



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:10 PM UTC

PDB ID : 5U05 / pdb_00005u05
EMDB ID : EMD-8475
Title : Cryo-EM structure of the E. coli CTP synthase tetramer
Authors : Lynch, E.M.; Hicks, D.R.; Kollman, J.M.
Deposited on : 2016-11-22
Resolution : 7.90 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

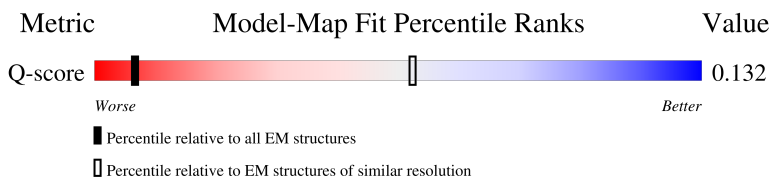
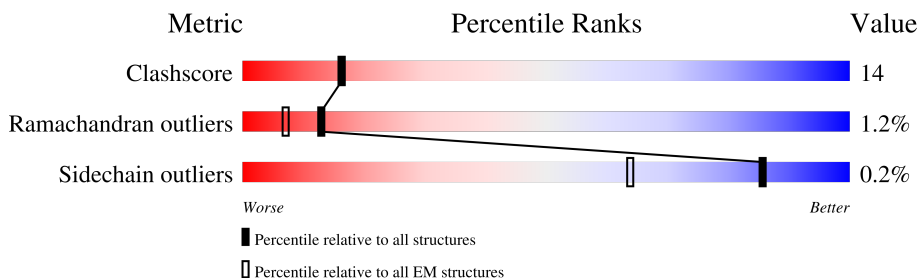
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	366 (7.40 - 8.40)

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	545	
1	B	545	
1	C	545	
1	D	545	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33336 atoms, of which 16692 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.

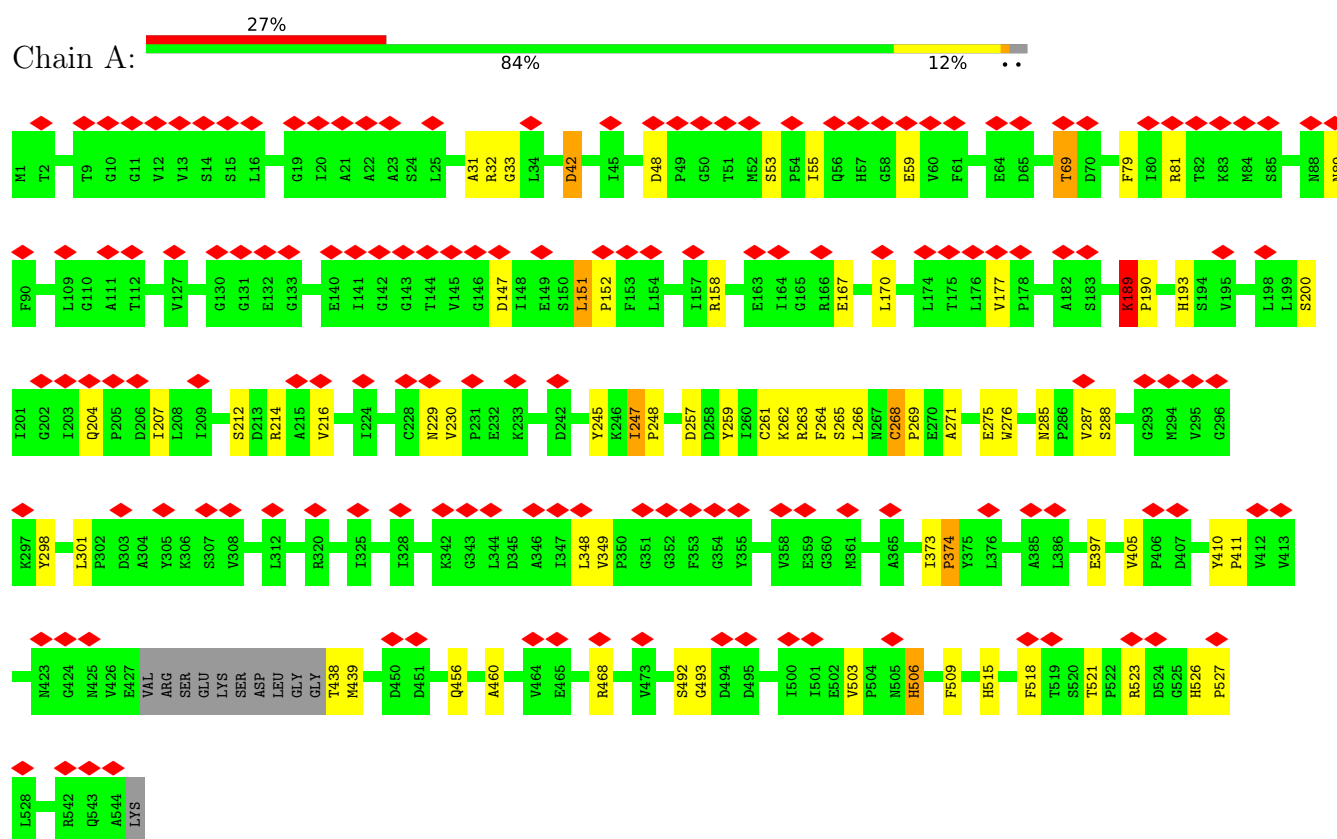
- Molecule 1 is a protein called CTP synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	534	Total	C	H	N	O	S	0	0
			8334	2629	4173	727	784	21		
1	B	534	Total	C	H	N	O	S	0	0
			8334	2629	4173	727	784	21		
1	C	534	Total	C	H	N	O	S	0	0
			8334	2629	4173	727	784	21		
1	D	534	Total	C	H	N	O	S	0	0
			8334	2629	4173	727	784	21		

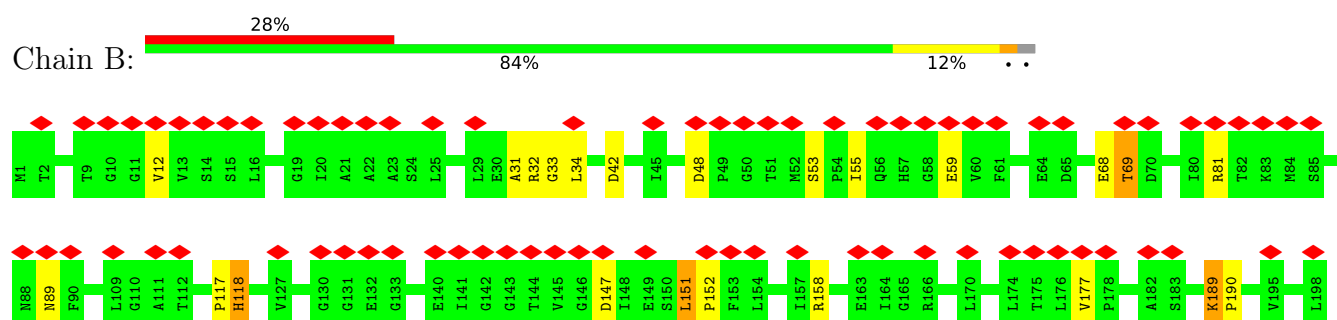
3 Residue-property plots

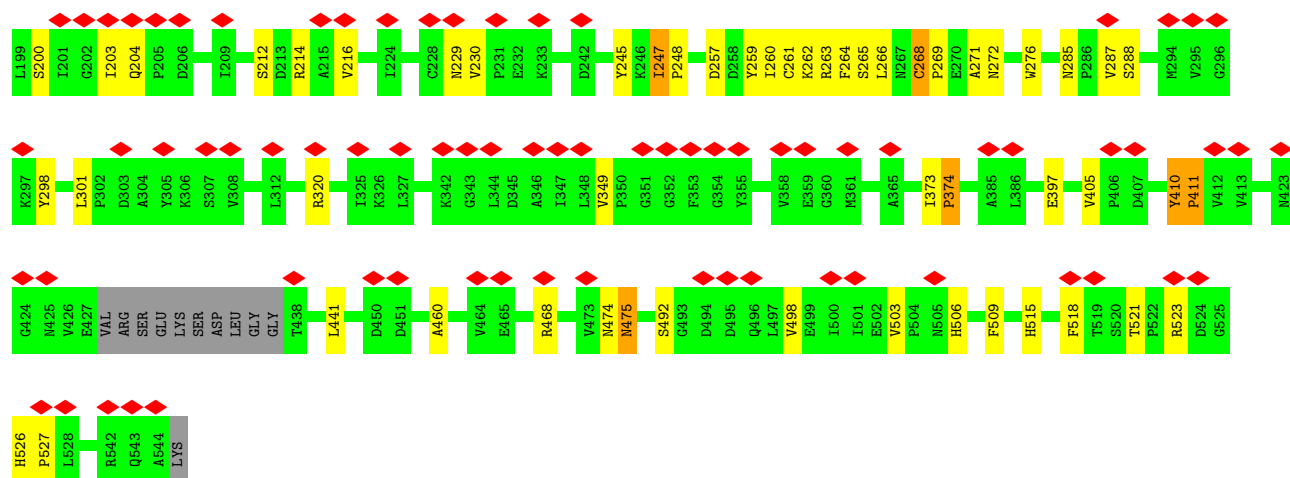
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CTP synthase

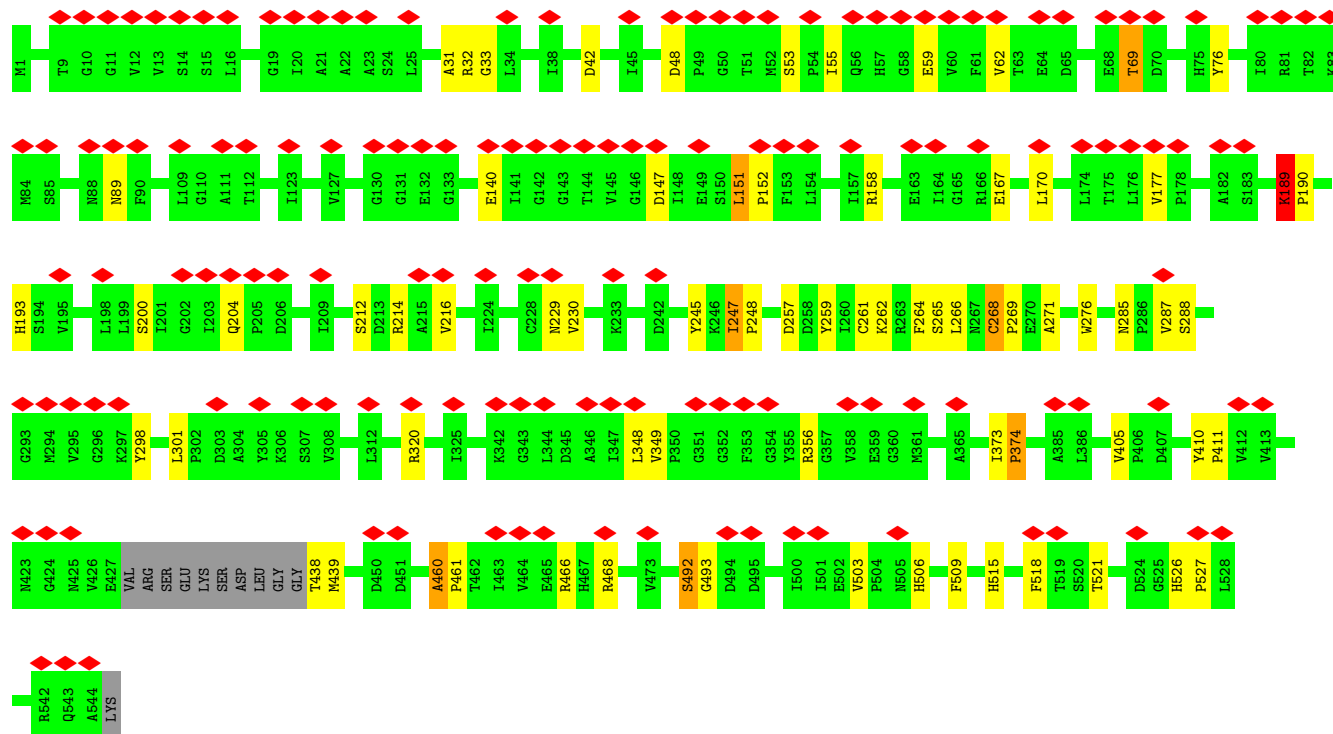
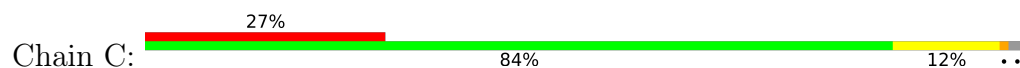


• Molecule 1: CTP synthase

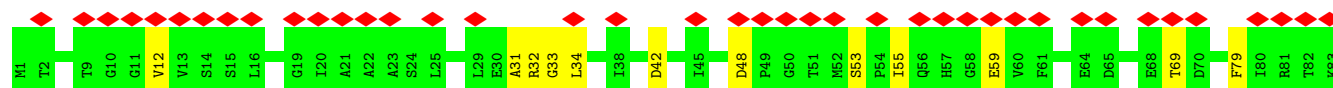
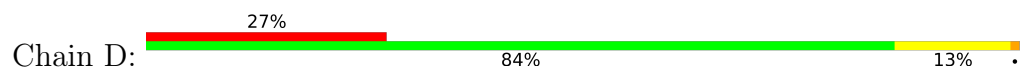


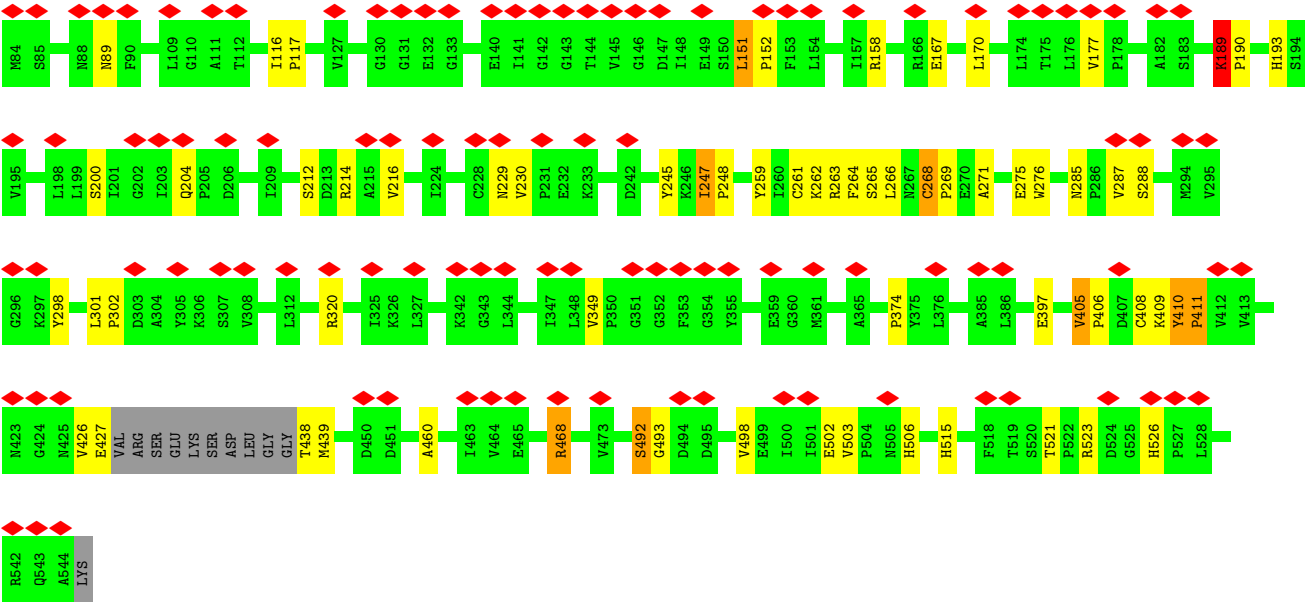


• Molecule 1: CTP synthase



• Molecule 1: CTP synthase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	6407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.222	Depositor
Minimum map value	-1.503	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.293	Depositor
Recommended contour level	1.3	Depositor
Map size ($\text{\AA}$)	221.76, 221.76, 221.76	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.26, 1.26, 1.26	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/4235	1.13	46/5734 (0.8%)
1	B	0.80	0/4235	1.13	44/5734 (0.8%)
1	C	0.81	0/4235	1.15	45/5734 (0.8%)
1	D	0.80	0/4235	1.13	48/5734 (0.8%)
All	All	0.80	0/16940	1.14	183/22936 (0.8%)

There are no bond length outliers.

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	VAL	CA-C-N	8.97	128.82	120.21
1	A	349	VAL	C-N-CA	8.97	128.82	120.21
1	C	349	VAL	CA-C-N	8.96	128.81	120.21
1	C	349	VAL	C-N-CA	8.96	128.81	120.21
1	B	48	ASP	CA-C-N	8.48	128.13	119.56
1	B	48	ASP	C-N-CA	8.48	128.13	119.56
1	A	48	ASP	CA-C-N	8.44	128.09	119.56
1	A	48	ASP	C-N-CA	8.44	128.09	119.56
1	C	48	ASP	CA-C-N	8.33	127.97	119.56
1	C	48	ASP	C-N-CA	8.33	127.97	119.56
1	D	526	HIS	CA-C-N	8.32	128.81	119.32
1	D	526	HIS	C-N-CA	8.32	128.81	119.32
1	D	460	ALA	CA-C-N	8.19	128.65	119.32
1	D	460	ALA	C-N-CA	8.19	128.65	119.32
1	B	460	ALA	CA-C-N	8.16	128.62	119.32
1	B	460	ALA	C-N-CA	8.16	128.62	119.32
1	D	48	ASP	CA-C-N	8.15	127.80	119.56
1	D	48	ASP	C-N-CA	8.15	127.80	119.56
1	A	42	ASP	CA-C-N	8.09	127.75	119.82
1	A	42	ASP	C-N-CA	8.09	127.75	119.82
1	A	460	ALA	CA-C-N	8.09	128.54	119.32
1	A	460	ALA	C-N-CA	8.09	128.54	119.32
1	C	460	ALA	CA-C-N	7.98	128.41	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	460	ALA	C-N-CA	7.98	128.41	119.32
1	D	268	CYS	CA-C-N	7.90	127.92	119.78
1	D	268	CYS	C-N-CA	7.90	127.92	119.78
1	B	301	LEU	CA-C-N	7.89	128.62	119.47
1	B	301	LEU	C-N-CA	7.89	128.62	119.47
1	C	53	SER	CA-C-N	7.89	127.81	119.05
1	C	53	SER	C-N-CA	7.89	127.81	119.05
1	A	53	SER	CA-C-N	7.87	127.78	119.05
1	A	53	SER	C-N-CA	7.87	127.78	119.05
1	D	349	VAL	CA-C-N	7.87	129.40	120.98
1	D	349	VAL	C-N-CA	7.87	129.40	120.98
1	C	301	LEU	CA-C-N	7.85	128.58	119.47
1	C	301	LEU	C-N-CA	7.85	128.58	119.47
1	B	405	VAL	CA-C-N	7.79	128.19	119.32
1	B	405	VAL	C-N-CA	7.79	128.19	119.32
1	C	268	CYS	CA-C-N	7.78	127.79	119.78
1	C	268	CYS	C-N-CA	7.78	127.79	119.78
1	B	349	VAL	CA-C-N	7.72	129.24	120.98
1	B	349	VAL	C-N-CA	7.72	129.24	120.98
1	D	53	SER	CA-C-N	7.70	127.59	119.05
1	D	53	SER	C-N-CA	7.70	127.59	119.05
1	B	268	CYS	CA-C-N	7.68	127.69	119.78
1	B	268	CYS	C-N-CA	7.68	127.69	119.78
1	A	268	CYS	CA-C-N	7.64	127.65	119.78
1	A	268	CYS	C-N-CA	7.64	127.65	119.78
1	A	405	VAL	CA-C-N	7.63	128.02	119.32
1	A	405	VAL	C-N-CA	7.63	128.02	119.32
1	D	42	ASP	CA-C-N	7.51	129.22	119.84
1	D	42	ASP	C-N-CA	7.51	129.22	119.84
1	B	204	GLN	CA-C-N	7.47	127.46	119.76
1	B	204	GLN	C-N-CA	7.47	127.46	119.76
1	C	515	HIS	CA-C-N	7.40	127.11	119.56
1	C	515	HIS	C-N-CA	7.40	127.11	119.56
1	A	515	HIS	CA-C-N	7.33	127.04	119.56
1	A	515	HIS	C-N-CA	7.33	127.04	119.56
1	C	204	GLN	CA-C-N	7.31	127.29	119.76
1	C	204	GLN	C-N-CA	7.31	127.29	119.76
1	D	216	VAL	CA-C-N	7.29	127.27	119.76
1	D	216	VAL	C-N-CA	7.29	127.27	119.76
1	A	204	GLN	CA-C-N	7.28	127.26	119.76
1	A	204	GLN	C-N-CA	7.28	127.26	119.76
1	C	503	VAL	CA-C-N	7.28	128.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	VAL	C-N-CA	7.28	128.94	119.84
1	D	204	GLN	CA-C-N	7.22	127.20	119.76
1	D	204	GLN	C-N-CA	7.22	127.20	119.76
1	B	503	VAL	CA-C-N	7.21	128.85	119.84
1	B	503	VAL	C-N-CA	7.21	128.85	119.84
1	D	515	HIS	CA-C-N	7.21	126.91	119.56
1	D	515	HIS	C-N-CA	7.21	126.91	119.56
1	C	285	ASN	CA-C-N	7.20	127.12	119.85
1	C	285	ASN	C-N-CA	7.20	127.12	119.85
1	B	216	VAL	CA-C-N	7.16	127.14	119.76
1	B	216	VAL	C-N-CA	7.16	127.14	119.76
1	D	177	VAL	CA-C-N	7.15	126.91	119.76
1	D	177	VAL	C-N-CA	7.15	126.91	119.76
1	D	503	VAL	CA-C-N	7.14	128.76	119.84
1	D	503	VAL	C-N-CA	7.14	128.76	119.84
1	D	301	LEU	CA-C-N	7.13	128.76	119.84
1	D	301	LEU	C-N-CA	7.13	128.76	119.84
1	C	42	ASP	CA-C-N	7.13	128.75	119.84
1	C	42	ASP	C-N-CA	7.13	128.75	119.84
1	A	503	VAL	CA-C-N	7.13	128.75	119.84
1	A	503	VAL	C-N-CA	7.13	128.75	119.84
1	C	216	VAL	CA-C-N	7.06	127.03	119.76
1	C	216	VAL	C-N-CA	7.06	127.03	119.76
1	C	405	VAL	CA-C-N	7.03	127.33	119.32
1	C	405	VAL	C-N-CA	7.03	127.33	119.32
1	B	515	HIS	CA-C-N	7.01	126.71	119.56
1	B	515	HIS	C-N-CA	7.01	126.71	119.56
1	B	42	ASP	CA-C-N	7.01	128.60	119.84
1	B	42	ASP	C-N-CA	7.01	128.60	119.84
1	B	53	SER	CA-C-N	7.00	126.71	119.64
1	B	53	SER	C-N-CA	7.00	126.71	119.64
1	A	216	VAL	CA-C-N	6.99	126.96	119.76
1	A	216	VAL	C-N-CA	6.99	126.96	119.76
1	B	177	VAL	CA-C-N	6.92	126.84	119.85
1	B	177	VAL	C-N-CA	6.92	126.84	119.85
1	C	506	HIS	CA-C-N	6.85	127.13	119.32
1	C	506	HIS	C-N-CA	6.85	127.13	119.32
1	A	177	VAL	CA-C-N	6.81	126.73	119.85
1	A	177	VAL	C-N-CA	6.81	126.73	119.85
1	C	177	VAL	CA-C-N	6.81	126.73	119.85
1	C	177	VAL	C-N-CA	6.81	126.73	119.85
1	A	521	THR	CA-C-N	6.80	126.42	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	THR	C-N-CA	6.80	126.42	119.56
1	A	301	LEU	CA-C-N	6.72	128.24	119.84
1	A	301	LEU	C-N-CA	6.72	128.24	119.84
1	B	506	HIS	CA-C-N	6.70	126.95	119.32
1	B	506	HIS	C-N-CA	6.70	126.95	119.32
1	B	526	HIS	CA-C-N	6.46	127.92	119.84
1	B	526	HIS	C-N-CA	6.46	127.92	119.84
1	B	151	LEU	CA-C-N	6.46	126.22	119.05
1	B	151	LEU	C-N-CA	6.46	126.22	119.05
1	B	285	ASN	CA-C-N	6.41	126.32	119.85
1	B	285	ASN	C-N-CA	6.41	126.32	119.85
1	A	285	ASN	CA-C-N	6.39	126.30	119.85
1	A	285	ASN	C-N-CA	6.39	126.30	119.85
1	D	506	HIS	CA-C-N	6.38	126.60	119.32
1	D	506	HIS	C-N-CA	6.38	126.60	119.32
1	A	151	LEU	CA-C-N	6.37	126.12	119.05
1	A	151	LEU	C-N-CA	6.37	126.12	119.05
1	C	526	HIS	CA-C-N	6.34	127.76	119.84
1	C	526	HIS	C-N-CA	6.34	127.76	119.84
1	A	506	HIS	CA-C-N	6.32	126.52	119.32
1	A	506	HIS	C-N-CA	6.32	126.52	119.32
1	D	151	LEU	CA-C-N	6.26	126.00	119.05
1	D	151	LEU	C-N-CA	6.26	126.00	119.05
1	A	526	HIS	CA-C-N	6.15	127.53	119.84
1	A	526	HIS	C-N-CA	6.15	127.53	119.84
1	D	405	VAL	CA-C-N	6.15	127.52	119.84
1	D	405	VAL	C-N-CA	6.15	127.52	119.84
1	D	285	ASN	CA-C-N	6.14	126.05	119.85
1	D	285	ASN	C-N-CA	6.14	126.05	119.85
1	D	189	LYS	CA-C-N	6.13	126.30	119.32
1	D	189	LYS	C-N-CA	6.13	126.30	119.32
1	C	521	THR	CA-C-N	6.12	125.74	119.56
1	C	521	THR	C-N-CA	6.12	125.74	119.56
1	C	230	VAL	CA-C-N	6.11	126.05	119.76
1	C	230	VAL	C-N-CA	6.11	126.05	119.76
1	C	151	LEU	CA-C-N	6.10	126.27	119.32
1	C	151	LEU	C-N-CA	6.10	126.27	119.32
1	C	189	LYS	CA-C-N	6.04	126.21	119.32
1	C	189	LYS	C-N-CA	6.04	126.21	119.32
1	A	189	LYS	CA-C-N	6.02	126.19	119.32
1	A	189	LYS	C-N-CA	6.02	126.19	119.32
1	D	230	VAL	CA-C-N	6.01	125.95	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	VAL	C-N-CA	6.01	125.95	119.76
1	D	521	THR	CA-C-N	5.93	125.56	119.56
1	D	521	THR	C-N-CA	5.93	125.56	119.56
1	B	230	VAL	CA-C-N	5.93	125.87	119.76
1	B	230	VAL	C-N-CA	5.93	125.87	119.76
1	A	230	VAL	CA-C-N	5.93	125.86	119.76
1	A	230	VAL	C-N-CA	5.93	125.86	119.76
1	D	247	ILE	CA-C-N	5.92	126.07	119.32
1	D	247	ILE	C-N-CA	5.92	126.07	119.32
1	B	521	THR	CA-C-N	5.92	125.54	119.56
1	B	521	THR	C-N-CA	5.92	125.54	119.56
1	C	247	ILE	CA-C-N	5.88	126.02	119.32
1	C	247	ILE	C-N-CA	5.88	126.02	119.32
1	A	247	ILE	CA-C-N	5.87	126.01	119.32
1	A	247	ILE	C-N-CA	5.87	126.01	119.32
1	B	189	LYS	CA-C-N	5.84	125.98	119.32
1	B	189	LYS	C-N-CA	5.84	125.98	119.32
1	B	247	ILE	CA-C-N	5.84	125.98	119.32
1	B	247	ILE	C-N-CA	5.84	125.98	119.32
1	D	79	PHE	CA-CB-CG	-5.64	108.16	113.80
1	C	69	THR	N-CA-C	5.62	115.53	108.45
1	A	410	TYR	CA-C-N	5.59	126.83	119.84
1	A	410	TYR	C-N-CA	5.59	126.83	119.84
1	B	69	THR	N-CA-C	5.50	115.38	108.45
1	D	410	TYR	CA-C-N	5.39	126.57	119.84
1	D	410	TYR	C-N-CA	5.39	126.57	119.84
1	A	69	THR	N-CA-C	5.38	115.23	108.45
1	C	410	TYR	CA-C-N	5.37	126.56	119.84
1	C	410	TYR	C-N-CA	5.37	126.56	119.84
1	B	203	ILE	N-CA-C	5.19	115.33	107.75
1	D	502	GLU	CA-C-N	-5.14	119.10	122.60
1	D	502	GLU	C-N-CA	-5.14	119.10	122.60
1	D	503	VAL	N-CA-C	5.13	112.23	107.56
1	A	503	VAL	N-CA-C	5.00	112.11	107.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4161	4173	4170	122	0
1	B	4161	4173	4166	121	0
1	C	4161	4173	4171	116	0
1	D	4161	4173	4170	125	0
All	All	16644	16692	16677	472	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 14.

All (472) 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:C:261:CYS:SG	1:C:266:LEU:HB2	1.29	1.67
1:D:263:ARG:HB2	1:D:264:PHE:CD2	1.09	1.62
1:D:245:TYR:HB3	1:D:276:TRP:CD1	1.32	1.62
1:A:263:ARG:HB2	1:A:264:PHE:CD2	1.08	1.61
1:B:263:ARG:HB2	1:B:264:PHE:CD2	1.14	1.60
1:A:263:ARG:CB	1:A:264:PHE:HD2	1.12	1.59
1:C:170:LEU:CD1	1:C:264:PHE:CZ	1.83	1.57
1:A:170:LEU:HD11	1:A:264:PHE:CE2	1.36	1.56
1:C:170:LEU:HD11	1:C:264:PHE:CE2	1.38	1.55
1:D:170:LEU:HD11	1:D:264:PHE:CE2	1.37	1.54
1:C:261:CYS:CB	1:C:266:LEU:HB2	1.35	1.54
1:B:245:TYR:CB	1:B:276:TRP:CD1	1.90	1.54
1:A:32:ARG:NE	1:A:268:CYS:CB	1.70	1.51
1:A:170:LEU:CD1	1:A:264:PHE:CZ	1.94	1.50
1:A:170:LEU:HD13	1:A:264:PHE:CZ	1.45	1.47
1:D:263:ARG:N	1:D:264:PHE:CA	1.68	1.47
1:D:32:ARG:C	1:D:269:PRO:HD2	1.10	1.46
1:B:32:ARG:NE	1:B:268:CYS:CB	1.80	1.45
1:D:263:ARG:CB	1:D:264:PHE:HD2	1.26	1.45
1:B:245:TYR:HB3	1:B:276:TRP:CD1	0.93	1.44
1:C:170:LEU:HD13	1:C:264:PHE:CZ	1.46	1.44
1:D:170:LEU:CD1	1:D:264:PHE:CZ	2.01	1.43
1:C:261:CYS:SG	1:C:266:LEU:CB	2.07	1.43
1:C:262:LYS:CA	1:C:265:SER:H	1.12	1.41
1:D:263:ARG:N	1:D:264:PHE:HA	1.09	1.41
1:B:32:ARG:NE	1:B:268:CYS:HB2	1.31	1.41
1:D:170:LEU:CD1	1:D:264:PHE:CE2	2.02	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:CD1	1:A:264:PHE:CE2	1.98	1.41
1:A:32:ARG:NE	1:A:268:CYS:HB2	1.23	1.39
1:D:170:LEU:HD13	1:D:264:PHE:CZ	1.54	1.39
1:B:263:ARG:CB	1:B:264:PHE:CD2	2.08	1.36
1:B:263:ARG:CB	1:B:264:PHE:HD2	1.38	1.34
1:C:245:TYR:HB3	1:C:276:TRP:CD1	1.61	1.34
1:A:32:ARG:CZ	1:A:268:CYS:HB2	1.56	1.33
1:D:32:ARG:C	1:D:269:PRO:CD	1.74	1.33
1:D:32:ARG:O	1:D:269:PRO:CG	1.74	1.33
1:D:33:GLY:CA	1:D:269:PRO:HG2	1.59	1.32
1:D:263:ARG:CB	1:D:264:PHE:CD2	2.02	1.32
1:B:32:ARG:HB3	1:B:268:CYS:CB	1.62	1.29
1:C:32:ARG:NE	1:C:268:CYS:CB	1.94	1.29
1:B:55:ILE:HD13	1:B:298:TYR:CD2	1.68	1.28
1:B:245:TYR:HB3	1:B:276:TRP:NE1	1.49	1.27
1:A:55:ILE:HB	1:A:298:TYR:CE2	1.68	1.26
1:B:32:ARG:CB	1:B:268:CYS:HB3	1.66	1.26
1:C:261:CYS:HA	1:C:266:LEU:CG	1.65	1.24
1:A:32:ARG:CD	1:A:268:CYS:HB3	1.68	1.24
1:D:245:TYR:CB	1:D:276:TRP:CD1	2.21	1.24
1:C:261:CYS:CB	1:C:266:LEU:CB	2.16	1.23
1:D:263:ARG:CA	1:D:264:PHE:HA	1.69	1.23
1:A:275:GLU:OE2	1:A:523:ARG:NH1	1.72	1.22
1:D:263:ARG:N	1:D:264:PHE:N	1.84	1.22
1:A:32:ARG:CG	1:A:268:CYS:HB3	1.68	1.22
1:A:262:LYS:N	1:A:264:PHE:N	1.65	1.22
1:B:262:LYS:N	1:B:264:PHE:N	1.66	1.18
1:D:32:ARG:HA	1:D:269:PRO:O	1.42	1.18
1:A:32:ARG:CB	1:A:268:CYS:HB3	1.73	1.18
1:A:32:ARG:HB3	1:A:268:CYS:CB	1.73	1.18
1:A:263:ARG:CB	1:A:264:PHE:CD2	1.96	1.17
1:C:55:ILE:HB	1:C:298:TYR:CE2	1.80	1.17
1:D:32:ARG:HB3	1:D:268:CYS:CB	1.74	1.17
1:D:55:ILE:HD13	1:D:298:TYR:CD2	1.79	1.16
1:C:170:LEU:HD11	1:C:264:PHE:CZ	1.58	1.16
1:D:55:ILE:HB	1:D:298:TYR:CE2	1.81	1.16
1:A:261:CYS:CB	1:A:266:LEU:H	1.59	1.16
1:C:262:LYS:CA	1:C:265:SER:N	1.89	1.16
1:D:261:CYS:CB	1:D:266:LEU:H	1.58	1.16
1:D:55:ILE:HD13	1:D:298:TYR:HD2	1.00	1.15
1:B:32:ARG:CZ	1:B:268:CYS:HB2	1.74	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:CYS:HB3	1:B:266:LEU:H	1.07	1.15
1:B:32:ARG:CG	1:B:268:CYS:HB3	1.74	1.15
1:C:32:ARG:NE	1:C:268:CYS:HB2	1.60	1.14
1:D:261:CYS:HA	1:D:266:LEU:CG	1.74	1.14
1:B:32:ARG:CD	1:B:268:CYS:HB3	1.76	1.14
1:D:32:ARG:C	1:D:269:PRO:CG	2.17	1.14
1:A:55:ILE:HD13	1:A:298:TYR:CD2	1.82	1.14
1:C:32:ARG:NE	1:C:268:CYS:HB3	1.56	1.13
1:C:170:LEU:CD1	1:C:264:PHE:CE2	2.11	1.13
1:C:32:ARG:HB3	1:C:268:CYS:HB3	1.31	1.12
1:B:55:ILE:HB	1:B:298:TYR:CE2	1.82	1.12
1:C:262:LYS:C	1:C:265:SER:N	2.06	1.12
1:A:261:CYS:HB3	1:A:266:LEU:N	1.48	1.11
1:A:261:CYS:HA	1:A:266:LEU:CG	1.70	1.11
1:D:261:CYS:HB3	1:D:266:LEU:N	1.37	1.10
1:B:32:ARG:NE	1:B:268:CYS:HB3	1.59	1.10
1:D:32:ARG:O	1:D:269:PRO:HD3	1.34	1.10
1:A:33:GLY:HA3	1:A:269:PRO:HG2	1.26	1.09
1:D:32:ARG:HB3	1:D:268:CYS:HB3	1.10	1.09
1:C:32:ARG:CZ	1:C:268:CYS:HB2	1.83	1.09
1:D:32:ARG:O	1:D:269:PRO:N	1.83	1.09
1:D:32:ARG:CB	1:D:268:CYS:HB3	1.58	1.09
1:D:245:TYR:CB	1:D:276:TRP:HD1	1.63	1.09
1:D:261:CYS:CA	1:D:266:LEU:HG	1.80	1.08
1:A:55:ILE:HD13	1:A:298:TYR:HD2	0.95	1.08
1:A:259:TYR:O	1:A:264:PHE:N	1.86	1.07
1:A:275:GLU:CD	1:A:523:ARG:HH11	1.62	1.07
1:D:33:GLY:HA3	1:D:269:PRO:CG	1.83	1.07
1:B:261:CYS:HA	1:B:266:LEU:HG	1.09	1.06
1:B:261:CYS:CB	1:B:266:LEU:H	1.67	1.06
1:C:261:CYS:CA	1:C:266:LEU:HG	1.86	1.05
1:B:245:TYR:CB	1:B:276:TRP:HD1	1.46	1.04
1:C:33:GLY:HA3	1:C:269:PRO:HG2	1.39	1.04
1:C:245:TYR:HB3	1:C:276:TRP:HD1	0.90	1.03
1:A:170:LEU:HD11	1:A:264:PHE:CD2	1.92	1.03
1:D:55:ILE:HB	1:D:298:TYR:CD2	1.92	1.03
1:B:32:ARG:HE	1:B:268:CYS:CB	1.53	1.03
1:B:261:CYS:HA	1:B:266:LEU:CG	1.85	1.03
1:C:32:ARG:HE	1:C:268:CYS:CB	1.59	1.03
1:A:261:CYS:CA	1:A:266:LEU:HG	1.87	1.02
1:D:262:LYS:C	1:D:264:PHE:CA	2.21	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:NE	1:A:268:CYS:HB3	1.50	1.02
1:C:32:ARG:HB3	1:C:268:CYS:CB	1.91	1.01
1:D:55:ILE:CD1	1:D:298:TYR:HD2	1.74	1.01
1:B:261:CYS:HB3	1:B:266:LEU:N	1.59	1.00
1:A:32:ARG:HB3	1:A:268:CYS:HB3	1.32	1.00
1:A:261:CYS:HB3	1:A:266:LEU:H	1.03	1.00
1:D:259:TYR:O	1:D:264:PHE:N	1.93	1.00
1:B:55:ILE:HD13	1:B:298:TYR:HD2	0.98	1.00
1:A:170:LEU:HD13	1:A:264:PHE:HZ	1.21	0.99
1:B:32:ARG:HB3	1:B:268:CYS:HB3	1.19	0.98
1:C:261:CYS:HB3	1:C:266:LEU:HB2	1.37	0.98
1:D:287:VAL:HG23	1:D:288:SER:N	1.79	0.98
1:B:55:ILE:CD1	1:B:298:TYR:HD2	1.76	0.98
1:B:262:LYS:C	1:B:265:SER:N	2.21	0.98
1:C:261:CYS:HB3	1:C:266:LEU:CB	1.89	0.98
1:A:262:LYS:CA	1:A:264:PHE:N	2.12	0.98
1:C:261:CYS:HB3	1:C:266:LEU:CA	1.94	0.97
1:D:263:ARG:HB2	1:D:264:PHE:CE2	2.00	0.97
1:A:32:ARG:HE	1:A:268:CYS:CB	1.51	0.97
1:C:261:CYS:HB3	1:C:266:LEU:H	1.29	0.97
1:C:32:ARG:CB	1:C:268:CYS:HB3	1.95	0.96
1:C:55:ILE:HB	1:C:298:TYR:CD2	1.99	0.96
1:C:261:CYS:HB3	1:C:266:LEU:N	1.79	0.96
1:A:263:ARG:HG3	1:A:264:PHE:CE2	2.00	0.95
1:C:245:TYR:CB	1:C:276:TRP:CD1	2.49	0.95
1:C:262:LYS:HA	1:C:265:SER:H	0.82	0.95
1:C:261:CYS:HA	1:C:266:LEU:HG	0.97	0.94
1:A:31:ALA:HB1	1:A:271:ALA:HA	1.46	0.94
1:D:32:ARG:HB3	1:D:268:CYS:CA	1.97	0.94
1:D:261:CYS:HB3	1:D:266:LEU:H	0.89	0.94
1:D:262:LYS:C	1:D:264:PHE:C	2.31	0.94
1:B:245:TYR:CB	1:B:276:TRP:NE1	2.16	0.93
1:D:32:ARG:O	1:D:269:PRO:CD	0.63	0.93
1:B:81:ARG:CZ	1:B:523:ARG:NH2	2.30	0.92
1:A:32:ARG:HB3	1:A:268:CYS:CA	2.00	0.92
1:A:263:ARG:CG	1:A:264:PHE:CD2	2.51	0.92
1:C:245:TYR:CB	1:C:276:TRP:HD1	1.80	0.92
1:D:170:LEU:HD11	1:D:264:PHE:CD2	2.04	0.92
1:A:262:LYS:H	1:A:264:PHE:N	1.66	0.92
1:C:262:LYS:C	1:C:265:SER:H	1.74	0.91
1:D:170:LEU:HD13	1:D:264:PHE:HZ	1.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:CYS:HA	1:A:266:LEU:HG	0.91	0.91
1:C:55:ILE:HD13	1:C:298:TYR:HD2	1.33	0.91
1:D:261:CYS:CB	1:D:266:LEU:N	2.22	0.91
1:D:245:TYR:HB3	1:D:276:TRP:NE1	1.85	0.91
1:C:261:CYS:SG	1:C:266:LEU:HD12	2.11	0.91
1:B:263:ARG:C	1:B:264:PHE:HA	1.79	0.91
1:A:261:CYS:CA	1:A:266:LEU:H	1.83	0.91
1:D:33:GLY:HA3	1:D:269:PRO:HG2	0.92	0.90
1:A:55:ILE:HB	1:A:298:TYR:HE2	1.37	0.90
1:A:33:GLY:CA	1:A:269:PRO:HG2	2.01	0.90
1:B:81:ARG:NH1	1:B:523:ARG:NH2	2.21	0.89
1:B:81:ARG:CZ	1:B:523:ARG:HH22	1.85	0.89
1:D:31:ALA:HB1	1:D:271:ALA:HA	1.52	0.89
1:B:32:ARG:HB3	1:B:268:CYS:CA	2.02	0.89
1:B:33:GLY:HA3	1:B:269:PRO:HG2	1.55	0.89
1:C:32:ARG:CD	1:C:268:CYS:HB3	2.02	0.89
1:B:263:ARG:HB2	1:B:264:PHE:CE2	2.04	0.88
1:B:55:ILE:HB	1:B:298:TYR:CD2	2.08	0.88
1:B:31:ALA:HB1	1:B:271:ALA:HA	1.53	0.87
1:C:261:CYS:SG	1:C:266:LEU:CD1	2.63	0.87
1:C:261:CYS:CA	1:C:266:LEU:CG	2.48	0.87
1:D:262:LYS:C	1:D:265:SER:N	2.18	0.87
1:A:262:LYS:C	1:A:265:SER:N	2.06	0.87
1:B:55:ILE:CD1	1:B:298:TYR:CD2	2.52	0.87
1:D:261:CYS:HA	1:D:266:LEU:HG	0.91	0.87
1:A:261:CYS:C	1:A:266:LEU:H	1.77	0.87
1:C:262:LYS:HA	1:C:265:SER:N	1.64	0.86
1:B:261:CYS:CA	1:B:266:LEU:H	1.89	0.85
1:B:59:GLU:OE2	1:B:468:ARG:NH1	2.09	0.85
1:C:32:ARG:NH2	1:C:268:CYS:HB2	1.92	0.85
1:C:59:GLU:OE2	1:C:468:ARG:NH1	2.09	0.84
1:A:55:ILE:CD1	1:A:298:TYR:HD2	1.85	0.84
1:D:33:GLY:N	1:D:269:PRO:HG2	1.91	0.84
1:B:68:GLU:OE2	1:B:441:LEU:CD2	2.26	0.84
1:B:32:ARG:HE	1:B:268:CYS:HB2	1.07	0.84
1:B:245:TYR:HD1	1:B:276:TRP:HE1	1.25	0.84
1:A:170:LEU:HD13	1:A:264:PHE:CE2	1.91	0.83
1:D:170:LEU:HD11	1:D:264:PHE:CZ	1.89	0.83
1:A:32:ARG:CG	1:A:268:CYS:CB	2.55	0.83
1:C:170:LEU:HD11	1:C:264:PHE:CD2	2.13	0.82
1:B:32:ARG:O	1:B:268:CYS:HA	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD11	1:A:264:PHE:CZ	1.83	0.81
1:A:32:ARG:NH2	1:A:268:CYS:HB2	1.95	0.81
1:A:59:GLU:OE2	1:A:468:ARG:NH1	2.13	0.81
1:C:261:CYS:C	1:C:266:LEU:H	1.88	0.81
1:C:55:ILE:HB	1:C:298:TYR:HE2	1.45	0.81
1:C:261:CYS:SG	1:C:266:LEU:HB3	2.20	0.81
1:B:259:TYR:O	1:B:264:PHE:N	2.14	0.81
1:A:55:ILE:HB	1:A:298:TYR:CD2	2.15	0.81
1:D:263:ARG:HG3	1:D:264:PHE:CE2	2.16	0.81
1:D:32:ARG:C	1:D:269:PRO:CB	2.54	0.81
1:A:261:CYS:C	1:A:266:LEU:N	2.35	0.80
1:C:170:LEU:HD13	1:C:264:PHE:HZ	1.01	0.80
1:A:32:ARG:CZ	1:A:268:CYS:CB	2.37	0.80
1:A:263:ARG:CG	1:A:264:PHE:CE2	2.65	0.80
1:C:259:TYR:O	1:C:264:PHE:N	2.15	0.80
1:C:32:ARG:CG	1:C:268:CYS:HB3	2.12	0.80
1:B:245:TYR:CD1	1:B:276:TRP:NE1	2.47	0.79
1:C:261:CYS:O	1:C:266:LEU:N	2.09	0.79
1:A:275:GLU:CD	1:A:523:ARG:NH1	2.28	0.79
1:B:261:CYS:C	1:B:266:LEU:H	1.87	0.79
1:D:245:TYR:O	1:D:276:TRP:CD1	2.36	0.79
1:A:32:ARG:HA	1:A:269:PRO:O	1.82	0.78
1:C:189:LYS:HE3	1:C:189:LYS:HA	1.64	0.78
1:C:32:ARG:CZ	1:C:268:CYS:CB	2.53	0.78
1:A:189:LYS:HE3	1:A:189:LYS:HA	1.64	0.77
1:C:261:CYS:CB	1:C:266:LEU:H	1.96	0.77
1:B:245:TYR:CG	1:B:276:TRP:NE1	2.52	0.77
1:D:32:ARG:CB	1:D:268:CYS:CB	2.47	0.76
1:D:189:LYS:HE3	1:D:189:LYS:HA	1.67	0.76
1:D:263:ARG:CG	1:D:264:PHE:CD2	2.69	0.76
1:B:262:LYS:H	1:B:264:PHE:N	1.83	0.75
1:D:263:ARG:CB	1:D:264:PHE:CE2	2.63	0.75
1:A:261:CYS:CA	1:A:266:LEU:N	2.47	0.75
1:D:59:GLU:OE2	1:D:468:ARG:NH1	2.21	0.74
1:A:263:ARG:CB	1:A:264:PHE:CE2	2.69	0.74
1:D:263:ARG:C	1:D:264:PHE:HA	2.13	0.73
1:D:287:VAL:HG22	1:D:320:ARG:O	1.89	0.73
1:B:81:ARG:NH1	1:B:523:ARG:HH22	1.81	0.73
1:C:32:ARG:HE	1:C:268:CYS:HB2	1.28	0.72
1:D:32:ARG:HA	1:D:269:PRO:C	2.13	0.72
1:B:32:ARG:CG	1:B:268:CYS:CB	2.61	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HE	1:A:268:CYS:HB2	1.11	0.72
1:C:261:CYS:HA	1:C:266:LEU:CD1	2.19	0.72
1:D:55:ILE:CD1	1:D:298:TYR:CD2	2.59	0.72
1:D:55:ILE:CB	1:D:298:TYR:CD2	2.71	0.72
1:B:55:ILE:CB	1:B:298:TYR:CE2	2.69	0.72
1:A:55:ILE:CD1	1:A:298:TYR:CD2	2.67	0.72
1:B:32:ARG:CB	1:B:268:CYS:CB	2.40	0.72
1:B:32:ARG:HA	1:B:269:PRO:O	1.90	0.71
1:C:32:ARG:HA	1:C:269:PRO:O	1.89	0.71
1:D:245:TYR:CB	1:D:276:TRP:NE1	2.48	0.71
1:D:33:GLY:N	1:D:269:PRO:CG	2.51	0.71
1:D:261:CYS:C	1:D:266:LEU:H	1.98	0.70
1:B:263:ARG:CB	1:B:264:PHE:CE2	2.70	0.70
1:D:263:ARG:CG	1:D:264:PHE:CE2	2.74	0.70
1:D:245:TYR:CA	1:D:276:TRP:CD1	2.75	0.70
1:C:55:ILE:HD13	1:C:298:TYR:CD2	2.23	0.70
1:A:32:ARG:HB3	1:A:268:CYS:HA	1.74	0.69
1:C:245:TYR:O	1:C:276:TRP:CD1	2.45	0.69
1:C:261:CYS:SG	1:C:266:LEU:CG	2.80	0.69
1:A:55:ILE:CB	1:A:298:TYR:CE2	2.63	0.69
1:A:287:VAL:HG23	1:A:288:SER:N	2.07	0.69
1:B:32:ARG:NH2	1:B:268:CYS:HB2	2.08	0.69
1:C:261:CYS:C	1:C:266:LEU:N	2.51	0.69
1:B:287:VAL:C	1:B:288:SER:N	2.52	0.68
1:D:261:CYS:C	1:D:266:LEU:N	2.51	0.68
1:A:33:GLY:HA3	1:A:269:PRO:CG	2.14	0.68
1:D:261:CYS:CA	1:D:266:LEU:H	2.05	0.68
1:A:193:HIS:CE1	1:C:147:ASP:OD1	2.46	0.68
1:D:245:TYR:HA	1:D:276:TRP:HE1	1.58	0.68
1:B:261:CYS:C	1:B:266:LEU:N	2.52	0.67
1:C:468:ARG:O	1:C:468:ARG:HG2	1.93	0.67
1:B:262:LYS:C	1:B:264:PHE:C	2.55	0.67
1:B:287:VAL:HG23	1:B:288:SER:N	2.09	0.67
1:D:245:TYR:CA	1:D:276:TRP:NE1	2.57	0.67
1:C:262:LYS:O	1:C:265:SER:N	2.28	0.66
1:D:287:VAL:C	1:D:288:SER:N	2.54	0.66
1:C:170:LEU:CD1	1:C:264:PHE:CE1	2.70	0.66
1:C:261:CYS:CA	1:C:266:LEU:CB	2.73	0.66
1:A:32:ARG:CB	1:A:268:CYS:CB	2.47	0.66
1:B:245:TYR:CG	1:B:276:TRP:CD1	2.82	0.65
1:D:33:GLY:CA	1:D:269:PRO:CG	2.52	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HE	1:A:268:CYS:C	2.05	0.65
1:D:245:TYR:HB3	1:D:276:TRP:HD1	0.84	0.64
1:B:261:CYS:CA	1:B:266:LEU:N	2.59	0.64
1:B:261:CYS:CA	1:B:266:LEU:HG	2.04	0.64
1:B:55:ILE:CB	1:B:298:TYR:CD2	2.81	0.63
1:D:287:VAL:CG2	1:D:288:SER:N	2.60	0.63
1:A:147:ASP:OD1	1:C:193:HIS:CE1	2.50	0.63
1:D:170:LEU:HD13	1:D:264:PHE:CE2	1.96	0.63
1:B:32:ARG:HB3	1:B:268:CYS:SG	2.39	0.63
1:A:32:ARG:CD	1:A:268:CYS:CB	2.47	0.62
1:B:245:TYR:HB3	1:B:276:TRP:HD1	0.80	0.62
1:B:32:ARG:HB3	1:B:268:CYS:HA	1.82	0.62
1:D:32:ARG:C	1:D:269:PRO:N	2.46	0.62
1:D:262:LYS:C	1:D:264:PHE:HA	2.02	0.62
1:C:31:ALA:HB1	1:C:271:ALA:HA	1.81	0.61
1:B:245:TYR:HB2	1:B:276:TRP:HD1	1.55	0.61
1:B:32:ARG:CZ	1:B:268:CYS:CB	2.53	0.61
1:B:55:ILE:HD13	1:B:298:TYR:CG	2.32	0.61
1:C:261:CYS:CB	1:C:266:LEU:CG	2.78	0.61
1:D:245:TYR:HA	1:D:276:TRP:NE1	2.15	0.61
1:A:158:ARG:NH1	1:D:229:ASN:HD21	1.98	0.61
1:C:170:LEU:HD21	1:C:264:PHE:HE2	1.65	0.61
1:D:405:VAL:HG12	1:D:405:VAL:O	2.01	0.61
1:C:287:VAL:C	1:C:288:SER:N	2.59	0.60
1:D:32:ARG:HB3	1:D:268:CYS:C	2.26	0.60
1:A:193:HIS:HE1	1:C:147:ASP:OD1	1.83	0.60
1:C:55:ILE:CD1	1:C:298:TYR:HD2	2.12	0.60
1:A:147:ASP:OD1	1:C:193:HIS:HE1	1.84	0.60
1:B:261:CYS:CB	1:B:266:LEU:N	2.36	0.59
1:A:263:ARG:HG3	1:A:264:PHE:HE2	1.62	0.59
1:B:55:ILE:CG1	1:B:298:TYR:CD2	2.85	0.59
1:B:68:GLU:OE2	1:B:441:LEU:HD21	1.99	0.59
1:A:81:ARG:NH2	1:A:523:ARG:HH12	2.00	0.59
1:D:261:CYS:CA	1:D:266:LEU:N	2.64	0.59
1:B:245:TYR:CA	1:B:276:TRP:CD1	2.82	0.59
1:B:263:ARG:C	1:B:264:PHE:CA	2.67	0.58
1:D:55:ILE:CG1	1:D:298:TYR:HD2	2.16	0.58
1:D:55:ILE:HB	1:D:298:TYR:HE2	1.59	0.58
1:B:34:LEU:CD1	1:B:266:LEU:HD13	2.33	0.58
1:D:245:TYR:C	1:D:276:TRP:CD1	2.82	0.58
1:A:200:SER:HA	1:D:200:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TYR:O	1:A:276:TRP:CD2	2.56	0.57
1:A:261:CYS:CA	1:A:266:LEU:CG	2.54	0.57
1:D:32:ARG:C	1:D:269:PRO:HB2	2.29	0.57
1:A:32:ARG:HE	1:A:268:CYS:CA	2.15	0.57
1:B:229:ASN:HD21	1:C:158:ARG:NH1	2.03	0.56
1:D:245:TYR:CA	1:D:276:TRP:HE1	2.16	0.56
1:D:261:CYS:O	1:D:266:LEU:N	2.28	0.56
1:A:32:ARG:HG3	1:A:268:CYS:SG	2.46	0.56
1:B:200:SER:HA	1:C:200:SER:HA	1.88	0.55
1:A:32:ARG:O	1:A:268:CYS:HA	2.06	0.55
1:B:245:TYR:CB	1:B:276:TRP:HE1	2.01	0.55
1:B:263:ARG:HG3	1:B:264:PHE:CE2	2.41	0.55
1:C:170:LEU:CD2	1:C:264:PHE:HE2	2.20	0.55
1:D:32:ARG:CA	1:D:269:PRO:O	2.35	0.55
1:B:59:GLU:CD	1:B:518:PHE:HZ	2.16	0.54
1:C:261:CYS:CA	1:C:266:LEU:H	2.19	0.54
1:A:492:SER:OG	1:A:493:GLY:N	2.40	0.54
1:B:261:CYS:CA	1:B:266:LEU:CG	2.69	0.54
1:C:245:TYR:CA	1:C:276:TRP:CD1	2.91	0.54
1:B:263:ARG:CG	1:B:264:PHE:CD2	2.89	0.53
1:D:34:LEU:HD11	1:D:268:CYS:SG	2.48	0.53
1:C:32:ARG:HH21	1:C:268:CYS:HB2	1.70	0.53
1:C:33:GLY:CA	1:C:269:PRO:HG2	2.25	0.53
1:B:55:ILE:CG1	1:B:298:TYR:HD2	2.21	0.53
1:C:32:ARG:HB3	1:C:268:CYS:CA	2.39	0.53
1:A:229:ASN:HD21	1:D:158:ARG:NH1	2.06	0.52
1:A:262:LYS:CB	1:A:264:PHE:N	2.71	0.52
1:C:170:LEU:CD2	1:C:264:PHE:CE2	2.93	0.52
1:D:32:ARG:CA	1:D:269:PRO:N	2.73	0.52
1:D:245:TYR:CB	1:D:276:TRP:HE1	2.22	0.51
1:B:69:THR:OG1	1:B:89:ASN:OD1	2.26	0.51
1:C:170:LEU:HD21	1:C:264:PHE:CE2	2.45	0.51
1:B:509:PHE:C	1:B:509:PHE:CD2	2.88	0.51
1:B:410:TYR:N	1:B:411:PRO:CD	2.73	0.51
1:A:59:GLU:CD	1:A:518:PHE:HZ	2.17	0.51
1:A:69:THR:OG1	1:A:89:ASN:OD1	2.29	0.51
1:D:492:SER:OG	1:D:493:GLY:N	2.41	0.51
1:A:275:GLU:OE1	1:A:523:ARG:NH1	2.43	0.51
1:A:55:ILE:CB	1:A:298:TYR:CD2	2.92	0.51
1:C:69:THR:OG1	1:C:89:ASN:OD1	2.29	0.51
1:B:68:GLU:OE2	1:B:441:LEU:HD22	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG22	1:C:320:ARG:O	2.11	0.50
1:B:32:ARG:HE	1:B:268:CYS:C	2.18	0.50
1:C:492:SER:OG	1:C:493:GLY:N	2.44	0.50
1:D:69:THR:OG1	1:D:89:ASN:OD1	2.28	0.50
1:B:147:ASP:OD1	1:D:193:HIS:CE1	2.65	0.49
1:A:262:LYS:HA	1:A:265:SER:CA	2.25	0.49
1:A:81:ARG:NH2	1:A:523:ARG:NH1	2.61	0.49
1:C:32:ARG:O	1:C:268:CYS:HA	2.13	0.49
1:C:55:ILE:CB	1:C:298:TYR:CD2	2.85	0.49
1:B:287:VAL:HG22	1:B:320:ARG:O	2.12	0.49
1:B:33:GLY:HA3	1:B:269:PRO:CG	2.36	0.48
1:D:55:ILE:HD13	1:D:298:TYR:CB	2.43	0.48
1:B:263:ARG:CG	1:B:264:PHE:CE2	2.96	0.48
1:C:212:SER:OG	1:C:214:ARG:O	2.31	0.48
1:A:262:LYS:O	1:A:265:SER:OG	2.22	0.48
1:B:474:ASN:O	1:B:475:ASN:CB	2.62	0.48
1:C:509:PHE:C	1:C:509:PHE:CD2	2.91	0.48
1:C:76:TYR:OH	1:C:140:GLU:OE1	2.30	0.48
1:A:212:SER:OG	1:A:214:ARG:O	2.32	0.48
1:C:189:LYS:HB3	1:C:190:PRO:HD3	1.95	0.48
1:B:33:GLY:CA	1:B:269:PRO:HG2	2.35	0.47
1:B:245:TYR:CA	1:B:276:TRP:NE1	2.77	0.47
1:A:261:CYS:HB3	1:A:266:LEU:O	2.15	0.47
1:D:275:GLU:OE2	1:D:523:ARG:NH1	2.47	0.47
1:A:55:ILE:CB	1:A:298:TYR:HE2	2.17	0.47
1:A:170:LEU:CD2	1:A:264:PHE:HE2	2.27	0.47
1:C:262:LYS:HA	1:C:265:SER:CA	2.43	0.47
1:A:509:PHE:C	1:A:509:PHE:CD2	2.92	0.47
1:C:287:VAL:HG23	1:C:288:SER:N	2.29	0.47
1:B:257:ASP:OD1	1:B:257:ASP:N	2.47	0.47
1:D:32:ARG:CA	1:D:269:PRO:CD	2.80	0.46
1:A:189:LYS:HB3	1:A:190:PRO:HD3	1.96	0.46
1:B:55:ILE:HD13	1:B:298:TYR:HB3	1.97	0.46
1:B:59:GLU:HG2	1:B:518:PHE:HE2	1.79	0.46
1:D:189:LYS:HB3	1:D:190:PRO:HD3	1.96	0.46
1:B:32:ARG:CB	1:B:268:CYS:SG	3.01	0.46
1:A:32:ARG:HB3	1:A:268:CYS:SG	2.55	0.46
1:B:55:ILE:HD13	1:B:298:TYR:CB	2.45	0.46
1:C:33:GLY:HA3	1:C:269:PRO:CG	2.27	0.46
1:D:212:SER:OG	1:D:214:ARG:O	2.31	0.46
1:B:147:ASP:OD1	1:D:193:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:SER:OG	1:B:214:ARG:O	2.31	0.46
1:C:245:TYR:HA	1:C:276:TRP:HE1	1.81	0.45
1:D:55:ILE:CG1	1:D:298:TYR:CD2	2.97	0.45
1:D:55:ILE:HD13	1:D:298:TYR:CG	2.41	0.45
1:D:261:CYS:HA	1:D:266:LEU:CD1	2.44	0.45
1:D:397:GLU:O	1:D:397:GLU:HG3	2.17	0.45
1:A:167:GLU:H	1:A:167:GLU:CD	2.23	0.45
1:A:438:THR:OG1	1:A:439:MET:N	2.50	0.45
1:A:170:LEU:CD2	1:A:264:PHE:CE2	3.00	0.45
1:A:189:LYS:HA	1:A:189:LYS:CE	2.40	0.45
1:D:263:ARG:CB	1:D:264:PHE:HA	2.38	0.45
1:C:167:GLU:H	1:C:167:GLU:CD	2.24	0.44
1:C:151:LEU:N	1:C:152:PRO:CD	2.80	0.44
1:B:373:ILE:O	1:B:374:PRO:C	2.60	0.44
1:A:245:TYR:O	1:A:276:TRP:CE3	2.71	0.44
1:D:263:ARG:HG3	1:D:264:PHE:HE2	1.77	0.44
1:C:373:ILE:O	1:C:374:PRO:C	2.61	0.44
1:A:42:ASP:C	1:A:42:ASP:OD1	2.61	0.43
1:C:189:LYS:HE3	1:C:189:LYS:CA	2.38	0.43
1:C:189:LYS:HA	1:C:189:LYS:CE	2.41	0.43
1:A:151:LEU:N	1:A:152:PRO:CD	2.81	0.43
1:A:397:GLU:O	1:A:397:GLU:HG3	2.19	0.43
1:A:257:ASP:N	1:A:257:ASP:OD1	2.48	0.43
1:B:32:ARG:HG3	1:B:268:CYS:SG	2.58	0.43
1:B:34:LEU:HD11	1:B:266:LEU:HD13	2.00	0.43
1:D:247:ILE:N	1:D:248:PRO:CD	2.81	0.43
1:A:170:LEU:CD1	1:A:264:PHE:CE1	2.81	0.43
1:B:151:LEU:N	1:B:152:PRO:CD	2.81	0.43
1:A:373:ILE:O	1:A:374:PRO:C	2.62	0.43
1:C:438:THR:OG1	1:C:439:MET:N	2.50	0.43
1:D:151:LEU:N	1:D:152:PRO:CD	2.82	0.43
1:A:262:LYS:HB2	1:A:264:PHE:N	2.34	0.43
1:B:55:ILE:HD12	1:B:55:ILE:HA	1.88	0.43
1:C:245:TYR:HA	1:C:276:TRP:NE1	2.34	0.43
1:C:257:ASP:OD1	1:C:257:ASP:N	2.48	0.43
1:B:32:ARG:HE	1:B:268:CYS:CA	2.25	0.43
1:B:59:GLU:HG2	1:B:518:PHE:CE2	2.53	0.43
1:D:438:THR:OG1	1:D:439:MET:N	2.50	0.43
1:A:247:ILE:N	1:A:248:PRO:CD	2.81	0.43
1:B:474:ASN:C	1:B:474:ASN:OD1	2.62	0.43
1:A:262:LYS:HA	1:A:265:SER:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:O	1:A:468:ARG:HG2	2.19	0.42
1:C:247:ILE:N	1:C:248:PRO:CD	2.81	0.42
1:C:261:CYS:CA	1:C:266:LEU:N	2.82	0.42
1:C:348:LEU:HD23	1:C:348:LEU:C	2.44	0.42
1:D:189:LYS:HA	1:D:189:LYS:CE	2.44	0.42
1:B:260:ILE:HA	1:B:264:PHE:CE2	2.37	0.42
1:A:79:PHE:CE2	1:A:276:TRP:CZ2	3.07	0.42
1:A:456:GLN:OE1	1:A:456:GLN:HA	2.18	0.42
1:B:158:ARG:NH1	1:C:229:ASN:HD21	2.17	0.42
1:C:32:ARG:HB3	1:C:268:CYS:SG	2.60	0.42
1:C:261:CYS:HB3	1:C:266:LEU:C	2.43	0.42
1:B:189:LYS:N	1:B:190:PRO:CD	2.83	0.42
1:A:207:ILE:HD11	1:A:264:PHE:HZ	1.85	0.42
1:B:247:ILE:N	1:B:248:PRO:CD	2.83	0.41
1:B:474:ASN:O	1:B:475:ASN:HB3	2.20	0.41
1:A:55:ILE:HD12	1:A:55:ILE:HA	1.92	0.41
1:D:32:ARG:HA	1:D:269:PRO:CA	2.50	0.41
1:A:348:LEU:HD23	1:A:348:LEU:C	2.45	0.41
1:D:408:CYS:O	1:D:409:LYS:HB2	2.20	0.41
1:A:79:PHE:CE2	1:A:276:TRP:HZ2	2.39	0.41
1:A:287:VAL:C	1:A:288:SER:N	2.79	0.41
1:B:117:PRO:O	1:B:118:HIS:HB2	2.20	0.41
1:B:397:GLU:O	1:B:397:GLU:HG3	2.19	0.41
1:C:62:VAL:O	1:C:466:ARG:NH1	2.54	0.41
1:D:55:ILE:CD1	1:D:298:TYR:HB3	2.50	0.41
1:D:167:GLU:H	1:D:167:GLU:CD	2.24	0.41
1:C:460:ALA:HA	1:C:461:PRO:HD3	1.92	0.41
1:A:506:HIS:CG	1:A:509:PHE:HB2	2.56	0.40
1:B:262:LYS:O	1:B:265:SER:N	2.52	0.40
1:B:272:ASN:C	1:B:272:ASN:OD1	2.64	0.40
1:D:116:ILE:HA	1:D:117:PRO:HA	1.92	0.40
1:C:59:GLU:CD	1:C:518:PHE:HZ	2.29	0.40
1:A:275:GLU:CD	1:A:523:ARG:HD3	2.46	0.40
1:D:410:TYR:N	1:D:411:PRO:CD	2.84	0.40
1:D:426:VAL:O	1:D:427:GLU:HB2	2.22	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	526/545 (96%)	501 (95%)	22 (4%)	3 (1%)	21	59
1	B	526/545 (96%)	494 (94%)	23 (4%)	9 (2%)	7	36
1	C	526/545 (96%)	495 (94%)	26 (5%)	5 (1%)	12	49
1	D	526/545 (96%)	496 (94%)	22 (4%)	8 (2%)	8	40
All	All	2104/2180 (96%)	1986 (94%)	93 (4%)	25 (1%)	13	44

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	B	374	PRO
1	C	374	PRO
1	C	492	SER
1	B	12	VAL
1	B	475	ASN
1	C	356	ARG
1	D	492	SER
1	A	411	PRO
1	B	411	PRO
1	C	411	PRO
1	D	12	VAL
1	D	302	PRO
1	D	411	PRO
1	D	468	ARG
1	B	492	SER
1	D	374	PRO
1	B	118	HIS
1	B	498	VAL
1	B	527	PRO
1	D	498	VAL
1	B	410	TYR

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Mol	Chain	Res	Type
1	C	527	PRO
1	D	406	PRO
1	A	527	PRO

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	452/461 (98%)	451 (100%)	1 (0%)	87	87
1	B	452/461 (98%)	452 (100%)	0	100	100
1	C	452/461 (98%)	451 (100%)	1 (0%)	87	87
1	D	452/461 (98%)	451 (100%)	1 (0%)	87	87
All	All	1808/1844 (98%)	1805 (100%)	3 (0%)	85	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	C	189	LYS
1	D	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	193	HIS
1	A	229	ASN
1	B	114	GLN
1	B	193	HIS
1	B	324	ASN
1	B	447	GLN
1	B	459	ASN
1	C	114	GLN
1	C	193	HIS

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Mol	Chain	Res	Type
1	D	114	GLN
1	D	193	HIS
1	D	475	ASN
1	D	496	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	A	2
1	C	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	263:ARG	C	264:PHE	N	4.01
1	A	263:ARG	C	264:PHE	N	3.86
1	C	263:ARG	C	264:PHE	N	3.71
1	B	263:ARG	C	264:PHE	N	3.61
1	A	287:VAL	C	288:SER	N	2.79
1	C	287:VAL	C	288:SER	N	2.59
1	D	287:VAL	C	288:SER	N	2.54
1	B	287:VAL	C	288:SER	N	2.52

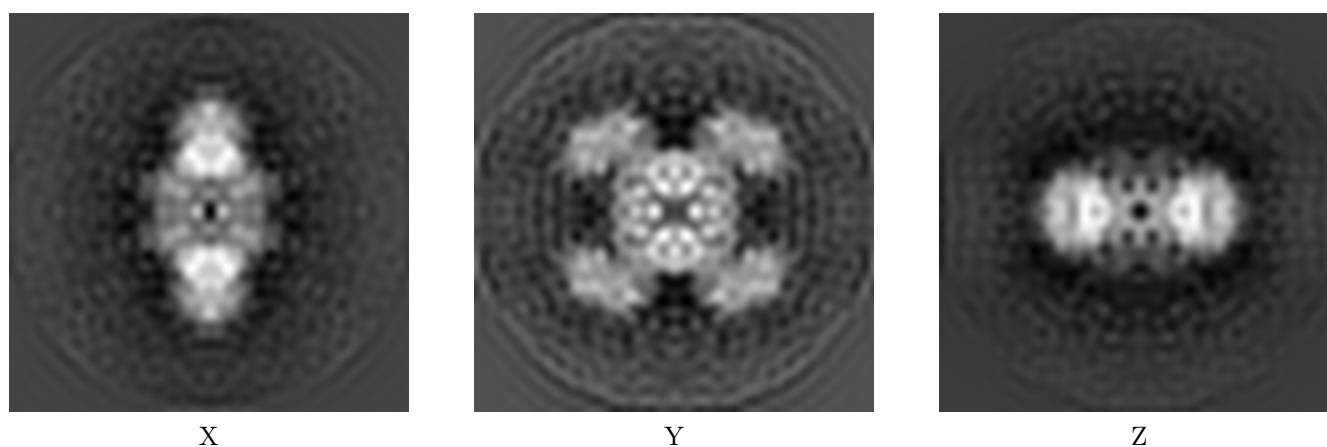
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8475. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

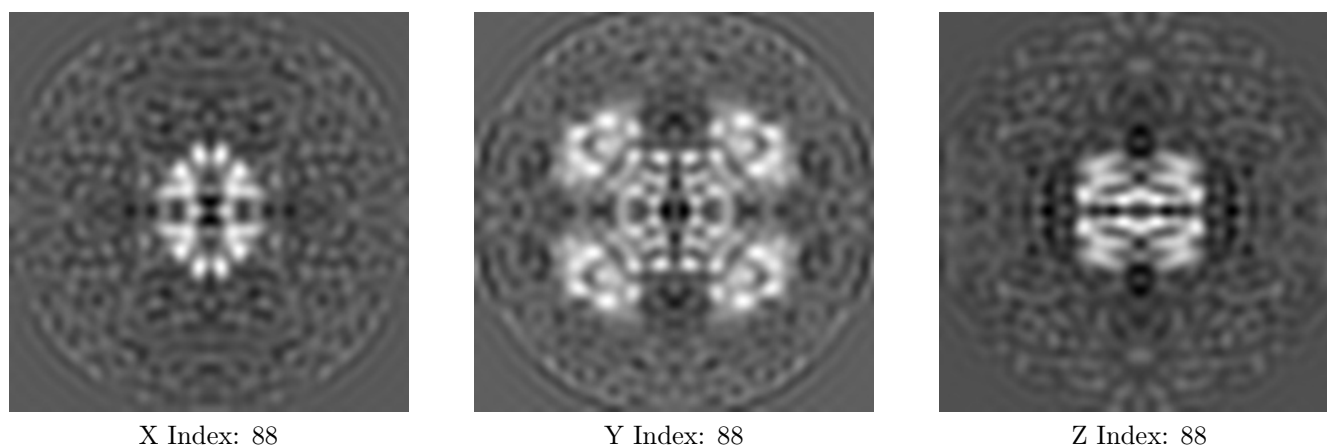
6.1.1 Primary map



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

6.2 Central slices [i](#)

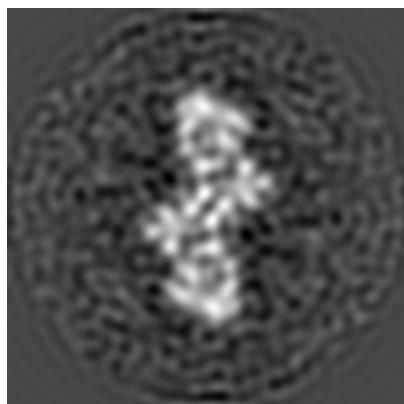
6.2.1 Primary map



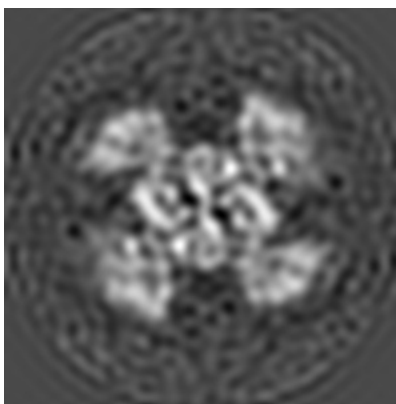
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

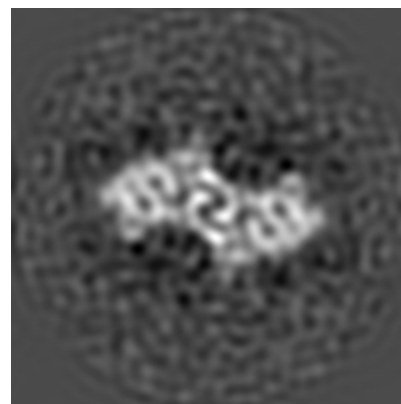
6.3.1 Primary map



X Index: 112



Y Index: 93

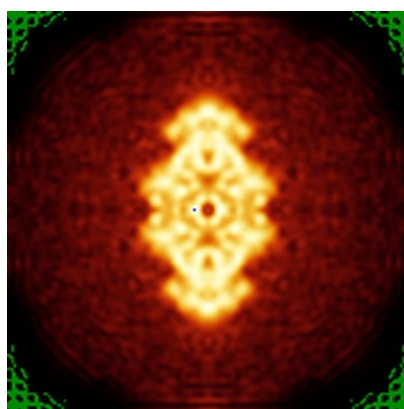


Z Index: 69

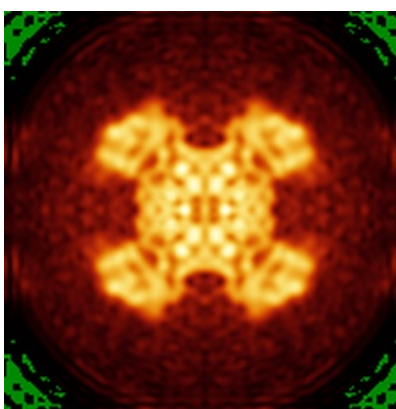
The images above show the largest variance slices of the map in three orthogonal directions.

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

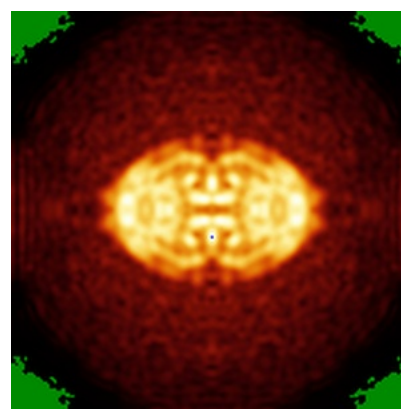
6.4.1 Primary map



X



Y

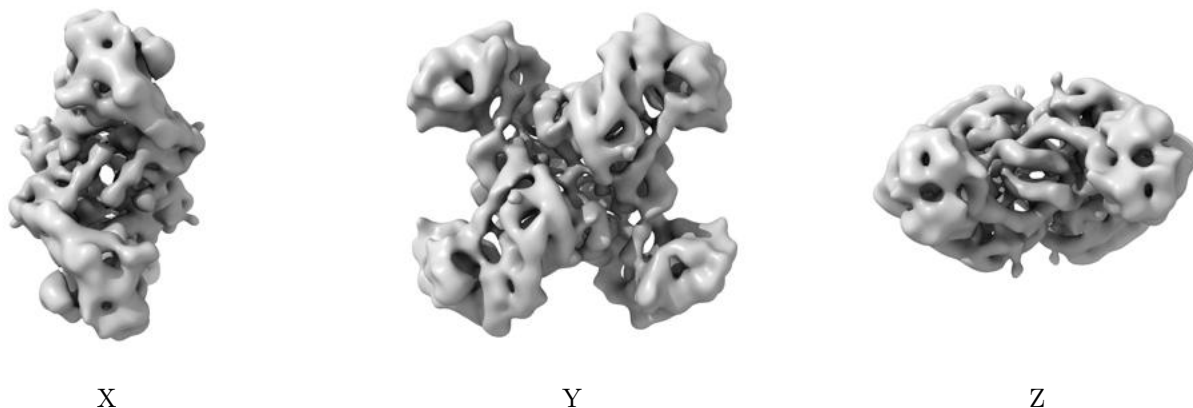


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

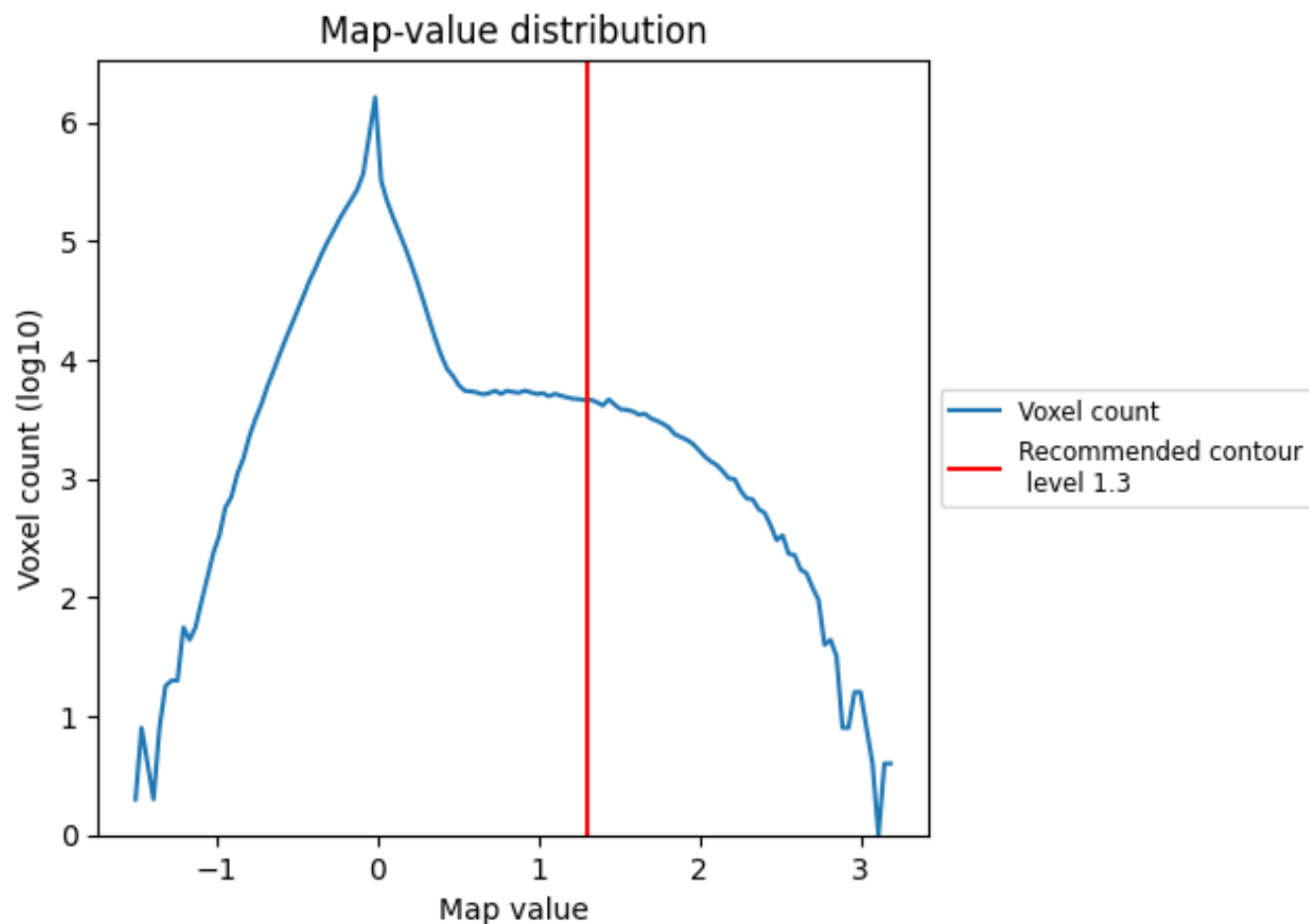
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

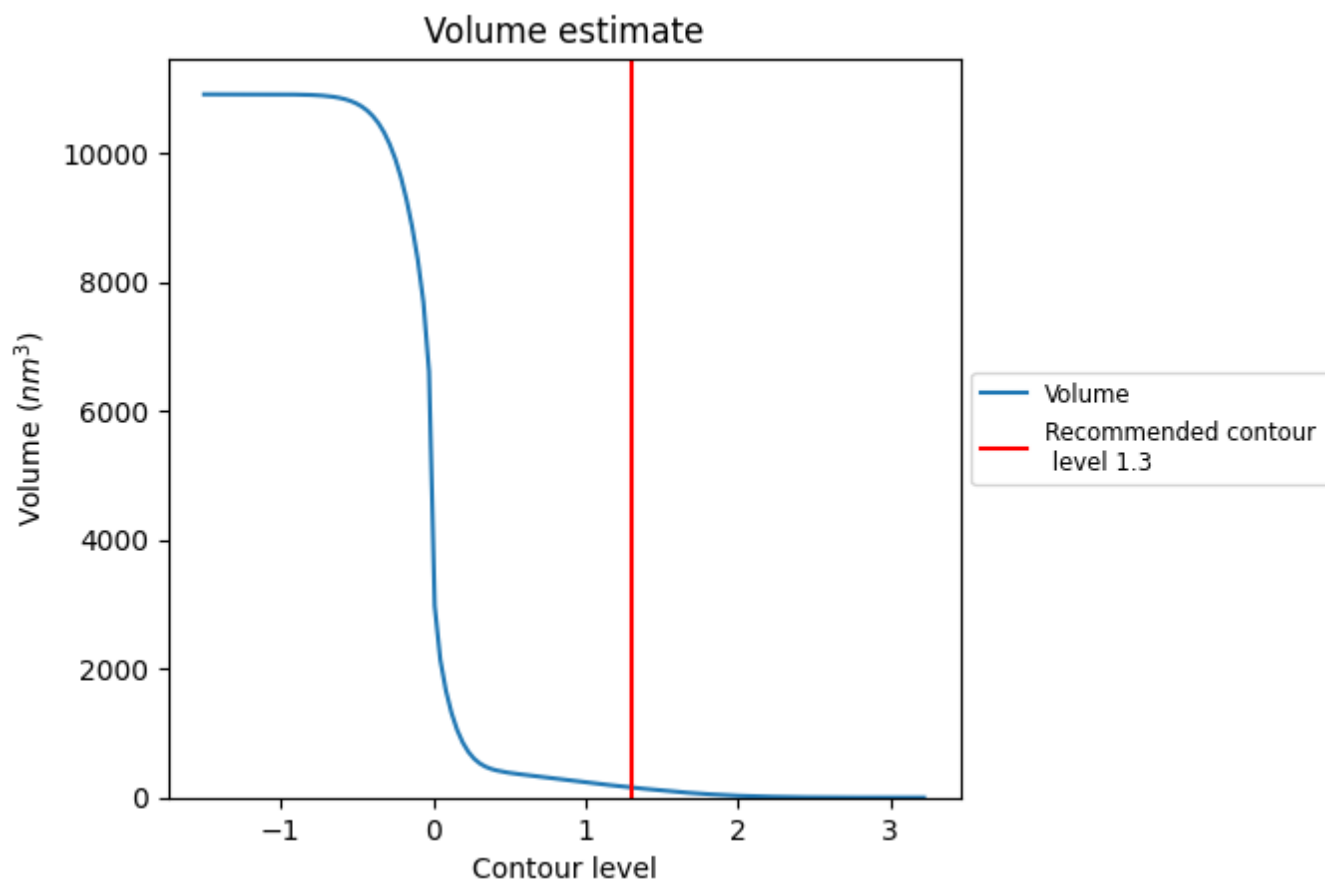
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

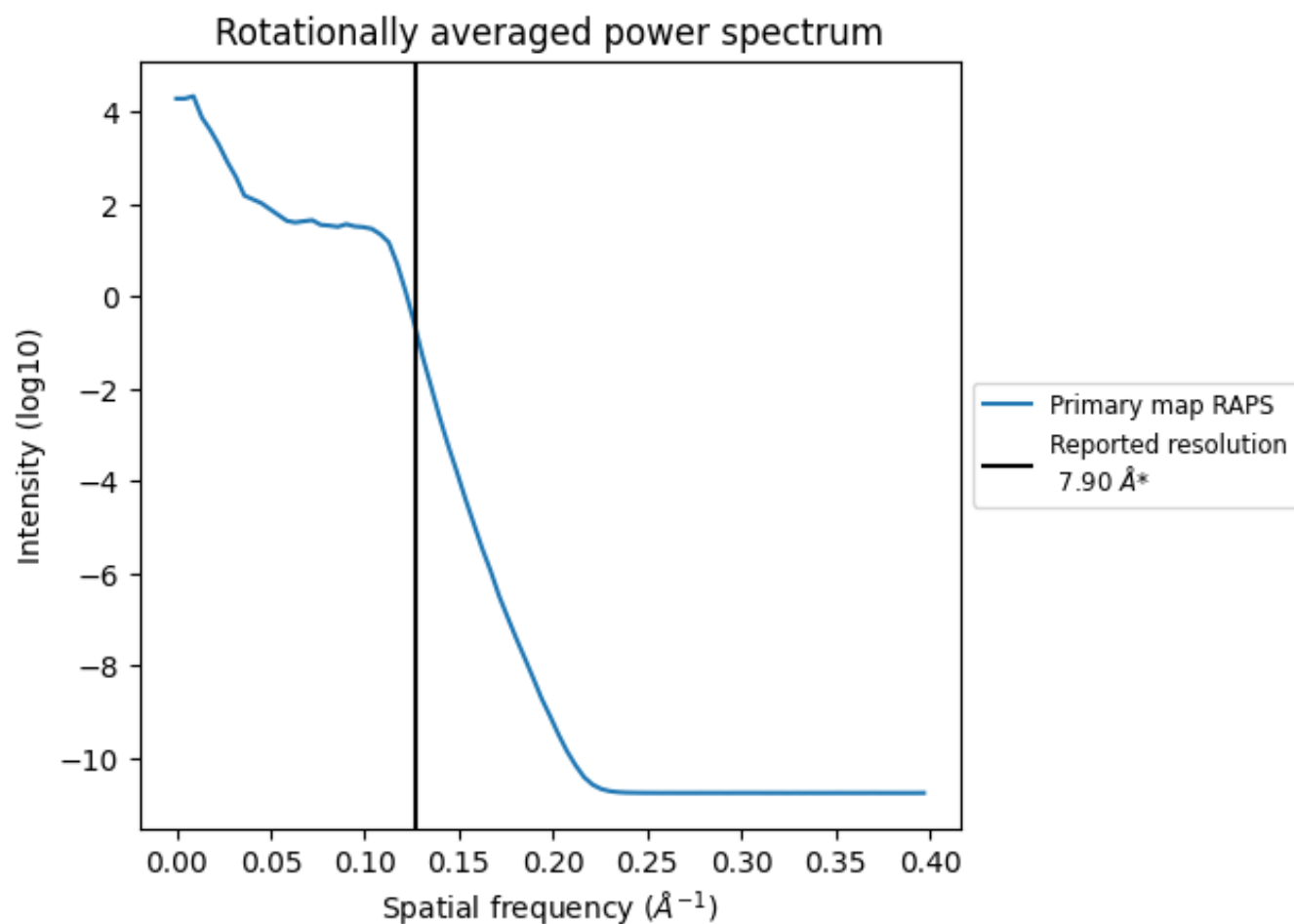
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 0.127 Å⁻¹

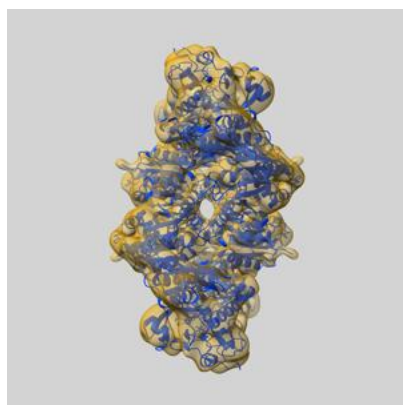
8 Fourier-Shell correlation ⓘ

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

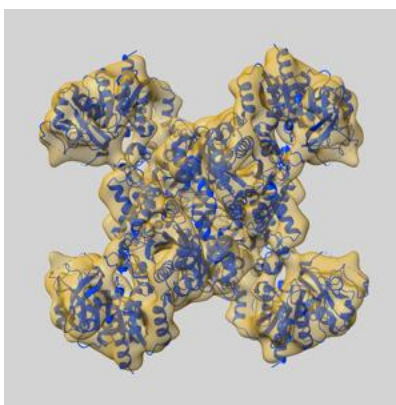
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8475 and PDB model 5U05. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

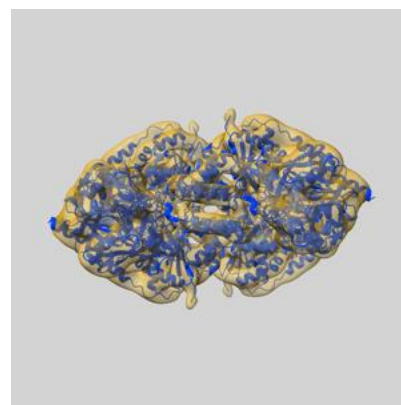
9.1 Map-model overlay [i](#)



X



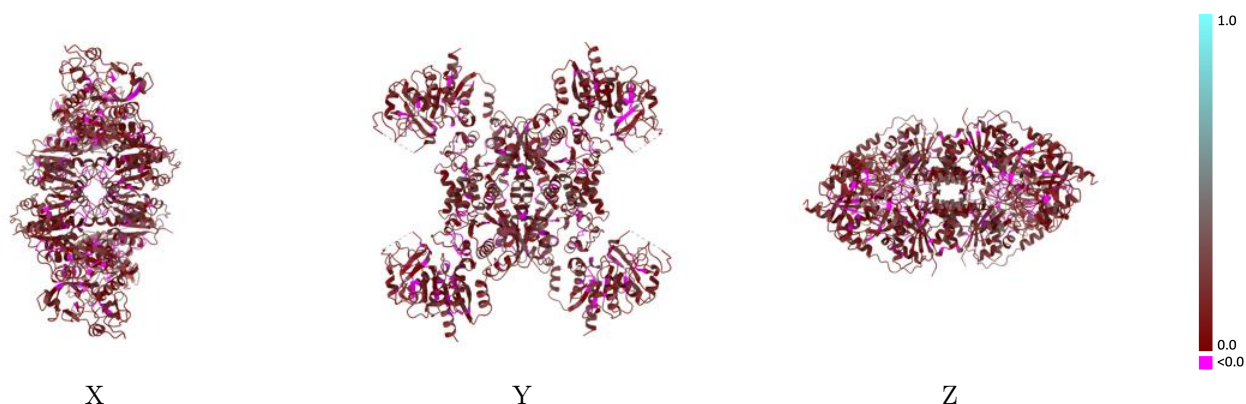
Y



Z

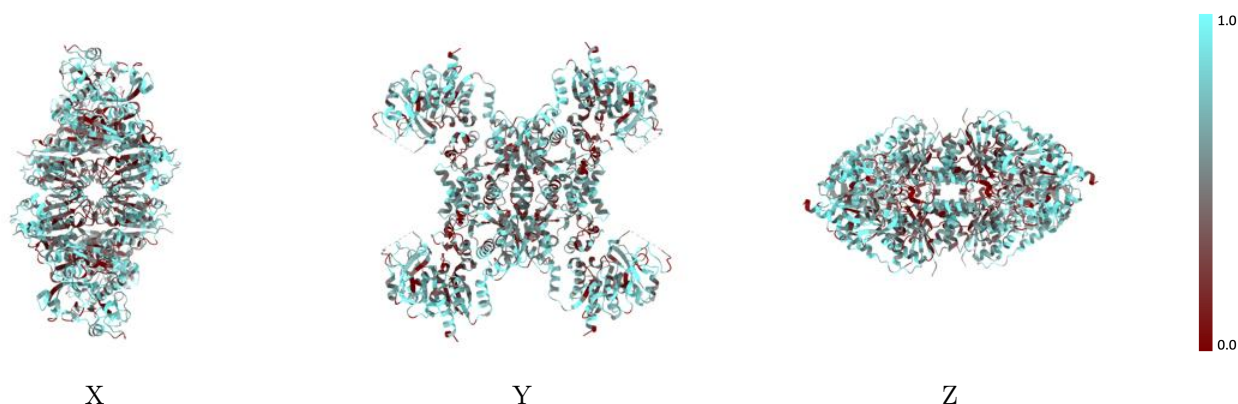
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



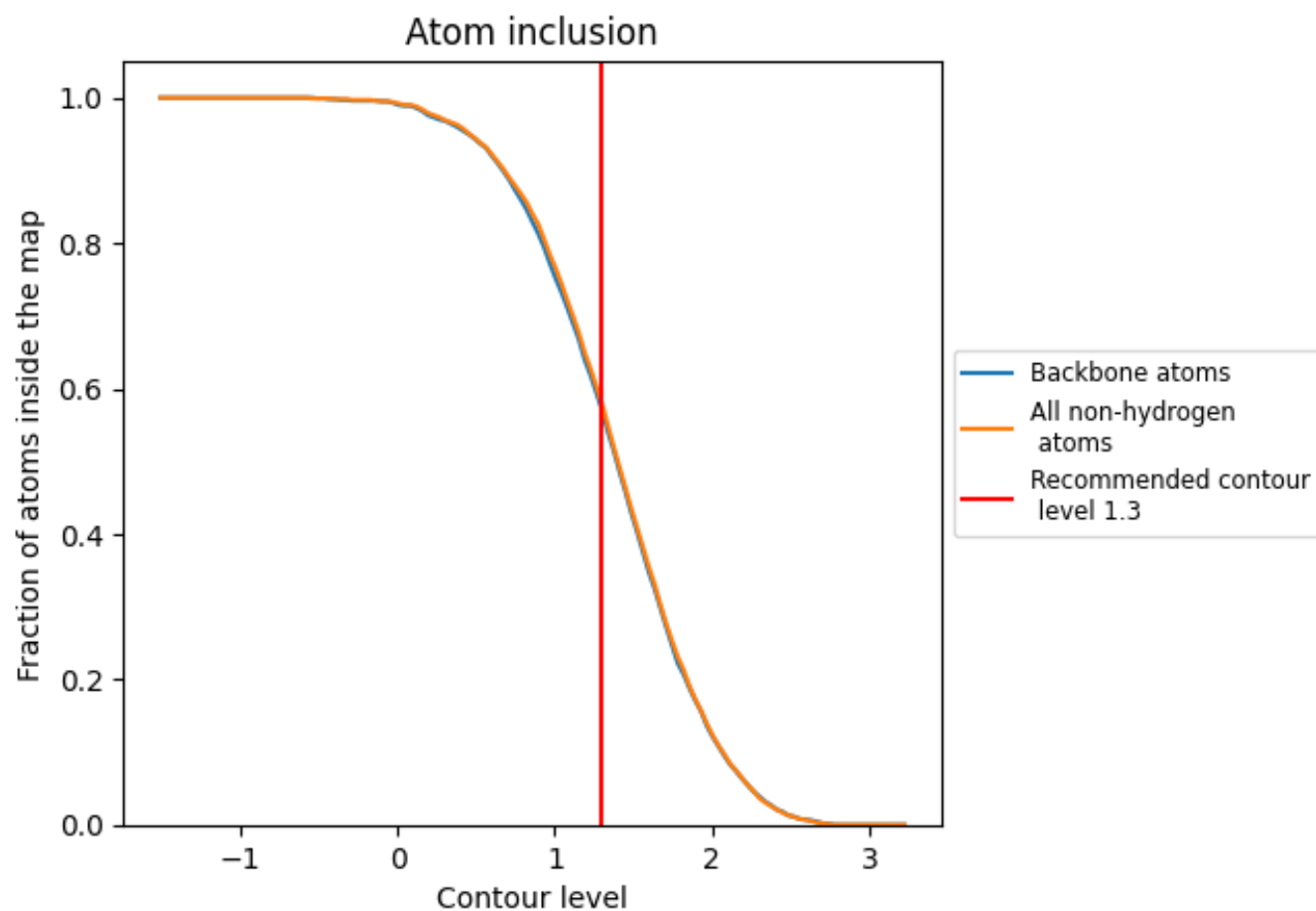
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5790	0.1320
A	0.5880	0.1320
B	0.5860	0.1330
C	0.5880	0.1300
D	0.5880	0.1320

