Full wwPDB EM Validation Report ⓘ

Jul 17, 2023 – 10:19 PM JST

PDB ID	:	8GRN
EMDB ID	:	EMD-34209
Title	:	AtOSCA1.1 extended state
Authors	:	Zhang, M.F.
Deposited on	:	2022-09-02
Resolution	:	2.50 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:

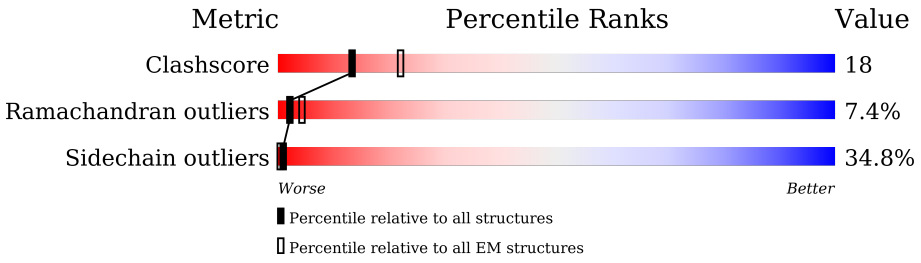
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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 <=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	772	10% 42% 28% 17% 5% 7%
1	B	772	9% 42% 29% 16% 5% 7%

2 Entry composition

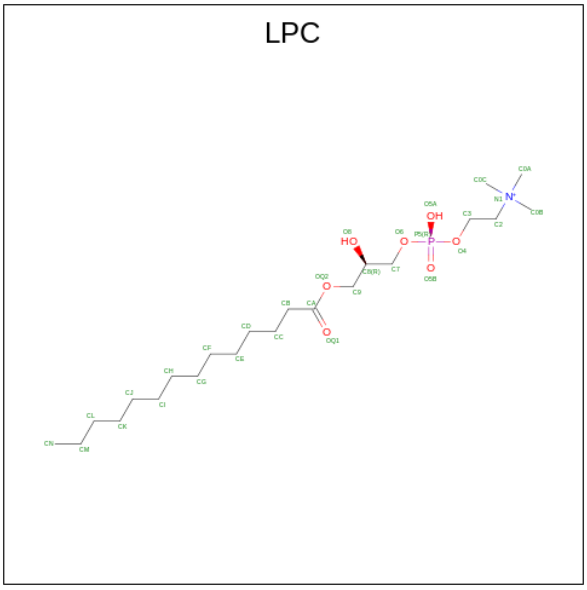
There are 2 unique types of molecules in this entry. The entry contains 11602 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein OSCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	716	Total	C	N	O	S	0	0
			5770	3802	948	994	26		
1	B	716	Total	C	N	O	S	0	0
			5770	3802	948	994	26		

- Molecule 2 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (three-letter code: LPC) (formula: $C_{22}H_{47}NO_7P$) (labeled as "Ligand of Interest" by depositor).



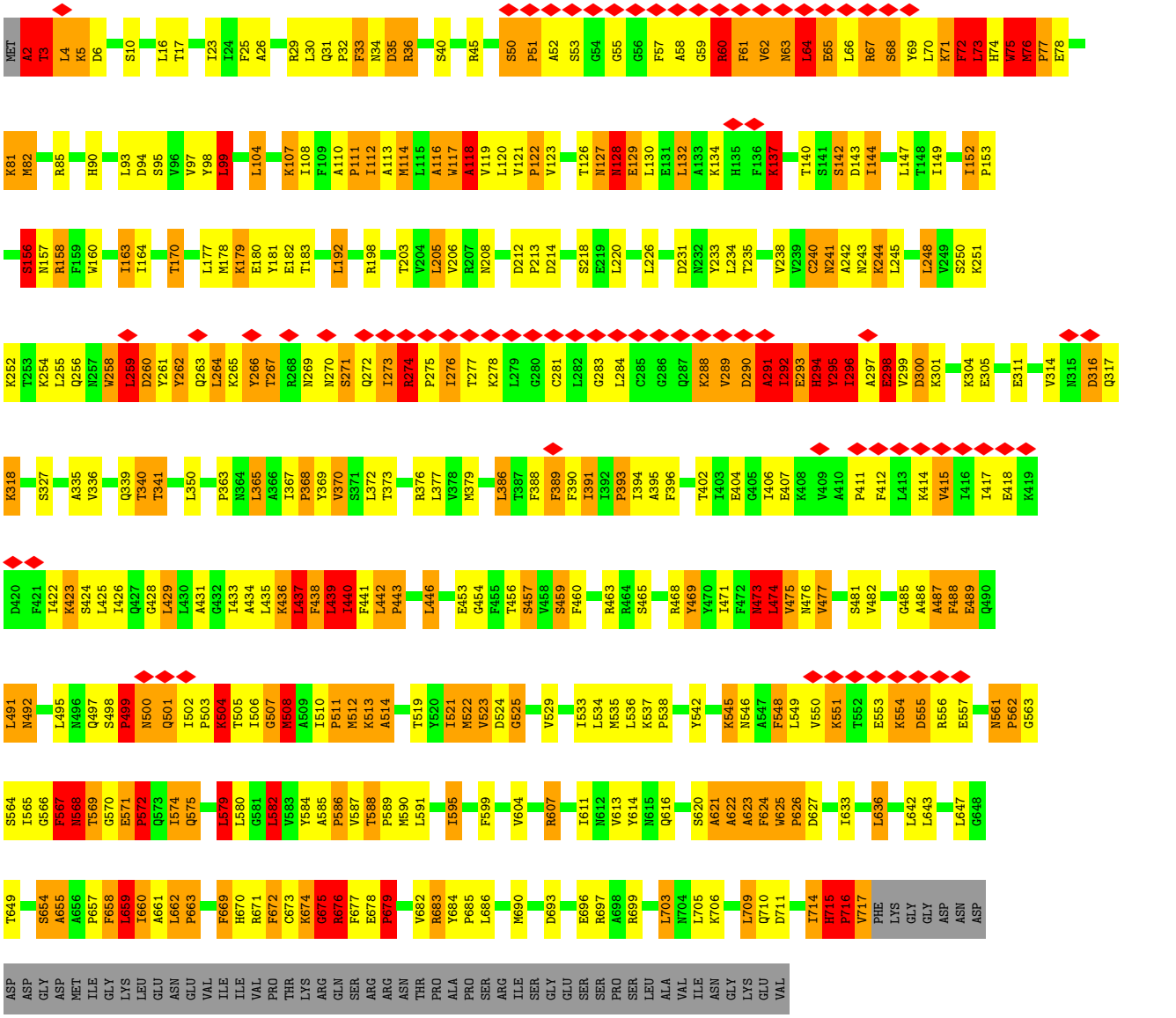
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	22	1	7	1	
2	B	1	Total	C	N	O	P	0
			31	22	1	7	1	

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.

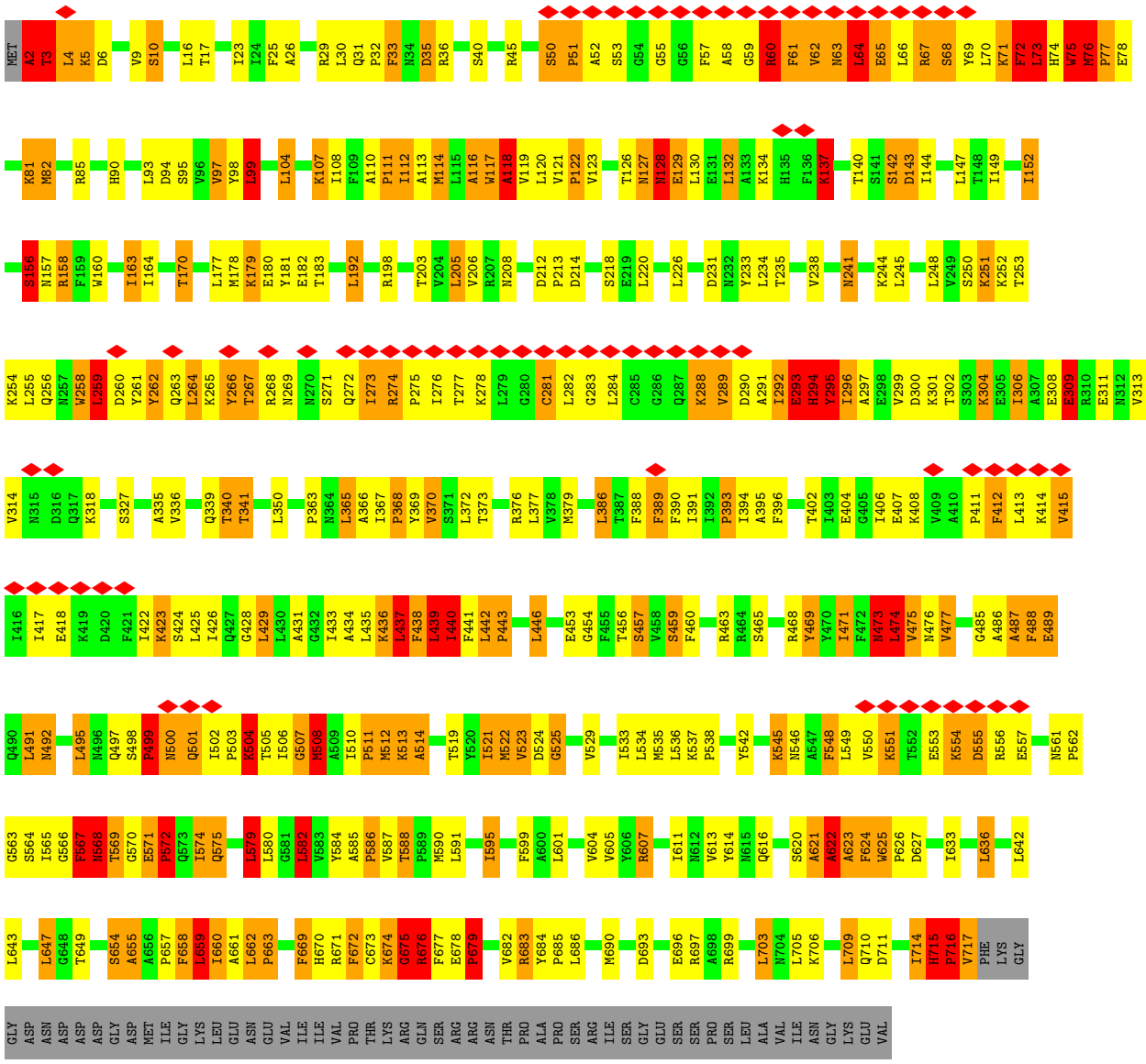
- Molecule 1: Protein OSCA1

Chain A:



• Molecule 1: Protein OSCA1

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	838000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.375	Depositor
Minimum map value	-2.032	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8489999, 0.8489999, 0.8489999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPC

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	1.61	63/5928 (1.1%)	1.48	95/8061 (1.2%)
1	B	1.55	55/5928 (0.9%)	1.42	80/8061 (1.0%)
All	All	1.58	118/11856 (1.0%)	1.45	175/16122 (1.1%)

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	9
1	B	0	7
All	All	0	16

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	ASN	C-O	19.58	1.60	1.23
1	A	623	ALA	C-O	16.66	1.55	1.23
1	B	623	ALA	C-O	16.66	1.55	1.23
1	A	437	LEU	C-O	15.37	1.52	1.23
1	B	437	LEU	C-O	15.37	1.52	1.23
1	A	440	ILE	C-O	14.02	1.50	1.23
1	B	440	ILE	C-O	14.02	1.50	1.23
1	A	507	GLY	C-O	10.92	1.41	1.23
1	B	507	GLY	C-O	10.92	1.41	1.23
1	A	655	ALA	C-O	10.87	1.44	1.23
1	B	655	ALA	C-O	10.87	1.44	1.23
1	A	676	ARG	C-O	10.63	1.43	1.23
1	B	676	ARG	C-O	10.63	1.43	1.23
1	A	369	TYR	C-O	10.44	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	TYR	C-O	10.44	1.43	1.23
1	A	500	ASN	C-O	9.82	1.42	1.23
1	B	500	ASN	C-O	9.82	1.42	1.23
1	A	293	GLU	C-O	9.46	1.41	1.23
1	A	511	PRO	C-O	9.21	1.41	1.23
1	B	511	PRO	C-O	9.21	1.41	1.23
1	A	438	PHE	C-O	8.46	1.39	1.23
1	B	438	PHE	C-O	8.46	1.39	1.23
1	A	428	GLY	C-O	8.41	1.37	1.23
1	B	428	GLY	C-O	8.41	1.37	1.23
1	A	241	ASN	N-CA	8.17	1.62	1.46
1	A	675	GLY	C-O	7.89	1.36	1.23
1	B	675	GLY	C-O	7.89	1.36	1.23
1	A	512	MET	C-O	7.89	1.38	1.23
1	B	512	MET	C-O	7.89	1.38	1.23
1	A	511	PRO	CA-C	7.73	1.68	1.52
1	B	511	PRO	CA-C	7.73	1.68	1.52
1	A	241	ASN	CA-C	7.71	1.73	1.52
1	A	98	TYR	C-O	7.51	1.37	1.23
1	B	98	TYR	C-O	7.51	1.37	1.23
1	A	582	LEU	C-O	7.33	1.37	1.23
1	B	582	LEU	C-O	7.33	1.37	1.23
1	A	291	ALA	C-O	7.33	1.37	1.23
1	A	294	HIS	C-O	7.19	1.37	1.23
1	A	118	ALA	C-O	6.99	1.36	1.23
1	B	118	ALA	C-O	6.99	1.36	1.23
1	A	434	ALA	C-O	6.90	1.36	1.23
1	B	434	ALA	C-O	6.90	1.36	1.23
1	A	436	LYS	C-O	6.72	1.36	1.23
1	B	436	LYS	C-O	6.72	1.36	1.23
1	A	298	GLU	N-CA	-6.71	1.32	1.46
1	A	107	LYS	C-O	6.65	1.35	1.23
1	B	107	LYS	C-O	6.65	1.35	1.23
1	A	655	ALA	CA-C	6.58	1.70	1.52
1	B	655	ALA	CA-C	6.58	1.70	1.52
1	A	508	MET	C-O	6.50	1.35	1.23
1	B	508	MET	C-O	6.50	1.35	1.23
1	A	428	GLY	CA-C	6.40	1.62	1.51
1	B	428	GLY	CA-C	6.40	1.62	1.51
1	A	510	ILE	C-O	6.40	1.35	1.23
1	B	510	ILE	C-O	6.40	1.35	1.23
1	A	370	VAL	C-O	6.36	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	VAL	C-O	6.36	1.35	1.23
1	A	660	ILE	C-O	6.34	1.35	1.23
1	B	660	ILE	C-O	6.34	1.35	1.23
1	A	658	PHE	C-O	6.28	1.35	1.23
1	B	658	PHE	C-O	6.28	1.35	1.23
1	A	715	HIS	C-N	6.23	1.46	1.34
1	B	715	HIS	C-N	6.23	1.46	1.34
1	A	521	ILE	C-O	-6.20	1.11	1.23
1	B	521	ILE	C-O	-6.20	1.11	1.23
1	A	489	GLU	C-O	6.19	1.35	1.23
1	B	489	GLU	C-O	6.19	1.35	1.23
1	A	431	ALA	C-O	6.15	1.35	1.23
1	B	431	ALA	C-O	6.15	1.35	1.23
1	A	439	LEU	C-O	6.14	1.35	1.23
1	B	439	LEU	C-O	6.14	1.35	1.23
1	A	504	LYS	C-O	6.06	1.34	1.23
1	B	504	LYS	C-O	6.06	1.34	1.23
1	A	659	LEU	C-O	6.05	1.34	1.23
1	B	659	LEU	C-O	6.05	1.34	1.23
1	A	81	LYS	N-CA	5.91	1.58	1.46
1	B	81	LYS	N-CA	5.91	1.58	1.46
1	A	525	GLY	CA-C	-5.89	1.42	1.51
1	B	525	GLY	CA-C	-5.89	1.42	1.51
1	A	655	ALA	N-CA	5.85	1.58	1.46
1	B	655	ALA	N-CA	5.85	1.58	1.46
1	A	298	GLU	C-O	5.71	1.34	1.23
1	A	388	PHE	C-O	5.70	1.34	1.23
1	B	388	PHE	C-O	5.70	1.34	1.23
1	A	457	SER	CA-CB	-5.68	1.44	1.52
1	B	457	SER	CA-CB	-5.68	1.44	1.52
1	A	488	PHE	C-O	5.60	1.33	1.23
1	B	488	PHE	C-O	5.60	1.33	1.23
1	A	116	ALA	CA-C	-5.58	1.38	1.52
1	B	116	ALA	CA-C	-5.58	1.38	1.52
1	A	469	TYR	C-O	-5.50	1.12	1.23
1	B	469	TYR	C-O	-5.50	1.12	1.23
1	A	473	ASN	C-O	-5.44	1.13	1.23
1	B	473	ASN	C-O	-5.44	1.13	1.23
1	A	623	ALA	CA-C	5.35	1.66	1.52
1	B	623	ALA	CA-C	5.35	1.66	1.52
1	A	459	SER	CA-CB	-5.33	1.45	1.52
1	B	459	SER	CA-CB	-5.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657	PRO	C-O	5.28	1.33	1.23
1	B	657	PRO	C-O	5.28	1.33	1.23
1	A	672	PHE	C-O	5.27	1.33	1.23
1	B	672	PHE	C-O	5.27	1.33	1.23
1	A	679	PRO	CA-CB	-5.26	1.43	1.53
1	B	679	PRO	CA-CB	-5.26	1.43	1.53
1	A	72	PHE	CA-C	-5.24	1.39	1.52
1	B	72	PHE	CA-C	-5.24	1.39	1.52
1	A	465	SER	CA-CB	-5.21	1.45	1.52
1	B	465	SER	CA-CB	-5.21	1.45	1.52
1	A	624	PHE	N-CA	-5.18	1.35	1.46
1	B	624	PHE	N-CA	-5.18	1.35	1.46
1	A	622	ALA	CA-CB	-5.10	1.41	1.52
1	B	622	ALA	CA-CB	-5.10	1.41	1.52
1	A	389	PHE	C-O	5.07	1.32	1.23
1	B	389	PHE	C-O	5.07	1.32	1.23
1	A	443	PRO	C-O	5.04	1.33	1.23
1	B	443	PRO	C-O	5.04	1.33	1.23
1	A	627	ASP	N-CA	5.03	1.56	1.46
1	B	627	ASP	N-CA	5.03	1.56	1.46

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	GLU	N-CA-C	-14.99	70.54	111.00
1	A	567	PHE	N-CA-C	-14.90	70.77	111.00
1	B	567	PHE	N-CA-C	-14.90	70.77	111.00
1	A	586	PRO	C-N-CA	10.88	148.90	121.70
1	B	586	PRO	C-N-CA	10.88	148.90	121.70
1	A	241	ASN	CA-C-O	10.61	142.39	120.10
1	A	316	ASP	N-CA-C	10.18	138.48	111.00
1	A	623	ALA	CA-C-O	9.22	139.47	120.10
1	B	623	ALA	CA-C-O	9.22	139.47	120.10
1	A	81	LYS	N-CA-C	8.95	135.17	111.00
1	B	81	LYS	N-CA-C	8.95	135.17	111.00
1	A	128	ASN	N-CA-C	8.95	135.15	111.00
1	B	128	ASN	N-CA-C	8.95	135.15	111.00
1	A	440	ILE	C-N-CA	-8.80	99.69	121.70
1	B	440	ILE	C-N-CA	-8.80	99.69	121.70
1	A	296	ILE	O-C-N	-8.65	108.85	122.70
1	A	622	ALA	O-C-N	-8.51	109.09	122.70
1	B	622	ALA	O-C-N	-8.51	109.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	443	PRO	CA-N-CD	-8.29	99.89	111.50
1	B	443	PRO	CA-N-CD	-8.29	99.89	111.50
1	A	291	ALA	N-CA-C	8.23	133.23	111.00
1	A	679	PRO	CA-N-CD	-8.22	100.00	111.50
1	B	679	PRO	CA-N-CD	-8.22	100.00	111.50
1	A	298	GLU	C-N-CA	-7.87	102.03	121.70
1	A	566	GLY	N-CA-C	-7.70	93.85	113.10
1	B	566	GLY	N-CA-C	-7.70	93.85	113.10
1	A	198	ARG	N-CA-C	-7.61	90.46	111.00
1	B	198	ARG	N-CA-C	-7.61	90.46	111.00
1	A	64	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	64	LEU	CA-CB-CG	7.45	132.44	115.30
1	A	454	GLY	N-CA-C	7.29	131.34	113.10
1	B	454	GLY	N-CA-C	7.29	131.34	113.10
1	A	240	CYS	O-C-N	-7.25	111.10	122.70
1	A	177	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	177	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	291	ALA	N-CA-C	7.20	130.43	111.00
1	A	241	ASN	N-CA-C	7.19	130.41	111.00
1	A	474	LEU	CA-CB-CG	7.14	131.72	115.30
1	A	567	PHE	N-CA-CB	7.14	123.45	110.60
1	B	474	LEU	CA-CB-CG	7.14	131.72	115.30
1	B	567	PHE	N-CA-CB	7.14	123.45	110.60
1	A	241	ASN	O-C-N	-7.13	111.30	122.70
1	A	233	TYR	N-CA-C	-7.05	91.96	111.00
1	B	233	TYR	N-CA-C	-7.05	91.96	111.00
1	A	244	LYS	C-N-CA	-6.99	104.22	121.70
1	A	586	PRO	CA-C-N	6.97	132.54	117.20
1	B	586	PRO	CA-C-N	6.97	132.54	117.20
1	A	241	ASN	C-N-CA	-6.96	104.29	121.70
1	A	259	LEU	CB-CG-CD2	6.95	122.82	111.00
1	A	620	SER	CB-CA-C	-6.91	96.97	110.10
1	B	620	SER	CB-CA-C	-6.91	96.97	110.10
1	A	586	PRO	CA-C-O	-6.72	104.08	120.20
1	B	586	PRO	CA-C-O	-6.72	104.08	120.20
1	A	716	PRO	CB-CA-C	-6.67	95.33	112.00
1	B	716	PRO	CB-CA-C	-6.67	95.33	112.00
1	A	234	LEU	CA-CB-CG	6.63	130.54	115.30
1	B	234	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	292	ILE	N-CA-C	6.43	128.35	111.00
1	A	2	ALA	N-CA-C	-6.40	93.72	111.00
1	B	2	ALA	N-CA-C	-6.40	93.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	PHE	CB-CA-C	-6.39	97.61	110.40
1	B	72	PHE	CB-CA-C	-6.39	97.61	110.40
1	A	294	HIS	N-CA-C	-6.39	93.74	111.00
1	A	499	PRO	O-C-N	-6.39	112.48	122.70
1	B	499	PRO	O-C-N	-6.39	112.48	122.70
1	A	663	PRO	CA-N-CD	-6.36	102.59	111.50
1	B	663	PRO	CA-N-CD	-6.36	102.59	111.50
1	A	439	LEU	CB-CA-C	6.33	122.23	110.20
1	B	439	LEU	CB-CA-C	6.33	122.23	110.20
1	A	368	PRO	O-C-N	-6.29	112.63	122.70
1	B	368	PRO	O-C-N	-6.29	112.63	122.70
1	A	429	LEU	CA-CB-CG	6.26	129.70	115.30
1	B	429	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	500	ASN	CA-C-O	6.24	133.21	120.10
1	B	500	ASN	CA-C-O	6.24	133.21	120.10
1	A	104	LEU	CA-CB-CG	6.24	129.64	115.30
1	B	104	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	579	LEU	CA-CB-CG	6.23	129.63	115.30
1	B	579	LEU	CA-CB-CG	6.23	129.63	115.30
1	B	260	ASP	N-CA-C	-6.14	94.41	111.00
1	A	63	ASN	N-CA-C	-6.10	94.54	111.00
1	B	63	ASN	N-CA-C	-6.10	94.54	111.00
1	A	636	LEU	CA-CB-CG	6.09	129.31	115.30
1	B	636	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	95	SER	N-CA-CB	-6.02	101.47	110.50
1	B	95	SER	N-CA-CB	-6.02	101.47	110.50
1	A	192	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	192	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	443	PRO	C-N-CA	-5.99	106.73	121.70
1	B	443	PRO	C-N-CA	-5.99	106.73	121.70
1	B	259	LEU	N-CA-C	5.93	127.01	111.00
1	A	205	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	205	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	226	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	226	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	623	ALA	CA-C-N	-5.84	104.34	117.20
1	B	623	ALA	CA-C-N	-5.84	104.34	117.20
1	A	156	SER	N-CA-C	5.78	126.60	111.00
1	B	156	SER	N-CA-C	5.78	126.60	111.00
1	A	511	PRO	O-C-N	-5.76	113.49	122.70
1	B	511	PRO	O-C-N	-5.76	113.49	122.70
1	A	81	LYS	C-N-CA	5.75	136.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	LYS	C-N-CA	5.75	136.08	121.70
1	A	97	VAL	CB-CA-C	5.73	122.28	111.40
1	B	97	VAL	CB-CA-C	5.73	122.28	111.40
1	A	393	PRO	CA-N-CD	-5.69	103.53	111.50
1	B	393	PRO	CA-N-CD	-5.69	103.53	111.50
1	A	572	PRO	CA-N-CD	-5.65	103.59	111.50
1	B	572	PRO	CA-N-CD	-5.65	103.59	111.50
1	A	260	ASP	N-CA-C	-5.58	95.92	111.00
1	A	489	GLU	CA-C-O	5.55	131.76	120.10
1	B	489	GLU	CA-C-O	5.55	131.76	120.10
1	A	514	ALA	CB-CA-C	-5.54	101.78	110.10
1	B	514	ALA	CB-CA-C	-5.54	101.78	110.10
1	A	716	PRO	CA-N-CD	-5.54	103.75	111.50
1	B	716	PRO	CA-N-CD	-5.54	103.75	111.50
1	A	534	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	534	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	440	ILE	CA-C-O	5.50	131.65	120.10
1	B	440	ILE	CA-C-O	5.50	131.65	120.10
1	A	591	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	591	LEU	CA-CB-CG	5.49	127.93	115.30
1	A	622	ALA	CA-C-N	5.48	129.25	117.20
1	B	622	ALA	CA-C-N	5.48	129.25	117.20
1	A	489	GLU	C-N-CA	-5.47	108.03	121.70
1	B	489	GLU	C-N-CA	-5.47	108.03	121.70
1	A	709	LEU	CA-CB-CG	5.45	127.82	115.30
1	B	709	LEU	CA-CB-CG	5.45	127.82	115.30
1	A	77	PRO	CA-N-CD	-5.44	103.89	111.50
1	B	77	PRO	CA-N-CD	-5.44	103.89	111.50
1	A	415	VAL	CB-CA-C	-5.42	101.10	111.40
1	B	415	VAL	CB-CA-C	-5.42	101.10	111.40
1	B	266	TYR	N-CA-C	-5.42	96.36	111.00
1	A	585	ALA	C-N-CA	-5.41	99.27	122.00
1	B	585	ALA	C-N-CA	-5.41	99.27	122.00
1	A	294	HIS	CB-CA-C	5.38	121.17	110.40
1	A	446	LEU	CA-CB-CG	5.36	127.64	115.30
1	B	446	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	316	ASP	CA-C-N	5.35	128.97	117.20
1	A	241	ASN	CA-C-N	-5.34	105.44	117.20
1	A	511	PRO	CA-C-O	5.31	132.94	120.20
1	B	511	PRO	CA-C-O	5.31	132.94	120.20
1	A	386	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	386	LEU	CA-CB-CG	5.30	127.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	99	LEU	CA-CB-CG	5.29	127.45	115.30
1	A	293	GLU	CB-CA-C	5.28	120.95	110.40
1	A	94	ASP	N-CA-CB	-5.27	101.11	110.60
1	B	94	ASP	N-CA-CB	-5.27	101.11	110.60
1	A	220	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	220	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	266	TYR	N-CA-C	-5.19	96.98	111.00
1	B	309	GLU	N-CA-C	-5.18	97.02	111.00
1	A	75	TRP	CA-CB-CG	5.16	123.51	113.70
1	B	75	TRP	CA-CB-CG	5.16	123.51	113.70
1	A	555	ASP	N-CA-C	-5.15	97.09	111.00
1	B	555	ASP	N-CA-C	-5.15	97.09	111.00
1	A	350	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	350	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	2	ALA	O-C-N	-5.10	114.54	122.70
1	B	2	ALA	O-C-N	-5.10	114.54	122.70
1	A	440	ILE	CA-C-N	-5.09	105.99	117.20
1	B	440	ILE	CA-C-N	-5.09	105.99	117.20
1	A	586	PRO	CA-N-CD	-5.09	104.37	111.50
1	B	586	PRO	CA-N-CD	-5.09	104.37	111.50
1	B	273	ILE	CB-CA-C	-5.05	101.49	111.60
1	A	658	PHE	C-N-CA	-5.05	109.08	121.70
1	B	658	PHE	C-N-CA	-5.05	109.08	121.70
1	A	655	ALA	N-CA-C	5.04	124.61	111.00
1	B	655	ALA	N-CA-C	5.04	124.61	111.00
1	A	273	ILE	CB-CA-C	-5.04	101.53	111.60
1	A	514	ALA	C-N-CA	-5.03	109.13	121.70
1	B	514	ALA	C-N-CA	-5.03	109.13	121.70
1	A	703	LEU	N-CA-C	5.02	124.56	111.00
1	B	703	LEU	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	THR	Mainchain
1	A	2	ALA	Mainchain
1	A	240	CYS	Mainchain
1	A	296	ILE	Mainchain
1	A	477	VAL	Mainchain
1	A	499	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	501	GLN	Mainchain
1	A	622	ALA	Mainchain
1	A	654	SER	Mainchain
1	B	126	THR	Mainchain
1	B	2	ALA	Mainchain
1	B	477	VAL	Mainchain
1	B	499	PRO	Mainchain
1	B	501	GLN	Mainchain
1	B	622	ALA	Mainchain
1	B	654	SER	Mainchain

5.2 Too-close contacts (i)

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	5770	0	5856	218	0
1	B	5770	0	5856	218	0
2	A	31	0	46	3	0
2	B	31	0	46	4	0
All	All	11602	0	11804	427	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 18.

All (427) 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:274:ARG:CD	1:B:289:VAL:HG13	1.92	1.00
1:A:295:TYR:O	1:A:297:ALA:N	1.96	0.99
1:B:293:GLU:OE2	1:B:296:ILE:HD12	1.68	0.93
1:B:407:GLU:HB3	1:B:414:LYS:HE2	1.52	0.92
1:A:407:GLU:HB3	1:A:414:LYS:HE2	1.52	0.92
1:A:686:LEU:HD22	1:B:340:THR:CG2	2.03	0.88
1:A:340:THR:CG2	1:B:686:LEU:HD22	2.03	0.87
1:B:259:LEU:HD23	1:B:294:HIS:CG	2.11	0.86
1:A:341:THR:HG21	1:B:683:ARG:HG2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:LEU:O	1:B:663:PRO:HD2	1.77	0.85
1:B:439:LEU:O	1:B:443:PRO:HD2	1.77	0.85
1:B:258:TRP:HB3	1:B:259:LEU:HD22	1.59	0.85
1:A:341:THR:CG2	1:B:683:ARG:HG2	2.07	0.84
1:A:659:LEU:O	1:A:663:PRO:HD2	1.77	0.84
1:A:683:ARG:HG2	1:B:341:THR:HG21	1.58	0.84
1:A:439:LEU:O	1:A:443:PRO:HD2	1.77	0.84
1:A:683:ARG:HG2	1:B:341:THR:CG2	2.07	0.84
1:B:414:LYS:HZ2	1:B:417:ILE:HG13	1.42	0.81
1:A:582:LEU:O	1:A:586:PRO:HD2	1.80	0.81
1:B:571:GLU:HG3	1:B:572:PRO:HD3	1.63	0.80
1:B:582:LEU:O	1:B:586:PRO:HD2	1.80	0.80
1:A:571:GLU:HG3	1:A:572:PRO:HD3	1.63	0.80
1:A:414:LYS:HZ2	1:A:417:ILE:HG13	1.47	0.80
1:A:340:THR:HG21	1:B:686:LEU:HD22	1.64	0.79
1:A:340:THR:HG21	1:B:686:LEU:CD2	2.13	0.79
1:A:686:LEU:HD22	1:B:340:THR:HG21	1.64	0.79
1:A:686:LEU:CD2	1:B:340:THR:HG21	2.13	0.79
1:A:178:MET:HB2	1:A:669:PHE:HE2	1.48	0.78
1:B:178:MET:HB2	1:B:669:PHE:HE2	1.48	0.78
1:B:274:ARG:HD3	1:B:289:VAL:HG13	1.65	0.77
1:A:297:ALA:HA	1:A:300:ASP:H	1.50	0.76
1:A:715:HIS:HB3	1:A:716:PRO:HD3	1.68	0.75
1:A:414:LYS:HZ2	1:A:417:ILE:HA	1.50	0.74
1:A:259:LEU:HD12	1:A:293:GLU:H	1.52	0.74
1:B:715:HIS:HB3	1:B:716:PRO:HD3	1.68	0.74
1:B:67:ARG:NH1	1:B:68:SER:O	2.22	0.73
1:B:274:ARG:NE	1:B:289:VAL:CG1	2.52	0.73
1:A:67:ARG:NH1	1:A:68:SER:O	2.22	0.73
1:B:3:THR:O	1:B:4:LEU:C	2.23	0.73
1:A:414:LYS:NZ	1:A:417:ILE:HG13	2.04	0.72
1:A:3:THR:O	1:A:4:LEU:C	2.23	0.72
1:B:414:LYS:NZ	1:B:417:ILE:HG13	2.04	0.72
1:A:715:HIS:CB	1:A:716:PRO:HD3	2.20	0.71
1:B:258:TRP:O	1:B:261:TYR:HB3	1.91	0.71
1:B:274:ARG:CD	1:B:289:VAL:CG1	2.66	0.70
1:A:297:ALA:N	1:A:299:VAL:H	1.90	0.70
1:A:107:LYS:O	1:A:111:PRO:HD2	1.91	0.69
1:B:715:HIS:CB	1:B:716:PRO:HD3	2.20	0.69
1:B:259:LEU:HB2	1:B:294:HIS:H	1.54	0.69
1:B:259:LEU:HD12	1:B:262:TYR:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ALA:HB2	1:A:584:TYR:CE1	2.28	0.69
1:B:514:ALA:HB2	1:B:584:TYR:CE1	2.28	0.68
1:B:107:LYS:O	1:B:111:PRO:HD2	1.91	0.68
1:B:274:ARG:HD3	1:B:289:VAL:CG1	2.24	0.68
1:B:389:PHE:O	1:B:393:PRO:HD2	1.94	0.68
1:B:67:ARG:HH11	1:B:68:SER:C	1.97	0.68
1:B:414:LYS:HZ2	1:B:417:ILE:HA	1.55	0.68
1:B:437:LEU:O	1:B:440:ILE:HG12	1.94	0.68
1:A:437:LEU:O	1:A:440:ILE:HG12	1.94	0.67
1:B:51:PRO:HB2	1:B:55:GLY:HA2	1.75	0.67
1:A:389:PHE:O	1:A:393:PRO:HD2	1.94	0.67
1:A:414:LYS:HZ2	1:A:417:ILE:CA	2.07	0.67
1:A:67:ARG:HH11	1:A:68:SER:C	1.97	0.67
1:A:51:PRO:HB2	1:A:55:GLY:HA2	1.75	0.67
1:A:297:ALA:H	1:A:299:VAL:H	1.42	0.66
1:B:274:ARG:NE	1:B:289:VAL:HG13	2.11	0.66
1:A:550:VAL:HG13	1:A:551:LYS:H	1.61	0.65
1:B:295:TYR:O	1:B:297:ALA:N	2.29	0.65
1:A:259:LEU:HD12	1:A:293:GLU:N	2.11	0.65
1:A:297:ALA:N	1:A:299:VAL:N	2.44	0.65
1:B:550:VAL:HG13	1:B:551:LYS:H	1.61	0.65
1:A:294:HIS:O	1:A:295:TYR:O	2.15	0.65
1:B:259:LEU:CB	1:B:294:HIS:H	2.10	0.65
1:A:259:LEU:HG	1:A:294:HIS:N	2.11	0.64
1:B:414:LYS:HZ2	1:B:417:ILE:CA	2.11	0.64
1:B:715:HIS:CG	1:B:716:PRO:HD3	2.33	0.64
1:B:584:TYR:HD1	1:B:588:THR:HG23	1.63	0.64
1:A:715:HIS:CG	1:A:716:PRO:HD3	2.33	0.63
1:A:584:TYR:HD1	1:A:588:THR:HG23	1.63	0.63
1:B:414:LYS:HB3	1:B:417:ILE:HA	1.81	0.62
1:B:390:PHE:HE1	1:B:438:PHE:HB3	1.63	0.62
1:B:58:ALA:HB1	1:B:60:ARG:HG3	1.82	0.61
1:A:390:PHE:HE1	1:A:438:PHE:HB3	1.63	0.61
1:A:414:LYS:HB3	1:A:417:ILE:HA	1.81	0.61
1:A:537:LYS:HB3	1:A:538:PRO:HD3	1.83	0.61
1:A:58:ALA:HB1	1:A:60:ARG:HG3	1.82	0.61
1:B:170:THR:HG21	1:B:662:LEU:HG	1.83	0.61
1:B:714:ILE:O	1:B:715:HIS:HB2	2.00	0.61
1:A:507:GLY:O	1:A:511:PRO:HD2	2.00	0.61
1:B:259:LEU:HB2	1:B:294:HIS:N	2.15	0.61
1:B:507:GLY:O	1:B:511:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:O	1:B:259:LEU:HD13	2.01	0.60
1:B:537:LYS:HB3	1:B:538:PRO:HD3	1.83	0.60
1:A:568:ASN:O	1:A:572:PRO:HD2	2.02	0.60
1:A:623:ALA:O	1:A:624:PHE:C	2.40	0.60
1:A:714:ILE:O	1:A:715:HIS:HB2	2.00	0.60
1:A:675:GLY:O	1:A:679:PRO:HD2	2.03	0.59
1:B:568:ASN:O	1:B:572:PRO:HD2	2.02	0.59
1:B:414:LYS:NZ	1:B:417:ILE:HA	2.17	0.59
1:A:170:THR:HG21	1:A:662:LEU:HG	1.83	0.59
1:A:241:ASN:O	1:A:242:ALA:C	2.37	0.59
1:B:623:ALA:O	1:B:624:PHE:C	2.40	0.59
1:A:2:ALA:O	1:A:3:THR:O	2.21	0.58
1:A:414:LYS:NZ	1:A:417:ILE:HA	2.17	0.58
1:B:675:GLY:O	1:B:679:PRO:HD2	2.03	0.58
1:A:340:THR:HG23	1:B:686:LEU:HD22	1.83	0.58
1:A:3:THR:HG23	1:A:142:SER:HB2	1.86	0.58
1:B:3:THR:HG23	1:B:142:SER:HB2	1.86	0.58
1:B:293:GLU:OE2	1:B:296:ILE:CD1	2.47	0.58
1:B:2:ALA:O	1:B:3:THR:O	2.21	0.57
1:B:117:TRP:O	1:B:118:ALA:C	2.41	0.57
1:B:571:GLU:HG3	1:B:572:PRO:CD	2.32	0.57
1:A:571:GLU:HG3	1:A:572:PRO:CD	2.32	0.57
1:B:108:ILE:O	1:B:112:ILE:HG23	2.05	0.57
1:B:293:GLU:O	1:B:294:HIS:C	2.41	0.57
1:A:2:ALA:O	1:A:3:THR:C	2.43	0.56
1:A:336:VAL:O	1:A:340:THR:HB	2.05	0.56
1:A:108:ILE:O	1:A:112:ILE:HG23	2.05	0.56
1:A:521:ILE:O	1:A:522:MET:C	2.42	0.56
1:B:336:VAL:O	1:B:340:THR:HB	2.05	0.56
1:B:275:PRO:HB3	1:B:283:GLY:HA2	1.87	0.56
1:B:365:LEU:HD13	1:B:456:THR:HG21	1.88	0.56
1:A:117:TRP:O	1:A:118:ALA:C	2.41	0.56
1:A:584:TYR:CD1	1:A:588:THR:HG23	2.40	0.56
1:A:255:LEU:HD13	1:A:298:GLU:HB3	1.87	0.55
1:B:584:TYR:CD1	1:B:588:THR:HG23	2.40	0.55
1:B:497:GLN:NE2	1:B:501:GLN:HE22	2.05	0.55
1:A:99:LEU:HD21	1:A:607:ARG:HG3	1.88	0.55
1:A:259:LEU:C	1:A:261:TYR:N	2.59	0.55
1:B:99:LEU:HD21	1:B:607:ARG:HG3	1.88	0.55
1:A:365:LEU:HD13	1:A:456:THR:HG21	1.88	0.55
1:A:440:ILE:O	1:A:441:PHE:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:O	1:B:3:THR:C	2.43	0.55
1:A:293:GLU:O	1:A:294:HIS:C	2.46	0.54
1:A:686:LEU:HD22	1:B:340:THR:HG23	1.83	0.54
1:B:440:ILE:O	1:B:441:PHE:C	2.45	0.54
1:A:474:LEU:HD12	1:A:579:LEU:HD11	1.89	0.54
1:A:259:LEU:HG	1:A:294:HIS:H	1.71	0.54
1:A:241:ASN:C	1:A:243:ASN:H	2.10	0.54
1:A:316:ASP:O	1:A:318:LYS:N	2.41	0.54
1:A:72:PHE:O	1:A:74:HIS:N	2.40	0.54
1:A:497:GLN:NE2	1:A:501:GLN:HE22	2.05	0.54
1:B:72:PHE:O	1:B:74:HIS:N	2.40	0.54
1:B:474:LEU:HD12	1:B:579:LEU:HD11	1.89	0.54
1:B:76:MET:HB3	1:B:77:PRO:CD	2.39	0.53
1:A:23:ILE:HD11	1:A:71:LYS:HD2	1.90	0.53
1:B:31:GLN:HB3	1:B:33:PHE:CZ	2.43	0.53
1:B:116:ALA:O	1:B:117:TRP:C	2.45	0.53
1:A:76:MET:HB3	1:A:77:PRO:CD	2.39	0.53
1:A:31:GLN:HB3	1:A:33:PHE:CZ	2.43	0.53
1:A:116:ALA:O	1:A:117:TRP:C	2.45	0.53
1:A:298:GLU:O	1:A:299:VAL:C	2.46	0.53
1:B:488:PHE:O	1:B:491:LEU:HB3	2.09	0.53
1:A:340:THR:HG21	1:B:686:LEU:HD21	1.91	0.53
1:B:521:ILE:O	1:B:522:MET:C	2.42	0.53
1:A:488:PHE:O	1:A:491:LEU:HB3	2.09	0.53
1:B:23:ILE:HD11	1:B:71:LYS:HD2	1.90	0.53
1:A:118:ALA:O	1:A:119:VAL:C	2.47	0.52
1:A:686:LEU:HD21	1:B:340:THR:HG21	1.91	0.52
1:B:568:ASN:N	1:B:568:ASN:HD22	2.06	0.52
1:A:241:ASN:O	1:A:243:ASN:N	2.43	0.52
1:A:293:GLU:HA	1:A:293:GLU:OE1	2.10	0.52
1:B:74:HIS:O	1:B:75:TRP:C	2.47	0.52
1:A:73:LEU:O	1:A:77:PRO:HD2	2.10	0.51
1:A:74:HIS:O	1:A:75:TRP:C	2.47	0.51
1:A:64:LEU:HD22	1:A:65:GLU:H	1.75	0.51
1:A:568:ASN:HD22	1:A:568:ASN:N	2.06	0.51
1:B:64:LEU:HD22	1:B:65:GLU:H	1.75	0.51
1:B:475:VAL:O	1:B:476:ASN:C	2.48	0.51
1:A:3:THR:O	1:A:5:LYS:N	2.43	0.51
1:B:73:LEU:O	1:B:77:PRO:HD2	2.10	0.51
1:A:563:GLY:O	1:A:564:SER:HB2	2.10	0.51
1:B:76:MET:HB3	1:B:77:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:CB	1:B:259:LEU:HD22	2.36	0.51
1:B:274:ARG:HD2	1:B:289:VAL:HG13	1.89	0.51
1:A:178:MET:HB2	1:A:669:PHE:CE2	2.38	0.51
1:B:61:PHE:HA	1:B:64:LEU:HB3	1.92	0.51
1:B:294:HIS:O	1:B:295:TYR:C	2.49	0.51
1:A:261:TYR:C	1:A:263:GLN:H	2.13	0.51
1:A:473:ASN:O	1:A:474:LEU:C	2.49	0.50
1:B:563:GLY:O	1:B:564:SER:HB2	2.10	0.50
1:B:118:ALA:O	1:B:122:PRO:HD2	2.12	0.50
1:B:3:THR:O	1:B:5:LYS:N	2.43	0.50
1:A:76:MET:HB3	1:A:77:PRO:HD2	1.93	0.50
1:A:297:ALA:CA	1:A:299:VAL:N	2.75	0.50
1:B:118:ALA:O	1:B:119:VAL:C	2.47	0.50
1:A:275:PRO:HB3	1:A:283:GLY:HA2	1.93	0.50
1:A:475:VAL:O	1:A:476:ASN:C	2.48	0.50
1:B:137:LYS:HG2	1:B:501:GLN:NE2	2.27	0.49
1:A:61:PHE:HA	1:A:64:LEU:HB3	1.92	0.49
1:A:674:LYS:O	1:A:675:GLY:C	2.49	0.49
1:B:259:LEU:HB3	1:B:293:GLU:HA	1.93	0.49
1:B:595:ILE:HG23	1:B:599:PHE:CE2	2.48	0.49
1:A:118:ALA:O	1:A:122:PRO:HD2	2.12	0.49
1:A:248:LEU:HD22	1:A:305:GLU:HG2	1.94	0.49
1:A:137:LYS:HG2	1:A:501:GLN:NE2	2.27	0.49
1:A:241:ASN:C	1:A:243:ASN:N	2.59	0.49
1:A:407:GLU:HB3	1:A:414:LYS:CE	2.36	0.49
1:A:595:ILE:HG23	1:A:599:PHE:CE2	2.48	0.49
1:B:674:LYS:O	1:B:675:GLY:C	2.49	0.49
1:B:259:LEU:CD1	1:B:262:TYR:CD2	2.96	0.49
1:B:633:ILE:HD11	1:B:669:PHE:HE1	1.78	0.49
1:A:414:LYS:HZ2	1:A:417:ILE:CG1	2.22	0.48
1:B:474:LEU:O	1:B:475:VAL:C	2.52	0.48
1:A:633:ILE:HD11	1:A:669:PHE:HE1	1.78	0.48
1:A:476:ASN:O	1:A:477:VAL:C	2.48	0.48
1:B:33:PHE:HE1	1:B:60:ARG:HB3	1.78	0.48
1:B:414:LYS:HZ2	1:B:417:ILE:CG1	2.19	0.48
1:A:683:ARG:HG2	1:B:341:THR:HG22	1.94	0.48
1:B:473:ASN:O	1:B:474:LEU:C	2.49	0.48
1:B:245:LEU:HD13	1:B:309:GLU:HB3	1.95	0.48
1:B:276:ILE:HB	1:B:282:LEU:HG	1.96	0.48
1:B:259:LEU:CB	1:B:293:GLU:HA	2.43	0.48
1:B:113:ALA:O	1:B:114:MET:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:C	1:B:259:LEU:HD13	2.34	0.48
1:B:571:GLU:O	1:B:572:PRO:C	2.51	0.48
1:B:716:PRO:HD2	1:B:717:VAL:HG22	1.96	0.48
1:A:258:TRP:HA	1:A:258:TRP:CE3	2.48	0.48
1:A:522:MET:O	1:A:523:VAL:C	2.52	0.48
1:B:258:TRP:HA	1:B:258:TRP:CE3	2.48	0.47
1:A:93:LEU:HD23	1:A:621:ALA:HB1	1.97	0.47
1:A:491:LEU:O	1:A:492:ASN:C	2.52	0.47
1:B:473:ASN:O	1:B:474:LEU:O	2.32	0.47
1:A:129:GLU:HG2	1:A:132:LEU:HD22	1.96	0.47
1:A:473:ASN:O	1:A:474:LEU:O	2.32	0.47
1:A:716:PRO:HD2	1:A:717:VAL:HG22	1.96	0.47
1:B:476:ASN:O	1:B:477:VAL:C	2.48	0.47
1:B:491:LEU:O	1:B:492:ASN:C	2.52	0.47
1:A:33:PHE:HE1	1:A:60:ARG:HB3	1.78	0.47
1:A:274:ARG:HA	1:A:288:LYS:HE2	1.97	0.47
1:B:522:MET:O	1:B:523:VAL:C	2.52	0.47
1:B:545:LYS:HB2	1:B:545:LYS:HE2	1.40	0.47
1:A:90:HIS:HE1	1:A:611:ILE:O	1.97	0.47
1:A:149:ILE:O	1:A:152:ILE:HG22	2.15	0.47
1:A:341:THR:HG22	1:B:683:ARG:HG2	1.94	0.47
1:A:295:TYR:C	1:A:297:ALA:N	2.66	0.47
1:B:500:ASN:C	1:B:502:ILE:N	2.68	0.47
1:B:514:ALA:CB	1:B:588:THR:HG21	2.45	0.47
1:B:655:ALA:O	1:B:658:PHE:HB2	2.15	0.46
1:A:390:PHE:CE1	1:A:438:PHE:HB3	2.49	0.46
1:B:90:HIS:HE1	1:B:611:ILE:O	1.97	0.46
1:A:244:LYS:O	1:A:245:LEU:C	2.52	0.46
1:A:655:ALA:O	1:A:658:PHE:HB2	2.15	0.46
1:B:129:GLU:HG2	1:B:132:LEU:HD22	1.96	0.46
1:A:442:LEU:HD22	1:A:442:LEU:HA	1.59	0.46
1:B:93:LEU:HD23	1:B:621:ALA:HB1	1.97	0.46
1:A:113:ALA:O	1:A:114:MET:C	2.51	0.46
1:A:514:ALA:CB	1:A:588:THR:HG21	2.45	0.46
1:B:63:ASN:O	1:B:65:GLU:N	2.48	0.46
1:B:149:ILE:O	1:B:152:ILE:HG22	2.15	0.46
1:A:270:ASN:HB3	1:A:271:SER:H	1.54	0.46
1:A:411:PRO:C	1:A:414:LYS:HD2	2.36	0.46
1:A:501:GLN:O	1:A:502:ILE:C	2.53	0.46
1:B:110:ALA:HB3	1:B:111:PRO:CD	2.46	0.46
1:B:662:LEU:O	1:B:663:PRO:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:O	1:A:475:VAL:C	2.52	0.46
1:B:259:LEU:HD11	1:B:262:TYR:CD2	2.51	0.46
1:B:684:TYR:HA	1:B:685:PRO:HD2	1.83	0.46
2:B:801:LPC:H32	2:B:801:LPC:H0A2	1.56	0.46
1:A:63:ASN:O	1:A:65:GLU:N	2.48	0.45
1:B:178:MET:HB2	1:B:669:PHE:CE2	2.38	0.45
1:B:633:ILE:HD11	1:B:669:PHE:CE1	2.51	0.45
1:B:263:GLN:HG3	1:B:264:LEU:HD23	1.98	0.45
1:B:281:CYS:HB3	1:B:282:LEU:H	1.51	0.45
1:A:259:LEU:HD13	1:A:262:TYR:HB2	1.97	0.45
1:A:276:ILE:HA	1:A:276:ILE:HD13	1.71	0.45
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.78	0.45
1:A:633:ILE:HD11	1:A:669:PHE:CE1	2.51	0.45
1:B:501:GLN:O	1:B:502:ILE:C	2.53	0.45
1:A:500:ASN:C	1:A:502:ILE:N	2.68	0.45
1:B:156:SER:HB2	1:B:157:ASN:H	1.26	0.45
1:B:259:LEU:HD23	1:B:294:HIS:ND1	2.29	0.45
1:A:110:ALA:HB3	1:A:111:PRO:CD	2.46	0.45
1:B:714:ILE:H	1:B:714:ILE:HG13	1.60	0.45
1:A:163:ILE:HG13	1:A:164:ILE:N	2.32	0.45
1:B:335:ALA:O	1:B:339:GLN:HG2	2.17	0.45
1:B:411:PRO:C	1:B:414:LYS:HD2	2.36	0.45
1:A:714:ILE:O	1:A:715:HIS:CB	2.64	0.45
1:B:508:MET:H	1:B:508:MET:HG2	1.54	0.45
2:B:801:LPC:HD1	2:B:801:LPC:HG1	1.71	0.45
1:A:107:LYS:O	1:A:108:ILE:C	2.55	0.44
1:A:290:ASP:O	1:A:291:ALA:HB2	2.18	0.44
1:B:408:LYS:HA	1:B:408:LYS:HD3	1.49	0.44
1:B:678:GLU:O	1:B:679:PRO:C	2.52	0.44
1:A:571:GLU:O	1:A:572:PRO:C	2.51	0.44
1:A:623:ALA:C	1:A:625:TRP:N	2.70	0.44
1:A:675:GLY:O	1:A:679:PRO:CD	2.65	0.44
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.78	0.44
1:A:474:LEU:O	1:A:475:VAL:O	2.36	0.44
1:A:662:LEU:O	1:A:663:PRO:C	2.54	0.44
2:A:801:LPC:H32	2:A:801:LPC:H0A2	1.56	0.44
1:A:523:VAL:O	1:A:524:ASP:C	2.55	0.44
1:A:662:LEU:HB3	1:A:663:PRO:CD	2.47	0.44
1:B:259:LEU:HD12	1:B:262:TYR:CB	2.43	0.44
1:B:662:LEU:HB3	1:B:663:PRO:CD	2.47	0.44
1:B:407:GLU:HB3	1:B:414:LYS:CE	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:MET:HE2	1:A:114:MET:HB2	1.80	0.44
1:A:179:LYS:O	1:A:182:GLU:HG3	2.18	0.44
2:A:801:LPC:HD1	2:A:801:LPC:HG1	1.71	0.44
2:B:801:LPC:HE1	2:B:801:LPC:HB1	1.53	0.44
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.78	0.44
1:B:107:LYS:O	1:B:108:ILE:C	2.55	0.44
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.90	0.44
1:B:523:VAL:O	1:B:524:ASP:C	2.55	0.44
1:A:335:ALA:O	1:A:339:GLN:HG2	2.17	0.44
1:B:474:LEU:HB3	1:B:475:VAL:H	1.71	0.44
1:B:486:ALA:O	1:B:487:ALA:C	2.56	0.44
1:A:52:ALA:HB3	1:A:57:PHE:HD2	1.83	0.43
1:B:121:VAL:O	1:B:122:PRO:C	2.55	0.43
1:A:25:PHE:O	1:A:26:ALA:C	2.55	0.43
1:A:259:LEU:HD12	1:A:292:ILE:HA	2.00	0.43
1:B:395:ALA:O	1:B:396:PHE:C	2.55	0.43
1:A:414:LYS:HD3	1:A:417:ILE:HA	2.01	0.43
1:B:179:LYS:O	1:B:182:GLU:HG3	2.18	0.43
1:B:274:ARG:HA	1:B:288:LYS:HE2	2.00	0.43
1:B:474:LEU:O	1:B:475:VAL:O	2.36	0.43
1:A:34:ASN:O	1:A:36:ARG:N	2.45	0.43
1:B:163:ILE:HG13	1:B:164:ILE:N	2.32	0.43
1:B:304:LYS:HD2	1:B:304:LYS:HA	1.43	0.43
1:A:156:SER:HB2	1:A:157:ASN:H	1.26	0.43
1:B:120:LEU:O	1:B:121:VAL:C	2.55	0.43
1:B:302:THR:O	1:B:306:ILE:HB	2.19	0.43
1:B:567:PHE:CZ	1:B:624:PHE:HB2	2.54	0.43
1:B:714:ILE:O	1:B:715:HIS:CB	2.64	0.43
2:A:801:LPC:H0B3	2:A:801:LPC:H31	0.77	0.43
1:B:25:PHE:O	1:B:26:ALA:C	2.55	0.43
1:B:675:GLY:O	1:B:679:PRO:CD	2.65	0.43
1:B:675:GLY:O	1:B:676:ARG:C	2.56	0.43
1:A:121:VAL:O	1:A:122:PRO:C	2.55	0.43
1:A:567:PHE:CZ	1:A:624:PHE:HB2	2.54	0.43
1:B:51:PRO:HB2	1:B:52:ALA:H	1.62	0.43
1:B:261:TYR:C	1:B:263:GLN:H	2.22	0.43
1:B:471:ILE:H	1:B:471:ILE:HG12	1.62	0.43
1:B:123:VAL:HG13	1:B:158:ARG:HD3	2.01	0.43
1:B:522:MET:O	1:B:523:VAL:O	2.37	0.43
1:B:568:ASN:O	1:B:572:PRO:CD	2.67	0.43
1:A:395:ALA:O	1:A:396:PHE:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LYS:HE2	1:A:545:LYS:HB2	1.40	0.43
1:A:568:ASN:O	1:A:569:THR:C	2.57	0.43
1:A:678:GLU:O	1:A:679:PRO:C	2.52	0.43
1:A:675:GLY:O	1:A:676:ARG:C	2.56	0.43
1:B:575:GLN:HE21	1:B:575:GLN:HB3	1.59	0.43
1:B:673:CYS:O	1:B:674:LYS:C	2.57	0.43
2:B:801:LPC:HM2	2:B:801:LPC:HJ1	1.66	0.43
1:B:251:LYS:O	1:B:255:LEU:HG	2.18	0.42
1:B:414:LYS:HD3	1:B:417:ILE:HA	2.01	0.42
1:A:522:MET:O	1:A:523:VAL:O	2.37	0.42
1:A:568:ASN:O	1:A:572:PRO:CD	2.67	0.42
1:B:406:ILE:CG1	1:B:488:PHE:HB3	2.49	0.42
1:A:82:MET:O	1:A:607:ARG:NH2	2.51	0.42
1:A:406:ILE:CG1	1:A:488:PHE:HB3	2.49	0.42
1:A:575:GLN:HE21	1:A:575:GLN:HB3	1.59	0.42
1:A:486:ALA:O	1:A:487:ALA:C	2.56	0.42
1:B:485:GLY:HA3	1:B:513:LYS:HD3	2.01	0.42
1:B:504:LYS:O	1:B:508:MET:HG2	2.20	0.42
1:A:74:HIS:O	1:A:78:GLU:HG2	2.20	0.42
1:A:504:LYS:O	1:A:508:MET:HG2	2.20	0.42
1:B:669:PHE:O	1:B:670:HIS:C	2.57	0.42
1:A:144:ILE:HD12	1:A:144:ILE:HA	1.71	0.42
1:A:658:PHE:O	1:A:659:LEU:C	2.58	0.42
1:A:672:PHE:O	1:A:673:CYS:C	2.58	0.42
1:B:623:ALA:C	1:B:625:TRP:N	2.70	0.42
1:B:662:LEU:HD12	1:B:662:LEU:HA	1.69	0.42
1:A:67:ARG:HH11	1:A:69:TYR:N	2.17	0.42
1:A:258:TRP:O	1:A:259:LEU:HD22	2.20	0.42
1:A:673:CYS:O	1:A:674:LYS:C	2.57	0.42
1:B:32:PRO:HG3	1:B:58:ALA:C	2.40	0.42
1:B:67:ARG:HH11	1:B:69:TYR:N	2.17	0.42
1:A:474:LEU:HB3	1:A:475:VAL:H	1.71	0.42
1:A:588:THR:HA	1:A:589:PRO:HD3	1.90	0.42
1:B:672:PHE:O	1:B:673:CYS:C	2.58	0.42
1:A:179:LYS:O	1:A:183:THR:HG23	2.20	0.42
1:A:423:LYS:HA	1:A:423:LYS:HD2	1.75	0.42
1:A:485:GLY:HA3	1:A:513:LYS:HD3	2.01	0.42
1:B:74:HIS:O	1:B:78:GLU:HG2	2.20	0.42
1:A:123:VAL:HG13	1:A:158:ARG:HD3	2.01	0.41
1:A:561:ASN:HA	1:A:562:PRO:HD3	1.85	0.41
1:B:52:ALA:HB3	1:B:57:PHE:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLY:O	1:B:529:VAL:HG22	2.20	0.41
1:A:625:TRP:O	1:A:626:PRO:C	2.58	0.41
1:B:435:LEU:HG	1:B:439:LEU:HD22	2.01	0.41
1:A:258:TRP:HA	1:A:258:TRP:HE3	1.83	0.41
1:A:570:GLY:O	1:A:574:ILE:HG13	2.20	0.41
1:A:684:TYR:HA	1:A:685:PRO:HD2	1.83	0.41
1:B:241:ASN:OD1	1:B:366:ALA:HB1	2.21	0.41
1:B:647:LEU:HD12	1:B:647:LEU:HA	1.86	0.41
1:A:60:ARG:HG3	1:A:60:ARG:H	1.46	0.41
1:A:120:LEU:O	1:A:121:VAL:C	2.55	0.41
1:A:259:LEU:HD23	1:A:294:HIS:ND1	2.36	0.41
1:A:288:LYS:H	1:A:288:LYS:HG3	1.61	0.41
1:A:435:LEU:HG	1:A:439:LEU:HD22	2.01	0.41
1:B:179:LYS:O	1:B:183:THR:HG23	2.20	0.41
1:B:390:PHE:CE1	1:B:438:PHE:HB3	2.49	0.41
1:B:412:PHE:HB3	1:B:413:LEU:H	1.61	0.41
1:A:36:ARG:H	1:A:36:ARG:HG3	1.68	0.41
1:A:72:PHE:HB3	1:A:73:LEU:H	0.98	0.41
1:A:660:ILE:O	1:A:661:ALA:C	2.58	0.41
1:B:50:SER:CB	1:B:51:PRO:HD2	2.51	0.41
1:B:367:ILE:HG21	1:B:367:ILE:HD13	1.83	0.41
1:A:137:LYS:HB2	1:A:137:LYS:HE2	1.60	0.41
1:A:669:PHE:O	1:A:670:HIS:C	2.57	0.41
1:B:82:MET:HE3	1:B:82:MET:HB3	1.59	0.41
1:B:97:VAL:HG21	1:B:622:ALA:HB2	2.03	0.41
1:B:601:LEU:O	1:B:605:VAL:HG13	2.21	0.41
1:A:437:LEU:O	1:A:438:PHE:C	2.59	0.41
1:A:367:ILE:HD13	1:A:367:ILE:HG21	1.83	0.41
1:A:390:PHE:O	1:A:391:ILE:C	2.60	0.41
1:A:525:GLY:O	1:A:529:VAL:HG22	2.20	0.41
1:B:568:ASN:O	1:B:569:THR:C	2.57	0.41
1:A:50:SER:CB	1:A:51:PRO:HD2	2.51	0.40
1:A:137:LYS:HG2	1:A:501:GLN:CD	2.41	0.40
1:B:137:LYS:HG2	1:B:501:GLN:CD	2.41	0.40
1:B:423:LYS:HA	1:B:423:LYS:HD2	1.75	0.40
1:A:32:PRO:HG3	1:A:58:ALA:C	2.40	0.40
1:A:137:LYS:HE2	1:A:137:LYS:HB3	1.84	0.40
1:A:264:LEU:HD22	1:A:264:LEU:HA	1.76	0.40
1:B:82:MET:O	1:B:607:ARG:NH2	2.51	0.40
1:B:142:SER:HB2	1:B:143:ASP:H	1.74	0.40
1:B:437:LEU:O	1:B:438:PHE:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLY:O	1:B:574:ILE:HG13	2.20	0.40
1:B:658:PHE:O	1:B:659:LEU:C	2.58	0.40
1:B:660:ILE:O	1:B:661:ALA:C	2.58	0.40
1:B:9:VAL:O	1:B:10:SER:C	2.57	0.40
1:A:60:ARG:HB2	1:A:61:PHE:H	1.27	0.40
1:A:442:LEU:O	1:A:443:PRO:C	2.59	0.40
1:A:481:SER:O	1:A:482:VAL:C	2.59	0.40
1:B:442:LEU:O	1:B:443:PRO:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	714/772 (92%)	555 (78%)	106 (15%)	53 (7%)	1 1
1	B	714/772 (92%)	556 (78%)	105 (15%)	53 (7%)	1 1
All	All	1428/1544 (92%)	1111 (78%)	211 (15%)	106 (7%)	2 1

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	51	PRO
1	A	128	ASN
1	A	156	SER
1	A	289	VAL
1	A	291	ALA
1	A	296	ILE
1	A	317	GLN
1	A	418	GLU
1	A	474	LEU

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Mol	Chain	Res	Type
1	A	523	VAL
1	A	567	PHE
1	A	568	ASN
1	A	614	TYR
1	A	621	ALA
1	A	703	LEU
1	A	715	HIS
1	A	716	PRO
1	B	3	THR
1	B	51	PRO
1	B	128	ASN
1	B	156	SER
1	B	289	VAL
1	B	293	GLU
1	B	296	ILE
1	B	418	GLU
1	B	474	LEU
1	B	523	VAL
1	B	567	PHE
1	B	568	ASN
1	B	614	TYR
1	B	621	ALA
1	B	703	LEU
1	B	715	HIS
1	B	716	PRO
1	A	62	VAL
1	A	64	LEU
1	A	72	PHE
1	A	137	LYS
1	A	208	ASN
1	A	213	PRO
1	A	295	TYR
1	A	368	PRO
1	A	475	VAL
1	A	487	ALA
1	A	562	PRO
1	A	674	LYS
1	A	675	GLY
1	B	62	VAL
1	B	64	LEU
1	B	72	PHE
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	208	ASN
1	B	213	PRO
1	B	368	PRO
1	B	475	VAL
1	B	487	ALA
1	B	562	PRO
1	B	674	LYS
1	B	675	GLY
1	A	35	ASP
1	A	73	LEU
1	A	118	ALA
1	A	267	THR
1	B	35	ASP
1	B	73	LEU
1	B	118	ALA
1	B	295	TYR
1	A	60	ARG
1	A	117	TRP
1	A	522	MET
1	A	554	LYS
1	A	555	ASP
1	A	561	ASN
1	A	565	ILE
1	A	613	VAL
1	B	60	ARG
1	B	117	TRP
1	B	267	THR
1	B	292	ILE
1	B	522	MET
1	B	554	LYS
1	B	555	ASP
1	B	561	ASN
1	B	565	ILE
1	B	613	VAL
1	A	127	ASN
1	A	453	GLU
1	B	127	ASN
1	B	294	HIS
1	B	453	GLU
1	A	4	LEU
1	A	59	GLY
1	A	76	MET

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Mol	Chain	Res	Type
1	A	473	ASN
1	A	499	PRO
1	A	548	PHE
1	B	4	LEU
1	B	59	GLY
1	B	76	MET
1	B	473	ASN
1	B	499	PRO
1	B	548	PHE
1	A	587	VAL
1	B	587	VAL
1	A	274	ARG

5.3.2 Protein sidechains (i)

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	618/666 (93%)	406 (66%)	212 (34%)	0 0
1	B	618/666 (93%)	400 (65%)	218 (35%)	0 0
All	All	1236/1332 (93%)	806 (65%)	430 (35%)	1 0

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	5	LYS
1	A	6	ASP
1	A	10	SER
1	A	16	LEU
1	A	17	THR
1	A	29	ARG
1	A	30	LEU
1	A	33	PHE
1	A	35	ASP
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	40	SER
1	A	45	ARG
1	A	50	SER
1	A	53	SER
1	A	60	ARG
1	A	61	PHE
1	A	62	VAL
1	A	64	LEU
1	A	65	GLU
1	A	66	LEU
1	A	67	ARG
1	A	68	SER
1	A	70	LEU
1	A	71	LYS
1	A	73	LEU
1	A	75	TRP
1	A	76	MET
1	A	81	LYS
1	A	82	MET
1	A	85	ARG
1	A	99	LEU
1	A	104	LEU
1	A	111	PRO
1	A	112	ILE
1	A	114	MET
1	A	122	PRO
1	A	127	ASN
1	A	128	ASN
1	A	129	GLU
1	A	132	LEU
1	A	134	LYS
1	A	137	LYS
1	A	140	THR
1	A	142	SER
1	A	143	ASP
1	A	144	ILE
1	A	147	LEU
1	A	152	ILE
1	A	156	SER
1	A	158	ARG
1	A	160	TRP
1	A	163	ILE

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Mol	Chain	Res	Type
1	A	170	THR
1	A	179	LYS
1	A	180	GLU
1	A	181	TYR
1	A	192	LEU
1	A	203	THR
1	A	205	LEU
1	A	206	VAL
1	A	212	ASP
1	A	214	ASP
1	A	218	SER
1	A	231	ASP
1	A	235	THR
1	A	238	VAL
1	A	248	LEU
1	A	250	SER
1	A	251	LYS
1	A	252	LYS
1	A	254	LYS
1	A	256	GLN
1	A	258	TRP
1	A	259	LEU
1	A	260	ASP
1	A	262	TYR
1	A	264	LEU
1	A	265	LYS
1	A	266	TYR
1	A	267	THR
1	A	269	ASN
1	A	271	SER
1	A	272	GLN
1	A	273	ILE
1	A	274	ARG
1	A	276	ILE
1	A	277	THR
1	A	278	LYS
1	A	281	CYS
1	A	284	LEU
1	A	288	LYS
1	A	289	VAL
1	A	290	ASP
1	A	292	ILE

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Mol	Chain	Res	Type
1	A	294	HIS
1	A	295	TYR
1	A	298	GLU
1	A	300	ASP
1	A	301	LYS
1	A	304	LYS
1	A	311	GLU
1	A	314	VAL
1	A	318	LYS
1	A	327	SER
1	A	340	THR
1	A	341	THR
1	A	363	PRO
1	A	365	LEU
1	A	370	VAL
1	A	372	LEU
1	A	373	THR
1	A	376	ARG
1	A	377	LEU
1	A	379	MET
1	A	386	LEU
1	A	391	ILE
1	A	394	ILE
1	A	402	THR
1	A	404	GLU
1	A	412	PHE
1	A	415	VAL
1	A	422	ILE
1	A	423	LYS
1	A	424	SER
1	A	425	LEU
1	A	426	ILE
1	A	429	LEU
1	A	433	ILE
1	A	436	LYS
1	A	437	LEU
1	A	439	LEU
1	A	440	ILE
1	A	442	LEU
1	A	446	LEU
1	A	457	SER
1	A	459	SER

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Mol	Chain	Res	Type
1	A	460	PHE
1	A	463	ARG
1	A	468	ARG
1	A	469	TYR
1	A	471	ILE
1	A	489	GLU
1	A	491	LEU
1	A	492	ASN
1	A	495	LEU
1	A	498	SER
1	A	503	PRO
1	A	504	LYS
1	A	505	THR
1	A	506	ILE
1	A	508	MET
1	A	512	MET
1	A	513	LYS
1	A	519	THR
1	A	533	ILE
1	A	535	MET
1	A	536	LEU
1	A	542	TYR
1	A	545	LYS
1	A	546	ASN
1	A	548	PHE
1	A	549	LEU
1	A	551	LYS
1	A	553	GLU
1	A	554	LYS
1	A	556	ARG
1	A	557	GLU
1	A	568	ASN
1	A	569	THR
1	A	571	GLU
1	A	572	PRO
1	A	574	ILE
1	A	575	GLN
1	A	579	LEU
1	A	580	LEU
1	A	582	LEU
1	A	588	THR
1	A	590	MET

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Mol	Chain	Res	Type
1	A	595	ILE
1	A	604	VAL
1	A	607	ARG
1	A	616	GLN
1	A	625	TRP
1	A	626	PRO
1	A	636	LEU
1	A	642	LEU
1	A	643	LEU
1	A	647	LEU
1	A	649	THR
1	A	654	SER
1	A	659	LEU
1	A	662	LEU
1	A	669	PHE
1	A	671	ARG
1	A	676	ARG
1	A	677	PHE
1	A	679	PRO
1	A	682	VAL
1	A	683	ARG
1	A	690	MET
1	A	693	ASP
1	A	696	GLU
1	A	697	ARG
1	A	699	ARG
1	A	705	LEU
1	A	706	LYS
1	A	709	LEU
1	A	710	GLN
1	A	711	ASP
1	A	714	ILE
1	A	717	VAL
1	B	3	THR
1	B	5	LYS
1	B	6	ASP
1	B	10	SER
1	B	16	LEU
1	B	17	THR
1	B	29	ARG
1	B	30	LEU
1	B	33	PHE

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Mol	Chain	Res	Type
1	B	35	ASP
1	B	36	ARG
1	B	40	SER
1	B	45	ARG
1	B	50	SER
1	B	53	SER
1	B	60	ARG
1	B	61	PHE
1	B	62	VAL
1	B	64	LEU
1	B	65	GLU
1	B	66	LEU
1	B	67	ARG
1	B	68	SER
1	B	70	LEU
1	B	71	LYS
1	B	73	LEU
1	B	75	TRP
1	B	76	MET
1	B	81	LYS
1	B	82	MET
1	B	85	ARG
1	B	99	LEU
1	B	104	LEU
1	B	111	PRO
1	B	112	ILE
1	B	114	MET
1	B	122	PRO
1	B	127	ASN
1	B	128	ASN
1	B	129	GLU
1	B	132	LEU
1	B	134	LYS
1	B	137	LYS
1	B	140	THR
1	B	142	SER
1	B	143	ASP
1	B	144	ILE
1	B	147	LEU
1	B	152	ILE
1	B	156	SER
1	B	158	ARG

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Mol	Chain	Res	Type
1	B	160	TRP
1	B	163	ILE
1	B	170	THR
1	B	179	LYS
1	B	180	GLU
1	B	181	TYR
1	B	192	LEU
1	B	203	THR
1	B	205	LEU
1	B	206	VAL
1	B	212	ASP
1	B	214	ASP
1	B	218	SER
1	B	231	ASP
1	B	235	THR
1	B	238	VAL
1	B	241	ASN
1	B	244	LYS
1	B	248	LEU
1	B	250	SER
1	B	251	LYS
1	B	252	LYS
1	B	253	THR
1	B	254	LYS
1	B	256	GLN
1	B	258	TRP
1	B	259	LEU
1	B	262	TYR
1	B	264	LEU
1	B	265	LYS
1	B	266	TYR
1	B	267	THR
1	B	268	ARG
1	B	269	ASN
1	B	271	SER
1	B	272	GLN
1	B	273	ILE
1	B	274	ARG
1	B	277	THR
1	B	278	LYS
1	B	281	CYS
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	288	LYS
1	B	290	ASP
1	B	292	ILE
1	B	293	GLU
1	B	294	HIS
1	B	295	TYR
1	B	299	VAL
1	B	300	ASP
1	B	301	LYS
1	B	304	LYS
1	B	306	ILE
1	B	308	GLU
1	B	309	GLU
1	B	311	GLU
1	B	313	VAL
1	B	314	VAL
1	B	318	LYS
1	B	327	SER
1	B	340	THR
1	B	341	THR
1	B	363	PRO
1	B	365	LEU
1	B	370	VAL
1	B	372	LEU
1	B	373	THR
1	B	376	ARG
1	B	377	LEU
1	B	379	MET
1	B	386	LEU
1	B	391	ILE
1	B	394	ILE
1	B	402	THR
1	B	404	GLU
1	B	412	PHE
1	B	415	VAL
1	B	422	ILE
1	B	423	LYS
1	B	424	SER
1	B	425	LEU
1	B	426	ILE
1	B	429	LEU
1	B	433	ILE

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Mol	Chain	Res	Type
1	B	436	LYS
1	B	437	LEU
1	B	439	LEU
1	B	440	ILE
1	B	442	LEU
1	B	446	LEU
1	B	457	SER
1	B	459	SER
1	B	460	PHE
1	B	463	ARG
1	B	468	ARG
1	B	469	TYR
1	B	471	ILE
1	B	489	GLU
1	B	491	LEU
1	B	492	ASN
1	B	495	LEU
1	B	498	SER
1	B	503	PRO
1	B	504	LYS
1	B	505	THR
1	B	506	ILE
1	B	508	MET
1	B	512	MET
1	B	513	LYS
1	B	519	THR
1	B	533	ILE
1	B	535	MET
1	B	536	LEU
1	B	542	TYR
1	B	545	LYS
1	B	546	ASN
1	B	548	PHE
1	B	549	LEU
1	B	551	LYS
1	B	553	GLU
1	B	554	LYS
1	B	556	ARG
1	B	557	GLU
1	B	568	ASN
1	B	569	THR
1	B	571	GLU

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Mol	Chain	Res	Type
1	B	572	PRO
1	B	574	ILE
1	B	575	GLN
1	B	579	LEU
1	B	580	LEU
1	B	582	LEU
1	B	588	THR
1	B	590	MET
1	B	595	ILE
1	B	604	VAL
1	B	607	ARG
1	B	616	GLN
1	B	625	TRP
1	B	626	PRO
1	B	636	LEU
1	B	642	LEU
1	B	643	LEU
1	B	647	LEU
1	B	649	THR
1	B	654	SER
1	B	659	LEU
1	B	662	LEU
1	B	669	PHE
1	B	671	ARG
1	B	676	ARG
1	B	677	PHE
1	B	679	PRO
1	B	682	VAL
1	B	683	ARG
1	B	690	MET
1	B	693	ASP
1	B	696	GLU
1	B	697	ARG
1	B	699	ARG
1	B	705	LEU
1	B	706	LYS
1	B	709	LEU
1	B	710	GLN
1	B	711	ASP
1	B	714	ILE
1	B	717	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	74	HIS
1	A	90	HIS
1	A	124	ASN
1	A	256	GLN
1	A	272	GLN
1	A	342	GLN
1	A	476	ASN
1	A	490	GLN
1	A	497	GLN
1	A	500	ASN
1	A	501	GLN
1	A	543	HIS
1	A	568	ASN
1	A	573	GLN
1	A	575	GLN
1	A	687	GLN
1	B	63	ASN
1	B	90	HIS
1	B	124	ASN
1	B	270	ASN
1	B	272	GLN
1	B	342	GLN
1	B	476	ASN
1	B	490	GLN
1	B	497	GLN
1	B	500	ASN
1	B	543	HIS
1	B	568	ASN
1	B	573	GLN
1	B	575	GLN
1	B	687	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	LPC	A	801	-	30,30,30	0.87	1 (3%)	35,37,37	2.35	7 (20%)
2	LPC	B	801	-	30,30,30	0.87	1 (3%)	35,37,37	2.35	7 (20%)

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
2	LPC	A	801	-	-	18/32/32/32	-
2	LPC	B	801	-	-	18/32/32/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	LPC	OQ2-CA	4.02	1.45	1.33
2	B	801	LPC	OQ2-CA	4.02	1.45	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	LPC	C0B-N1-C2	-6.32	84.05	109.92
2	B	801	LPC	C0B-N1-C2	-6.32	84.05	109.92
2	A	801	LPC	C0A-N1-C2	-6.15	84.75	109.92
2	B	801	LPC	C0A-N1-C2	-6.15	84.75	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	LPC	C0C-N1-C2	-6.14	84.81	109.92
2	B	801	LPC	C0C-N1-C2	-6.14	84.81	109.92
2	A	801	LPC	C0C-N1-C0B	4.09	119.48	108.97
2	B	801	LPC	C0C-N1-C0B	4.09	119.48	108.97
2	A	801	LPC	C0B-N1-C0A	4.04	119.35	108.97
2	B	801	LPC	C0B-N1-C0A	4.04	119.35	108.97
2	A	801	LPC	C0C-N1-C0A	3.70	118.48	108.97
2	B	801	LPC	C0C-N1-C0A	3.70	118.48	108.97
2	A	801	LPC	OQ2-CA-CB	2.38	119.36	111.91
2	B	801	LPC	OQ2-CA-CB	2.38	119.36	111.91

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	LPC	C3-O4-P5-O6
2	A	801	LPC	C7-O6-P5-O4
2	A	801	LPC	C7-O6-P5-O5A
2	A	801	LPC	C7-O6-P5-O5B
2	A	801	LPC	C7-C8-C9-OQ2
2	B	801	LPC	C3-O4-P5-O6
2	B	801	LPC	C7-O6-P5-O4
2	B	801	LPC	C7-O6-P5-O5A
2	B	801	LPC	C7-O6-P5-O5B
2	B	801	LPC	C7-C8-C9-OQ2
2	A	801	LPC	CJ-CK-CL-CM
2	B	801	LPC	CJ-CK-CL-CM
2	A	801	LPC	O8-C8-C9-OQ2
2	B	801	LPC	O8-C8-C9-OQ2
2	A	801	LPC	CB-CC-CD-CE
2	B	801	LPC	CB-CC-CD-CE
2	A	801	LPC	CD-CE-CF-CG
2	B	801	LPC	CD-CE-CF-CG
2	A	801	LPC	CB-CA-OQ2-C9
2	B	801	LPC	CB-CA-OQ2-C9
2	A	801	LPC	CG-CH-CI-CJ
2	B	801	LPC	CG-CH-CI-CJ
2	A	801	LPC	CI-CJ-CK-CL
2	B	801	LPC	CI-CJ-CK-CL
2	A	801	LPC	CH-CI-CJ-CK
2	B	801	LPC	CH-CI-CJ-CK
2	A	801	LPC	CE-CF-CG-CH

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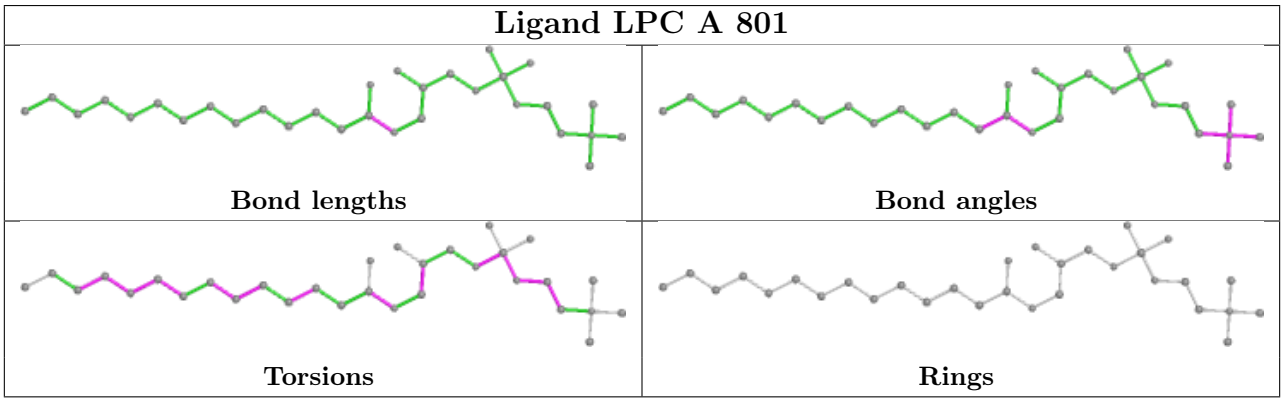
Mol	Chain	Res	Type	Atoms
2	B	801	LPC	CE-CF-CG-CH
2	A	801	LPC	OQ1-CA-OQ2-C9
2	B	801	LPC	OQ1-CA-OQ2-C9
2	A	801	LPC	C3-O4-P5-O5B
2	B	801	LPC	C3-O4-P5-O5B
2	A	801	LPC	N1-C2-C3-O4
2	B	801	LPC	N1-C2-C3-O4
2	A	801	LPC	C2-C3-O4-P5
2	B	801	LPC	C2-C3-O4-P5

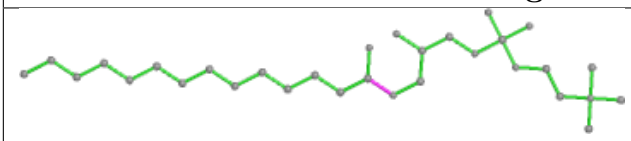
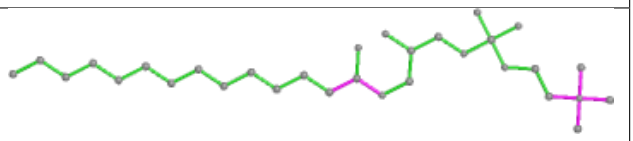
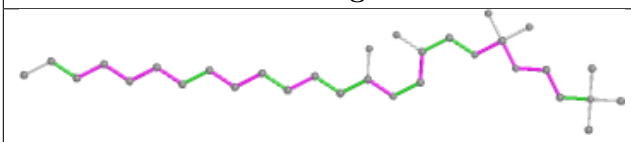
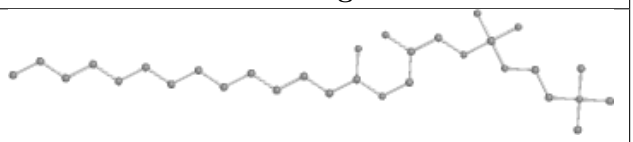
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	LPC	3	0
2	B	801	LPC	4	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 then 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 LPC B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

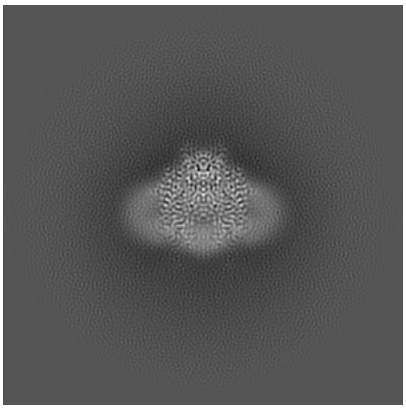
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34209. These allow visual inspection of the internal detail of the map and identification of artifacts.

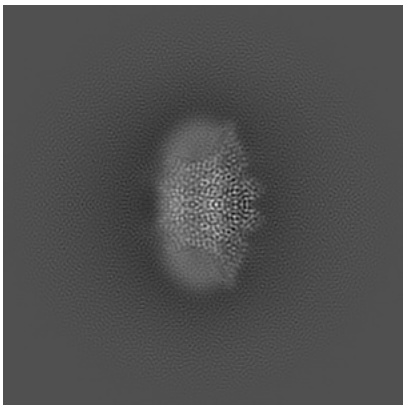
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

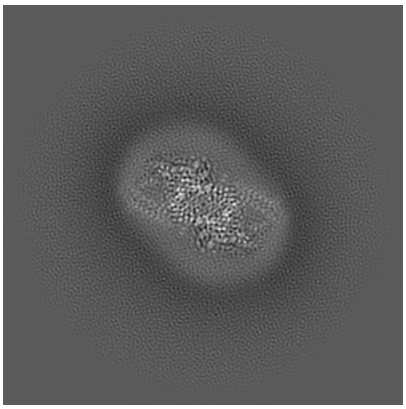
6.1.1 Primary map



X

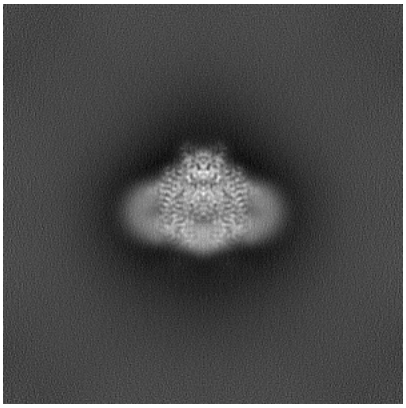


Y

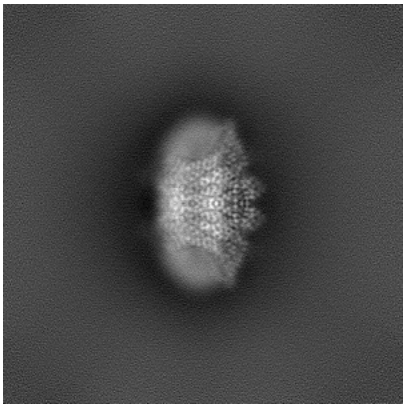


Z

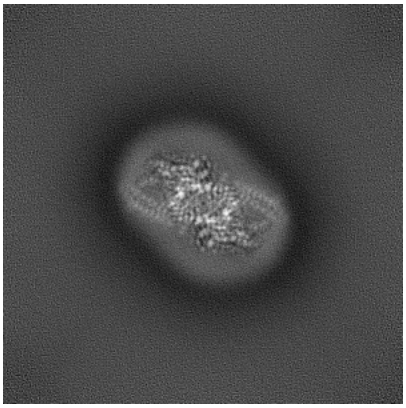
6.1.2 Raw map



X



Y

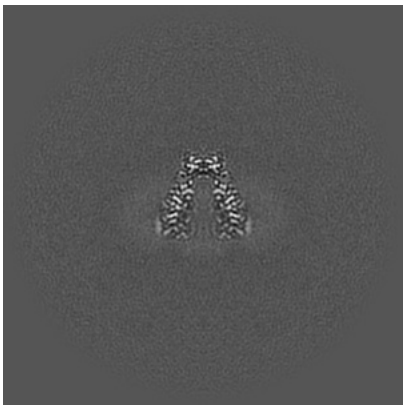


Z

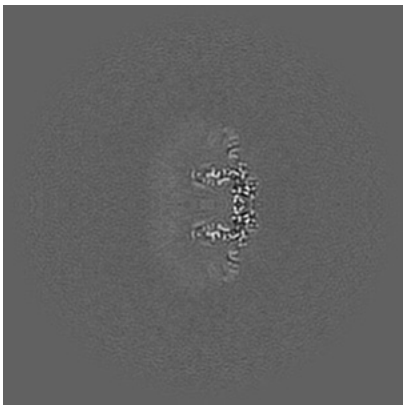
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

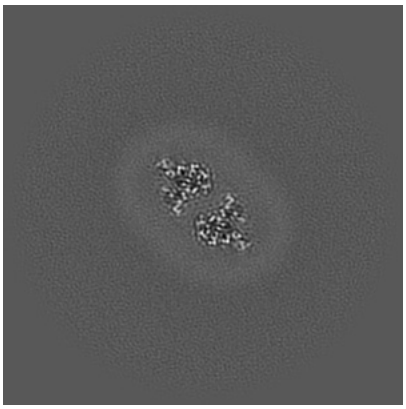
6.2.1 Primary map



X Index: 200

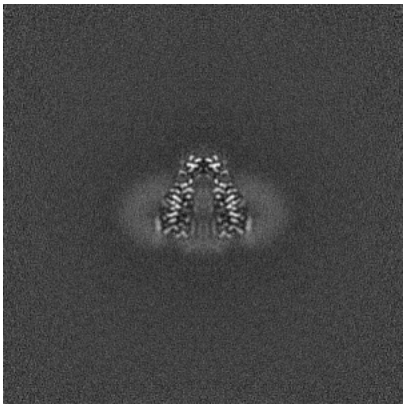


Y Index: 200

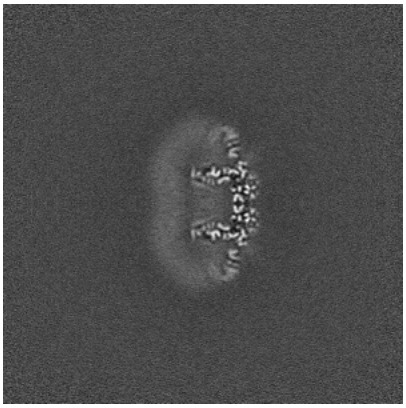


Z Index: 200

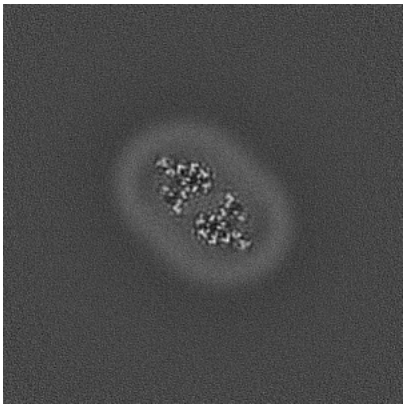
6.2.2 Raw map



X Index: 200



Y Index: 200

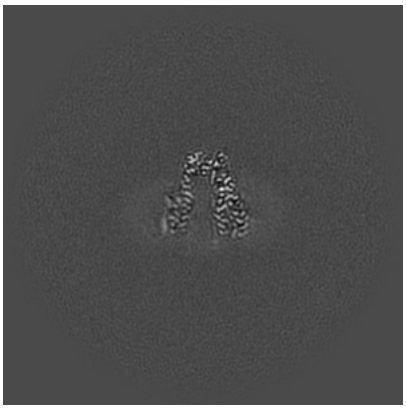


Z Index: 200

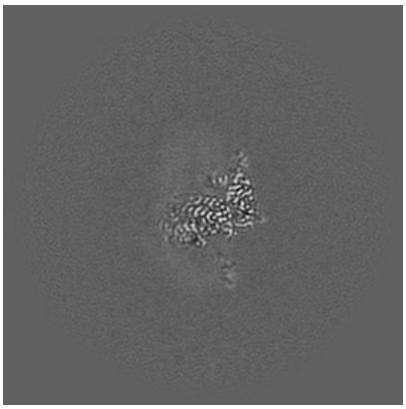
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

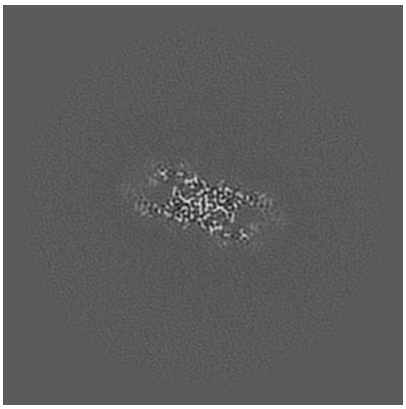
6.3.1 Primary map



X Index: 195

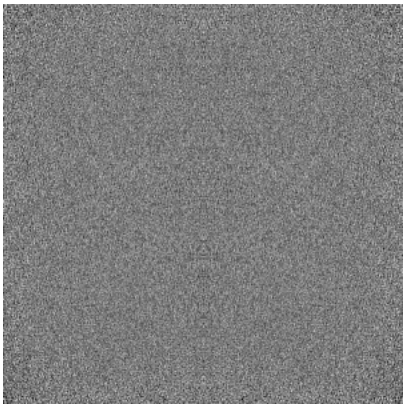


Y Index: 215

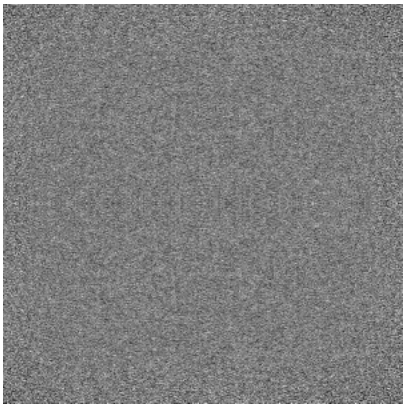


Z Index: 232

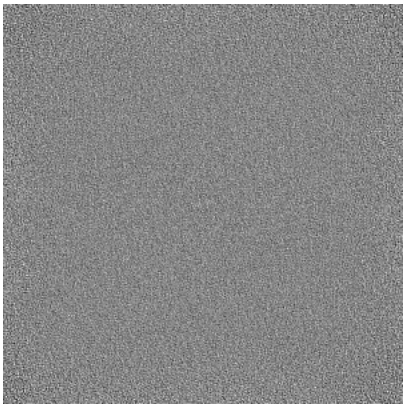
6.3.2 Raw map



X Index: 0



Y Index: 0

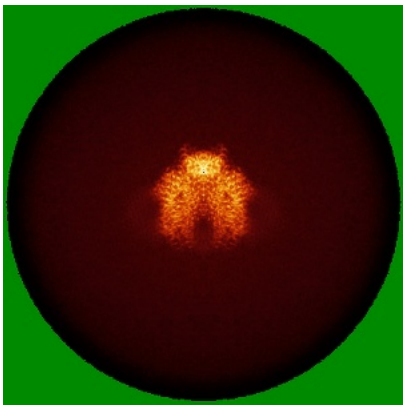


Z Index: 0

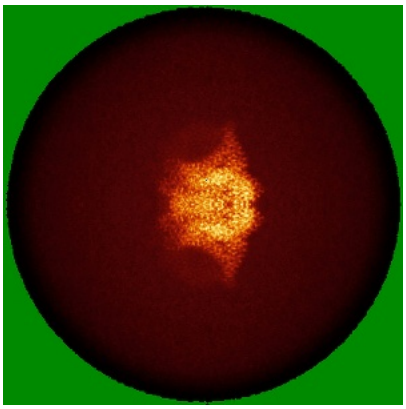
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

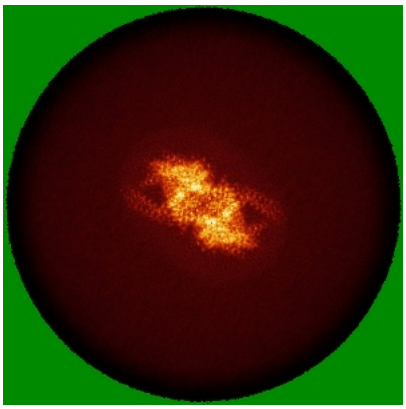
6.4.1 Primary map



X

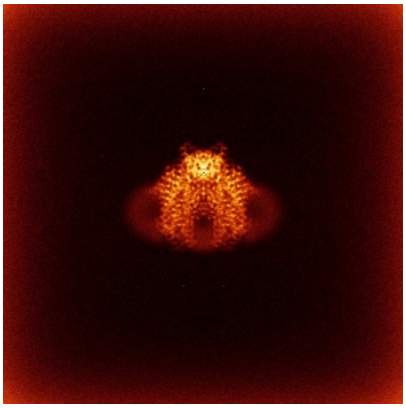


Y

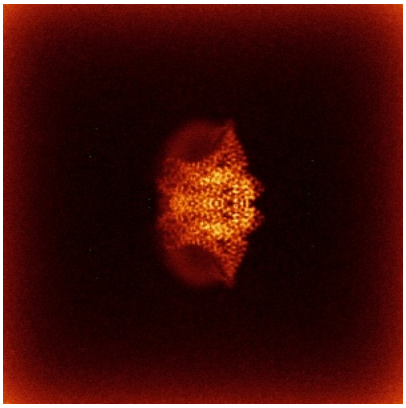


Z

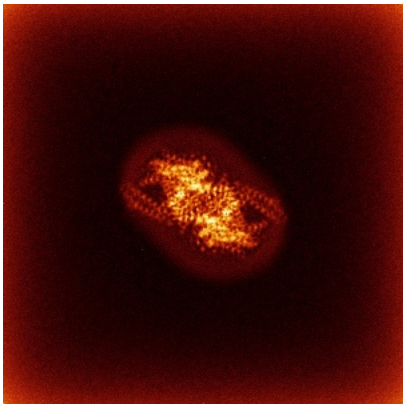
6.4.2 Raw map



X



Y

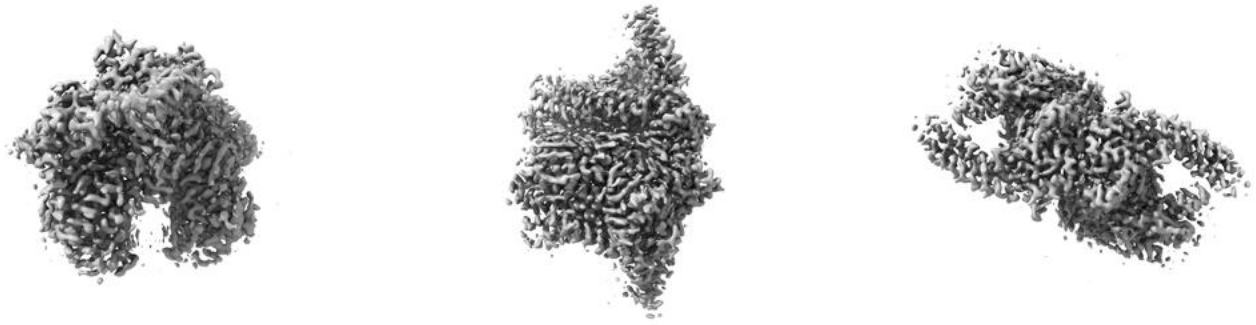


Z

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 0.4. 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.

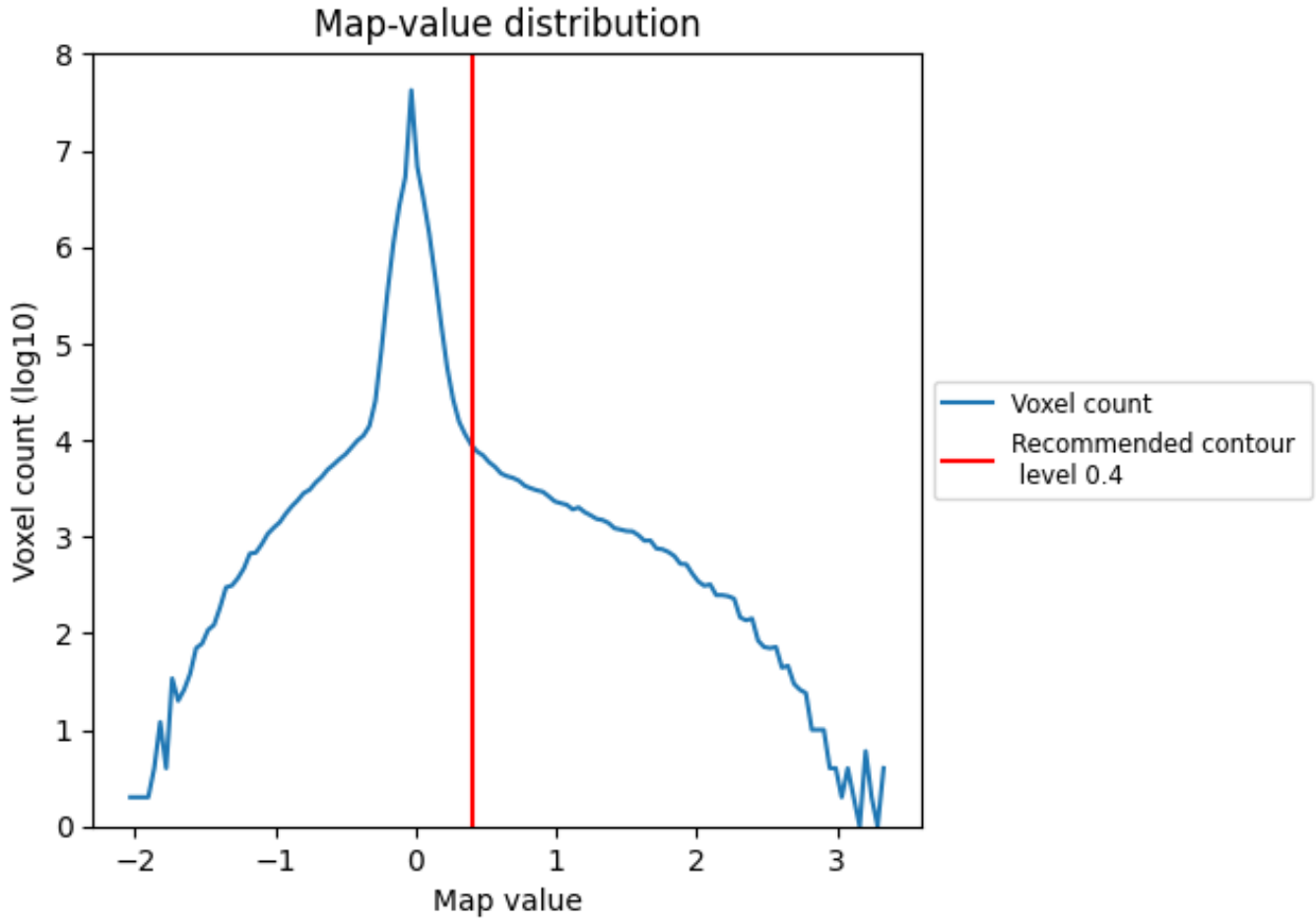
6.6 Mask visualisation (i)

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

7 Map analysis

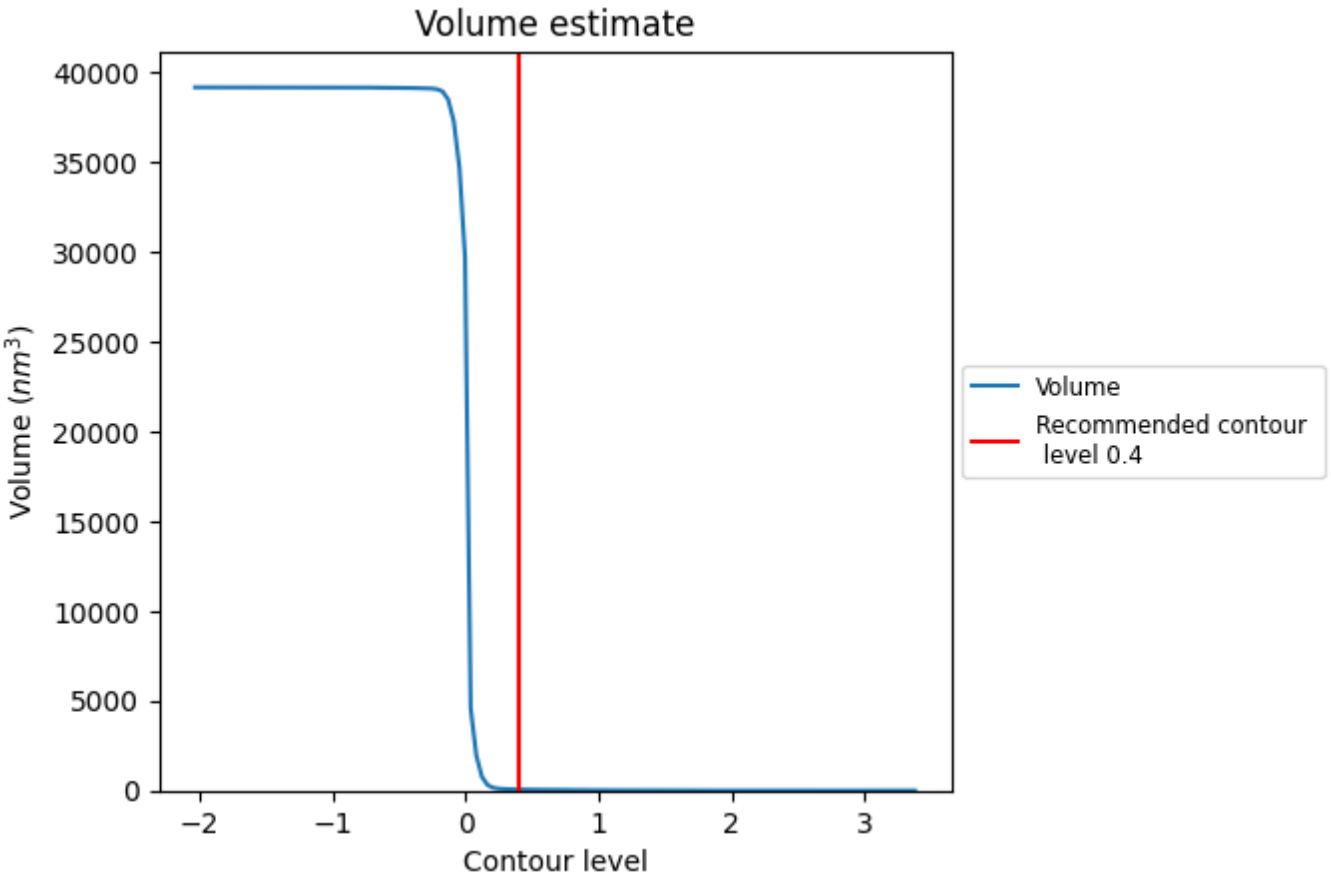
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

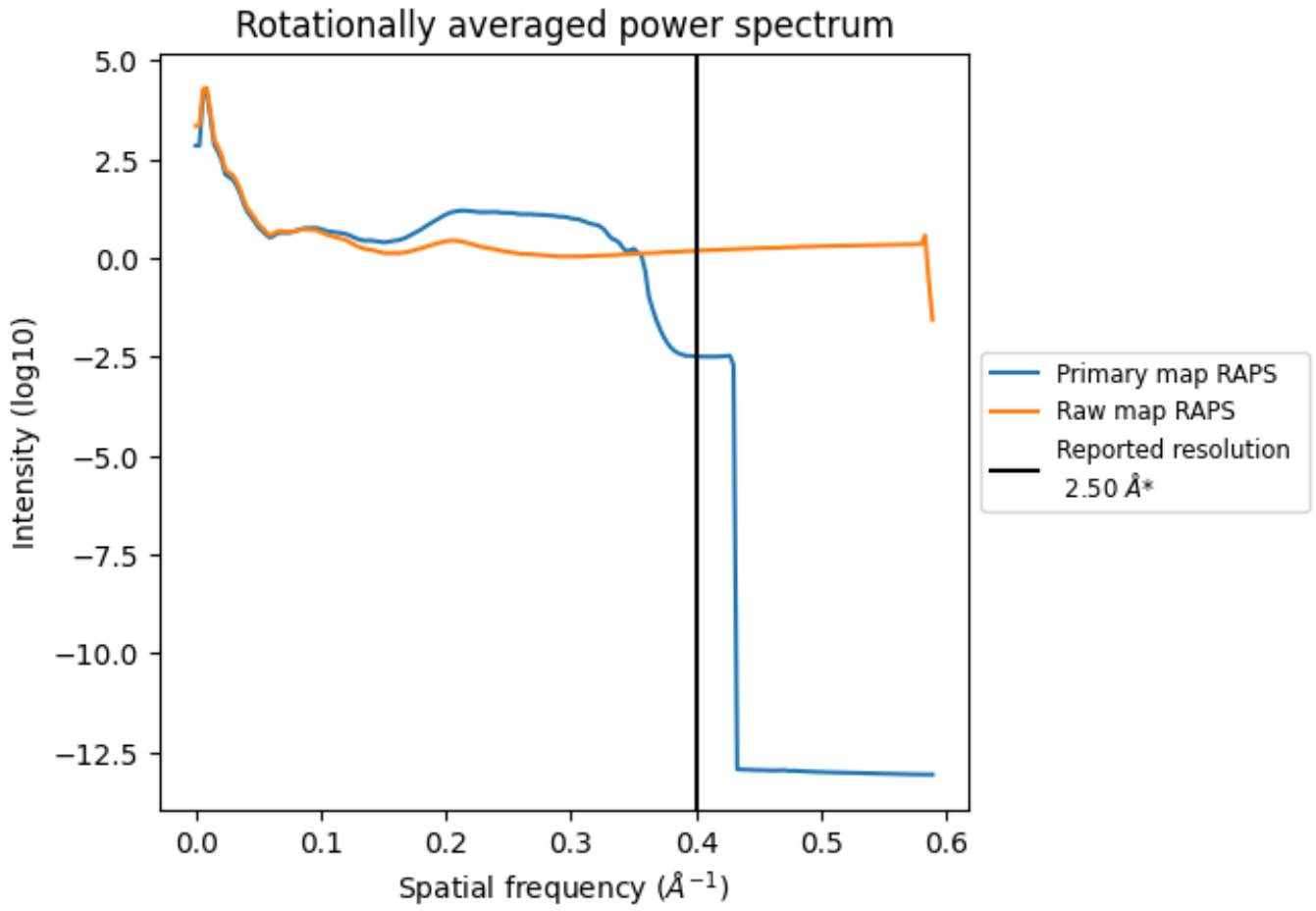
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 55 kDa.

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

7.3 Rotationally averaged power spectrum (i)

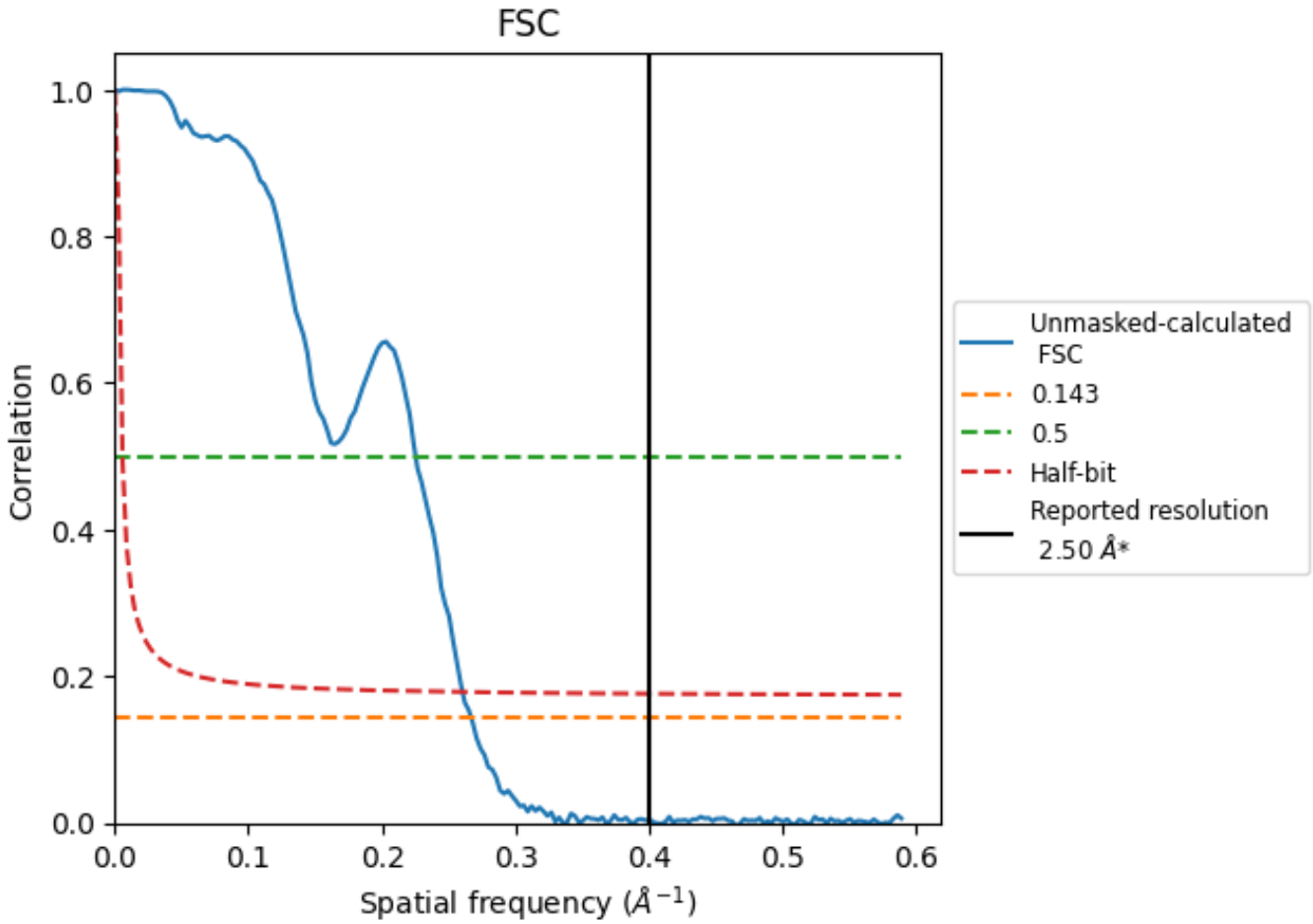


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

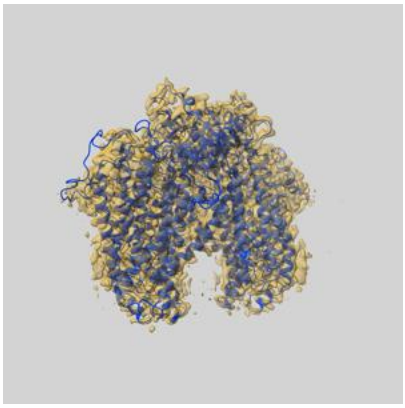
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	4.44	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.5 by more than 10 %

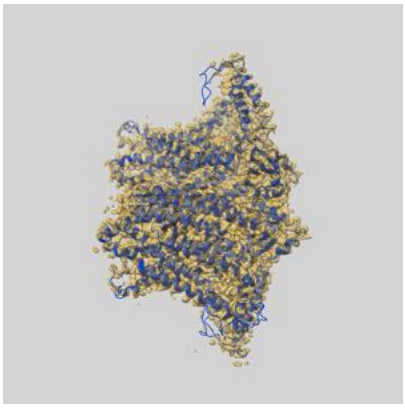
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34209 and PDB model 8GRN. Per-residue inclusion information can be found in section 3 on page 4.

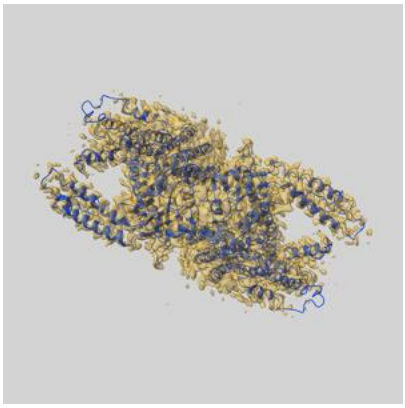
9.1 Map-model overlay



X



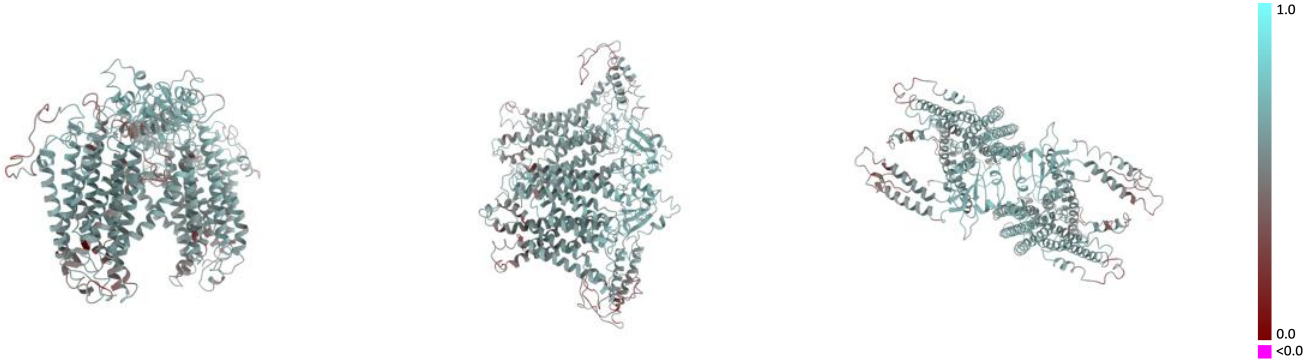
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

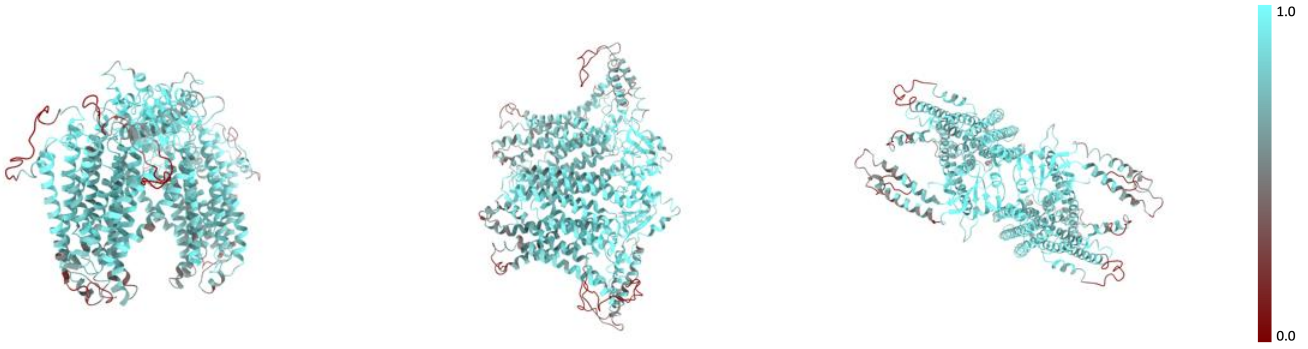
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

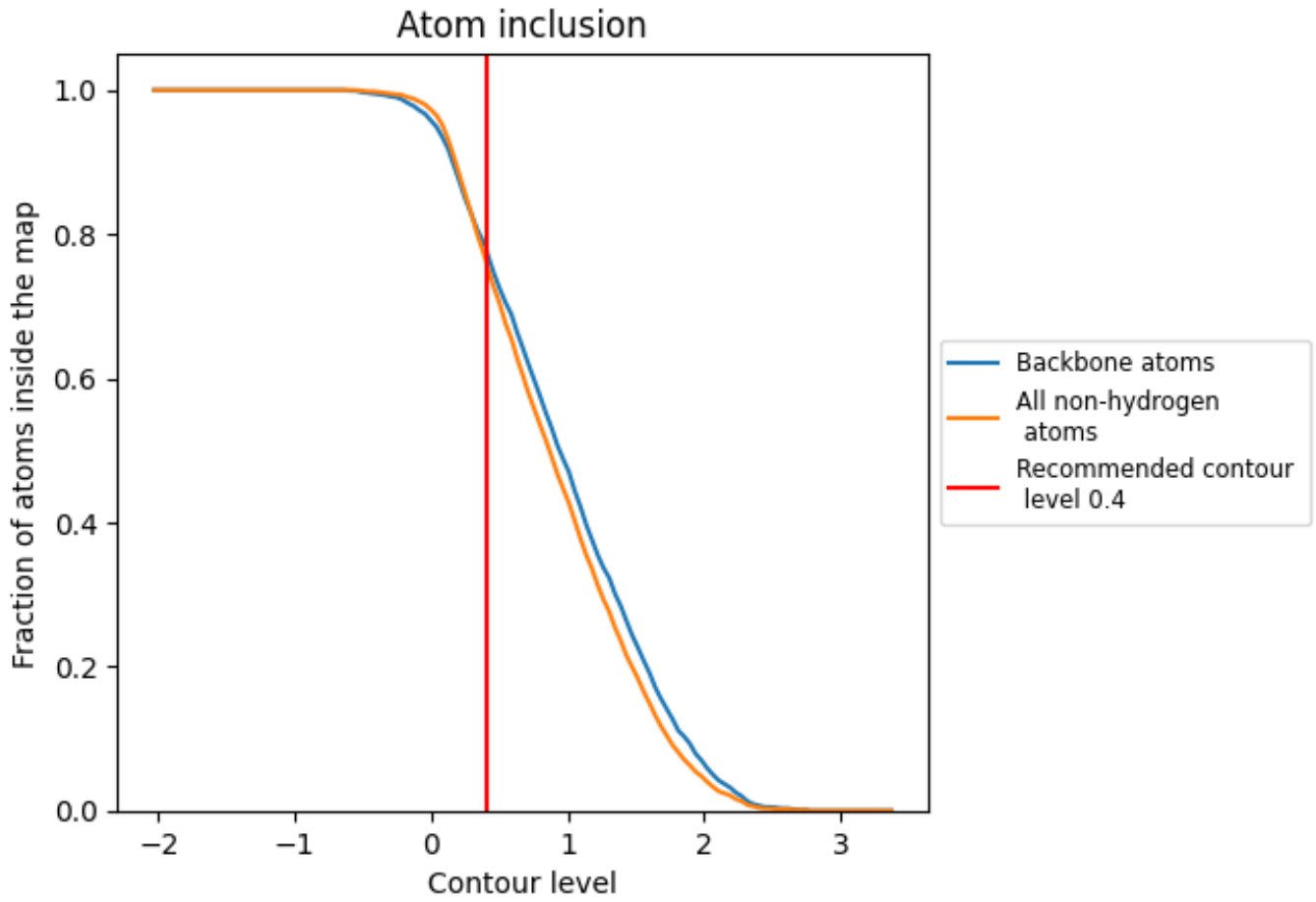
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5650
A	0.7630	0.5640
B	0.7640	0.5660