



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 3J25 / pdb_00003j25
EMDB ID : EMD-2183
Title : Structural basis for TetM-mediated tetracycline resistance
Authors : Doenhoefer, A.; Franckenberg, S.; Wickles, S.; Berninghausen, O.; Beckmann, R.; Wilson, D.N.
Deposited on : 2012-08-22
Resolution : 7.20 Å(reported)
Based on initial model : 2WRI

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

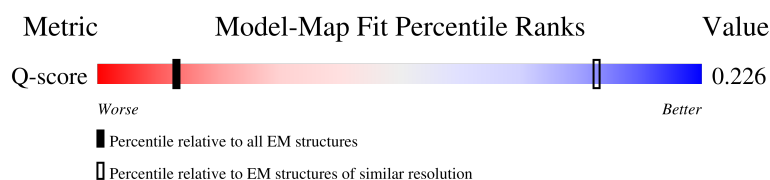
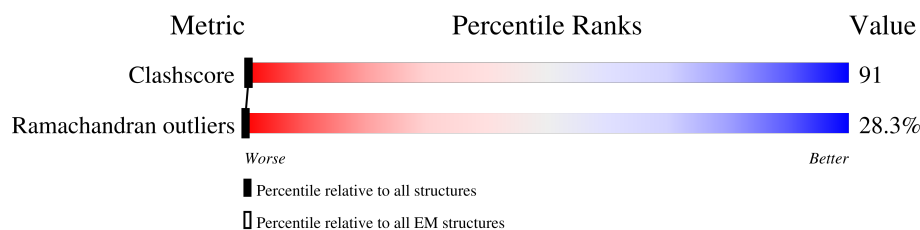
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

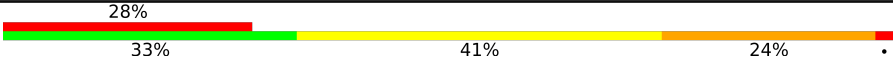
The reported resolution of this entry is 7.20 Å.

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	-
Q-score	-	25397	444 (6.70 - 7.70)

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	638	

2 Entry composition [i](#)

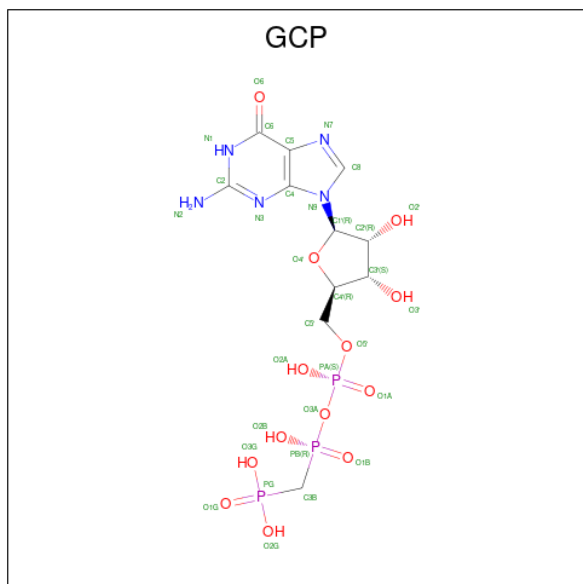
There are 2 unique types of molecules in this entry. The entry contains 3186 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tetracycline resistance protein tetM.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	638	Total	C	N	O	0	0
			3154	1877	638	639		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

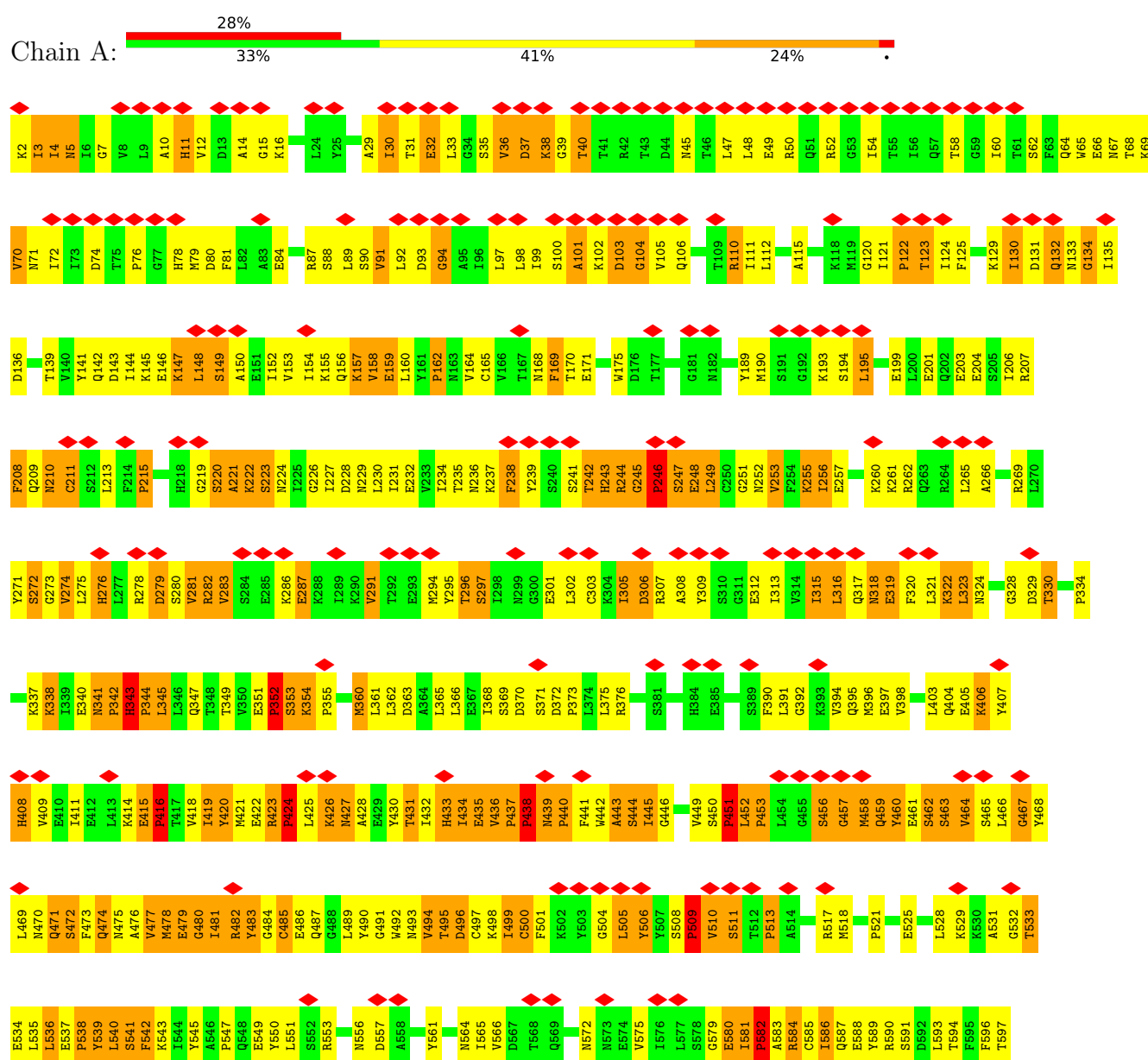


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

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

• Molecule 1: Tetracycline resistance protein tetM





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52701	Depositor
Resolution determination method	Not provided	
CTF correction method	The volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	75000	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	0.695	Depositor
Minimum map value	-0.609	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	455.36322, 455.36322, 455.36322	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2374, 1.2374, 1.2374	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.40	50/3153 (1.6%)	1.75	142/4389 (3.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	604	LEU	C-N	8.65	1.45	1.33
1	A	251	GLY	CA-C	-8.10	1.42	1.51
1	A	229	ASN	N-CA	7.96	1.55	1.46
1	A	94	GLY	CA-C	-7.66	1.45	1.51
1	A	302	LEU	CA-C	-7.56	1.43	1.52
1	A	291	VAL	C-N	-7.21	1.23	1.33
1	A	596	PHE	CA-C	-7.05	1.43	1.52
1	A	543	LYS	C-N	6.96	1.42	1.33
1	A	144	ILE	N-CA	-6.80	1.39	1.46
1	A	368	ILE	C-N	6.77	1.43	1.33
1	A	347	GLN	N-CA	-6.66	1.38	1.46
1	A	303	CYS	CA-C	-6.56	1.44	1.52
1	A	550	TYR	C-N	6.54	1.42	1.34
1	A	580	GLU	C-N	6.49	1.40	1.33
1	A	84	GLU	CA-C	-6.46	1.44	1.52
1	A	231	ILE	N-CA	-6.42	1.39	1.46
1	A	210	ASN	CA-C	-6.41	1.43	1.52
1	A	397	GLU	C-O	-6.40	1.16	1.24
1	A	587	GLN	CA-C	-6.36	1.45	1.52
1	A	144	ILE	CA-C	-6.30	1.45	1.52
1	A	235	THR	CA-C	-6.09	1.44	1.52
1	A	605	THR	N-CA	-5.99	1.38	1.46
1	A	110	ARG	CA-C	-5.94	1.44	1.52
1	A	553	ARG	N-CA	-5.91	1.38	1.46
1	A	565	ILE	CA-C	-5.89	1.45	1.52
1	A	365	LEU	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	LEU	C-N	-5.80	1.25	1.33
1	A	582	PRO	CA-CB	-5.78	1.45	1.53
1	A	557	ASP	N-CA	-5.74	1.39	1.46
1	A	361	LEU	CA-C	-5.56	1.45	1.52
1	A	633	TYR	N-CA	-5.53	1.39	1.46
1	A	550	TYR	CA-C	5.49	1.60	1.52
1	A	362	LEU	N-CA	-5.48	1.39	1.46
1	A	201	GLU	C-N	5.48	1.41	1.33
1	A	366	LEU	C-N	5.47	1.41	1.33
1	A	557	ASP	CA-C	5.46	1.60	1.52
1	A	232	GLU	C-N	5.43	1.40	1.33
1	A	145	LYS	CA-C	-5.41	1.45	1.52
1	A	232	GLU	CA-C	-5.35	1.45	1.52
1	A	262	ARG	N-CA	-5.33	1.37	1.47
1	A	208	PHE	N-CA	-5.32	1.40	1.46
1	A	564	ASN	CA-C	-5.31	1.45	1.53
1	A	591	SER	CA-C	-5.27	1.45	1.52
1	A	88	SER	CA-C	-5.21	1.46	1.52
1	A	587	GLN	C-N	5.20	1.40	1.33
1	A	575	VAL	N-CA	-5.20	1.40	1.46
1	A	361	LEU	N-CA	-5.15	1.40	1.46
1	A	345	LEU	CA-C	5.14	1.59	1.52
1	A	489	LEU	CA-C	-5.09	1.46	1.52
1	A	565	ILE	C-N	5.04	1.39	1.33

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ALA	CA-C-N	10.08	133.79	120.28
1	A	115	ALA	C-N-CA	10.08	133.79	120.28
1	A	547	PRO	N-CA-CB	9.93	112.78	103.15
1	A	566	VAL	N-CA-C	-9.48	95.49	108.96
1	A	343	HIS	CA-C-N	9.18	131.32	119.84
1	A	343	HIS	C-N-CA	9.18	131.32	119.84
1	A	343	HIS	N-CA-C	8.90	129.49	109.81
1	A	269	ARG	CA-C-O	8.90	130.08	120.38
1	A	231	ILE	CA-C-N	8.84	132.47	120.54
1	A	231	ILE	C-N-CA	8.84	132.47	120.54
1	A	143	ASP	CA-C-N	8.18	131.16	120.60
1	A	143	ASP	C-N-CA	8.18	131.16	120.60
1	A	561	TYR	CB-CA-C	8.16	121.26	111.22
1	A	249	LEU	N-CA-C	-7.87	96.57	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	GLN	CA-C-N	7.78	131.04	120.54
1	A	587	GLN	C-N-CA	7.78	131.04	120.54
1	A	226	GLY	CA-C-N	7.66	130.36	120.56
1	A	226	GLY	C-N-CA	7.66	130.36	120.56
1	A	517	ARG	CA-C-N	7.59	130.31	120.44
1	A	517	ARG	C-N-CA	7.59	130.31	120.44
1	A	373	PRO	N-CA-CB	7.58	110.40	103.20
1	A	93	ASP	CA-C-O	-7.55	112.92	120.70
1	A	437	PRO	N-CA-CB	7.55	110.40	103.08
1	A	204	GLU	CA-C-O	-7.40	112.58	120.42
1	A	110	ARG	CA-C-N	7.40	135.28	121.97
1	A	110	ARG	C-N-CA	7.40	135.28	121.97
1	A	587	GLN	CA-C-O	-7.25	113.39	121.00
1	A	590	ARG	N-CA-C	7.25	119.81	111.11
1	A	582	PRO	N-CA-CB	7.24	110.85	103.25
1	A	334	PRO	N-CA-CB	7.23	110.39	103.52
1	A	624	PRO	N-CA-CB	7.09	110.41	102.60
1	A	586	ILE	CA-C-N	7.09	130.01	120.65
1	A	586	ILE	C-N-CA	7.09	130.01	120.65
1	A	594	THR	CB-CA-C	-7.07	98.66	110.68
1	A	261	LYS	CB-CA-C	-7.04	100.12	110.96
1	A	139	THR	O-C-N	6.90	129.43	122.12
1	A	603	CYS	CB-CA-C	-6.86	96.77	110.42
1	A	438	PRO	N-CA-CB	6.86	110.45	103.25
1	A	513	PRO	N-CA-CB	6.85	110.44	103.25
1	A	122	PRO	N-CA-CB	6.83	110.42	103.25
1	A	509	PRO	N-CA-CB	6.83	110.42	103.25
1	A	76	PRO	N-CA-CB	6.82	110.42	103.25
1	A	215	PRO	N-CA-CB	6.82	110.41	103.25
1	A	451	PRO	N-CA-CB	6.81	110.41	103.25
1	A	617	PRO	N-CA-CB	6.81	110.40	103.25
1	A	355	PRO	N-CA-CB	6.81	110.40	103.25
1	A	246	PRO	N-CA-CB	6.80	110.39	103.25
1	A	424	PRO	N-CA-CB	6.80	110.39	103.25
1	A	352	PRO	N-CA-CB	6.79	110.38	103.25
1	A	162	PRO	N-CA-CB	6.78	110.37	103.25
1	A	621	PRO	N-CA-CB	6.78	110.37	103.25
1	A	453	PRO	N-CA-CB	6.78	110.37	103.25
1	A	440	PRO	N-CA-CB	6.77	110.36	103.25
1	A	630	LYS	CA-C-N	6.75	129.20	120.56
1	A	630	LYS	C-N-CA	6.75	129.20	120.56
1	A	521	PRO	N-CA-CB	6.66	110.41	103.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	PRO	N-CA-CB	6.63	110.21	103.25
1	A	210	ASN	N-CA-C	6.60	120.44	112.38
1	A	230	LEU	O-C-N	-6.55	115.18	122.12
1	A	588	GLU	CA-C-N	6.55	129.29	120.65
1	A	588	GLU	C-N-CA	6.55	129.29	120.65
1	A	345	LEU	N-CA-C	6.50	124.64	110.80
1	A	204	GLU	CA-C-N	6.47	128.96	120.28
1	A	204	GLU	C-N-CA	6.47	128.96	120.28
1	A	141	TYR	N-CA-C	6.46	119.15	111.33
1	A	581	ILE	CA-C-N	6.46	127.92	119.84
1	A	581	ILE	C-N-CA	6.46	127.92	119.84
1	A	545	TYR	CB-CA-C	-6.44	100.48	110.78
1	A	141	TYR	CA-C-O	-6.42	113.70	120.63
1	A	84	GLU	N-CA-C	-6.33	105.48	113.72
1	A	91	VAL	CA-C-O	-6.31	112.89	120.78
1	A	89	LEU	CA-C-N	6.29	133.55	121.54
1	A	89	LEU	C-N-CA	6.29	133.55	121.54
1	A	112	LEU	CA-C-N	6.27	128.68	120.28
1	A	112	LEU	C-N-CA	6.27	128.68	120.28
1	A	93	ASP	CB-CA-C	-6.27	101.00	110.90
1	A	361	LEU	CA-C-N	6.27	128.59	120.44
1	A	361	LEU	C-N-CA	6.27	128.59	120.44
1	A	229	ASN	CA-C-O	6.21	127.10	120.70
1	A	416	PRO	N-CA-CB	6.14	109.70	103.25
1	A	398	VAL	CA-C-N	6.08	129.06	120.42
1	A	398	VAL	C-N-CA	6.08	129.06	120.42
1	A	396	MET	CA-C-N	6.08	129.24	120.79
1	A	396	MET	C-N-CA	6.08	129.24	120.79
1	A	586	ILE	N-CA-CB	5.98	117.94	110.47
1	A	631	VAL	N-CA-CB	5.97	118.21	110.57
1	A	87	ARG	N-CA-C	-5.95	104.73	112.23
1	A	206	ILE	CA-C-N	5.95	128.73	120.29
1	A	206	ILE	C-N-CA	5.95	128.73	120.29
1	A	203	GLU	CA-C-N	5.92	128.70	120.29
1	A	203	GLU	C-N-CA	5.92	128.70	120.29
1	A	111	ILE	CA-C-O	-5.90	113.40	120.78
1	A	395	GLN	CA-C-N	5.90	130.67	120.58
1	A	395	GLN	C-N-CA	5.90	130.67	120.58
1	A	227	ILE	CA-C-N	5.90	128.18	120.28
1	A	227	ILE	C-N-CA	5.90	128.18	120.28
1	A	547	PRO	CA-C-O	-5.76	114.83	121.86
1	A	84	GLU	CA-C-N	5.74	130.15	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	GLU	C-N-CA	5.74	130.15	121.65
1	A	142	GLN	CB-CA-C	-5.69	101.34	110.79
1	A	397	GLU	O-C-N	5.68	128.16	122.08
1	A	230	LEU	CA-C-O	5.67	126.76	120.63
1	A	204	GLU	CB-CA-C	-5.65	101.24	110.85
1	A	199	GLU	N-CA-C	5.65	118.20	111.71
1	A	226	GLY	N-CA-C	-5.63	107.55	115.32
1	A	146	GLU	N-CA-C	5.62	117.26	111.03
1	A	474	GLN	N-CA-C	-5.60	105.71	112.54
1	A	45	ASN	N-CA-C	5.57	119.55	112.87
1	A	397	GLU	N-CA-CB	5.56	118.27	109.82
1	A	581	ILE	N-CA-CB	5.50	118.90	111.21
1	A	124	ILE	CA-C-N	-5.45	114.34	122.74
1	A	124	ILE	C-N-CA	-5.45	114.34	122.74
1	A	363	ASP	CA-C-N	5.44	127.51	120.44
1	A	363	ASP	C-N-CA	5.44	127.51	120.44
1	A	556	ASN	CB-CA-C	-5.42	101.64	110.85
1	A	93	ASP	CA-C-N	-5.35	118.01	121.65
1	A	93	ASP	C-N-CA	-5.35	118.01	121.65
1	A	593	LEU	CA-C-N	5.35	127.71	120.38
1	A	593	LEU	C-N-CA	5.35	127.71	120.38
1	A	204	GLU	O-C-N	5.34	128.24	122.15
1	A	291	VAL	O-C-N	-5.34	115.89	122.57
1	A	549	GLU	CB-CA-C	-5.24	101.94	110.85
1	A	344	PRO	CA-C-N	5.24	131.54	121.54
1	A	344	PRO	C-N-CA	5.24	131.54	121.54
1	A	551	LEU	N-CA-CB	-5.23	102.17	110.22
1	A	144	ILE	N-CA-CB	-5.22	104.72	110.51
1	A	605	THR	N-CA-CB	5.21	119.30	110.49
1	A	593	LEU	CA-C-O	-5.21	115.33	121.07
1	A	541	SER	N-CA-C	-5.21	104.91	113.50
1	A	261	LYS	N-CA-CB	5.20	117.50	109.91
1	A	231	ILE	N-CA-C	5.20	115.41	110.42
1	A	115	ALA	N-CA-C	5.19	117.02	111.36
1	A	360	MET	CA-C-N	5.15	127.14	120.44
1	A	360	MET	C-N-CA	5.15	127.14	120.44
1	A	589	TYR	CA-C-N	5.11	127.44	120.54
1	A	589	TYR	C-N-CA	5.11	127.44	120.54
1	A	234	ILE	CA-C-N	5.10	127.11	120.28
1	A	234	ILE	C-N-CA	5.10	127.11	120.28
1	A	597	THR	N-CA-CB	5.09	117.70	110.98
1	A	228	ASP	CB-CA-C	-5.07	102.37	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	N-CA-C	5.06	117.46	111.33
1	A	593	LEU	CB-CA-C	-5.04	102.90	110.92

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	3154	0	1361	417	0
2	A	32	0	14	6	0
All	All	3186	0	1375	417	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 91.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:MET:CB	1:A:630:LYS:HA	1.63	1.29
1:A:623:ARG:CB	1:A:624:PRO:HA	1.60	1.27
1:A:538:PRO:CB	1:A:583:ALA:CB	2.14	1.25
1:A:470:ASN:HA	1:A:473:PHE:CB	1.67	1.23
1:A:541:SER:O	1:A:579:GLY:O	1.58	1.22
1:A:539:TYR:HA	1:A:582:PRO:O	1.06	1.21
1:A:540:LEU:HA	1:A:607:LEU:CB	1.70	1.21
1:A:424:PRO:N	1:A:534:GLU:CB	2.05	1.18
1:A:189:TYR:O	1:A:193:LYS:N	1.78	1.16
1:A:464:VAL:O	1:A:466:LEU:N	1.78	1.15
1:A:80:ASP:CB	1:A:394:VAL:CB	2.25	1.14
1:A:463:SER:HA	1:A:464:VAL:CB	1.68	1.14
1:A:243:HIS:HA	1:A:308:ALA:CB	1.78	1.13
1:A:584:ARG:CB	1:A:585:CYS:HA	1.79	1.12
1:A:538:PRO:CB	1:A:583:ALA:HB2	1.76	1.12
1:A:266:ALA:O	1:A:313:ILE:O	1.68	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ALA:HB3	1:A:316:LEU:CB	1.81	1.11
1:A:435:GLU:CB	1:A:440:PRO:CB	2.31	1.08
1:A:537:GLU:N	1:A:610:TYR:O	1.85	1.08
1:A:539:TYR:CA	1:A:582:PRO:O	2.01	1.08
1:A:266:ALA:CB	1:A:316:LEU:CB	2.31	1.08
1:A:48:LEU:O	1:A:52:ARG:CB	2.02	1.07
1:A:249:LEU:HA	1:A:273:GLY:CA	1.83	1.07
1:A:272:SER:HA	1:A:308:ALA:HA	1.35	1.07
1:A:4:ILE:CB	1:A:70:VAL:HA	1.84	1.07
1:A:623:ARG:CB	1:A:624:PRO:CA	2.30	1.05
1:A:341:ASN:O	1:A:343:HIS:N	1.90	1.04
1:A:538:PRO:CB	1:A:583:ALA:HB3	1.87	1.04
1:A:584:ARG:CB	1:A:585:CYS:CA	2.33	1.04
1:A:424:PRO:CA	1:A:534:GLU:CB	2.35	1.03
1:A:4:ILE:O	1:A:239:TYR:HA	1.57	1.02
1:A:539:TYR:HA	1:A:582:PRO:C	1.84	1.02
1:A:157:LYS:HA	1:A:168:ASN:O	1.61	1.01
1:A:518:MET:CB	1:A:630:LYS:CA	2.40	0.99
1:A:4:ILE:HA	1:A:69:LYS:O	1.59	0.99
1:A:243:HIS:HA	1:A:308:ALA:HB1	1.43	0.98
1:A:540:LEU:CB	1:A:606:GLU:O	2.11	0.98
1:A:537:GLU:CB	1:A:610:TYR:O	2.12	0.97
1:A:459:GLN:O	1:A:498:LYS:CB	2.12	0.97
1:A:541:SER:O	1:A:542:PHE:C	2.07	0.97
1:A:540:LEU:CA	1:A:607:LEU:CB	2.42	0.96
1:A:38:LYS:CB	1:A:40:THR:H	1.78	0.96
1:A:349:THR:N	1:A:414:LYS:O	2.00	0.95
1:A:266:ALA:HB3	1:A:315:ILE:O	1.67	0.94
1:A:189:TYR:O	1:A:193:LYS:O	1.87	0.93
1:A:541:SER:HA	1:A:580:GLU:HA	1.50	0.93
1:A:249:LEU:HA	1:A:273:GLY:HA3	1.48	0.92
1:A:484:GLY:HA2	1:A:487:GLN:O	1.69	0.91
1:A:470:ASN:CA	1:A:473:PHE:CB	2.48	0.91
1:A:485:CYS:CB	1:A:494:VAL:CB	2.49	0.91
1:A:536:LEU:O	1:A:612:VAL:CB	1.74	0.91
1:A:243:HIS:HA	1:A:308:ALA:HB2	1.49	0.90
1:A:428:ALA:O	1:A:449:VAL:CB	2.19	0.90
1:A:460:TYR:CB	1:A:461:GLU:CB	2.49	0.90
1:A:122:PRO:CB	1:A:209:GLN:HA	2.01	0.90
1:A:249:LEU:HA	1:A:273:GLY:HA2	1.53	0.89
1:A:440:PRO:HA	1:A:441:PHE:C	1.97	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:SER:O	1:A:542:PHE:O	1.90	0.89
1:A:422:GLU:HA	1:A:534:GLU:O	1.73	0.89
1:A:189:TYR:O	1:A:193:LYS:C	2.16	0.88
1:A:584:ARG:CB	1:A:586:ILE:N	2.37	0.88
1:A:424:PRO:HA	1:A:534:GLU:CB	2.05	0.85
1:A:464:VAL:C	1:A:466:LEU:H	1.84	0.85
1:A:243:HIS:CA	1:A:308:ALA:HB1	2.05	0.85
1:A:248:GLU:O	1:A:272:SER:O	1.95	0.85
1:A:446:GLY:O	1:A:500:CYS:O	1.95	0.85
1:A:584:ARG:CB	1:A:585:CYS:C	2.50	0.83
1:A:48:LEU:O	1:A:52:ARG:N	2.12	0.82
1:A:340:GLU:O	1:A:342:PRO:N	2.13	0.81
1:A:463:SER:CA	1:A:464:VAL:CB	2.52	0.81
1:A:10:ALA:O	1:A:11:HIS:CB	2.29	0.81
1:A:478:MET:O	1:A:481:ILE:CB	2.30	0.80
1:A:38:LYS:CB	1:A:40:THR:O	2.30	0.80
1:A:432:ILE:CB	1:A:444:SER:O	2.30	0.79
1:A:474:GLN:O	1:A:477:VAL:CB	2.30	0.79
1:A:480:GLY:O	1:A:483:TYR:CB	2.30	0.79
1:A:486:GLU:O	1:A:492:TRP:N	2.16	0.79
1:A:158:VAL:O	1:A:168:ASN:CB	2.30	0.79
1:A:451:PRO:O	1:A:452:LEU:CB	2.31	0.79
1:A:160:LEU:CB	1:A:164:VAL:O	2.31	0.79
1:A:458:MET:O	1:A:459:GLN:CB	2.31	0.79
1:A:14:ALA:H	2:A:701:GCP:C3B	1.97	0.78
1:A:266:ALA:CB	1:A:315:ILE:O	2.30	0.78
1:A:439:ASN:O	1:A:441:PHE:CB	2.31	0.78
1:A:434:ILE:O	1:A:435:GLU:CB	2.32	0.77
1:A:433:HIS:O	1:A:434:ILE:CB	2.31	0.77
1:A:541:SER:C	1:A:579:GLY:O	2.27	0.77
1:A:329:ASP:O	1:A:330:THR:CB	2.31	0.77
1:A:155:LYS:O	1:A:170:THR:O	2.02	0.77
1:A:243:HIS:CB	1:A:308:ALA:HB1	2.14	0.77
1:A:36:VAL:O	1:A:37:ASP:O	2.03	0.77
1:A:432:ILE:O	1:A:433:HIS:CB	2.33	0.76
1:A:535:LEU:CB	1:A:613:THR:HA	2.16	0.76
1:A:621:PRO:O	1:A:622:ARG:CB	2.32	0.76
1:A:536:LEU:H	1:A:613:THR:HA	1.49	0.76
1:A:189:TYR:O	1:A:193:LYS:CA	2.33	0.76
1:A:462:SER:O	1:A:463:SER:CB	2.33	0.76
1:A:532:GLY:O	1:A:533:THR:CB	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLN:C	1:A:473:PHE:H	1.92	0.75
1:A:337:LYS:O	1:A:338:LYS:CB	2.33	0.75
1:A:11:HIS:CB	1:A:98:LEU:CB	2.65	0.75
1:A:156:GLN:C	1:A:169:PHE:HA	2.12	0.75
1:A:438:PRO:O	1:A:439:ASN:CB	2.33	0.75
1:A:243:HIS:CA	1:A:308:ALA:CB	2.62	0.74
1:A:65:TRP:C	1:A:67:ASN:H	1.95	0.74
1:A:471:GLN:C	1:A:473:PHE:N	2.43	0.74
1:A:422:GLU:CA	1:A:534:GLU:O	2.35	0.74
1:A:156:GLN:O	1:A:169:PHE:CB	2.36	0.73
1:A:606:GLU:O	1:A:607:LEU:CB	2.36	0.73
1:A:64:GLN:CB	1:A:69:LYS:CB	2.66	0.73
1:A:122:PRO:O	1:A:123:THR:CB	2.37	0.73
1:A:477:VAL:O	1:A:478:MET:C	2.32	0.73
1:A:122:PRO:CB	1:A:209:GLN:O	2.36	0.72
1:A:539:TYR:CA	1:A:582:PRO:C	2.57	0.72
1:A:38:LYS:CB	1:A:40:THR:N	2.53	0.72
1:A:249:LEU:CA	1:A:273:GLY:HA3	2.19	0.72
1:A:484:GLY:O	1:A:485:CYS:C	2.32	0.72
1:A:3:ILE:O	1:A:4:ILE:CB	2.37	0.72
1:A:266:ALA:N	1:A:315:ILE:O	2.23	0.72
1:A:536:LEU:H	1:A:613:THR:CA	2.01	0.72
1:A:322:LYS:O	1:A:323:LEU:C	2.33	0.71
1:A:422:GLU:CB	1:A:492:TRP:CB	2.68	0.71
1:A:340:GLU:O	1:A:341:ASN:C	2.34	0.71
1:A:243:HIS:O	1:A:244:ARG:C	2.33	0.71
1:A:282:ARG:O	1:A:283:VAL:C	2.33	0.71
1:A:538:PRO:C	1:A:583:ALA:N	2.37	0.71
1:A:158:VAL:O	1:A:159:GLU:CB	2.38	0.70
1:A:537:GLU:CA	1:A:610:TYR:O	2.40	0.70
1:A:14:ALA:H	2:A:701:GCP:H3B1	1.54	0.70
1:A:369:SER:HA	1:A:375:LEU:CB	2.22	0.70
1:A:279:ASP:CB	1:A:286:LYS:CB	2.69	0.69
1:A:4:ILE:CB	1:A:70:VAL:CA	2.65	0.69
1:A:155:LYS:C	1:A:170:THR:O	2.36	0.69
1:A:536:LEU:C	1:A:610:TYR:O	2.35	0.69
1:A:305:ILE:O	1:A:306:ASP:CB	2.40	0.69
1:A:430:TYR:O	1:A:431:THR:CB	2.40	0.69
1:A:207:ARG:CB	1:A:213:LEU:CB	2.71	0.69
1:A:535:LEU:O	1:A:536:LEU:CB	2.41	0.68
1:A:249:LEU:CB	1:A:273:GLY:HA3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:THR:O	1:A:496:ASP:CB	2.41	0.68
1:A:628:ILE:O	1:A:629:ASP:C	2.36	0.68
1:A:122:PRO:C	1:A:208:PHE:O	2.37	0.68
1:A:418:VAL:C	1:A:420:TYR:H	2.02	0.68
1:A:130:ILE:C	1:A:132:GLN:H	2.03	0.67
1:A:122:PRO:CB	1:A:209:GLN:CA	2.72	0.67
1:A:341:ASN:C	1:A:343:HIS:H	1.97	0.67
1:A:271:TYR:O	1:A:272:SER:CB	2.42	0.67
1:A:481:ILE:O	1:A:482:ARG:C	2.35	0.67
1:A:431:THR:CB	1:A:432:ILE:HA	2.25	0.67
1:A:456:SER:C	1:A:458:MET:H	2.02	0.67
1:A:457:GLY:O	1:A:458:MET:C	2.37	0.67
1:A:493:ASN:O	1:A:494:VAL:C	2.37	0.67
1:A:352:PRO:O	1:A:353:SER:CB	2.43	0.66
1:A:623:ARG:CB	1:A:624:PRO:CB	2.73	0.66
1:A:390:PHE:C	1:A:392:GLY:H	2.02	0.66
1:A:440:PRO:HA	1:A:441:PHE:O	1.96	0.66
1:A:249:LEU:CA	1:A:273:GLY:CA	2.70	0.65
1:A:423:ARG:C	1:A:534:GLU:CB	2.69	0.65
1:A:426:LYS:O	1:A:427:ASN:CB	2.44	0.65
1:A:477:VAL:O	1:A:479:GLU:N	2.30	0.65
1:A:479:GLU:O	1:A:481:ILE:N	2.30	0.65
1:A:242:THR:O	1:A:244:ARG:N	2.30	0.65
1:A:243:HIS:O	1:A:245:GLY:N	2.30	0.65
1:A:403:LEU:O	1:A:405:GLU:N	2.30	0.65
1:A:484:GLY:O	1:A:486:GLU:N	2.30	0.65
1:A:147:LYS:O	1:A:149:SER:N	2.30	0.65
1:A:444:SER:O	1:A:445:ILE:CB	2.45	0.65
1:A:156:GLN:CB	1:A:169:PHE:O	2.46	0.64
1:A:471:GLN:O	1:A:473:PHE:N	2.30	0.64
1:A:486:GLU:O	1:A:491:GLY:HA2	1.96	0.64
1:A:484:GLY:CA	1:A:487:GLN:O	2.44	0.64
1:A:613:THR:O	1:A:615:GLY:N	2.30	0.64
1:A:463:SER:O	1:A:501:PHE:O	2.15	0.64
1:A:471:GLN:O	1:A:474:GLN:N	2.30	0.64
1:A:456:SER:O	1:A:458:MET:N	2.30	0.64
1:A:102:LYS:C	1:A:104:GLY:H	2.05	0.64
1:A:241:SER:O	1:A:242:THR:C	2.41	0.63
1:A:65:TRP:O	1:A:67:ASN:N	2.30	0.63
1:A:407:TYR:O	1:A:408:HIS:CB	2.46	0.63
1:A:436:VAL:O	1:A:438:PRO:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ARG:O	1:A:628:ILE:C	2.39	0.63
1:A:390:PHE:O	1:A:392:GLY:N	2.32	0.63
1:A:459:GLN:O	1:A:460:TYR:CB	2.47	0.63
1:A:470:ASN:O	1:A:474:GLN:N	2.32	0.63
1:A:48:LEU:O	1:A:52:ARG:CA	2.46	0.62
1:A:540:LEU:CB	1:A:607:LEU:CB	2.77	0.62
1:A:421:MET:HA	1:A:493:ASN:N	2.14	0.62
1:A:15:GLY:O	1:A:16:LYS:CB	2.47	0.62
1:A:30:ILE:HA	1:A:33:LEU:O	2.00	0.62
1:A:422:GLU:HA	1:A:534:GLU:C	2.25	0.62
1:A:280:SER:O	1:A:281:VAL:CB	2.48	0.61
1:A:626:SER:O	1:A:627:ARG:CB	2.46	0.61
1:A:242:THR:O	1:A:243:HIS:C	2.43	0.61
1:A:14:ALA:H	2:A:701:GCP:H3B2	1.65	0.61
1:A:318:ASN:O	1:A:320:PHE:N	2.32	0.61
1:A:37:ASP:O	1:A:38:LYS:CB	2.48	0.61
1:A:518:MET:HA	1:A:630:LYS:CB	2.31	0.61
1:A:612:VAL:C	1:A:614:THR:H	2.09	0.61
1:A:481:ILE:O	1:A:483:TYR:N	2.34	0.61
1:A:472:SER:O	1:A:475:ASN:CB	2.49	0.61
1:A:403:LEU:C	1:A:405:GLU:H	2.09	0.60
1:A:418:VAL:O	1:A:420:TYR:N	2.30	0.60
1:A:479:GLU:O	1:A:480:GLY:C	2.44	0.60
1:A:148:LEU:C	1:A:150:ALA:H	2.07	0.60
1:A:479:GLU:C	1:A:481:ILE:N	2.52	0.60
1:A:14:ALA:N	2:A:701:GCP:H3B1	2.17	0.60
1:A:39:GLY:O	1:A:40:THR:CB	2.47	0.60
1:A:31:THR:O	1:A:32:GLU:CB	2.50	0.60
1:A:4:ILE:CA	1:A:69:LYS:O	2.42	0.60
1:A:468:TYR:O	1:A:471:GLN:CB	2.49	0.60
1:A:157:LYS:N	1:A:169:PHE:HA	2.16	0.60
1:A:421:MET:HA	1:A:493:ASN:H	1.67	0.59
1:A:456:SER:C	1:A:458:MET:N	2.59	0.59
1:A:538:PRO:CB	1:A:583:ALA:N	2.65	0.59
1:A:528:LEU:O	1:A:531:ALA:N	2.35	0.59
1:A:100:SER:HA	1:A:129:LYS:O	2.03	0.59
1:A:38:LYS:CA	1:A:40:THR:H	2.16	0.59
1:A:610:TYR:O	1:A:611:HIS:C	2.44	0.59
1:A:155:LYS:CB	1:A:156:GLN:CA	2.80	0.59
1:A:467:GLY:O	1:A:469:LEU:N	2.30	0.59
1:A:222:LYS:C	1:A:224:ASN:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:GLN:HA	1:A:497:CYS:O	2.01	0.59
1:A:122:PRO:CA	1:A:208:PHE:O	2.51	0.58
1:A:260:LYS:CB	1:A:406:LYS:CB	2.81	0.58
1:A:155:LYS:CB	1:A:156:GLN:HA	2.32	0.58
1:A:432:ILE:CB	1:A:445:ILE:O	2.51	0.58
1:A:490:TYR:HA	1:A:620:GLN:O	2.02	0.58
1:A:390:PHE:C	1:A:392:GLY:N	2.60	0.58
1:A:210:ASN:O	1:A:211:CYS:CB	2.51	0.58
1:A:403:LEU:C	1:A:405:GLU:N	2.60	0.58
1:A:148:LEU:O	1:A:150:ALA:N	2.37	0.57
1:A:584:ARG:CA	1:A:585:CYS:C	2.77	0.57
1:A:4:ILE:O	1:A:5:ASN:CB	2.52	0.57
1:A:296:THR:O	1:A:297:SER:C	2.47	0.57
1:A:79:MET:O	1:A:81:PHE:N	2.30	0.57
1:A:48:LEU:O	1:A:49:GLU:C	2.45	0.57
1:A:436:VAL:C	1:A:438:PRO:N	2.60	0.57
1:A:156:GLN:C	1:A:169:PHE:CB	2.78	0.57
1:A:584:ARG:CB	1:A:586:ILE:H	2.15	0.57
1:A:133:ASN:O	1:A:134:GLY:C	2.48	0.56
1:A:442:TRP:O	1:A:443:ALA:C	2.48	0.56
1:A:221:ALA:O	1:A:224:ASN:N	2.32	0.56
1:A:440:PRO:CA	1:A:441:PHE:C	2.73	0.56
1:A:536:LEU:H	1:A:613:THR:N	2.03	0.56
1:A:54:ILE:CB	2:A:701:GCP:O3G	2.54	0.56
1:A:352:PRO:O	1:A:411:ILE:CB	2.53	0.56
1:A:431:THR:CB	1:A:432:ILE:CA	2.84	0.56
1:A:481:ILE:C	1:A:483:TYR:N	2.64	0.56
1:A:130:ILE:O	1:A:132:GLN:N	2.39	0.55
1:A:450:SER:O	1:A:451:PRO:C	2.50	0.55
1:A:484:GLY:C	1:A:486:GLU:N	2.64	0.55
1:A:360:MET:CB	1:A:408:HIS:O	2.55	0.55
1:A:156:GLN:C	1:A:169:PHE:CA	2.79	0.55
1:A:148:LEU:C	1:A:150:ALA:N	2.62	0.55
1:A:281:VAL:O	1:A:282:ARG:C	2.49	0.55
1:A:64:GLN:HA	1:A:69:LYS:HA	1.89	0.54
1:A:504:GLY:O	1:A:505:LEU:CB	2.54	0.54
1:A:147:LYS:C	1:A:149:SER:N	2.65	0.54
1:A:432:ILE:CB	1:A:444:SER:C	2.80	0.54
1:A:485:CYS:C	1:A:494:VAL:H	2.16	0.54
1:A:536:LEU:N	1:A:613:THR:HA	2.20	0.54
1:A:318:ASN:O	1:A:319:GLU:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:CB	1:A:209:GLN:C	2.81	0.54
1:A:36:VAL:O	1:A:37:ASP:C	2.51	0.54
1:A:518:MET:CB	1:A:630:LYS:CB	2.85	0.54
1:A:419:ILE:O	1:A:420:TYR:CB	2.55	0.53
1:A:249:LEU:CB	1:A:273:GLY:CA	2.87	0.53
1:A:470:ASN:C	1:A:473:PHE:CB	2.81	0.53
1:A:160:LEU:CB	1:A:165:CYS:HA	2.39	0.53
1:A:249:LEU:CB	1:A:274:VAL:H	2.21	0.53
1:A:351:GLU:O	1:A:411:ILE:CB	2.57	0.53
1:A:541:SER:CA	1:A:579:GLY:O	2.57	0.52
1:A:583:ALA:O	1:A:584:ARG:C	2.51	0.52
1:A:275:LEU:O	1:A:276:HIS:CB	2.57	0.52
1:A:48:LEU:C	1:A:52:ARG:CB	2.79	0.52
1:A:424:PRO:CB	1:A:534:GLU:CB	2.88	0.52
1:A:440:PRO:HA	1:A:441:PHE:CB	2.39	0.52
1:A:286:LYS:O	1:A:287:GLU:CB	2.57	0.52
1:A:222:LYS:C	1:A:224:ASN:N	2.67	0.52
1:A:539:TYR:O	1:A:540:LEU:CB	2.57	0.52
1:A:294:MET:CB	1:A:312:GLU:H	2.23	0.51
1:A:459:GLN:CA	1:A:497:CYS:O	2.58	0.51
1:A:509:PRO:O	1:A:510:VAL:CB	2.58	0.51
1:A:30:ILE:C	1:A:32:GLU:H	2.18	0.51
1:A:38:LYS:CB	1:A:40:THR:C	2.83	0.51
1:A:480:GLY:C	1:A:483:TYR:CB	2.83	0.51
1:A:353:SER:O	1:A:354:LYS:C	2.53	0.51
1:A:221:ALA:O	1:A:222:LYS:C	2.54	0.51
1:A:318:ASN:C	1:A:320:PHE:N	2.69	0.51
1:A:120:GLY:O	1:A:121:ILE:C	2.53	0.51
1:A:422:GLU:N	1:A:534:GLU:O	2.44	0.51
1:A:420:TYR:O	1:A:422:GLU:N	2.38	0.51
1:A:65:TRP:C	1:A:67:ASN:N	2.62	0.51
1:A:485:CYS:CB	1:A:494:VAL:H	2.23	0.51
1:A:97:LEU:N	1:A:125:PHE:O	2.44	0.50
1:A:129:LYS:O	1:A:130:ILE:CB	2.58	0.50
1:A:252:ASN:O	1:A:253:VAL:C	2.52	0.50
1:A:583:ALA:O	1:A:584:ARG:O	2.30	0.50
1:A:219:GLY:O	1:A:220:SER:O	2.30	0.50
1:A:296:THR:O	1:A:297:SER:O	2.30	0.50
1:A:484:GLY:O	1:A:487:GLN:O	2.30	0.50
1:A:627:ARG:O	1:A:628:ILE:O	2.30	0.50
1:A:147:LYS:O	1:A:148:LEU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:CA	1:A:583:ALA:HB2	2.37	0.49
1:A:351:GLU:O	1:A:352:PRO:O	2.30	0.49
1:A:485:CYS:O	1:A:492:TRP:C	2.55	0.49
1:A:538:PRO:CB	1:A:583:ALA:H	2.25	0.49
1:A:418:VAL:C	1:A:420:TYR:N	2.68	0.49
1:A:629:ASP:O	1:A:630:LYS:C	2.54	0.49
1:A:194:SER:O	1:A:195:LEU:CB	2.60	0.49
1:A:349:THR:H	1:A:415:GLU:HA	1.76	0.49
1:A:405:GLU:O	1:A:406:LYS:O	2.30	0.49
1:A:102:LYS:O	1:A:104:GLY:N	2.46	0.49
1:A:415:GLU:O	1:A:416:PRO:CB	2.61	0.49
1:A:510:VAL:O	1:A:511:SER:CB	2.60	0.49
1:A:244:ARG:O	1:A:245:GLY:O	2.30	0.49
1:A:423:ARG:O	1:A:424:PRO:O	2.30	0.49
1:A:35:SER:O	1:A:36:VAL:O	2.30	0.49
1:A:617:PRO:C	1:A:619:CYS:H	2.21	0.49
1:A:103:ASP:O	1:A:105:VAL:N	2.45	0.48
1:A:278:ARG:O	1:A:279:ASP:CB	2.60	0.48
1:A:370:ASP:C	1:A:372:ASP:H	2.21	0.48
1:A:450:SER:O	1:A:451:PRO:O	2.30	0.48
1:A:457:GLY:O	1:A:458:MET:O	2.30	0.48
1:A:628:ILE:O	1:A:629:ASP:O	2.30	0.48
1:A:100:SER:H	1:A:103:ASP:CB	2.26	0.48
1:A:478:MET:C	1:A:481:ILE:CB	2.85	0.48
1:A:541:SER:CA	1:A:580:GLU:HA	2.34	0.48
1:A:534:GLU:O	1:A:535:LEU:C	2.55	0.48
1:A:295:TYR:O	1:A:296:THR:O	2.30	0.48
1:A:432:ILE:O	1:A:444:SER:O	2.32	0.48
1:A:612:VAL:O	1:A:614:THR:N	2.46	0.48
1:A:36:VAL:C	1:A:37:ASP:O	2.55	0.48
1:A:102:LYS:C	1:A:104:GLY:N	2.71	0.48
1:A:219:GLY:O	1:A:220:SER:C	2.57	0.48
1:A:460:TYR:CB	1:A:461:GLU:CA	2.91	0.48
1:A:253:VAL:CB	1:A:324:ASN:O	2.61	0.47
1:A:353:SER:O	1:A:354:LYS:O	2.31	0.47
1:A:237:LYS:O	1:A:238:PHE:CB	2.63	0.47
1:A:443:ALA:O	1:A:444:SER:C	2.58	0.47
1:A:535:LEU:CA	1:A:613:THR:HA	2.43	0.47
1:A:349:THR:N	1:A:415:GLU:HA	2.30	0.47
1:A:62:SER:HA	1:A:71:ASN:HA	1.96	0.47
1:A:156:GLN:N	1:A:170:THR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:C	1:A:481:ILE:H	2.22	0.47
1:A:482:ARG:HA	1:A:485:CYS:CB	2.45	0.47
1:A:247:SER:O	1:A:248:GLU:O	2.33	0.46
1:A:2:LYS:CB	1:A:68:THR:CB	2.93	0.46
1:A:528:LEU:O	1:A:529:LYS:C	2.58	0.46
1:A:47:LEU:O	1:A:48:LEU:CB	2.64	0.46
1:A:133:ASN:O	1:A:135:ILE:N	2.49	0.46
1:A:477:VAL:C	1:A:479:GLU:N	2.71	0.46
1:A:275:LEU:O	1:A:291:VAL:CB	2.64	0.46
1:A:155:LYS:CB	1:A:156:GLN:CB	2.93	0.46
1:A:423:ARG:CB	1:A:495:THR:O	2.64	0.46
1:A:505:LEU:O	1:A:506:TYR:CB	2.64	0.46
1:A:525:GLU:O	1:A:528:LEU:CB	2.64	0.46
1:A:275:LEU:O	1:A:291:VAL:HA	2.16	0.46
1:A:58:THR:HA	1:A:74:ASP:O	2.16	0.46
1:A:535:LEU:N	1:A:613:THR:HA	2.31	0.46
1:A:612:VAL:C	1:A:614:THR:N	2.74	0.45
1:A:222:LYS:O	1:A:224:ASN:N	2.49	0.45
1:A:482:ARG:O	1:A:483:TYR:C	2.59	0.45
1:A:130:ILE:C	1:A:132:GLN:N	2.69	0.45
1:A:420:TYR:O	1:A:535:LEU:O	2.34	0.45
1:A:246:PRO:O	1:A:247:SER:CB	2.64	0.45
1:A:464:VAL:C	1:A:466:LEU:N	2.48	0.45
1:A:463:SER:C	1:A:501:PHE:O	2.60	0.45
1:A:249:LEU:CA	1:A:273:GLY:HA2	2.34	0.45
1:A:535:LEU:CB	1:A:613:THR:CA	2.92	0.44
1:A:223:SER:O	1:A:224:ASN:C	2.61	0.44
1:A:538:PRO:CB	1:A:583:ALA:CA	2.92	0.44
1:A:154:ILE:CB	1:A:175:TRP:HA	2.48	0.44
1:A:266:ALA:CA	1:A:315:ILE:O	2.65	0.44
1:A:480:GLY:O	1:A:481:ILE:O	2.36	0.44
1:A:486:GLU:O	1:A:491:GLY:CA	2.62	0.44
1:A:50:ARG:C	1:A:52:ARG:N	2.75	0.44
1:A:14:ALA:N	2:A:701:GCP:C3B	2.73	0.44
1:A:7:GLY:HA2	1:A:94:GLY:O	2.18	0.44
1:A:147:LYS:C	1:A:149:SER:H	2.26	0.44
1:A:474:GLN:C	1:A:477:VAL:CB	2.91	0.44
1:A:541:SER:O	1:A:579:GLY:C	2.48	0.43
1:A:189:TYR:C	1:A:193:LYS:H	2.15	0.43
1:A:266:ALA:HB2	1:A:316:LEU:CB	2.40	0.43
1:A:499:ILE:O	1:A:500:CYS:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:C	1:A:315:ILE:O	2.61	0.43
1:A:486:GLU:O	1:A:491:GLY:C	2.61	0.43
1:A:255:LYS:O	1:A:256:ILE:CB	2.67	0.43
1:A:537:GLU:CB	1:A:610:TYR:C	2.87	0.43
1:A:48:LEU:C	1:A:50:ARG:N	2.73	0.42
1:A:518:MET:CA	1:A:630:LYS:CB	2.97	0.42
1:A:617:PRO:C	1:A:619:CYS:N	2.78	0.42
1:A:351:GLU:O	1:A:352:PRO:C	2.61	0.42
1:A:266:ALA:HB3	1:A:315:ILE:C	2.40	0.42
1:A:190:MET:HA	1:A:193:LYS:O	2.20	0.42
1:A:100:SER:N	1:A:103:ASP:CB	2.83	0.42
1:A:471:GLN:O	1:A:472:SER:C	2.60	0.42
1:A:4:ILE:CB	1:A:70:VAL:CB	2.98	0.41
1:A:100:SER:O	1:A:101:ALA:C	2.62	0.41
1:A:154:ILE:CB	1:A:175:TRP:CB	2.98	0.41
1:A:440:PRO:CA	1:A:441:PHE:CB	2.99	0.41
1:A:476:ALA:O	1:A:479:GLU:CB	2.68	0.41
1:A:328:GLY:O	1:A:329:ASP:CB	2.68	0.41
1:A:484:GLY:O	1:A:486:GLU:C	2.63	0.41
1:A:493:ASN:O	1:A:494:VAL:O	2.37	0.41
1:A:425:LEU:C	1:A:451:PRO:CB	2.94	0.41
1:A:475:ASN:C	1:A:477:VAL:N	2.78	0.41
1:A:155:LYS:HA	1:A:156:GLN:HA	1.96	0.41
1:A:321:LEU:O	1:A:322:LYS:O	2.39	0.41
1:A:189:TYR:C	1:A:193:LYS:O	2.61	0.40
1:A:470:ASN:O	1:A:473:PHE:CB	2.69	0.40
1:A:50:ARG:O	1:A:52:ARG:N	2.54	0.40
1:A:170:THR:O	1:A:171:GLU:CB	2.69	0.40
1:A:257:GLU:CB	1:A:371:SER:HA	2.52	0.40
1:A:295:TYR:O	1:A:296:THR:C	2.64	0.40
1:A:307:ARG:C	1:A:309:TYR:N	2.78	0.40
1:A:469:LEU:C	1:A:471:GLN:H	2.29	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	636/638 (100%)	328 (52%)	128 (20%)	180 (28%)	0 0

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	4	ILE
1	A	5	ASN
1	A	11	HIS
1	A	12	VAL
1	A	32	GLU
1	A	37	ASP
1	A	40	THR
1	A	60	ILE
1	A	66	GLU
1	A	99	ILE
1	A	132	GLN
1	A	147	LYS
1	A	148	LEU
1	A	159	GLU
1	A	162	PRO
1	A	220	SER
1	A	236	ASN
1	A	238	PHE
1	A	242	THR
1	A	243	HIS
1	A	244	ARG
1	A	246	PRO
1	A	255	LYS
1	A	272	SER
1	A	276	HIS
1	A	279	ASP
1	A	283	VAL
1	A	296	THR
1	A	297	SER
1	A	306	ASP
1	A	319	GLU
1	A	322	LYS
1	A	323	LEU

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Mol	Chain	Res	Type
1	A	338	LYS
1	A	342	PRO
1	A	343	HIS
1	A	344	PRO
1	A	345	LEU
1	A	352	PRO
1	A	353	SER
1	A	406	LYS
1	A	416	PRO
1	A	423	ARG
1	A	424	PRO
1	A	427	ASN
1	A	431	THR
1	A	433	HIS
1	A	434	ILE
1	A	435	GLU
1	A	436	VAL
1	A	438	PRO
1	A	439	ASN
1	A	444	SER
1	A	445	ILE
1	A	451	PRO
1	A	452	LEU
1	A	458	MET
1	A	459	GLN
1	A	462	SER
1	A	463	SER
1	A	464	VAL
1	A	465	SER
1	A	471	GLN
1	A	477	VAL
1	A	478	MET
1	A	479	GLU
1	A	481	ILE
1	A	483	TYR
1	A	485	CYS
1	A	494	VAL
1	A	496	ASP
1	A	506	TYR
1	A	508	SER
1	A	509	PRO
1	A	513	PRO

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Mol	Chain	Res	Type
1	A	533	THR
1	A	536	LEU
1	A	581	ILE
1	A	584	ARG
1	A	605	THR
1	A	612	VAL
1	A	614	THR
1	A	616	GLU
1	A	617	PRO
1	A	621	PRO
1	A	622	ARG
1	A	623	ARG
1	A	624	PRO
1	A	627	ARG
1	A	628	ILE
1	A	629	ASP
1	A	29	ALA
1	A	36	VAL
1	A	38	LYS
1	A	70	VAL
1	A	92	LEU
1	A	101	ALA
1	A	103	ASP
1	A	104	GLY
1	A	123	THR
1	A	130	ILE
1	A	131	ASP
1	A	149	SER
1	A	152	ILE
1	A	157	LYS
1	A	158	VAL
1	A	169	PHE
1	A	195	LEU
1	A	211	CYS
1	A	222	LYS
1	A	245	GLY
1	A	248	GLU
1	A	253	VAL
1	A	281	VAL
1	A	282	ARG
1	A	315	ILE
1	A	318	ASN

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Mol	Chain	Res	Type
1	A	330	THR
1	A	376	ARG
1	A	391	LEU
1	A	404	GLN
1	A	415	GLU
1	A	419	ILE
1	A	453	PRO
1	A	457	GLY
1	A	480	GLY
1	A	482	ARG
1	A	499	ILE
1	A	500	CYS
1	A	511	SER
1	A	540	LEU
1	A	542	PHE
1	A	582	PRO
1	A	607	LEU
1	A	618	VAL
1	A	619	CYS
1	A	630	LYS
1	A	72	ILE
1	A	78	HIS
1	A	90	SER
1	A	106	GLN
1	A	136	ASP
1	A	153	VAL
1	A	215	PRO
1	A	223	SER
1	A	247	SER
1	A	408	HIS
1	A	437	PRO
1	A	460	TYR
1	A	472	SER
1	A	510	VAL
1	A	572	ASN
1	A	604	LEU
1	A	611	HIS
1	A	625	ASN
1	A	30	ILE
1	A	110	ARG
1	A	134	GLY
1	A	256	ILE

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Mol	Chain	Res	Type
1	A	301	GLU
1	A	317	GLN
1	A	341	ASN
1	A	409	VAL
1	A	420	TYR
1	A	426	LYS
1	A	443	ALA
1	A	456	SER
1	A	221	ALA
1	A	316	LEU
1	A	354	LYS
1	A	495	THR
1	A	505	LEU
1	A	539	TYR
1	A	287	GLU
1	A	599	GLY
1	A	274	VAL
1	A	91	VAL
1	A	305	ILE
1	A	467	GLY

5.3.2 Protein sidechains [i](#)

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

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](#)

1 ligand is 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	GCP	A	701	-	32,34,34	1.58	6 (18%)	49,54,54	1.17	5 (10%)

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	GCP	A	701	-	-	11/19/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GCP	PA-O3A	-4.22	1.54	1.59
2	A	701	GCP	C5-N7	-3.70	1.31	1.39
2	A	701	GCP	C6-N1	3.25	1.44	1.38
2	A	701	GCP	C4-N3	2.75	1.40	1.34
2	A	701	GCP	PG-O3G	-2.48	1.49	1.55
2	A	701	GCP	PG-O1G	-2.13	1.45	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GCP	C2-N1-C6	-3.26	119.19	125.11
2	A	701	GCP	O2G-PG-O1G	-2.57	105.73	112.39
2	A	701	GCP	O2'-C2'-C3'	2.26	119.06	111.82
2	A	701	GCP	N1-C2-N3	2.22	127.39	123.32
2	A	701	GCP	C6-C5-C4	-2.15	115.60	118.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

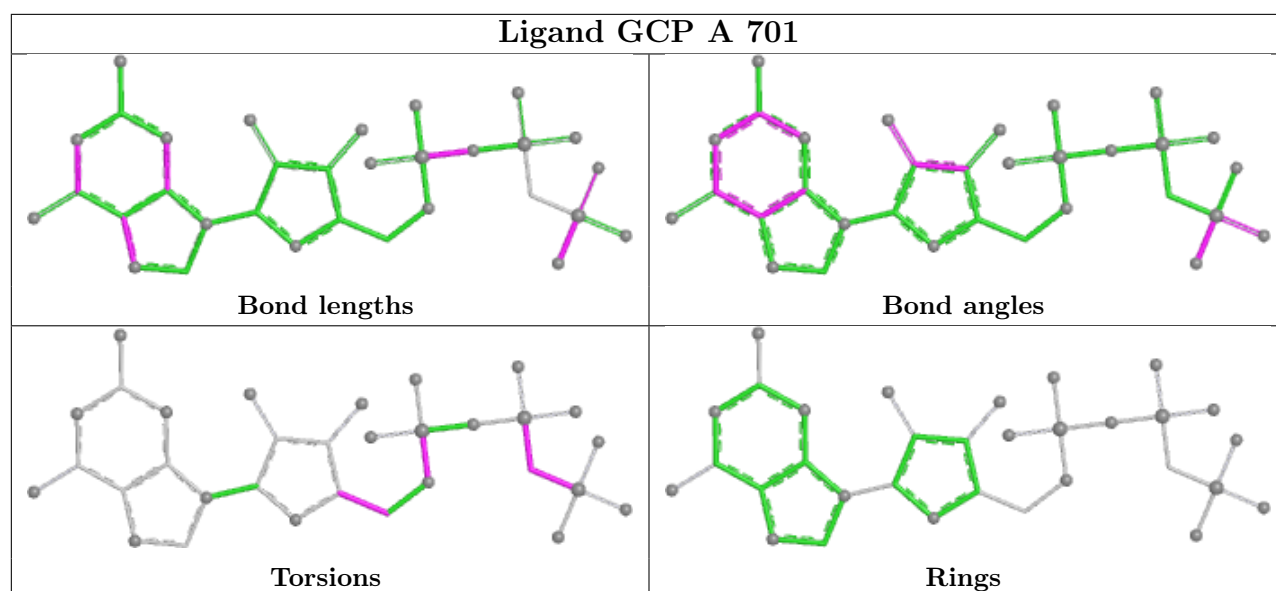
Mol	Chain	Res	Type	Atoms
2	A	701	GCP	PB-C3B-PG-O1G
2	A	701	GCP	PG-C3B-PB-O1B
2	A	701	GCP	PG-C3B-PB-O2B
2	A	701	GCP	PG-C3B-PB-O3A
2	A	701	GCP	C5'-O5'-PA-O3A
2	A	701	GCP	C5'-O5'-PA-O1A
2	A	701	GCP	C5'-O5'-PA-O2A
2	A	701	GCP	O4'-C4'-C5'-O5'
2	A	701	GCP	C3'-C4'-C5'-O5'
2	A	701	GCP	PB-C3B-PG-O2G
2	A	701	GCP	PB-C3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GCP	6	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

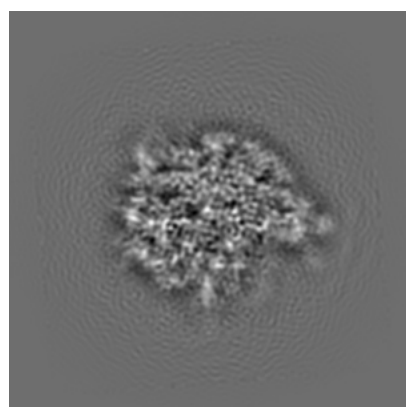
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2183. These allow visual inspection of the internal detail of the map and identification of artifacts.

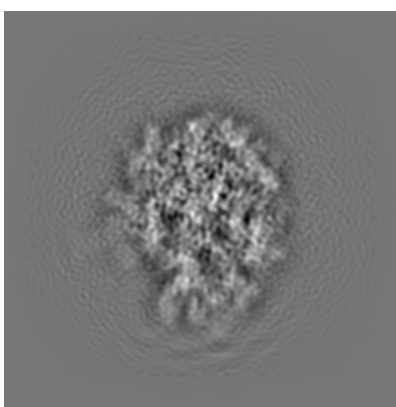
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

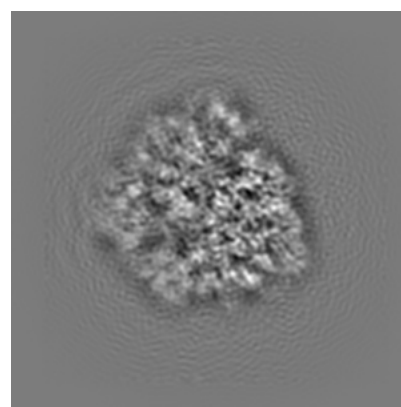
6.1.1 Primary map



X



Y

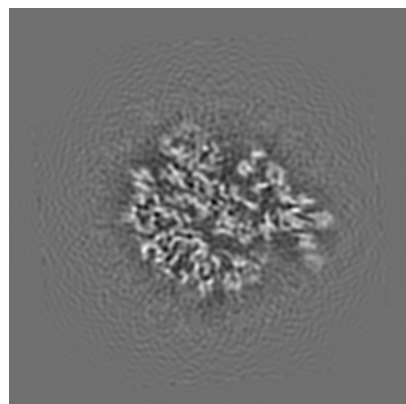


Z

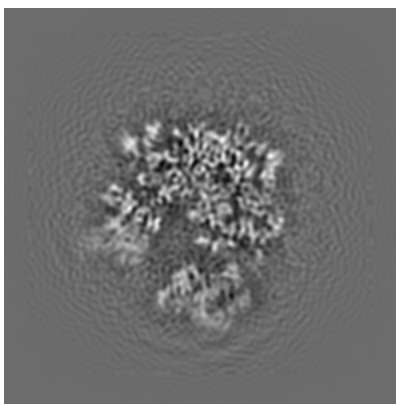
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

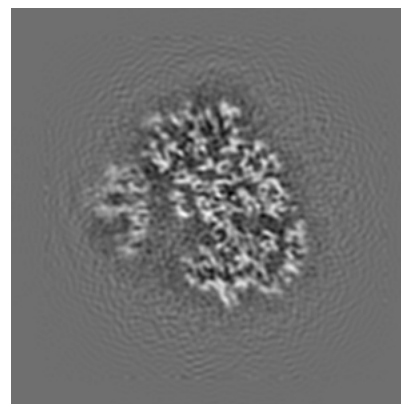
6.2.1 Primary map



X Index: 184



Y Index: 184

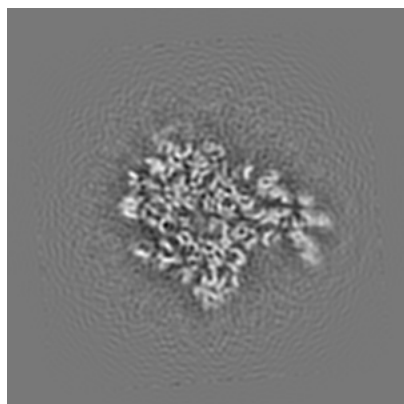


Z Index: 184

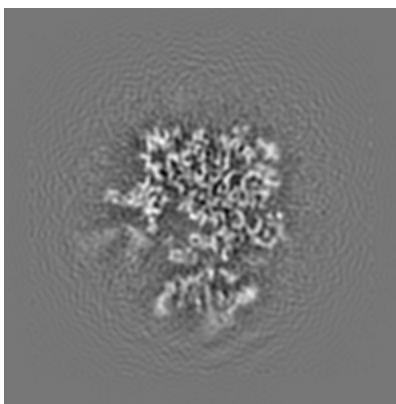
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

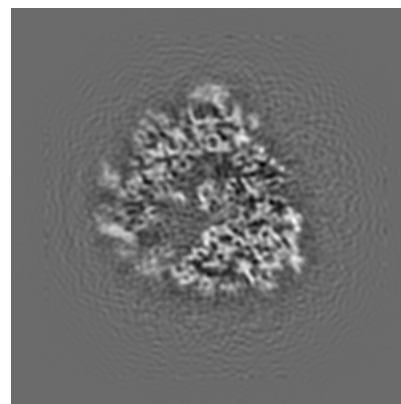
6.3.1 Primary map



X Index: 191



Y Index: 192

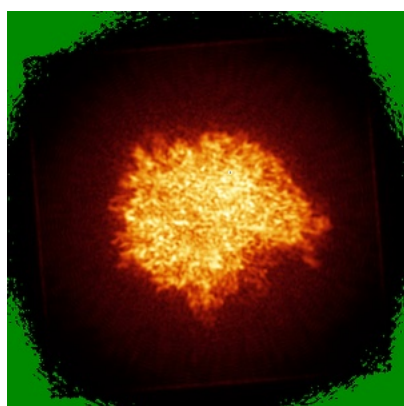


Z Index: 173

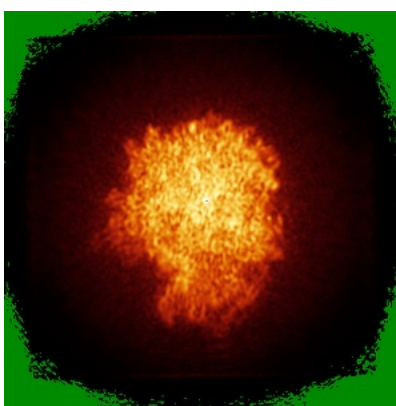
The images above show the largest variance slices of the map in three orthogonal directions.

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

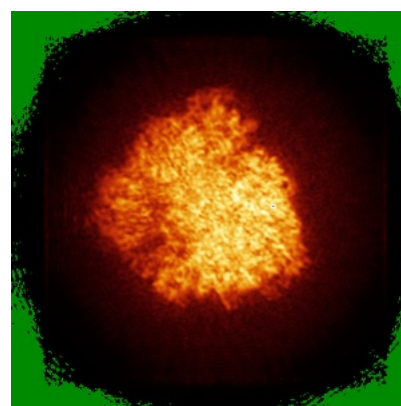
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

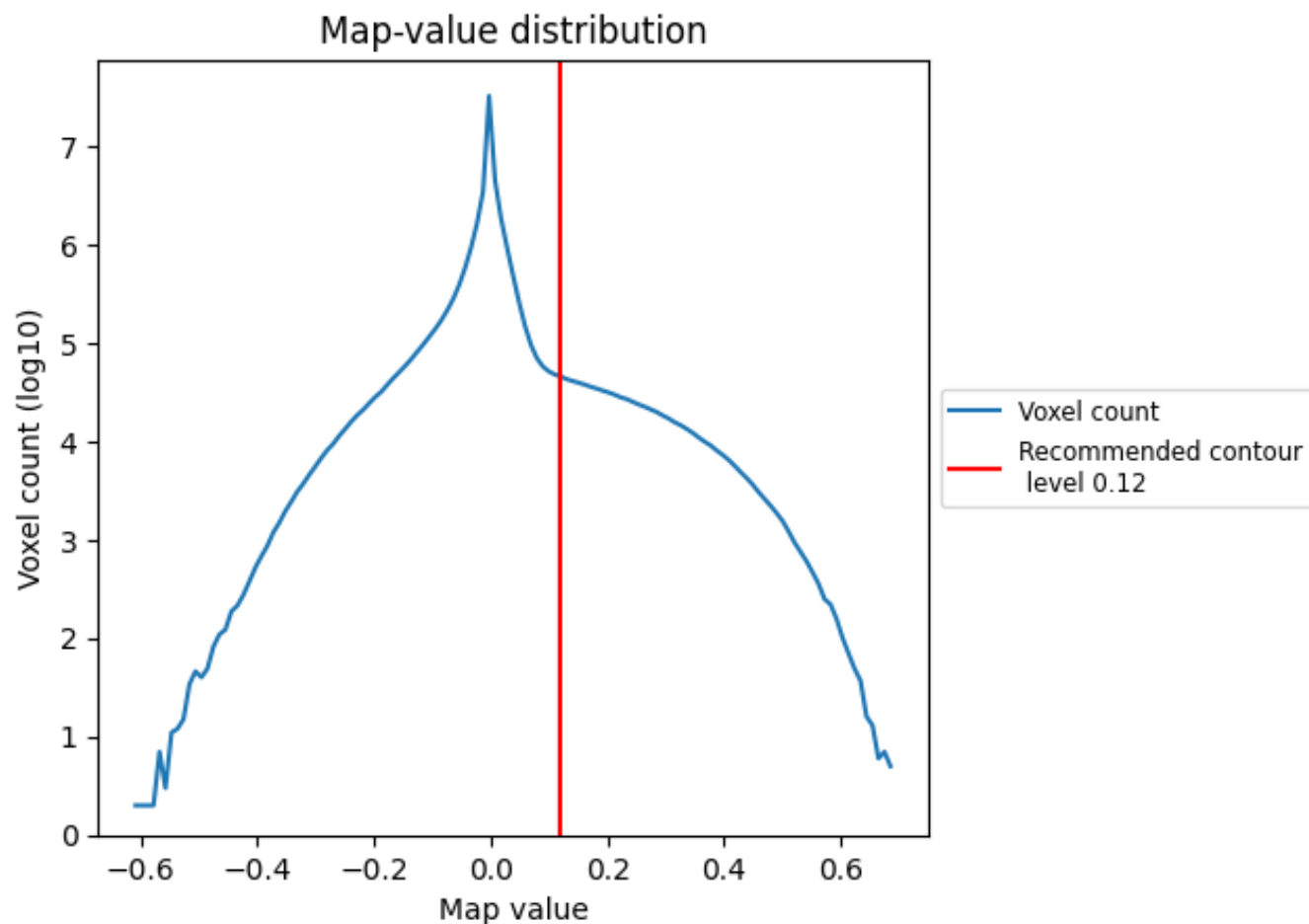
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

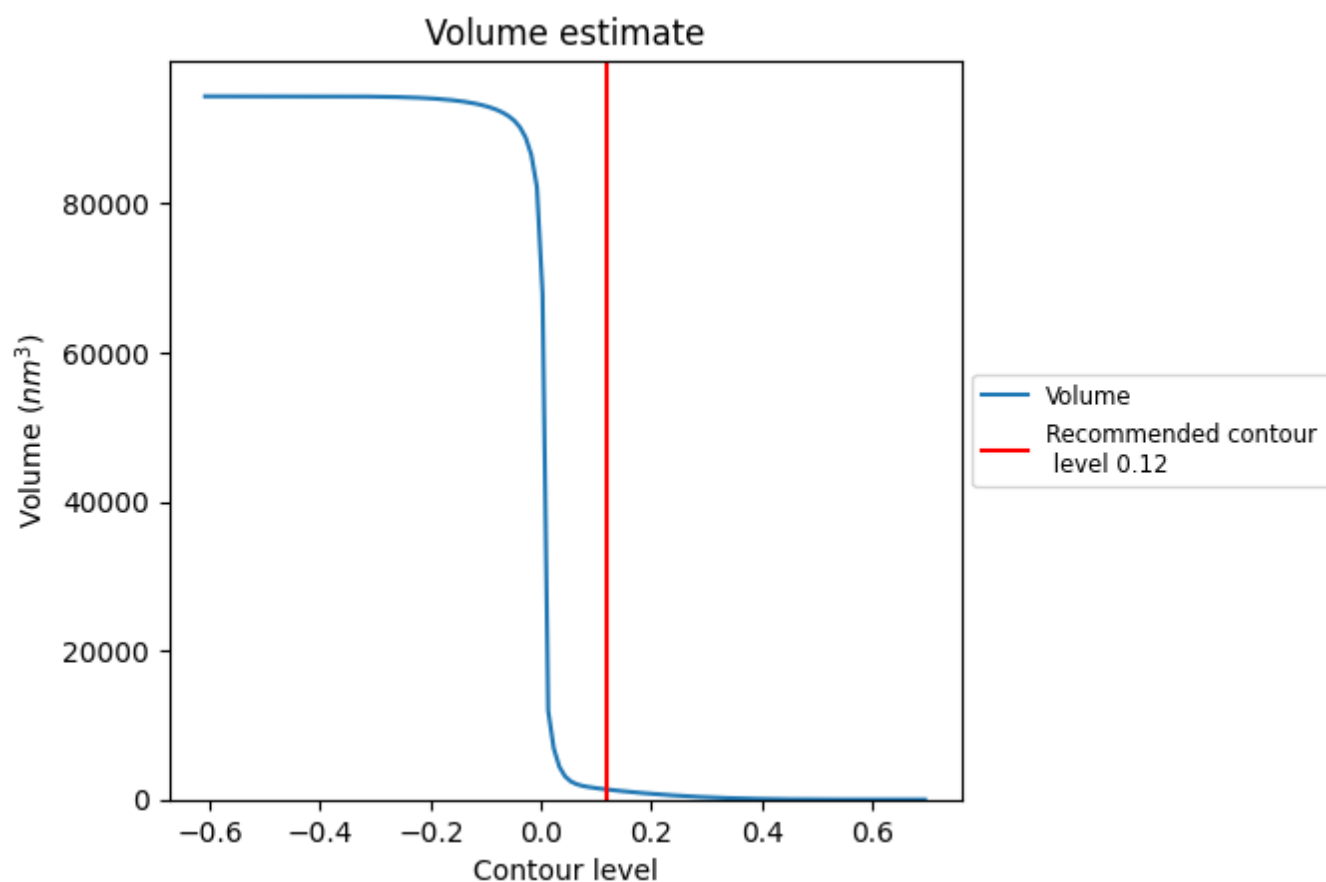
This section contains the results of statistical analysis of the map.

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.

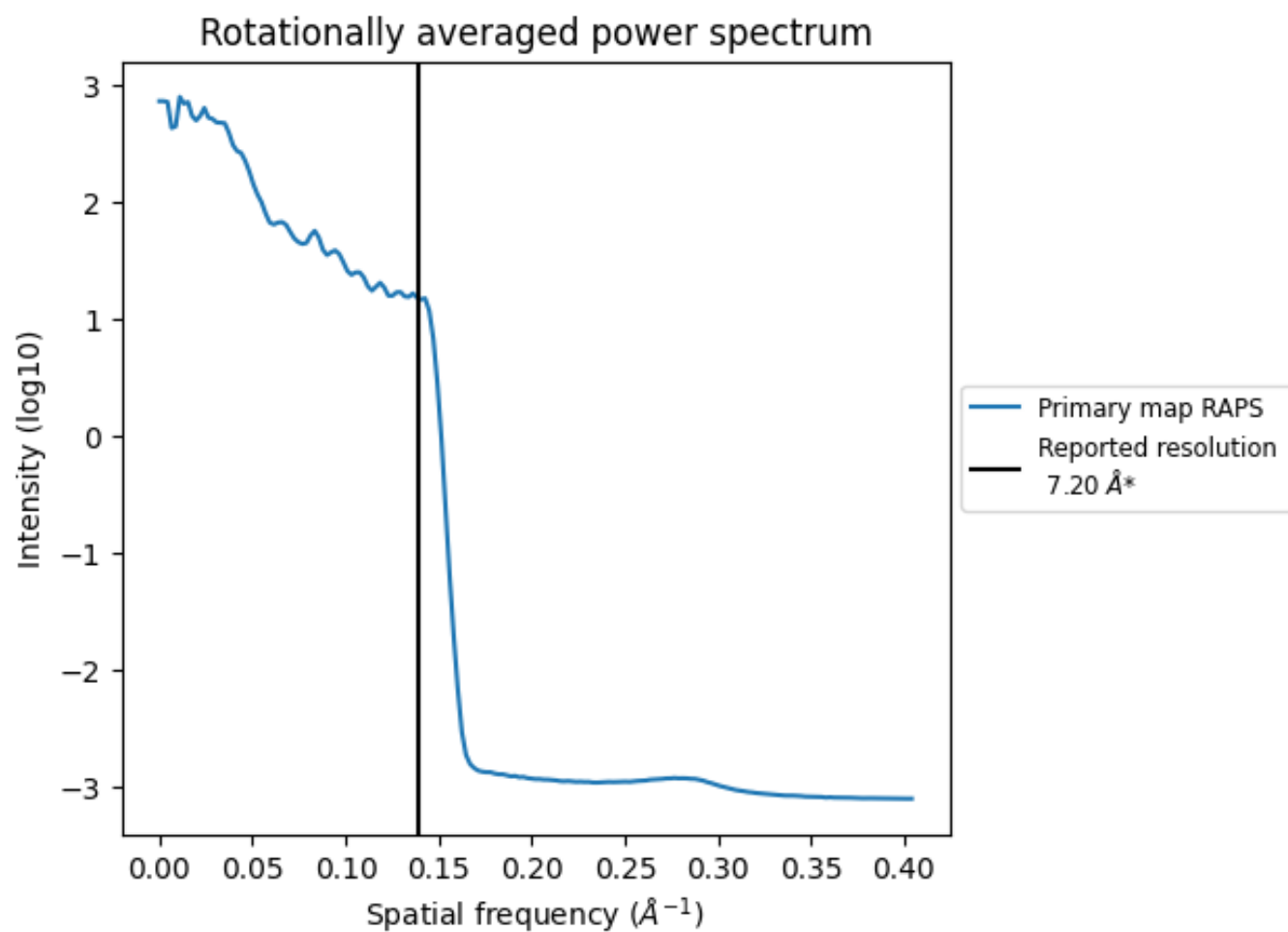
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1348 nm³; this corresponds to an approximate mass of 1218 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 0.139 Å⁻¹

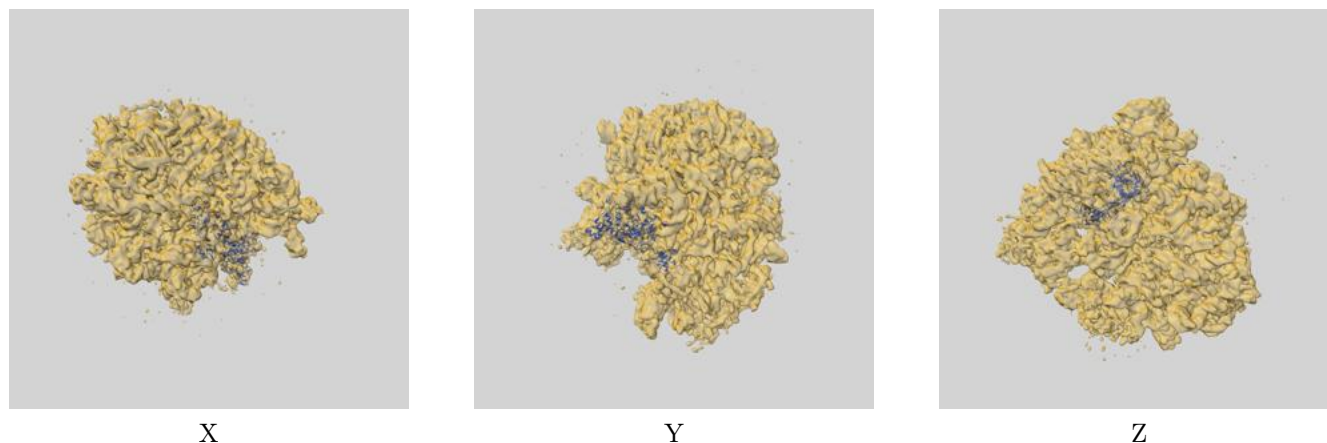
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

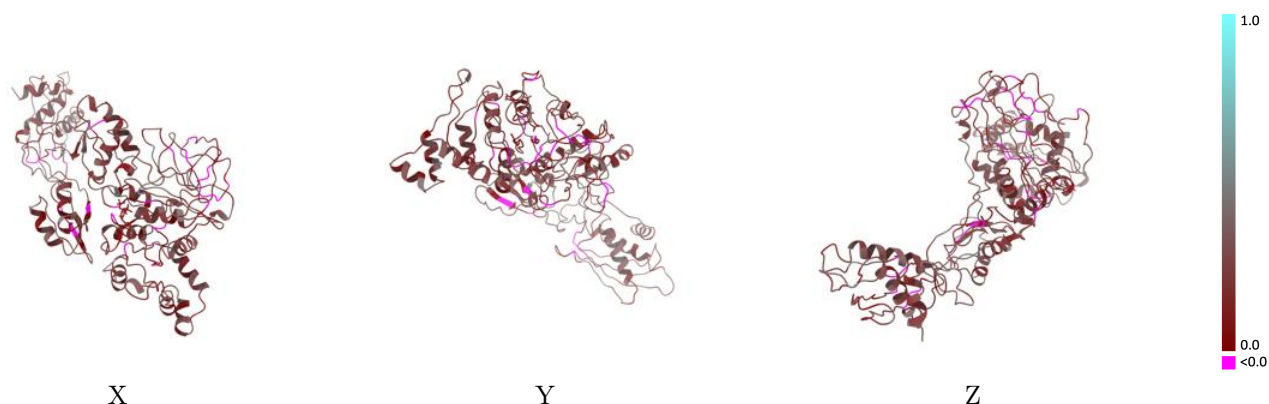
This section contains information regarding the fit between EMDB map EMD-2183 and PDB model 3J25. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



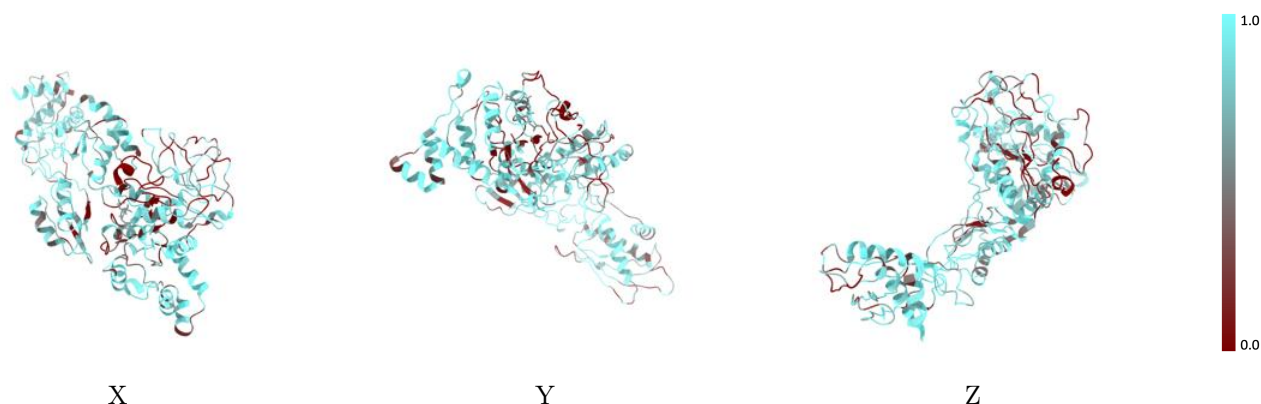
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



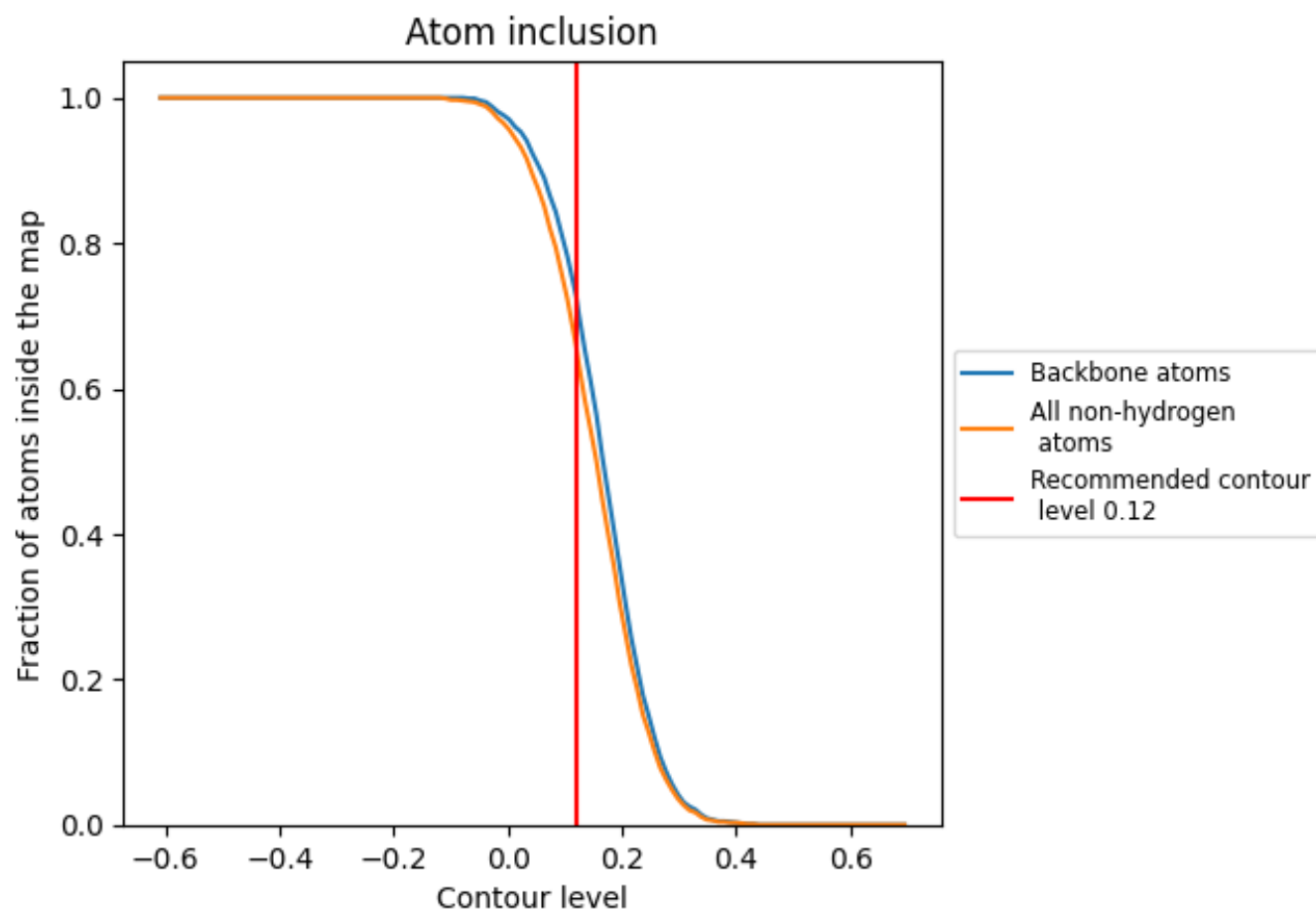
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.2260
A	0.6580	0.2260

