



Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 01:44 PM EDT

PDB ID : 8DMG
EMDB ID : EMD-27536
Title : CYP102A1 in Closed Conformation
Authors : Su, M.; Xu, H.
Deposited on : 2022-07-08
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

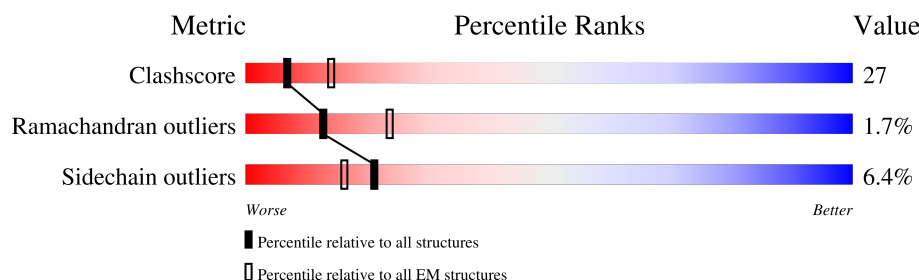
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1037	
1	B	1037	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1C6	A	1102	-	-	X	-
3	1C6	B	1102	-	-	X	-
7	PG4	A	1109	-	-	X	-
7	PG4	B	1109	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16844 atoms, of which 202 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1034	Total	C	H	N	O	S	4	0
			8236	5165	101	1386	1549	35		
1	B	1034	Total	C	H	N	O	S	4	0
			8238	5165	101	1386	1551	35		

There are 26 discrepancies between the modelled and reference sequences:

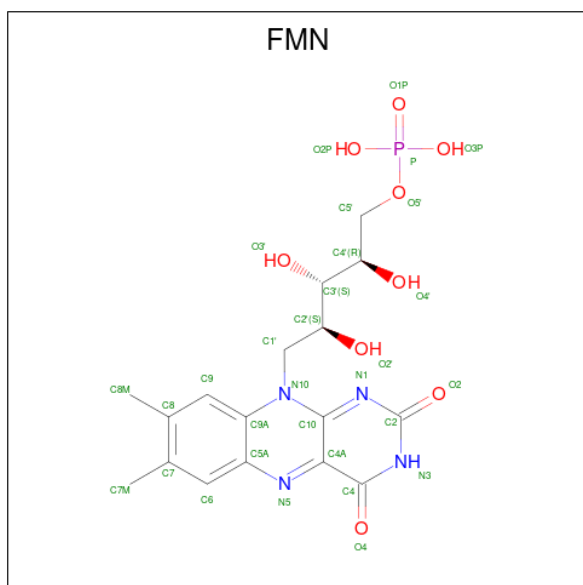
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	conflict	UNP P14779
A	?	-	GLY	deletion	UNP P14779
A	?	-	GLY	deletion	UNP P14779
A	?	-	ILE	deletion	UNP P14779
A	?	-	PRO	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	PRO	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	THR	deletion	UNP P14779
A	?	-	GLU	deletion	UNP P14779
A	?	-	GLN	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	ALA	deletion	UNP P14779
B	82	PHE	ALA	conflict	UNP P14779
B	?	-	GLY	deletion	UNP P14779
B	?	-	GLY	deletion	UNP P14779
B	?	-	ILE	deletion	UNP P14779
B	?	-	PRO	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	PRO	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	THR	deletion	UNP P14779
B	?	-	GLU	deletion	UNP P14779
B	?	-	GLN	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	ALA	deletion	UNP P14779

- # HEM

1C6

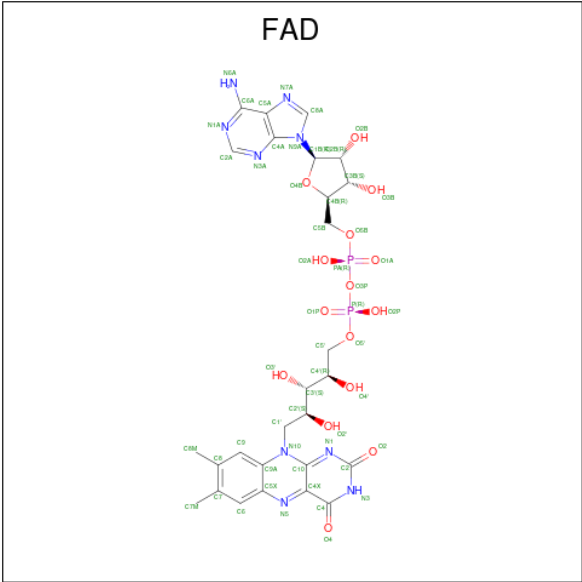
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 23	C 17	N 3	O 2	S 1	0
3	B	1	Total 23	C 17	N 3	O 2	S 1	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



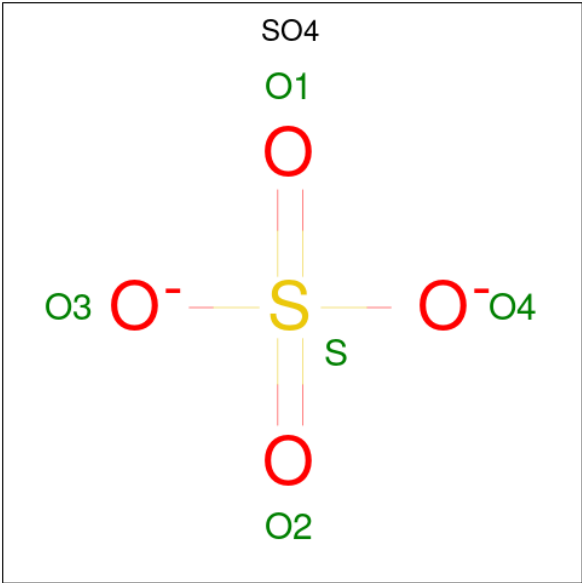
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 17	N 4	O 9	P 1	0
4	B	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
5	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	O S	0
			5	4 1	
6	A	1	Total	O S	0
			5	4 1	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	S	0
			5	4	1	
6	B	1	Total	O	S	0
			5	4	1	
6	B	1	Total	O	S	0
			5	4	1	
6	B	1	Total	O	S	0
			5	4	1	

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).

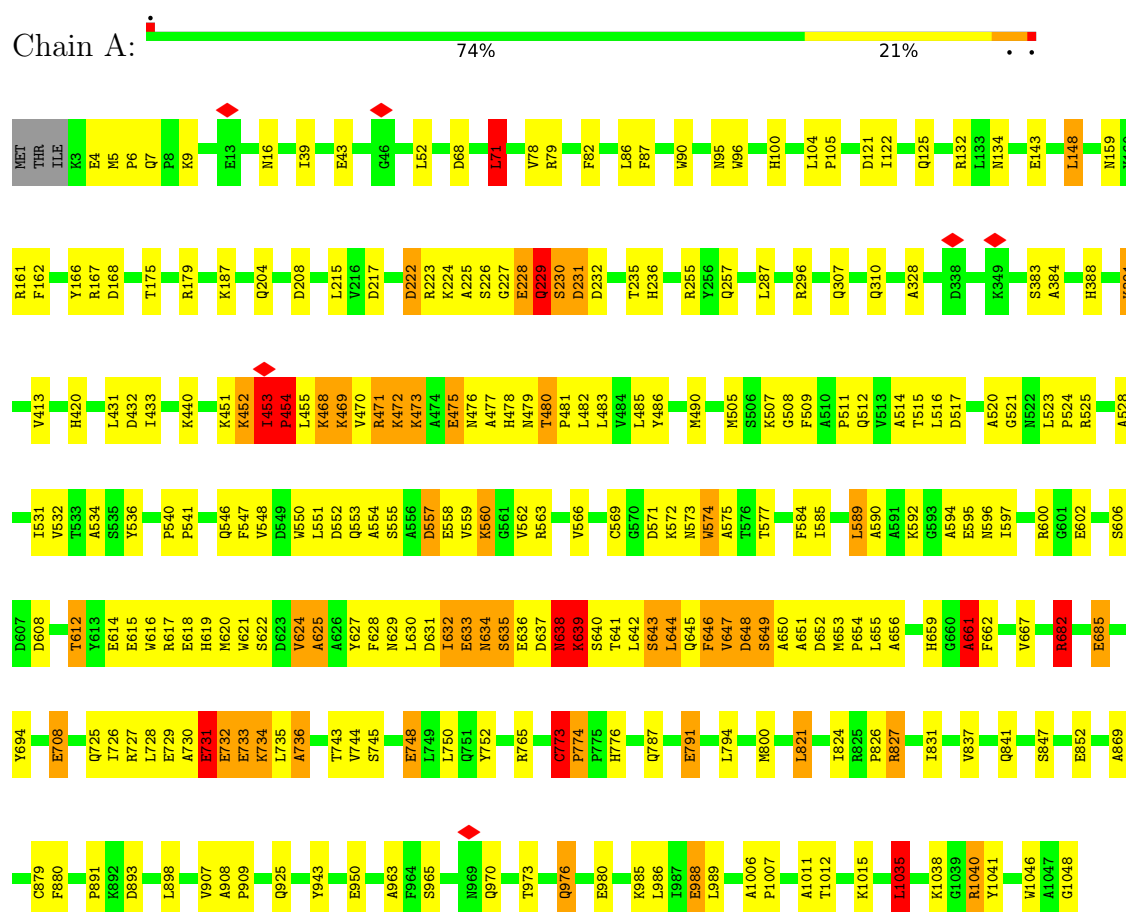


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			13	8	5	
7	A	1	Total	C	O	0
			7	4	3	
7	B	1	Total	C	O	0
			13	8	5	
7	B	1	Total	C	O	0
			7	4	3	

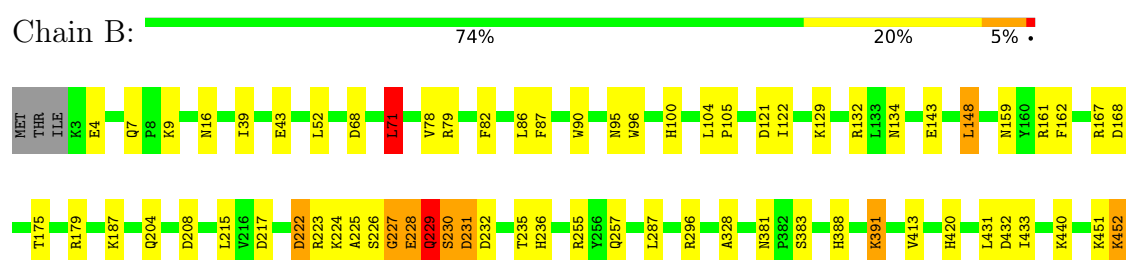
3 Residue-property plots

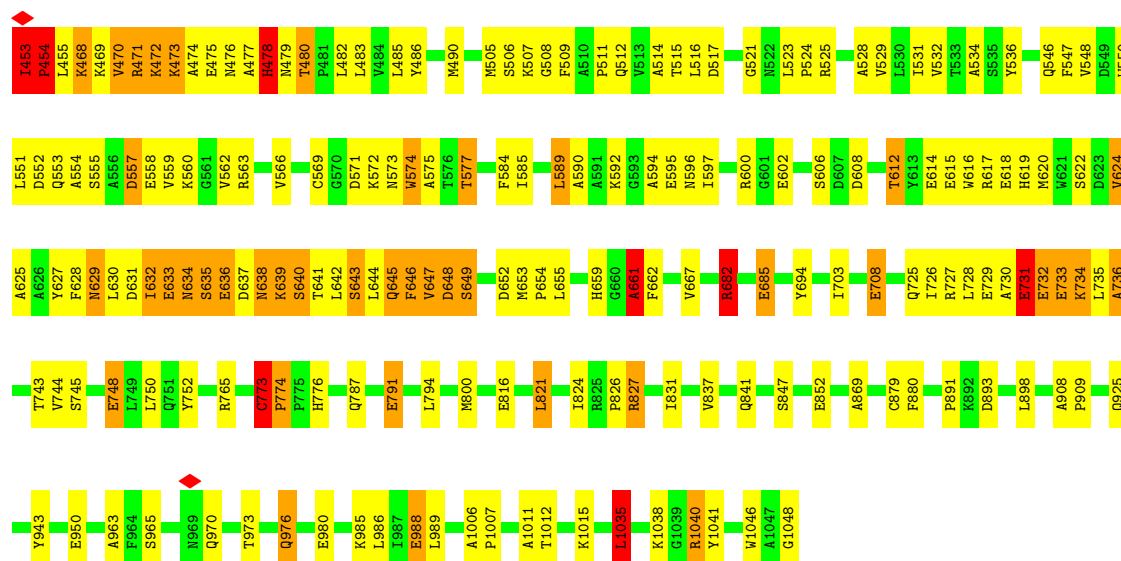
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.460	Depositor
Minimum map value	-1.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	363.6, 363.6, 363.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.02, 2.02, 2.02	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 1C6, PG4, FAD, FMN, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	16/8317 (0.2%)	1.12	43/11271 (0.4%)
1	B	1.13	18/8318 (0.2%)	1.11	44/11272 (0.4%)
All	All	1.13	34/16635 (0.2%)	1.12	87/22543 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	ALA	C-N	-20.86	0.86	1.34
1	B	661	ALA	C-N	-20.85	0.86	1.34
1	A	774	PRO	N-CD	14.87	1.68	1.47
1	B	774	PRO	N-CD	14.80	1.68	1.47
1	B	478	HIS	CA-CB	10.68	1.77	1.53
1	A	988	GLU	CG-CD	8.98	1.65	1.51
1	B	988	GLU	CG-CD	8.93	1.65	1.51
1	A	454	PRO	CA-C	8.58	1.70	1.52
1	B	454	PRO	CA-C	8.57	1.70	1.52
1	A	454	PRO	N-CA	8.36	1.61	1.47
1	B	454	PRO	N-CA	8.34	1.61	1.47
1	B	478	HIS	N-CA	8.13	1.62	1.46
1	A	733	GLU	N-CA	7.75	1.61	1.46
1	B	733	GLU	N-CA	7.73	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	748	GLU	CG-CD	7.24	1.62	1.51
1	B	748	GLU	CG-CD	7.21	1.62	1.51
1	A	454	PRO	N-CD	-6.10	1.39	1.47
1	B	454	PRO	N-CD	-6.10	1.39	1.47
1	A	143	GLU	CG-CD	5.94	1.60	1.51
1	B	143	GLU	CG-CD	5.89	1.60	1.51
1	B	1011	ALA	CA-CB	5.78	1.64	1.52
1	A	1011	ALA	CA-CB	5.72	1.64	1.52
1	B	791	GLU	CG-CD	5.54	1.60	1.51
1	A	791	GLU	CG-CD	5.50	1.60	1.51
1	B	708	GLU	CG-CD	5.35	1.59	1.51
1	A	708	GLU	CG-CD	5.33	1.59	1.51
1	A	9	LYS	CE-NZ	5.28	1.62	1.49
1	B	9	LYS	CE-NZ	5.26	1.62	1.49
1	B	950	GLU	CB-CG	5.15	1.61	1.52
1	A	950	GLU	CB-CG	5.15	1.61	1.52
1	A	734	LYS	N-CA	-5.11	1.36	1.46
1	B	734	LYS	N-CA	-5.11	1.36	1.46
1	A	852	GLU	CB-CG	5.08	1.61	1.52
1	B	852	GLU	CB-CG	5.04	1.61	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	736	ALA	N-CA-CB	29.28	151.10	110.10
1	B	736	ALA	N-CA-CB	29.28	151.10	110.10
1	A	453	ILE	C-N-CD	-24.46	66.79	120.60
1	B	453	ILE	C-N-CD	-24.45	66.81	120.60
1	A	734	LYS	N-CA-CB	-21.83	71.30	110.60
1	B	734	LYS	N-CA-CB	-21.83	71.30	110.60
1	B	661	ALA	O-C-N	-16.38	96.49	122.70
1	A	661	ALA	O-C-N	-16.38	96.49	122.70
1	A	638	ASN	N-CA-C	-13.55	74.41	111.00
1	A	227	GLY	N-CA-C	-12.17	82.69	113.10
1	B	227	GLY	N-CA-C	-12.16	82.70	113.10
1	B	453	ILE	N-CA-C	-11.13	80.94	111.00
1	A	453	ILE	N-CA-C	-11.12	80.98	111.00
1	A	661	ALA	CA-C-N	9.38	137.85	117.20
1	B	661	ALA	CA-C-N	9.37	137.82	117.20
1	A	661	ALA	C-N-CA	9.14	144.54	121.70
1	B	661	ALA	C-N-CA	9.10	144.45	121.70
1	A	229	GLN	N-CA-C	-9.06	86.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	GLN	N-CA-C	-9.05	86.57	111.00
1	A	1040	ARG	NE-CZ-NH2	8.61	124.60	120.30
1	B	736	ALA	N-CA-C	-8.59	87.81	111.00
1	A	736	ALA	N-CA-C	-8.57	87.86	111.00
1	B	1040	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	B	682	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	121	ASP	CB-CG-OD1	8.14	125.62	118.30
1	A	121	ASP	CB-CG-OD1	8.12	125.61	118.30
1	B	453	ILE	O-C-N	-8.10	105.72	121.10
1	A	682	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	453	ILE	O-C-N	-8.07	105.76	121.10
1	B	79	ARG	CG-CD-NE	7.93	128.45	111.80
1	A	79	ARG	CG-CD-NE	7.91	128.41	111.80
1	A	774	PRO	N-CA-CB	7.74	112.59	103.30
1	B	79	ARG	N-CA-CB	7.74	124.53	110.60
1	B	774	PRO	N-CA-CB	7.73	112.58	103.30
1	A	79	ARG	N-CA-CB	7.72	124.50	110.60
1	A	774	PRO	CA-N-CD	-7.43	101.10	111.50
1	B	774	PRO	CA-N-CD	-7.41	101.13	111.50
1	B	79	ARG	CB-CA-C	-6.96	96.48	110.40
1	A	79	ARG	CB-CA-C	-6.95	96.50	110.40
1	B	68	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	68	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	732	GLU	O-C-N	-6.78	111.85	122.70
1	A	732	GLU	O-C-N	-6.75	111.89	122.70
1	B	79	ARG	CA-CB-CG	6.71	128.17	113.40
1	A	79	ARG	CA-CB-CG	6.71	128.17	113.40
1	B	68	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	1040	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	68	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	1040	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	71	LEU	CB-CG-CD1	6.60	122.22	111.00
1	A	71	LEU	CB-CG-CD1	6.60	122.22	111.00
1	A	648	ASP	N-CA-C	-6.32	93.95	111.00
1	A	296	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	648	ASP	N-CA-C	-6.26	94.10	111.00
1	B	296	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	827	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	647	VAL	N-CA-C	-5.99	94.82	111.00
1	B	827	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	574	TRP	C-N-CA	5.96	136.60	121.70
1	A	574	TRP	C-N-CA	5.94	136.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	765	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	893	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	893	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	773	CYS	C-N-CD	5.50	139.95	128.40
1	A	432	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	773	CYS	C-N-CD	5.49	139.92	128.40
1	B	432	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	296	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	296	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	454	PRO	N-CA-C	5.38	126.08	112.10
1	B	454	PRO	N-CA-C	5.37	126.07	112.10
1	B	79	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	1035	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	1035	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	79	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	B	733	GLU	C-N-CA	-5.23	108.62	121.70
1	A	733	GLU	C-N-CA	-5.22	108.65	121.70
1	B	478	HIS	CA-C-O	5.20	131.02	120.10
1	B	633	GLU	N-CA-C	-5.11	97.21	111.00
1	A	633	GLU	N-CA-C	-5.10	97.24	111.00
1	A	96	TRP	CA-CB-CG	-5.07	104.07	113.70
1	B	647	VAL	N-CA-C	-5.05	97.36	111.00
1	B	96	TRP	CA-CB-CG	-5.05	104.10	113.70
1	B	475	GLU	N-CA-C	-5.04	97.40	111.00
1	B	391	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	A	391	LYS	CD-CE-NZ	-5.00	100.20	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	LYS	Mainchain
1	A	661	ALA	Mainchain
1	B	224	LYS	Mainchain
1	B	661	ALA	Mainchain

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	8135	101	7896	532	0
1	B	8137	101	7894	573	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	23	0	19	10	0
3	B	23	0	19	11	0
4	A	31	0	19	0	0
4	B	31	0	19	1	0
5	A	53	0	31	4	0
5	B	53	0	31	4	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0
7	A	20	0	27	8	0
7	B	20	0	27	8	0
All	All	16642	202	16042	895	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 27.

All (895) 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:478:HIS:CB	1:B:478:HIS:CA	1.77	1.61
1:B:478:HIS:CA	1:B:479:ASN:HA	1.33	1.54
1:B:478:HIS:HA	1:B:479:ASN:CA	1.11	1.53
1:B:1046:TRP:CD1	1:B:1048:GLY:C	1.83	1.53
1:A:645:GLN:HB3	1:B:728:LEU:C	1.16	1.48
1:A:1046:TRP:CD1	1:A:1048:GLY:C	1.83	1.48
1:A:229:GLN:C	1:B:471:ARG:HH22	1.13	1.47
1:B:774:PRO:N	1:B:774:PRO:CD	1.68	1.47
1:A:472:LYS:CE	1:B:231:ASP:HB2	1.44	1.45
1:A:472:LYS:NZ	1:B:231:ASP:CA	1.79	1.41
1:B:1046:TRP:HD1	1:B:1048:GLY:C	1.18	1.40
1:A:774:PRO:CD	1:A:774:PRO:N	1.68	1.38
1:A:1048:GLY:O	5:A:1104:FAD:H1'2	1.21	1.38
1:A:472:LYS:HZ2	1:B:231:ASP:CG	1.23	1.37
1:A:645:GLN:HB3	1:B:729:GLU:N	1.40	1.37
1:B:1048:GLY:O	5:B:1104:FAD:H1'2	1.21	1.36
1:A:472:LYS:HZ1	1:B:231:ASP:CA	1.31	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:O	1:A:662:PHE:N	1.58	1.35
1:B:661:ALA:O	1:B:662:PHE:N	1.58	1.33
1:A:1046:TRP:HD1	1:A:1048:GLY:C	1.18	1.32
1:A:229:GLN:C	1:B:471:ARG:NH2	1.79	1.32
1:A:643:SER:N	1:B:732:GLU:OE2	1.64	1.31
1:A:643:SER:OG	1:B:732:GLU:CG	1.77	1.30
1:A:231:ASP:H	1:B:471:ARG:CZ	1.41	1.30
1:A:383:SER:HB2	1:B:546:GLN:NE2	1.44	1.28
1:A:229:GLN:HB2	1:B:471:ARG:NH2	1.46	1.28
1:A:727:ARG:O	1:B:646:PHE:N	1.65	1.27
1:A:645:GLN:HB3	1:B:728:LEU:CA	1.65	1.26
1:A:472:LYS:CE	1:B:231:ASP:OD2	1.83	1.24
1:A:645:GLN:CB	1:B:728:LEU:C	2.05	1.23
1:A:383:SER:CB	1:B:546:GLN:HB3	1.67	1.23
1:A:644:LEU:CA	1:B:729:GLU:O	1.87	1.22
1:A:641:THR:O	1:B:732:GLU:CD	1.76	1.22
1:A:643:SER:OG	1:B:732:GLU:HG2	1.04	1.21
1:A:645:GLN:O	1:B:728:LEU:HD23	1.36	1.20
1:A:642:LEU:CA	1:B:732:GLU:OE2	1.88	1.19
1:A:645:GLN:CG	1:B:727:ARG:O	1.90	1.18
1:A:472:LYS:HE3	1:B:231:ASP:OD2	1.35	1.18
1:A:728:LEU:CD2	1:B:645:GLN:O	1.91	1.18
1:A:728:LEU:HD23	1:B:645:GLN:O	1.44	1.18
1:A:645:GLN:CB	1:B:729:GLU:N	2.07	1.17
1:A:727:ARG:HB3	1:B:647:VAL:HB	1.17	1.16
1:A:641:THR:C	1:B:732:GLU:OE1	1.80	1.16
1:A:642:LEU:C	1:B:732:GLU:OE2	1.81	1.15
1:A:231:ASP:H	1:B:471:ARG:NH1	1.41	1.15
1:A:507:LYS:HG2	1:A:632:ILE:HG21	1.25	1.13
1:A:643:SER:OG	1:B:731:GLU:OE1	1.65	1.13
1:A:642:LEU:HA	1:B:732:GLU:OE2	1.47	1.13
1:A:645:GLN:HG3	1:B:727:ARG:O	0.96	1.12
1:A:229:GLN:CB	1:B:471:ARG:NH2	2.14	1.11
1:A:231:ASP:H	1:B:471:ARG:NH2	1.49	1.11
1:B:661:ALA:C	1:B:662:PHE:CA	2.19	1.11
1:B:478:HIS:HA	1:B:479:ASN:N	1.62	1.10
1:A:472:LYS:HZ2	1:B:231:ASP:HB3	1.07	1.10
1:B:452:LYS:HE2	1:B:455:LEU:H	0.99	1.10
1:A:661:ALA:C	1:A:662:PHE:CA	2.19	1.09
1:B:478:HIS:C	1:B:509:PHE:HA	1.71	1.09
1:A:472:LYS:NZ	1:B:231:ASP:CG	1.86	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HE2	1:A:455:LEU:H	0.99	1.08
1:A:644:LEU:N	1:B:729:GLU:O	1.88	1.06
1:B:478:HIS:CA	1:B:479:ASN:CA	2.05	1.05
1:A:78:VAL:CG1	1:A:82:PHE:CD2	2.40	1.05
1:A:1048:GLY:O	5:A:1104:FAD:C1'	2.05	1.05
1:A:231:ASP:N	1:B:471:ARG:NH2	2.03	1.04
1:A:655:LEU:HD21	1:A:826:PRO:HD3	1.12	1.04
1:A:507:LYS:CG	1:A:632:ILE:HG21	1.88	1.04
1:B:78:VAL:CG1	1:B:82:PHE:CD2	2.40	1.04
1:B:1048:GLY:O	5:B:1104:FAD:C1'	2.05	1.04
1:A:472:LYS:CE	1:B:231:ASP:CB	2.14	1.03
1:A:773:CYS:SG	1:A:776:HIS:CG	2.52	1.03
1:A:383:SER:HB2	1:B:546:GLN:HB3	1.34	1.02
1:B:773:CYS:SG	1:B:776:HIS:CG	2.52	1.02
1:A:451:LYS:O	1:A:454:PRO:N	1.94	1.01
1:A:661:ALA:CA	1:A:662:PHE:N	2.24	1.00
1:B:661:ALA:CA	1:B:662:PHE:N	2.24	1.00
1:B:507:LYS:CB	1:B:632:ILE:HG21	1.92	1.00
1:B:451:LYS:O	1:B:454:PRO:N	1.94	1.00
1:A:727:ARG:O	1:B:645:GLN:HG3	1.59	1.00
1:A:229:GLN:HB2	1:B:471:ARG:CZ	1.91	0.99
1:B:637:ASP:C	1:B:639:LYS:H	1.62	0.99
1:A:132:ARG:O	1:B:161:ARG:HD2	1.62	0.99
1:A:384:ALA:H	1:B:546:GLN:HE22	1.09	0.99
1:A:231:ASP:N	1:B:471:ARG:NH1	2.11	0.99
1:A:231:ASP:N	1:B:471:ARG:CZ	2.26	0.98
1:B:735:LEU:HD12	1:B:736:ALA:N	1.79	0.98
1:A:980:GLU:CB	1:A:980:GLU:OE2	2.12	0.98
1:A:647:VAL:HB	1:B:727:ARG:HB3	1.44	0.98
1:A:472:LYS:CE	1:B:231:ASP:CG	2.30	0.97
1:B:980:GLU:OE2	1:B:980:GLU:CB	2.12	0.97
1:A:472:LYS:NZ	1:B:231:ASP:HB3	1.62	0.97
1:A:735:LEU:HD12	1:A:736:ALA:N	1.79	0.97
1:A:229:GLN:CA	1:B:471:ARG:NH2	2.26	0.97
1:A:643:SER:O	1:B:730:ALA:HB2	1.15	0.97
1:B:507:LYS:HD3	1:B:632:ILE:HD12	1.44	0.97
1:B:478:HIS:C	1:B:479:ASN:HA	1.86	0.96
1:B:217:ASP:OD1	1:B:255:ARG:NH1	1.98	0.96
1:A:217:ASP:OD1	1:A:255:ARG:NH1	1.98	0.96
1:A:645:GLN:CB	1:B:728:LEU:HA	1.96	0.95
1:A:452:LYS:C	1:A:454:PRO:N	2.16	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:SER:CB	1:B:546:GLN:CB	2.44	0.95
1:B:478:HIS:CA	1:B:479:ASN:N	2.22	0.95
1:B:452:LYS:O	1:B:454:PRO:N	1.99	0.95
1:A:645:GLN:CB	1:B:728:LEU:CA	2.43	0.94
1:B:478:HIS:N	1:B:631:ASP:OD2	2.00	0.94
1:B:478:HIS:O	1:B:509:PHE:HA	1.68	0.94
1:A:452:LYS:O	1:A:454:PRO:N	1.99	0.94
1:B:452:LYS:HE2	1:B:455:LEU:N	1.82	0.94
1:A:645:GLN:O	1:B:728:LEU:CD2	2.15	0.93
3:B:1102:1C6:H3	3:B:1102:1C6:H8	1.50	0.93
1:A:134:ASN:HD21	1:B:161:ARG:N	1.66	0.93
1:A:383:SER:CB	1:B:546:GLN:NE2	2.32	0.93
1:A:452:LYS:HE2	1:A:455:LEU:N	1.82	0.92
1:B:655:LEU:HD22	1:B:824:ILE:O	1.69	0.92
1:A:231:ASP:N	1:B:471:ARG:HH22	1.65	0.92
1:A:384:ALA:N	1:B:546:GLN:HE22	1.68	0.92
1:A:230:SER:N	1:B:471:ARG:HH22	1.68	0.92
1:A:645:GLN:HE21	1:A:646:PHE:H	1.08	0.92
1:A:383:SER:HB2	1:B:546:GLN:HE21	1.23	0.91
3:A:1102:1C6:H8	3:A:1102:1C6:H3	1.50	0.91
1:A:452:LYS:HB3	1:A:455:LEU:HG	1.51	0.91
1:B:661:ALA:C	1:B:662:PHE:N	0.86	0.91
1:A:727:ARG:HB3	1:B:647:VAL:CB	1.99	0.90
1:A:161:ARG:N	1:B:134:ASN:HD21	1.69	0.90
1:A:661:ALA:C	1:A:662:PHE:N	0.86	0.90
1:A:590:ALA:HA	1:A:594:ALA:HB2	1.53	0.90
1:A:643:SER:CB	1:B:732:GLU:HG2	2.01	0.90
1:A:659:HIS:HB3	1:A:880:PHE:CD1	2.07	0.90
1:B:452:LYS:C	1:B:454:PRO:N	2.16	0.90
1:A:161:ARG:H	1:B:134:ASN:HD21	0.98	0.90
1:B:452:LYS:HB3	1:B:455:LEU:HG	1.51	0.90
1:A:452:LYS:HE3	1:A:468:LYS:HG2	1.53	0.89
1:B:452:LYS:O	1:B:453:ILE:C	2.10	0.89
1:A:229:GLN:HB2	1:B:471:ARG:HH21	1.28	0.89
1:A:452:LYS:O	1:A:453:ILE:C	2.10	0.89
1:A:472:LYS:NZ	1:B:231:ASP:CB	0.82	0.89
1:A:728:LEU:HD22	1:B:645:GLN:O	1.71	0.89
1:A:734:LYS:O	1:A:736:ALA:O	1.91	0.89
1:B:659:HIS:HB3	1:B:880:PHE:CD1	2.07	0.89
1:A:644:LEU:HA	1:B:729:GLU:O	1.73	0.89
1:B:78:VAL:CG1	1:B:82:PHE:HD2	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:LYS:O	1:B:736:ALA:O	1.91	0.89
1:B:634:ASN:C	1:B:636:GLU:H	1.71	0.89
1:B:590:ALA:HA	1:B:594:ALA:HB2	1.53	0.89
1:A:731:GLU:OE1	1:B:643:SER:HB3	1.72	0.88
1:A:472:LYS:HZ2	1:B:231:ASP:CB	0.37	0.88
1:A:645:GLN:HB3	1:B:728:LEU:HA	1.51	0.88
1:A:645:GLN:HG3	1:B:727:ARG:C	1.94	0.88
1:A:644:LEU:C	1:B:729:GLU:O	2.11	0.88
1:A:134:ASN:HD21	1:B:161:ARG:H	1.16	0.88
1:B:452:LYS:HE3	1:B:468:LYS:HG2	1.53	0.88
1:A:383:SER:HB3	1:B:546:GLN:HB3	1.55	0.87
1:A:384:ALA:N	1:B:546:GLN:NE2	2.21	0.87
1:A:78:VAL:CG1	1:A:82:PHE:HD2	1.86	0.87
1:B:773:CYS:SG	1:B:776:HIS:ND1	2.48	0.86
1:A:383:SER:HB2	1:B:546:GLN:CB	2.04	0.86
1:A:773:CYS:SG	1:A:776:HIS:ND1	2.48	0.86
1:A:472:LYS:CD	1:B:231:ASP:OD2	2.24	0.86
1:A:731:GLU:N	1:B:643:SER:CB	2.30	0.85
1:A:231:ASP:N	1:B:471:ARG:HH12	1.74	0.85
1:A:161:ARG:H	1:B:134:ASN:ND2	1.74	0.84
1:B:507:LYS:CG	1:B:632:ILE:HG21	2.06	0.84
1:B:470:VAL:HG22	1:B:472:LYS:H	1.39	0.84
1:A:659:HIS:HB3	1:A:880:PHE:CE1	2.13	0.84
1:B:7:GLN:HE21	1:B:16:ASN:HD21	1.25	0.84
1:A:634:ASN:C	1:A:636:GLU:H	1.79	0.84
1:A:546:GLN:OE1	1:B:381:ASN:HB2	1.75	0.83
1:A:645:GLN:C	1:B:728:LEU:HA	1.98	0.83
1:B:659:HIS:HB3	1:B:880:PHE:CE1	2.13	0.83
1:A:383:SER:HB2	1:B:546:GLN:CD	1.97	0.83
1:B:478:HIS:C	1:B:480:THR:H	1.81	0.83
1:A:661:ALA:HA	1:A:879:CYS:O	1.79	0.83
1:A:134:ASN:ND2	1:B:161:ARG:H	1.77	0.83
1:A:517:ASP:HB2	1:A:546:GLN:HB2	1.61	0.83
1:A:727:ARG:O	1:B:645:GLN:CG	2.28	0.82
1:A:168[B]:ASP:OD1	1:B:167:ARG:HA	1.80	0.82
1:B:507:LYS:HG2	1:B:632:ILE:HG21	1.59	0.82
1:B:632:ILE:HG12	1:B:632:ILE:O	1.80	0.82
1:A:472:LYS:HZ1	1:B:231:ASP:N	1.77	0.82
1:B:661:ALA:HA	1:B:879:CYS:O	1.79	0.82
1:A:7:GLN:HE21	1:A:16:ASN:HD21	1.25	0.82
1:A:78:VAL:HG12	1:A:82:PHE:HD2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASP:HB2	1:B:546:GLN:HB2	1.61	0.81
1:B:507:LYS:CD	1:B:632:ILE:HD12	2.11	0.81
1:A:734:LYS:HG2	1:A:736:ALA:O	1.81	0.80
1:A:477:ALA:HB1	1:A:479:ASN:CB	2.11	0.80
1:A:451:LYS:C	1:A:453:ILE:N	2.29	0.80
1:A:472:LYS:NZ	1:B:231:ASP:N	2.30	0.80
1:B:734:LYS:HG2	1:B:736:ALA:O	1.81	0.80
1:B:451:LYS:C	1:B:453:ILE:N	2.29	0.80
1:B:478:HIS:C	1:B:480:THR:N	2.35	0.80
1:A:731:GLU:OE1	1:B:643:SER:CB	2.30	0.80
1:A:976:GLN:H	1:A:976:GLN:HE21	1.26	0.80
1:B:478:HIS:C	1:B:509:PHE:CA	2.50	0.80
1:B:976:GLN:HE21	1:B:976:GLN:H	1.26	0.80
1:B:637:ASP:C	1:B:639:LYS:N	2.28	0.80
1:A:507:LYS:CB	1:A:632:ILE:HG21	2.12	0.79
1:A:645:GLN:O	1:B:728:LEU:HA	1.82	0.79
1:A:645:GLN:HE21	1:A:646:PHE:N	1.79	0.79
1:B:78:VAL:HG12	1:B:82:PHE:HD2	1.45	0.79
1:B:477:ALA:O	1:B:479:ASN:N	2.16	0.79
1:A:638:ASN:O	1:A:640:SER:N	2.16	0.78
1:A:231:ASP:HB2	1:B:471:ARG:CZ	2.13	0.78
1:A:478:HIS:N	1:A:479:ASN:N	2.31	0.78
1:A:643:SER:O	1:B:730:ALA:CB	2.07	0.78
1:B:16:ASN:HD22	1:B:43:GLU:H	1.31	0.78
1:A:16:ASN:HD22	1:A:43:GLU:H	1.31	0.78
1:A:229:GLN:CB	1:B:471:ARG:HH21	1.88	0.78
1:A:726:ILE:CG2	1:B:648:ASP:OD1	2.33	0.77
1:A:727:ARG:C	1:B:645:GLN:HG3	2.04	0.77
1:A:638:ASN:O	1:A:639:LYS:C	2.21	0.77
1:A:223:ARG:HA	1:A:226:SER:CB	2.15	0.76
1:A:726:ILE:HA	1:B:648:ASP:HA	1.65	0.76
1:A:477:ALA:HB1	1:A:479:ASN:HB3	1.67	0.76
1:B:223:ARG:HA	1:B:226:SER:CB	2.16	0.76
1:B:478:HIS:CG	1:B:479:ASN:N	2.54	0.76
1:B:730:ALA:HB1	1:B:732:GLU:HG2	1.64	0.76
1:A:729:GLU:H	1:B:645:GLN:N	1.09	0.76
1:A:643:SER:C	1:B:730:ALA:CA	2.48	0.76
1:A:645:GLN:N	1:B:729:GLU:H	1.84	0.75
1:B:634:ASN:C	1:B:636:GLU:N	2.39	0.75
1:B:659:HIS:CB	1:B:880:PHE:CE1	2.69	0.75
1:B:744:VAL:HG23	1:B:748:GLU:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:TRP:NE1	1:B:1048:GLY:C	2.39	0.75
1:A:659:HIS:CB	1:A:880:PHE:CE1	2.69	0.75
1:A:230:SER:N	1:B:471:ARG:NH2	2.30	0.75
1:A:726:ILE:HG22	1:B:648:ASP:HA	1.69	0.75
1:A:1046:TRP:NE1	1:A:1048:GLY:C	2.40	0.75
1:B:478:HIS:C	1:B:508:GLY:O	2.24	0.75
1:A:645:GLN:CA	1:B:728:LEU:HA	2.16	0.75
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.69	0.75
1:A:451:LYS:O	1:A:453:ILE:N	2.20	0.74
1:A:744:VAL:HG23	1:A:748:GLU:HG3	1.67	0.74
1:B:661:ALA:O	1:B:662:PHE:CA	2.28	0.74
1:A:632:ILE:CG1	1:A:635:SER:H	2.00	0.74
1:B:451:LYS:O	1:B:453:ILE:N	2.20	0.74
1:A:661:ALA:O	1:A:662:PHE:CA	2.28	0.74
1:A:645:GLN:HB2	1:B:729:GLU:CB	2.18	0.74
1:B:507:LYS:HA	1:B:632:ILE:CG2	2.18	0.74
1:A:452:LYS:HB3	1:A:455:LEU:CG	2.18	0.74
1:B:78:VAL:HG11	1:B:82:PHE:CD2	2.23	0.73
1:A:647:VAL:CB	1:B:727:ARG:HB3	2.18	0.73
1:A:1046:TRP:HD1	1:A:1048:GLY:CA	2.01	0.73
1:B:1046:TRP:HD1	1:B:1048:GLY:CA	2.01	0.73
1:A:645:GLN:HB2	1:B:729:GLU:N	2.02	0.73
1:A:727:ARG:O	1:B:647:VAL:N	2.19	0.73
1:A:86:LEU:H	1:A:257:GLN:HE22	1.37	0.73
1:B:507:LYS:HB3	1:B:632:ILE:HG21	1.71	0.73
1:A:478:HIS:N	1:A:631:ASP:OD2	2.21	0.73
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.69	0.72
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.24	0.72
1:B:86:LEU:H	1:B:257:GLN:HE22	1.37	0.72
1:B:478:HIS:CB	1:B:479:ASN:N	2.53	0.72
1:B:452:LYS:HB3	1:B:455:LEU:CG	2.18	0.72
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.24	0.72
1:A:78:VAL:HG12	1:A:82:PHE:CD2	2.20	0.72
1:A:730:ALA:O	1:A:731:GLU:HB3	1.89	0.72
1:A:472:LYS:HD2	1:B:231:ASP:OD2	1.88	0.71
1:A:451:LYS:C	1:A:453:ILE:H	1.94	0.71
1:A:727:ARG:HG2	1:B:645:GLN:HG3	1.71	0.71
1:B:645:GLN:NE2	1:B:646:PHE:H	1.87	0.71
1:B:229:GLN:O	1:B:230:SER:C	2.29	0.71
1:B:682:ARG:HD2	1:B:869:ALA:HA	1.71	0.71
1:A:646:PHE:N	1:B:727:ARG:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:ALA:O	1:B:731:GLU:HB3	1.89	0.71
1:B:550:TRP:O	1:B:554:ALA:HB3	1.91	0.71
1:A:383:SER:OG	1:B:517:ASP:O	2.09	0.70
1:A:682:ARG:HD2	1:A:869:ALA:HA	1.71	0.70
1:A:641:THR:O	1:B:732:GLU:OE1	0.71	0.70
1:A:548:VAL:HG13	1:A:584:PHE:CE2	2.26	0.70
1:A:727:ARG:CB	1:B:647:VAL:HB	2.10	0.70
1:A:963:ALA:HB1	1:A:973:THR:HG22	1.72	0.70
1:B:451:LYS:C	1:B:453:ILE:H	1.94	0.70
1:A:78:VAL:HG11	1:A:82:PHE:CD2	2.23	0.70
1:A:642:LEU:HD12	1:A:643:SER:H	1.56	0.70
1:A:667:VAL:HG22	1:A:685:GLU:HB3	1.74	0.70
1:B:507:LYS:CA	1:B:632:ILE:HG21	2.22	0.70
1:A:229:GLN:O	1:A:230:SER:C	2.29	0.70
1:A:550:TRP:O	1:A:554:ALA:HB3	1.91	0.70
1:A:643:SER:C	1:B:730:ALA:HA	2.10	0.70
1:A:230:SER:CA	1:B:471:ARG:HH12	2.04	0.70
1:B:667:VAL:HG22	1:B:685:GLU:HB3	1.74	0.70
1:A:482:LEU:O	1:A:511:PRO:HA	1.92	0.70
1:B:7:GLN:HE21	1:B:16:ASN:ND2	1.89	0.70
1:B:963:ALA:HB1	1:B:973:THR:HG22	1.72	0.70
1:B:482:LEU:O	1:B:511:PRO:HA	1.92	0.70
1:B:523:LEU:HD23	1:B:562:VAL:HG11	1.74	0.70
1:B:1035:LEU:HD13	1:B:1041:TYR:HB2	1.74	0.69
1:A:7:GLN:HE21	1:A:16:ASN:ND2	1.89	0.69
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.56	0.69
1:A:523:LEU:HD23	1:A:562:VAL:HG11	1.74	0.69
1:A:1035:LEU:HD13	1:A:1041:TYR:HB2	1.74	0.69
1:B:773:CYS:SG	1:B:776:HIS:CE1	2.86	0.69
1:A:645:GLN:HG2	1:B:727:ARG:HG2	1.73	0.69
1:B:548:VAL:HG13	1:B:584:PHE:CE2	2.26	0.69
1:A:632:ILE:HG13	1:A:635:SER:H	1.57	0.69
1:A:773:CYS:SG	1:A:776:HIS:CE1	2.86	0.69
1:A:773:CYS:HB3	1:A:776:HIS:HB2	1.73	0.69
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.56	0.69
1:A:472:LYS:HZ1	1:B:231:ASP:HA	1.47	0.69
1:A:528:ALA:HA	1:A:563:ARG:O	1.93	0.69
1:B:773:CYS:HB3	1:B:776:HIS:HB2	1.73	0.68
1:B:472:LYS:HZ2	1:B:474:ALA:HA	1.58	0.68
1:A:383:SER:CB	1:B:546:GLN:HE21	2.02	0.68
1:A:645:GLN:NE2	1:A:646:PHE:H	1.88	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ASP:HA	1:A:639:LYS:HB3	1.74	0.68
1:B:528:ALA:HA	1:B:563:ARG:O	1.93	0.68
1:A:470:VAL:HG13	1:A:471:ARG:H	1.58	0.68
1:A:229:GLN:HG2	1:A:230:SER:H	1.59	0.68
1:A:726:ILE:HG22	1:B:648:ASP:CB	2.23	0.68
1:A:1015:LYS:HD3	7:A:1109:PG4:H81	1.75	0.68
1:B:229:GLN:HG2	1:B:230:SER:H	1.59	0.67
1:A:485:LEU:HD22	1:A:515:THR:O	1.95	0.67
1:B:452:LYS:HB2	1:B:454:PRO:HA	1.76	0.67
1:B:655:LEU:HD11	1:B:826:PRO:HD3	1.76	0.67
1:B:222:ASP:O	1:B:226:SER:N	2.28	0.67
1:B:223:ARG:HD3	1:B:228:GLU:HB3	1.76	0.67
1:A:659:HIS:CG	1:A:880:PHE:CZ	2.83	0.67
1:A:727:ARG:O	1:B:646:PHE:CA	2.42	0.67
1:A:731:GLU:OE1	1:B:642:LEU:O	2.13	0.67
1:B:452:LYS:O	1:B:454:PRO:CA	2.43	0.67
1:A:727:ARG:N	1:B:647:VAL:O	2.28	0.66
1:B:659:HIS:CG	1:B:880:PHE:CZ	2.83	0.66
1:A:452:LYS:HD3	1:A:468:LYS:NZ	2.10	0.66
1:A:608:ASP:OD1	1:B:794:LEU:CD1	2.44	0.66
1:A:643:SER:OG	1:B:732:GLU:CD	2.34	0.66
1:B:645:GLN:OE1	1:B:645:GLN:HA	1.91	0.66
1:B:1015:LYS:HD3	7:B:1109:PG4:H81	1.75	0.66
1:A:223:ARG:HD3	1:A:228:GLU:HB3	1.76	0.66
1:A:452:LYS:O	1:A:454:PRO:CA	2.43	0.66
1:A:728:LEU:HD23	1:B:645:GLN:C	2.16	0.66
1:A:222:ASP:O	1:A:226:SER:N	2.28	0.66
1:B:478:HIS:O	1:B:480:THR:CG2	2.44	0.66
1:A:661:ALA:CA	1:A:879:CYS:O	2.43	0.66
1:A:452:LYS:HB2	1:A:454:PRO:HA	1.76	0.66
1:B:485:LEU:HD22	1:B:515:THR:O	1.95	0.66
1:A:732:GLU:H	1:B:643:SER:CB	2.09	0.66
1:B:477:ALA:O	1:B:478:HIS:CG	2.49	0.66
1:B:478:HIS:N	1:B:479:ASN:HA	2.10	0.65
1:B:452:LYS:HD3	1:B:468:LYS:NZ	2.10	0.65
1:B:507:LYS:HA	1:B:632:ILE:HG21	1.78	0.65
1:A:634:ASN:C	1:A:636:GLU:N	2.44	0.65
1:A:731:GLU:N	1:B:643:SER:HB3	1.74	0.65
1:B:507:LYS:HD3	1:B:632:ILE:CD1	2.25	0.65
1:A:520:ALA:O	1:B:383:SER:HA	1.96	0.65
1:B:661:ALA:CA	1:B:879:CYS:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLN:C	1:B:727:ARG:O	2.34	0.65
1:A:469:LYS:HG3	1:A:471:ARG:HH22	1.62	0.65
1:B:630:LEU:C	1:B:631:ASP:N	2.50	0.65
1:B:179:ARG:NH1	1:B:204:GLN:OE1	2.28	0.65
1:A:168[B]:ASP:OD1	1:B:167:ARG:HG2	1.96	0.65
1:B:78:VAL:HG12	1:B:82:PHE:CD2	2.20	0.65
1:B:175:THR:HG22	1:B:179:ARG:HH21	1.62	0.65
1:B:470:VAL:HG13	1:B:471:ARG:H	1.62	0.65
1:A:471:ARG:HG2	1:A:472:LYS:N	2.12	0.64
1:A:1015:LYS:CD	7:A:1109:PG4:H81	2.27	0.64
1:B:507:LYS:CG	1:B:632:ILE:HD12	2.27	0.64
1:B:478:HIS:C	1:B:508:GLY:C	2.56	0.64
1:B:478:HIS:HB3	1:B:480:THR:N	2.12	0.64
1:A:452:LYS:HD2	1:A:455:LEU:HG	1.80	0.64
1:B:452:LYS:CE	1:B:468:LYS:H	2.11	0.64
1:B:452:LYS:HD2	1:B:455:LEU:HG	1.80	0.64
1:A:452:LYS:HD3	1:A:468:LYS:HZ2	1.63	0.64
1:A:452:LYS:CE	1:A:468:LYS:H	2.11	0.64
1:A:100:HIS:CE1	1:A:104:LEU:HD11	2.33	0.64
1:B:1015:LYS:CD	7:B:1109:PG4:H81	2.27	0.64
1:A:655:LEU:HD21	1:A:826:PRO:CD	2.08	0.64
1:A:175:THR:HG22	1:A:179:ARG:HH21	1.62	0.63
1:A:179:ARG:NH1	1:A:204:GLN:OE1	2.28	0.63
1:A:635:SER:C	1:A:637:ASP:H	2.01	0.63
1:A:1046:TRP:CD1	1:A:1048:GLY:O	2.46	0.63
1:B:452:LYS:O	1:B:453:ILE:O	2.16	0.63
1:B:563:ARG:HG2	1:B:595:GLU:CB	2.28	0.63
1:A:655:LEU:CD2	1:A:826:PRO:HD3	2.08	0.63
1:B:659:HIS:ND1	1:B:880:PHE:CZ	2.66	0.63
1:B:637:ASP:O	1:B:639:LYS:N	2.32	0.63
1:B:734:LYS:O	1:B:734:LYS:HG2	1.97	0.63
1:A:452:LYS:O	1:A:453:ILE:O	2.16	0.63
1:B:229:GLN:C	1:B:231:ASP:N	2.52	0.63
1:A:563:ARG:HG2	1:A:595:GLU:CB	2.28	0.63
1:A:726:ILE:HG22	1:B:648:ASP:CG	2.19	0.63
1:A:507:LYS:HG2	1:A:632:ILE:CG2	2.16	0.63
1:A:229:GLN:CA	1:B:471:ARG:HH21	2.04	0.63
1:A:1035:LEU:HD22	1:A:1040:ARG:HB2	1.81	0.62
1:B:100:HIS:CE1	1:B:104:LEU:HD11	2.33	0.62
1:B:645:GLN:HE21	1:B:647:VAL:HG23	1.64	0.62
1:A:659:HIS:ND1	1:A:880:PHE:CZ	2.66	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:LEU:HD22	1:B:1040:ARG:HB2	1.81	0.62
1:A:734:LYS:O	1:A:734:LYS:HG2	1.97	0.62
1:B:478:HIS:CA	1:B:631:ASP:OD2	2.46	0.62
1:B:773:CYS:SG	1:B:776:HIS:CD2	2.92	0.62
1:A:477:ALA:C	1:A:479:ASN:N	2.52	0.62
1:A:571:ASP:OD1	1:A:573:ASN:HB2	2.00	0.62
1:A:595:GLU:OE2	1:A:627:TYR:OH	2.18	0.62
1:A:773:CYS:SG	1:A:776:HIS:CD2	2.92	0.62
1:B:478:HIS:CA	1:B:480:THR:H	2.13	0.62
1:B:659:HIS:CG	1:B:880:PHE:CE1	2.88	0.62
1:B:1046:TRP:CD1	1:B:1048:GLY:O	2.46	0.62
1:A:546:GLN:OE1	1:B:381:ASN:CB	2.44	0.61
1:A:659:HIS:CG	1:A:880:PHE:CE1	2.88	0.61
1:B:223:ARG:C	1:B:226:SER:H	2.03	0.61
1:B:637:ASP:HA	1:B:639:LYS:HG3	1.81	0.61
1:A:642:LEU:CA	1:B:732:GLU:CD	2.68	0.61
1:B:477:ALA:C	1:B:631:ASP:OD2	2.39	0.61
1:B:563:ARG:HG2	1:B:595:GLU:HB3	1.82	0.61
1:B:571:ASP:OD1	1:B:573:ASN:HB2	2.00	0.61
1:B:734:LYS:CG	1:B:736:ALA:O	2.49	0.61
1:A:78:VAL:HG11	1:A:82:PHE:CE2	2.36	0.61
1:A:647:VAL:HG21	1:B:727:ARG:HD2	1.81	0.61
1:B:735:LEU:HD12	1:B:735:LEU:C	2.20	0.61
1:A:482:LEU:HB2	1:A:509:PHE:CD2	2.35	0.61
1:B:482:LEU:HB2	1:B:509:PHE:CD2	2.35	0.61
1:A:734:LYS:CG	1:A:736:ALA:O	2.48	0.61
1:B:595:GLU:OE2	1:B:627:TYR:OH	2.18	0.61
1:A:516:LEU:HD21	1:A:531:ILE:HG23	1.82	0.61
1:A:563:ARG:HG2	1:A:595:GLU:HB3	1.83	0.61
1:A:655:LEU:HD22	1:A:824:ILE:O	2.01	0.61
1:A:223:ARG:C	1:A:226:SER:H	2.04	0.60
1:A:646:PHE:CA	1:B:727:ARG:O	2.49	0.60
1:A:787:GLN:HE21	1:A:791:GLU:CD	2.04	0.60
1:B:787:GLN:HE21	1:B:791:GLU:CD	2.04	0.60
1:A:643:SER:CB	1:B:731:GLU:OE1	2.48	0.60
1:A:635:SER:C	1:A:637:ASP:N	2.52	0.60
1:A:642:LEU:C	1:B:732:GLU:CD	2.60	0.60
1:A:735:LEU:HD12	1:A:735:LEU:C	2.20	0.60
1:B:616:TRP:O	1:B:620:MET:HB2	2.02	0.60
1:A:616:TRP:O	1:A:620:MET:HB2	2.02	0.60
1:B:452:LYS:HB2	1:B:454:PRO:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:HG11	1:B:82:PHE:CE2	2.36	0.60
1:B:478:HIS:HB3	1:B:480:THR:H	1.66	0.60
1:B:516:LEU:HD21	1:B:531:ILE:HG23	1.82	0.60
1:B:634:ASN:O	1:B:636:GLU:N	2.35	0.60
1:A:452:LYS:HB2	1:A:454:PRO:CA	2.31	0.60
1:B:477:ALA:C	1:B:479:ASN:N	2.56	0.60
1:B:659:HIS:CB	1:B:880:PHE:CD1	2.83	0.60
1:A:659:HIS:HB3	1:A:880:PHE:CG	2.37	0.59
1:B:229:GLN:O	1:B:231:ASP:N	2.35	0.59
1:B:451:LYS:O	1:B:452:LYS:C	2.40	0.59
1:A:229:GLN:O	1:A:231:ASP:N	2.35	0.59
1:A:729:GLU:N	1:B:645:GLN:N	1.91	0.59
1:B:478:HIS:CA	1:B:480:THR:N	2.66	0.59
1:A:659:HIS:NE2	1:A:826:PRO:HG3	2.18	0.59
1:B:629:ASN:H	1:B:629:ASN:HD22	1.51	0.59
1:B:478:HIS:CA	1:B:508:GLY:O	2.51	0.59
1:B:659:HIS:HB3	1:B:880:PHE:CG	2.37	0.59
1:B:659:HIS:NE2	1:B:826:PRO:HG3	2.18	0.59
1:A:451:LYS:O	1:A:452:LYS:C	2.40	0.59
1:A:659:HIS:CB	1:A:880:PHE:CD1	2.83	0.59
1:A:478:HIS:CA	1:A:479:ASN:N	2.66	0.59
1:B:87[A]:PHE:HZ	3:B:1102:1C6:CE2	2.16	0.59
1:B:452:LYS:CB	1:B:455:LEU:HG	2.29	0.59
1:B:478:HIS:CB	1:B:480:THR:H	2.16	0.59
1:B:473:LYS:H	1:B:473:LYS:HZ3	1.51	0.59
1:A:78:VAL:HG13	1:A:82:PHE:CD2	2.38	0.58
1:A:87[A]:PHE:HZ	3:A:1102:1C6:CE2	2.16	0.58
1:A:477:ALA:HB1	1:A:479:ASN:N	2.18	0.58
1:A:727:ARG:HG2	1:B:645:GLN:CG	2.31	0.58
1:A:637:ASP:OD2	1:A:640:SER:HB3	2.02	0.58
1:B:478:HIS:N	1:B:479:ASN:N	2.51	0.58
1:B:230:SER:O	1:B:232:ASP:N	2.36	0.58
1:A:477:ALA:HB1	1:A:479:ASN:CA	2.33	0.58
1:A:478:HIS:HB2	1:A:629:ASN:OD1	2.04	0.58
1:A:1012:THR:HA	7:A:1109:PG4:H82	1.85	0.58
1:B:1012:THR:HA	7:B:1109:PG4:H82	1.85	0.58
1:A:223:ARG:HG3	1:A:228:GLU:OE2	2.03	0.58
1:A:223:ARG:O	1:A:226:SER:N	2.37	0.58
1:B:223:ARG:HG3	1:B:228:GLU:OE2	2.03	0.58
1:B:473:LYS:HZ3	1:B:473:LYS:N	2.01	0.58
1:A:523:LEU:HD11	1:A:547:PHE:HE1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LEU:HG	1:A:644:LEU:HG	1.86	0.58
1:B:523:LEU:HD11	1:B:547:PHE:HE1	1.69	0.58
1:A:161:ARG:HD2	1:B:132:ARG:O	2.04	0.58
1:A:230:SER:O	1:A:232:ASP:N	2.36	0.58
1:B:478:HIS:O	1:B:480:THR:HG22	2.04	0.58
1:A:475:GLU:HB2	1:A:476:ASN:OD1	2.04	0.57
1:A:648:ASP:HA	1:B:726:ILE:HA	1.86	0.57
1:A:472:LYS:CD	1:B:231:ASP:HB2	2.30	0.57
1:A:731:GLU:N	1:B:643:SER:HB2	2.06	0.57
1:B:223:ARG:O	1:B:226:SER:N	2.37	0.57
1:A:168[B]:ASP:OD1	1:B:167:ARG:CA	2.51	0.57
1:A:87[A]:PHE:CZ	3:A:1102:1C6:CE2	2.88	0.57
1:A:647:VAL:HG12	1:A:649:SER:HB3	1.87	0.57
1:A:653:MET:SD	1:A:752:TYR:CD2	2.98	0.57
1:B:653:MET:SD	1:B:752:TYR:CD2	2.97	0.57
1:A:452:LYS:CD	1:A:455:LEU:HG	2.35	0.57
1:A:472:LYS:HZ1	1:B:231:ASP:CB	1.28	0.57
3:B:1102:1C6:H3	3:B:1102:1C6:C2	2.31	0.57
1:A:452:LYS:CB	1:A:455:LEU:HG	2.29	0.57
1:A:726:ILE:HA	1:B:647:VAL:O	2.04	0.57
1:B:87[A]:PHE:CZ	3:B:1102:1C6:CE2	2.88	0.56
1:A:478:HIS:O	1:A:480:THR:N	2.37	0.56
1:B:452:LYS:CD	1:B:455:LEU:HG	2.35	0.56
1:B:472:LYS:HD2	1:B:473:LYS:NZ	2.19	0.56
1:B:635:SER:O	1:B:636:GLU:C	2.44	0.56
1:B:735:LEU:CD1	1:B:736:ALA:N	2.64	0.56
1:A:632:ILE:HG12	1:A:635:SER:H	1.68	0.56
1:B:506:SER:HB3	1:B:638:ASN:HB2	1.88	0.56
1:B:647:VAL:HG12	1:B:649:SER:HB3	1.87	0.56
1:A:787:GLN:NE2	1:A:791:GLU:OE1	2.38	0.56
1:A:794:LEU:HD12	1:B:608:ASP:OD1	2.05	0.56
1:B:635:SER:HG	1:B:637:ASP:H	1.54	0.56
1:A:485:LEU:HA	1:A:514:ALA:O	2.05	0.56
1:B:645:GLN:NE2	1:B:647:VAL:HG23	2.20	0.56
1:B:655:LEU:HD23	1:B:703:ILE:HG23	1.87	0.56
1:B:891:PRO:CD	1:B:898:LEU:HD21	2.36	0.56
1:A:891:PRO:CD	1:A:898:LEU:HD21	2.36	0.56
1:A:168[B]:ASP:OD1	1:B:167:ARG:CG	2.54	0.55
1:B:478:HIS:O	1:B:480:THR:HG23	2.06	0.55
1:B:507:LYS:HA	1:B:632:ILE:HG22	1.88	0.55
1:B:507:LYS:CA	1:B:632:ILE:CG2	2.82	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:ALA:HA	1:B:880:PHE:HB3	1.89	0.55
1:A:229:GLN:C	1:A:231:ASP:N	2.52	0.55
1:B:162:PHE:HE1	1:B:215:LEU:CD2	2.19	0.55
1:A:78:VAL:CG1	1:A:82:PHE:CE2	2.89	0.55
1:A:645:GLN:CB	1:B:729:GLU:H	2.14	0.55
1:B:478:HIS:N	1:B:508:GLY:O	2.38	0.55
1:A:646:PHE:CG	1:A:646:PHE:O	2.60	0.55
1:A:726:ILE:HB	1:B:648:ASP:OD1	2.06	0.55
1:A:661:ALA:HA	1:A:880:PHE:HB3	1.88	0.55
1:A:732:GLU:HB3	1:B:641:THR:HG22	1.88	0.55
1:B:78:VAL:HG13	1:B:82:PHE:CD2	2.38	0.55
1:B:478:HIS:N	1:B:479:ASN:CA	2.70	0.55
1:B:485:LEU:HA	1:B:514:ALA:O	2.05	0.55
1:B:976:GLN:H	1:B:976:GLN:NE2	2.01	0.55
1:A:645:GLN:HG3	1:A:646:PHE:N	2.22	0.55
1:A:635:SER:O	1:A:636:GLU:HB3	2.07	0.54
1:A:645:GLN:CG	1:B:728:LEU:C	2.74	0.54
1:A:654:PRO:O	1:A:655:LEU:C	2.38	0.54
1:A:728:LEU:HB3	1:B:645:GLN:N	2.22	0.54
1:A:735:LEU:CD1	1:A:736:ALA:N	2.64	0.54
1:A:223:ARG:HD3	1:A:226:SER:CB	2.38	0.54
1:A:608:ASP:OD1	1:B:794:LEU:HD11	2.08	0.54
1:A:645:GLN:HB3	1:B:729:GLU:H	1.62	0.54
1:B:645:GLN:HE21	1:B:647:VAL:N	2.06	0.54
1:B:78:VAL:CG1	1:B:82:PHE:CE2	2.89	0.54
1:B:452:LYS:HE2	1:B:468:LYS:H	1.72	0.54
1:A:230:SER:C	1:B:471:ARG:HH12	2.10	0.54
1:A:642:LEU:HD12	1:A:643:SER:N	2.22	0.54
1:A:794:LEU:CD1	1:B:608:ASP:OD1	2.55	0.54
1:B:71:LEU:HD22	1:B:90:TRP:CE2	2.42	0.54
1:A:383:SER:OG	1:B:546:GLN:CB	2.56	0.54
1:A:383:SER:OG	1:B:546:GLN:HB2	2.08	0.54
1:A:168[B]:ASP:OD1	1:B:167:ARG:CB	2.56	0.54
1:A:472:LYS:NZ	1:B:231:ASP:HB2	0.38	0.54
1:A:647:VAL:HG12	1:A:649:SER:CB	2.38	0.54
1:B:223:ARG:HD3	1:B:226:SER:CB	2.38	0.54
1:B:655:LEU:CD2	1:B:824:ILE:O	2.52	0.54
1:A:71:LEU:HD22	1:A:90:TRP:CE2	2.42	0.53
1:A:551:LEU:HD11	1:A:589:LEU:HD13	1.90	0.53
1:A:643:SER:OG	1:B:732:GLU:CB	2.51	0.53
1:A:726:ILE:HG22	1:B:648:ASP:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:SER:O	1:B:638:ASN:N	2.31	0.53
1:A:471:ARG:HB3	1:A:471:ARG:CZ	2.39	0.53
1:A:1015:LYS:HB3	7:A:1109:PG4:H81	1.91	0.53
1:B:1015:LYS:HB3	7:B:1109:PG4:H81	1.91	0.53
1:B:452:LYS:HD3	1:B:468:LYS:HZ2	1.74	0.53
1:A:642:LEU:HA	1:B:732:GLU:CD	2.27	0.53
1:B:647:VAL:HG12	1:B:649:SER:CB	2.39	0.53
1:A:637:ASP:OD1	1:A:638:ASN:N	2.39	0.53
1:B:661:ALA:O	1:B:662:PHE:HA	2.09	0.53
1:A:162:PHE:HE1	1:A:215:LEU:CD2	2.19	0.53
1:A:383:SER:HB2	1:B:546:GLN:CG	2.38	0.52
1:A:452:LYS:HE2	1:A:468:LYS:H	1.72	0.52
1:B:478:HIS:HA	1:B:479:ASN:HA	0.52	0.52
1:B:478:HIS:CD2	1:B:479:ASN:N	2.78	0.52
1:B:629:ASN:H	1:B:629:ASN:ND2	2.06	0.52
1:B:420:HIS:CE1	1:B:453:ILE:HG21	2.45	0.52
1:A:469:LYS:HE2	1:A:470:VAL:N	2.25	0.52
1:A:635:SER:O	1:A:637:ASP:N	2.42	0.52
1:A:645:GLN:CD	1:A:647:VAL:HG23	2.30	0.52
1:A:661:ALA:O	1:A:662:PHE:HA	2.09	0.52
1:B:787:GLN:NE2	1:B:791:GLU:OE1	2.38	0.52
1:A:230:SER:HA	1:B:471:ARG:HH12	1.72	0.52
1:A:659:HIS:HB3	1:A:880:PHE:CZ	2.45	0.52
1:B:551:LEU:HD11	1:B:589:LEU:HD13	1.90	0.52
1:B:1006:ALA:HB3	1:B:1007:PRO:HD3	1.92	0.52
1:A:507:LYS:CB	1:A:632:ILE:CG2	2.87	0.52
1:A:726:ILE:CA	1:B:648:ASP:HA	2.39	0.52
1:B:659:HIS:HB3	1:B:880:PHE:CZ	2.45	0.52
1:A:744:VAL:CG2	1:A:748:GLU:HG3	2.39	0.52
1:A:585:ILE:O	1:A:589:LEU:HB2	2.09	0.51
1:B:431:LEU:HD21	1:B:433:ILE:HD11	1.91	0.51
1:A:1006:ALA:HB3	1:A:1007:PRO:HD3	1.92	0.51
1:B:477:ALA:O	1:B:478:HIS:ND1	2.43	0.51
1:A:420:HIS:CE1	1:A:453:ILE:HG21	2.45	0.51
1:A:431:LEU:HD21	1:A:433:ILE:HD11	1.91	0.51
1:A:452:LYS:O	1:A:454:PRO:C	2.49	0.51
3:A:1102:1C6:H3	3:A:1102:1C6:C2	2.31	0.51
1:B:563:ARG:HG2	1:B:595:GLU:CG	2.41	0.51
1:A:632:ILE:HG13	1:A:635:SER:N	2.25	0.51
1:B:733:GLU:CD	1:B:734:LYS:N	2.64	0.51
1:A:87[A]:PHE:CE2	3:A:1102:1C6:H11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:HIS:HB2	1:A:631:ASP:OD1	2.10	0.51
1:A:482:LEU:HB2	1:A:509:PHE:HD2	1.73	0.51
1:A:563:ARG:HG2	1:A:595:GLU:CG	2.41	0.51
1:A:646:PHE:HA	1:B:727:ARG:O	2.11	0.51
1:B:452:LYS:O	1:B:454:PRO:C	2.49	0.51
1:B:482:LEU:HB2	1:B:509:PHE:HD2	1.73	0.51
1:B:478:HIS:ND1	1:B:631:ASP:OD1	2.28	0.51
1:B:646:PHE:O	1:B:648:ASP:N	2.43	0.51
1:A:726:ILE:CG2	1:B:648:ASP:CG	2.78	0.51
1:A:469:LYS:HE2	1:A:470:VAL:H	1.75	0.51
1:A:597:ILE:HG22	1:A:597:ILE:O	2.11	0.51
1:A:618:GLU:HA	1:A:618:GLU:OE1	2.11	0.51
1:B:571:ASP:HB3	1:B:574:TRP:HE3	1.76	0.51
1:A:87[A]:PHE:CE2	3:A:1102:1C6:C1	2.94	0.51
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.44	0.51
1:A:1012:THR:HA	7:A:1109:PG4:H61	1.93	0.51
1:A:452:LYS:NZ	1:A:454:PRO:HA	2.26	0.50
1:A:642:LEU:HD12	1:B:732:GLU:OE2	2.11	0.50
1:A:733:GLU:CD	1:A:734:LYS:N	2.64	0.50
1:B:585:ILE:O	1:B:589:LEU:HB2	2.09	0.50
1:A:632:ILE:HD13	1:A:632:ILE:O	2.10	0.50
1:A:645:GLN:CG	1:B:727:ARG:C	2.66	0.50
1:B:635:SER:O	1:B:636:GLU:HG2	2.11	0.50
1:B:87[A]:PHE:CE2	3:B:1102:1C6:H11	2.46	0.50
1:B:87[A]:PHE:CE2	3:B:1102:1C6:C1	2.94	0.50
1:B:179:ARG:NH1	1:B:208:ASP:OD1	2.44	0.50
1:B:618:GLU:OE1	1:B:618:GLU:HA	2.11	0.50
1:A:166:TYR:CE2	1:B:129:LYS:HB2	2.47	0.50
1:B:597:ILE:HG22	1:B:597:ILE:O	2.11	0.50
1:A:477:ALA:HA	1:A:631:ASP:OD2	2.11	0.50
1:A:646:PHE:O	1:A:648:ASP:N	2.45	0.50
1:A:976:GLN:H	1:A:976:GLN:NE2	2.01	0.50
1:B:478:HIS:CA	1:B:478:HIS:CG	2.83	0.50
1:A:230:SER:O	1:A:235:THR:OG1	2.30	0.50
1:B:478:HIS:HD1	1:B:631:ASP:CG	2.11	0.50
1:A:104:LEU:N	1:A:105:PRO:CD	2.75	0.50
1:A:479:ASN:HA	1:A:508:GLY:O	2.12	0.50
1:B:452:LYS:NZ	1:B:454:PRO:HA	2.26	0.50
1:B:1012:THR:HA	7:B:1109:PG4:H61	1.93	0.50
1:B:725:GLN:OE1	1:B:743:THR:HG22	2.13	0.49
1:B:104:LEU:N	1:B:105:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:SER:O	1:B:235:THR:OG1	2.30	0.49
1:B:744:VAL:CG2	1:B:748:GLU:HG3	2.39	0.49
1:A:469:LYS:CG	1:A:471:ARG:HH22	2.25	0.49
1:A:725:GLN:OE1	1:A:743:THR:HG22	2.13	0.49
1:A:472:LYS:HZ3	1:B:231:ASP:HB2	0.66	0.49
1:A:232:ASP:O	1:A:236:HIS:HD2	1.96	0.49
1:A:645:GLN:CG	1:B:728:LEU:CA	2.90	0.49
1:A:726:ILE:CB	1:B:648:ASP:OD1	2.60	0.49
1:A:727:ARG:HD2	1:B:647:VAL:HG21	1.94	0.49
1:A:507:LYS:HA	1:A:632:ILE:CG2	2.43	0.49
1:B:507:LYS:HG2	1:B:632:ILE:HD12	1.95	0.49
1:A:571:ASP:HB3	1:A:574:TRP:HE3	1.76	0.49
1:A:479:ASN:N	1:A:479:ASN:OD1	2.46	0.48
1:B:452:LYS:HD3	1:B:468:LYS:HZ3	1.76	0.48
1:B:452:LYS:CE	1:B:468:LYS:HG2	2.35	0.48
1:B:232:ASP:O	1:B:236:HIS:HD2	1.96	0.48
1:B:478:HIS:HA	1:B:479:ASN:C	2.15	0.48
1:A:483:LEU:HD12	1:A:512:GLN:O	2.14	0.48
1:A:486:TYR:HA	1:A:532:VAL:O	2.13	0.48
1:B:483:LEU:HD12	1:B:512:GLN:O	2.14	0.48
1:B:523:LEU:HD11	1:B:547:PHE:CE1	2.48	0.48
1:A:523:LEU:HD11	1:A:547:PHE:CE1	2.48	0.48
1:A:571:ASP:HB3	1:A:574:TRP:CE3	2.48	0.48
1:A:614:GLU:HA	1:A:617:ARG:NH2	2.28	0.48
1:A:231:ASP:CB	1:B:471:ARG:CZ	2.90	0.48
1:A:520:ALA:O	1:B:383:SER:CA	2.61	0.48
1:B:87[A]:PHE:CE2	3:B:1102:1C6:CZ	2.97	0.48
1:B:87[A]:PHE:HE2	3:B:1102:1C6:C1	2.26	0.48
1:B:472:LYS:NZ	1:B:473:LYS:HE2	2.28	0.48
1:B:478:HIS:C	1:B:509:PHE:N	2.67	0.48
1:B:505:MET:HG3	1:B:511:PRO:HG2	1.96	0.48
1:B:653:MET:SD	1:B:752:TYR:CE2	3.07	0.48
1:A:472:LYS:CD	1:B:231:ASP:CB	2.89	0.48
1:A:726:ILE:CG2	1:B:648:ASP:HA	2.41	0.48
1:B:223:ARG:CD	1:B:228:GLU:HB3	2.44	0.48
1:B:472:LYS:HZ2	1:B:473:LYS:HE2	1.79	0.48
1:A:166:TYR:CZ	1:B:129:LYS:HA	2.49	0.47
1:A:559:VAL:HG22	1:A:592:LYS:O	2.14	0.47
1:A:638:ASN:O	1:A:641:THR:HG23	2.14	0.47
1:B:473:LYS:O	1:B:474:ALA:HB3	2.14	0.47
1:B:735:LEU:HD12	1:B:736:ALA:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:HB2	1:B:471:ARG:NE	2.25	0.47
1:B:472:LYS:NZ	1:B:474:ALA:HA	2.28	0.47
2:A:1101:HEM:CMB	2:A:1101:HEM:HBB2	2.44	0.47
1:B:486:TYR:HA	1:B:532:VAL:O	2.13	0.47
1:B:517:ASP:HA	1:B:547:PHE:HB2	1.96	0.47
1:B:571:ASP:HB3	1:B:574:TRP:CE3	2.48	0.47
2:B:1101:HEM:CMB	2:B:1101:HEM:HBB2	2.44	0.47
1:A:735:LEU:HD12	1:A:736:ALA:CA	2.44	0.47
1:B:559:VAL:HG22	1:B:592:LYS:O	2.15	0.47
1:B:614:GLU:HA	1:B:617:ARG:NH2	2.28	0.47
1:A:87[A]:PHE:CE2	3:A:1102:1C6:CZ	2.97	0.47
1:A:132:ARG:O	1:B:161:ARG:CD	2.50	0.47
1:A:547:PHE:O	1:A:550:TRP:HE3	1.96	0.47
1:A:653:MET:SD	1:A:752:TYR:CE2	3.08	0.47
1:A:229:GLN:O	1:B:471:ARG:NH2	2.30	0.47
1:A:452:LYS:HE3	1:A:468:LYS:CG	2.37	0.47
1:A:534:ALA:HA	1:A:569:CYS:O	2.15	0.47
1:A:625:ALA:HB1	1:A:630:LEU:HD13	1.97	0.47
1:A:726:ILE:HG22	1:B:648:ASP:OD1	2.09	0.47
1:A:87[A]:PHE:HE2	3:A:1102:1C6:C1	2.26	0.47
1:B:547:PHE:O	1:B:550:TRP:HE3	1.96	0.47
1:A:732:GLU:N	1:B:643:SER:OG	2.46	0.47
1:B:479:ASN:HA	1:B:508:GLY:O	2.15	0.47
1:A:480:THR:HA	1:A:481:PRO:HD3	1.70	0.47
1:A:517:ASP:HA	1:A:547:PHE:HB2	1.96	0.47
1:B:548:VAL:HG13	1:B:584:PHE:HE2	1.78	0.47
1:B:478:HIS:CB	1:B:480:THR:HG22	2.45	0.46
1:B:478:HIS:O	1:B:480:THR:N	2.43	0.46
1:B:1015:LYS:HB3	7:B:1109:PG4:C8	2.45	0.46
1:B:452:LYS:C	1:B:453:ILE:HG12	2.36	0.46
1:B:452:LYS:HE3	1:B:468:LYS:CG	2.37	0.46
1:B:635:SER:C	1:B:637:ASP:N	2.66	0.46
1:A:475:GLU:N	1:A:475:GLU:CD	2.67	0.46
1:A:726:ILE:HG21	1:B:648:ASP:OD1	2.14	0.46
1:A:827:ARG:HD2	5:A:1104:FAD:O1P	2.16	0.46
1:A:1015:LYS:HB3	7:A:1109:PG4:C8	2.45	0.46
1:A:452:LYS:C	1:A:453:ILE:HG12	2.36	0.46
1:A:452:LYS:HE3	1:A:468:LYS:H	1.80	0.46
1:A:475:GLU:CD	1:A:475:GLU:H	2.17	0.46
1:A:638:ASN:C	1:A:640:SER:N	2.68	0.46
1:B:452:LYS:HE3	1:B:468:LYS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HD12	1:A:52:LEU:CD2	2.46	0.46
1:B:478:HIS:CA	1:B:479:ASN:C	2.79	0.46
1:A:452:LYS:CE	1:A:468:LYS:HG2	2.35	0.46
1:A:505:MET:HG3	1:A:511:PRO:HG2	1.96	0.46
1:A:634:ASN:O	1:A:636:GLU:N	2.40	0.46
1:B:628:PHE:HB2	1:B:629:ASN:H	1.37	0.46
1:A:644:LEU:CD2	1:B:816:GLU:HA	2.46	0.46
1:A:735:LEU:O	1:A:736:ALA:C	2.54	0.46
1:B:745:SER:OG	1:B:748:GLU:HG2	2.15	0.46
1:A:230:SER:C	1:B:471:ARG:HH22	2.17	0.46
1:A:624:VAL:HG13	1:A:628:PHE:CE1	2.51	0.46
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.98	0.46
1:B:534:ALA:HA	1:B:569:CYS:O	2.15	0.46
1:B:637:ASP:OD2	1:B:640:SER:HB3	2.16	0.46
1:B:735:LEU:O	1:B:736:ALA:C	2.54	0.46
1:A:134:ASN:ND2	1:B:161:ARG:N	2.44	0.46
1:A:469:LYS:HG3	1:A:471:ARG:NH2	2.29	0.46
1:A:490:MET:HE3	1:A:536:TYR:HE2	1.81	0.46
1:A:166:TYR:HE2	1:B:129:LYS:HB2	1.80	0.45
1:A:548:VAL:HG13	1:A:584:PHE:HE2	1.78	0.45
1:B:87[A]:PHE:CZ	3:B:1102:1C6:CZ	2.99	0.45
1:B:624:VAL:HG13	1:B:628:PHE:CE1	2.51	0.45
1:B:827:ARG:HD2	5:B:1104:FAD:O1P	2.16	0.45
1:A:745:SER:OG	1:A:748:GLU:HG2	2.16	0.45
1:B:635:SER:OG	1:B:637:ASP:N	2.50	0.45
1:A:87[A]:PHE:CZ	3:A:1102:1C6:CZ	2.99	0.45
1:A:470:VAL:HG22	1:A:471:ARG:N	2.30	0.45
1:B:39:ILE:HD12	1:B:52:LEU:CD2	2.46	0.45
1:B:507:LYS:HB3	1:B:632:ILE:CG2	2.45	0.45
1:B:557:ASP:OD1	1:B:557:ASP:N	2.48	0.45
1:A:1038:LYS:HE3	7:A:1108:PG4:H11	1.98	0.45
1:B:490:MET:HE3	1:B:536:TYR:HE2	1.81	0.45
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.98	0.45
1:A:477:ALA:O	1:A:478:HIS:CG	2.69	0.45
1:B:655:LEU:HD21	1:B:826:PRO:HD3	1.98	0.45
1:A:231:ASP:HB2	1:B:471:ARG:NH2	2.31	0.45
1:A:727:ARG:HB3	1:B:647:VAL:CG2	2.45	0.45
1:A:731:GLU:OE1	1:B:643:SER:OG	2.34	0.45
1:A:472:LYS:NZ	1:B:231:ASP:H	2.10	0.45
1:A:486:TYR:O	1:A:516:LEU:N	2.50	0.45
1:B:507:LYS:HG2	1:B:632:ILE:CG2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:HD23	1:A:524:PRO:CG	2.47	0.44
1:A:560:LYS:HB3	1:A:560:LYS:HE3	1.75	0.44
1:B:645:GLN:C	1:B:646:PHE:CD2	2.91	0.44
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.99	0.44
1:B:455:LEU:O	1:B:468:LYS:C	2.54	0.44
1:B:639:LYS:O	1:B:640:SER:C	2.55	0.44
3:B:1102:1C6:H8	3:B:1102:1C6:C3	2.34	0.44
1:A:223:ARG:CD	1:A:228:GLU:HB3	2.44	0.44
1:B:122:ILE:HG22	1:B:148:LEU:HD12	1.99	0.44
1:A:222:ASP:O	1:A:225:ALA:HB3	2.18	0.44
1:A:328:ALA:HB1	3:A:1102:1C6:N1	2.33	0.44
1:B:222:ASP:O	1:B:225:ALA:HB3	2.18	0.44
1:B:1038:LYS:HE3	7:B:1108:PG4:H11	1.98	0.44
1:B:602:GLU:O	1:B:612:THR:HG21	2.18	0.44
1:B:615:GLU:O	1:B:619:HIS:ND1	2.51	0.44
1:A:5:MET:HA	1:A:6:PRO:HD3	1.88	0.44
1:A:452:LYS:CD	1:A:468:LYS:HZ2	2.31	0.44
1:A:521:GLY:HA2	1:A:550:TRP:CZ2	2.53	0.44
1:A:602:GLU:O	1:A:612:THR:HG21	2.18	0.44
1:A:615:GLU:O	1:A:619:HIS:ND1	2.51	0.44
1:B:328:ALA:HB1	3:B:1102:1C6:N1	2.33	0.44
1:B:483:LEU:HD23	1:B:524:PRO:CG	2.47	0.44
1:B:646:PHE:CD1	1:B:646:PHE:C	2.92	0.44
1:A:473:LYS:HA	1:A:473:LYS:HD2	1.47	0.43
1:A:727:ARG:O	1:B:645:GLN:CB	2.66	0.43
1:A:1048:GLY:C	5:A:1104:FAD:C1'	2.83	0.43
1:B:521:GLY:HA2	1:B:550:TRP:CZ2	2.53	0.43
1:A:167:ARG:HG2	1:B:168[B]:ASP:OD1	2.18	0.43
1:A:730:ALA:O	1:A:731:GLU:CB	2.62	0.43
1:A:655:LEU:O	1:A:656:ALA:C	2.55	0.43
1:B:473:LYS:CE	1:B:474:ALA:H	2.31	0.43
1:B:1015:LYS:CG	7:B:1109:PG4:H81	2.48	0.43
1:A:471:ARG:HB3	1:A:471:ARG:NH1	2.33	0.43
1:A:483:LEU:HD23	1:A:524:PRO:HG3	2.00	0.43
1:B:483:LEU:HD23	1:B:524:PRO:HG3	2.00	0.43
1:A:555:SER:HB3	1:A:592:LYS:HE3	2.00	0.43
1:A:225:ALA:O	1:A:226:SER:C	2.56	0.43
1:A:455:LEU:O	1:A:468:LYS:C	2.54	0.43
1:A:472:LYS:HE3	1:B:231:ASP:CG	2.14	0.43
1:A:726:ILE:HA	1:B:648:ASP:CA	2.44	0.43
1:B:685:GLU:HG2	1:B:841:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:HZ3	1:B:231:ASP:CB	1.26	0.43
1:B:645:GLN:HE21	1:B:646:PHE:H	1.62	0.43
1:B:963:ALA:CB	1:B:973:THR:HG22	2.45	0.43
1:A:963:ALA:CB	1:A:973:THR:HG22	2.45	0.42
1:A:1015:LYS:CG	7:A:1109:PG4:H81	2.48	0.42
1:A:540:PRO:HA	1:A:541:PRO:HD3	1.94	0.42
1:A:602:GLU:O	1:A:612:THR:CG2	2.68	0.42
1:A:643:SER:N	1:B:732:GLU:CD	2.61	0.42
1:B:478:HIS:CB	1:B:480:THR:N	2.77	0.42
1:B:908:ALA:HB3	1:B:909:PRO:HD3	2.01	0.42
1:B:225:ALA:O	1:B:226:SER:C	2.56	0.42
1:B:451:LYS:O	1:B:454:PRO:CD	2.65	0.42
1:A:168[B]:ASP:HB2	1:B:168[B]:ASP:HB2	2.01	0.42
1:A:646:PHE:C	1:A:648:ASP:N	2.73	0.42
1:A:231:ASP:HB2	1:B:471:ARG:NE	2.34	0.42
1:A:455:LEU:HD12	1:A:468:LYS:N	2.35	0.42
1:A:469:LYS:O	1:A:471:ARG:NH2	2.53	0.42
1:B:555:SER:HB3	1:B:592:LYS:HE3	2.00	0.42
1:A:563:ARG:HD3	1:A:627:TYR:OH	2.19	0.42
1:A:624:VAL:O	1:A:628:PHE:HD1	2.03	0.42
1:A:647:VAL:HB	1:B:727:ARG:CB	2.33	0.42
1:A:685:GLU:HG2	1:A:841:GLN:OE1	2.19	0.42
1:B:486:TYR:O	1:B:516:LEU:N	2.50	0.42
1:B:645:GLN:NE2	1:B:646:PHE:N	2.62	0.42
1:A:566:VAL:O	1:A:600:ARG:HA	2.20	0.42
1:A:650:ALA:O	1:A:651:ALA:C	2.57	0.42
1:A:970:GLN:HA	1:A:970:GLN:OE1	2.20	0.42
1:A:1046:TRP:HD1	1:A:1048:GLY:N	2.18	0.42
1:B:1046:TRP:HD1	1:B:1048:GLY:N	2.17	0.42
1:B:636:GLU:O	1:B:637:ASP:C	2.59	0.42
1:B:652:ASP:O	1:B:653:MET:C	2.58	0.42
1:A:95:ASN:HD22	1:A:95:ASN:HA	1.68	0.42
1:B:566:VAL:O	1:B:600:ARG:HA	2.20	0.42
1:A:168[A]:ASP:HB2	1:B:167:ARG:HA	2.02	0.41
1:A:507:LYS:HB3	1:A:632:ILE:HG21	1.97	0.41
1:A:509:PHE:C	1:A:511:PRO:HD3	2.41	0.41
1:A:907:VAL:HG22	1:A:907:VAL:O	2.20	0.41
1:A:908:ALA:HB3	1:A:909:PRO:HD3	2.01	0.41
1:B:229:GLN:HG2	1:B:230:SER:N	2.31	0.41
1:B:624:VAL:O	1:B:628:PHE:HD1	2.03	0.41
1:B:1048:GLY:C	5:B:1104:FAD:C1'	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LYS:NZ	1:A:632:ILE:CD1	2.83	0.41
1:A:732:GLU:N	1:B:643:SER:CB	2.79	0.41
1:B:507:LYS:CB	1:B:632:ILE:CG2	2.82	0.41
1:B:509:PHE:C	1:B:511:PRO:HD3	2.41	0.41
1:B:517:ASP:CB	1:B:546:GLN:HB2	2.41	0.41
1:A:647:VAL:CG2	1:B:727:ARG:HB3	2.49	0.41
1:B:563:ARG:HD3	1:B:627:TYR:OH	2.19	0.41
1:B:602:GLU:O	1:B:612:THR:CG2	2.68	0.41
1:B:645:GLN:CD	1:B:646:PHE:H	2.24	0.41
1:B:970:GLN:OE1	1:B:970:GLN:HA	2.20	0.41
1:A:452:LYS:O	1:A:453:ILE:HG12	2.20	0.41
1:B:455:LEU:HD12	1:B:468:LYS:N	2.35	0.41
1:B:473:LYS:HE2	1:B:474:ALA:H	1.85	0.41
1:B:730:ALA:O	1:B:731:GLU:CB	2.62	0.41
1:A:734:LYS:C	1:A:736:ALA:O	2.57	0.41
1:B:452:LYS:HB2	1:B:452:LYS:HZ3	1.86	0.41
1:A:477:ALA:CB	1:A:479:ASN:HB3	2.46	0.41
1:A:485:LEU:HB3	1:A:516:LEU:HD23	2.02	0.41
1:A:563:ARG:HA	1:A:595:GLU:CB	2.50	0.41
1:B:452:LYS:O	1:B:453:ILE:HG12	2.19	0.41
1:B:733:GLU:OE2	1:B:734:LYS:N	2.54	0.41
1:A:608:ASP:OD1	1:B:794:LEU:HD12	2.19	0.41
1:A:731:GLU:OE1	1:A:732:GLU:HB3	2.20	0.41
1:B:653:MET:HA	1:B:654:PRO:HD3	1.92	0.41
1:A:167:ARG:HA	1:B:168[B]:ASP:OD1	2.21	0.41
1:A:383:SER:CA	1:B:546:GLN:NE2	2.83	0.41
1:A:452:LYS:HB2	1:A:452:LYS:HZ3	1.85	0.41
1:A:557:ASP:OD1	1:A:557:ASP:N	2.48	0.41
1:A:628:PHE:HB2	1:A:629:ASN:H	1.52	0.41
1:A:632:ILE:HG12	1:A:634:ASN:N	2.35	0.41
1:A:694:TYR:CE2	1:A:831:ILE:HG21	2.56	0.41
1:A:731:GLU:H	1:B:643:SER:HB2	1.85	0.41
1:B:523:LEU:HA	1:B:524:PRO:HD3	1.89	0.41
1:A:733:GLU:OE2	1:A:734:LYS:N	2.54	0.41
1:B:694:TYR:CE2	1:B:831:ILE:HG21	2.56	0.41
1:B:731:GLU:O	1:B:731:GLU:HG2	2.16	0.41
1:B:735:LEU:C	1:B:735:LEU:CD1	2.88	0.41
1:B:800:MET:HE1	1:B:821:LEU:HD13	2.02	0.41
1:A:652:ASP:O	1:A:653:MET:C	2.58	0.40
1:A:800:MET:HE1	1:A:821:LEU:HD13	2.03	0.40
1:B:485:LEU:HB3	1:B:516:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLN:O	1:A:310[A]:GLN:HB2	2.22	0.40
1:B:223:ARG:C	1:B:225:ALA:N	2.75	0.40
1:B:478:HIS:O	1:B:509:PHE:CA	2.52	0.40
1:B:645:GLN:HE21	1:B:647:VAL:CG2	2.31	0.40
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.19	0.40
1:B:479:ASN:N	1:B:479:ASN:OD1	2.53	0.40
1:B:529:VAL:O	1:B:529:VAL:HG13	2.21	0.40
1:B:563:ARG:HA	1:B:595:GLU:CB	2.50	0.40
1:A:125:GLN:HG2	1:B:132:ARG:NH1	2.36	0.40
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.20	0.40
1:A:621:TRP:HA	1:A:621:TRP:CE3	2.57	0.40
1:B:577:THR:HB	4:B:1103:FMN:O4	2.22	0.40
1:B:642:LEU:HA	1:B:642:LEU:HD12	1.63	0.40
1:A:451:LYS:O	1:A:454:PRO:CD	2.65	0.40
1:A:589:LEU:HD12	1:A:589:LEU:HA	1.82	0.40
1:B:95:ASN:HD22	1:B:95:ASN:HA	1.68	0.40
1:B:226:SER:O	1:B:227:GLY:C	2.53	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	1034/1037 (100%)	958 (93%)	60 (6%)	16 (2%)	10	46
1	B	1032/1037 (100%)	950 (92%)	64 (6%)	18 (2%)	9	43
All	All	2066/2074 (100%)	1908 (92%)	124 (6%)	34 (2%)	13	45

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASP

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Mol	Chain	Res	Type
1	A	452	LYS
1	A	454	PRO
1	A	472	LYS
1	A	558	GLU
1	A	575	ALA
1	A	638	ASN
1	A	639	LYS
1	A	731	GLU
1	B	231	ASP
1	B	452	LYS
1	B	454	PRO
1	B	558	GLU
1	B	575	ALA
1	B	646	PHE
1	B	731	GLU
1	A	230	SER
1	A	596	ASN
1	B	230	SER
1	B	596	ASN
1	A	552	ASP
1	B	472	LYS
1	B	552	ASP
1	B	638	ASN
1	A	625	ALA
1	B	625	ALA
1	B	640	SER
1	A	468	LYS
1	B	468	LYS
1	B	470	VAL
1	A	773	CYS
1	B	773	CYS
1	A	453	ILE
1	B	453	ILE

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	853/882 (97%)	800 (94%)	53 (6%)	18	45
1	B	853/882 (97%)	797 (93%)	56 (7%)	16	43
All	All	1706/1764 (97%)	1597 (94%)	109 (6%)	21	44

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	71	LEU
1	A	148	LEU
1	A	159	ASN
1	A	187	LYS
1	A	222	ASP
1	A	228	GLU
1	A	229	GLN
1	A	287	LEU
1	A	440	LYS
1	A	453	ILE
1	A	469	LYS
1	A	471	ARG
1	A	473	LYS
1	A	475	GLU
1	A	480	THR
1	A	525	ARG
1	A	553	GLN
1	A	557	ASP
1	A	560	LYS
1	A	572	LYS
1	A	577	THR
1	A	589	LEU
1	A	606	SER
1	A	612	THR
1	A	622	SER
1	A	624	VAL
1	A	632	ILE
1	A	633	GLU
1	A	634	ASN
1	A	635	SER
1	A	639	LYS
1	A	643	SER
1	A	644	LEU
1	A	646	PHE

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Mol	Chain	Res	Type
1	A	649	SER
1	A	682	ARG
1	A	685	GLU
1	A	708	GLU
1	A	731	GLU
1	A	750	LEU
1	A	821	LEU
1	A	837	VAL
1	A	847	SER
1	A	925	GLN
1	A	943	TYR
1	A	965	SER
1	A	976	GLN
1	A	985	LYS
1	A	986	LEU
1	A	988	GLU
1	A	989	LEU
1	A	1035	LEU
1	B	4	GLU
1	B	71	LEU
1	B	148	LEU
1	B	159	ASN
1	B	187	LYS
1	B	222	ASP
1	B	228	GLU
1	B	229	GLN
1	B	287	LEU
1	B	440	LYS
1	B	453	ILE
1	B	469	LYS
1	B	471	ARG
1	B	473	LYS
1	B	476	ASN
1	B	478	HIS
1	B	480	THR
1	B	525	ARG
1	B	553	GLN
1	B	557	ASP
1	B	560	LYS
1	B	572	LYS
1	B	577	THR
1	B	589	LEU

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Mol	Chain	Res	Type
1	B	606	SER
1	B	612	THR
1	B	622	SER
1	B	624	VAL
1	B	629	ASN
1	B	632	ILE
1	B	633	GLU
1	B	634	ASN
1	B	635	SER
1	B	636	GLU
1	B	639	LYS
1	B	643	SER
1	B	644	LEU
1	B	645	GLN
1	B	649	SER
1	B	682	ARG
1	B	685	GLU
1	B	708	GLU
1	B	731	GLU
1	B	750	LEU
1	B	821	LEU
1	B	837	VAL
1	B	847	SER
1	B	925	GLN
1	B	943	TYR
1	B	965	SER
1	B	976	GLN
1	B	985	LYS
1	B	986	LEU
1	B	988	GLU
1	B	989	LEU
1	B	1035	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	95	ASN
1	A	100	HIS
1	A	134	ASN
1	A	159	ASN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	236	HIS
1	A	253	ASN
1	A	257	GLN
1	A	283	ASN
1	A	388	HIS
1	A	403	GLN
1	A	478	HIS
1	A	479	ASN
1	A	519	HIS
1	A	573	ASN
1	A	645	GLN
1	A	665	ASN
1	A	787	GLN
1	A	923	GLN
1	A	976	GLN
1	A	992	GLN
1	B	16	ASN
1	B	95	ASN
1	B	100	HIS
1	B	134	ASN
1	B	159	ASN
1	B	201	ASN
1	B	236	HIS
1	B	253	ASN
1	B	257	GLN
1	B	283	ASN
1	B	388	HIS
1	B	403	GLN
1	B	476	ASN
1	B	479	ASN
1	B	519	HIS
1	B	546	GLN
1	B	573	ASN
1	B	645	GLN
1	B	665	ASN
1	B	787	GLN
1	B	923	GLN
1	B	976	GLN
1	B	992	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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$
3	1C6	A	1102	-	23,25,25	3.25	7 (30%)	28,35,35	2.45	11 (39%)
2	HEM	B	1101	1	41,50,50	1.88	6 (14%)	45,82,82	2.12	13 (28%)
4	FMN	A	1103	-	33,33,33	1.36	4 (12%)	48,50,50	1.89	13 (27%)
7	PG4	A	1108	-	12,12,12	0.78	0	11,11,11	1.05	0
7	PG4	A	1109	-	6,6,12	1.47	1 (16%)	5,5,11	1.58	1 (20%)
7	PG4	B	1108	-	12,12,12	0.78	0	11,11,11	1.05	0
6	SO4	A	1106	-	4,4,4	0.15	0	6,6,6	1.20	1 (16%)
7	PG4	B	1109	-	6,6,12	1.47	1 (16%)	5,5,11	1.58	1 (20%)
3	1C6	B	1102	-	23,25,25	3.26	7 (30%)	28,35,35	2.45	11 (39%)
6	SO4	B	1105	-	4,4,4	0.47	0	6,6,6	1.22	1 (16%)
6	SO4	B	1106	-	4,4,4	0.30	0	6,6,6	0.83	0
2	HEM	A	1101	1	41,50,50	1.88	6 (14%)	45,82,82	2.11	13 (28%)
6	SO4	A	1105	-	4,4,4	0.40	0	6,6,6	1.15	1 (16%)
5	FAD	B	1104	-	53,58,58	1.48	6 (11%)	68,89,89	1.52	14 (20%)
5	FAD	A	1104	-	53,58,58	1.47	6 (11%)	68,89,89	1.52	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1107	-	4,4,4	0.30	0	6,6,6	0.32	0
4	FMN	B	1103	-	33,33,33	1.35	4 (12%)	48,50,50	1.89	13 (27%)
6	SO4	B	1107	-	4,4,4	0.31	0	6,6,6	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1C6	A	1102	-	-	6/7/9/9	0/3/3/3
2	HEM	B	1101	1	-	2/12/54/54	-
4	FMN	A	1103	-	-	5/18/18/18	0/3/3/3
7	PG4	A	1108	-	-	8/10/10/10	-
7	PG4	A	1109	-	-	3/4/4/10	-
7	PG4	B	1108	-	-	8/10/10/10	-
7	PG4	B	1109	-	-	3/4/4/10	-
3	1C6	B	1102	-	-	6/7/9/9	0/3/3/3
2	HEM	A	1101	1	-	2/12/54/54	-
5	FAD	B	1104	-	-	0/30/50/50	0/6/6/6
5	FAD	A	1104	-	-	0/30/50/50	0/6/6/6
4	FMN	B	1103	-	-	5/18/18/18	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	1C6	CD1-CG	11.01	1.50	1.39
3	A	1102	1C6	CD1-CG	10.96	1.50	1.39
2	A	1101	HEM	C3D-C2D	6.73	1.51	1.36
2	B	1101	HEM	C3D-C2D	6.72	1.51	1.36
3	A	1102	1C6	CE1-CD1	6.39	1.50	1.39
3	B	1102	1C6	CE1-CD1	6.37	1.50	1.39
2	A	1101	HEM	C3C-C2C	-5.34	1.33	1.40
2	B	1101	HEM	C3C-C2C	-5.30	1.33	1.40
3	B	1102	1C6	CE1-CZ	5.18	1.49	1.40
3	A	1102	1C6	CE1-CZ	5.14	1.49	1.40
3	A	1102	1C6	CB-S	-4.88	1.71	1.82
3	B	1102	1C6	CB-S	-4.87	1.71	1.82
5	B	1104	FAD	C4X-N5	4.61	1.39	1.30
5	A	1104	FAD	C4X-N5	4.55	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	FMN	P-O5'	-4.24	1.46	1.60
4	B	1103	FMN	P-O5'	-4.22	1.46	1.60
5	B	1104	FAD	C2A-N3A	3.60	1.37	1.32
5	A	1104	FAD	C2A-N3A	3.59	1.37	1.32
5	A	1104	FAD	C1'-C2'	3.08	1.57	1.52
4	A	1103	FMN	C5A-N5	-3.07	1.33	1.39
5	B	1104	FAD	C1'-C2'	3.07	1.57	1.52
4	B	1103	FMN	C5A-N5	-3.05	1.33	1.39
5	B	1104	FAD	C8M-C8	2.91	1.56	1.51
5	A	1104	FAD	C8M-C8	2.87	1.56	1.51
4	A	1103	FMN	O5'-C5'	2.56	1.54	1.44
2	A	1101	HEM	O1A-CGA	2.56	1.30	1.22
4	B	1103	FMN	O5'-C5'	2.55	1.54	1.44
2	B	1101	HEM	O1A-CGA	2.54	1.30	1.22
5	A	1104	FAD	C10-N1	2.39	1.38	1.33
5	B	1104	FAD	C10-N1	2.38	1.38	1.33
2	B	1101	HEM	C4D-ND	-2.31	1.36	1.40
3	B	1102	1C6	CF1-S	-2.31	1.71	1.75
2	A	1101	HEM	C4D-ND	-2.31	1.36	1.40
3	A	1102	1C6	CF1-S	-2.30	1.71	1.75
4	B	1103	FMN	C10-N10	2.29	1.42	1.37
4	A	1103	FMN	C10-N10	2.27	1.42	1.37
5	B	1104	FAD	C5A-N7A	-2.22	1.31	1.39
5	A	1104	FAD	C5A-N7A	-2.20	1.31	1.39
3	B	1102	1C6	CZ2-CS2	-2.20	1.38	1.41
3	A	1102	1C6	CZ2-CS2	-2.20	1.38	1.41
2	A	1101	HEM	CMD-C2D	2.10	1.55	1.50
2	B	1101	HEM	CMD-C2D	2.10	1.55	1.50
7	B	1109	PG4	C7-C8	2.05	1.60	1.49
3	A	1102	1C6	CE3-CZ3	2.05	1.40	1.37
2	A	1101	HEM	C1A-CHA	-2.04	1.35	1.41
2	B	1101	HEM	C1A-CHA	-2.04	1.35	1.41
7	A	1109	PG4	C7-C8	2.03	1.60	1.49
3	B	1102	1C6	CE3-CZ3	2.02	1.40	1.37

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	HEM	C4D-ND-C1D	6.29	111.57	105.07
2	A	1101	HEM	C4D-ND-C1D	6.25	111.53	105.07
3	A	1102	1C6	CE2-N1-CG	5.64	124.86	117.75
3	B	1102	1C6	CE2-N1-CG	5.63	124.85	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	FMN	O4'-C4'-C3'	-5.33	96.15	109.10
4	A	1103	FMN	O4'-C4'-C3'	-5.31	96.20	109.10
3	B	1102	1C6	CD1-CG-N1	-5.06	118.99	123.95
3	A	1102	1C6	CD1-CG-N1	-5.06	119.00	123.95
2	B	1101	HEM	C4C-CHD-C1D	4.68	128.73	122.56
2	A	1101	HEM	C4C-CHD-C1D	4.66	128.71	122.56
3	B	1102	1C6	CZ-CE1-CD1	-4.51	117.74	121.53
3	A	1102	1C6	CZ-CE1-CD1	-4.49	117.75	121.53
3	A	1102	1C6	O2-CE1-CD1	4.44	125.06	118.83
3	B	1102	1C6	O2-CE1-CD1	4.44	125.06	118.83
3	A	1102	1C6	CB-CG-CD1	4.44	124.47	120.29
3	B	1102	1C6	CB-CG-CD1	4.41	124.44	120.29
4	B	1103	FMN	C4-N3-C2	-4.12	118.03	125.64
4	A	1103	FMN	C4-N3-C2	-4.11	118.05	125.64
2	B	1101	HEM	CHA-C4D-ND	4.11	129.45	124.38
2	A	1101	HEM	CHA-C4D-ND	4.07	129.41	124.38
2	A	1101	HEM	CBA-CAA-C2A	-3.84	106.07	112.62
2	B	1101	HEM	CBA-CAA-C2A	-3.81	106.11	112.62
2	A	1101	HEM	CMA-C3A-C4A	-3.69	122.78	128.46
2	B	1101	HEM	CMA-C3A-C4A	-3.68	122.80	128.46
4	B	1103	FMN	C5A-N5-C4A	3.51	123.91	118.07
4	A	1103	FMN	C5A-N5-C4A	3.50	123.89	118.07
4	B	1103	FMN	O5'-C5'-C4'	-3.31	100.53	109.36
2	B	1101	HEM	CBD-CAD-C3D	-3.30	103.46	112.63
4	A	1103	FMN	O5'-C5'-C4'	-3.29	100.57	109.36
2	A	1101	HEM	CBD-CAD-C3D	-3.29	103.48	112.63
5	A	1104	FAD	P-O3P-PA	-3.25	121.69	132.83
5	B	1104	FAD	P-O3P-PA	-3.24	121.70	132.83
4	A	1103	FMN	C4'-C3'-C2'	-3.19	106.73	113.36
4	B	1103	FMN	C4'-C3'-C2'	-3.19	106.74	113.36
5	B	1104	FAD	N3A-C2A-N1A	-3.08	123.86	128.68
3	A	1102	1C6	CZ-CE2-N1	-3.06	121.98	125.11
5	A	1104	FAD	C4X-C4-N3	3.04	120.92	113.19
4	B	1103	FMN	C4-C4A-N5	3.04	122.56	118.23
2	B	1101	HEM	C4B-C3B-C2B	3.04	109.53	107.11
5	A	1104	FAD	N3A-C2A-N1A	-3.03	123.94	128.68
3	A	1102	1C6	CB-S-CF1	-3.03	99.09	102.42
4	A	1103	FMN	C4-C4A-N5	3.02	122.53	118.23
3	B	1102	1C6	CZ-CE2-N1	-3.02	122.02	125.11
5	B	1104	FAD	C4X-C4-N3	3.02	120.85	113.19
2	A	1101	HEM	C4B-C3B-C2B	3.02	109.51	107.11
3	B	1102	1C6	CB-S-CF1	-3.01	99.11	102.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1104	FAD	C4A-C5A-N7A	-2.93	106.34	109.40
5	B	1104	FAD	C4A-C5A-N7A	-2.93	106.35	109.40
5	A	1104	FAD	C4-N3-C2	-2.92	120.25	125.64
5	B	1104	FAD	C4-N3-C2	-2.90	120.28	125.64
5	B	1104	FAD	C9A-C5X-N5	-2.87	119.32	122.43
5	A	1104	FAD	C9A-C5X-N5	-2.85	119.33	122.43
4	B	1103	FMN	C4A-C4-N3	2.82	120.36	113.19
4	A	1103	FMN	C4A-C4-N3	2.81	120.32	113.19
5	A	1104	FAD	O4B-C1B-C2B	-2.79	102.84	106.93
5	B	1104	FAD	O4B-C1B-C2B	-2.75	102.90	106.93
5	A	1104	FAD	C5X-C9A-N10	2.75	120.80	117.95
5	B	1104	FAD	C5X-C9A-N10	2.75	120.79	117.95
4	A	1103	FMN	O2P-P-O5'	2.70	113.91	106.73
6	A	1106	SO4	O4-S-O3	2.69	120.56	109.06
2	A	1101	HEM	O1A-CGA-CBA	-2.69	114.44	123.08
2	B	1101	HEM	O1A-CGA-CBA	-2.68	114.47	123.08
4	B	1103	FMN	O2P-P-O5'	2.67	113.85	106.73
4	B	1103	FMN	O3P-P-O5'	2.64	113.75	106.73
4	A	1103	FMN	O3P-P-O5'	2.63	113.72	106.73
3	B	1102	1C6	C4-O3-CZ3	2.61	123.18	117.51
3	A	1102	1C6	C4-O3-CZ3	2.60	123.16	117.51
4	B	1103	FMN	C9A-C5A-N5	-2.55	119.66	122.43
3	B	1102	1C6	CE3-CX2-NV	2.52	138.03	130.83
5	A	1104	FAD	O3B-C3B-C4B	-2.52	103.76	111.05
3	A	1102	1C6	CE3-CX2-NV	2.52	138.03	130.83
5	B	1104	FAD	O3B-C3B-C4B	-2.52	103.77	111.05
4	A	1103	FMN	C9A-C5A-N5	-2.50	119.72	122.43
5	A	1104	FAD	O2'-C2'-C3'	-2.48	103.07	109.10
5	B	1104	FAD	O2'-C2'-C3'	-2.48	103.08	109.10
6	A	1105	SO4	O4-S-O1	2.45	122.09	109.31
6	B	1105	SO4	O3-S-O2	2.45	122.08	109.31
2	A	1101	HEM	C4B-CHC-C1C	2.41	125.74	122.56
2	B	1101	HEM	C4B-CHC-C1C	2.40	125.72	122.56
4	B	1103	FMN	C10-C4A-N5	-2.37	119.83	124.86
4	A	1103	FMN	C10-C4A-N5	-2.36	119.84	124.86
4	B	1103	FMN	O5'-P-O1P	2.34	113.03	106.47
2	A	1101	HEM	CMA-C3A-C2A	2.33	129.34	124.94
4	A	1103	FMN	O5'-P-O1P	2.33	113.00	106.47
2	B	1101	HEM	CMA-C3A-C2A	2.32	129.32	124.94
2	A	1101	HEM	C1B-NB-C4B	2.32	107.47	105.07
2	B	1101	HEM	C1B-NB-C4B	2.30	107.45	105.07
3	A	1102	1C6	CE2-CZ-CE1	2.25	118.99	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	1C6	CE2-CZ-CE1	2.23	118.97	116.27
5	B	1104	FAD	C9A-C9-C8	2.22	123.77	119.30
5	A	1104	FAD	C9A-C9-C8	2.19	123.72	119.30
5	A	1104	FAD	O4-C4-C4X	-2.19	120.80	126.60
2	A	1101	HEM	C1D-C2D-C3D	-2.17	104.67	106.96
2	B	1101	HEM	C1D-C2D-C3D	-2.17	104.67	106.96
5	B	1104	FAD	O4-C4-C4X	-2.17	120.85	126.60
2	B	1101	HEM	CBB-CAB-C3B	-2.16	116.87	127.62
2	A	1101	HEM	CBB-CAB-C3B	-2.16	116.89	127.62
5	A	1104	FAD	C7M-C7-C8	-2.15	116.33	120.74
4	A	1103	FMN	C6-C5A-N5	2.15	122.27	118.51
4	B	1103	FMN	C6-C5A-N5	2.14	122.26	118.51
5	B	1104	FAD	C1'-C2'-C3'	2.14	115.76	109.79
5	B	1104	FAD	C7M-C7-C8	-2.14	116.36	120.74
5	A	1104	FAD	C1'-C2'-C3'	2.13	115.73	109.79
3	A	1102	1C6	C3-CD1-CG	-2.06	120.89	122.69
3	B	1102	1C6	C3-CD1-CG	-2.05	120.90	122.69
7	A	1109	PG4	O4-C6-C5	2.03	118.99	110.07
7	B	1109	PG4	O4-C6-C5	2.03	118.99	110.07

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1108	PG4	O1-C1-C2-O2
7	A	1109	PG4	O3-C5-C6-O4
7	B	1108	PG4	O1-C1-C2-O2
7	B	1109	PG4	O3-C5-C6-O4
3	A	1102	1C6	CD1-CE1-O2-C2
3	B	1102	1C6	CD1-CE1-O2-C2
7	A	1108	PG4	O4-C7-C8-O5
7	B	1108	PG4	O4-C7-C8-O5
3	B	1102	1C6	CH2-CZ3-O3-C4
3	A	1102	1C6	CH2-CZ3-O3-C4
4	A	1103	FMN	O3'-C3'-C4'-C5'
4	B	1103	FMN	O3'-C3'-C4'-C5'
3	B	1102	1C6	CE3-CZ3-O3-C4
3	A	1102	1C6	CE3-CZ3-O3-C4
7	A	1109	PG4	O4-C7-C8-O5
7	B	1109	PG4	O4-C7-C8-O5
7	B	1109	PG4	C8-C7-O4-C6
7	A	1109	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
3	A	1102	1C6	S-CB-CG-N1
3	B	1102	1C6	S-CB-CG-N1
4	A	1103	FMN	C2'-C3'-C4'-C5'
4	B	1103	FMN	C2'-C3'-C4'-C5'
7	A	1108	PG4	C6-C5-O3-C4
7	B	1108	PG4	C6-C5-O3-C4
7	B	1108	PG4	C5-C6-O4-C7
7	A	1108	PG4	C5-C6-O4-C7
7	B	1108	PG4	C8-C7-O4-C6
7	A	1108	PG4	C8-C7-O4-C6
7	A	1108	PG4	C3-C4-O3-C5
7	B	1108	PG4	C3-C4-O3-C5
4	A	1103	FMN	C1'-C2'-C3'-O3'
4	B	1103	FMN	C1'-C2'-C3'-O3'
3	A	1102	1C6	CZ-CE1-O2-C2
3	B	1102	1C6	CZ-CE1-O2-C2
7	A	1108	PG4	C4-C3-O2-C2
7	B	1108	PG4	C4-C3-O2-C2
4	A	1103	FMN	O3'-C3'-C4'-O4'
4	B	1103	FMN	O3'-C3'-C4'-O4'
4	A	1103	FMN	O2'-C2'-C3'-O3'
4	B	1103	FMN	O2'-C2'-C3'-O3'
3	A	1102	1C6	S-CB-CG-CD1
3	B	1102	1C6	S-CB-CG-CD1
2	A	1101	HEM	CAD-CBD-CGD-O2D
2	B	1101	HEM	CAD-CBD-CGD-O2D
2	A	1101	HEM	CAD-CBD-CGD-O1D
2	B	1101	HEM	CAD-CBD-CGD-O1D
7	A	1108	PG4	O3-C5-C6-O4
7	B	1108	PG4	O3-C5-C6-O4

There are no ring outliers.

11 monomers are involved in 48 short contacts:

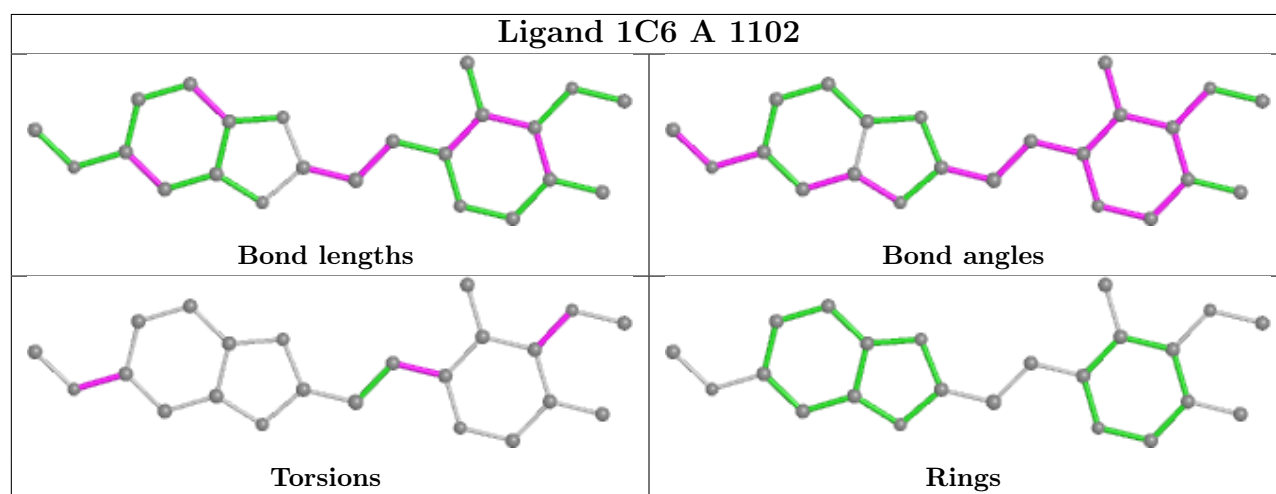
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	1C6	10	0
2	B	1101	HEM	1	0
7	A	1108	PG4	1	0
7	A	1109	PG4	7	0
7	B	1108	PG4	1	0
7	B	1109	PG4	7	0
3	B	1102	1C6	11	0

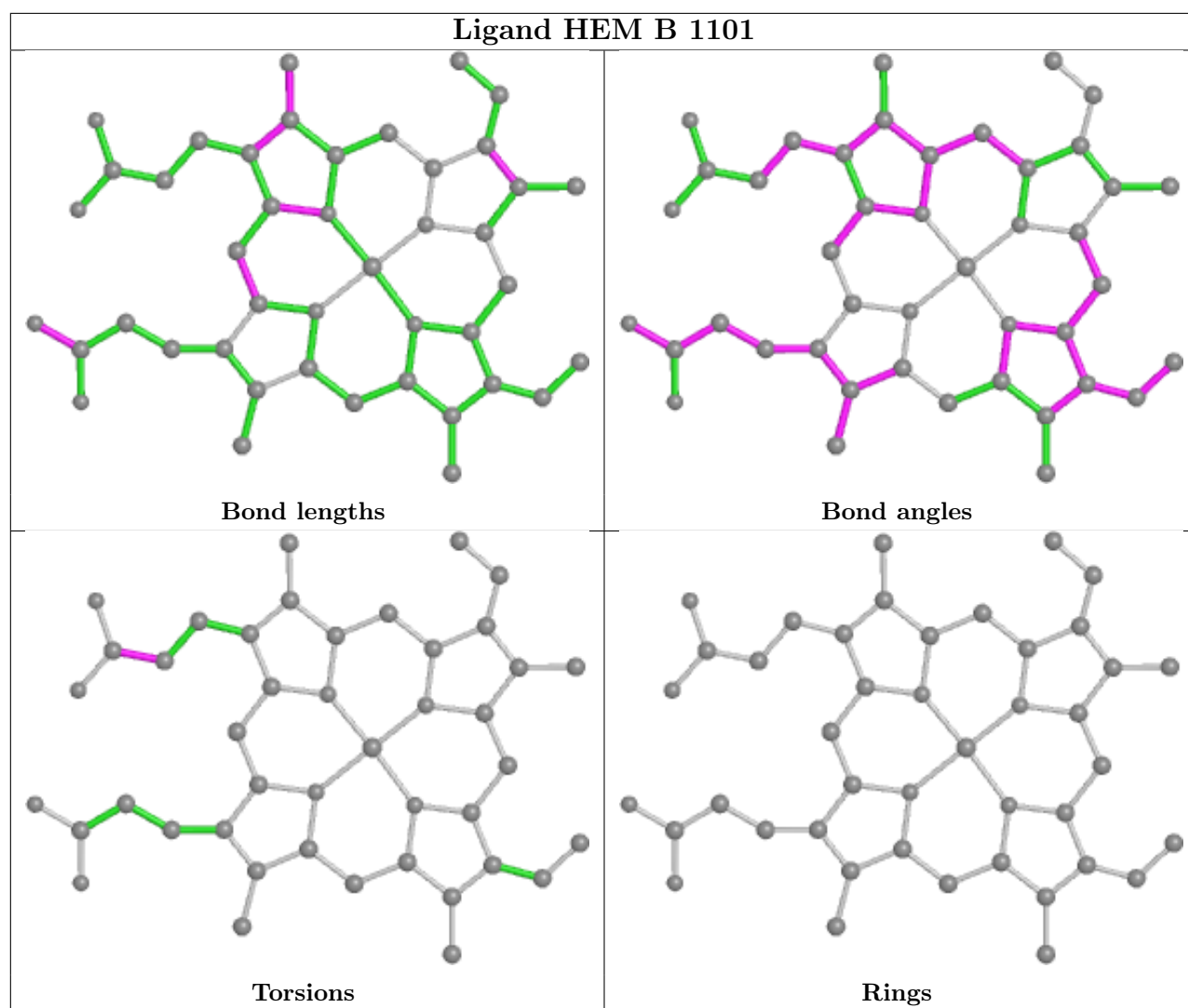
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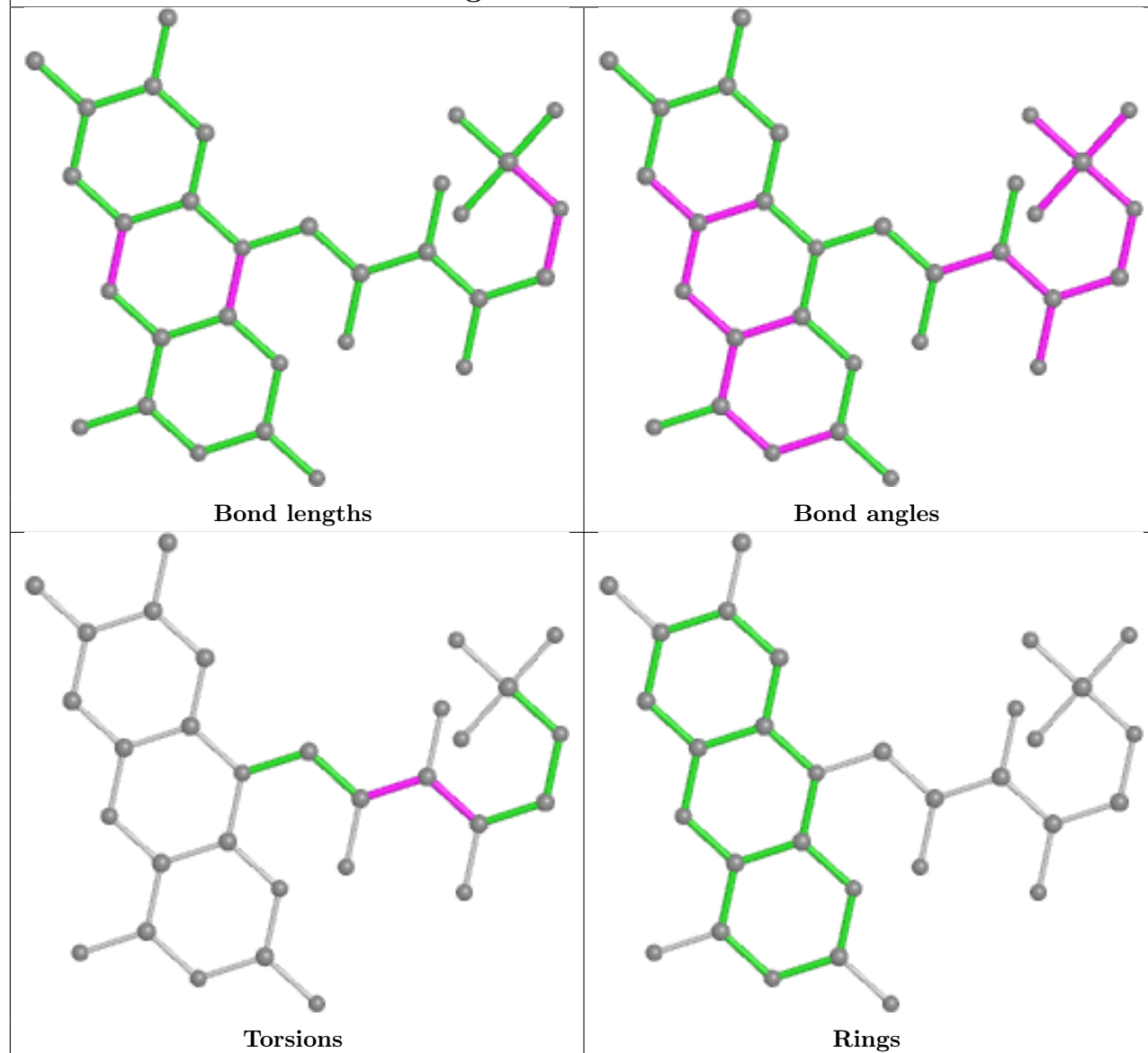
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	HEM	1	0
5	B	1104	FAD	4	0
5	A	1104	FAD	4	0
4	B	1103	FMN	1	0

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

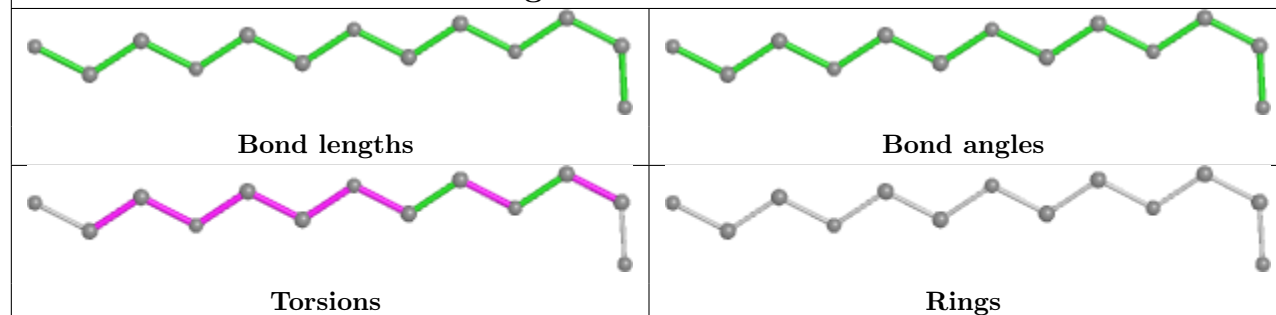


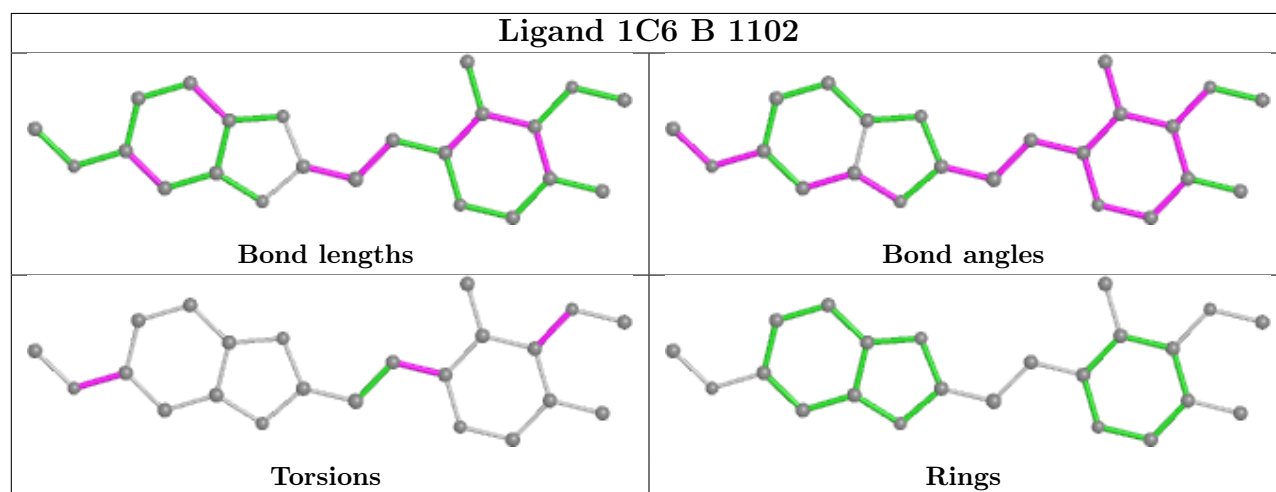
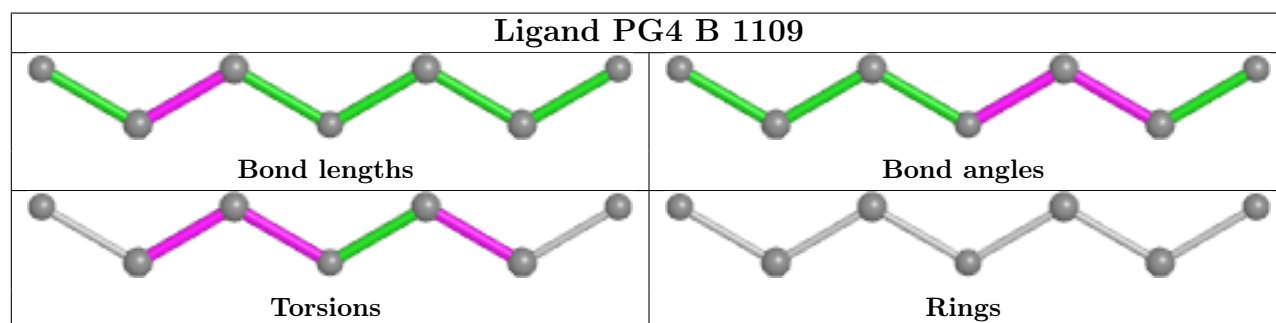
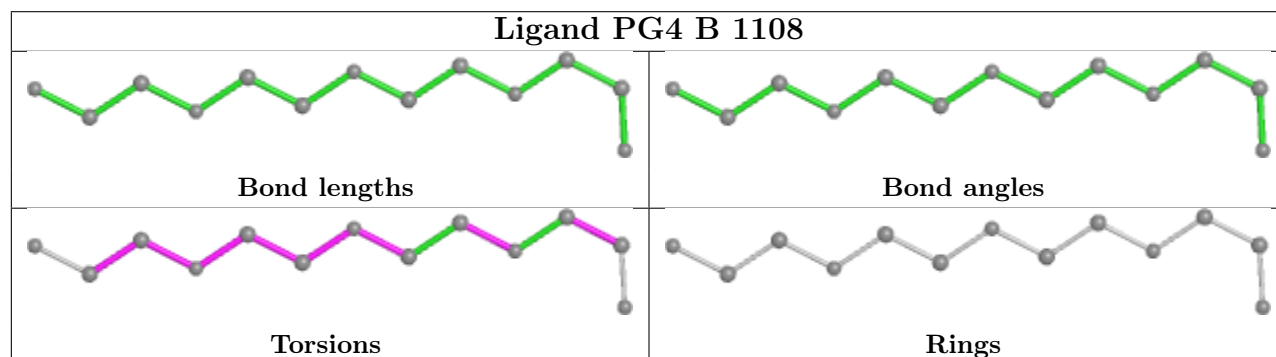
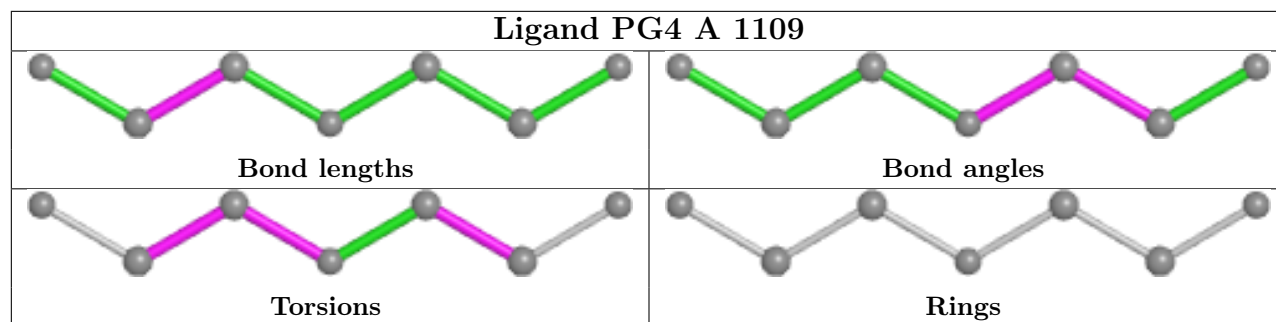


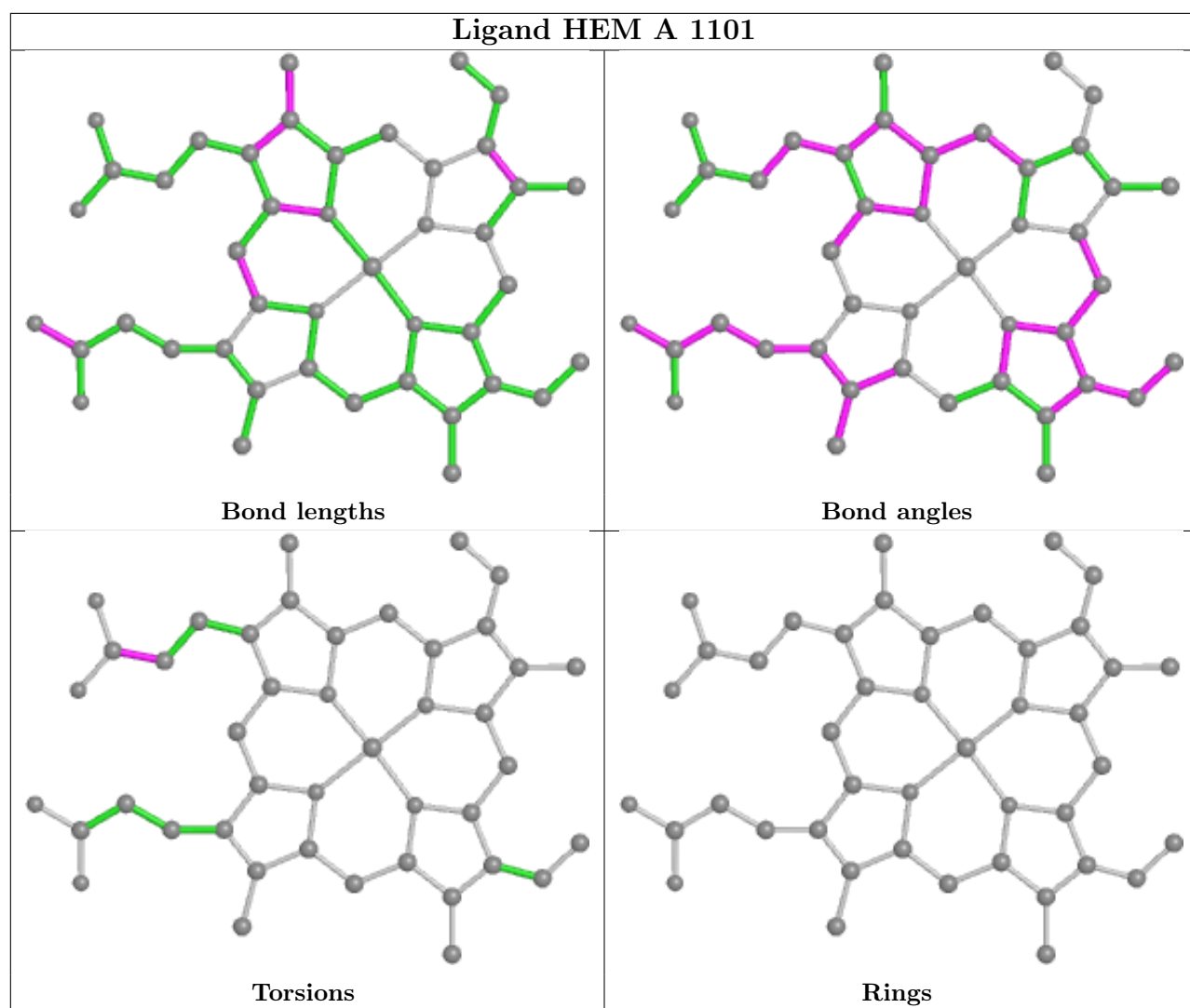
Ligand FMN A 1103

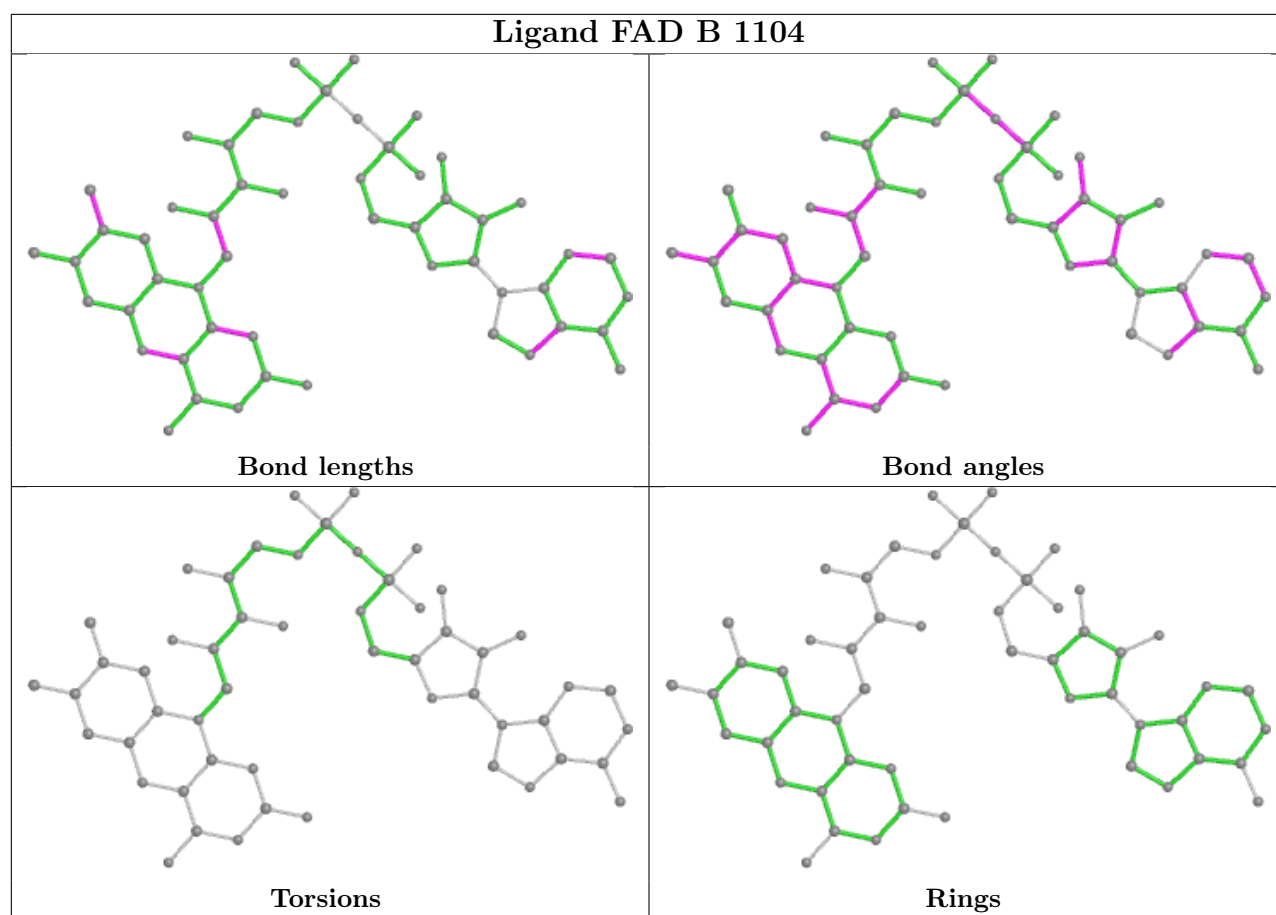


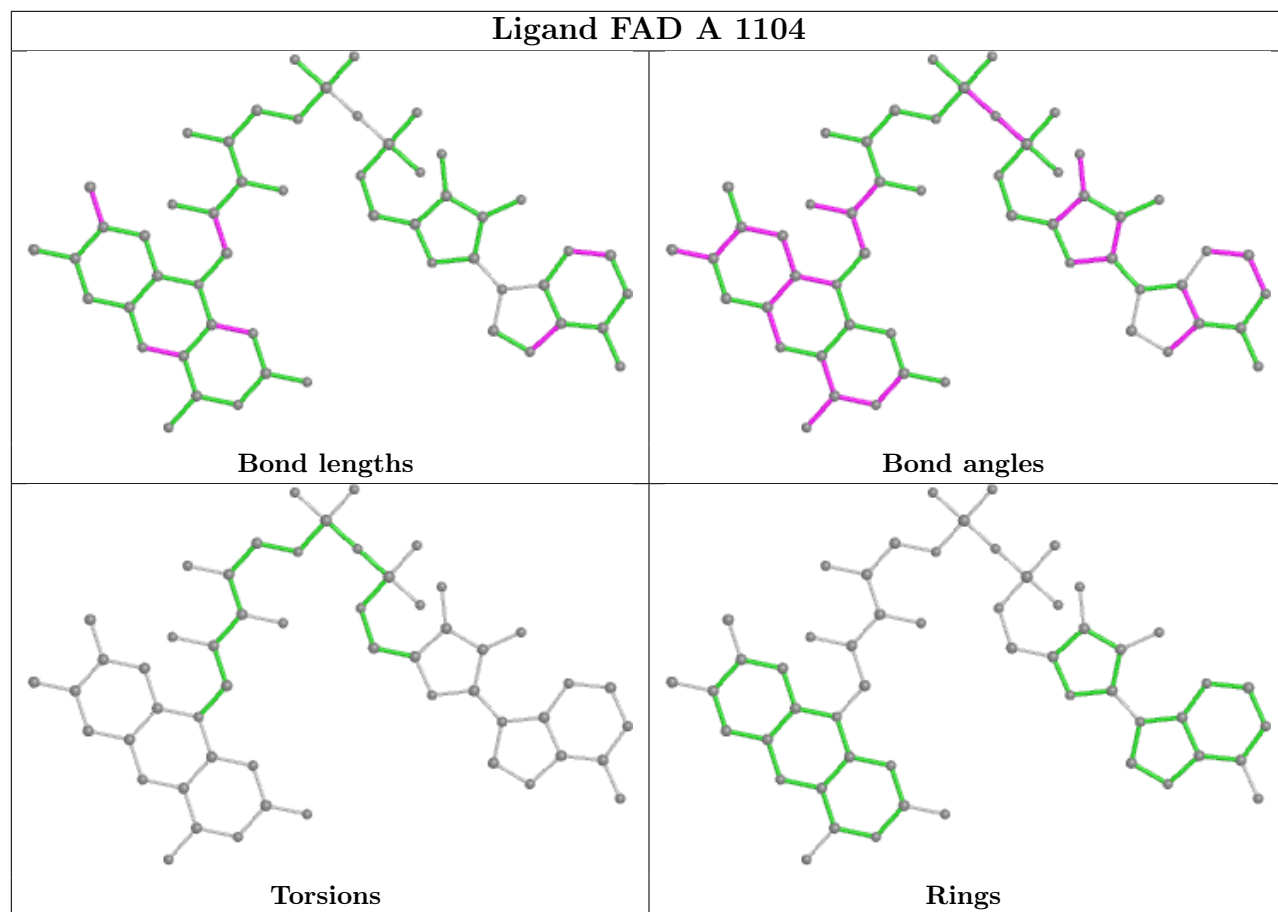
Ligand PG4 A 1108

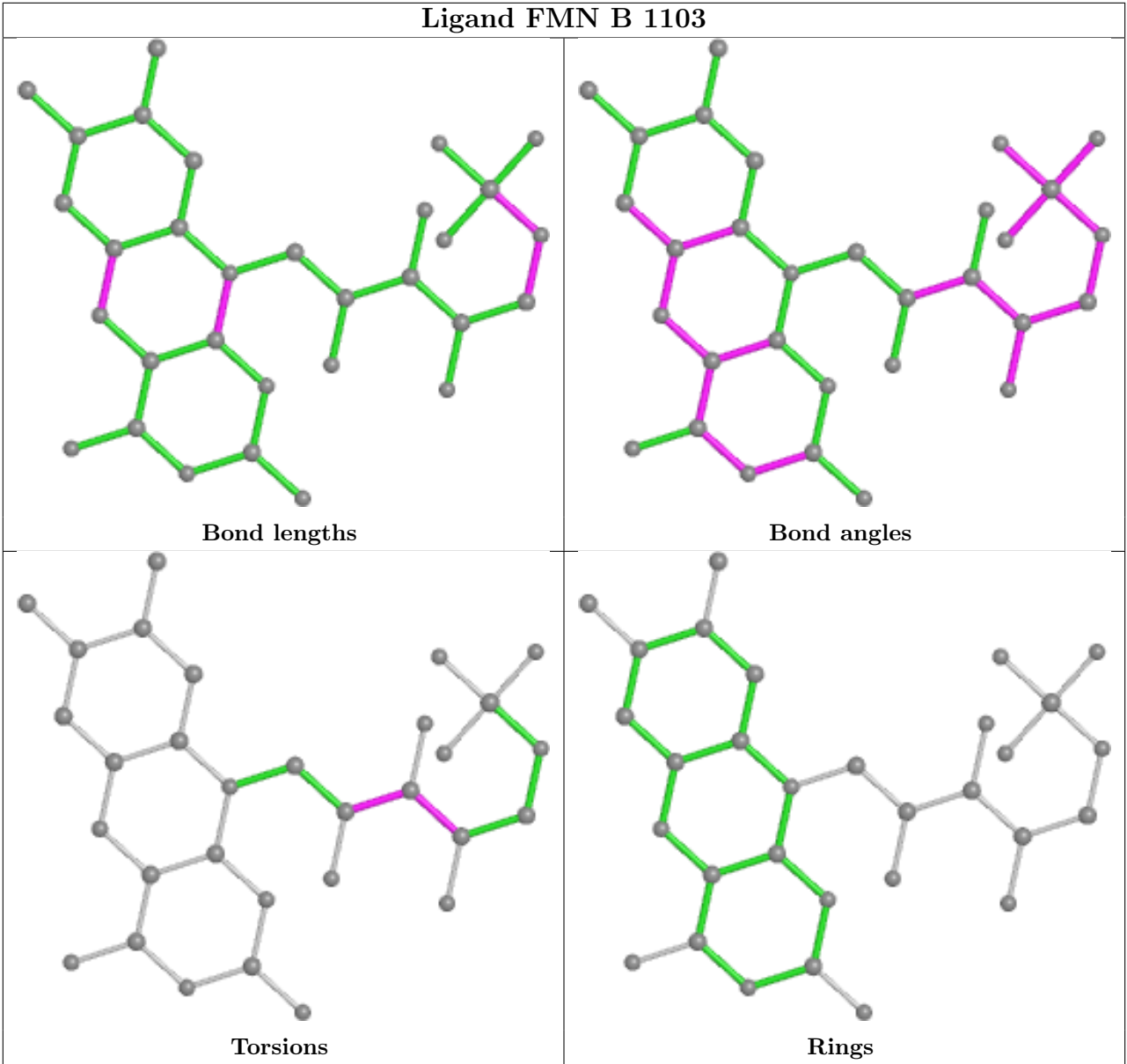












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	478:HIS	C	479:ASN	N	3.49
1	A	478:HIS	C	479:ASN	N	2.89
1	B	630:LEU	C	631:ASP	N	2.50
1	A	661:ALA	C	662:PHE	N	0.86
1	B	661:ALA	C	662:PHE	N	0.86

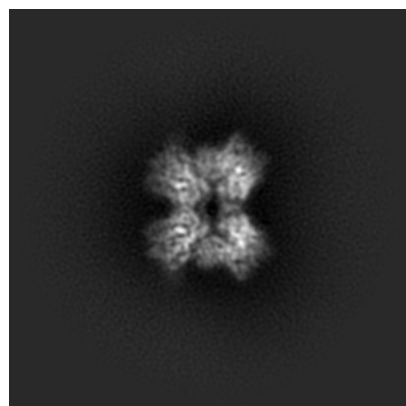
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27536. These allow visual inspection of the internal detail of the map and identification of artifacts.

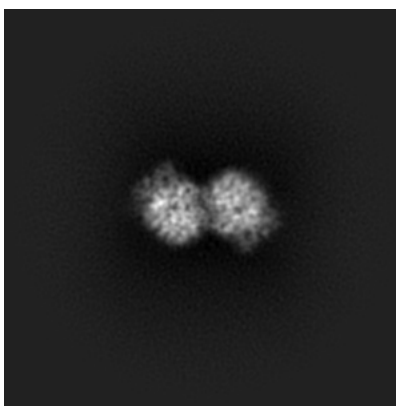
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

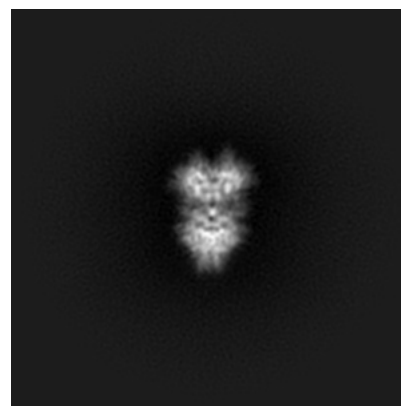
6.1.1 Primary map



X

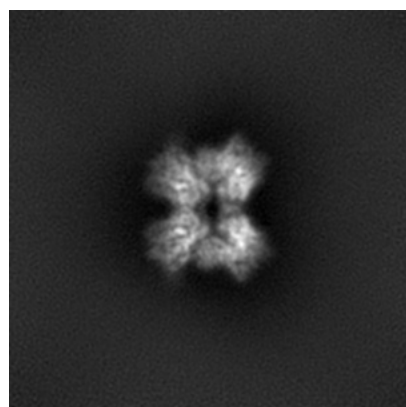


Y

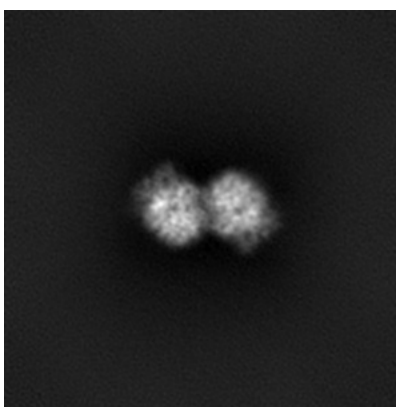


Z

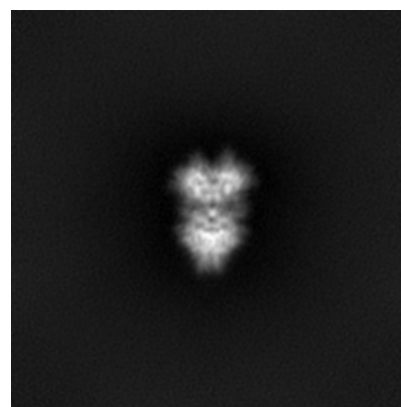
6.1.2 Raw map



X



Y

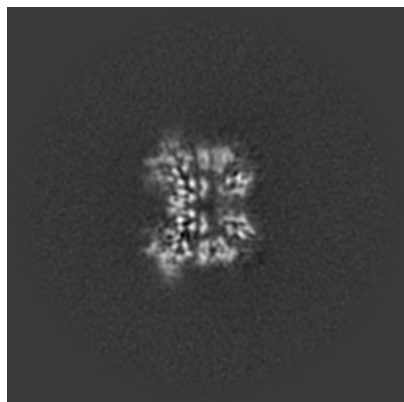


Z

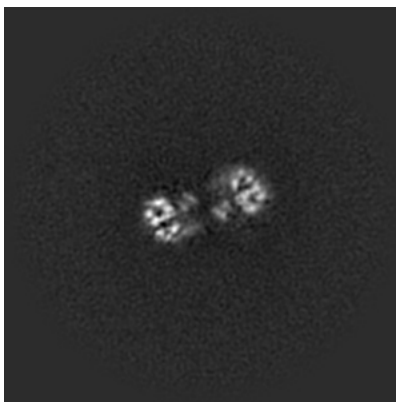
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

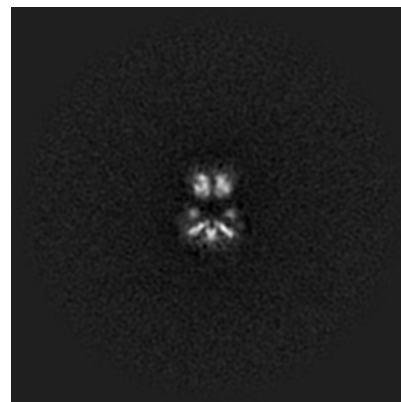
6.2.1 Primary map



X Index: 90

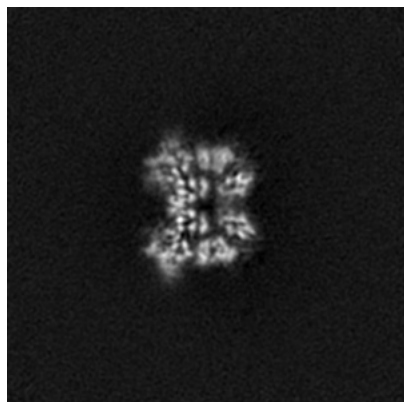


Y Index: 90

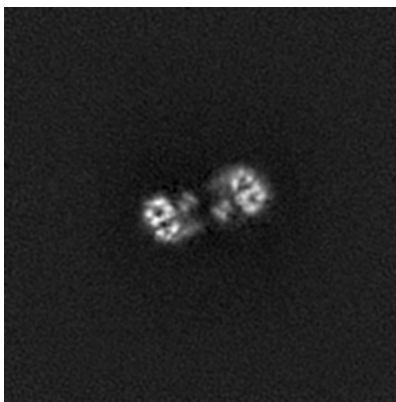


Z Index: 90

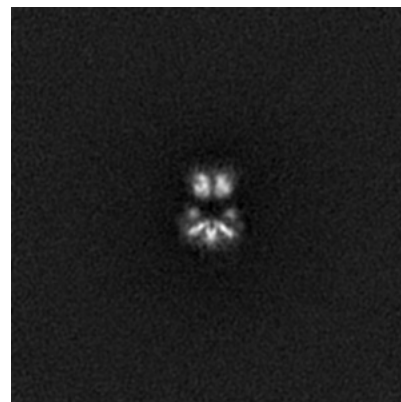
6.2.2 Raw map



X Index: 90



Y Index: 90

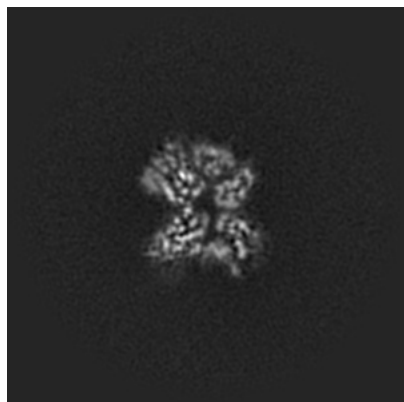


Z Index: 90

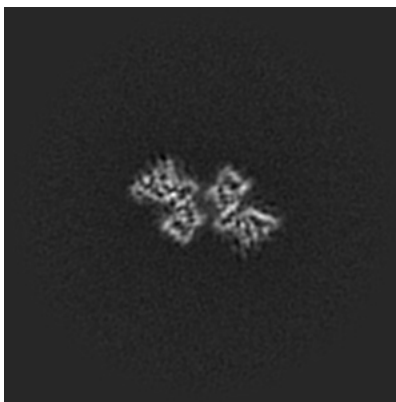
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 93

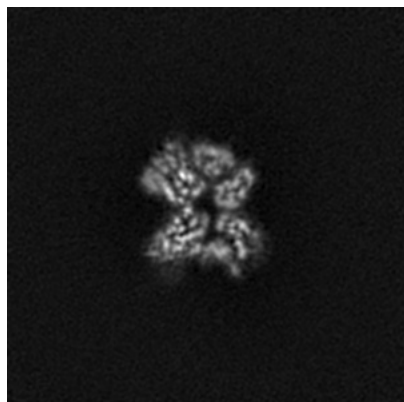


Y Index: 104

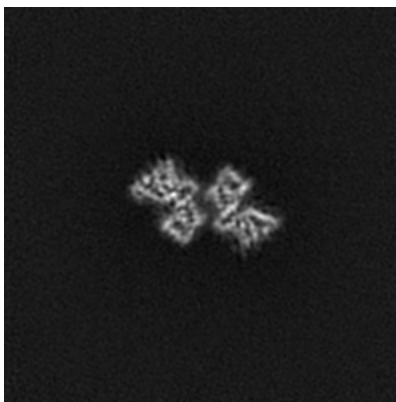


Z Index: 80

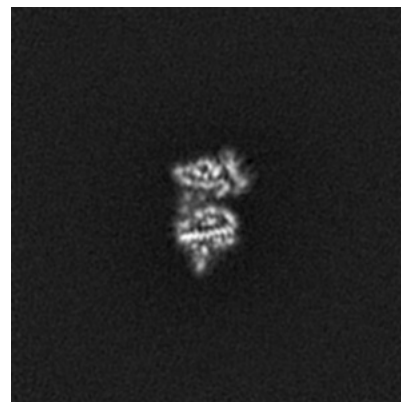
6.3.2 Raw map



X Index: 93



Y Index: 104

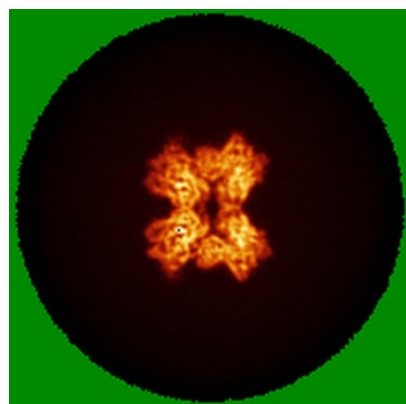


Z Index: 80

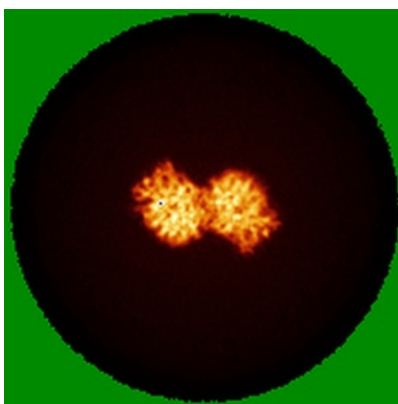
The images above show the largest variance slices of the map in three orthogonal directions.

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

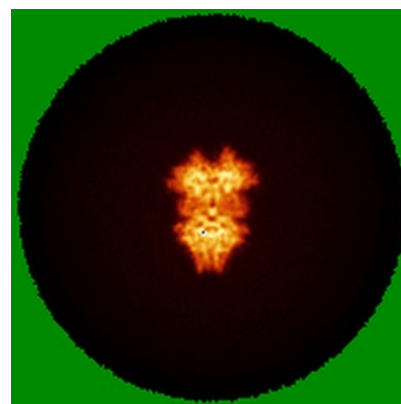
6.4.1 Primary map



X

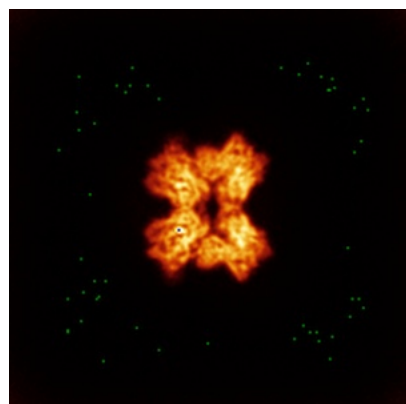


Y

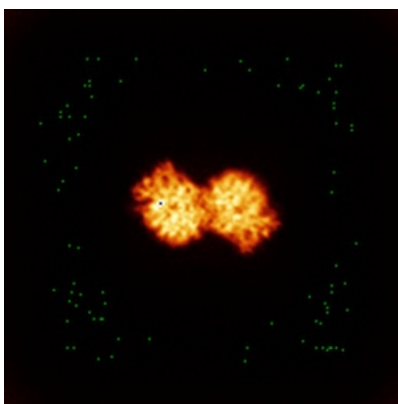


Z

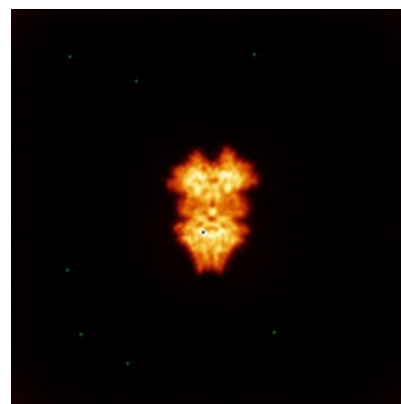
6.4.2 Raw map



X



Y



Z

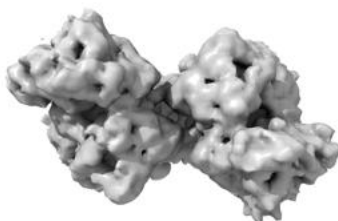
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

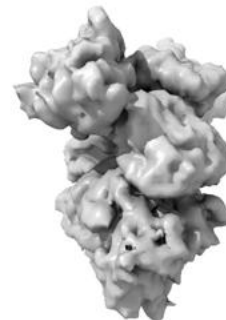
6.5.1 Primary map



X



Y



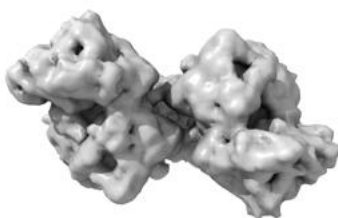
Z

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

6.5.2 Raw map



X



Y



Z

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

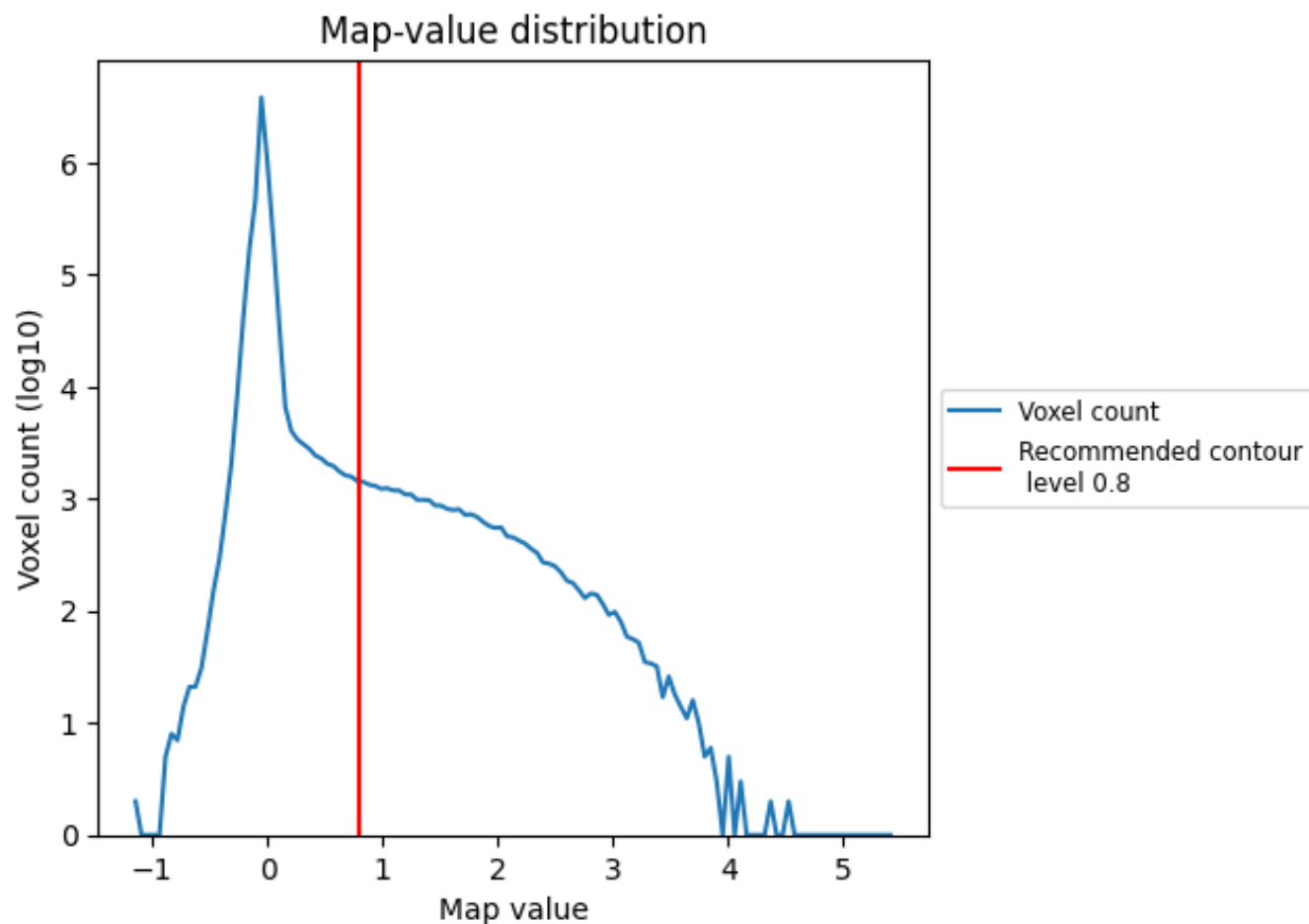
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

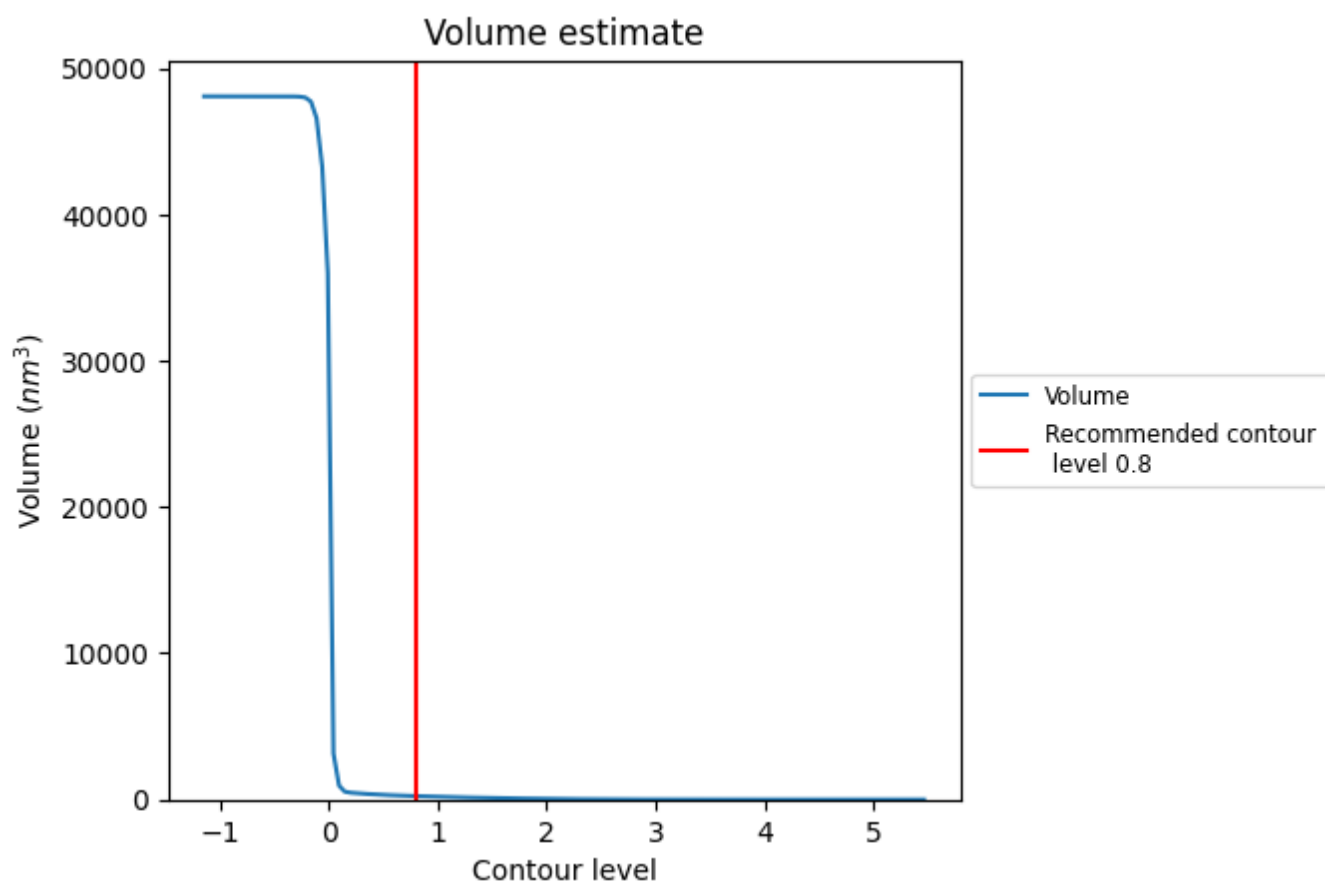
This section contains the results of statistical analysis of the map.

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.

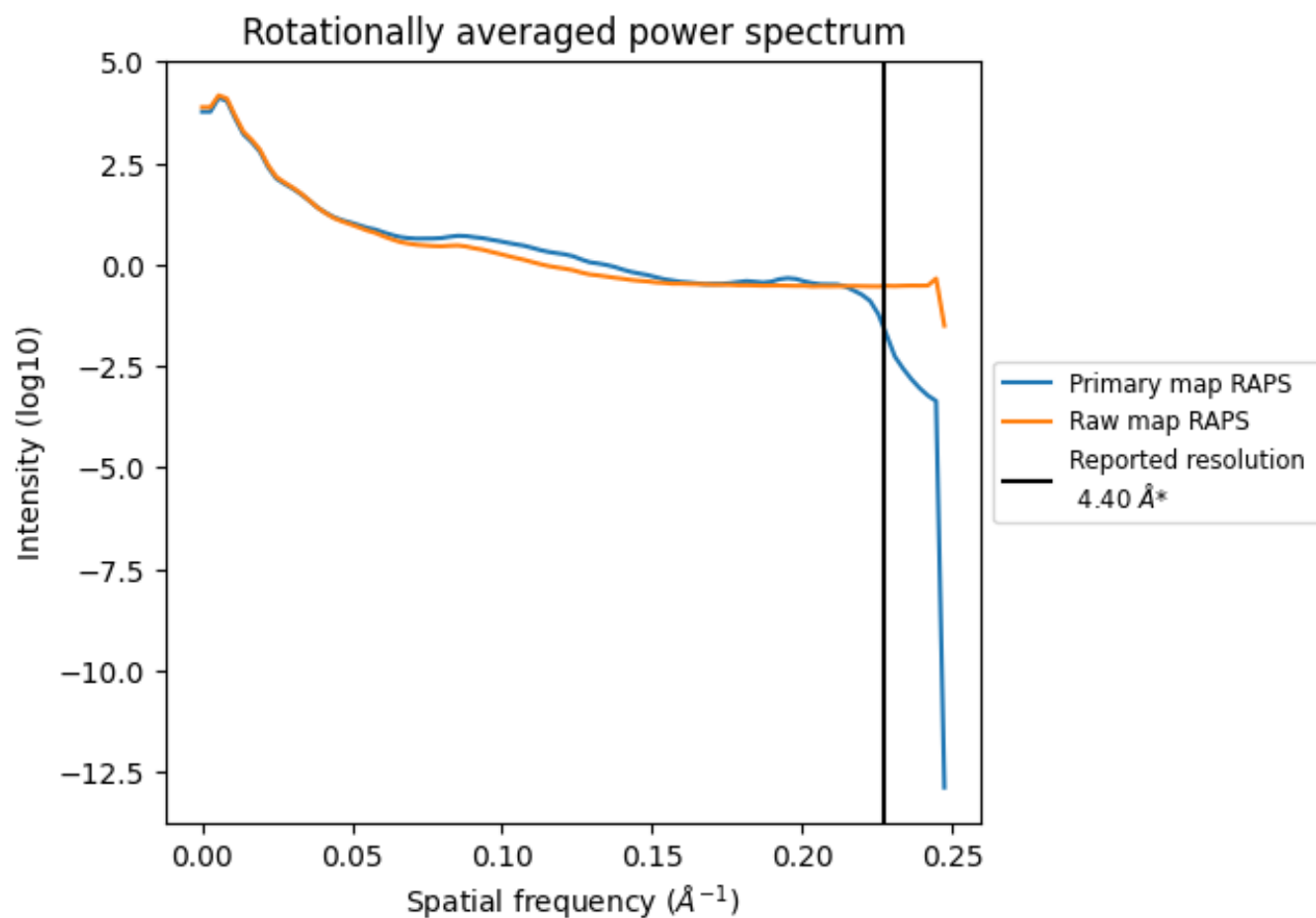
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 236 nm³; this corresponds to an approximate mass of 214 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 ⓘ

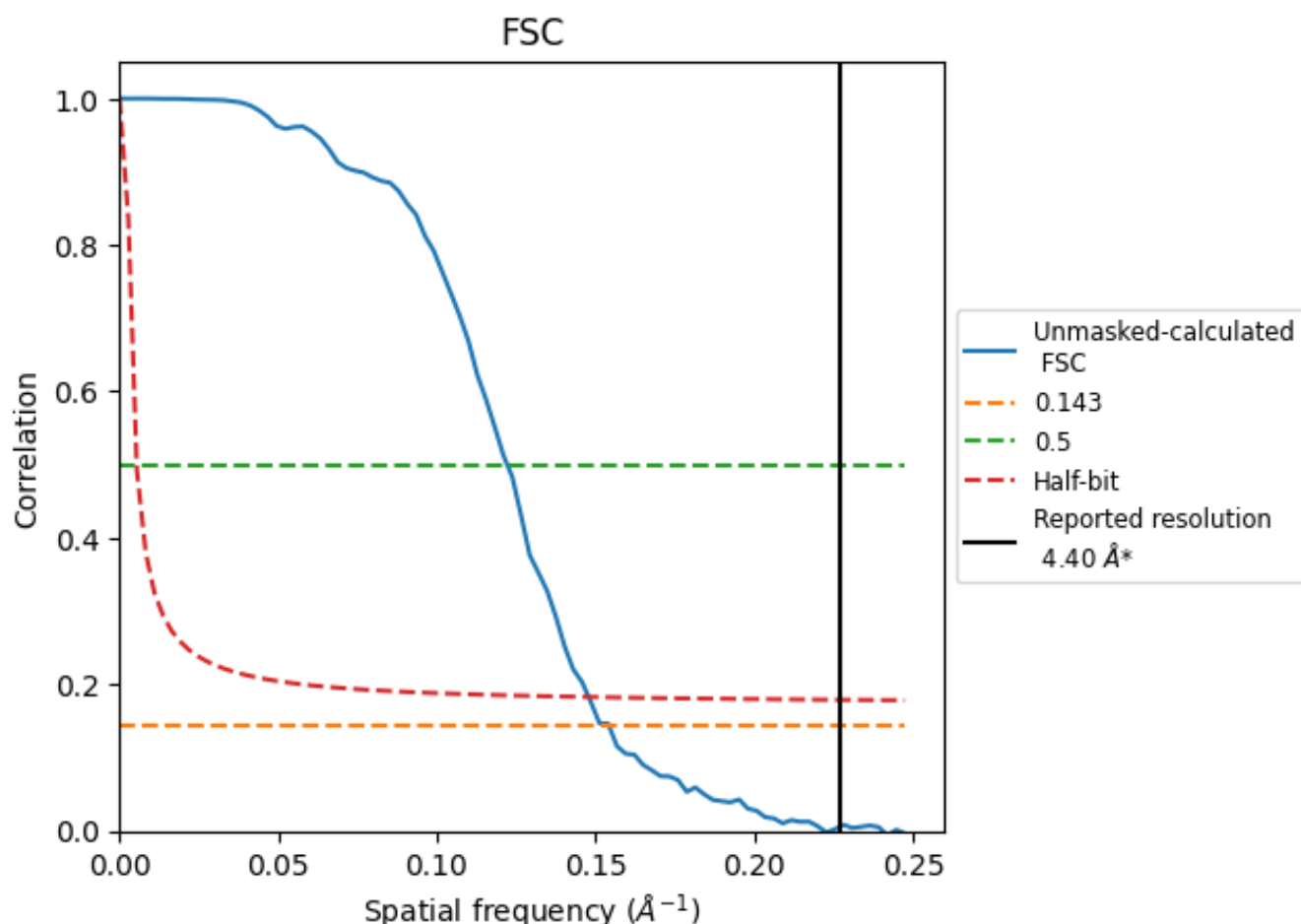


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

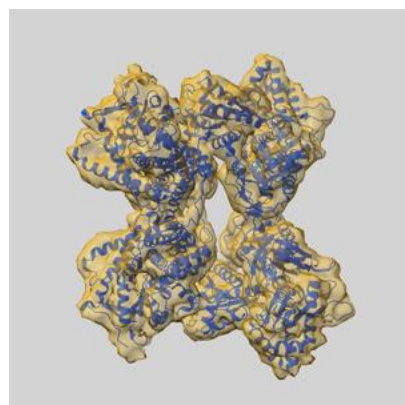
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.48	8.18	6.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.48 differs from the reported value 4.4 by more than 10 %

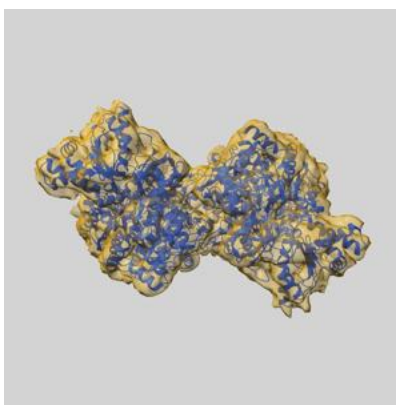
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27536 and PDB model 8DMG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

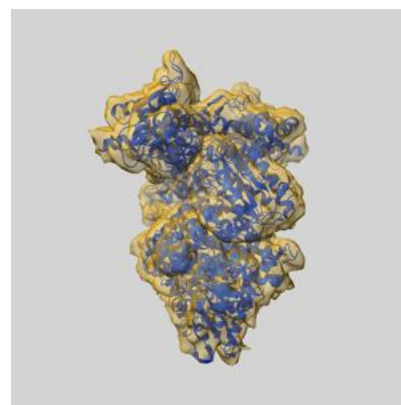
9.1 Map-model overlay [i](#)



X



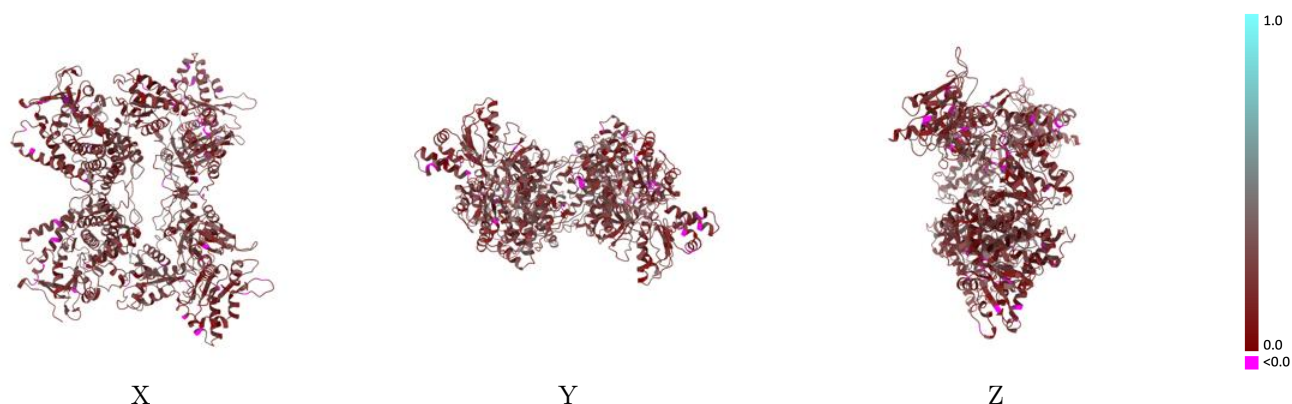
Y



Z

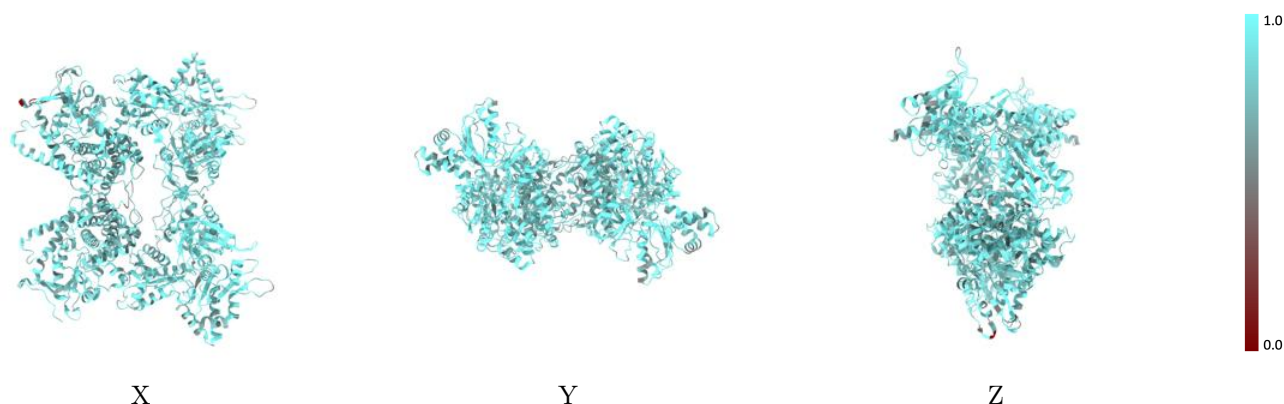
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



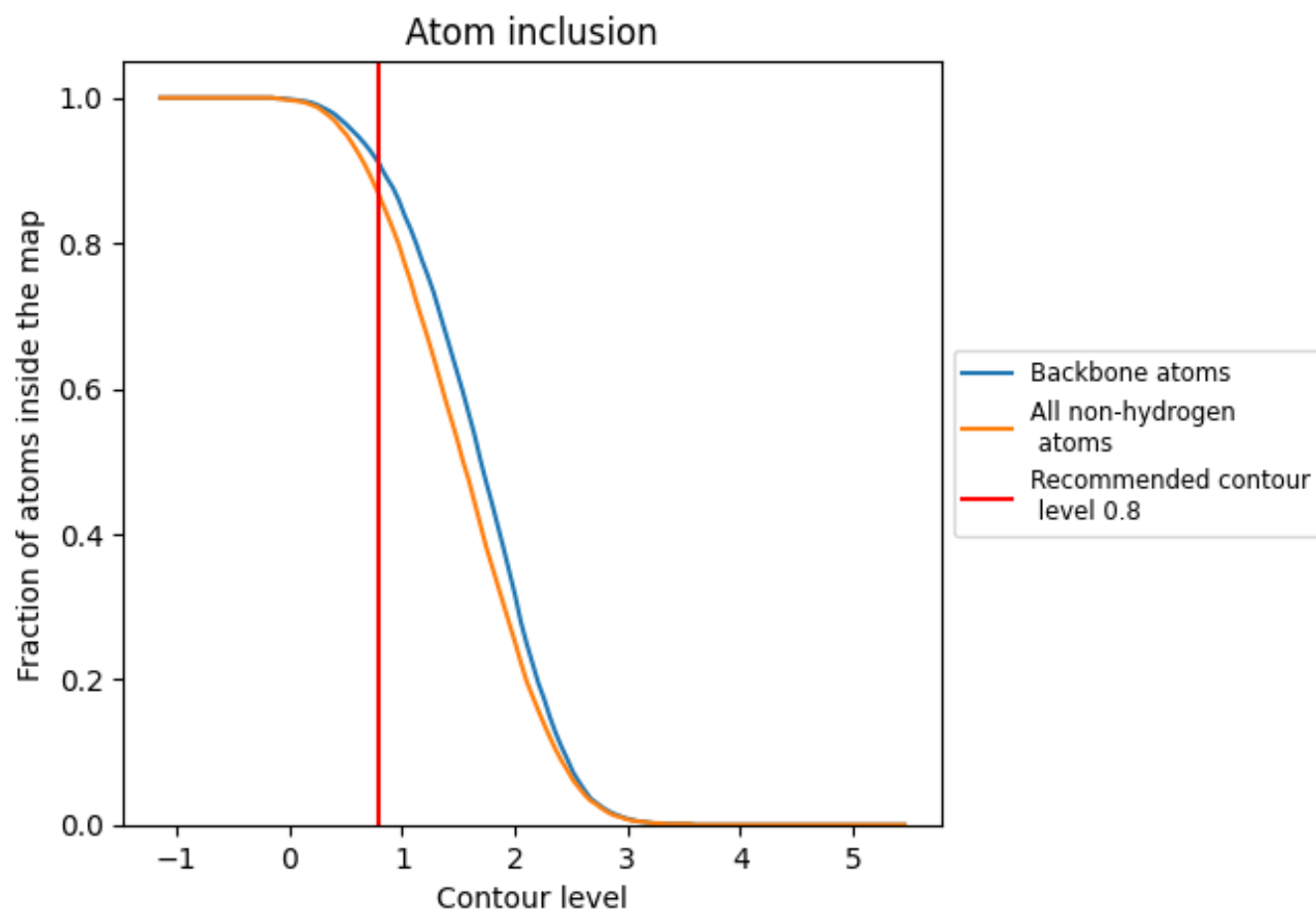
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8650	<div></div> 0.2160
A	<div></div> 0.8620	<div></div> 0.2130
B	<div></div> 0.8740	<div></div> 0.2190

