Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 04:58 PM JST

PDB ID	:	24CH / pdb_000024ch
EMDB ID	:	EMD-69437
Title	:	Cryo-EM structure of the NADPH-bound ClbB's polyketide synthase module involved in the colibactin biosynthesis
Deposited on	:	2026-02-27
Resolution	:	2.46 Å(reported)
Based on initial model	:	.

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

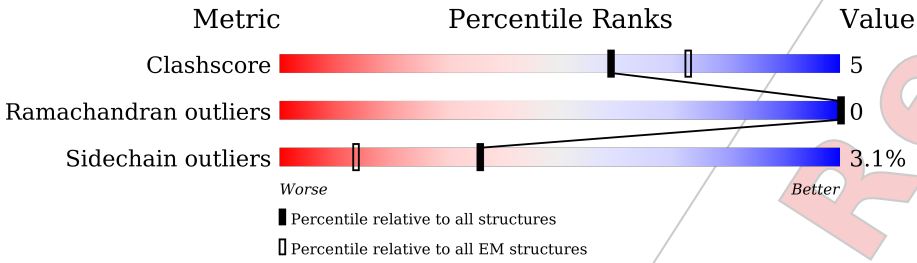
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13

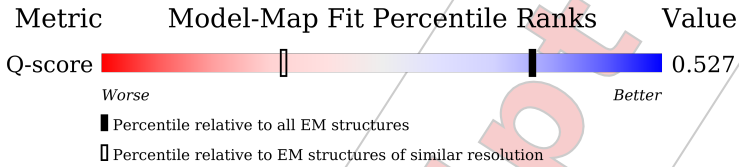
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.46 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	6014 (1.96 - 2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2164	79% 12% 9%
1	B	2164	80% 11% 9%

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30532 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 Colibactin hybrid non-ribosomal peptide synthetase/type I polyketide synthase ClbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1972	Total	C	N	O	S	0	0
			15170	9557	2694	2840	79		
1	B	1972	Total	C	N	O	S	0	0
			15170	9557	2694	2840	79		

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1043	MET	-	initiating methionine	UNP Q0P7J2
A	1044	GLY	-	expression tag	UNP Q0P7J2
A	1045	SER	-	expression tag	UNP Q0P7J2
A	1046	SER	-	expression tag	UNP Q0P7J2
A	1047	HIS	-	expression tag	UNP Q0P7J2
A	1048	HIS	-	expression tag	UNP Q0P7J2
A	1049	HIS	-	expression tag	UNP Q0P7J2
A	1050	HIS	-	expression tag	UNP Q0P7J2
A	1051	HIS	-	expression tag	UNP Q0P7J2
A	1052	HIS	-	expression tag	UNP Q0P7J2
A	1053	SER	-	expression tag	UNP Q0P7J2
A	1054	SER	-	expression tag	UNP Q0P7J2
A	1055	GLY	-	expression tag	UNP Q0P7J2
A	1056	LEU	-	expression tag	UNP Q0P7J2
A	1057	VAL	-	expression tag	UNP Q0P7J2
A	1058	PRO	-	expression tag	UNP Q0P7J2
A	1059	ARG	-	expression tag	UNP Q0P7J2
A	1060	GLY	-	expression tag	UNP Q0P7J2
A	1061	SER	-	expression tag	UNP Q0P7J2
A	1062	HIS	-	expression tag	UNP Q0P7J2
A	1063	MET	-	expression tag	UNP Q0P7J2
A	1064	ALA	-	expression tag	UNP Q0P7J2
A	1065	SER	-	expression tag	UNP Q0P7J2
A	1066	MET	-	expression tag	UNP Q0P7J2
A	1067	THR	-	expression tag	UNP Q0P7J2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	GLY	-	expression tag	UNP Q0P7J2
A	1069	GLY	-	expression tag	UNP Q0P7J2
A	1070	GLN	-	expression tag	UNP Q0P7J2
A	1071	GLN	-	expression tag	UNP Q0P7J2
A	1072	MET	-	expression tag	UNP Q0P7J2
A	1073	GLY	-	expression tag	UNP Q0P7J2
A	1074	ARG	-	expression tag	UNP Q0P7J2
A	1075	GLY	-	expression tag	UNP Q0P7J2
A	1076	SER	-	expression tag	UNP Q0P7J2
A	1077	GLU	-	expression tag	UNP Q0P7J2
A	1078	PHE	-	expression tag	UNP Q0P7J2
A	1079	GLU	-	expression tag	UNP Q0P7J2
A	1080	LEU	-	expression tag	UNP Q0P7J2
A	1081	ARG	-	expression tag	UNP Q0P7J2
A	1082	ARG	-	expression tag	UNP Q0P7J2
A	1083	GLN	-	expression tag	UNP Q0P7J2
A	1084	ALA	-	expression tag	UNP Q0P7J2
A	1085	CYS	-	expression tag	UNP Q0P7J2
B	1043	MET	-	initiating methionine	UNP Q0P7J2
B	1044	GLY	-	expression tag	UNP Q0P7J2
B	1045	SER	-	expression tag	UNP Q0P7J2
B	1046	SER	-	expression tag	UNP Q0P7J2
B	1047	HIS	-	expression tag	UNP Q0P7J2
B	1048	HIS	-	expression tag	UNP Q0P7J2
B	1049	HIS	-	expression tag	UNP Q0P7J2
B	1050	HIS	-	expression tag	UNP Q0P7J2
B	1051	HIS	-	expression tag	UNP Q0P7J2
B	1052	HIS	-	expression tag	UNP Q0P7J2
B	1053	SER	-	expression tag	UNP Q0P7J2
B	1054	SER	-	expression tag	UNP Q0P7J2
B	1055	GLY	-	expression tag	UNP Q0P7J2
B	1056	LEU	-	expression tag	UNP Q0P7J2
B	1057	VAL	-	expression tag	UNP Q0P7J2
B	1058	PRO	-	expression tag	UNP Q0P7J2
B	1059	ARG	-	expression tag	UNP Q0P7J2
B	1060	GLY	-	expression tag	UNP Q0P7J2
B	1061	SER	-	expression tag	UNP Q0P7J2
B	1062	HIS	-	expression tag	UNP Q0P7J2
B	1063	MET	-	expression tag	UNP Q0P7J2
B	1064	ALA	-	expression tag	UNP Q0P7J2
B	1065	SER	-	expression tag	UNP Q0P7J2
B	1066	MET	-	expression tag	UNP Q0P7J2

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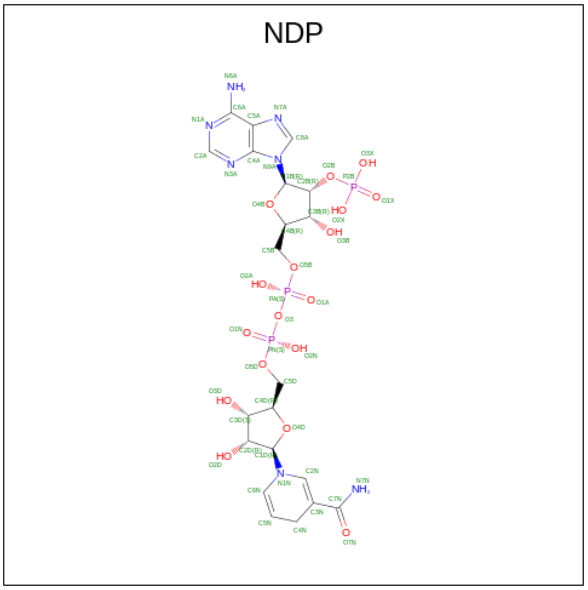
Chain	Residue	Modelled	Actual	Comment	Reference
B	1067	THR	-	expression tag	UNP Q0P7J2
B	1068	GLY	-	expression tag	UNP Q0P7J2
B	1069	GLY	-	expression tag	UNP Q0P7J2
B	1070	GLN	-	expression tag	UNP Q0P7J2
B	1071	GLN	-	expression tag	UNP Q0P7J2
B	1072	MET	-	expression tag	UNP Q0P7J2
B	1073	GLY	-	expression tag	UNP Q0P7J2
B	1074	ARG	-	expression tag	UNP Q0P7J2
B	1075	GLY	-	expression tag	UNP Q0P7J2
B	1076	SER	-	expression tag	UNP Q0P7J2
B	1077	GLU	-	expression tag	UNP Q0P7J2
B	1078	PHE	-	expression tag	UNP Q0P7J2
B	1079	GLU	-	expression tag	UNP Q0P7J2
B	1080	LEU	-	expression tag	UNP Q0P7J2
B	1081	ARG	-	expression tag	UNP Q0P7J2
B	1082	ARG	-	expression tag	UNP Q0P7J2
B	1083	GLN	-	expression tag	UNP Q0P7J2
B	1084	ALA	-	expression tag	UNP Q0P7J2
B	1085	CYS	-	expression tag	UNP Q0P7J2

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	48	21	7	17	3	0

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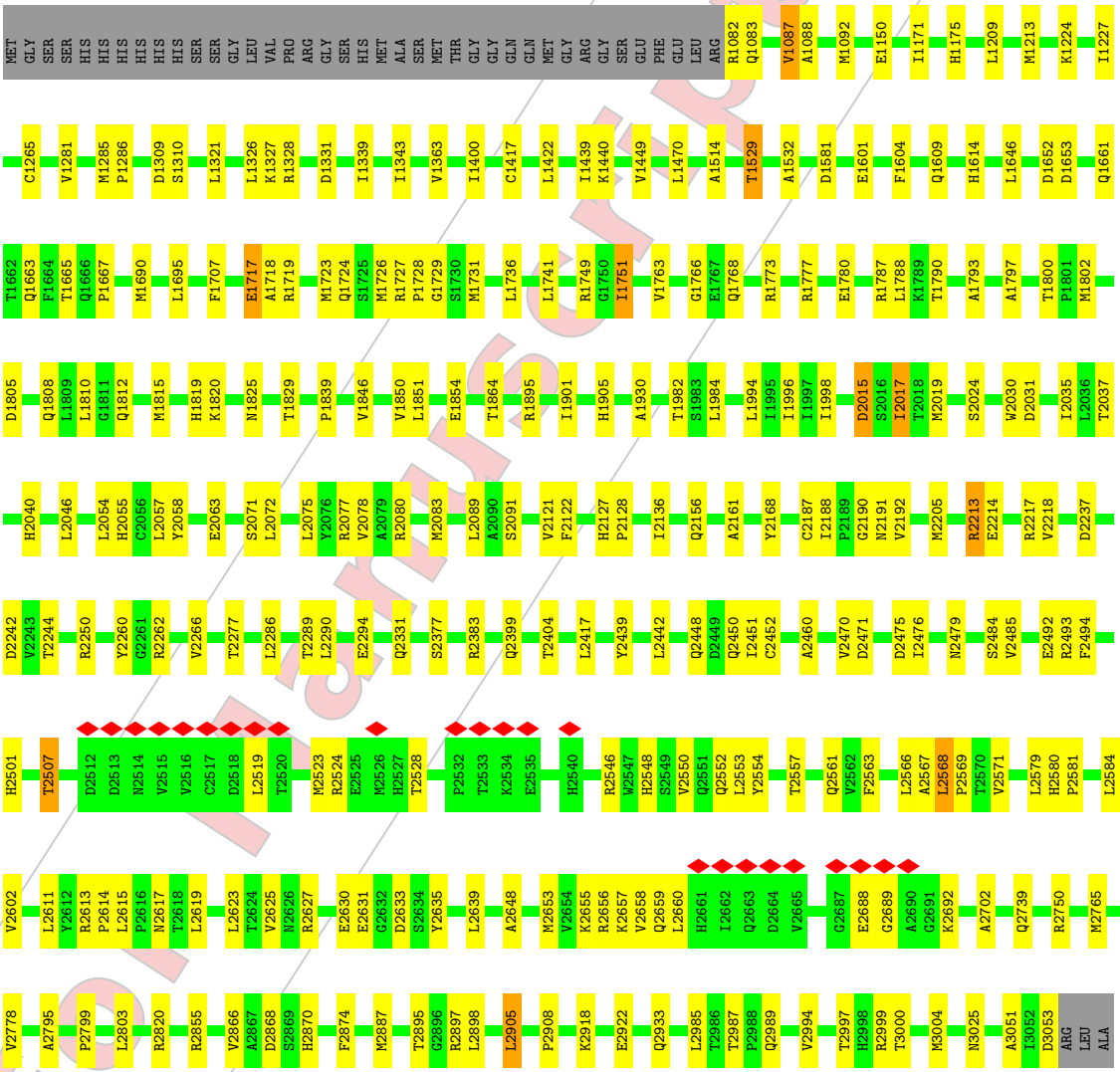
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

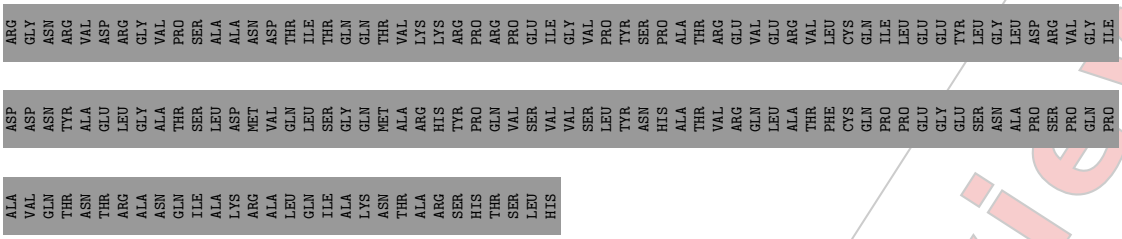
3 Residue-property plots (i)

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

• Molecule 1: Colibactin hybrid non-ribosomal peptide synthetase/type I polyketide synthase ClbB

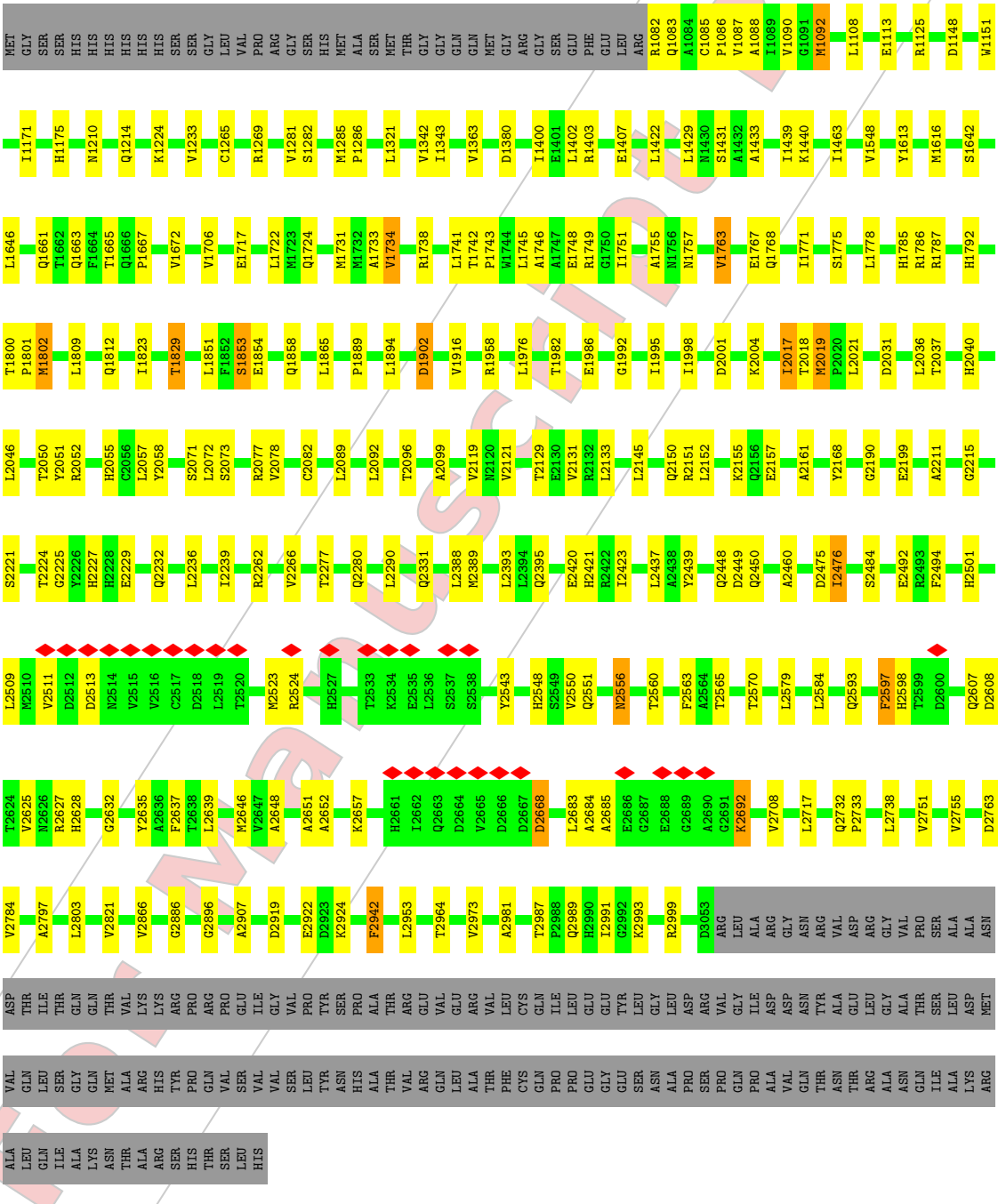
Chain A:





• Molecule 1: Colibactin hybrid non-ribosomal peptide synthetase/type I polyketide synthase ClbB

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	392982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58.85	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/15490	0.31	0/21088
1	B	0.13	0/15490	0.32	0/21088
All	All	0.12	0/30980	0.31	0/42176

There are no bond length outliers.

There are no bond angle outliers.

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	15170	0	15048	140	0
1	B	15170	0	15048	137	0
2	A	96	0	52	0	0
2	B	96	0	52	0	0
All	All	30532	0	30200	277	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 5.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ARG:HA	1:B:1085:CYS:SG	1.78	1.23
1:B:1085:CYS:HA	1:B:1269:ARG:HE	1.44	0.82
1:A:2492:GLU:HG2	1:A:2494:PHE:H	1.47	0.78
1:B:2623:LEU:HD11	1:B:2635:TYR:HB3	1.65	0.78
1:B:1082:ARG:HA	1:B:1085:CYS:HG	1.51	0.75
1:A:1087:VAL:HG21	1:A:1326:LEU:HB3	1.67	0.74
1:B:2607:GLN:HB2	1:B:2652:ALA:HB3	1.70	0.73
1:A:1787:ARG:NH1	1:A:1788:LEU:O	2.24	0.71
1:B:1986:GLU:HB2	1:B:2150:GLN:HB3	1.73	0.70
1:B:1082:ARG:CA	1:B:1085:CYS:SG	2.71	0.68
1:A:2623:LEU:HD11	1:A:2635:TYR:HB3	1.76	0.67
1:B:1082:ARG:O	1:B:1086:PRO:HD3	1.95	0.66
1:B:2987:THR:HG22	1:B:2989:GLN:H	1.60	0.66
1:B:1998:ILE:HG22	1:B:2021:LEU:HD23	1.78	0.65
1:B:2161:ALA:HB3	1:B:2168:TYR:HB2	1.77	0.65
1:B:1087:VAL:HB	1:B:1343:ILE:HB	1.78	0.64
1:A:1614:HIS:NE2	1:A:1652:ASP:O	2.31	0.64
1:A:1663:GLN:HE22	1:A:1724:GLN:HE21	1.46	0.63
1:A:2855:ARG:NH2	1:A:2868:ASP:OD2	2.31	0.63
1:A:2613:ARG:HG2	1:A:2614:PRO:HD2	1.81	0.63
1:B:1778:LEU:HD22	1:B:1785:HIS:CG	2.33	0.63
1:A:2460:ALA:HB3	1:A:2501:HIS:HD2	1.63	0.62
1:B:1125:ARG:O	1:B:1958:ARG:NH1	2.32	0.62
1:B:2190:GLY:N	1:B:2215:GLY:O	2.32	0.61
1:B:1281:VAL:HG23	1:B:1321:LEU:HB3	1.83	0.61
1:A:1727:ARG:NH1	1:A:1727:ARG:O	2.33	0.60
1:A:2601:SER:HB2	1:A:2657:LYS:HG2	1.84	0.60
1:A:1994:LEU:HD21	1:A:2017:ILE:HD11	1.83	0.60
1:B:1082:ARG:HD2	1:B:1083:GLN:N	2.16	0.60
1:B:1402:LEU:HD12	1:B:1463:ILE:HD13	1.83	0.60
1:B:2037:THR:O	1:B:2040:HIS:ND1	2.32	0.60
1:B:1992:GLY:O	1:B:2052:ARG:NH2	2.35	0.59
1:A:1736:LEU:HD21	1:A:1741:LEU:HD13	1.85	0.59
1:A:2639:LEU:HD23	1:A:2648:ALA:HB3	1.84	0.58
1:A:2630:GLU:O	1:A:2657:LYS:NZ	2.36	0.58
1:A:2987:THR:HG22	1:A:2989:GLN:H	1.68	0.58
1:A:2030:TRP:HE3	1:A:2035:ILE:HG22	1.68	0.57
1:B:2199:GLU:HB3	1:B:2229:GLU:HG2	1.86	0.57
1:A:2015:ASP:N	1:A:2015:ASP:OD1	2.36	0.57
1:B:2421:HIS:HD2	1:B:2543:TYR:HE1	1.53	0.57
1:A:2999:ARG:HB2	1:A:3004:MET:HE2	1.86	0.56
1:B:2548:HIS:HE1	1:B:2570:THR:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1642:SER:OG	1:B:1717:GLU:OE2	2.22	0.56
1:A:1422:LEU:HD13	1:A:1440:LYS:HD2	1.86	0.56
1:A:2568:LEU:HD12	1:A:2569:PRO:HD2	1.88	0.56
1:B:1745:LEU:O	1:B:1749:ARG:NH2	2.38	0.56
1:A:2895:THR:HG21	1:A:2918:LYS:HD3	1.86	0.56
1:B:2919:ASP:HA	1:B:2922:GLU:HG2	1.87	0.56
1:A:2377:SER:O	1:A:2383:ARG:NH1	2.36	0.56
1:A:2568:LEU:HB2	1:A:2617:ASN:HD21	1.71	0.55
1:B:1829:THR:HG23	1:B:1858:GLN:HE21	1.70	0.55
1:A:1901:ILE:HG23	1:A:1905:HIS:HB3	1.86	0.55
1:A:2205:MET:HE3	1:A:3025:ASN:HB3	1.87	0.55
1:B:2439:TYR:OH	1:B:2449:ASP:OD1	2.23	0.55
1:B:2684:ALA:HA	1:B:2692:LYS:HE3	1.88	0.55
1:A:1707:PHE:HE1	1:A:1815:MET:HG2	1.70	0.55
1:A:2553:LEU:HD22	1:A:2563:PHE:HB3	1.89	0.55
1:A:1601:GLU:HB2	1:A:1864:THR:HG22	1.87	0.55
1:A:2550:VAL:HG12	1:A:2567:ALA:HB2	1.89	0.55
1:B:2556:ASN:OD1	1:B:2556:ASN:N	2.39	0.55
1:B:1108:LEU:HD12	1:B:1113:GLU:HB2	1.88	0.54
1:A:2037:THR:O	1:A:2040:HIS:ND1	2.37	0.54
1:B:2732:GLN:HG2	1:B:2733:PRO:HD2	1.89	0.54
1:B:2973:VAL:HG21	1:B:2981:ALA:HB2	1.90	0.54
1:B:1087:VAL:HG21	1:B:1265:CYS:SG	2.48	0.54
1:B:1995:ILE:HG22	1:B:2055:HIS:HB2	1.88	0.54
1:B:2227:HIS:ND1	1:B:2229:GLU:OE1	2.41	0.54
1:A:2417:LEU:HD23	1:A:2581:PRO:HG2	1.90	0.53
1:B:1282:SER:HB2	1:B:1431:SER:HB2	1.90	0.53
1:B:1757:ASN:O	1:B:1853:SER:OG	2.24	0.53
1:B:2492:GLU:HG2	1:B:2494:PHE:H	1.73	0.53
1:A:1808:GLN:O	1:A:1812:GLN:NE2	2.36	0.53
1:A:1088:ALA:HB1	1:A:1339:ILE:HG23	1.90	0.52
1:A:2588:SER:HB2	1:A:2653:MET:HE1	1.90	0.52
1:A:2557:THR:HB	1:A:2561:GLN:HB3	1.92	0.52
1:A:2868:ASP:OD1	1:A:2870:HIS:N	2.40	0.52
1:B:1854:GLU:OE1	1:B:1854:GLU:N	2.42	0.52
1:B:1616:MET:HE3	1:B:1672:VAL:HG21	1.91	0.52
1:A:1087:VAL:HG13	1:A:1343:ILE:HB	1.90	0.52
1:B:2763:ASP:OD1	1:B:2763:ASP:N	2.40	0.52
1:B:2121:VAL:HG21	1:B:2331:GLN:O	2.10	0.52
1:A:2290:LEU:O	1:A:2294:GLU:HG2	2.09	0.52
1:B:1755:ALA:HB3	1:B:1763:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2918:LYS:NZ	1:A:2922:GLU:OE2	2.38	0.52
1:A:1309:ASP:OD1	1:A:1310:SER:N	2.42	0.52
1:A:2633:ASP:HB3	1:A:2655:LYS:HB2	1.92	0.52
1:B:1085:CYS:HB2	1:B:1086:PRO:HD3	1.90	0.52
1:B:2420:GLU:HG3	1:B:2543:TYR:CD2	2.44	0.52
1:B:2475:ASP:OD1	1:B:2475:ASP:N	2.42	0.51
1:A:2063:GLU:CD	1:A:2063:GLU:H	2.19	0.51
1:A:1209:LEU:HG	1:A:1213:MET:HE2	1.93	0.51
1:B:1087:VAL:O	1:B:1342:VAL:HA	2.11	0.51
1:A:2630:GLU:HG2	1:A:2631:GLU:HG3	1.93	0.51
1:A:2656:ARG:HE	1:A:2658:VAL:HG12	1.76	0.51
1:B:1663:GLN:HE22	1:B:1724:GLN:HE21	1.58	0.51
1:B:2072:LEU:HD23	1:B:2290:LEU:HD11	1.93	0.51
1:B:1380:ASP:OD1	1:B:1380:ASP:N	2.44	0.50
1:B:1403:ARG:O	1:B:1407:GLU:HG2	2.10	0.50
1:A:1777:ARG:NH1	1:A:1780:GLU:OE2	2.45	0.50
1:A:2448:GLN:NE2	1:A:2450:GLN:O	2.36	0.50
1:A:2523:MET:O	1:A:2561:GLN:NE2	2.45	0.50
1:A:1854:GLU:OE1	1:A:1854:GLU:N	2.45	0.50
1:A:1082:ARG:HD3	1:A:1082:ARG:C	2.37	0.50
1:B:2450:GLN:N	1:B:2450:GLN:OE1	2.45	0.50
1:B:2548:HIS:CE1	1:B:2570:THR:HB	2.46	0.50
1:B:2896:GLY:O	1:B:2924:LYS:NZ	2.45	0.50
1:A:2213:ARG:HG3	1:A:2214:GLU:H	1.77	0.49
1:B:2388:LEU:O	1:B:2389:MET:HG2	2.11	0.49
1:A:1731:MET:HB2	1:A:1790:THR:HG21	1.95	0.49
1:A:1825:ASN:HB3	1:A:1850:VAL:HG12	1.93	0.49
1:B:1422:LEU:HD13	1:B:1440:LYS:HD2	1.94	0.49
1:A:1281:VAL:HG23	1:A:1321:LEU:HB3	1.94	0.49
1:A:2024:SER:OG	1:A:2030:TRP:NE1	2.43	0.48
1:B:2784:VAL:HG21	1:B:2953:LEU:HB2	1.95	0.48
1:A:2765:MET:HE2	1:A:2795:ALA:HB1	1.95	0.48
1:B:1092:MET:HE2	1:B:1439:ILE:HG12	1.94	0.48
1:B:1731:MET:H	1:B:1787:ARG:HH12	1.59	0.48
1:A:2452:CYS:SG	1:A:2507:THR:HG23	2.53	0.48
1:B:1738:ARG:HA	1:B:1741:LEU:HG	1.94	0.48
1:A:2417:LEU:HD12	1:A:2417:LEU:H	1.79	0.48
1:A:2546:ARG:HG2	1:A:2548:HIS:CE1	2.48	0.48
1:A:2566:LEU:HB2	1:A:2619:LEU:HD23	1.94	0.48
1:A:1749:ARG:O	1:A:1773:ARG:NH2	2.46	0.48
1:B:1734:VAL:HG12	1:B:1785:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2608:ASP:HB2	1:B:2651:ALA:HB3	1.94	0.48
1:B:1082:ARG:O	1:B:1086:PRO:CD	2.61	0.48
1:B:1429:LEU:O	1:B:1433:ALA:HB2	2.14	0.48
1:B:2096:THR:HG21	1:B:2099:ALA:HB2	1.95	0.48
1:A:2524:ARG:HE	1:A:2553:LEU:HD13	1.77	0.48
1:B:2073:SER:O	1:B:2077:ARG:HG3	2.14	0.48
1:B:1148:ASP:HB3	1:B:1151:TRP:CD1	2.49	0.47
1:A:2442:LEU:HD13	1:A:2451:ILE:HG21	1.95	0.47
1:B:1082:ARG:HD2	1:B:1082:ARG:C	2.39	0.47
1:B:1285:MET:HB3	1:B:1286:PRO:HD3	1.96	0.47
1:A:1224:LYS:O	1:A:1227:ILE:HG22	2.14	0.47
1:A:1895:ARG:HD2	1:A:1901:ILE:O	2.14	0.47
1:B:2211:ALA:HB2	1:B:2236:LEU:HD21	1.96	0.47
1:B:2046:LEU:HD22	1:B:2050:THR:HG22	1.97	0.47
1:B:1210:ASN:O	1:B:1214:GLN:HG2	2.15	0.47
1:A:2080:ARG:HH21	1:A:2083:MET:HE3	1.80	0.47
1:A:2161:ALA:HB3	1:A:2168:TYR:HB2	1.97	0.47
1:A:1646:LEU:HD11	1:A:1667:PRO:HB2	1.97	0.47
1:A:2528:THR:HA	1:A:2553:LEU:O	2.15	0.47
1:B:2058:TYR:CD1	1:B:2078:VAL:HG21	2.50	0.47
1:B:2598:HIS:HB3	1:B:2657:LYS:HD2	1.97	0.47
1:B:1986:GLU:HB3	1:B:2151:ARG:H	1.80	0.46
1:A:2187:CYS:HA	1:A:2191:ASN:HD21	1.78	0.46
1:B:1661:GLN:O	1:B:1665:THR:HG23	2.16	0.46
1:A:1417:CYS:HB3	1:A:1470:LEU:HD23	1.96	0.46
1:B:2476:ILE:HA	1:B:2484:SER:O	2.14	0.46
1:A:1087:VAL:HG23	1:A:1327:LYS:O	2.15	0.46
1:A:1609:GLN:HB2	1:A:1695:LEU:HD12	1.97	0.46
1:A:2190:GLY:O	1:A:2262:ARG:NH1	2.49	0.46
1:B:2092:LEU:O	1:B:2131:VAL:HA	2.16	0.46
1:A:2580:HIS:HD2	1:A:2581:PRO:HD2	1.80	0.46
1:B:2221:SER:HA	1:B:2239:ILE:O	2.16	0.46
1:B:2448:GLN:NE2	1:B:2509:LEU:O	2.48	0.46
1:B:2685:ALA:H	1:B:2692:LYS:HB3	1.80	0.46
1:A:1810:LEU:HB3	1:A:1839:PRO:HB3	1.98	0.46
1:B:2001:ASP:N	1:B:2001:ASP:OD1	2.48	0.46
1:A:1653:ASP:OD1	1:A:1653:ASP:N	2.48	0.46
1:B:1088:ALA:O	1:B:1090:VAL:HG13	2.15	0.46
1:B:1775:SER:HA	1:B:1778:LEU:CD2	2.46	0.46
1:B:2017:ILE:HG22	1:B:2018:THR:H	1.80	0.46
1:A:2075:LEU:HG	1:A:2122:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:CYS:O	1:B:1087:VAL:HG23	2.16	0.45
1:B:1733:ALA:HB3	1:B:1786:ARG:HB3	1.97	0.45
1:B:1800:THR:HG23	1:B:1801:PRO:HD3	1.98	0.45
1:B:2623:LEU:HD13	1:B:2637:PHE:HB3	1.97	0.45
1:A:2702:ALA:HA	1:A:2750:ARG:HH22	1.81	0.45
1:A:2874:PHE:HE1	1:A:2898:LEU:HD12	1.82	0.45
1:A:1728:PRO:HA	1:A:1768:GLN:HE22	1.80	0.45
1:B:1746:ALA:HA	1:B:1749:ARG:HH22	1.81	0.45
1:B:2639:LEU:HD23	1:B:2648:ALA:HB3	1.99	0.45
1:B:2668:ASP:OD1	1:B:2668:ASP:N	2.49	0.45
1:B:2797:ALA:HB1	1:B:2993:LYS:HG3	1.98	0.45
1:A:1328:ARG:NH1	1:A:1331:ASP:OD2	2.50	0.45
1:A:2072:LEU:HD23	1:A:2290:LEU:HD11	1.97	0.45
1:A:2237:ASP:OD2	1:A:2260:TYR:OH	2.28	0.45
1:B:1742:THR:OG1	1:B:1743:PRO:HD3	2.15	0.45
1:A:2552:GLN:HG3	1:A:2554:TYR:HB2	1.99	0.45
1:B:1083:GLN:O	1:B:1086:PRO:HD2	2.17	0.45
1:B:1802:MET:HE3	1:B:1802:MET:HB2	1.75	0.45
1:B:1363:VAL:HG22	1:B:1400:ILE:HG23	1.98	0.45
1:A:1150:GLU:N	1:A:1150:GLU:OE1	2.49	0.45
1:A:2524:ARG:HB3	1:A:2553:LEU:HD21	1.99	0.45
1:B:2460:ALA:HB3	1:B:2501:HIS:CD2	2.52	0.45
1:A:1604:PHE:HB2	1:A:1690:MET:HG2	1.99	0.44
1:A:2476:ILE:HG22	1:A:2485:VAL:HG22	1.99	0.44
1:A:2625:VAL:HG22	1:A:2635:TYR:HE1	1.82	0.44
1:A:2479:ASN:OD1	1:A:2484:SER:N	2.51	0.44
1:A:1661:GLN:O	1:A:1665:THR:HG23	2.17	0.44
1:A:2739:GLN:HB2	1:A:2770:GLY:HA2	1.98	0.44
1:B:1224:LYS:HE3	1:B:1224:LYS:HB3	1.84	0.44
1:B:1768:GLN:O	1:B:1771:ILE:HG13	2.17	0.44
1:B:1865:LEU:HD23	1:B:1889:PRO:HG2	1.99	0.44
1:B:2593:GLN:HA	1:B:2597:PHE:CZ	2.53	0.44
1:A:1087:VAL:CG1	1:A:1343:ILE:HB	2.48	0.44
1:B:2509:LEU:HD21	1:B:2612:TYR:HE1	1.81	0.44
1:B:1171:ILE:HG22	1:B:1175:HIS:CE1	2.53	0.43
1:B:1775:SER:HA	1:B:1778:LEU:HD23	2.00	0.43
1:B:2627:ARG:NH2	1:B:2632:GLY:HA3	2.33	0.43
1:A:1717:GLU:HG3	1:A:1718:ALA:N	2.33	0.43
1:A:2121:VAL:HG21	1:A:2331:GLN:O	2.17	0.43
1:A:2820:ARG:HB3	1:A:2887:MET:HG3	1.99	0.43
1:A:2908:PRO:HA	1:A:2933:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2625:VAL:HG11	1:B:2628:HIS:NE2	2.33	0.43
1:A:1751:ILE:HG22	1:A:1766:GLY:HA3	2.01	0.43
1:A:3051:ALA:O	1:A:3053:ASP:N	2.49	0.43
1:B:2393:LEU:HD12	1:B:2437:LEU:HD21	2.00	0.43
1:A:1087:VAL:HG11	1:A:1265:CYS:SG	2.59	0.43
1:A:2399:GLN:HB3	1:A:2404:THR:HG22	2.00	0.43
1:A:1723:MET:HG2	1:A:1802:MET:SD	2.59	0.43
1:B:2082:CYS:SG	1:B:2089:LEU:HD12	2.59	0.43
1:B:2683:LEU:HA	1:B:2692:LYS:O	2.18	0.43
1:A:2579:LEU:HD12	1:A:2611:LEU:HD22	2.00	0.43
1:B:1402:LEU:HD23	1:B:1402:LEU:HA	1.89	0.43
1:B:1775:SER:O	1:B:1778:LEU:HG	2.18	0.43
1:A:2286:LEU:O	1:A:2289:THR:HG22	2.19	0.43
1:A:2897:ARG:H	1:A:2897:ARG:HG2	1.61	0.43
1:B:1085:CYS:HA	1:B:1269:ARG:NE	2.23	0.42
1:B:2523:MET:SD	1:B:2523:MET:N	2.90	0.42
1:B:2612:TYR:HE2	1:B:2646:MET:HE2	1.83	0.42
1:A:1529:THR:HG22	1:A:1532:ALA:H	1.82	0.42
1:B:2119:VAL:HG21	1:B:2133:LEU:HD12	2.01	0.42
1:A:2156:GLN:OE1	1:A:2156:GLN:N	2.44	0.42
1:A:2887:MET:HE1	1:A:2905:LEU:HD22	2.00	0.42
1:B:1902:ASP:OD1	1:B:1902:ASP:N	2.50	0.42
1:A:2471:ASP:OD2	1:A:2493:ARG:NH1	2.51	0.42
1:B:2036:LEU:HD13	1:B:2036:LEU:HA	1.92	0.42
1:B:2524:ARG:HE	1:B:2563:PHE:HB2	1.84	0.42
1:B:1812:GLN:OE1	1:B:1812:GLN:N	2.51	0.42
1:A:2799:PRO:O	1:A:2803:LEU:HB2	2.20	0.42
1:B:1613:TYR:CE2	1:B:1616:MET:HA	2.54	0.42
1:B:1722:LEU:HB3	1:B:1802:MET:HE2	2.02	0.42
1:A:1729:GLY:HA2	1:A:1793:ALA:HB2	2.02	0.41
1:A:2127:HIS:HB3	1:A:2128:PRO:HD3	2.02	0.41
1:B:1894:LEU:HD23	1:B:1894:LEU:HA	1.91	0.41
1:B:2019:MET:HE3	1:B:2019:MET:HB2	1.62	0.41
1:A:2058:TYR:CD1	1:A:2078:VAL:HG21	2.55	0.41
1:B:2051:TYR:HD2	1:B:2052:ARG:HH21	1.68	0.41
1:A:1087:VAL:CG2	1:A:1326:LEU:HB3	2.43	0.41
1:A:1797:ALA:O	1:A:1800:THR:OG1	2.30	0.41
1:A:2054:LEU:HB3	1:A:2089:LEU:HD13	2.03	0.41
1:B:1851:LEU:HB3	1:B:1854:GLU:CD	2.45	0.41
1:A:1092:MET:HE2	1:A:1439:ILE:HG23	2.03	0.41
1:A:1171:ILE:HG22	1:A:1175:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:VAL:HG22	1:A:1400:ILE:HG23	2.01	0.41
1:A:1614:HIS:NE2	1:A:1653:ASP:HA	2.35	0.41
1:A:2439:TYR:CE1	1:A:2611:LEU:HD23	2.55	0.41
1:A:2985:LEU:HD23	1:A:2985:LEU:HA	1.82	0.41
1:B:2886:GLY:HA3	1:B:2907:ALA:HB2	2.02	0.41
1:A:1514:ALA:HB1	1:A:1930:ALA:O	2.21	0.41
1:A:2242:ASP:OD1	1:A:2244:THR:HG22	2.21	0.41
1:B:2803:LEU:HD23	1:B:2942:PHE:HE2	1.86	0.41
1:A:2602:VAL:HG22	1:A:2659:GLN:HE21	1.85	0.41
1:B:2190:GLY:O	1:B:2262:ARG:NH1	2.53	0.41
1:B:2232:GLN:N	1:B:2232:GLN:OE1	2.54	0.41
1:A:1285:MET:HB3	1:A:1286:PRO:HD3	2.02	0.41
1:A:1719:ARG:CZ	1:A:1846:VAL:HG22	2.50	0.41
1:A:2030:TRP:HB2	1:A:2077:ARG:NH1	2.36	0.41
1:B:1646:LEU:HD11	1:B:1667:PRO:HB2	2.03	0.41
1:B:2224:THR:OG1	1:B:2225:GLY:N	2.54	0.41
1:A:1082:ARG:HD3	1:A:1082:ARG:O	2.20	0.41
1:A:1819:HIS:O	1:A:1820:LYS:HG3	2.21	0.41
1:A:2192:VAL:HA	1:A:2217:ARG:O	2.21	0.41
1:B:2551:GLN:NE2	1:B:2565:THR:OG1	2.53	0.41
1:A:2689:GLY:O	1:A:2692:LYS:HG2	2.21	0.40
1:B:2511:VAL:HG12	1:B:2513:ASP:H	1.85	0.40
1:A:1805:ASP:N	1:A:1805:ASP:OD1	2.55	0.40
1:A:1984:LEU:HD23	1:A:1984:LEU:HA	1.84	0.40
1:A:2692:LYS:HD2	1:A:2692:LYS:HA	1.82	0.40
1:A:2997:THR:HB	1:A:3004:MET:HE3	2.03	0.40
1:A:2055:HIS:ND1	1:A:2091:SER:OG	2.35	0.40
1:A:2688:GLU:O	1:A:2692:LYS:HD3	2.22	0.40
1:B:2155:LYS:HE2	1:B:2155:LYS:HB2	1.94	0.40
1:B:2560:THR:O	1:B:2625:VAL:HG23	2.21	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	1970/2164 (91%)	1891 (96%)	79 (4%)	0	100	100
1	B	1970/2164 (91%)	1875 (95%)	95 (5%)	0	100	100
All	All	3940/4328 (91%)	3766 (96%)	174 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1606/1766 (91%)	1563 (97%)	43 (3%)	39	54
1	B	1606/1766 (91%)	1551 (97%)	55 (3%)	32	47
All	All	3212/3532 (91%)	3114 (97%)	98 (3%)	36	50

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1083	GLN
1	A	1087	VAL
1	A	1449	VAL
1	A	1529	THR
1	A	1581	ASP
1	A	1717	GLU
1	A	1726	MET
1	A	1751	ILE
1	A	1763	VAL
1	A	1829	THR
1	A	1851	LEU
1	A	1982	THR
1	A	1996	ILE
1	A	1998	ILE
1	A	2015	ASP

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Mol	Chain	Res	Type
1	A	2017	ILE
1	A	2019	MET
1	A	2031	ASP
1	A	2046	LEU
1	A	2057	LEU
1	A	2071	SER
1	A	2136	ILE
1	A	2188	ILE
1	A	2213	ARG
1	A	2218	VAL
1	A	2250	ARG
1	A	2266	VAL
1	A	2277	THR
1	A	2470	VAL
1	A	2475	ASP
1	A	2507	THR
1	A	2519	LEU
1	A	2568	LEU
1	A	2571	VAL
1	A	2584	LEU
1	A	2615	LEU
1	A	2627	ARG
1	A	2660	LEU
1	A	2778	VAL
1	A	2866	VAL
1	A	2905	LEU
1	A	2994	VAL
1	A	3000	THR
1	B	1092	MET
1	B	1233	VAL
1	B	1548	VAL
1	B	1706	VAL
1	B	1734	VAL
1	B	1748	GLU
1	B	1751	ILE
1	B	1763	VAL
1	B	1767	GLU
1	B	1792	HIS
1	B	1802	MET
1	B	1809	LEU
1	B	1823	ILE
1	B	1829	THR

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Mol	Chain	Res	Type
1	B	1853	SER
1	B	1902	ASP
1	B	1916	VAL
1	B	1976	LEU
1	B	1982	THR
1	B	2004	LYS
1	B	2017	ILE
1	B	2019	MET
1	B	2031	ASP
1	B	2057	LEU
1	B	2071	SER
1	B	2129	THR
1	B	2145	LEU
1	B	2152	LEU
1	B	2157	GLU
1	B	2266	VAL
1	B	2277	THR
1	B	2280	GLN
1	B	2395	GLN
1	B	2423	ILE
1	B	2476	ILE
1	B	2550	VAL
1	B	2556	ASN
1	B	2579	LEU
1	B	2584	LEU
1	B	2597	PHE
1	B	2613	ARG
1	B	2668	ASP
1	B	2692	LYS
1	B	2708	VAL
1	B	2717	LEU
1	B	2738	LEU
1	B	2751	VAL
1	B	2755	VAL
1	B	2778	VAL
1	B	2821	VAL
1	B	2866	VAL
1	B	2942	PHE
1	B	2964	THR
1	B	2991	ILE
1	B	2999	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1083	GLN
1	A	1229	ASN
1	A	1263	GLN
1	A	1425	ASN
1	A	1666	GLN
1	A	1724	GLN
1	A	1784	GLN
1	A	1808	GLN
1	A	1844	GLN
1	A	1883	ASN
1	A	2006	GLN
1	A	2139	GLN
1	A	2184	GLN
1	A	2240	HIS
1	A	2280	GLN
1	A	2308	ASN
1	A	2501	HIS
1	A	2540	HIS
1	A	2617	ASN
1	A	2663	GLN
1	A	2774	GLN
1	A	2892	ASN
1	A	2955	GLN
1	B	1311	GLN
1	B	1390	HIS
1	B	1425	ASN
1	B	1474	GLN
1	B	1498	ASN
1	B	1624	GLN
1	B	1724	GLN
1	B	1760	HIS
1	B	1785	HIS
1	B	1848	ASN
1	B	1858	GLN
1	B	1928	GLN
1	B	2006	GLN
1	B	2007	GLN
1	B	2032	ASN
1	B	2038	HIS
1	B	2070	GLN
1	B	2184	GLN
1	B	2280	GLN

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Mol	Chain	Res	Type
1	B	2514	ASN
1	B	2548	HIS
1	B	2551	GLN
1	B	2598	HIS
1	B	2661	HIS
1	B	2663	GLN
1	B	2731	GLN
1	B	2774	GLN
1	B	2824	HIS
1	B	2892	ASN

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	A	3301	-	49,52,52	1.99	13 (26%)	66,80,80	2.16	12 (18%)
2	NDP	A	3302	-	49,52,52	1.98	13 (26%)	66,80,80	2.17	17 (25%)
2	NDP	B	3301	-	49,52,52	1.98	14 (28%)	66,80,80	2.16	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NDP	B	3302	-	49,52,52	1.97	13 (26%)	66,80,80	2.18	18 (27%)

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	NDP	A	3301	-	-	11/34/77/77	0/5/5/5
2	NDP	A	3302	-	-	11/34/77/77	0/5/5/5
2	NDP	B	3301	-	-	12/34/77/77	0/5/5/5
2	NDP	B	3302	-	-	10/34/77/77	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3302	NDP	C6A-N6A	4.62	1.45	1.34
2	B	3302	NDP	C6A-N6A	4.59	1.45	1.34
2	A	3301	NDP	C6A-N6A	4.58	1.45	1.34
2	B	3301	NDP	C6A-N6A	4.57	1.45	1.34
2	B	3302	NDP	C7N-N7N	4.57	1.45	1.33
2	A	3301	NDP	C7N-N7N	4.56	1.45	1.33
2	B	3301	NDP	C7N-N7N	4.56	1.45	1.33
2	A	3302	NDP	C7N-N7N	4.56	1.45	1.33
2	B	3301	NDP	C5A-N7A	4.38	1.47	1.39
2	A	3301	NDP	C5A-N7A	4.38	1.47	1.39
2	A	3302	NDP	C5A-N7A	4.32	1.47	1.39
2	B	3302	NDP	C5A-N7A	4.28	1.47	1.39
2	A	3302	NDP	P2B-O2B	3.48	1.65	1.59
2	B	3302	NDP	P2B-O2B	3.47	1.65	1.59
2	A	3301	NDP	C6N-N1N	3.42	1.45	1.37
2	A	3301	NDP	P2B-O2B	3.42	1.65	1.59
2	B	3301	NDP	C6N-N1N	3.40	1.45	1.37
2	B	3302	NDP	C6N-N1N	3.40	1.45	1.37
2	A	3302	NDP	C6N-N1N	3.40	1.45	1.37
2	B	3301	NDP	P2B-O2B	3.37	1.65	1.59
2	A	3302	NDP	C5A-C4A	3.18	1.44	1.39
2	B	3302	NDP	C5A-C4A	3.15	1.44	1.39
2	A	3301	NDP	C5A-C4A	3.07	1.44	1.39
2	B	3301	NDP	C5A-C4A	3.05	1.44	1.39
2	A	3301	NDP	C8A-N9A	-2.72	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3301	NDP	C8A-N9A	-2.68	1.32	1.37
2	A	3302	NDP	C8A-N9A	-2.68	1.32	1.37
2	B	3302	NDP	C8A-N9A	-2.65	1.32	1.37
2	A	3301	NDP	O7N-C7N	-2.49	1.18	1.24
2	B	3302	NDP	O7N-C7N	-2.48	1.18	1.24
2	B	3301	NDP	O7N-C7N	-2.48	1.18	1.24
2	A	3302	NDP	O7N-C7N	-2.47	1.18	1.24
2	A	3301	NDP	C3B-C2B	-2.46	1.47	1.52
2	B	3301	NDP	C3B-C2B	-2.42	1.47	1.52
2	B	3302	NDP	O4D-C1D	2.34	1.47	1.42
2	A	3302	NDP	O4B-C1B	2.32	1.47	1.42
2	B	3302	NDP	O4B-C1B	2.32	1.47	1.42
2	A	3302	NDP	O4D-C1D	2.30	1.47	1.42
2	B	3301	NDP	O4D-C1D	2.29	1.47	1.42
2	A	3301	NDP	O4B-C1B	2.28	1.47	1.42
2	B	3301	NDP	O4B-C1B	2.27	1.47	1.42
2	B	3302	NDP	C3B-C2B	-2.24	1.47	1.52
2	A	3301	NDP	O4D-C1D	2.23	1.47	1.42
2	A	3301	NDP	P2B-O3X	-2.20	1.46	1.54
2	B	3301	NDP	P2B-O3X	-2.18	1.46	1.54
2	A	3302	NDP	P2B-O2X	-2.18	1.46	1.54
2	B	3302	NDP	P2B-O3X	-2.17	1.46	1.54
2	A	3302	NDP	C3B-C2B	-2.17	1.48	1.52
2	B	3302	NDP	P2B-O2X	-2.17	1.46	1.54
2	A	3301	NDP	P2B-O2X	-2.16	1.46	1.54
2	A	3302	NDP	P2B-O3X	-2.16	1.46	1.54
2	B	3301	NDP	P2B-O2X	-2.14	1.46	1.54
2	B	3301	NDP	C8A-N7A	2.03	1.35	1.31

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3301	NDP	C4A-N9A-C8A	8.67	115.13	105.73
2	B	3301	NDP	C4A-N9A-C8A	8.63	115.08	105.73
2	B	3302	NDP	C4A-N9A-C8A	8.44	114.88	105.73
2	A	3302	NDP	C4A-N9A-C8A	8.41	114.84	105.73
2	A	3302	NDP	C5A-C4A-N3A	-6.09	118.81	126.75
2	B	3302	NDP	C5A-C4A-N3A	-6.02	118.89	126.75
2	B	3302	NDP	N3A-C4A-N9A	5.96	136.91	127.08
2	A	3302	NDP	N3A-C4A-N9A	5.95	136.89	127.08
2	A	3301	NDP	C5A-C4A-N3A	-5.87	119.09	126.75
2	B	3301	NDP	C5A-C4A-N3A	-5.87	119.09	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3301	NDP	N3A-C4A-N9A	5.78	136.60	127.08
2	B	3301	NDP	N3A-C4A-N9A	5.74	136.53	127.08
2	A	3301	NDP	C4A-C5A-N7A	-4.22	105.48	110.62
2	B	3301	NDP	C4A-C5A-N7A	-4.21	105.49	110.62
2	A	3302	NDP	C4A-C5A-N7A	-4.11	105.61	110.62
2	B	3302	NDP	C4A-C5A-N7A	-4.03	105.71	110.62
2	B	3301	NDP	N9A-C8A-N7A	-3.95	108.51	113.91
2	A	3301	NDP	N9A-C8A-N7A	-3.95	108.52	113.91
2	A	3302	NDP	C2A-N3A-C4A	3.84	120.83	111.75
2	B	3301	NDP	C2A-N3A-C4A	3.84	120.82	111.75
2	A	3301	NDP	C2A-N3A-C4A	3.83	120.79	111.75
2	B	3302	NDP	C2A-N3A-C4A	3.81	120.74	111.75
2	B	3301	NDP	N3A-C2A-N1A	-3.79	122.68	128.60
2	A	3301	NDP	N3A-C2A-N1A	-3.78	122.69	128.60
2	B	3302	NDP	N9A-C8A-N7A	-3.75	108.79	113.91
2	A	3302	NDP	N9A-C8A-N7A	-3.72	108.82	113.91
2	A	3302	NDP	N3A-C2A-N1A	-3.69	122.82	128.60
2	B	3302	NDP	N3A-C2A-N1A	-3.63	122.93	128.60
2	B	3301	NDP	C6A-C5A-N7A	3.18	137.95	132.02
2	A	3301	NDP	C6A-C5A-N7A	3.17	137.92	132.02
2	A	3302	NDP	C6A-C5A-N7A	2.99	137.60	132.02
2	B	3302	NDP	C6A-C5A-N7A	2.95	137.51	132.02
2	B	3302	NDP	C3D-C2D-C1D	2.90	106.93	101.43
2	B	3301	NDP	PN-O3-PA	-2.72	123.50	132.83
2	B	3302	NDP	PN-O3-PA	-2.67	123.65	132.83
2	A	3302	NDP	PN-O3-PA	-2.67	123.66	132.83
2	A	3302	NDP	C3D-C2D-C1D	2.53	106.23	101.43
2	A	3301	NDP	PN-O3-PA	-2.48	124.33	132.83
2	A	3302	NDP	C2B-C3B-C4B	2.46	107.34	101.99
2	A	3302	NDP	C3B-C2B-C1B	2.43	107.46	102.89
2	B	3302	NDP	C3B-C2B-C1B	2.43	107.45	102.89
2	B	3302	NDP	C2B-C3B-C4B	2.41	107.22	101.99
2	B	3301	NDP	O2N-PN-O1N	-2.30	100.89	112.24
2	A	3302	NDP	O2A-PA-O1A	-2.28	100.98	112.24
2	A	3301	NDP	O2A-PA-O1A	-2.27	101.03	112.24
2	B	3302	NDP	O2N-PN-O1N	-2.27	101.03	112.24
2	A	3301	NDP	O2N-PN-O1N	-2.27	101.04	112.24
2	A	3302	NDP	O2N-PN-O1N	-2.22	101.26	112.24
2	B	3301	NDP	O2A-PA-O1A	-2.21	101.30	112.24
2	B	3302	NDP	C1B-N9A-C8A	-2.21	122.14	127.14
2	B	3302	NDP	C2D-C3D-C4D	2.20	106.91	102.64
2	B	3302	NDP	O2A-PA-O1A	-2.19	101.41	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3301	NDP	C5A-N7A-C8A	2.15	106.56	103.51
2	A	3302	NDP	C1B-N9A-C8A	-2.14	122.30	127.14
2	B	3301	NDP	C5A-N7A-C8A	2.13	106.54	103.51
2	B	3302	NDP	C2B-C1B-N9A	-2.12	109.95	113.53
2	A	3302	NDP	C2D-C3D-C4D	2.11	106.74	102.64
2	A	3302	NDP	C5A-N7A-C8A	2.05	106.42	103.51
2	B	3302	NDP	C5A-N7A-C8A	2.05	106.42	103.51
2	B	3301	NDP	C4A-N9A-C1B	-2.01	121.81	126.59

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3301	NDP	C2N-C3N-C7N-O7N
2	A	3301	NDP	C2N-C3N-C7N-N7N
2	A	3302	NDP	C2B-O2B-P2B-O1X
2	A	3302	NDP	C2B-C1B-N9A-C8A
2	A	3302	NDP	PA-O3-PN-O5D
2	A	3302	NDP	O4D-C1D-N1N-C2N
2	A	3302	NDP	C2N-C3N-C7N-N7N
2	B	3301	NDP	C5B-O5B-PA-O1A
2	B	3301	NDP	C5B-O5B-PA-O2A
2	B	3301	NDP	C5D-O5D-PN-O3
2	B	3301	NDP	C5D-O5D-PN-O1N
2	B	3301	NDP	C5D-O5D-PN-O2N
2	B	3301	NDP	C2N-C3N-C7N-N7N
2	B	3302	NDP	C4B-C5B-O5B-PA
2	B	3302	NDP	C2B-O2B-P2B-O1X
2	B	3302	NDP	C2N-C3N-C7N-N7N
2	B	3302	NDP	O4D-C1D-N1N-C2N
2	A	3301	NDP	O4D-C4D-C5D-O5D
2	A	3301	NDP	C3D-C4D-C5D-O5D
2	A	3302	NDP	C4B-C5B-O5B-PA
2	A	3302	NDP	C2B-C1B-N9A-C4A
2	B	3301	NDP	O4B-C4B-C5B-O5B
2	A	3301	NDP	O4D-C1D-N1N-C6N
2	B	3302	NDP	C2B-C1B-N9A-C8A
2	B	3301	NDP	O4D-C1D-N1N-C6N
2	A	3301	NDP	O4B-C4B-C5B-O5B
2	A	3301	NDP	C5B-O5B-PA-O3
2	B	3302	NDP	C2B-O2B-P2B-O3X
2	A	3301	NDP	C5B-O5B-PA-O1A

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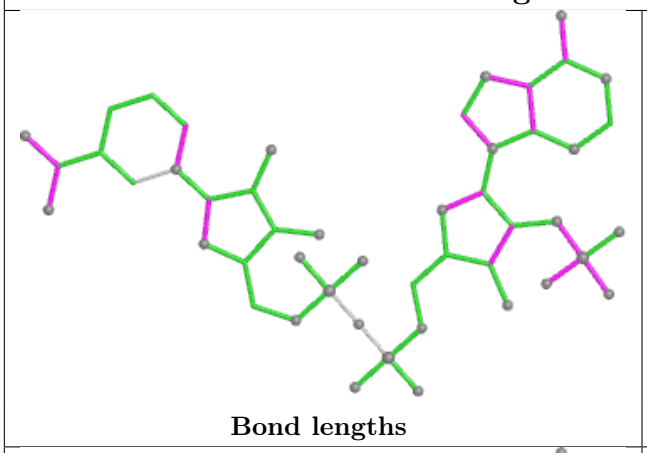
Mol	Chain	Res	Type	Atoms
2	A	3301	NDP	C5D-O5D-PN-O1N
2	A	3302	NDP	C3D-C4D-C5D-O5D
2	B	3301	NDP	C3B-C4B-C5B-O5B
2	A	3302	NDP	C2N-C3N-C7N-O7N
2	B	3301	NDP	C2N-C3N-C7N-O7N
2	B	3302	NDP	C2N-C3N-C7N-O7N
2	A	3301	NDP	PN-O3-PA-O2A
2	B	3302	NDP	C2B-C1B-N9A-C4A
2	A	3302	NDP	O4D-C4D-C5D-O5D
2	B	3302	NDP	O4B-C4B-C5B-O5B
2	B	3301	NDP	PN-O3-PA-O5B
2	B	3302	NDP	O4B-C1B-N9A-C8A
2	A	3301	NDP	C2B-O2B-P2B-O3X
2	B	3301	NDP	C5B-O5B-PA-O3
2	A	3302	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

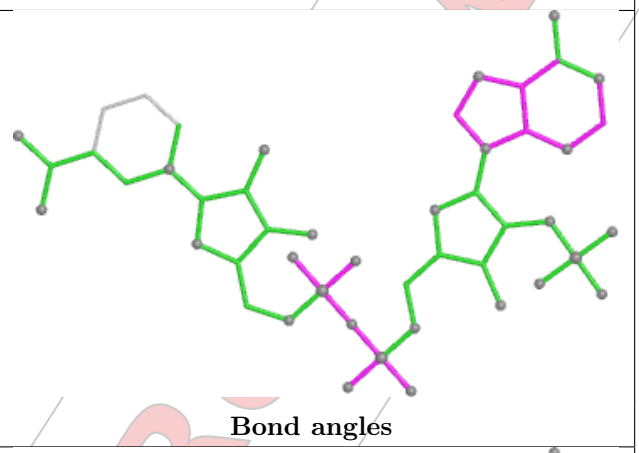
No monomer is involved in short contacts.

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

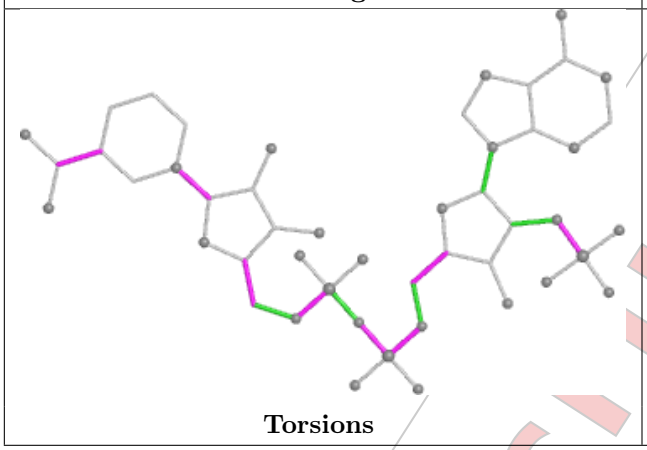
Ligand NDP A 3301



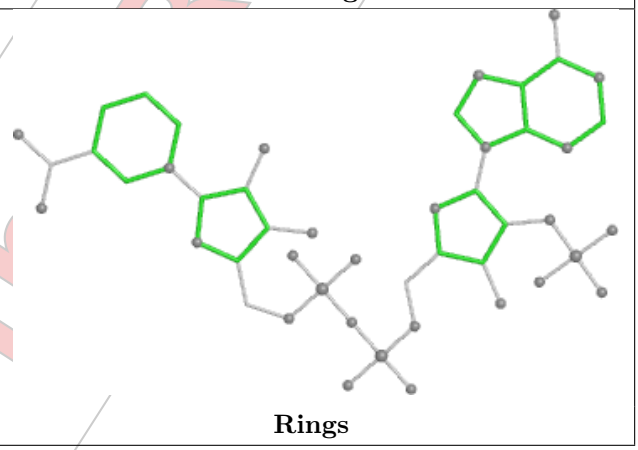
Bond lengths



Bond angles

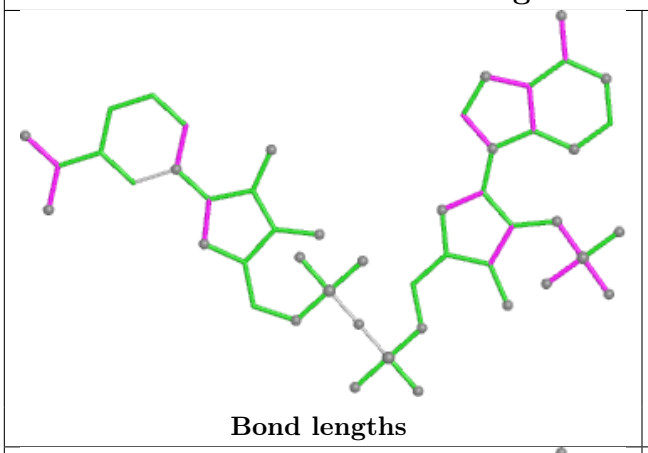


Torsions

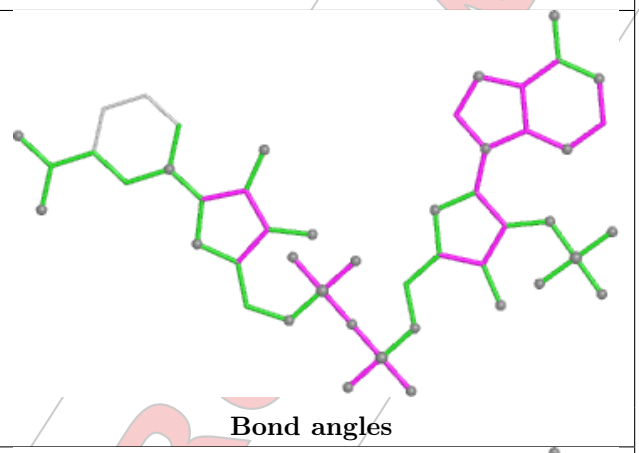


Rings

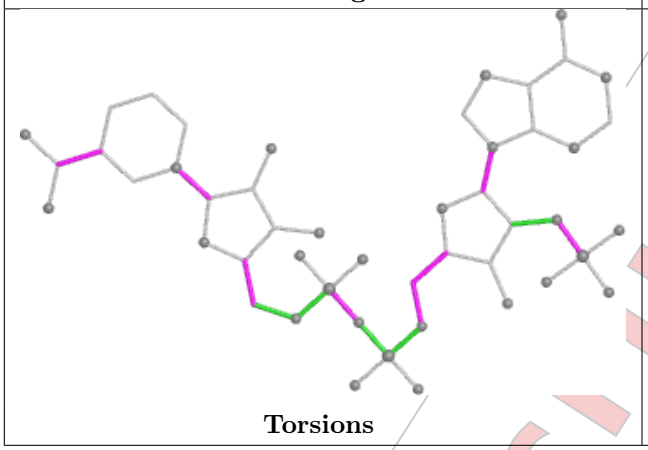
Ligand NDP A 3302



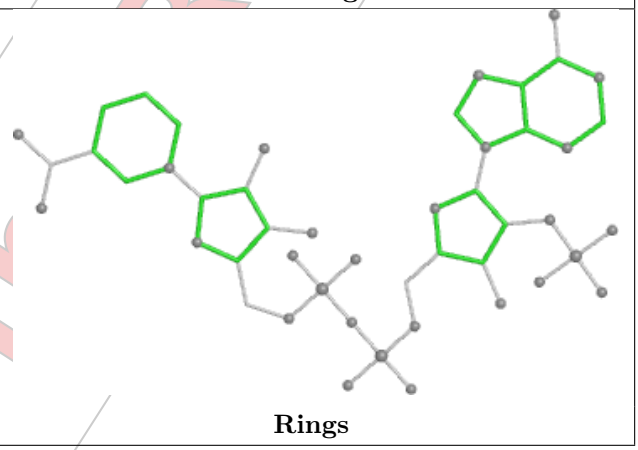
Bond lengths



Bond angles

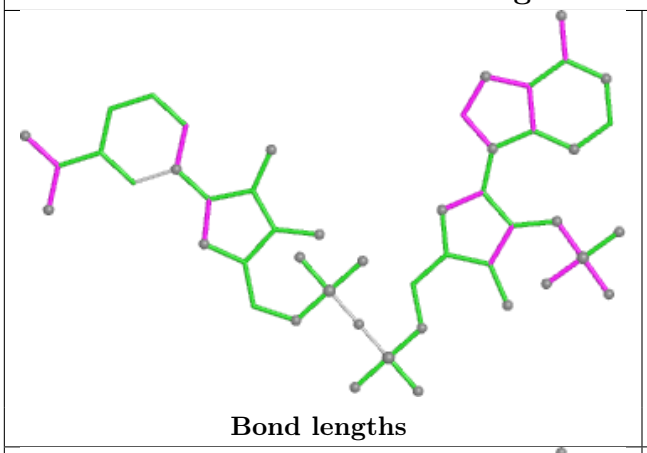


Torsions

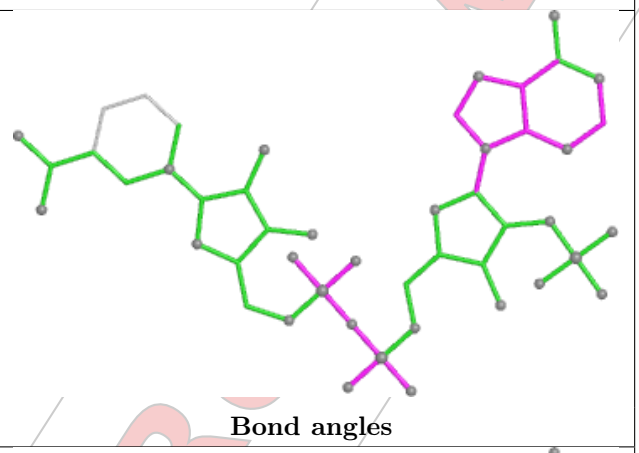


Rings

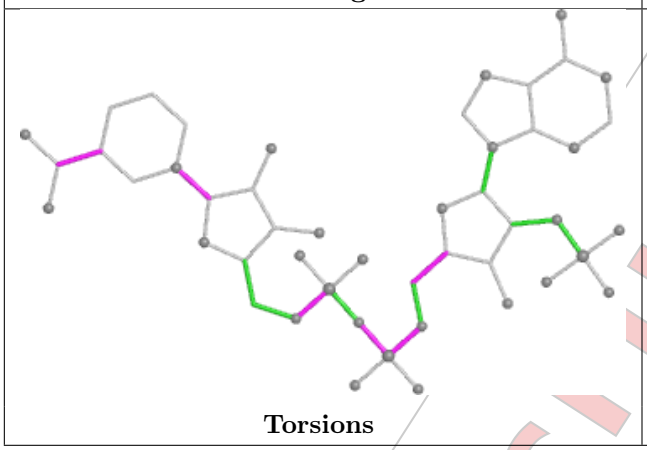
Ligand NDP B 3301



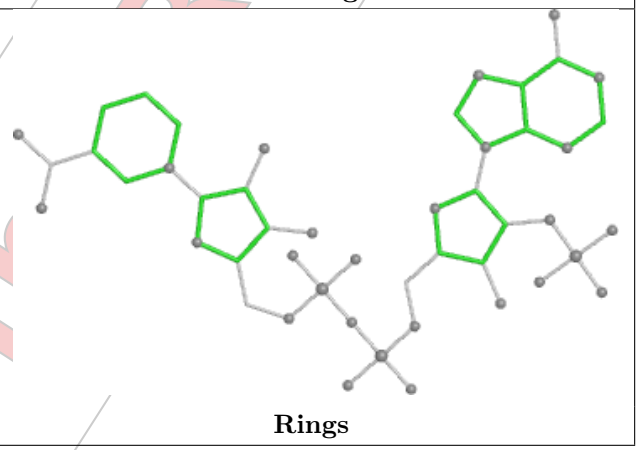
Bond lengths



Bond angles

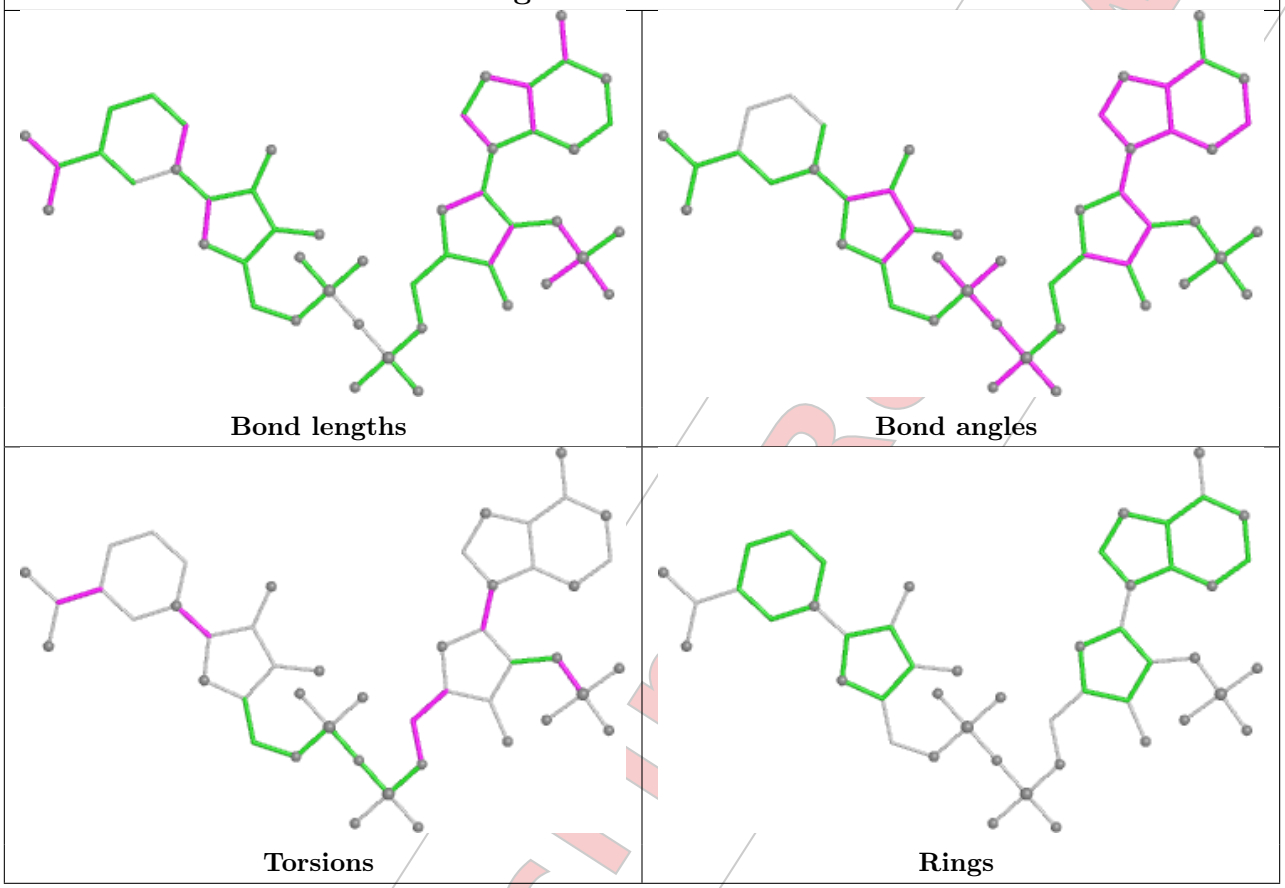


Torsions



Rings

Ligand NDP B 3302



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.

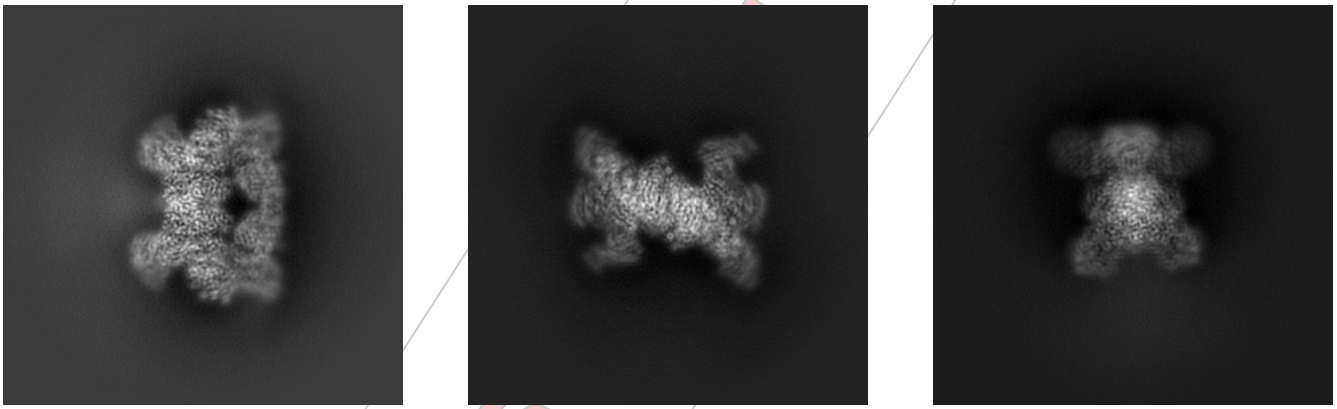
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69437. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

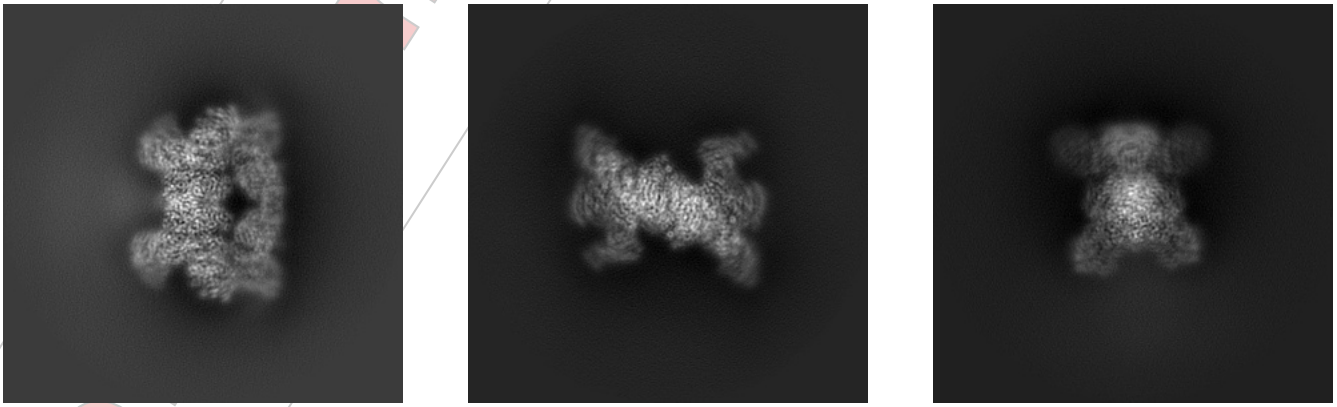
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

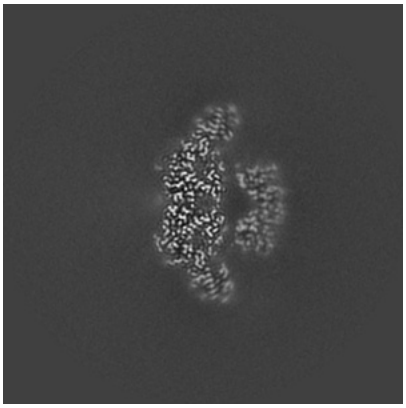


X Y Z

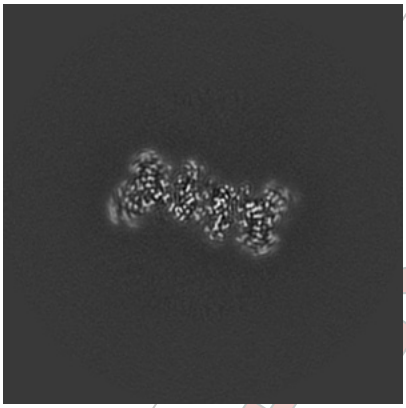
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

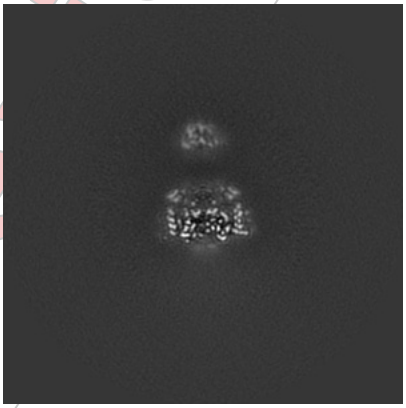
6.2.1 Primary map



X Index: 160

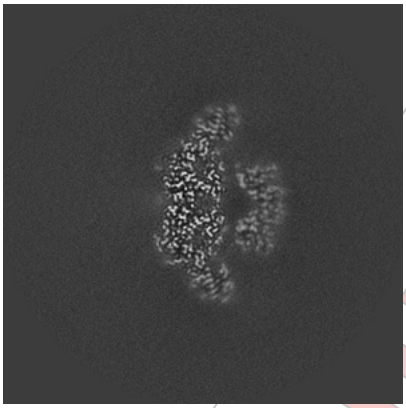


Y Index: 160

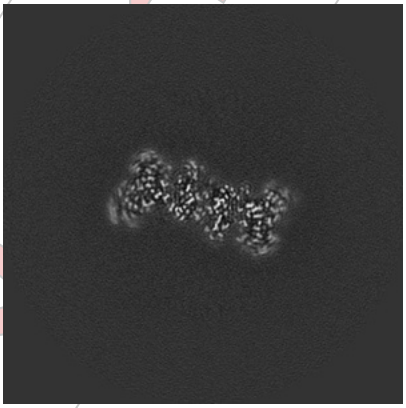


Z Index: 160

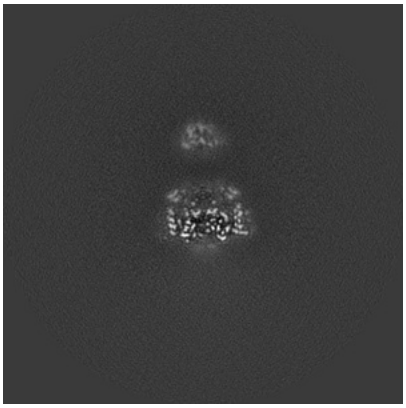
6.2.2 Raw map



X Index: 160



Y Index: 160

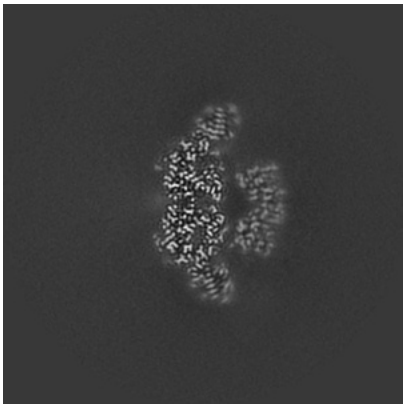


Z Index: 160

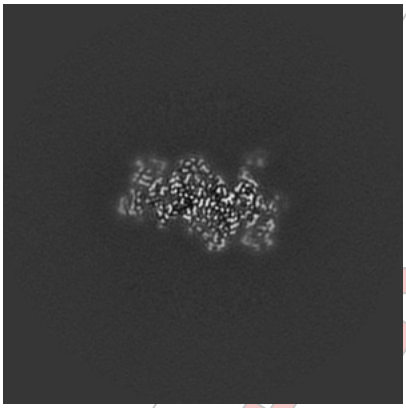
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

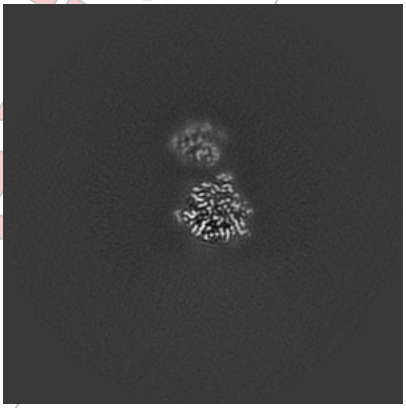
6.3.1 Primary map



X Index: 161

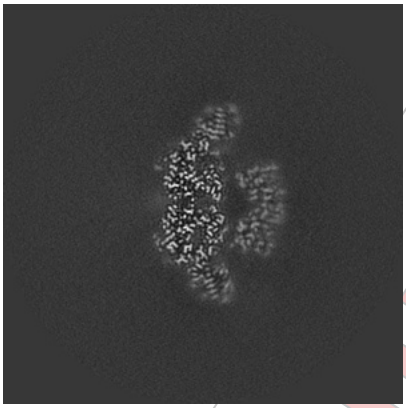


Y Index: 151

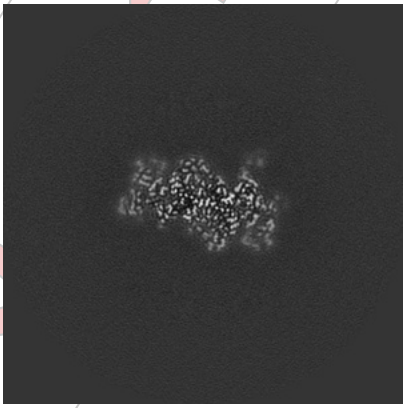


Z Index: 149

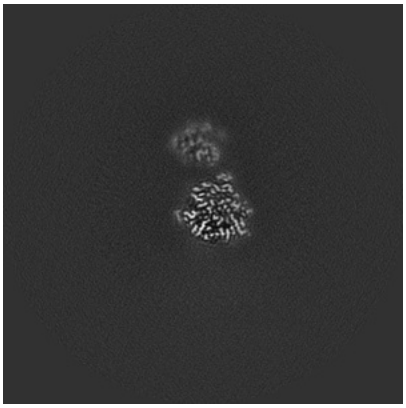
6.3.2 Raw map



X Index: 161



Y Index: 151



Z Index: 149

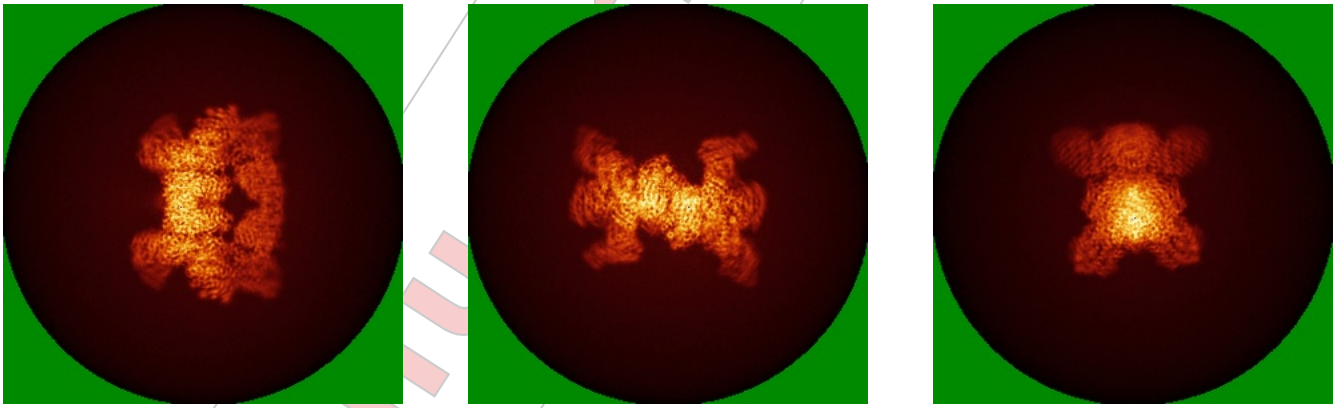
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map

X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

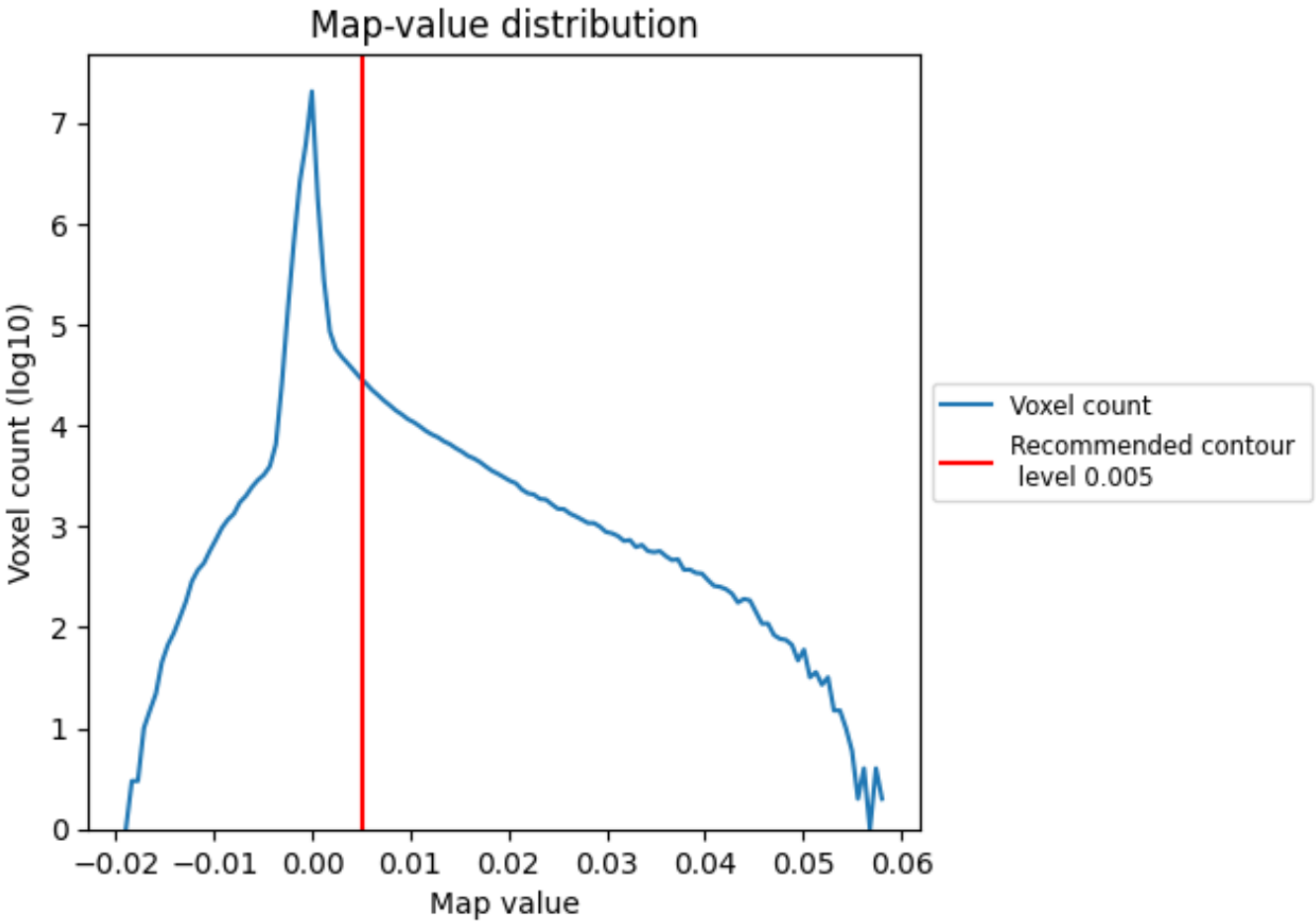
6.6 Mask visualisation (i)

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

7 Map analysis

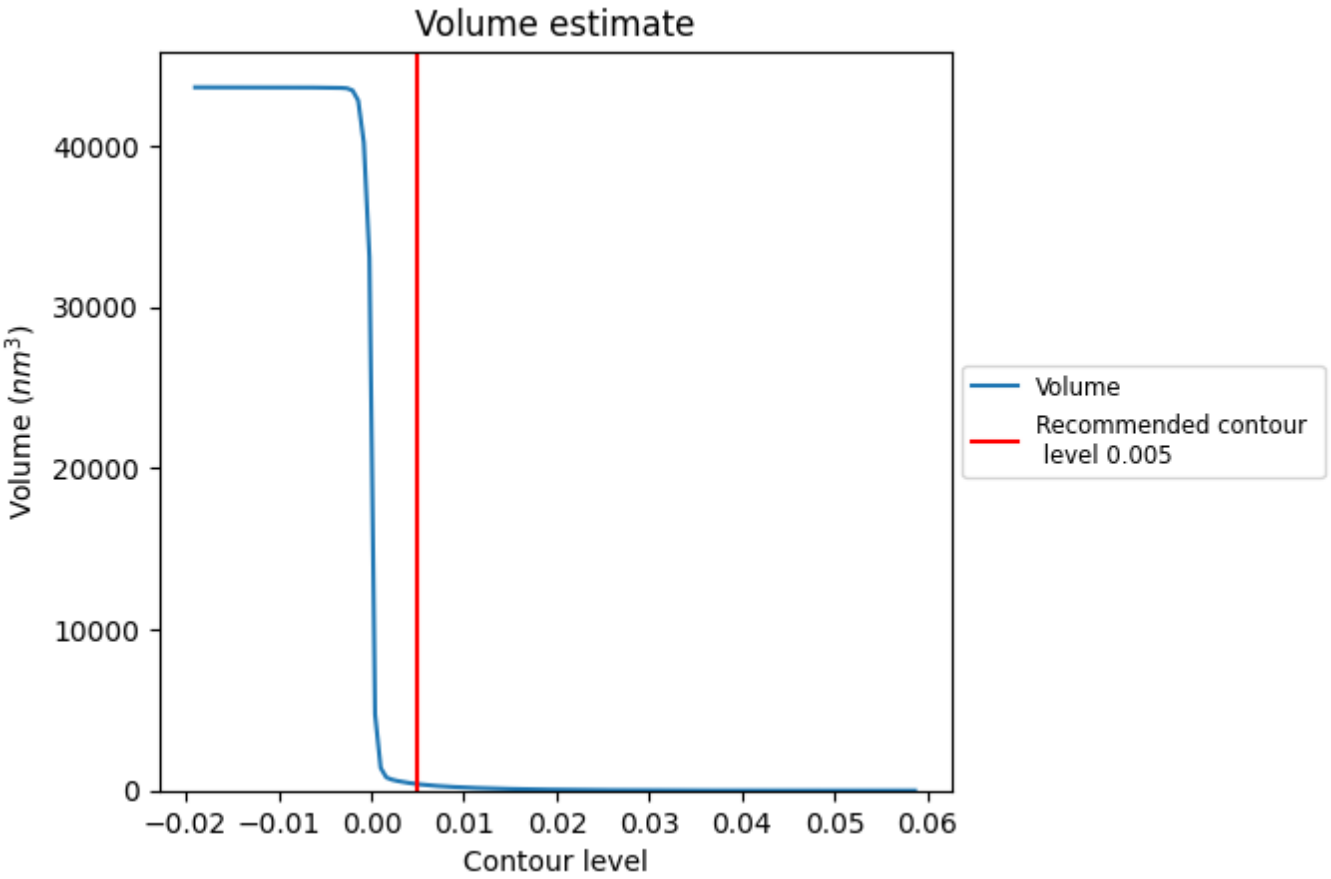
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

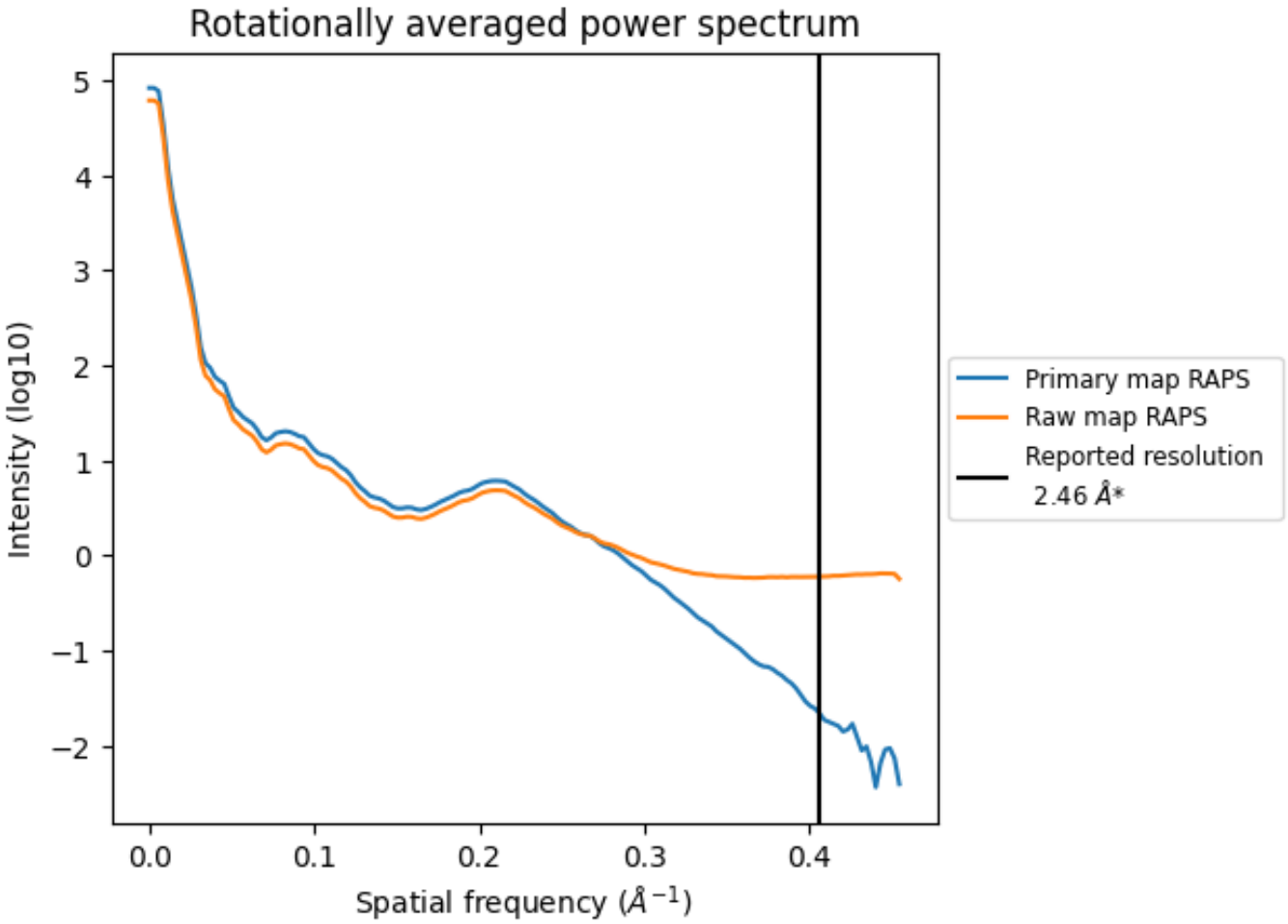
7.2 Volume estimate (i)



The volume at the recommended contour level is 402 nm^3; this corresponds to an approximate mass of 363 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

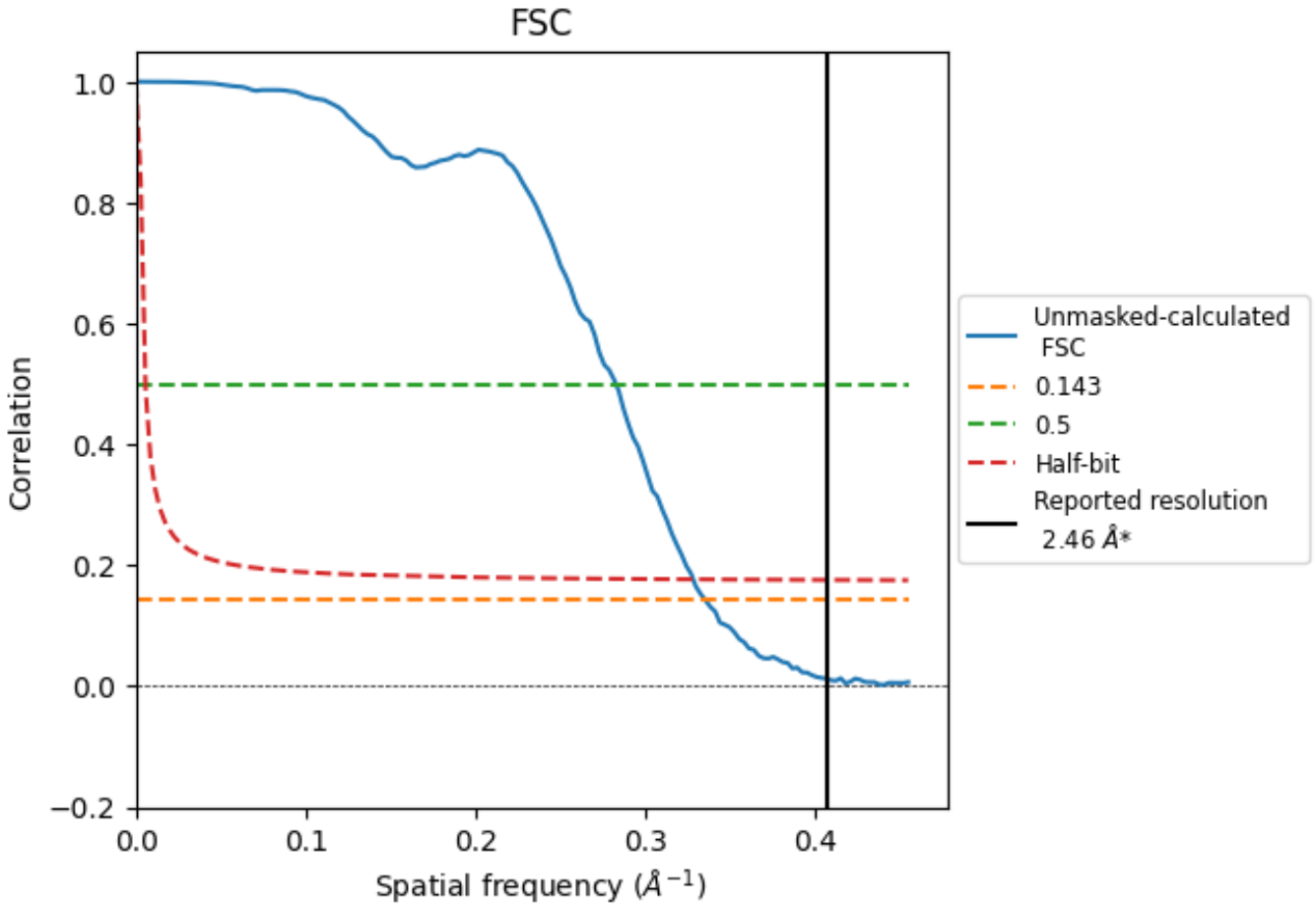


*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8.2 Resolution estimates (i)

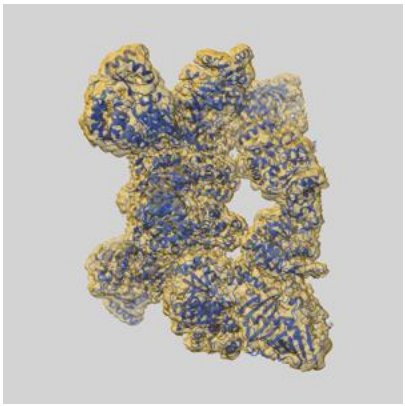
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.54	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.46 by more than 10 %

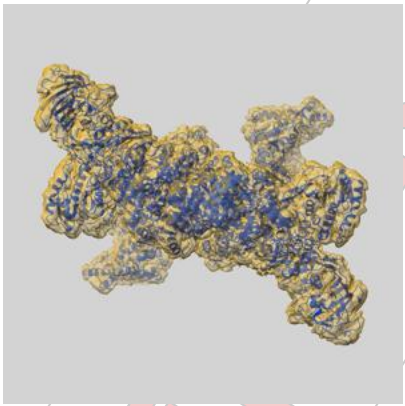
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69437 and PDB model 24CH. Per-residue inclusion information can be found in section 3 on page 7.

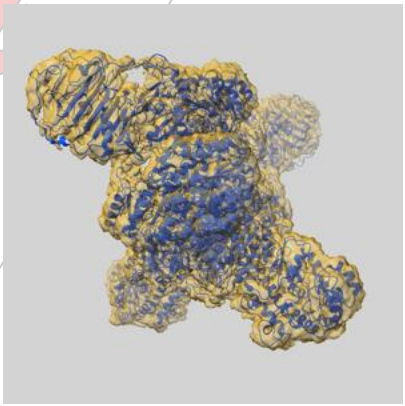
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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

X Y Z

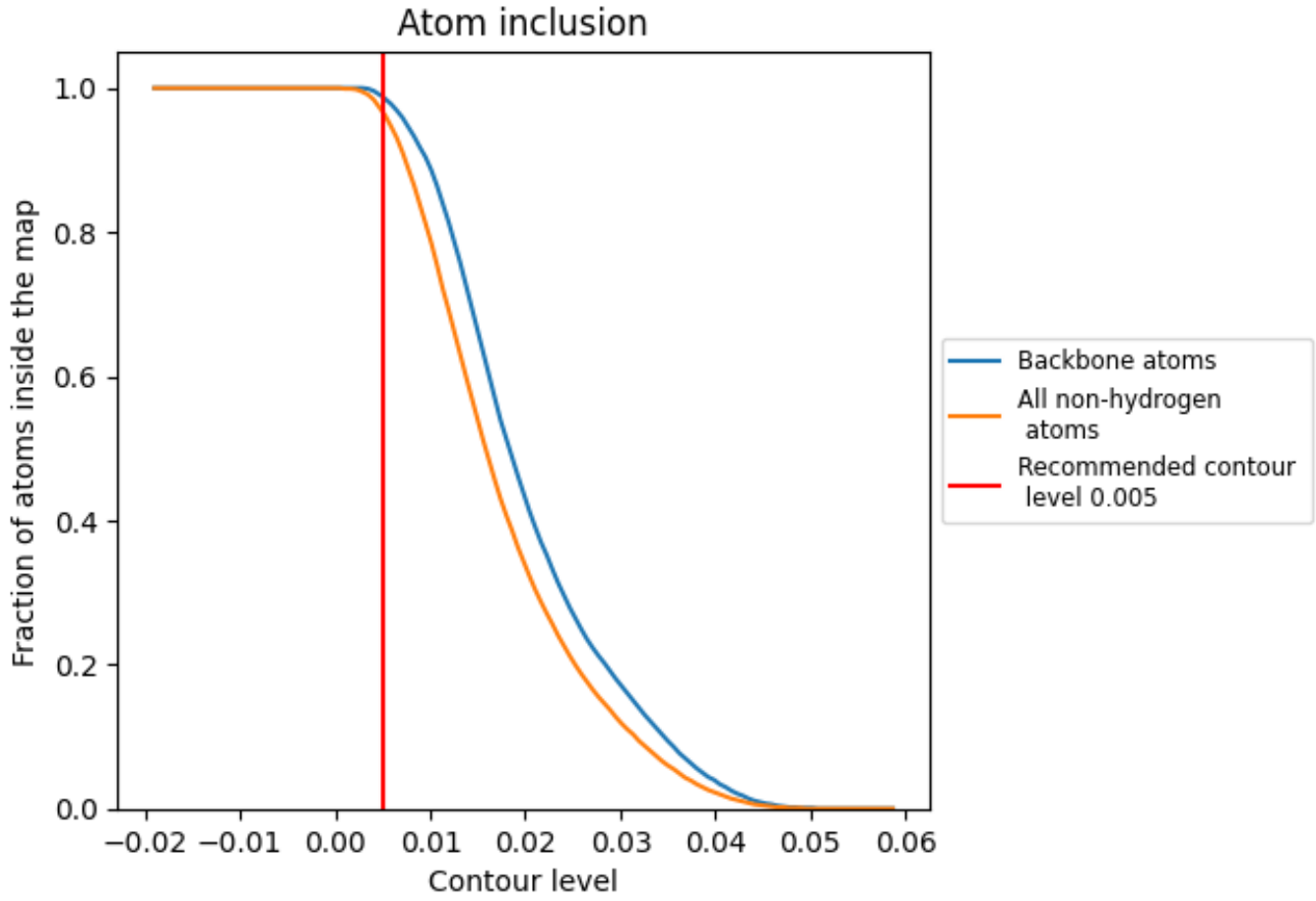
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.5270
A	0.9680	0.5280
B	0.9670	0.5260