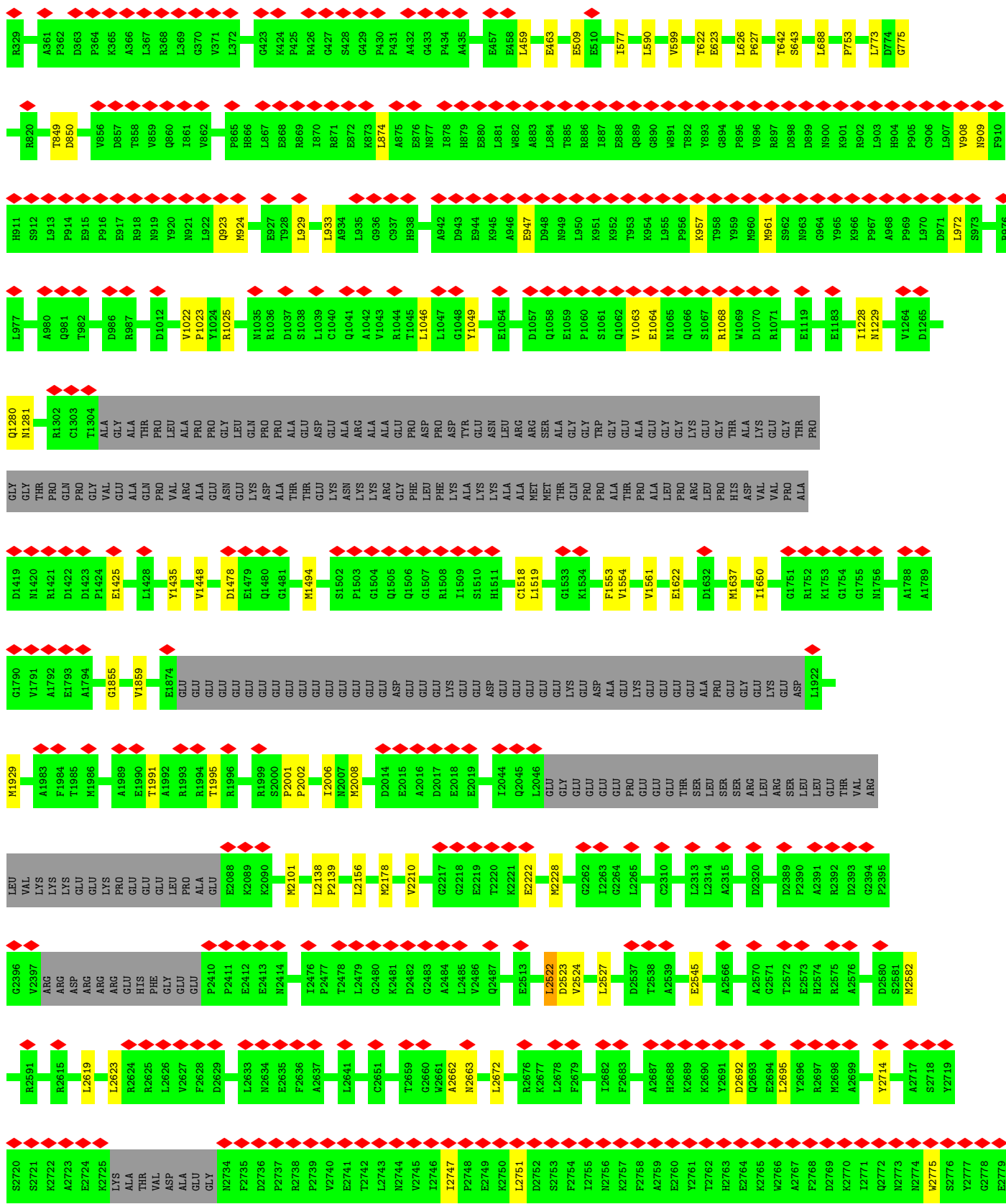




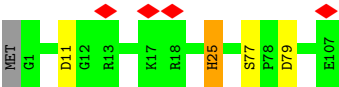




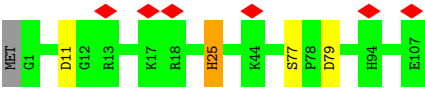
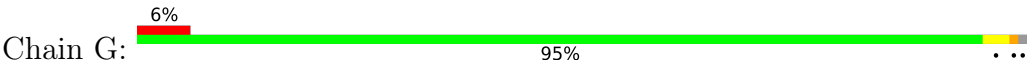




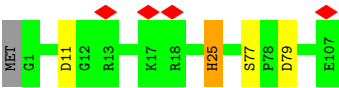




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	82421	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 ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.634	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.051	Depositor
Map value standard deviation	0.278	Depositor
Recommended contour level	1.14	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, CA, POV

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	0.48	31/35885 (0.1%)	0.62	120/48603 (0.2%)
1	B	0.36	14/35885 (0.0%)	0.53	15/48603 (0.0%)
1	C	0.42	26/35885 (0.1%)	0.58	64/48603 (0.1%)
1	D	0.53	44/35885 (0.1%)	0.67	180/48603 (0.4%)
2	E	0.31	1/851 (0.1%)	0.51	2/1146 (0.2%)
2	F	0.31	1/851 (0.1%)	0.51	2/1146 (0.2%)
2	G	0.31	1/851 (0.1%)	0.51	2/1146 (0.2%)
2	H	0.31	1/851 (0.1%)	0.51	2/1146 (0.2%)
All	All	0.45	119/146944 (0.1%)	0.60	387/198996 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	4

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4650	HIS	CE1-NE2	-8.90	1.23	1.32
1	A	4812	HIS	CE1-NE2	-8.83	1.23	1.32
1	D	4812	HIS	CE1-NE2	-8.82	1.23	1.32
1	C	4886	HIS	ND1-CE1	-8.80	1.23	1.32
1	D	4650	HIS	ND1-CE1	-8.78	1.23	1.32
1	A	4650	HIS	ND1-CE1	-8.74	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4832	HIS	ND1-CE1	-8.74	1.23	1.32
1	D	4832	HIS	ND1-CE1	-8.74	1.23	1.32
1	D	4812	HIS	ND1-CE1	-8.74	1.23	1.32
1	A	4812	HIS	ND1-CE1	-8.73	1.23	1.32
1	A	4650	HIS	CE1-NE2	-8.71	1.23	1.32
1	D	4886	HIS	ND1-CE1	-8.66	1.23	1.32
1	A	4563	ARG	CZ-NH2	-8.30	1.22	1.33
1	A	4892	ARG	CZ-NH2	-8.30	1.22	1.33
1	D	4860	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	4944	ARG	CZ-NH2	-8.26	1.22	1.33
1	B	4944	ARG	CZ-NH2	-8.26	1.22	1.33
1	D	4944	ARG	CZ-NH2	-8.25	1.22	1.33
1	D	4812	HIS	CD2-NE2	-8.24	1.28	1.37
1	D	4892	ARG	CZ-NH2	-8.24	1.22	1.33
1	A	4824	ARG	CZ-NH2	-8.21	1.22	1.33
1	D	4824	ARG	CZ-NH2	-8.21	1.22	1.33
1	D	4650	HIS	CD2-NE2	-8.20	1.28	1.37
1	A	4650	HIS	CD2-NE2	-8.10	1.28	1.37
1	C	4832	HIS	ND1-CE1	-8.01	1.24	1.32
1	A	4812	HIS	CD2-NE2	-8.01	1.29	1.37
1	C	4913	ARG	CZ-NH2	-7.97	1.23	1.33
1	D	4563	ARG	CZ-NH2	-7.95	1.23	1.33
1	C	4860	ARG	CZ-NH2	-7.88	1.23	1.33
1	C	4944	ARG	CZ-NH2	-7.36	1.23	1.33
1	C	4892	ARG	CZ-NH2	-7.32	1.24	1.33
1	A	4886	HIS	ND1-CE1	-7.20	1.25	1.32
1	A	4570	ALA	CA-CB	-7.10	1.42	1.53
1	A	4586	PRO	CA-CB	-7.10	1.47	1.53
1	D	4855	ALA	CA-CB	-7.08	1.42	1.53
1	A	4654	ALA	CA-CB	-7.05	1.42	1.53
1	D	4586	PRO	CA-CB	-6.98	1.47	1.53
1	A	4642	ALA	CA-CB	-6.95	1.42	1.53
1	A	4817	ALA	CA-CB	-6.95	1.42	1.53
1	B	4892	ARG	CZ-NH2	-6.95	1.24	1.33
1	B	4832	HIS	ND1-CE1	-6.90	1.25	1.32
1	D	4905	ALA	CA-CB	-6.89	1.42	1.53
1	D	4817	ALA	CA-CB	-6.87	1.42	1.53
1	D	4845	ALA	CA-CB	-6.82	1.42	1.53
1	C	4845	ALA	CA-CB	-6.82	1.42	1.53
1	B	4944	ARG	CZ-NH1	-6.74	1.23	1.32
1	A	4563	ARG	CZ-NH1	-6.71	1.23	1.32
1	A	4892	ARG	CZ-NH1	-6.69	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4860	ARG	CZ-NH1	-6.67	1.23	1.32
1	D	4892	ARG	CZ-NH1	-6.67	1.23	1.32
1	D	4824	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	4824	ARG	CZ-NH1	-6.65	1.23	1.32
1	C	4855	ALA	CA-CB	-6.65	1.43	1.53
1	A	4944	ARG	CZ-NH1	-6.64	1.23	1.32
1	D	4944	ARG	CZ-NH1	-6.62	1.23	1.32
1	D	4572	ALA	CA-CB	-6.62	1.43	1.53
1	D	4570	ALA	CA-CB	-6.62	1.43	1.53
1	B	4886	HIS	ND1-CE1	-6.58	1.25	1.32
1	C	4824	ARG	CZ-NH2	-6.57	1.25	1.33
1	D	4642	ALA	CA-CB	-6.56	1.43	1.53
1	D	4654	ALA	CA-CB	-6.54	1.43	1.53
1	D	4893	ALA	CA-CB	-6.46	1.42	1.53
1	C	4913	ARG	CZ-NH1	-6.45	1.23	1.32
1	C	4860	ARG	CZ-NH1	-6.44	1.23	1.32
1	D	4563	ARG	CZ-NH1	-6.43	1.23	1.32
1	C	4905	ALA	CA-CB	-6.41	1.43	1.53
1	A	4793	GLY	N-CA	-6.33	1.38	1.45
1	D	4890	GLY	N-CA	-6.24	1.38	1.45
1	D	4819	GLY	N-CA	-6.21	1.38	1.45
1	C	4842	GLY	N-CA	-6.17	1.38	1.45
1	D	4842	GLY	N-CA	-6.16	1.38	1.45
1	A	4941	GLY	N-CA	-6.15	1.38	1.45
1	B	4941	GLY	N-CA	-6.15	1.38	1.45
1	C	4941	GLY	N-CA	-6.15	1.38	1.45
1	D	4941	GLY	N-CA	-6.12	1.38	1.45
1	A	4819	GLY	N-CA	-6.12	1.38	1.45
1	A	4802	GLY	N-CA	-6.11	1.38	1.45
1	D	4802	GLY	N-CA	-6.08	1.38	1.45
1	D	4894	GLY	N-CA	-5.97	1.38	1.45
1	C	4894	GLY	N-CA	-5.93	1.38	1.45
1	D	4793	GLY	N-CA	-5.92	1.38	1.45
1	C	4944	ARG	CZ-NH1	-5.87	1.24	1.32
1	D	4834	GLY	N-CA	-5.83	1.38	1.45
1	A	4834	GLY	N-CA	-5.74	1.38	1.45
1	B	4824	ARG	CZ-NH2	-5.72	1.26	1.33
1	C	4892	ARG	CZ-NH1	-5.71	1.24	1.32
1	D	4895	GLY	N-CA	-5.70	1.38	1.45
1	C	4895	GLY	N-CA	-5.70	1.38	1.45
1	D	4898	GLY	N-CA	-5.60	1.38	1.45
1	D	4944	ARG	CD-NE	-5.57	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4906	GLY	N-CA	-5.57	1.38	1.45
1	B	4944	ARG	CD-NE	-5.56	1.38	1.46
1	B	4892	ARG	CZ-NH1	-5.55	1.25	1.32
1	A	4944	ARG	CD-NE	-5.55	1.38	1.46
1	C	4913	ARG	CD-NE	-5.52	1.38	1.46
1	C	4898	GLY	N-CA	-5.51	1.38	1.45
1	C	4906	GLY	N-CA	-5.50	1.38	1.45
1	A	4892	ARG	CD-NE	-5.41	1.38	1.46
1	D	4892	ARG	CD-NE	-5.34	1.38	1.46
1	D	4824	ARG	CD-NE	-5.32	1.38	1.46
1	A	4563	ARG	CD-NE	-5.30	1.38	1.46
1	D	4860	ARG	CD-NE	-5.28	1.38	1.46
1	C	4944	ARG	CD-NE	-5.26	1.38	1.46
1	A	4824	ARG	CD-NE	-5.25	1.38	1.46
1	C	4860	ARG	CD-NE	-5.23	1.39	1.46
1	D	4563	ARG	CD-NE	-5.21	1.39	1.46
1	B	4894	GLY	N-CA	-5.20	1.39	1.45
1	B	4650	HIS	ND1-CE1	-5.17	1.27	1.32
1	C	4824	ARG	CZ-NH1	-5.13	1.25	1.32
1	B	4650	HIS	CE1-NE2	-5.12	1.27	1.32
1	B	4812	HIS	ND1-CE1	-5.12	1.27	1.32
2	E	25	HIS	CE1-NE2	-5.08	1.27	1.32
2	H	25	HIS	CE1-NE2	-5.07	1.27	1.32
2	F	25	HIS	CE1-NE2	-5.06	1.27	1.32
2	G	25	HIS	CE1-NE2	-5.05	1.27	1.32
1	C	4834	GLY	N-CA	-5.04	1.39	1.45
1	B	4812	HIS	CE1-NE2	-5.02	1.27	1.32
1	C	4892	ARG	CD-NE	-5.01	1.39	1.46
1	A	4895	GLY	N-CA	-5.01	1.39	1.45

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4920	PHE	CA-CB-CG	7.58	121.38	113.80
1	C	4920	PHE	CA-CB-CG	7.55	121.35	113.80
1	D	4899	ASP	CA-CB-CG	7.53	120.13	112.60
1	D	4627	MET	CA-C-N	7.50	130.29	122.27
1	D	4627	MET	C-N-CA	7.50	130.29	122.27
1	A	4627	MET	CA-C-N	7.45	130.24	122.27
1	A	4627	MET	C-N-CA	7.45	130.24	122.27
1	A	4571	PHE	CA-CB-CG	7.23	121.03	113.80
1	D	4571	PHE	CA-CB-CG	7.19	120.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4809	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	4574	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	4650	HIS	CA-CB-CG	7.15	120.95	113.80
1	A	4945	ASP	CA-CB-CG	7.12	119.72	112.60
1	D	4574	ASN	CA-CB-CG	7.11	119.71	112.60
1	D	4945	ASP	CA-CB-CG	7.10	119.70	112.60
1	D	4917	ASP	CA-CB-CG	7.05	119.65	112.60
1	C	4917	ASP	CA-CB-CG	7.02	119.62	112.60
1	D	4650	HIS	CA-CB-CG	7.01	120.81	113.80
1	D	4809	PHE	CA-CB-CG	7.01	120.81	113.80
1	D	4862	PHE	CA-CB-CG	7.01	120.81	113.80
1	D	4903	ASP	CA-CB-CG	7.01	119.61	112.60
1	D	4886	HIS	CA-CB-CG	7.00	120.80	113.80
1	D	4579	PHE	CA-CB-CG	6.98	120.78	113.80
1	C	4886	HIS	CA-CB-CG	6.98	120.78	113.80
1	A	4579	PHE	CA-CB-CG	6.95	120.75	113.80
1	B	4920	PHE	CA-CB-CG	6.95	120.75	113.80
1	D	4885	PHE	CA-CB-CG	6.93	120.73	113.80
1	C	4862	PHE	CA-CB-CG	6.93	120.73	113.80
1	D	4877	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	4575	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	4877	ASP	CA-CB-CG	6.89	119.50	112.60
1	C	4885	PHE	CA-CB-CG	6.88	120.69	113.80
1	D	4864	ASN	CA-CB-CG	6.88	119.48	112.60
1	D	4907	ASP	CA-CB-CG	6.84	119.44	112.60
1	D	4575	PHE	CA-CB-CG	6.81	120.61	113.80
1	C	4907	ASP	CA-CB-CG	6.77	119.37	112.60
1	C	4864	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	4812	HIS	CA-CB-CG	6.74	120.54	113.80
1	A	4920	PHE	CA-CB-CG	6.73	120.53	113.80
1	D	4832	HIS	CA-CB-CG	6.60	120.40	113.80
1	D	4812	HIS	CA-CB-CG	6.59	120.39	113.80
1	A	4832	HIS	CA-CB-CG	6.59	120.39	113.80
1	D	4815	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	4815	ASP	CA-CB-CG	6.49	119.09	112.60
2	H	25	HIS	ND1-CG-CD2	-6.48	99.62	106.10
2	G	25	HIS	ND1-CG-CD2	-6.47	99.63	106.10
2	F	25	HIS	ND1-CG-CD2	-6.45	99.65	106.10
2	E	25	HIS	ND1-CG-CD2	-6.43	99.67	106.10
1	B	4917	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	4655	PHE	CA-CB-CG	6.36	120.16	113.80
1	D	4921	PHE	CA-CB-CG	6.35	120.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4921	PHE	CA-CB-CG	6.33	120.14	113.80
1	D	4581	LYS	CA-C-N	6.28	130.98	123.19
1	D	4581	LYS	C-N-CA	6.28	130.98	123.19
1	D	4655	PHE	CA-CB-CG	6.24	120.04	113.80
1	C	4856	PHE	CA-CB-CG	6.21	120.00	113.80
1	D	4563	ARG	CD-NE-CZ	6.12	132.96	124.40
1	A	4581	LYS	CA-C-N	6.11	130.77	123.19
1	A	4581	LYS	C-N-CA	6.11	130.77	123.19
1	A	4917	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	4888	TYR	CA-C-N	6.11	129.56	122.35
1	D	4888	TYR	C-N-CA	6.11	129.56	122.35
1	A	4563	ARG	CD-NE-CZ	6.07	132.89	124.40
1	C	4945	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	4824	ARG	CD-NE-CZ	6.02	132.82	124.40
1	D	4824	ARG	CD-NE-CZ	6.02	132.83	124.40
1	D	4878	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	4921	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	4899	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	4878	ASP	CA-CB-CG	5.74	118.33	112.60
1	D	4920	PHE	CA-C-N	5.63	127.76	120.44
1	D	4920	PHE	C-N-CA	5.63	127.76	120.44
1	D	4795	TYR	CA-C-N	5.62	127.75	120.44
1	D	4795	TYR	C-N-CA	5.62	127.75	120.44
1	C	4920	PHE	CA-C-N	5.61	127.73	120.44
1	C	4920	PHE	C-N-CA	5.61	127.73	120.44
1	A	4819	GLY	CA-C-N	5.59	129.62	121.80
1	A	4819	GLY	C-N-CA	5.59	129.62	121.80
1	D	4628	VAL	CA-C-N	5.58	131.33	122.62
1	D	4628	VAL	C-N-CA	5.58	131.33	122.62
1	D	4874	MET	CA-C-N	5.58	127.76	120.28
1	D	4874	MET	C-N-CA	5.58	127.76	120.28
1	C	4832	HIS	CA-CB-CG	5.58	119.38	113.80
1	D	4917	ASP	CA-C-N	5.57	127.58	120.56
1	D	4917	ASP	C-N-CA	5.57	127.58	120.56
1	D	4819	GLY	CA-C-N	5.57	129.59	121.80
1	D	4819	GLY	C-N-CA	5.57	129.59	121.80
1	A	4628	VAL	CA-C-N	5.55	131.28	122.62
1	A	4628	VAL	C-N-CA	5.55	131.28	122.62
1	A	4795	TYR	CA-C-N	5.55	127.66	120.44
1	A	4795	TYR	C-N-CA	5.55	127.66	120.44
1	C	4899	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	4845	ALA	CA-C-N	5.53	127.52	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4845	ALA	C-N-CA	5.53	127.52	120.56
1	C	4896	GLY	CA-C-N	5.52	128.03	120.46
1	C	4896	GLY	C-N-CA	5.52	128.03	120.46
1	D	4896	GLY	CA-C-N	5.52	128.02	120.46
1	D	4896	GLY	C-N-CA	5.52	128.02	120.46
1	A	4921	PHE	CA-CB-CG	5.50	119.31	113.80
1	C	4884	LEU	CA-C-N	5.50	127.59	120.44
1	C	4884	LEU	C-N-CA	5.50	127.59	120.44
1	C	4917	ASP	CA-C-N	5.50	127.49	120.56
1	C	4917	ASP	C-N-CA	5.50	127.49	120.56
1	C	4845	ALA	CA-C-N	5.48	127.47	120.56
1	C	4845	ALA	C-N-CA	5.48	127.47	120.56
1	A	4837	LEU	CA-C-N	5.48	127.57	120.56
1	A	4837	LEU	C-N-CA	5.48	127.57	120.56
1	D	4832	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
1	C	4886	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
1	D	4884	LEU	CA-C-N	5.42	127.49	120.44
1	D	4884	LEU	C-N-CA	5.42	127.49	120.44
1	C	4824	ARG	CD-NE-CZ	5.41	131.98	124.40
1	D	4890	GLY	CA-C-N	5.40	127.47	120.56
1	D	4890	GLY	C-N-CA	5.40	127.47	120.56
1	C	4907	ASP	CA-C-N	5.40	128.05	120.28
1	C	4907	ASP	C-N-CA	5.40	128.05	120.28
1	D	4886	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	A	4832	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	A	4892	ARG	CD-NE-CZ	5.37	131.92	124.40
1	D	4572	ALA	CA-C-N	5.37	127.33	120.56
1	D	4572	ALA	C-N-CA	5.37	127.33	120.56
1	A	4890	GLY	CA-C-N	5.36	127.42	120.56
1	A	4890	GLY	C-N-CA	5.36	127.42	120.56
1	D	4657	CYS	CA-C-N	5.36	127.32	120.56
1	D	4657	CYS	C-N-CA	5.36	127.32	120.56
1	D	4892	ARG	CD-NE-CZ	5.36	131.90	124.40
1	B	4920	PHE	CA-C-N	5.35	127.40	120.44
1	B	4920	PHE	C-N-CA	5.35	127.40	120.44
1	C	4941	GLY	CA-C-N	5.35	127.39	120.44
1	C	4941	GLY	C-N-CA	5.35	127.39	120.44
1	D	4941	GLY	CA-C-N	5.34	127.39	120.44
1	D	4941	GLY	C-N-CA	5.34	127.39	120.44
2	F	25	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	C	4890	GLY	CA-C-N	5.34	127.40	120.56
1	C	4890	GLY	C-N-CA	5.34	127.40	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4907	ASP	CA-C-N	5.34	127.97	120.28
1	D	4907	ASP	C-N-CA	5.34	127.97	120.28
1	D	4812	HIS	ND1-CG-CD2	-5.34	100.76	106.10
1	A	4941	GLY	CA-C-N	5.34	127.38	120.44
1	A	4941	GLY	C-N-CA	5.34	127.38	120.44
1	D	4650	HIS	ND1-CG-CD2	-5.34	100.76	106.10
1	D	4794	TRP	CA-C-N	5.34	127.38	120.44
1	D	4794	TRP	C-N-CA	5.34	127.38	120.44
1	C	4859	PHE	CA-C-N	5.33	127.96	120.28
1	C	4859	PHE	C-N-CA	5.33	127.96	120.28
1	D	4793	GLY	CA-C-N	5.33	127.42	120.28
1	D	4793	GLY	C-N-CA	5.33	127.42	120.28
1	C	4860	ARG	CD-NE-CZ	5.32	131.85	124.40
2	H	25	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
1	A	4657	CYS	CA-C-N	5.32	127.26	120.56
1	A	4657	CYS	C-N-CA	5.32	127.26	120.56
1	D	4860	ARG	CD-NE-CZ	5.31	131.83	124.40
1	A	4572	ALA	CA-C-N	5.31	127.25	120.56
1	A	4572	ALA	C-N-CA	5.31	127.25	120.56
1	C	4849	TYR	N-CA-CB	5.30	117.70	110.01
1	D	4649	LEU	CA-C-N	5.30	127.33	120.44
1	D	4649	LEU	C-N-CA	5.30	127.33	120.44
1	D	4642	ALA	CA-C-N	5.29	127.32	120.44
1	D	4642	ALA	C-N-CA	5.29	127.32	120.44
1	A	4575	PHE	CA-C-N	5.29	127.71	120.46
1	A	4575	PHE	C-N-CA	5.29	127.71	120.46
1	A	4791	TYR	N-CA-CB	5.29	117.68	110.01
1	A	4649	LEU	CA-C-N	5.29	127.31	120.44
1	A	4649	LEU	C-N-CA	5.29	127.31	120.44
1	A	4886	HIS	CA-CB-CG	5.29	119.09	113.80
1	B	4943	LEU	CA-C-N	5.29	127.32	120.44
1	B	4943	LEU	C-N-CA	5.29	127.32	120.44
1	A	4650	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	4812	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	B	4917	ASP	CA-C-N	5.28	127.22	120.56
1	B	4917	ASP	C-N-CA	5.28	127.22	120.56
1	D	4832	HIS	CG-CD2-NE2	5.28	112.48	107.20
2	G	25	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	D	4651	THR	CA-C-N	5.28	127.31	120.44
1	D	4651	THR	C-N-CA	5.28	127.31	120.44
1	D	4943	LEU	CA-C-N	5.28	127.30	120.44
1	D	4943	LEU	C-N-CA	5.28	127.30	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4791	TYR	N-CA-CB	5.28	117.66	110.01
1	A	4943	LEU	CA-C-N	5.28	127.30	120.44
1	A	4943	LEU	C-N-CA	5.28	127.30	120.44
1	A	4642	ALA	CA-C-N	5.27	127.30	120.44
1	A	4642	ALA	C-N-CA	5.27	127.30	120.44
1	C	4886	HIS	CG-CD2-NE2	5.26	112.46	107.20
1	D	4575	PHE	CA-C-N	5.26	127.67	120.46
1	D	4575	PHE	C-N-CA	5.26	127.67	120.46
2	E	25	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	D	4632	LEU	CA-C-N	5.26	131.34	123.23
1	D	4632	LEU	C-N-CA	5.26	131.34	123.23
1	D	4645	CYS	CA-C-N	5.26	127.33	120.28
1	D	4645	CYS	C-N-CA	5.26	127.33	120.28
1	A	4652	LEU	CA-C-N	5.26	127.19	120.56
1	A	4652	LEU	C-N-CA	5.26	127.19	120.56
1	C	4886	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	D	4832	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	D	4823	LEU	CA-C-N	5.25	127.27	120.44
1	D	4823	LEU	C-N-CA	5.25	127.27	120.44
1	D	4886	HIS	CG-CD2-NE2	5.25	112.45	107.20
1	C	4885	PHE	CA-C-N	5.25	127.26	120.44
1	C	4885	PHE	C-N-CA	5.25	127.26	120.44
1	A	4832	HIS	ND1-CG-CD2	-5.24	100.86	106.10
1	C	4848	VAL	CA-C-N	5.24	127.25	120.44
1	C	4848	VAL	C-N-CA	5.24	127.25	120.44
1	D	4568	PHE	CA-C-N	5.24	127.30	120.28
1	D	4568	PHE	C-N-CA	5.24	127.30	120.28
1	D	4899	ASP	CA-C-N	5.23	129.58	120.68
1	D	4899	ASP	C-N-CA	5.23	129.58	120.68
1	D	4652	LEU	CA-C-N	5.23	127.15	120.56
1	D	4652	LEU	C-N-CA	5.23	127.15	120.56
1	D	4849	TYR	N-CA-CB	5.23	117.59	110.01
1	A	4645	CYS	CA-C-N	5.22	127.28	120.28
1	A	4645	CYS	C-N-CA	5.22	127.28	120.28
1	D	4885	PHE	CA-C-N	5.22	127.23	120.44
1	D	4885	PHE	C-N-CA	5.22	127.23	120.44
1	D	4886	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	D	4942	GLU	CA-C-N	5.22	127.27	120.28
1	D	4942	GLU	C-N-CA	5.22	127.27	120.28
1	D	4641	PRO	CA-C-N	5.21	127.27	120.28
1	D	4641	PRO	C-N-CA	5.21	127.27	120.28
1	C	4855	ALA	CA-C-N	5.21	127.22	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4855	ALA	C-N-CA	5.21	127.22	120.44
1	D	4576	ILE	CA-C-N	5.21	127.78	120.28
1	D	4576	ILE	C-N-CA	5.21	127.78	120.28
1	D	4838	VAL	CA-C-N	5.21	127.21	120.44
1	D	4838	VAL	C-N-CA	5.21	127.21	120.44
1	A	4832	HIS	CG-CD2-NE2	5.21	112.41	107.20
1	A	4568	PHE	CA-C-N	5.21	127.26	120.28
1	A	4568	PHE	C-N-CA	5.21	127.26	120.28
1	A	4651	THR	CA-C-N	5.20	127.20	120.44
1	A	4651	THR	C-N-CA	5.20	127.20	120.44
1	A	4632	LEU	CA-C-N	5.20	131.24	123.23
1	A	4632	LEU	C-N-CA	5.20	131.24	123.23
1	A	4942	GLU	CA-C-N	5.20	127.25	120.28
1	A	4942	GLU	C-N-CA	5.20	127.25	120.28
1	D	4574	ASN	CA-C-N	5.20	127.20	120.44
1	D	4574	ASN	C-N-CA	5.20	127.20	120.44
1	D	4650	HIS	CA-C-N	5.20	127.20	120.44
1	D	4650	HIS	C-N-CA	5.20	127.20	120.44
1	A	4832	HIS	N-CA-CB	5.20	117.55	110.01
1	C	4838	VAL	CA-C-N	5.20	127.20	120.44
1	C	4838	VAL	C-N-CA	5.20	127.20	120.44
1	B	4945	ASP	CA-CB-CG	5.19	117.79	112.60
1	D	4946	GLN	CA-C-N	5.19	127.19	120.44
1	D	4946	GLN	C-N-CA	5.19	127.19	120.44
1	A	4946	GLN	CA-C-N	5.19	127.18	120.44
1	A	4946	GLN	C-N-CA	5.19	127.18	120.44
1	D	4832	HIS	N-CA-CB	5.19	117.53	110.01
1	C	4883	TYR	N-CA-CB	5.18	117.53	110.01
1	A	4641	PRO	CA-C-N	5.18	127.22	120.28
1	A	4641	PRO	C-N-CA	5.18	127.22	120.28
1	A	4812	HIS	CA-C-N	5.18	127.74	120.28
1	A	4812	HIS	C-N-CA	5.18	127.74	120.28
1	D	4654	ALA	CA-C-N	5.18	127.17	120.44
1	D	4654	ALA	C-N-CA	5.18	127.17	120.44
1	A	4576	ILE	CA-C-N	5.18	127.73	120.28
1	A	4576	ILE	C-N-CA	5.18	127.73	120.28
1	B	4919	THR	CA-C-N	5.18	127.17	120.44
1	B	4919	THR	C-N-CA	5.18	127.17	120.44
1	D	4570	ALA	CA-C-N	5.18	127.17	120.44
1	D	4570	ALA	C-N-CA	5.18	127.17	120.44
1	A	4574	ASN	CA-C-N	5.17	127.17	120.44
1	A	4574	ASN	C-N-CA	5.17	127.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4883	TYR	N-CA-CB	5.17	117.51	110.01
1	D	4848	VAL	CA-C-N	5.17	127.16	120.44
1	D	4848	VAL	C-N-CA	5.17	127.16	120.44
1	A	4823	LEU	CA-C-N	5.17	127.16	120.44
1	A	4823	LEU	C-N-CA	5.17	127.16	120.44
1	C	4900	GLU	CA-C-N	5.17	129.52	122.34
1	C	4900	GLU	C-N-CA	5.17	129.52	122.34
1	D	4812	HIS	CA-C-N	5.16	127.71	120.28
1	D	4812	HIS	C-N-CA	5.16	127.71	120.28
1	D	4854	VAL	CA-C-N	5.16	127.15	120.44
1	D	4854	VAL	C-N-CA	5.16	127.15	120.44
1	A	4654	ALA	CA-C-N	5.16	127.15	120.44
1	A	4654	ALA	C-N-CA	5.16	127.15	120.44
1	A	4883	TYR	CA-C-N	5.16	127.20	120.28
1	A	4883	TYR	C-N-CA	5.16	127.20	120.28
1	D	4860	ARG	CA-CB-CG	5.16	124.42	114.10
1	A	4820	VAL	CA-C-N	5.16	127.19	120.28
1	A	4820	VAL	C-N-CA	5.16	127.19	120.28
1	D	4652	LEU	N-CA-CB	5.15	117.48	110.01
1	C	4901	ILE	CA-C-N	5.15	128.52	120.75
1	C	4901	ILE	C-N-CA	5.15	128.52	120.75
1	D	4901	ILE	CA-C-N	5.15	128.52	120.75
1	D	4901	ILE	C-N-CA	5.15	128.52	120.75
1	D	4883	TYR	CA-C-N	5.15	127.18	120.28
1	D	4883	TYR	C-N-CA	5.15	127.18	120.28
1	D	4900	GLU	CA-C-N	5.15	129.49	122.34
1	D	4900	GLU	C-N-CA	5.15	129.49	122.34
1	D	4566	ALA	CA-C-N	5.14	127.12	120.44
1	D	4566	ALA	C-N-CA	5.14	127.12	120.44
1	D	4789	PHE	CA-C-N	5.14	127.12	120.44
1	D	4789	PHE	C-N-CA	5.14	127.12	120.44
1	A	4567	LEU	N-CA-CB	5.13	117.45	110.01
1	D	4824	ARG	CA-C-N	5.13	127.11	120.44
1	D	4824	ARG	C-N-CA	5.13	127.11	120.44
1	C	4856	PHE	N-CA-CB	5.13	117.44	110.01
1	D	4791	TYR	CA-C-N	5.12	127.14	120.28
1	D	4791	TYR	C-N-CA	5.12	127.14	120.28
1	D	4898	GLY	CA-C-N	5.12	127.09	120.44
1	D	4898	GLY	C-N-CA	5.12	127.09	120.44
1	A	4570	ALA	CA-C-N	5.11	127.09	120.44
1	A	4570	ALA	C-N-CA	5.11	127.09	120.44
1	B	4941	GLY	CA-C-N	5.11	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4941	GLY	C-N-CA	5.11	127.09	120.44
1	D	4571	PHE	CA-C-N	5.11	127.09	120.44
1	D	4571	PHE	C-N-CA	5.11	127.09	120.44
1	A	4566	ALA	CA-C-N	5.11	127.09	120.44
1	A	4566	ALA	C-N-CA	5.11	127.09	120.44
1	D	4919	THR	CA-C-N	5.11	127.09	120.44
1	D	4919	THR	C-N-CA	5.11	127.09	120.44
1	A	4789	PHE	CA-C-N	5.11	127.08	120.44
1	A	4789	PHE	C-N-CA	5.11	127.08	120.44
1	D	4835	LYS	N-CA-CB	5.11	117.42	110.01
1	A	4920	PHE	CA-C-N	5.11	127.08	120.44
1	A	4920	PHE	C-N-CA	5.11	127.08	120.44
1	C	4864	ASN	N-CA-CB	5.11	117.47	110.57
1	C	4892	ARG	CD-NE-CZ	5.11	131.55	124.40
1	D	4864	ASN	N-CA-CB	5.11	117.47	110.57
1	A	4835	LYS	N-CA-CB	5.11	117.41	110.01
1	C	4943	LEU	CA-C-N	5.10	127.07	120.44
1	C	4943	LEU	C-N-CA	5.10	127.07	120.44
1	C	4860	ARG	CA-CB-CG	5.10	124.29	114.10
1	A	4652	LEU	N-CA-CB	5.09	117.40	110.01
1	D	4567	LEU	N-CA-CB	5.09	117.39	110.01
1	C	4888	TYR	CA-C-N	5.09	128.35	122.35
1	C	4888	TYR	C-N-CA	5.09	128.35	122.35
1	D	4562	LEU	CA-C-N	5.09	127.05	120.44
1	D	4562	LEU	C-N-CA	5.09	127.05	120.44
1	A	4824	ARG	CA-C-N	5.08	127.05	120.44
1	A	4824	ARG	C-N-CA	5.08	127.05	120.44
1	A	4650	HIS	N-CA-CB	5.08	117.37	110.01
1	A	4655	PHE	N-CA-CB	5.08	117.37	110.01
1	D	4643	LEU	N-CA-CB	5.08	117.37	110.01
1	B	4944	ARG	N-CA-CB	5.07	117.37	110.01
1	D	4637	GLY	CA-C-N	5.07	130.42	122.11
1	D	4637	GLY	C-N-CA	5.07	130.42	122.11
1	D	4655	PHE	N-CA-CB	5.07	117.36	110.01
1	D	4944	ARG	N-CA-CB	5.07	117.36	110.01
1	A	4643	LEU	N-CA-CB	5.06	117.35	110.01
1	D	4653	VAL	CA-C-N	5.06	127.06	120.28
1	D	4653	VAL	C-N-CA	5.06	127.06	120.28
1	D	4790	LEU	CA-C-N	5.06	127.02	120.44
1	D	4790	LEU	C-N-CA	5.06	127.02	120.44
1	D	4879	MET	CA-C-N	5.06	127.02	120.44
1	D	4879	MET	C-N-CA	5.06	127.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4573	ILE	CA-C-N	5.06	127.06	120.28
1	A	4573	ILE	C-N-CA	5.06	127.06	120.28
1	D	4816	ILE	CA-C-N	5.06	127.02	120.44
1	D	4816	ILE	C-N-CA	5.06	127.02	120.44
1	D	4573	ILE	CA-C-N	5.06	127.06	120.28
1	D	4573	ILE	C-N-CA	5.06	127.06	120.28
1	A	4791	TYR	CA-C-N	5.05	127.05	120.28
1	A	4791	TYR	C-N-CA	5.05	127.05	120.28
1	A	4944	ARG	N-CA-CB	5.05	117.34	110.01
1	A	4799	SER	N-CA-CB	5.05	117.33	110.01
1	A	4562	LEU	CA-C-N	5.04	127.00	120.44
1	A	4562	LEU	C-N-CA	5.04	127.00	120.44
1	C	4881	THR	CA-C-N	5.04	127.00	120.44
1	C	4881	THR	C-N-CA	5.04	127.00	120.44
1	D	4569	LEU	CA-C-N	5.04	127.00	120.44
1	D	4569	LEU	C-N-CA	5.04	127.00	120.44
1	D	4650	HIS	N-CA-CB	5.04	117.31	110.01
1	D	4880	MET	CA-C-N	5.04	126.98	120.44
1	D	4880	MET	C-N-CA	5.04	126.98	120.44
1	D	4902	GLU	N-CA-CB	5.04	117.44	110.04
1	C	4902	GLU	N-CA-CB	5.03	117.43	110.04
1	C	4910	GLU	CA-C-N	5.03	126.98	120.44
1	C	4910	GLU	C-N-CA	5.03	126.98	120.44
1	D	4942	GLU	N-CA-CB	5.03	117.30	110.01
1	D	4910	GLU	CA-C-N	5.02	126.97	120.44
1	D	4910	GLU	C-N-CA	5.02	126.97	120.44
1	A	4637	GLY	CA-C-N	5.02	130.34	122.11
1	A	4637	GLY	C-N-CA	5.02	130.34	122.11
1	A	4917	ASP	CA-C-N	5.02	126.88	120.56
1	A	4917	ASP	C-N-CA	5.02	126.88	120.56
1	A	4816	ILE	CA-C-N	5.02	126.96	120.44
1	A	4816	ILE	C-N-CA	5.02	126.96	120.44
1	A	4653	VAL	CA-C-N	5.01	127.00	120.28
1	A	4653	VAL	C-N-CA	5.01	127.00	120.28
1	A	4569	LEU	CA-C-N	5.01	126.95	120.44
1	A	4569	LEU	C-N-CA	5.01	126.95	120.44
1	D	4799	SER	N-CA-CB	5.01	117.27	110.01
1	A	4884	LEU	N-CA-CB	5.01	117.48	110.12
1	A	4824	ARG	CA-CB-CG	5.01	124.11	114.10
1	D	4824	ARG	CA-CB-CG	5.01	124.11	114.10
1	D	4834	GLY	CA-C-N	5.01	126.95	120.44
1	D	4834	GLY	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	25	HIS	Sidechain
2	F	25	HIS	Sidechain
2	G	25	HIS	Sidechain
2	H	25	HIS	Sidechain

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	34734	34715	132	0
1	B	35088	34734	34715	129	0
1	C	35088	34734	34715	129	0
1	D	35088	34734	34715	130	0
2	E	832	829	831	2	0
2	F	832	829	831	2	0
2	G	832	829	831	2	0
2	H	832	829	831	2	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	104	164	164	0	0
5	B	104	164	164	0	0
5	C	104	164	164	0	0
5	D	104	164	164	0	0
All	All	144104	142908	142840	528	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 2.

All (528) 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:B:3372:VAL:HG21	1:B:3401:LEU:HD11	1.45	0.98
1:C:3372:VAL:HG21	1:C:3401:LEU:HD11	1.45	0.95
1:D:3372:VAL:HG21	1:D:3401:LEU:HD11	1.45	0.95
1:A:3372:VAL:HG21	1:A:3401:LEU:HD11	1.45	0.95
1:A:849:THR:HG22	1:A:850:ASP:H	1.52	0.75
1:C:849:THR:HG22	1:C:850:ASP:H	1.52	0.74
1:D:849:THR:HG22	1:D:850:ASP:H	1.52	0.74
1:B:849:THR:HG22	1:B:850:ASP:H	1.52	0.73
1:D:1637:MET:HE3	1:D:1650:ILE:HD13	1.74	0.70
1:C:1637:MET:HE3	1:C:1650:ILE:HD13	1.74	0.70
1:A:1637:MET:HE3	1:A:1650:ILE:HD13	1.74	0.70
1:B:1637:MET:HE3	1:B:1650:ILE:HD13	1.74	0.69
1:B:2008:MET:HE2	1:B:2008:MET:HA	1.75	0.69
1:B:3528:THR:HG23	1:B:3573:MET:CE	2.23	0.69
1:A:2008:MET:HE2	1:A:2008:MET:HA	1.75	0.68
1:C:3528:THR:HG23	1:C:3573:MET:CE	2.23	0.68
1:A:3528:THR:HG23	1:A:3573:MET:CE	2.23	0.68
1:C:2008:MET:HE2	1:C:2008:MET:HA	1.75	0.68
1:D:2008:MET:HE2	1:D:2008:MET:HA	1.75	0.68
1:D:3528:THR:HG23	1:D:3573:MET:CE	2.23	0.67
1:D:323:LEU:O	1:D:325:THR:HG23	1.94	0.67
1:A:323:LEU:O	1:A:325:THR:HG23	1.95	0.67
1:B:323:LEU:O	1:B:325:THR:HG23	1.95	0.66
1:C:323:LEU:O	1:C:325:THR:HG23	1.95	0.66
1:A:3337:ARG:O	1:A:3340:VAL:HG22	1.99	0.63
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.81	0.63
1:B:3337:ARG:O	1:B:3340:VAL:HG22	1.99	0.62
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.81	0.62
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.81	0.62
1:C:874:LEU:HD21	1:C:1046:LEU:HD21	1.82	0.62
1:D:874:LEU:HD21	1:D:1046:LEU:HD21	1.81	0.62
1:C:4231:MET:HA	1:C:4231:MET:HE2	1.82	0.62
1:D:3337:ARG:O	1:D:3340:VAL:HG22	1.99	0.62
1:C:3337:ARG:O	1:C:3340:VAL:HG22	1.99	0.62
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.81	0.62
1:C:1637:MET:HE2	1:C:1650:ILE:HG21	1.82	0.61
1:B:4231:MET:HE2	1:B:4231:MET:HA	1.82	0.61
1:A:1637:MET:HE2	1:A:1650:ILE:HG21	1.82	0.61
1:B:1637:MET:HE2	1:B:1650:ILE:HG21	1.82	0.61
1:D:1637:MET:HE2	1:D:1650:ILE:HG21	1.82	0.61
1:D:4231:MET:HE2	1:D:4231:MET:HA	1.82	0.61
1:B:874:LEU:HD21	1:B:1046:LEU:HD21	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3368:ARG:O	1:A:3372:VAL:HG23	2.01	0.60
1:A:874:LEU:HD21	1:A:1046:LEU:HD21	1.82	0.60
1:B:3368:ARG:O	1:B:3372:VAL:HG23	2.01	0.60
1:D:3368:ARG:O	1:D:3372:VAL:HG23	2.01	0.60
1:A:4231:MET:HE2	1:A:4231:MET:HA	1.82	0.60
1:C:3563:VAL:HG13	1:C:3564:GLU:HG3	1.84	0.60
1:A:3563:VAL:HG13	1:A:3564:GLU:HG3	1.84	0.60
1:B:874:LEU:HD21	1:B:1046:LEU:CD2	2.32	0.59
1:C:3368:ARG:O	1:C:3372:VAL:HG23	2.01	0.59
1:C:874:LEU:HD21	1:C:1046:LEU:CD2	2.32	0.59
1:D:874:LEU:HD21	1:D:1046:LEU:CD2	2.32	0.59
1:D:3467:MET:O	1:D:3471:THR:HG22	2.02	0.59
1:A:874:LEU:HD21	1:A:1046:LEU:CD2	2.32	0.59
1:B:3467:MET:O	1:B:3471:THR:HG22	2.02	0.59
1:C:3467:MET:O	1:C:3471:THR:HG22	2.02	0.59
1:B:3563:VAL:HG13	1:B:3564:GLU:HG3	1.84	0.59
1:D:3563:VAL:HG13	1:D:3564:GLU:HG3	1.84	0.59
1:A:3467:MET:O	1:A:3471:THR:HG22	2.02	0.58
1:A:3723:MET:HE1	1:A:3792:ALA:HB3	1.85	0.58
1:D:3723:MET:HE1	1:D:3792:ALA:HB3	1.85	0.58
1:C:3723:MET:HE1	1:C:3792:ALA:HB3	1.85	0.58
1:B:3644:LEU:HD12	1:B:3645:PRO:CD	2.34	0.58
1:C:1637:MET:CE	1:C:1650:ILE:HG21	2.34	0.57
1:A:1637:MET:CE	1:A:1650:ILE:HG21	2.34	0.57
1:B:1637:MET:CE	1:B:1650:ILE:HG21	2.34	0.57
1:D:1637:MET:CE	1:D:1650:ILE:HG21	2.34	0.57
1:D:3644:LEU:HD12	1:D:3645:PRO:CD	2.34	0.57
1:A:3644:LEU:HD12	1:A:3645:PRO:CD	2.34	0.57
1:B:3723:MET:HE1	1:B:3792:ALA:HB3	1.85	0.57
1:C:3644:LEU:HD12	1:C:3645:PRO:CD	2.34	0.57
1:A:2967:MET:HE1	1:A:3049:LEU:HD13	1.87	0.56
1:B:3391:GLU:O	1:B:3394:VAL:HG22	2.05	0.56
1:C:2178:MET:CE	1:C:2210:VAL:HG11	2.36	0.56
1:A:3391:GLU:O	1:A:3394:VAL:HG22	2.05	0.56
1:A:2178:MET:CE	1:A:2210:VAL:HG11	2.36	0.56
1:C:3315:LEU:HD12	1:C:3315:LEU:O	2.06	0.56
1:D:1622:GLU:OE1	1:D:1622:GLU:N	2.39	0.56
1:D:2967:MET:HE1	1:D:3049:LEU:HD13	1.87	0.56
1:A:236:ALA:C	1:A:237:ASP:OD1	2.49	0.56
1:B:2967:MET:HE1	1:B:3049:LEU:HD13	1.87	0.56
1:B:236:ALA:C	1:B:237:ASP:OD1	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2178:MET:CE	1:D:2210:VAL:HG11	2.36	0.56
1:D:3315:LEU:HD12	1:D:3315:LEU:O	2.06	0.56
1:C:3391:GLU:O	1:C:3394:VAL:HG22	2.05	0.56
1:C:1622:GLU:N	1:C:1622:GLU:OE1	2.39	0.56
1:D:3391:GLU:O	1:D:3394:VAL:HG22	2.05	0.56
1:A:1622:GLU:N	1:A:1622:GLU:OE1	2.39	0.56
1:B:1622:GLU:OE1	1:B:1622:GLU:N	2.39	0.56
1:B:3315:LEU:HD12	1:B:3315:LEU:O	2.06	0.56
1:A:3315:LEU:HD12	1:A:3315:LEU:O	2.06	0.55
1:B:2178:MET:CE	1:B:2210:VAL:HG11	2.36	0.55
1:C:2967:MET:HE1	1:C:3049:LEU:HD13	1.87	0.55
1:D:236:ALA:C	1:D:237:ASP:OD1	2.49	0.55
1:C:236:ALA:C	1:C:237:ASP:OD1	2.49	0.55
1:D:2178:MET:HE2	1:D:2210:VAL:HG11	1.89	0.54
1:C:2178:MET:HE2	1:C:2210:VAL:HG11	1.89	0.54
1:C:3353:LEU:HD12	1:C:3353:LEU:H	1.73	0.54
1:B:3353:LEU:H	1:B:3353:LEU:HD12	1.73	0.53
1:A:3353:LEU:HD12	1:A:3353:LEU:H	1.73	0.53
1:A:2178:MET:HE2	1:A:2210:VAL:HG11	1.89	0.53
1:D:3353:LEU:HD12	1:D:3353:LEU:H	1.73	0.53
1:B:2522:LEU:HD11	1:B:2582:MET:SD	2.49	0.53
1:A:2522:LEU:HD11	1:A:2582:MET:SD	2.49	0.53
1:A:4731:ILE:HG23	1:A:4732:PHE:CD1	2.44	0.53
1:C:2522:LEU:HD11	1:C:2582:MET:SD	2.49	0.53
1:D:4731:ILE:HG23	1:D:4732:PHE:CD1	2.44	0.53
1:C:4731:ILE:HG23	1:C:4732:PHE:CD1	2.44	0.52
1:D:2522:LEU:HD11	1:D:2582:MET:SD	2.49	0.52
1:B:2178:MET:HE2	1:B:2210:VAL:HG11	1.89	0.52
1:C:509:GLU:OE1	1:C:509:GLU:N	2.42	0.52
1:B:509:GLU:N	1:B:509:GLU:OE1	2.42	0.52
1:D:2523:ASP:OD1	1:D:2524:VAL:HG13	2.10	0.52
1:A:2523:ASP:OD1	1:A:2524:VAL:HG13	2.10	0.52
1:B:4731:ILE:HG23	1:B:4732:PHE:CD1	2.44	0.52
1:A:3644:LEU:HD12	1:A:3645:PRO:HD2	1.91	0.52
1:D:3644:LEU:HD12	1:D:3645:PRO:HD2	1.91	0.52
1:A:509:GLU:N	1:A:509:GLU:OE1	2.42	0.52
1:C:1494:MET:HE1	1:C:1553:PHE:CD2	2.45	0.52
1:D:509:GLU:N	1:D:509:GLU:OE1	2.42	0.52
1:A:1494:MET:HE1	1:A:1553:PHE:CD2	2.45	0.51
1:B:3644:LEU:HD12	1:B:3645:PRO:HD2	1.91	0.51
1:D:1494:MET:HE1	1:D:1553:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2523:ASP:OD1	1:C:2524:VAL:HG13	2.10	0.51
1:D:3528:THR:HG23	1:D:3573:MET:HE2	1.93	0.51
1:C:309:THR:HG22	1:C:309:THR:O	2.10	0.51
1:C:3644:LEU:HD12	1:C:3645:PRO:HD2	1.91	0.51
1:A:4871:GLU:O	1:A:4871:GLU:HG2	2.11	0.51
1:D:4954:MET:HA	1:D:4954:MET:HE3	1.93	0.51
1:B:1494:MET:HE1	1:B:1553:PHE:CD2	2.45	0.51
1:B:3528:THR:HG23	1:B:3573:MET:HE2	1.93	0.51
1:D:4871:GLU:O	1:D:4871:GLU:HG2	2.11	0.51
1:A:3136:LEU:HD12	1:A:3140:LEU:HD23	1.93	0.51
1:C:4871:GLU:O	1:C:4871:GLU:HG2	2.11	0.51
1:A:1228:ILE:HG23	1:A:1229:ASN:N	2.26	0.51
1:A:3528:THR:HG23	1:A:3573:MET:HE2	1.93	0.51
1:B:3136:LEU:HD12	1:B:3140:LEU:HD23	1.93	0.51
1:C:4954:MET:HE3	1:C:4954:MET:HA	1.93	0.51
2:E:11:ASP:C	2:E:11:ASP:OD1	2.54	0.51
1:B:1228:ILE:HG23	1:B:1229:ASN:N	2.26	0.50
1:C:1228:ILE:HG23	1:C:1229:ASN:N	2.26	0.50
1:C:3372:VAL:HG21	1:C:3401:LEU:CD1	2.31	0.50
2:H:11:ASP:C	2:H:11:ASP:OD1	2.54	0.50
1:B:309:THR:O	1:B:309:THR:HG22	2.10	0.50
1:C:3226:GLU:O	1:C:3227:ARG:HB2	2.12	0.50
1:D:3136:LEU:HD12	1:D:3140:LEU:HD23	1.93	0.50
1:A:309:THR:HG22	1:A:309:THR:O	2.10	0.50
1:A:4954:MET:HE3	1:A:4954:MET:HA	1.93	0.50
1:B:4871:GLU:HG2	1:B:4871:GLU:O	2.11	0.50
1:C:3528:THR:HG23	1:C:3573:MET:HE2	1.93	0.50
1:B:2672:LEU:HD12	1:B:2672:LEU:H	1.77	0.50
1:A:3372:VAL:HG21	1:A:3401:LEU:CD1	2.31	0.50
1:B:2523:ASP:OD1	1:B:2524:VAL:HG13	2.10	0.50
1:B:3226:GLU:O	1:B:3227:ARG:HB2	2.12	0.50
1:D:908:VAL:HG13	1:D:909:ASN:H	1.77	0.50
1:D:1228:ILE:HG23	1:D:1229:ASN:N	2.26	0.50
1:B:2971:GLN:OE1	1:B:2971:GLN:O	2.30	0.50
1:C:908:VAL:HG13	1:C:909:ASN:H	1.77	0.50
1:D:3226:GLU:O	1:D:3227:ARG:HB2	2.12	0.50
1:A:2672:LEU:HD12	1:A:2672:LEU:H	1.77	0.50
1:B:908:VAL:HG13	1:B:909:ASN:H	1.77	0.50
1:C:2672:LEU:HD12	1:C:2672:LEU:H	1.77	0.50
1:C:2971:GLN:O	1:C:2971:GLN:OE1	2.30	0.50
1:D:309:THR:O	1:D:309:THR:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4954:MET:HE3	1:B:4954:MET:HA	1.93	0.49
1:D:2672:LEU:HD12	1:D:2672:LEU:H	1.77	0.49
2:G:11:ASP:OD1	2:G:11:ASP:C	2.54	0.49
1:C:3136:LEU:HD12	1:C:3140:LEU:HD23	1.93	0.49
1:D:2858:GLN:N	1:D:2859:PRO:CD	2.76	0.49
2:E:79:ASP:OD1	2:E:79:ASP:C	2.56	0.49
2:F:11:ASP:OD1	2:F:11:ASP:C	2.54	0.49
1:B:2858:GLN:N	1:B:2859:PRO:CD	2.76	0.49
1:C:2858:GLN:N	1:C:2859:PRO:CD	2.76	0.49
2:H:79:ASP:OD1	2:H:79:ASP:C	2.56	0.49
1:A:908:VAL:HG13	1:A:909:ASN:H	1.77	0.49
1:A:3226:GLU:O	1:A:3227:ARG:HB2	2.12	0.49
1:D:1022:VAL:HG22	1:D:1023:PRO:HD2	1.95	0.49
1:A:2967:MET:HE1	1:A:3049:LEU:CD1	2.43	0.48
1:A:2971:GLN:OE1	1:A:2971:GLN:O	2.30	0.48
2:G:79:ASP:C	2:G:79:ASP:OD1	2.56	0.48
1:A:2858:GLN:N	1:A:2859:PRO:CD	2.76	0.48
1:C:1022:VAL:HG22	1:C:1023:PRO:HD2	1.95	0.48
1:D:2971:GLN:OE1	1:D:2971:GLN:O	2.30	0.48
1:B:3372:VAL:HG21	1:B:3401:LEU:CD1	2.31	0.48
2:F:79:ASP:OD1	2:F:79:ASP:C	2.56	0.48
1:C:2874:MET:HE1	1:C:2938:THR:HA	1.96	0.48
1:B:463:GLU:OE1	1:B:463:GLU:HA	2.14	0.48
1:B:2874:MET:HE1	1:B:2938:THR:HA	1.96	0.48
1:D:3372:VAL:HG21	1:D:3401:LEU:CD1	2.30	0.48
1:D:2967:MET:HE1	1:D:3049:LEU:CD1	2.43	0.48
1:A:463:GLU:HA	1:A:463:GLU:OE1	2.14	0.48
1:C:3989:VAL:HG11	1:C:4047:MET:HE2	1.95	0.48
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.95	0.48
1:C:2967:MET:HE1	1:C:3049:LEU:CD1	2.43	0.48
1:C:2527:LEU:HD12	1:C:2527:LEU:O	2.14	0.48
1:D:3989:VAL:HG11	1:D:4047:MET:HE2	1.95	0.48
1:B:2967:MET:HE1	1:B:3049:LEU:CD1	2.43	0.48
1:B:2527:LEU:HD12	1:B:2527:LEU:O	2.14	0.47
1:A:2874:MET:HE1	1:A:2938:THR:HA	1.96	0.47
1:B:3877:ASP:OD1	1:B:3877:ASP:N	2.48	0.47
1:B:3989:VAL:HG11	1:B:4047:MET:HE2	1.95	0.47
1:D:2527:LEU:HD12	1:D:2527:LEU:O	2.14	0.47
1:A:1063:VAL:HG13	1:A:1064:GLU:N	2.30	0.47
1:D:2874:MET:HE1	1:D:2938:THR:HA	1.96	0.47
1:A:1228:ILE:HG23	1:A:1229:ASN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:VAL:HG22	1:B:1023:PRO:HD2	1.95	0.47
1:B:2101:MET:HE2	1:B:2101:MET:HA	1.97	0.47
1:D:463:GLU:OE1	1:D:463:GLU:HA	2.14	0.47
1:A:929:LEU:O	1:A:933:LEU:HD12	2.15	0.47
1:C:849:THR:HG22	1:C:850:ASP:N	2.27	0.47
1:A:2527:LEU:O	1:A:2527:LEU:HD12	2.14	0.47
1:A:3239:MET:HE3	1:A:3239:MET:HA	1.97	0.47
1:A:3989:VAL:HG11	1:A:4047:MET:HE2	1.95	0.47
1:D:1063:VAL:HG13	1:D:1064:GLU:N	2.30	0.47
1:D:3239:MET:HE3	1:D:3239:MET:HA	1.97	0.47
1:D:3423:TRP:CD1	1:D:3423:TRP:N	2.83	0.47
1:A:2101:MET:HA	1:A:2101:MET:HE2	1.97	0.47
1:B:1228:ILE:HG23	1:B:1229:ASN:H	1.80	0.47
1:D:2101:MET:HA	1:D:2101:MET:HE2	1.97	0.47
1:B:1063:VAL:HG13	1:B:1064:GLU:N	2.30	0.47
1:C:1228:ILE:HG23	1:C:1229:ASN:H	1.80	0.47
1:C:3877:ASP:N	1:C:3877:ASP:OD1	2.48	0.47
1:A:3423:TRP:N	1:A:3423:TRP:CD1	2.83	0.46
1:C:2101:MET:HE2	1:C:2101:MET:HA	1.97	0.46
1:C:3423:TRP:CD1	1:C:3423:TRP:N	2.83	0.46
1:D:3877:ASP:OD1	1:D:3877:ASP:N	2.48	0.46
1:C:929:LEU:O	1:C:933:LEU:HD12	2.15	0.46
1:C:3239:MET:HE3	1:C:3239:MET:HA	1.97	0.46
1:C:3397:GLU:O	1:C:3401:LEU:HG	2.16	0.46
1:A:2751:LEU:H	1:A:2751:LEU:HD23	1.80	0.46
1:A:3877:ASP:OD1	1:A:3877:ASP:N	2.48	0.46
1:B:2751:LEU:HD23	1:B:2751:LEU:H	1.80	0.46
1:B:3397:GLU:O	1:B:3401:LEU:HG	2.16	0.46
1:D:929:LEU:O	1:D:933:LEU:HD12	2.15	0.46
1:B:3239:MET:HA	1:B:3239:MET:HE3	1.97	0.46
1:C:463:GLU:HA	1:C:463:GLU:OE1	2.14	0.46
1:C:1063:VAL:HG13	1:C:1064:GLU:N	2.30	0.46
1:D:1228:ILE:HG23	1:D:1229:ASN:H	1.80	0.46
1:B:929:LEU:O	1:B:933:LEU:HD12	2.15	0.46
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.31	0.46
1:D:577:ILE:O	1:D:577:ILE:HG22	2.16	0.46
1:D:2751:LEU:H	1:D:2751:LEU:HD23	1.80	0.46
1:A:3397:GLU:O	1:A:3401:LEU:HG	2.16	0.46
1:C:3690:VAL:HG22	1:C:3690:VAL:O	2.16	0.46
1:B:2006:ILE:HD11	1:B:3641:LEU:HD21	1.98	0.46
1:D:3690:VAL:HG22	1:D:3690:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ILE:HG22	1:A:577:ILE:O	2.16	0.46
1:B:908:VAL:HG13	1:B:909:ASN:N	2.31	0.46
1:B:3723:MET:HE1	1:B:3792:ALA:CB	2.46	0.46
1:A:3690:VAL:HG22	1:A:3690:VAL:O	2.16	0.45
1:B:3690:VAL:HG22	1:B:3690:VAL:O	2.16	0.45
1:C:577:ILE:HG22	1:C:577:ILE:O	2.16	0.45
1:C:2006:ILE:HD11	1:C:3641:LEU:HD21	1.98	0.45
1:D:3397:GLU:O	1:D:3401:LEU:HG	2.16	0.45
1:B:577:ILE:HG22	1:B:577:ILE:O	2.16	0.45
1:D:947:GLU:HG3	1:D:1049:TYR:CD1	2.51	0.45
1:D:3391:GLU:O	1:D:3395:ARG:HG3	2.17	0.45
1:A:3723:MET:HE1	1:A:3792:ALA:CB	2.46	0.45
1:A:3867:ASN:O	1:A:3868:ARG:C	2.59	0.45
1:A:947:GLU:HG3	1:A:1049:TYR:CD1	2.51	0.45
1:B:3867:ASN:O	1:B:3868:ARG:C	2.59	0.45
1:C:947:GLU:HG3	1:C:1049:TYR:CD1	2.51	0.45
1:C:2662:ALA:C	1:C:2663:ASN:OD1	2.59	0.45
1:A:2662:ALA:C	1:A:2663:ASN:OD1	2.59	0.45
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.31	0.45
1:C:908:VAL:HG13	1:C:909:ASN:N	2.31	0.45
1:C:2751:LEU:HD23	1:C:2751:LEU:H	1.80	0.45
1:C:3723:MET:HE1	1:C:3792:ALA:CB	2.46	0.45
1:D:2662:ALA:C	1:D:2663:ASN:OD1	2.59	0.45
1:D:3867:ASN:O	1:D:3868:ARG:C	2.59	0.45
1:B:2662:ALA:C	1:B:2663:ASN:OD1	2.59	0.45
1:C:3391:GLU:O	1:C:3395:ARG:HG3	2.16	0.45
1:C:3883:ASP:C	1:C:3883:ASP:OD1	2.60	0.45
1:A:908:VAL:HG13	1:A:909:ASN:N	2.31	0.45
1:B:3423:TRP:N	1:B:3423:TRP:CD1	2.83	0.45
1:B:3509:LEU:O	1:B:3513:THR:HG23	2.17	0.45
1:D:2006:ILE:HD11	1:D:3641:LEU:HD21	1.98	0.45
1:D:3883:ASP:OD1	1:D:3883:ASP:C	2.60	0.45
1:B:947:GLU:HG3	1:B:1049:TYR:CD1	2.51	0.45
1:A:2619:LEU:O	1:A:2623:LEU:HD13	2.17	0.45
1:B:3133:THR:HG23	1:B:3134:VAL:HG23	1.99	0.45
1:C:3509:LEU:O	1:C:3513:THR:HG23	2.17	0.45
1:A:849:THR:HG22	1:A:850:ASP:N	2.27	0.45
1:B:1280:GLN:O	1:B:1281:ASN:OD1	2.35	0.45
1:D:2619:LEU:O	1:D:2623:LEU:HD13	2.17	0.45
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.31	0.45
1:A:2006:ILE:HD11	1:A:3641:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2619:LEU:O	1:C:2623:LEU:HD13	2.17	0.44
1:C:3133:THR:HG23	1:C:3134:VAL:HG23	1.99	0.44
1:C:3666:ASP:OD1	1:C:3666:ASP:C	2.60	0.44
1:D:2228:MET:SD	1:D:2228:MET:C	3.01	0.44
1:D:3723:MET:HE1	1:D:3792:ALA:CB	2.46	0.44
1:A:2228:MET:SD	1:A:2228:MET:C	3.01	0.44
1:B:3666:ASP:C	1:B:3666:ASP:OD1	2.60	0.44
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.31	0.44
1:B:2228:MET:C	1:B:2228:MET:SD	3.01	0.44
1:D:908:VAL:HG13	1:D:909:ASN:N	2.31	0.44
1:D:3265:GLU:HG2	1:D:3266:MET:SD	2.57	0.44
1:A:1280:GLN:O	1:A:1281:ASN:OD1	2.35	0.44
1:A:3265:GLU:HG2	1:A:3266:MET:SD	2.57	0.44
1:A:3391:GLU:O	1:A:3395:ARG:HG3	2.16	0.44
1:A:3644:LEU:HD12	1:A:3645:PRO:HD3	1.99	0.44
1:C:3867:ASN:O	1:C:3868:ARG:C	2.59	0.44
1:A:3865:VAL:O	1:A:3865:VAL:HG13	2.17	0.44
1:B:3883:ASP:OD1	1:B:3883:ASP:C	2.60	0.44
1:D:3644:LEU:HD12	1:D:3645:PRO:HD3	1.99	0.44
1:B:3865:VAL:HG13	1:B:3865:VAL:O	2.17	0.44
1:B:4725:LEU:HD22	1:B:4743:MET:HE1	2.00	0.44
1:C:4954:MET:HE3	1:C:4954:MET:CA	2.48	0.44
1:D:3509:LEU:O	1:D:3513:THR:HG23	2.17	0.44
1:A:3780:LEU:HD21	1:A:3816:MET:SD	2.57	0.44
1:A:3883:ASP:OD1	1:A:3883:ASP:C	2.60	0.44
1:C:3265:GLU:HG2	1:C:3266:MET:SD	2.57	0.44
1:C:4725:LEU:HD22	1:C:4743:MET:HE1	2.00	0.44
1:A:3133:THR:HG23	1:A:3134:VAL:HG23	1.99	0.44
1:B:2619:LEU:O	1:B:2623:LEU:HD13	2.17	0.44
1:C:3528:THR:HG23	1:C:3573:MET:HE3	2.00	0.44
1:C:3780:LEU:HD21	1:C:3816:MET:SD	2.57	0.44
1:D:3133:THR:HG23	1:D:3134:VAL:HG23	1.99	0.44
1:D:3780:LEU:HD21	1:D:3816:MET:SD	2.58	0.44
1:D:4954:MET:HE3	1:D:4954:MET:CA	2.48	0.44
1:B:3391:GLU:O	1:B:3395:ARG:HG3	2.16	0.44
1:B:3780:LEU:HD21	1:B:3816:MET:SD	2.57	0.44
1:C:2228:MET:SD	1:C:2228:MET:C	3.01	0.44
1:B:3192:GLU:OE1	1:B:3192:GLU:O	2.37	0.43
1:C:1280:GLN:O	1:C:1281:ASN:OD1	2.35	0.43
1:C:3865:VAL:HG13	1:C:3865:VAL:O	2.17	0.43
1:D:3865:VAL:HG13	1:D:3865:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3644:LEU:HD12	1:B:3645:PRO:HD3	1.99	0.43
1:A:4954:MET:HE3	1:A:4954:MET:CA	2.48	0.43
1:D:3528:THR:HG23	1:D:3573:MET:HE3	2.00	0.43
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.01	0.43
1:B:2714:TYR:CD1	1:B:2714:TYR:C	2.96	0.43
1:B:3265:GLU:HG2	1:B:3266:MET:SD	2.57	0.43
1:B:4954:MET:HE3	1:B:4954:MET:CA	2.48	0.43
1:D:1280:GLN:O	1:D:1281:ASN:OD1	2.35	0.43
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	2.01	0.43
1:A:3509:LEU:O	1:A:3513:THR:HG23	2.17	0.43
1:A:3192:GLU:O	1:A:3192:GLU:OE1	2.37	0.43
1:A:4725:LEU:HD22	1:A:4743:MET:HE1	2.00	0.43
1:C:1991:THR:O	1:C:1995:THR:HG23	2.19	0.43
1:C:3192:GLU:OE1	1:C:3192:GLU:O	2.36	0.43
1:D:1855:GLY:O	1:D:1859:VAL:HG23	2.19	0.43
1:D:3666:ASP:OD1	1:D:3666:ASP:C	2.60	0.43
1:A:4244:GLU:OE1	1:A:4244:GLU:HA	2.19	0.43
1:C:2001:PRO:HG2	1:C:3864:THR:HG21	2.00	0.43
1:D:2714:TYR:C	1:D:2714:TYR:CD1	2.96	0.43
1:D:4244:GLU:OE1	1:D:4244:GLU:HA	2.19	0.43
1:A:2714:TYR:CD1	1:A:2714:TYR:C	2.96	0.43
1:B:1068:ARG:NE	1:B:1068:ARG:HA	2.34	0.43
1:C:3644:LEU:HD12	1:C:3645:PRO:HD3	1.99	0.43
1:D:2001:PRO:HG2	1:D:3864:THR:HG21	2.00	0.43
1:A:1991:THR:O	1:A:1995:THR:HG23	2.19	0.43
1:B:2001:PRO:HG2	1:B:3864:THR:HG21	2.00	0.43
1:C:1068:ARG:HA	1:C:1068:ARG:NE	2.34	0.43
1:C:2714:TYR:CD1	1:C:2714:TYR:C	2.96	0.43
1:A:1281:ASN:OD1	1:A:1281:ASN:C	2.62	0.43
1:A:2858:GLN:O	1:A:2859:PRO:C	2.62	0.43
1:A:3666:ASP:OD1	1:A:3666:ASP:C	2.60	0.43
1:A:4224:GLU:OE1	1:A:4224:GLU:O	2.37	0.43
1:B:1281:ASN:OD1	1:B:1281:ASN:C	2.62	0.43
1:B:2858:GLN:O	1:B:2859:PRO:C	2.62	0.43
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	2.01	0.43
1:D:1068:ARG:HA	1:D:1068:ARG:NE	2.34	0.43
1:A:1068:ARG:HA	1:A:1068:ARG:NE	2.34	0.42
1:A:2001:PRO:HG2	1:A:3864:THR:HG21	2.00	0.42
1:B:2138:LEU:N	1:B:2139:PRO:CD	2.82	0.42
1:B:2971:GLN:OE1	1:B:2974:ILE:HD11	2.19	0.42
1:B:3050:VAL:O	1:B:3050:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4224:GLU:O	1:B:4224:GLU:OE1	2.37	0.42
1:C:1855:GLY:O	1:C:1859:VAL:HG23	2.19	0.42
1:C:3398:PHE:HA	1:C:3401:LEU:HD12	2.01	0.42
1:B:849:THR:O	1:B:850:ASP:CB	2.67	0.42
1:C:2138:LEU:N	1:C:2139:PRO:CD	2.82	0.42
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	2.01	0.42
1:D:78:LEU:O	1:D:78:LEU:HD12	2.19	0.42
1:A:3206:LEU:HD12	1:A:3280:TYR:CE2	2.54	0.42
1:A:3528:THR:HG23	1:A:3573:MET:HE3	2.00	0.42
1:B:459:LEU:N	1:B:459:LEU:HD22	2.35	0.42
1:B:1855:GLY:O	1:B:1859:VAL:HG23	2.18	0.42
1:C:849:THR:O	1:C:850:ASP:CB	2.67	0.42
1:A:78:LEU:HD12	1:A:78:LEU:O	2.20	0.42
1:B:78:LEU:O	1:B:78:LEU:HD12	2.19	0.42
1:B:1991:THR:O	1:B:1995:THR:HG23	2.19	0.42
1:C:2971:GLN:OE1	1:C:2974:ILE:HD11	2.19	0.42
1:D:3192:GLU:O	1:D:3192:GLU:OE1	2.37	0.42
1:A:2819:TRP:C	1:A:2820:GLU:HG3	2.45	0.42
1:B:4244:GLU:HA	1:B:4244:GLU:OE1	2.19	0.42
1:C:590:LEU:HD21	1:C:599:VAL:HB	2.02	0.42
1:D:923:GLN:HB2	1:D:924:MET:HE2	2.02	0.42
1:D:4224:GLU:O	1:D:4224:GLU:OE1	2.37	0.42
1:D:4725:LEU:HD22	1:D:4743:MET:HE1	2.00	0.42
1:A:923:GLN:HB2	1:A:924:MET:HE2	2.02	0.42
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.01	0.42
1:C:459:LEU:N	1:C:459:LEU:HD22	2.35	0.42
1:D:2545:GLU:H	1:D:2545:GLU:CD	2.28	0.42
1:B:623:GLU:HA	1:B:623:GLU:OE1	2.20	0.42
1:B:2819:TRP:C	1:B:2820:GLU:HG3	2.45	0.42
1:B:3398:PHE:HA	1:B:3401:LEU:HD12	2.01	0.42
1:D:590:LEU:HD21	1:D:599:VAL:HB	2.02	0.42
1:A:2138:LEU:N	1:A:2139:PRO:CD	2.82	0.42
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	2.01	0.42
1:C:2858:GLN:O	1:C:2859:PRO:C	2.62	0.42
1:C:3206:LEU:HD12	1:C:3280:TYR:CE2	2.54	0.42
1:C:4224:GLU:OE1	1:C:4224:GLU:O	2.37	0.42
1:C:4244:GLU:OE1	1:C:4244:GLU:HA	2.19	0.42
1:D:623:GLU:OE1	1:D:623:GLU:HA	2.20	0.42
1:D:2138:LEU:N	1:D:2139:PRO:CD	2.82	0.42
1:A:292:ALA:HB2	1:A:312:THR:HG22	2.02	0.42
1:A:1855:GLY:O	1:A:1859:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:HB2	1:B:312:THR:HG22	2.02	0.42
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	2.01	0.42
1:C:2545:GLU:CD	1:C:2545:GLU:H	2.28	0.42
1:C:3050:VAL:HG22	1:C:3050:VAL:O	2.19	0.42
1:D:2819:TRP:C	1:D:2820:GLU:HG3	2.45	0.42
1:D:3050:VAL:O	1:D:3050:VAL:HG22	2.19	0.42
1:D:3398:PHE:HA	1:D:3401:LEU:HD12	2.01	0.42
1:A:1518:CYS:C	1:A:1519:LEU:HD12	2.45	0.42
1:B:1425:GLU:CD	1:B:1425:GLU:C	2.88	0.42
1:B:2964:LEU:HD11	1:B:3038:MET:HB3	2.01	0.42
1:B:3206:LEU:HD12	1:B:3280:TYR:CE2	2.54	0.42
1:C:292:ALA:HB2	1:C:312:THR:HG22	2.02	0.42
1:D:1281:ASN:OD1	1:D:1281:ASN:C	2.62	0.42
1:D:2971:GLN:OE1	1:D:2974:ILE:HD11	2.19	0.42
1:A:849:THR:O	1:A:850:ASP:CB	2.67	0.41
1:C:1281:ASN:OD1	1:C:1281:ASN:C	2.62	0.41
1:D:1991:THR:O	1:D:1995:THR:HG23	2.19	0.41
1:D:2692:ASP:OD2	1:D:2695:LEU:HD13	2.20	0.41
1:D:3424:LEU:HD23	1:D:3424:LEU:O	2.20	0.41
1:A:2545:GLU:CD	1:A:2545:GLU:H	2.28	0.41
1:A:2964:LEU:HD11	1:A:3038:MET:HB3	2.02	0.41
1:A:2971:GLN:OE1	1:A:2974:ILE:HD11	2.19	0.41
1:C:623:GLU:OE1	1:C:623:GLU:HA	2.20	0.41
1:D:1518:CYS:C	1:D:1519:LEU:HD12	2.45	0.41
1:A:459:LEU:N	1:A:459:LEU:HD22	2.35	0.41
1:A:3132:THR:HA	1:A:3136:LEU:HB3	2.02	0.41
1:A:3239:MET:N	1:A:3239:MET:SD	2.93	0.41
1:B:3132:THR:HA	1:B:3136:LEU:HB3	2.02	0.41
1:B:4772:ASP:OD1	1:B:4772:ASP:C	2.63	0.41
1:C:2692:ASP:OD2	1:C:2695:LEU:HD13	2.20	0.41
1:D:2858:GLN:O	1:D:2859:PRO:C	2.62	0.41
1:D:2964:LEU:HD11	1:D:3038:MET:HB3	2.02	0.41
1:D:3132:THR:HA	1:D:3136:LEU:HB3	2.03	0.41
1:D:3239:MET:SD	1:D:3239:MET:N	2.93	0.41
1:A:623:GLU:OE1	1:A:623:GLU:HA	2.20	0.41
1:B:1478:ASP:C	1:B:1478:ASP:OD1	2.64	0.41
1:B:2545:GLU:H	1:B:2545:GLU:CD	2.28	0.41
1:B:3424:LEU:O	1:B:3424:LEU:HD23	2.20	0.41
1:C:78:LEU:HD12	1:C:78:LEU:O	2.20	0.41
1:C:1478:ASP:OD1	1:C:1478:ASP:C	2.63	0.41
1:C:2819:TRP:C	1:C:2820:GLU:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3132:THR:HA	1:C:3136:LEU:HB3	2.02	0.41
1:D:292:ALA:HB2	1:D:312:THR:HG22	2.02	0.41
1:A:2692:ASP:OD2	1:A:2695:LEU:HD13	2.20	0.41
1:A:3050:VAL:HG22	1:A:3050:VAL:O	2.19	0.41
1:B:590:LEU:HD21	1:B:599:VAL:HB	2.02	0.41
1:B:688:LEU:HD21	1:B:775:GLY:HA3	2.03	0.41
1:B:3239:MET:SD	1:B:3239:MET:N	2.93	0.41
1:C:688:LEU:HD21	1:C:775:GLY:HA3	2.03	0.41
1:C:908:VAL:O	1:C:961:MET:HE1	2.21	0.41
1:C:1425:GLU:C	1:C:1425:GLU:CD	2.88	0.41
1:C:2964:LEU:HD11	1:C:3038:MET:HB3	2.02	0.41
1:D:3206:LEU:HD12	1:D:3280:TYR:CE2	2.54	0.41
1:A:642:THR:HG22	1:A:643:SER:N	2.35	0.41
1:B:642:THR:HG22	1:B:643:SER:N	2.35	0.41
1:C:3239:MET:N	1:C:3239:MET:SD	2.93	0.41
1:D:1425:GLU:C	1:D:1425:GLU:CD	2.88	0.41
1:A:3398:PHE:HA	1:A:3401:LEU:HD12	2.01	0.41
1:B:923:GLN:HB2	1:B:924:MET:HE2	2.02	0.41
1:B:2692:ASP:OD2	1:B:2695:LEU:HD13	2.20	0.41
1:D:459:LEU:HD22	1:D:459:LEU:N	2.35	0.41
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	2.01	0.41
1:A:127:MET:HE2	1:A:127:MET:HA	2.03	0.41
1:A:590:LEU:HD21	1:A:599:VAL:HB	2.02	0.41
1:A:1425:GLU:C	1:A:1425:GLU:CD	2.88	0.41
1:A:3424:LEU:HD23	1:A:3424:LEU:O	2.20	0.41
1:D:753:PRO:HG3	1:D:773:LEU:HD21	2.03	0.41
1:A:753:PRO:HG3	1:A:773:LEU:HD21	2.03	0.41
1:A:1108:GLU:O	1:A:1108:GLU:CG	2.69	0.41
1:A:2002:PRO:HB2	1:A:3652:MET:HE1	2.03	0.41
1:B:127:MET:HA	1:B:127:MET:HE2	2.03	0.41
1:B:626:LEU:N	1:B:627:PRO:HD2	2.36	0.41
1:B:4224:GLU:OE1	1:B:4224:GLU:C	2.64	0.41
1:C:127:MET:HE2	1:C:127:MET:HA	2.03	0.41
1:C:3424:LEU:O	1:C:3424:LEU:HD23	2.20	0.41
1:D:127:MET:HE2	1:D:127:MET:HA	2.03	0.41
1:D:642:THR:HG22	1:D:643:SER:N	2.35	0.41
1:D:688:LEU:HD21	1:D:775:GLY:HA3	2.03	0.41
1:D:1478:ASP:OD1	1:D:1478:ASP:C	2.64	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.36	0.41
1:B:849:THR:HG22	1:B:850:ASP:N	2.27	0.41
1:B:1518:CYS:C	1:B:1519:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:THR:HG22	1:C:643:SER:N	2.35	0.41
1:C:1518:CYS:C	1:C:1519:LEU:HD12	2.45	0.41
1:C:3392:LEU:HD13	1:C:3395:ARG:HD3	2.03	0.41
1:D:2002:PRO:HB2	1:D:3652:MET:HE1	2.03	0.41
1:D:3276:MET:HE2	1:D:3276:MET:HB3	1.98	0.41
1:D:4224:GLU:OE1	1:D:4224:GLU:C	2.64	0.41
1:B:3137:LEU:HB3	1:B:3138:PRO:HD3	2.03	0.40
1:D:2751:LEU:HG	1:D:2751:LEU:O	2.21	0.40
1:D:3612:PRO:O	1:D:3614:LYS:N	2.54	0.40
1:A:688:LEU:HD21	1:A:775:GLY:HA3	2.03	0.40
1:A:4772:ASP:OD1	1:A:4772:ASP:C	2.64	0.40
1:B:2751:LEU:O	1:B:2751:LEU:HG	2.21	0.40
1:B:3392:LEU:HD13	1:B:3395:ARG:HD3	2.03	0.40
1:B:3528:THR:HG23	1:B:3573:MET:HE3	2.00	0.40
1:D:908:VAL:O	1:D:961:MET:HE1	2.21	0.40
1:D:3392:LEU:HD13	1:D:3395:ARG:HD3	2.03	0.40
1:B:2926:LEU:C	1:B:2926:LEU:HD23	2.47	0.40
1:C:3313:ASN:OD1	1:C:3313:ASN:C	2.64	0.40
1:A:972:LEU:HD12	1:A:972:LEU:C	2.47	0.40
1:A:1153:ILE:HD11	1:A:1155:LEU:HD21	2.04	0.40
1:A:2008:MET:HE2	1:A:2008:MET:CA	2.50	0.40
1:A:2926:LEU:C	1:A:2926:LEU:HD23	2.47	0.40
1:B:3409:TYR:N	1:B:3410:PRO:HD2	2.37	0.40
1:C:753:PRO:HG3	1:C:773:LEU:HD21	2.03	0.40
1:C:923:GLN:HB2	1:C:924:MET:HE2	2.02	0.40
1:C:961:MET:HE2	1:C:965:TYR:O	2.22	0.40
1:C:4772:ASP:OD1	1:C:4772:ASP:C	2.64	0.40
1:D:972:LEU:HD12	1:D:972:LEU:C	2.47	0.40
1:A:908:VAL:O	1:A:961:MET:HE1	2.21	0.40
1:A:961:MET:HE2	1:A:965:TYR:O	2.22	0.40
1:A:1478:ASP:OD1	1:A:1478:ASP:C	2.64	0.40
1:C:626:LEU:N	1:C:627:PRO:HD2	2.36	0.40
1:C:4224:GLU:OE1	1:C:4224:GLU:C	2.64	0.40
1:D:626:LEU:N	1:D:627:PRO:HD2	2.36	0.40
1:D:849:THR:O	1:D:850:ASP:CB	2.67	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%)	4255 (97%)	120 (3%)	1 (0%)	100	100
1	B	4376/5037 (87%)	4255 (97%)	120 (3%)	1 (0%)	100	100
1	C	4376/5037 (87%)	4253 (97%)	122 (3%)	1 (0%)	100	100
1	D	4376/5037 (87%)	4253 (97%)	122 (3%)	1 (0%)	100	100
2	E	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	G	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
All	All	17924/20580 (87%)	17404 (97%)	516 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3613	TYR
1	B	3613	TYR
1	C	3613	TYR
1	D	3613	TYR

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%)	3805 (99%)	22 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	3827/4276 (90%)	3805 (99%)	22 (1%)	78	79
1	C	3827/4276 (90%)	3805 (99%)	22 (1%)	78	79
1	D	3827/4276 (90%)	3805 (99%)	22 (1%)	78	79
2	E	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	F	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	G	89/90 (99%)	88 (99%)	1 (1%)	65	73
2	H	89/90 (99%)	88 (99%)	1 (1%)	65	73
All	All	15664/17464 (90%)	15572 (99%)	92 (1%)	76	79

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	155	LYS
1	A	622	THR
1	A	957	LYS
1	A	1025	ARG
1	A	1435	TYR
1	A	1561	VAL
1	A	1929	MET
1	A	2156	LEU
1	A	2222	GLU
1	A	2522	LEU
1	A	2747	ILE
1	A	2775	TRP
1	A	3564	GLU
1	A	3723	MET
1	A	3766	GLN
1	A	3944	GLU
1	A	4070	ASP
1	A	4636	THR
1	A	4749	GLU
1	A	4882	CYS
1	A	5035	GLN
1	B	31	GLU
1	B	155	LYS
1	B	622	THR
1	B	957	LYS
1	B	1025	ARG
1	B	1435	TYR

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Mol	Chain	Res	Type
1	B	1561	VAL
1	B	1929	MET
1	B	2156	LEU
1	B	2222	GLU
1	B	2522	LEU
1	B	2747	ILE
1	B	2775	TRP
1	B	3564	GLU
1	B	3723	MET
1	B	3766	GLN
1	B	3944	GLU
1	B	4070	ASP
1	B	4636	THR
1	B	4749	GLU
1	B	4882	CYS
1	B	5035	GLN
1	C	31	GLU
1	C	155	LYS
1	C	622	THR
1	C	957	LYS
1	C	1025	ARG
1	C	1435	TYR
1	C	1561	VAL
1	C	1929	MET
1	C	2156	LEU
1	C	2222	GLU
1	C	2522	LEU
1	C	2747	ILE
1	C	2775	TRP
1	C	3564	GLU
1	C	3723	MET
1	C	3766	GLN
1	C	3944	GLU
1	C	4070	ASP
1	C	4636	THR
1	C	4749	GLU
1	C	4882	CYS
1	C	5035	GLN
1	D	31	GLU
1	D	155	LYS
1	D	622	THR
1	D	957	LYS

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Mol	Chain	Res	Type
1	D	1025	ARG
1	D	1435	TYR
1	D	1561	VAL
1	D	1929	MET
1	D	2156	LEU
1	D	2222	GLU
1	D	2522	LEU
1	D	2747	ILE
1	D	2775	TRP
1	D	3564	GLU
1	D	3723	MET
1	D	3766	GLN
1	D	3944	GLU
1	D	4070	ASP
1	D	4636	THR
1	D	4880	MET
1	D	4882	CYS
1	D	5035	GLN
2	E	77	SER
2	F	77	SER
2	G	77	SER
2	H	77	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	405	HIS
1	A	461	HIS
1	A	681	HIS
1	A	720	HIS
1	A	838	HIS
1	A	974	HIS
1	A	1066	GLN
1	A	1133	HIS
1	A	1229	ASN
1	A	1231	GLN
1	A	1458	HIS
1	A	1460	HIS
1	A	1719	HIS
1	A	1775	HIS
1	A	1824	GLN

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Mol	Chain	Res	Type
1	A	2011	HIS
1	A	2194	HIS
1	A	2284	ASN
1	A	2441	HIS
1	A	3150	HIS
1	A	3268	HIS
1	A	3870	ASN
1	A	3927	GLN
1	A	4806	ASN
1	A	4886	HIS
1	B	218	HIS
1	B	255	HIS
1	B	405	HIS
1	B	461	HIS
1	B	681	HIS
1	B	765	GLN
1	B	838	HIS
1	B	974	HIS
1	B	1066	GLN
1	B	1133	HIS
1	B	1229	ASN
1	B	1231	GLN
1	B	1300	HIS
1	B	1460	HIS
1	B	1719	HIS
1	B	1775	HIS
1	B	1824	GLN
1	B	2011	HIS
1	B	2194	HIS
1	B	2284	ASN
1	B	2441	HIS
1	B	3150	HIS
1	B	3268	HIS
1	B	3869	GLN
1	B	3870	ASN
1	B	3927	GLN
1	B	4806	ASN
1	B	4886	HIS
1	C	255	HIS
1	C	405	HIS
1	C	461	HIS
1	C	838	HIS

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Mol	Chain	Res	Type
1	C	974	HIS
1	C	1066	GLN
1	C	1133	HIS
1	C	1229	ASN
1	C	1231	GLN
1	C	1458	HIS
1	C	1460	HIS
1	C	1719	HIS
1	C	1775	HIS
1	C	1824	GLN
1	C	2011	HIS
1	C	2194	HIS
1	C	2284	ASN
1	C	2441	HIS
1	C	3150	HIS
1	C	3268	HIS
1	C	3869	GLN
1	C	3870	ASN
1	C	3927	GLN
1	C	4806	ASN
1	C	4886	HIS
1	D	151	HIS
1	D	218	HIS
1	D	255	HIS
1	D	405	HIS
1	D	461	HIS
1	D	681	HIS
1	D	765	GLN
1	D	838	HIS
1	D	974	HIS
1	D	1133	HIS
1	D	1229	ASN
1	D	1231	GLN
1	D	1460	HIS
1	D	1719	HIS
1	D	1775	HIS
1	D	1824	GLN
1	D	2011	HIS
1	D	2194	HIS
1	D	2284	ASN
1	D	2441	HIS
1	D	3150	HIS

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Mol	Chain	Res	Type
1	D	3268	HIS
1	D	3621	HIS
1	D	3870	ASN
1	D	3927	GLN
1	D	4806	ASN
2	F	94	HIS
2	G	94	HIS
2	H	94	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	POV	B	5104	-	51,51,51	0.74	0	57,59,59	0.64	1 (1%)
5	POV	D	5103	-	51,51,51	0.73	0	57,59,59	0.63	1 (1%)
5	POV	A	5104	-	51,51,51	0.86	2 (3%)	57,59,59	0.57	1 (1%)
5	POV	B	5103	-	51,51,51	0.83	2 (3%)	57,59,59	0.54	1 (1%)
5	POV	C	5103	-	51,51,51	0.83	2 (3%)	57,59,59	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	POV	D	5104	-	51,51,51	0.85	2 (3%)	57,59,59	0.53	1 (1%)
5	POV	C	5104	-	51,51,51	0.74	0	57,59,59	0.60	1 (1%)
5	POV	A	5103	-	51,51,51	0.75	0	57,59,59	0.64	1 (1%)

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	POV	B	5104	-	-	11/55/55/55	-
5	POV	D	5103	-	-	11/55/55/55	-
5	POV	A	5104	-	-	11/55/55/55	-
5	POV	B	5103	-	-	11/55/55/55	-
5	POV	C	5103	-	-	12/55/55/55	-
5	POV	D	5104	-	-	12/55/55/55	-
5	POV	C	5104	-	-	11/55/55/55	-
5	POV	A	5103	-	-	12/55/55/55	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	POV	C1-C2	2.34	1.57	1.50
5	A	5104	POV	C1-C2	2.30	1.57	1.50
5	D	5104	POV	C1-C2	2.29	1.57	1.50
5	B	5103	POV	C1-C2	2.25	1.57	1.50
5	A	5104	POV	C3-C2	2.09	1.57	1.50
5	D	5104	POV	C3-C2	2.07	1.57	1.50
5	C	5103	POV	C3-C2	2.06	1.57	1.50
5	B	5103	POV	C3-C2	2.05	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5104	POV	C2-O21-C21	3.01	125.19	117.79
5	A	5103	POV	C2-O21-C21	2.94	125.04	117.79
5	D	5103	POV	C2-O21-C21	2.81	124.71	117.79
5	C	5104	POV	C2-O21-C21	2.61	124.21	117.79
5	A	5104	POV	C2-O21-C21	2.38	123.64	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5103	POV	C2-O21-C21	2.27	123.39	117.79
5	D	5104	POV	C2-O21-C21	2.23	123.29	117.79
5	C	5103	POV	C2-O21-C21	2.21	123.23	117.79

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5103	POV	C11-O12-P-O11
5	A	5103	POV	C11-O12-P-O13
5	A	5103	POV	C11-O12-P-O14
5	A	5103	POV	C2-C1-O11-P
5	A	5103	POV	C12-C11-O12-P
5	A	5103	POV	C22-C21-O21-C2
5	A	5103	POV	O22-C21-O21-C2
5	A	5104	POV	C2-C1-O11-P
5	A	5104	POV	O12-C11-C12-N
5	A	5104	POV	C12-C11-O12-P
5	B	5103	POV	C2-C1-O11-P
5	B	5103	POV	O12-C11-C12-N
5	B	5103	POV	C12-C11-O12-P
5	B	5104	POV	C11-O12-P-O11
5	B	5104	POV	C11-O12-P-O13
5	B	5104	POV	C11-O12-P-O14
5	B	5104	POV	C2-C1-O11-P
5	B	5104	POV	C12-C11-O12-P
5	B	5104	POV	C22-C21-O21-C2
5	B	5104	POV	O22-C21-O21-C2
5	C	5103	POV	C2-C1-O11-P
5	C	5103	POV	O12-C11-C12-N
5	C	5103	POV	C12-C11-O12-P
5	C	5104	POV	C11-O12-P-O11
5	C	5104	POV	C11-O12-P-O13
5	C	5104	POV	C11-O12-P-O14
5	C	5104	POV	C2-C1-O11-P
5	C	5104	POV	C12-C11-O12-P
5	C	5104	POV	C22-C21-O21-C2
5	C	5104	POV	O22-C21-O21-C2
5	D	5103	POV	C11-O12-P-O11
5	D	5103	POV	C11-O12-P-O13
5	D	5103	POV	C11-O12-P-O14
5	D	5103	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
5	D	5103	POV	C12-C11-O12-P
5	D	5103	POV	C22-C21-O21-C2
5	D	5103	POV	O22-C21-O21-C2
5	D	5104	POV	C2-C1-O11-P
5	D	5104	POV	O12-C11-C12-N
5	D	5104	POV	C12-C11-O12-P
5	A	5103	POV	O11-C1-C2-C3
5	B	5104	POV	O11-C1-C2-C3
5	C	5104	POV	O11-C1-C2-C3
5	D	5104	POV	C1-C2-C3-O31
5	D	5103	POV	O11-C1-C2-C3
5	A	5104	POV	C1-C2-C3-O31
5	B	5103	POV	C1-C2-C3-O31
5	C	5103	POV	C1-C2-C3-O31
5	A	5103	POV	O11-C1-C2-O21
5	C	5104	POV	O11-C1-C2-O21
5	D	5103	POV	O11-C1-C2-O21
5	B	5104	POV	O11-C1-C2-O21
5	A	5104	POV	O21-C2-C3-O31
5	B	5103	POV	O21-C2-C3-O31
5	C	5103	POV	O21-C2-C3-O31
5	D	5104	POV	O21-C2-C3-O31
5	A	5103	POV	O12-C11-C12-N
5	B	5104	POV	O12-C11-C12-N
5	C	5104	POV	O12-C11-C12-N
5	D	5103	POV	O12-C11-C12-N
5	B	5104	POV	C24-C25-C26-C27
5	A	5104	POV	C1-C2-O21-C21
5	A	5104	POV	C3-C2-O21-C21
5	C	5103	POV	C3-C2-O21-C21
5	D	5104	POV	C1-C2-O21-C21
5	A	5104	POV	C1-O11-P-O12
5	A	5104	POV	C11-O12-P-O11
5	B	5103	POV	C1-O11-P-O12
5	B	5103	POV	C11-O12-P-O11
5	C	5103	POV	C1-O11-P-O12
5	C	5103	POV	C11-O12-P-O11
5	D	5104	POV	C1-O11-P-O12
5	D	5104	POV	C11-O12-P-O11
5	A	5103	POV	C24-C25-C26-C27
5	D	5103	POV	C24-C25-C26-C27
5	B	5103	POV	C1-C2-O21-C21

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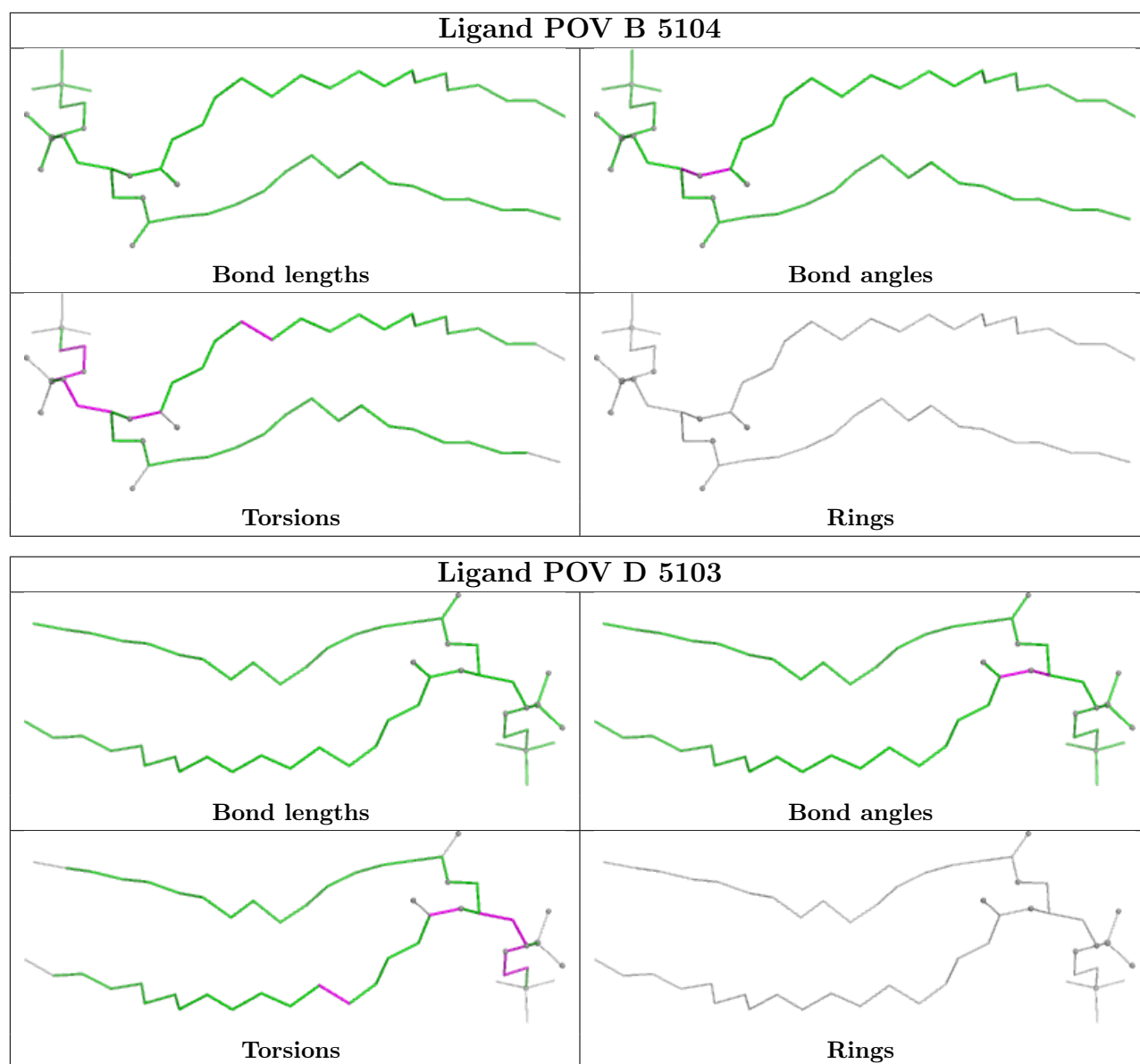
Continued from previous page...

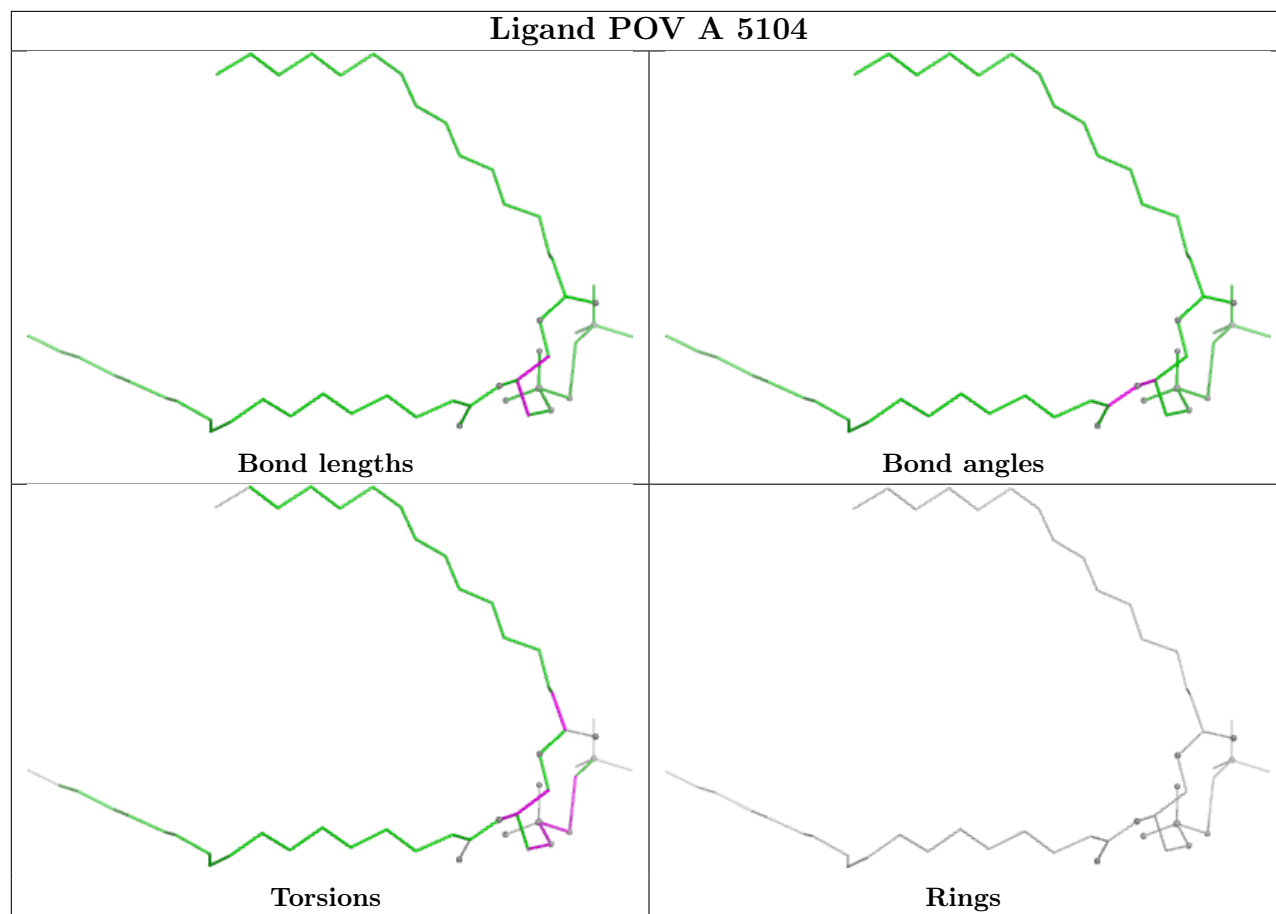
Mol	Chain	Res	Type	Atoms
5	B	5103	POV	C3-C2-O21-C21
5	C	5103	POV	C1-C2-O21-C21
5	D	5104	POV	C3-C2-O21-C21
5	C	5104	POV	C24-C25-C26-C27
5	B	5103	POV	O31-C31-C32-C33
5	C	5103	POV	O31-C31-C32-C33
5	D	5104	POV	O31-C31-C32-C33
5	A	5104	POV	O31-C31-C32-C33
5	A	5104	POV	C11-O12-P-O14
5	C	5103	POV	C11-O12-P-O14
5	D	5104	POV	C11-O12-P-O14
5	A	5103	POV	C35-C36-C37-C38
5	D	5104	POV	O32-C31-C32-C33
5	B	5103	POV	O32-C31-C32-C33
5	C	5103	POV	O32-C31-C32-C33

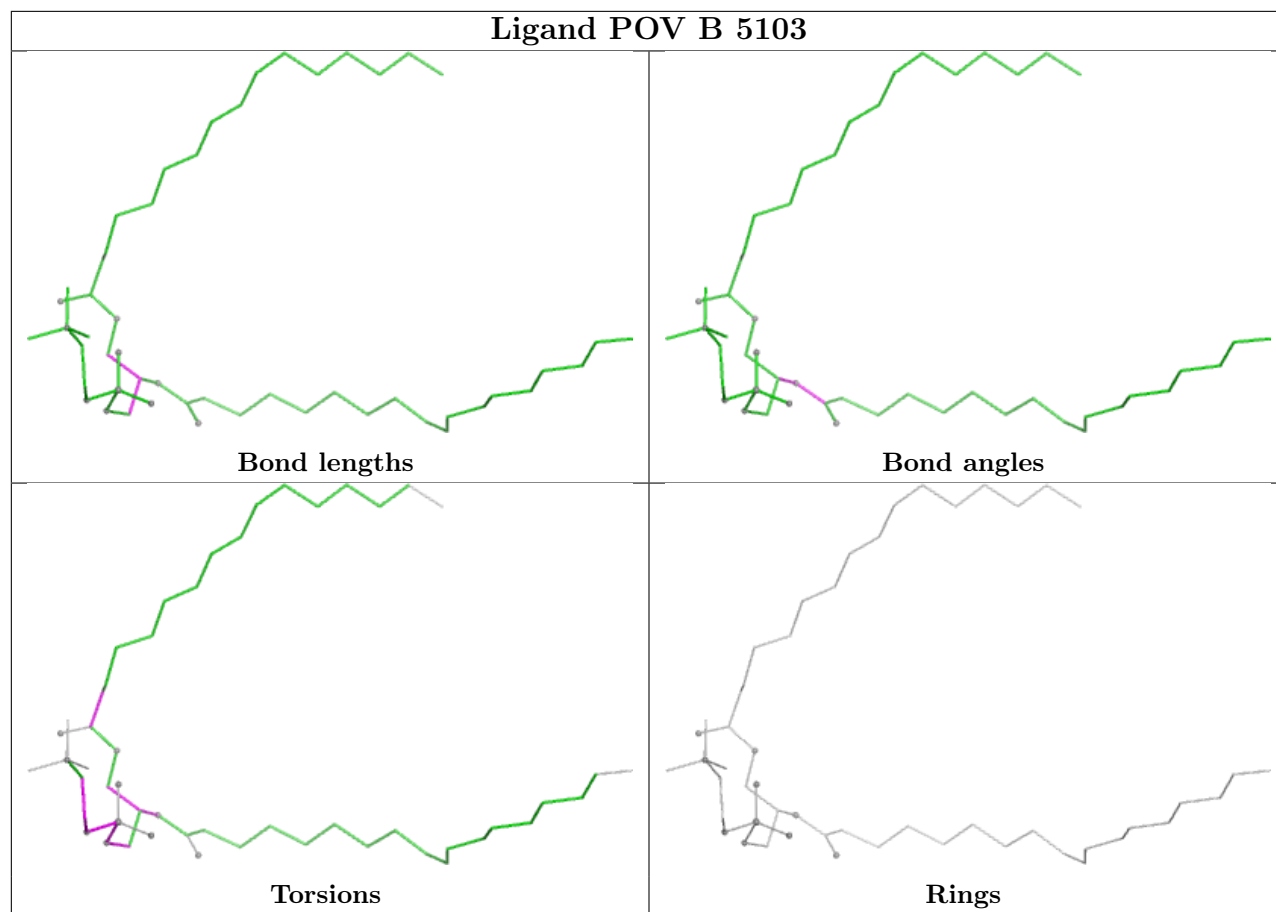
There are no ring outliers.

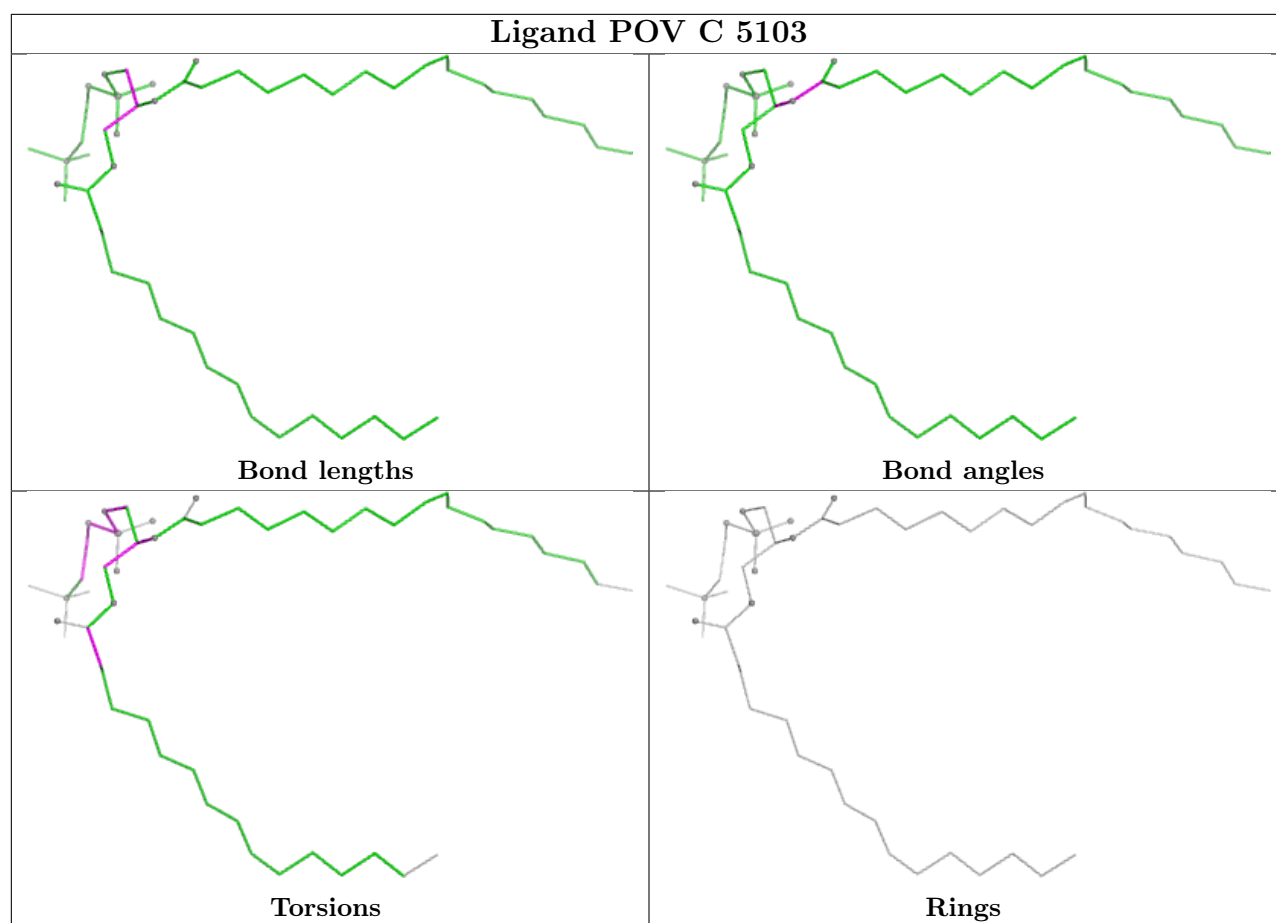
No monomer is involved in short contacts.

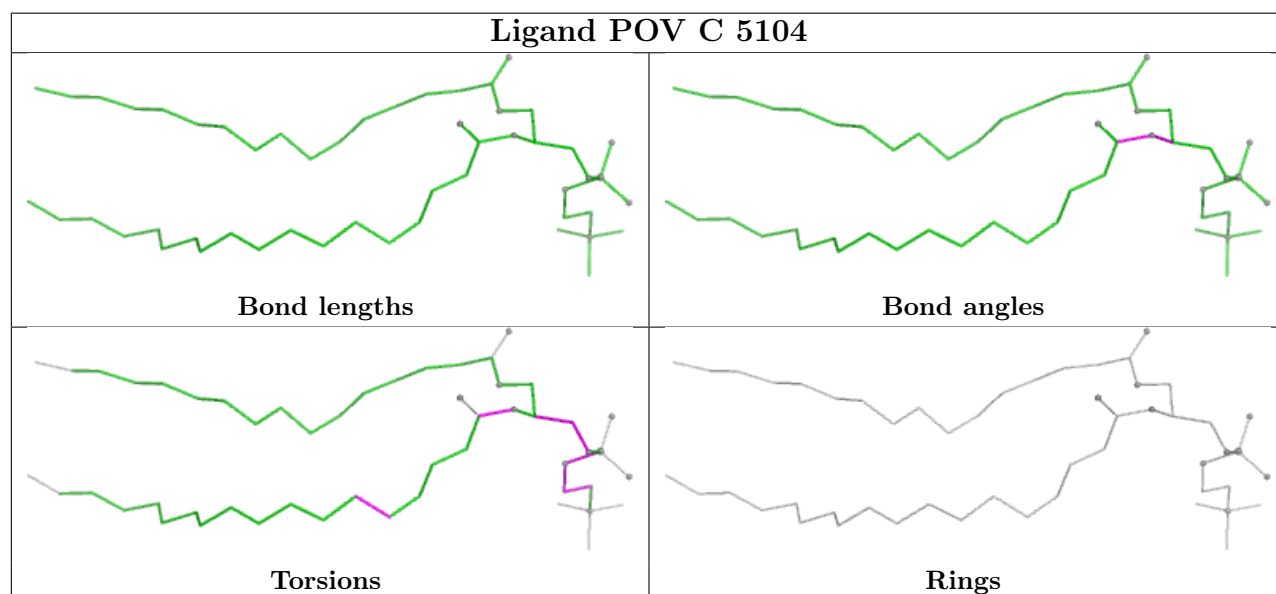
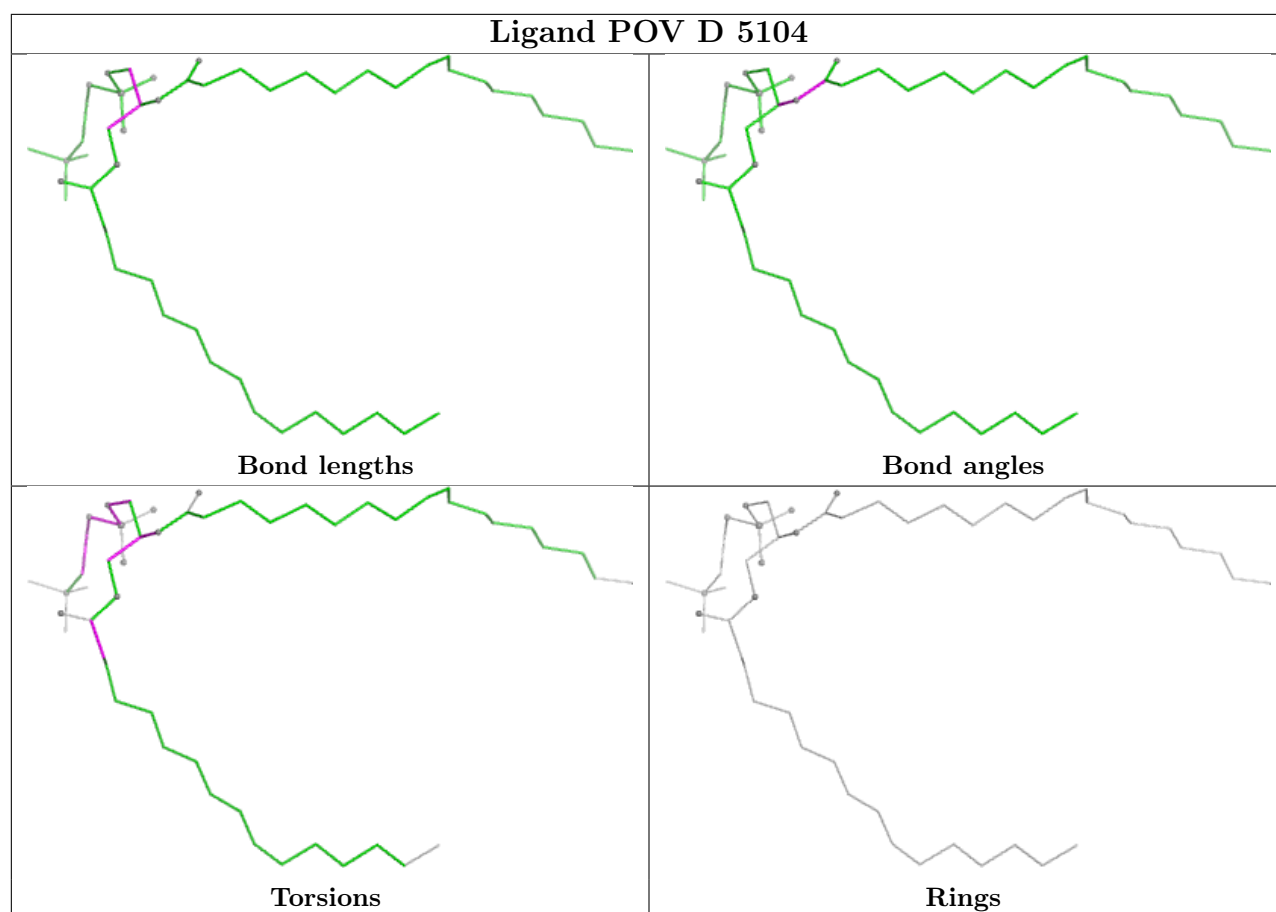
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

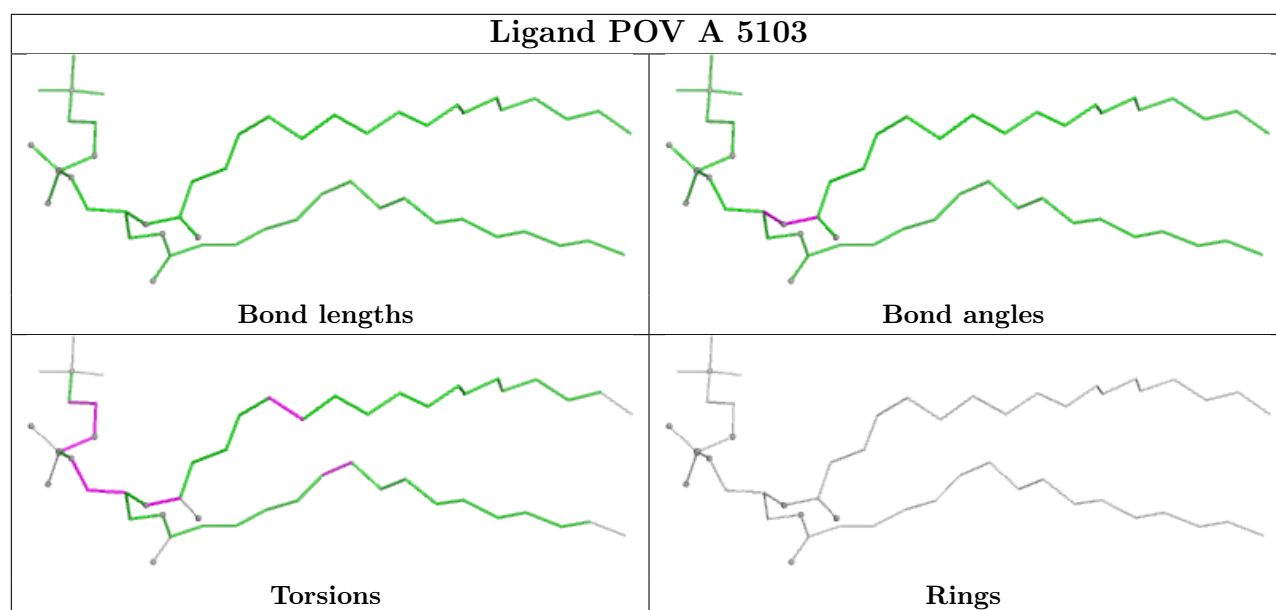












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

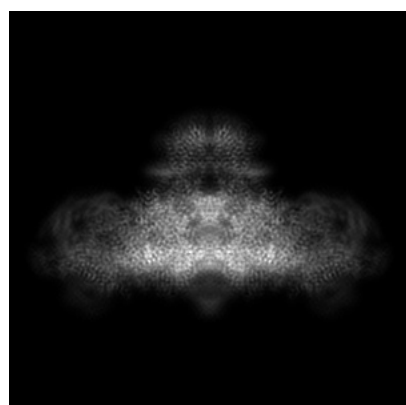
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54509. These allow visual inspection of the internal detail of the map and identification of artifacts.

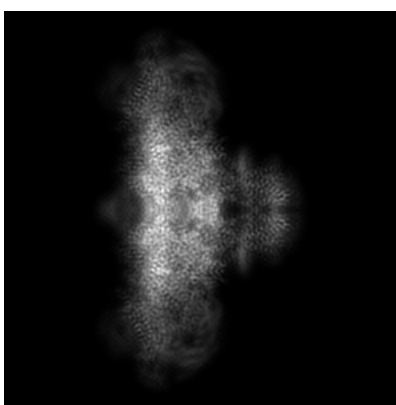
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

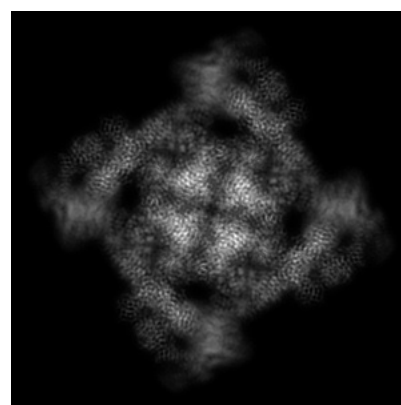
6.1.1 Primary map



X



Y

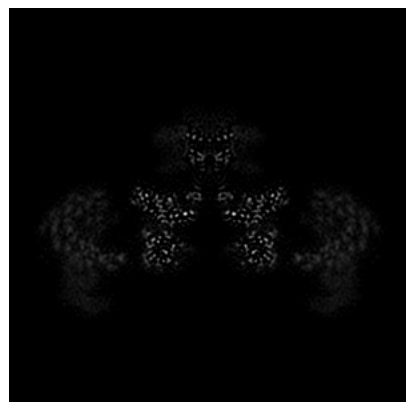


Z

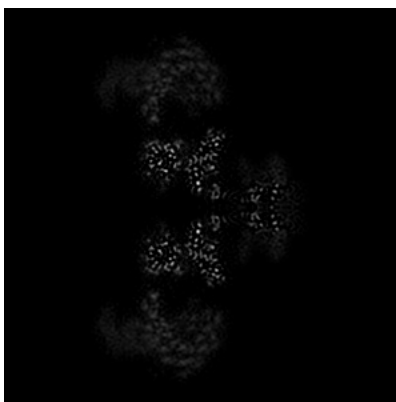
The images above show the map projected in three orthogonal directions.

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](#)

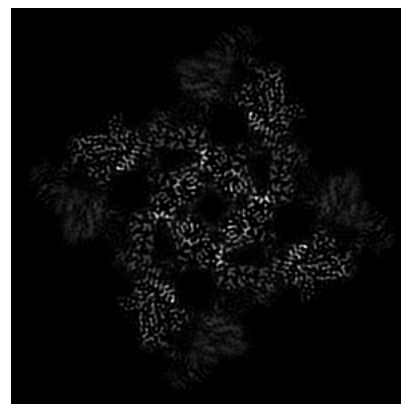
6.3.1 Primary map



X Index: 168



Y Index: 132

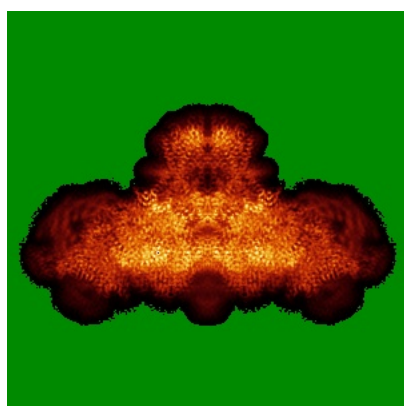


Z Index: 119

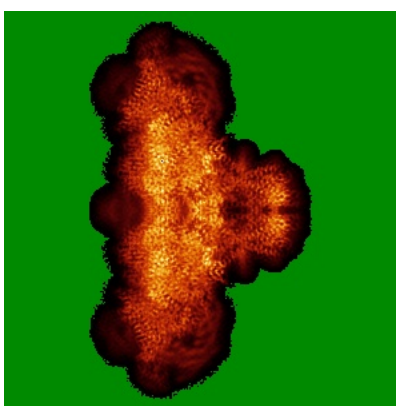
The images above show the largest variance slices of the map in three orthogonal directions.

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

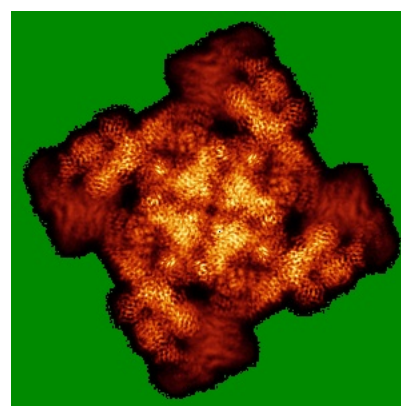
6.4.1 Primary map



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 1.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

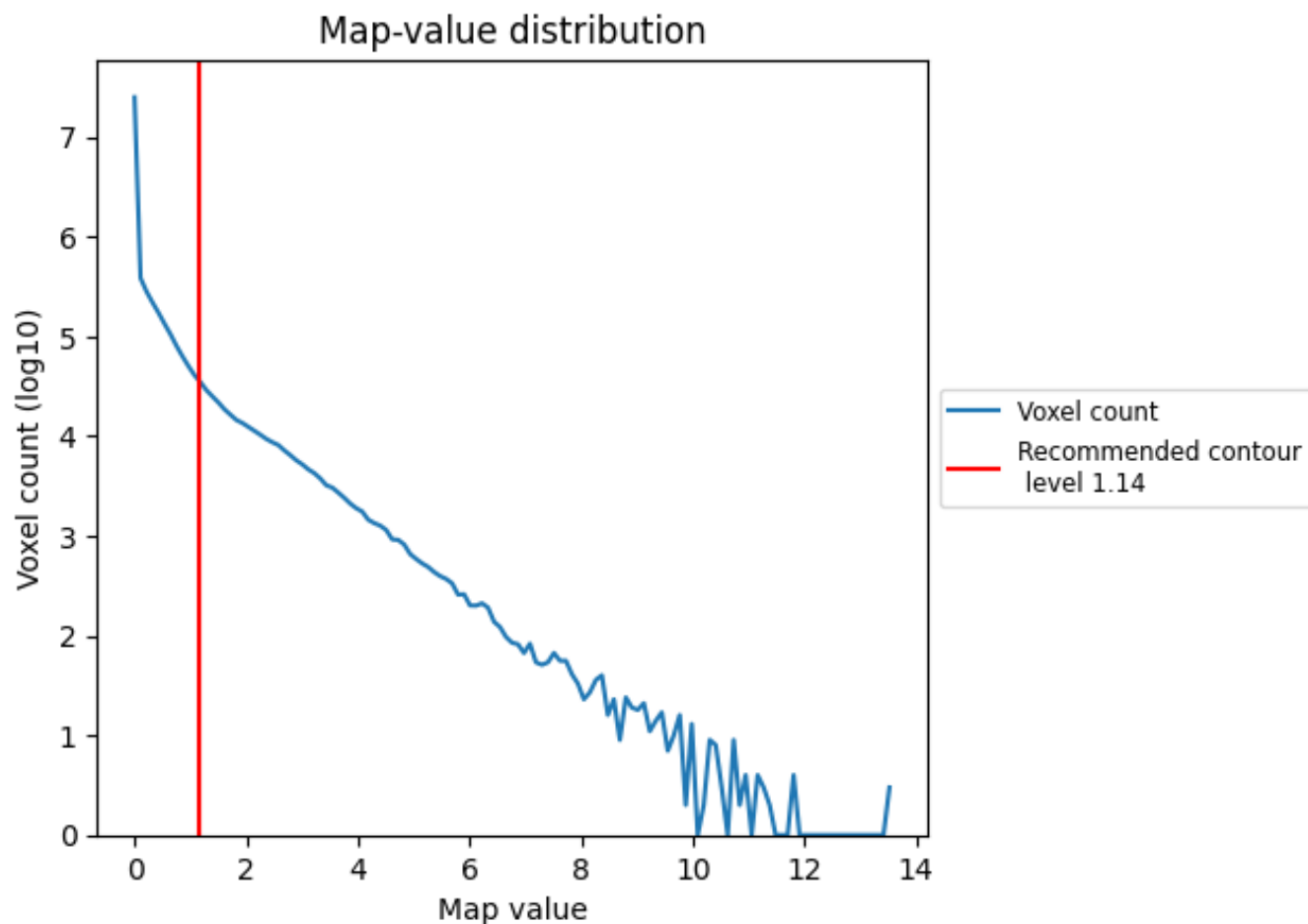
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

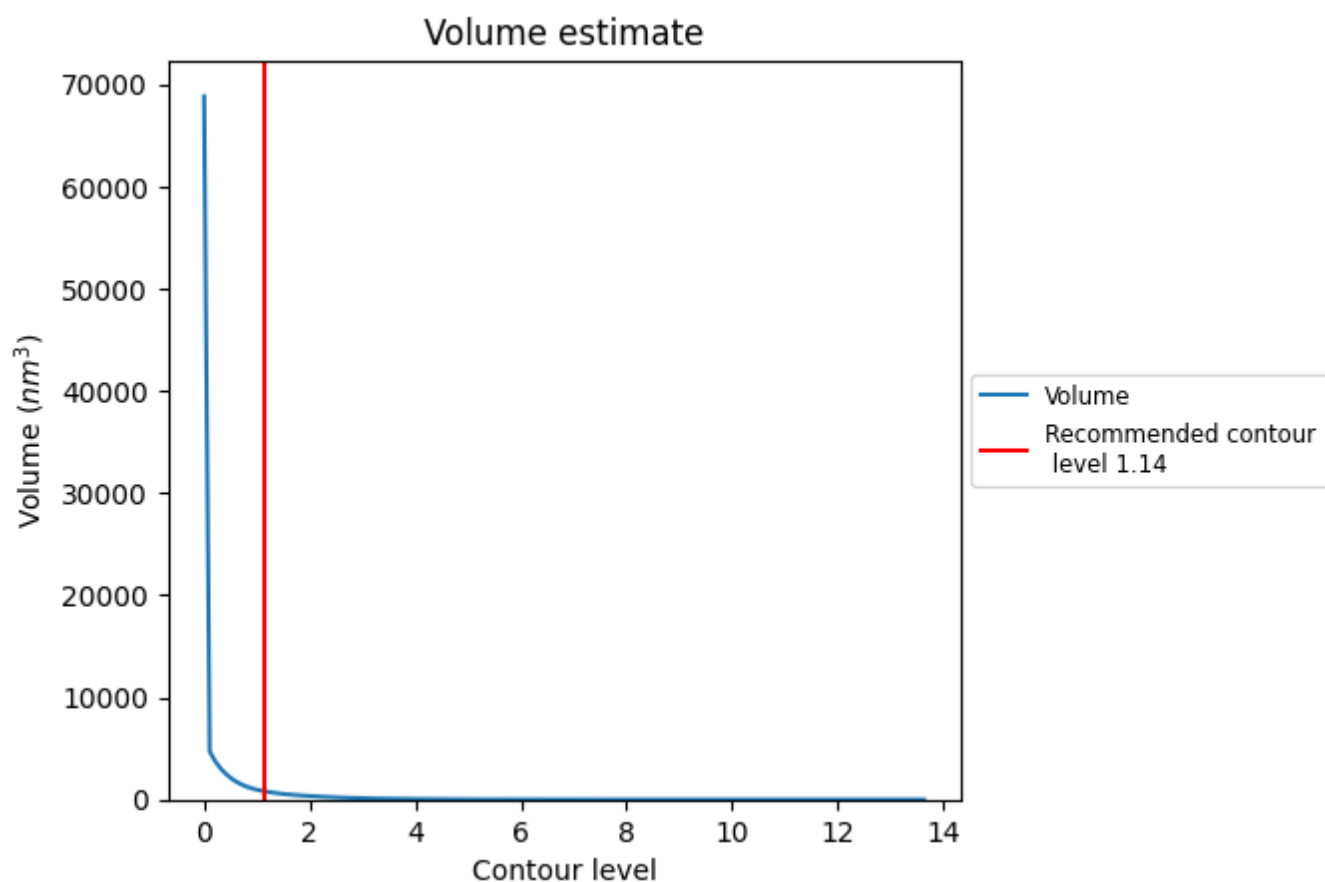
This section contains the results of statistical analysis of the map.

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.

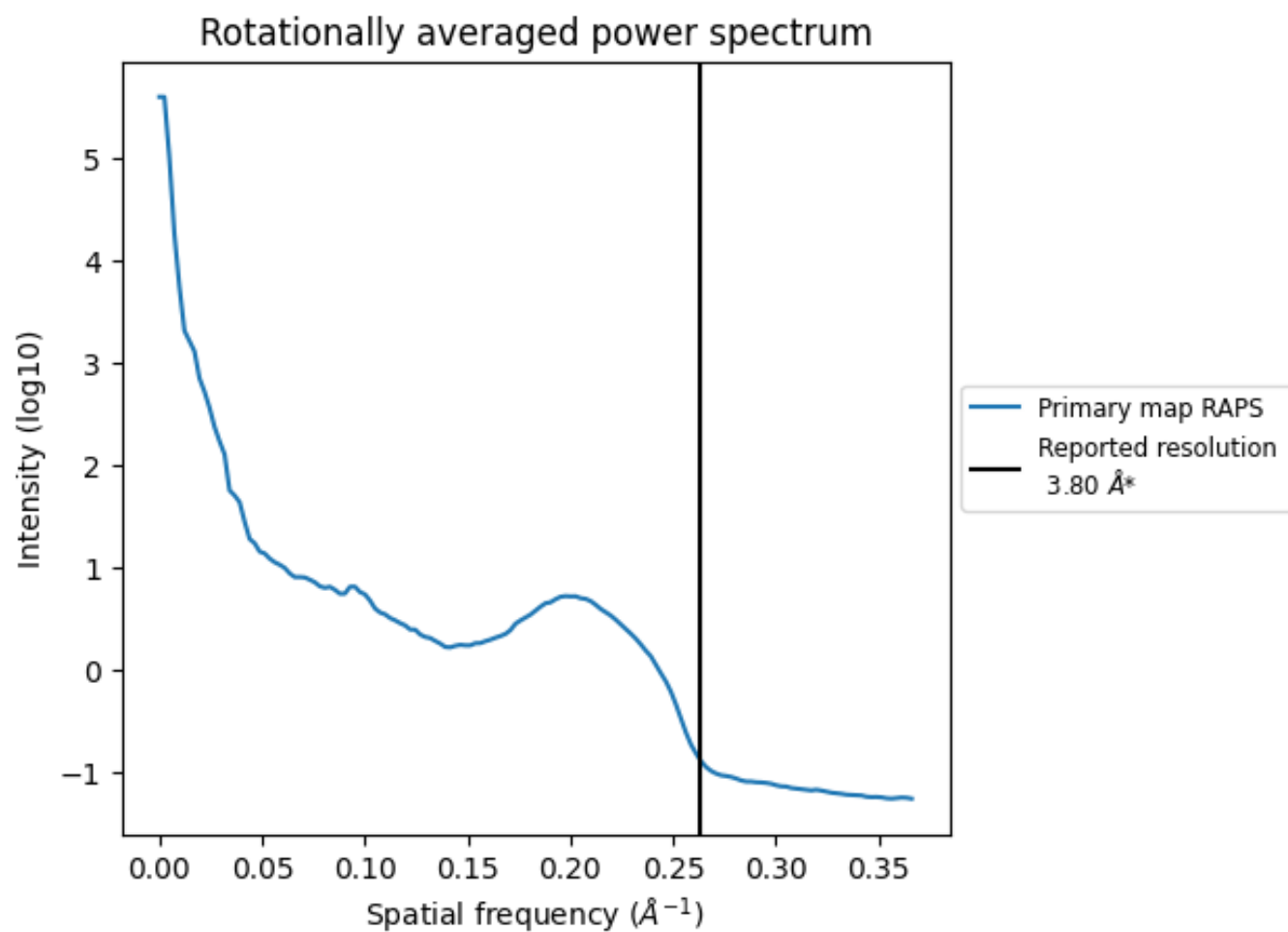
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 813 nm³; this corresponds to an approximate mass of 735 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 0.263 Å⁻¹

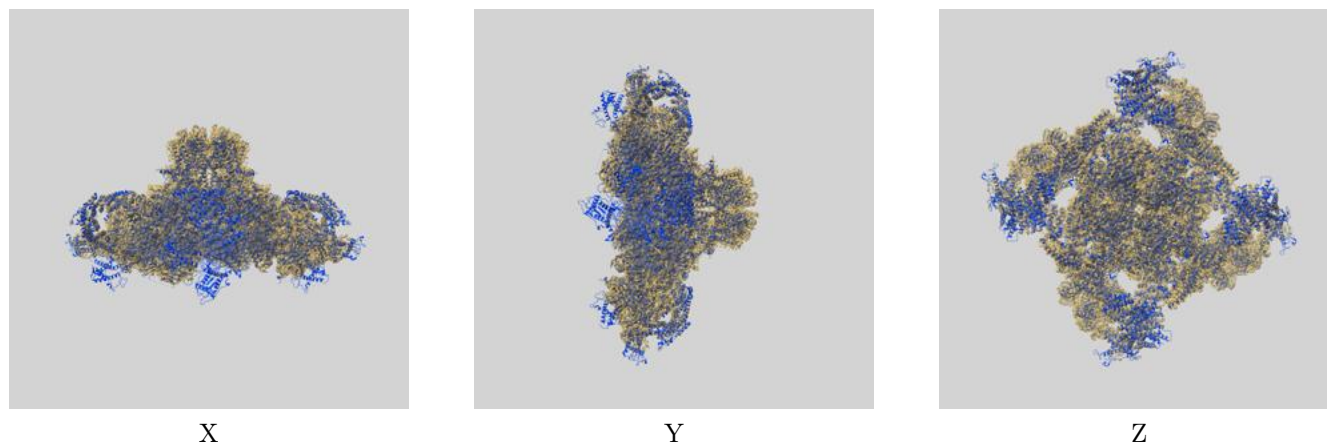
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

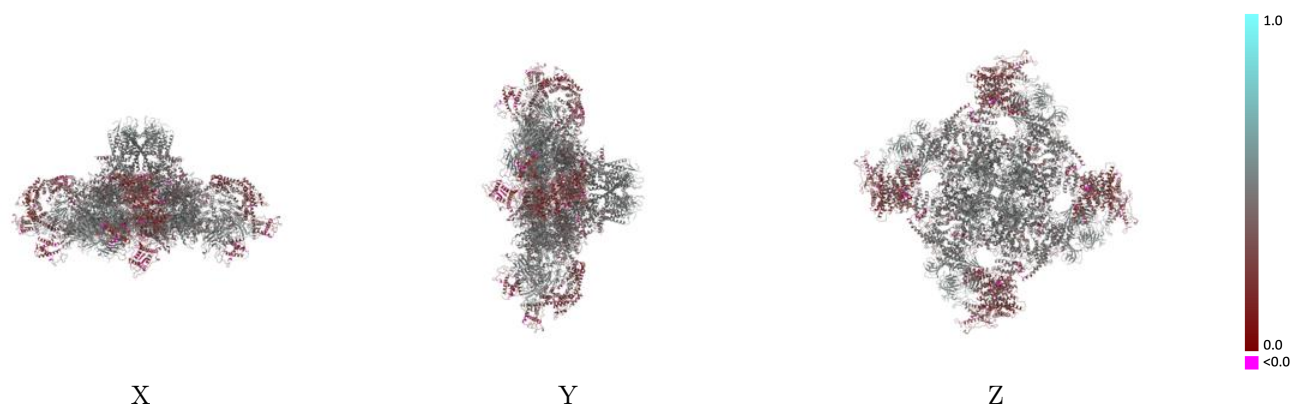
This section contains information regarding the fit between EMDB map EMD-54509 and PDB model 9S2S. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



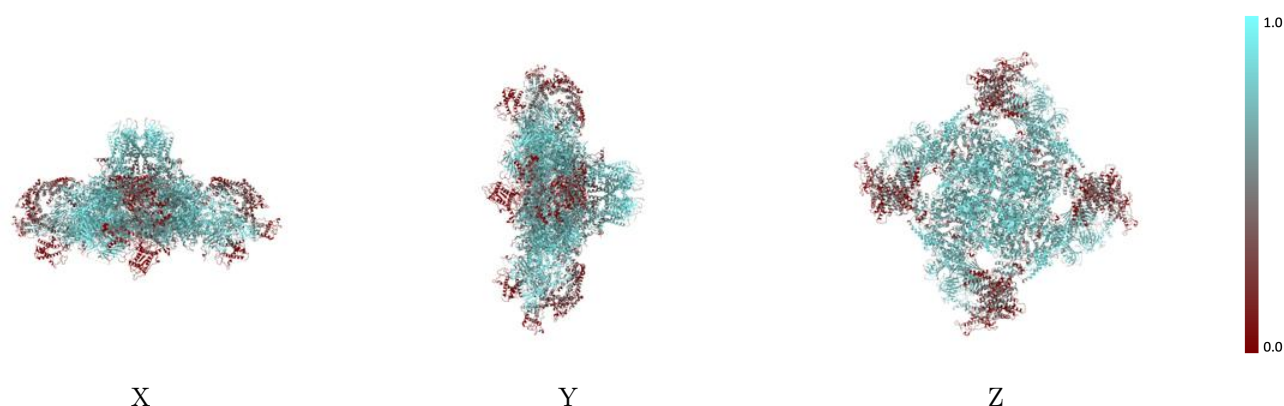
The images above show the 3D surface view of the map at the recommended contour level 1.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



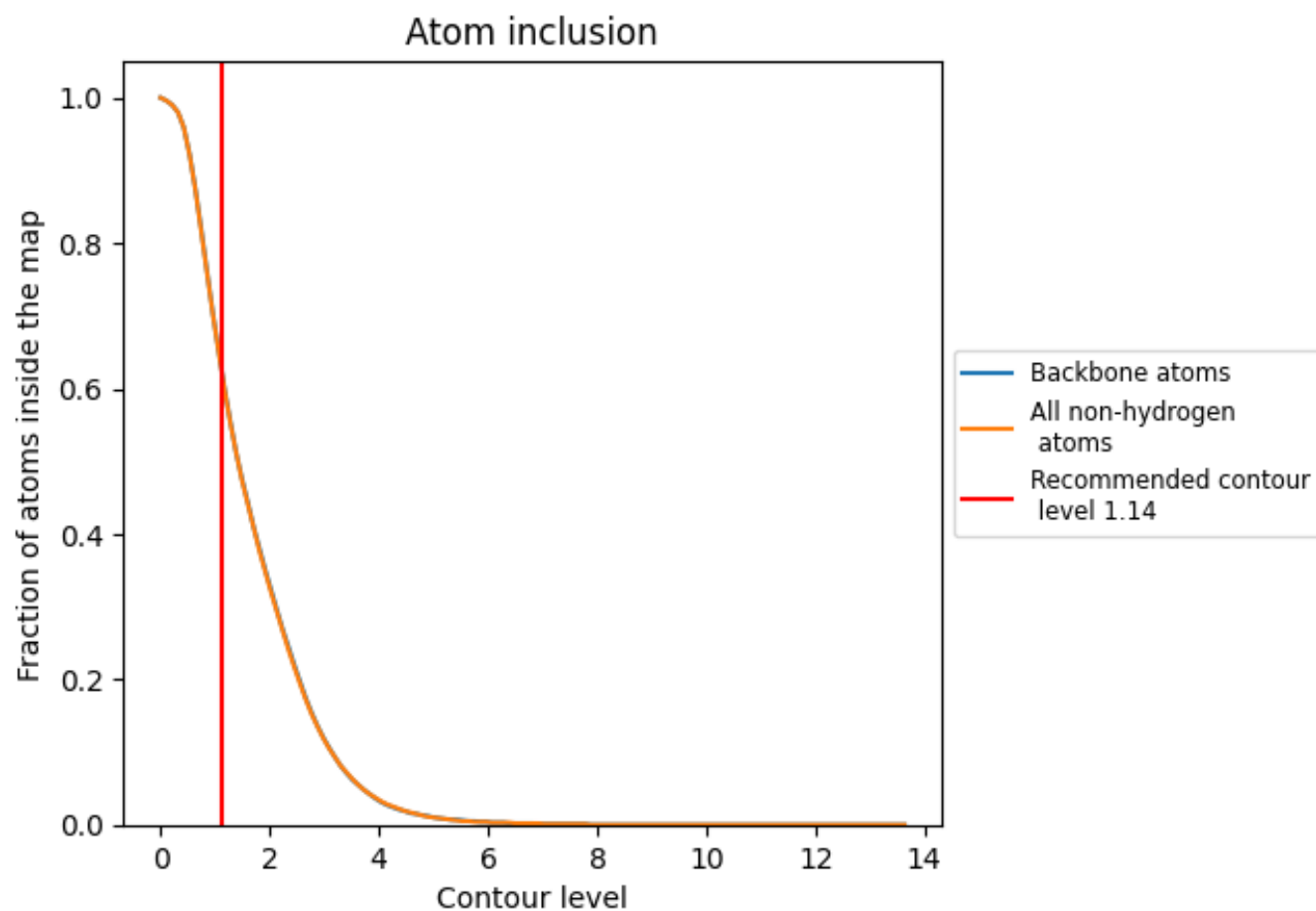
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 62% of all backbone atoms, 61% 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 (1.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.4100
A	0.6140	0.4090
B	0.6140	0.4090
C	0.6140	0.4090
D	0.6260	0.4060
E	0.7610	0.4790
F	0.7610	0.4800
G	0.7600	0.4810
H	0.7820	0.4760

1.0

0.0

<0.0