



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 9BDE / pdb_00009bde
EMDB ID : EMD-44450
Title : Middle Region of Apolipoprotein B 100 bound to Low Density Lipoprotein Receptor
Authors : Dearborn, A.D.; Reimund, M.; Graziano, G.; Lei, H.; Kumar, A.; Neufeld, E.B.; Remaley, A.T.; Marcotrigiano, J.
Deposited on : 2024-04-11
Resolution : 4.18 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

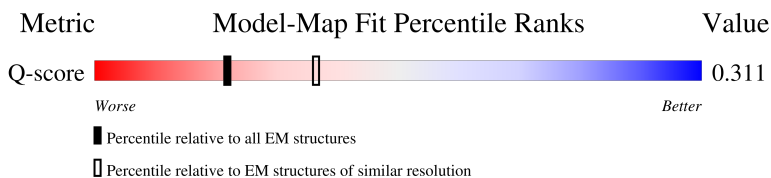
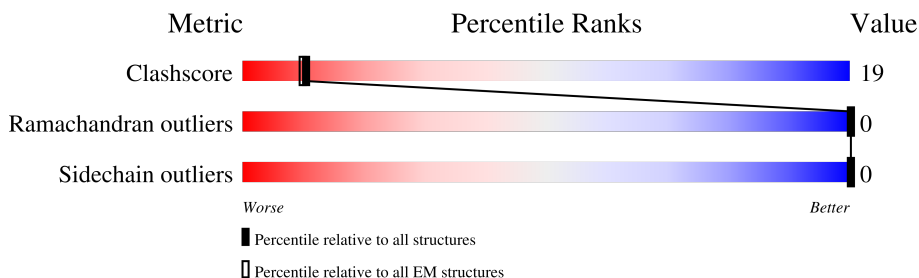
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.18 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	5389 (3.68 - 4.68)

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	H	234	
2	A	4563	
3	L	219	
4	B	545	

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Mol	Chain	Length	Quality of chain
5	N	131	 65% 30% 5%
6	R	860	 6% 19% 13% 68%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17216 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 Legobody 8D3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	177	Total	C	N	O	S	0	0
			1289	818	213	250	8		

- Molecule 2 is a protein called Apolipoprotein B 100.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1121	Total	C	N	O	S	0	0
			8453	5327	1437	1677	12		

- Molecule 3 is a protein called Legobody 8D3 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	180	Total	C	N	O	S	0	0
			1244	780	201	258	5		

- Molecule 4 is a protein called Maltose/maltodextrin-binding periplasmic protein,Immunoglobulin G-binding protein A,Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	466	Total	C	N	O	S	0	0
			3396	2161	545	686	4		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0AEX9
B	361	ALA	GLN	conflict	UNP P02976
B	362	LEU	ASN	conflict	UNP P02976
B	365	ALA	TYR	conflict	UNP P02976
B	366	GLN	GLU	conflict	UNP P02976
B	369	ILE	HIS	conflict	UNP P02976
B	370	MET	LEU	conflict	UNP P02976
B	404	GLU	ASP	conflict	UNP P02976

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Chain	Residue	Modelled	Actual	Comment	Reference
B	405	HIS	ALA	conflict	UNP P02976
B	410	GLY	-	linker	UNP P02976
B	411	GLY	-	linker	UNP P02976
B	412	SER	-	linker	UNP P02976
B	413	GLY	-	linker	UNP P02976
B	414	GLY	-	linker	UNP P02976
B	415	ALA	-	linker	UNP P02976
B	416	GLY	-	linker	UNP P02976
B	417	SER	-	linker	UNP P02976
B	418	GLY	-	linker	UNP P02976
B	468	GLY	-	linker	UNP P02976
B	469	GLY	-	linker	UNP P02976
B	470	GLY	-	linker	UNP P02976
B	471	SER	-	linker	UNP P02976
B	472	GLY	-	linker	UNP P02976
B	473	GLY	-	linker	UNP P02976
B	474	GLY	-	linker	UNP P02976
B	475	SER	-	linker	UNP P02976
B	476	GLY	-	linker	UNP P02976
B	477	GLY	-	linker	UNP P02976
B	478	SER	-	linker	UNP P02976
B	537	GLY	-	expression tag	UNP P19909
B	538	SER	-	expression tag	UNP P19909
B	539	GLY	-	expression tag	UNP P19909
B	540	HIS	-	expression tag	UNP P19909
B	541	HIS	-	expression tag	UNP P19909
B	542	HIS	-	expression tag	UNP P19909
B	543	HIS	-	expression tag	UNP P19909
B	544	HIS	-	expression tag	UNP P19909
B	545	HIS	-	expression tag	UNP P19909

- Molecule 5 is a protein called ApoB100 nanobody 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	124	Total	C	N	O	S	0	0
			859	538	153	164	4		

- Molecule 6 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	272	Total	C	N	O	S	0	0
			1898	1125	322	407	44		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	R	7	Total	Ca	0
			7	7	





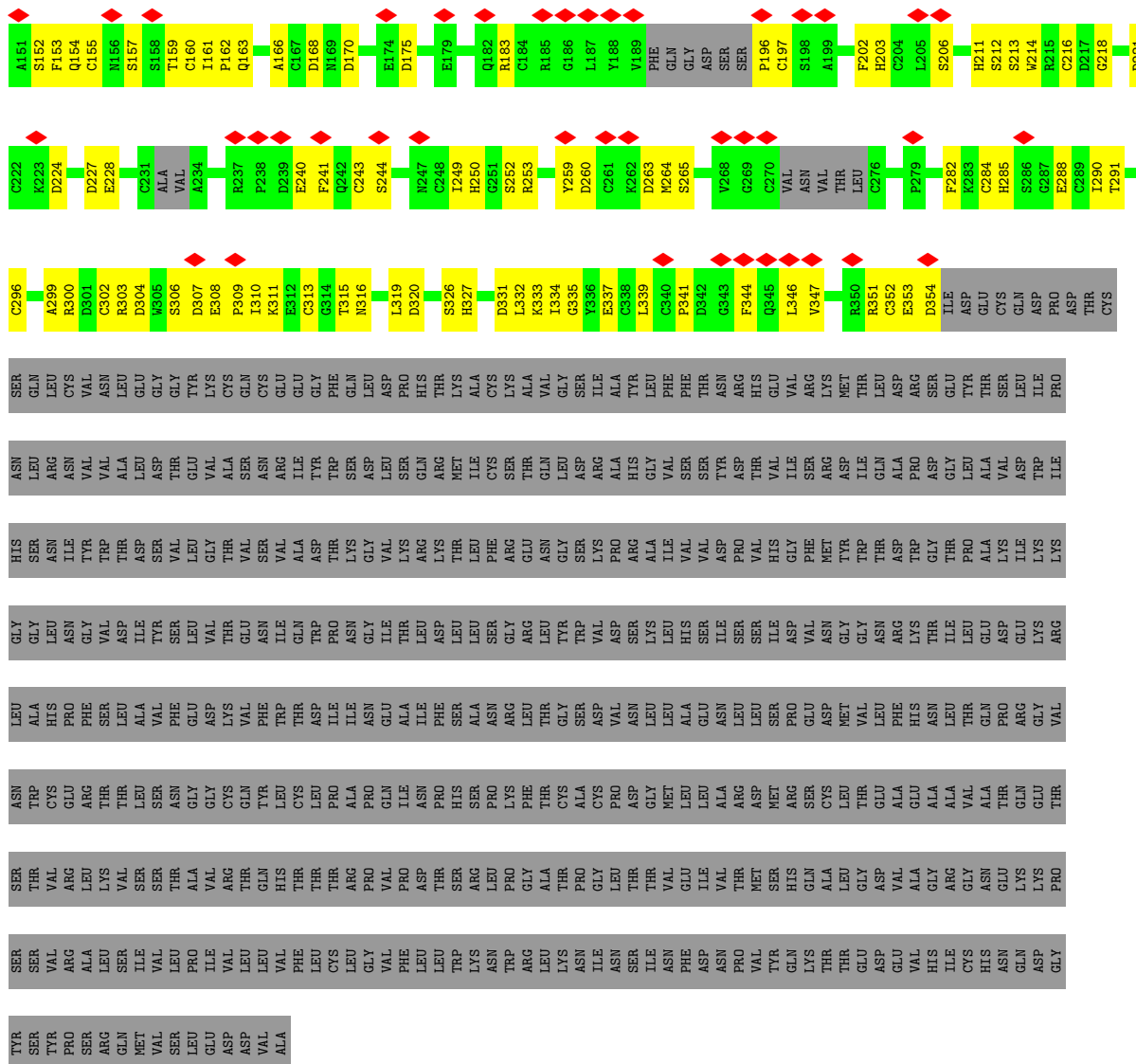


[illegible]

- Molecule 3: Legobody 8D3 Fab light chain

Chain L: 56% 26% 18%

V196	C199	Q204	GLY	LEU	SER	PRO	V210	M215	ARG	GLY	CYS	E110	LLE	LVS	ARG	THR	VAL	ALA	ALA	PRO	SER	V120	Q129	S132	V138	C139	L140	L141	N143	F144	Y145	E148	ALA	LVS	VAL	GLN	TRP	LVS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	Q165	T177	L180	S181	S182	T183	L184	T185	LEU	SER	SER	LVS	ALA	D190	H194	K195																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	527598	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.494	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.76, 557.76, 557.76	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6600001, 1.6600001, 1.6600001	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: NAG, CA

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	H	0.13	0/1320	0.33	0/1803
2	A	0.11	0/8603	0.30	0/11684
3	L	0.11	0/1267	0.32	0/1743
4	B	0.10	0/3468	0.27	0/4753
5	N	0.14	0/877	0.37	0/1196
6	R	0.12	0/1932	0.36	0/2622
All	All	0.11	0/17467	0.31	0/23801

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1289	0	1173	56	0
2	A	8453	0	8047	302	0
3	L	1244	0	1077	40	0
4	B	3396	0	3063	136	0
5	N	859	0	767	27	0
6	R	1898	0	1496	85	0
7	A	70	0	65	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	7	0	0	0	0
All	All	17216	0	15688	623	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 19.

All (623) 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)
2:A:3060:PHE:HB2	2:A:3064:LEU:HB2	1.64	0.77
2:A:2931:TRP:NE1	2:A:2933:CYS:SG	2.58	0.77
1:H:20:LEU:HD23	1:H:83:MET:HE1	1.64	0.77
1:H:22:CYS:HB3	1:H:79:LEU:HB3	1.66	0.77
2:A:3017:PHE:HB3	2:A:3039:PHE:HB3	1.67	0.77
4:B:69:GLY:HA3	4:B:333:ASN:HB2	1.65	0.77
2:A:1965:GLU:HB2	2:A:1984:LYS:HB2	1.66	0.76
2:A:3389:ARG:HE	2:A:3392:GLY:HA3	1.50	0.76
6:R:284:CYS:SG	6:R:303:ARG:N	2.61	0.74
2:A:3020:ARG:HH21	2:A:3034:LYS:HE2	1.53	0.74
2:A:3590:GLU:HB2	2:A:3597:SER:HB2	1.70	0.73
1:H:107:GLY:HA3	3:L:56:TRP:HE1	1.54	0.73
2:A:3075:ALA:HB3	2:A:3086:SER:HB3	1.71	0.73
4:B:455:VAL:O	4:B:459:ALA:N	2.21	0.72
4:B:117:ILE:HG12	4:B:245:VAL:HG12	1.72	0.72
2:A:2862:THR:HG22	2:A:2863:GLU:H	1.55	0.72
2:A:3410:HIS:HA	2:A:3427:THR:HA	1.72	0.71
1:H:73:ASP:O	1:H:77:ASN:N	2.24	0.70
6:R:299:ALA:N	6:R:308:GLU:OE1	2.24	0.70
2:A:2881:LEU:HB3	2:A:2914:LEU:HB2	1.74	0.69
2:A:3341:PHE:HB3	2:A:3352:THR:HB	1.74	0.69
3:L:138:VAL:HA	3:L:183:THR:HA	1.74	0.69
4:B:305:LEU:HD23	4:B:308:TYR:HB2	1.73	0.69
6:R:327:HIS:HB3	6:R:341:PRO:HG2	1.74	0.69
2:A:3437:ARG:HB3	2:A:3463:ASP:HB3	1.72	0.69
1:H:210:HIS:O	1:H:214:ASN:N	2.25	0.69
1:H:154:ASP:HA	1:H:185:LEU:HD13	1.74	0.69
4:B:119:ASN:HB2	4:B:218:PHE:HE1	1.58	0.69
2:A:3565:HIS:NE2	2:A:3567:THR:OG1	2.27	0.68
2:A:3517:ALA:HA	2:A:3530:VAL:HG23	1.76	0.68
2:A:2008:GLU:HA	2:A:2057:PHE:HB3	1.75	0.68
2:A:3608:SER:H	2:A:3612:ASP:HA	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:MET:HB3	1:H:113:TRP:HE1	1.58	0.68
6:R:332:LEU:HD23	6:R:333:LYS:H	1.59	0.68
2:A:2988:ILE:HB	2:A:3004:ALA:HB3	1.74	0.68
2:A:3358:ASN:HA	7:A:4601:NAG:H4	1.76	0.68
2:A:3493:GLU:HG2	2:A:3518:ASN:HD21	1.59	0.67
4:B:287:THR:HG23	4:B:290:GLY:H	1.58	0.67
4:B:456:LEU:O	4:B:459:ALA:HB3	1.94	0.67
2:A:3344:LYS:NZ	6:R:170:ASP:OD2	2.27	0.67
2:A:3343:PHE:HB3	2:A:3350:LEU:HB2	1.75	0.67
2:A:3621:ALA:HB3	2:A:3632:ARG:HB2	1.77	0.67
2:A:2844:LEU:HB2	2:A:2851:GLU:HB3	1.76	0.67
4:B:451:GLN:O	4:B:454:ASN:HB3	1.93	0.67
2:A:2881:LEU:HD23	2:A:2914:LEU:HD12	1.76	0.66
2:A:3502:GLY:H	2:A:3509:TYR:HD2	1.41	0.66
6:R:309:PRO:HG2	6:R:334:ILE:HD12	1.76	0.66
2:A:1909:ALA:HB3	2:A:1931:PHE:HB2	1.77	0.66
4:B:432:ASN:ND2	4:B:466:GLN:O	2.28	0.66
2:A:1890:LEU:HA	2:A:1915:GLY:HA2	1.78	0.65
4:B:372:ASN:ND2	4:B:403:ASN:O	2.29	0.65
5:N:5:GLN:N	5:N:22:CYS:SG	2.69	0.65
4:B:377:GLN:NE2	5:N:15:GLY:O	2.27	0.65
2:A:3052:ASN:HB3	2:A:3072:ASN:HB2	1.78	0.65
2:A:2858:ALA:HB3	2:A:2869:LEU:HB2	1.79	0.65
2:A:3097:LYS:HB3	2:A:3120:GLU:HB2	1.77	0.65
4:B:215:GLU:OE1	4:B:219:ASN:ND2	2.30	0.65
2:A:3547:LYS:O	2:A:3565:HIS:ND1	2.30	0.64
4:B:281:LEU:HA	4:B:285:LEU:HB2	1.79	0.64
1:H:51:ILE:HD11	1:H:55:SER:HA	1.79	0.64
2:A:1844:SER:HA	2:A:1849:ALA:HA	1.78	0.64
2:A:2889:TYR:HB3	2:A:2906:LEU:HB2	1.79	0.64
1:H:162:VAL:HG21	1:H:188:LEU:HD11	1.80	0.64
4:B:453:THR:O	4:B:456:LEU:HB3	1.97	0.64
6:R:326:SER:OG	6:R:339:LEU:O	2.15	0.64
2:A:2723:ILE:HD12	2:A:2724:PRO:HD2	1.80	0.64
3:L:59:THR:O	3:L:60:ARG:NH1	2.30	0.64
2:A:2066:VAL:HA	2:A:2753:PRO:HA	1.80	0.63
2:A:1981:TRP:HB3	2:A:1983:LEU:HD13	1.81	0.63
2:A:2820:ASN:HD21	2:A:2847:GLY:H	1.46	0.63
4:B:209:THR:HA	4:B:213:ILE:HD11	1.80	0.63
2:A:3518:ASN:ND2	2:A:3520:TYR:OH	2.31	0.63
2:A:3433:ILE:HG22	2:A:3435:ILE:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:452:SER:O	4:B:456:LEU:N	2.32	0.62
2:A:3121:ALA:HB3	2:A:3167:GLN:HE21	1.63	0.62
2:A:3386:ARG:HE	6:R:214:TRP:HZ3	1.46	0.62
6:R:218:GLY:N	6:R:228:GLU:OE2	2.31	0.62
2:A:2012:ARG:HH12	2:A:2014:LEU:HB2	1.63	0.62
4:B:312:LEU:HD22	4:B:318:ILE:HG21	1.82	0.62
4:B:442:ILE:HD12	6:R:92:GLN:HB2	1.81	0.62
4:B:451:GLN:O	4:B:455:VAL:N	2.30	0.62
4:B:526:ASP:O	4:B:530:LYS:N	2.32	0.62
2:A:3072:ASN:HA	2:A:3089:VAL:HG12	1.81	0.62
2:A:3394:LYS:NZ	6:R:213:SER:O	2.31	0.62
2:A:3421:MET:N	2:A:3448:THR:OG1	2.33	0.62
2:A:3401:LEU:HD21	2:A:3406:VAL:HG12	1.80	0.62
2:A:3489:TYR:OH	6:R:303:ARG:O	2.18	0.62
2:A:3065:THR:OG1	6:R:125:GLN:NE2	2.32	0.61
2:A:3665:LEU:HB2	2:A:3702:LEU:HD12	1.80	0.61
2:A:1940:PHE:HB2	2:A:1972:LEU:HB2	1.83	0.61
2:A:3339:TYR:HB3	2:A:3354:ALA:HB3	1.82	0.61
2:A:3703:ARG:NH1	2:A:3888:GLU:O	2.33	0.61
6:R:128:CYS:N	6:R:139:ASP:O	2.29	0.61
4:B:118:TYR:N	4:B:244:GLY:O	2.34	0.61
6:R:310:ILE:HA	6:R:313:CYS:HB2	1.82	0.61
4:B:193:LEU:HD11	4:B:348:VAL:HG12	1.82	0.61
2:A:3656:LYS:HG2	2:A:3711:THR:HG23	1.81	0.61
6:R:114:PHE:N	6:R:122:ILE:O	2.33	0.61
2:A:2823:ALA:HB2	2:A:2844:LEU:HD13	1.83	0.60
6:R:241:PHE:N	6:R:249:ILE:O	2.33	0.60
2:A:3386:ARG:HH12	2:A:3396:ALA:N	1.99	0.60
6:R:123:SER:OG	6:R:125:GLN:OE1	2.18	0.60
1:H:162:VAL:HG22	1:H:208:VAL:HG12	1.83	0.60
2:A:3416:LEU:HD12	2:A:3421:MET:HG3	1.83	0.60
4:B:122:LEU:HD23	4:B:140:LEU:HD21	1.82	0.60
2:A:1999:TYR:OH	2:A:2004:LYS:NZ	2.31	0.60
4:B:521:GLY:CA	4:B:535:THR:O	2.49	0.60
2:A:3436:LEU:HD12	2:A:3464:PHE:HD1	1.66	0.60
2:A:3052:ASN:OD1	2:A:3053:GLU:N	2.35	0.60
2:A:1925:GLY:HA2	2:A:1950:THR:HA	1.83	0.60
2:A:2813:GLN:HB2	2:A:2825:LYS:HB2	1.83	0.59
2:A:3432:GLN:OE1	2:A:3437:ARG:NE	2.31	0.59
2:A:2959:LEU:HB3	2:A:2974:LEU:HB2	1.84	0.59
2:A:1994:GLN:HE21	2:A:2009:LEU:HG	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3637:VAL:HB	2:A:3644:PHE:HB3	1.85	0.59
4:B:140:LEU:HD23	4:B:147:ALA:HA	1.85	0.59
5:N:51:ILE:HB	5:N:70:ILE:HG21	1.84	0.59
2:A:3351:ASN:OD1	2:A:3352:THR:N	2.36	0.58
2:A:2422:MET:SD	2:A:2422:MET:N	2.76	0.58
4:B:258:PRO:HD2	4:B:328:GLY:HA2	1.85	0.58
6:R:244:SER:N	6:R:263:ASP:OD2	2.35	0.58
1:H:179:VAL:O	1:H:181:GLN:NE2	2.36	0.58
2:A:1907:ILE:HB	2:A:1933:LEU:HB2	1.85	0.58
2:A:1977:GLN:OE1	2:A:2000:ASN:ND2	2.28	0.58
2:A:2814:LEU:HD11	2:A:2824:LEU:HG	1.86	0.58
2:A:3432:GLN:NE2	2:A:3433:ILE:O	2.36	0.58
4:B:485:LEU:HD22	4:B:532:PHE:H	1.68	0.58
1:H:66:GLY:C	4:B:458:GLU:HG3	2.29	0.58
2:A:1849:ALA:O	2:A:1872:ILE:N	2.37	0.58
2:A:3495:SER:HA	2:A:3516:GLU:HA	1.86	0.57
6:R:157:SER:N	6:R:175:ASP:OD2	2.36	0.57
3:L:27:GLN:HE21	5:N:118:GLN:HG2	1.70	0.57
2:A:3437:ARG:O	2:A:3463:ASP:N	2.29	0.57
4:B:117:ILE:HD12	4:B:228:ASN:HB2	1.85	0.57
6:R:116:CYS:SG	6:R:117:HIS:N	2.77	0.57
4:B:482:THR:HA	4:B:499:LYS:HA	1.86	0.57
6:R:168:ASP:N	6:R:170:ASP:OD1	2.37	0.57
6:R:284:CYS:HB3	6:R:288:GLU:N	2.19	0.57
2:A:3509:TYR:HB2	2:A:3538:ILE:HD13	1.86	0.57
4:B:159:TRP:HA	4:B:162:ILE:HG12	1.87	0.57
2:A:3559:ILE:HB	2:A:3591:LEU:HB3	1.85	0.57
2:A:3361:ASP:OD1	2:A:3362:ILE:N	2.38	0.56
4:B:162:ILE:HB	4:B:193:LEU:HD22	1.85	0.56
2:A:2762:LEU:HB2	2:A:2773:ALA:HB3	1.87	0.56
2:A:3630:LYS:HA	2:A:3651:SER:HA	1.87	0.56
2:A:2779:ASN:HB3	2:A:2789:ILE:HA	1.87	0.56
2:A:2894:ASN:HA	2:A:2901:SER:HA	1.86	0.56
2:A:3516:GLU:OE2	2:A:3531:LYS:N	2.38	0.56
2:A:2438:GLU:O	2:A:2442:LYS:NZ	2.39	0.56
2:A:3384:THR:OG1	2:A:3396:ALA:O	2.19	0.56
4:B:521:GLY:HA2	4:B:535:THR:O	2.05	0.56
6:R:67:THR:OG1	6:R:68:CYS:N	2.36	0.56
2:A:1866:HIS:HB2	2:A:1883:THR:HG23	1.88	0.56
2:A:3363:VAL:HA	2:A:3385:THR:O	2.05	0.56
6:R:284:CYS:HB3	6:R:288:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:152:SER:HA	6:R:162:PRO:HA	1.88	0.56
2:A:1843:SER:OG	2:A:1850:SER:OG	2.24	0.56
2:A:2436:VAL:HG21	2:A:2725:THR:HG22	1.87	0.56
4:B:93:PHE:HB2	4:B:330:ILE:HD11	1.88	0.56
4:B:281:LEU:O	4:B:286:LEU:N	2.26	0.56
3:L:70:GLY:HA3	3:L:79:LEU:HD12	1.88	0.56
4:B:486:VAL:HG22	4:B:495:GLU:HB3	1.87	0.56
2:A:3177:TYR:HA	2:A:3337:ILE:HG23	1.89	0.55
4:B:91:TYR:H	4:B:304:ALA:HB1	1.71	0.55
4:B:89:LYS:NZ	4:B:286:LEU:O	2.40	0.55
2:A:2453:GLU:HA	2:A:2456:ALA:HB3	1.87	0.55
2:A:3471:SER:HB2	2:A:3504:VAL:HG12	1.87	0.55
3:L:18:ARG:HA	3:L:82:ASN:HA	1.88	0.55
1:H:62:ASP:OD1	1:H:63:THR:N	2.39	0.55
2:A:3665:LEU:O	2:A:3702:LEU:N	2.40	0.55
4:B:69:GLY:O	4:B:73:GLN:NE2	2.38	0.55
2:A:3614:PRO:HB2	2:A:3638:ARG:HB2	1.88	0.55
2:A:3631:ILE:HG23	2:A:3650:LEU:HB3	1.88	0.55
2:A:3619:GLU:HB3	2:A:3634:LYS:HB3	1.89	0.55
2:A:2991:GLN:HG2	2:A:3001:VAL:HG23	1.89	0.54
2:A:3099:ASN:HB3	2:A:3118:ASN:HB2	1.89	0.54
4:B:130:TRP:N	4:B:250:THR:O	2.31	0.54
2:A:1953:HIS:HB3	2:A:1959:SER:HA	1.88	0.54
2:A:3651:SER:HB2	2:A:3658:HIS:HB2	1.89	0.54
2:A:1894:ASN:HA	2:A:1911:THR:HA	1.89	0.54
2:A:3076:LEU:HA	2:A:3085:ALA:HA	1.89	0.54
4:B:136:LEU:HD12	4:B:147:ALA:HB1	1.89	0.54
4:B:455:VAL:HA	4:B:458:GLU:OE1	2.08	0.54
2:A:1897:ARG:NH2	2:A:2730:ASP:O	2.40	0.54
2:A:3066:GLY:HA2	2:A:3094:ASN:HD21	1.72	0.54
2:A:3119:GLY:H	2:A:3169:PHE:HB2	1.71	0.54
6:R:153:PHE:N	6:R:161:ILE:O	2.39	0.54
6:R:351:ARG:NE	6:R:353:GLU:OE2	2.41	0.54
4:B:116:LEU:HD13	4:B:249:PRO:HD3	1.89	0.54
2:A:3069:ASP:HB2	2:A:3092:ARG:HH21	1.73	0.54
6:R:153:PHE:HB2	6:R:163:GLN:HE22	1.72	0.54
4:B:420:GLN:HE22	4:B:421:GLN:HE21	1.55	0.54
3:L:139:CYS:N	3:L:182:SER:O	2.38	0.54
3:L:144:PHE:N	3:L:177:THR:OG1	2.41	0.54
2:A:1941:THR:HG21	2:A:2736:LEU:HD11	1.89	0.53
2:A:3095:GLN:HB2	2:A:3122:ASN:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:THR:OG1	1:H:121:VAL:N	2.39	0.53
1:H:165:ASN:HA	1:H:205:ILE:HB	1.90	0.53
2:A:2853:LYS:HZ3	2:A:2855:ASN:HB2	1.72	0.53
4:B:243:TYR:OH	4:B:317:ARG:NH2	2.42	0.53
4:B:451:GLN:O	4:B:455:VAL:HG23	2.09	0.53
2:A:1910:HIS:HB2	2:A:1930:LYS:HD2	1.89	0.53
2:A:2959:LEU:HD23	2:A:2974:LEU:HD12	1.91	0.53
2:A:3634:LYS:O	2:A:3635:ASN:ND2	2.41	0.53
4:B:372:ASN:ND2	4:B:403:ASN:OD1	2.40	0.53
6:R:214:TRP:NE1	6:R:221:ASP:OD2	2.42	0.53
2:A:3551:ALA:HB3	2:A:3562:LEU:HB3	1.90	0.53
3:L:22:SER:HA	3:L:78:THR:HA	1.89	0.53
6:R:332:LEU:HD23	6:R:333:LYS:N	2.23	0.53
2:A:2984:SER:N	2:A:3008:ALA:O	2.42	0.53
4:B:452:SER:HA	4:B:455:VAL:HB	1.91	0.53
2:A:2801:LEU:HB3	2:A:2803:VAL:HG22	1.91	0.53
2:A:3653:ASP:OD1	2:A:3654:GLN:N	2.41	0.53
2:A:3884:THR:O	2:A:3886:ARG:NH1	2.42	0.53
4:B:116:LEU:HD11	4:B:225:MET:HG3	1.89	0.53
5:N:11:LEU:HA	5:N:120:THR:O	2.09	0.53
2:A:2961:ASN:OD1	2:A:2972:GLN:NE2	2.35	0.53
2:A:3031:GLY:HA3	2:A:3056:LEU:HA	1.91	0.53
2:A:3453:THR:HA	2:A:3484:GLU:HG3	1.90	0.53
6:R:197:CYS:SG	6:R:203:HIS:ND1	2.80	0.53
3:L:145:TYR:HA	3:L:177:THR:HA	1.91	0.52
4:B:459:ALA:O	4:B:462:LEU:HG	2.09	0.52
6:R:300:ARG:NH1	6:R:302:CYS:O	2.43	0.52
4:B:100:TYR:HB2	4:B:105:ILE:HD13	1.90	0.52
4:B:117:ILE:N	4:B:226:THR:O	2.41	0.52
4:B:86:PHE:O	4:B:95:TRP:NE1	2.42	0.52
6:R:128:CYS:SG	6:R:143:CYS:N	2.82	0.52
4:B:119:ASN:HD21	4:B:121:ASP:HB3	1.74	0.52
4:B:448:ASP:OD1	4:B:448:ASP:N	2.41	0.52
6:R:282:PHE:HB3	6:R:291:THR:OG1	2.10	0.52
2:A:3427:THR:HB	2:A:3442:GLN:HB3	1.91	0.52
3:L:39:LEU:HB2	3:L:57:ALA:HB2	1.91	0.52
4:B:91:TYR:O	4:B:94:THR:OG1	2.28	0.52
4:B:100:TYR:N	4:B:103:LYS:O	2.41	0.52
5:N:19:ARG:HH21	5:N:80:TYR:HD2	1.58	0.52
6:R:100:ASP:N	6:R:100:ASP:OD1	2.42	0.52
1:H:157:PRO:HD2	1:H:210:HIS:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3365:HIS:CE1	2:A:3382:GLU:HG2	2.45	0.52
2:A:1879:ILE:HD13	2:A:1900:MET:HE1	1.92	0.51
2:A:2017:LEU:HG	2:A:2049:PRO:HA	1.92	0.51
2:A:3560:TYR:CE2	6:R:311:LYS:HA	2.45	0.51
1:H:99:ARG:NH2	5:N:125:GLU:OE2	2.42	0.51
2:A:1866:HIS:HE2	2:A:1868:LEU:HB2	1.74	0.51
2:A:2920:ALA:HA	2:A:2949:THR:HA	1.91	0.51
2:A:3486:LEU:HD13	2:A:3489:TYR:HB3	1.92	0.51
2:A:3643:SER:OG	2:A:3645:GLN:NE2	2.43	0.51
3:L:83:SER:O	3:L:85:GLN:NE2	2.43	0.51
2:A:3599:LEU:HD22	2:A:3601:GLN:HE22	1.76	0.51
4:B:178:ASP:OD1	4:B:178:ASP:N	2.43	0.51
4:B:200:ILE:HD12	4:B:207:ALA:HA	1.92	0.51
6:R:227:ASP:OD1	6:R:227:ASP:N	2.43	0.51
5:N:61:ALA:HB3	5:N:64:VAL:HG12	1.92	0.51
2:A:1952:HIS:H	2:A:1960:ILE:HG22	1.75	0.51
2:A:3490:PHE:H	2:A:3522:ASN:HA	1.76	0.51
1:H:50:TYR:OH	1:H:99:ARG:NH2	2.42	0.51
1:H:73:ASP:O	1:H:77:ASN:CA	2.58	0.51
4:B:302:ALA:HA	4:B:312:LEU:HD13	1.93	0.51
6:R:285:HIS:HB3	6:R:304:ASP:HB2	1.92	0.51
2:A:2876:LYS:HB2	2:A:2882:THR:HG22	1.92	0.51
6:R:155:CYS:SG	6:R:159:THR:OG1	2.65	0.51
2:A:2050:GLN:HG3	2:A:2767:PRO:HG2	1.91	0.51
6:R:154:GLN:O	6:R:183:ARG:NH2	2.44	0.50
2:A:2017:LEU:HD11	2:A:2050:GLN:HB2	1.93	0.50
2:A:3348:ILE:HA	2:A:3372:SER:HB2	1.92	0.50
4:B:98:VAL:HG21	4:B:108:PRO:HD3	1.94	0.50
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.34	0.50
2:A:2404:LEU:HD13	2:A:2407:LEU:HD12	1.93	0.50
5:N:91:THR:HG22	5:N:121:VAL:H	1.77	0.50
6:R:259:TYR:HB3	6:R:264:MET:HE1	1.94	0.50
2:A:3059:ARG:HB3	2:A:3065:THR:HG22	1.93	0.50
2:A:2003:ASP:OD1	2:A:2004:LYS:N	2.44	0.50
2:A:3113:ALA:H	2:A:3175:ALA:HB3	1.74	0.50
4:B:111:VAL:HG23	4:B:262:VAL:HG22	1.92	0.50
4:B:119:ASN:HB2	4:B:218:PHE:CE1	2.42	0.50
5:N:5:GLN:N	5:N:23:VAL:O	2.45	0.50
1:H:38:ARG:NH1	1:H:90:ASP:OD1	2.45	0.50
3:L:194:HIS:ND1	3:L:196:VAL:O	2.34	0.50
4:B:149:MET:HE1	4:B:213:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:167:GLY:HA3	4:B:189:ALA:HB2	1.94	0.50
4:B:492:LEU:H	4:B:519:VAL:HG11	1.77	0.50
6:R:202:PHE:H	6:R:211:HIS:HA	1.75	0.50
2:A:2081:PHE:HD2	2:A:2409:PHE:HB2	1.77	0.50
2:A:3386:ARG:HH12	2:A:3396:ALA:H	1.58	0.50
2:A:3588:THR:OG1	2:A:3590:GLU:OE2	2.30	0.50
5:N:52:SER:HB2	5:N:56:GLY:O	2.12	0.50
2:A:3052:ASN:N	2:A:3072:ASN:O	2.45	0.50
2:A:1960:ILE:HD11	2:A:1988:ASN:HB2	1.93	0.49
2:A:1985:THR:O	2:A:1991:GLU:HA	2.12	0.49
2:A:3067:LYS:O	2:A:3092:ARG:NH1	2.44	0.49
2:A:3622:LEU:HD13	2:A:3631:ILE:HB	1.94	0.49
6:R:250:HIS:NE2	6:R:252:SER:OG	2.44	0.49
6:R:351:ARG:NH2	6:R:352:CYS:O	2.39	0.49
6:R:250:HIS:H	6:R:253:ARG:HE	1.60	0.49
2:A:1942:PHE:O	2:A:1944:HIS:ND1	2.44	0.49
4:B:119:ASN:ND2	4:B:121:ASP:HB3	2.26	0.49
2:A:3152:LEU:HD21	2:A:3155:LYS:HB3	1.93	0.49
2:A:2843:MET:HE1	2:A:2845:PHE:HB2	1.95	0.49
2:A:3093:PHE:HB3	2:A:3096:TYR:HB2	1.95	0.49
3:L:25:SER:N	3:L:75:THR:OG1	2.46	0.49
2:A:3127:ASN:N	2:A:3151:SER:OG	2.46	0.49
2:A:3433:ILE:HB	2:A:3436:LEU:HB3	1.94	0.49
3:L:14:SER:OG	3:L:15:ALA:N	2.46	0.49
3:L:55:TYR:HD2	3:L:56:TRP:CD1	2.31	0.49
6:R:90:ASP:OD1	6:R:91:GLY:N	2.45	0.49
2:A:2093:GLU:O	2:A:2097:ARG:NH2	2.45	0.49
2:A:3489:TYR:OH	6:R:300:ARG:NH1	2.43	0.49
5:N:35:GLY:HA3	5:N:105:PHE:HE2	1.77	0.49
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.95	0.49
2:A:3054:GLY:HA3	2:A:3070:PHE:HB2	1.94	0.49
3:L:180:LEU:HD23	3:L:181:SER:N	2.28	0.49
1:H:37:VAL:HG23	1:H:47:TRP:HA	1.94	0.49
2:A:1850:SER:HA	2:A:1871:ASP:HA	1.94	0.49
2:A:2089:ILE:O	2:A:2093:GLU:N	2.45	0.49
4:B:372:ASN:HD22	4:B:407:ALA:HB2	1.77	0.49
3:L:68:PHE:HA	3:L:81:ILE:HD12	1.95	0.48
3:L:69:THR:OG1	3:L:80:THR:O	2.29	0.48
4:B:394:GLU:OE1	4:B:394:GLU:N	2.45	0.48
6:R:89:CYS:N	6:R:100:ASP:O	2.27	0.48
2:A:2817:PRO:HG2	2:A:2819:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2856:THR:HB	2:A:2871:ASN:HB3	1.94	0.48
6:R:136:ASP:OD1	6:R:138:SER:OG	2.31	0.48
2:A:3704:VAL:HA	2:A:3889:VAL:HG22	1.95	0.48
4:B:182:VAL:HG21	4:B:369:ILE:HD13	1.94	0.48
4:B:483:TYR:N	4:B:498:THR:O	2.45	0.48
2:A:3336:ASN:HA	2:A:3357:PHE:HA	1.94	0.48
1:H:213:SER:OG	1:H:215:THR:OG1	2.25	0.48
2:A:2974:LEU:HD22	2:A:2988:ILE:HD12	1.94	0.48
4:B:260:VAL:H	4:B:331:MET:HE3	1.78	0.48
5:N:67:ARG:HB3	5:N:84:ASN:O	2.14	0.48
2:A:2762:LEU:HD12	2:A:2764:ILE:HD11	1.95	0.48
5:N:47:TRP:CD1	5:N:105:PHE:HD2	2.32	0.48
2:A:3438:MET:HA	2:A:3462:TYR:HA	1.95	0.48
3:L:129:GLN:O	3:L:132:SER:OG	2.26	0.48
4:B:291:LEU:HD21	4:B:303:VAL:HG11	1.95	0.48
4:B:399:ALA:O	4:B:403:ASN:N	2.46	0.48
4:B:438:ARG:O	4:B:442:ILE:HG12	2.13	0.48
5:N:18:LEU:HD21	5:N:83:MET:HE3	1.94	0.48
5:N:32:VAL:HG22	5:N:98:ALA:HB1	1.95	0.48
6:R:84:PRO:HG2	6:R:86:PHE:CE2	2.49	0.48
2:A:1888:ASP:OD1	2:A:1888:ASP:N	2.44	0.48
2:A:2993:ASP:HA	2:A:2999:HIS:HA	1.96	0.48
2:A:3037:LEU:HB2	2:A:3050:THR:HG22	1.95	0.48
5:N:60:TYR:HB2	5:N:65:LYS:HD2	1.95	0.48
2:A:2851:GLU:OE1	2:A:2876:LYS:HD3	2.14	0.47
3:L:120:VAL:HG12	3:L:142:ASN:H	1.79	0.47
1:H:108:TYR:HE1	3:L:55:TYR:CZ	2.33	0.47
2:A:3656:LYS:HA	2:A:3712:LYS:H	1.79	0.47
1:H:33:GLY:O	1:H:34:MET:HE2	2.13	0.47
2:A:2764:ILE:HD12	2:A:2764:ILE:H	1.79	0.47
2:A:3447:ASN:ND2	2:A:3451:LYS:O	2.47	0.47
2:A:2435:PHE:HA	2:A:2438:GLU:HG2	1.96	0.47
2:A:3067:LYS:N	2:A:3094:ASN:OD1	2.38	0.47
2:A:3466:SER:HB2	2:A:3471:SER:H	1.79	0.47
2:A:3467:SER:HA	7:A:4605:NAG:H81	1.96	0.47
2:A:3405:PHE:HA	2:A:3432:GLN:HB3	1.96	0.47
4:B:485:LEU:HD21	4:B:510:PHE:CD2	2.50	0.47
4:B:90:LEU:H	4:B:95:TRP:HZ2	1.61	0.47
4:B:110:ALA:HB3	4:B:263:LEU:HD23	1.97	0.47
2:A:1963:ALA:O	2:A:1986:GLN:N	2.43	0.47
2:A:1980:THR:OG1	2:A:1982:LYS:NZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2401:VAL:HG23	2:A:2402:LYS:HD2	1.97	0.47
2:A:3560:TYR:CD2	6:R:311:LYS:HA	2.49	0.47
2:A:3629:GLN:HB2	2:A:3652:ASN:HB3	1.95	0.47
4:B:109:ILE:HB	4:B:263:LEU:HG	1.96	0.47
4:B:155:PRO:HA	4:B:158:THR:HG22	1.95	0.47
6:R:315:THR:OG1	6:R:316:ASN:N	2.48	0.47
1:H:50:TYR:HD2	1:H:59:TYR:HD2	1.63	0.47
4:B:247:VAL:HG23	4:B:324:ASN:HD21	1.80	0.47
5:N:99:ALA:HB3	5:N:105:PHE:HE1	1.80	0.47
1:H:73:ASP:O	1:H:77:ASN:HA	2.15	0.47
1:H:210:HIS:O	1:H:214:ASN:CA	2.63	0.47
2:A:1871:ASP:OD1	2:A:1872:ILE:N	2.48	0.47
2:A:2946:ILE:HG13	2:A:2959:LEU:HD13	1.95	0.47
4:B:118:TYR:CD1	4:B:126:PRO:HG3	2.50	0.47
2:A:3440:PHE:HE1	2:A:3458:MET:HG2	1.80	0.46
3:L:96:GLN:HE21	3:L:102:THR:HB	1.80	0.46
4:B:159:TRP:CD1	4:B:162:ILE:HD11	2.50	0.46
2:A:1931:PHE:HA	2:A:1944:HIS:HB2	1.96	0.46
4:B:148:LEU:HD13	4:B:225:MET:HG2	1.97	0.46
2:A:3119:GLY:O	2:A:3169:PHE:N	2.46	0.46
6:R:153:PHE:N	6:R:163:GLN:OE1	2.48	0.46
6:R:206:SER:HB3	6:R:224:ASP:HB3	1.98	0.46
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.51	0.46
2:A:1963:ALA:HB3	2:A:1986:GLN:HB3	1.96	0.46
2:A:2930:LYS:HA	2:A:2938:ASP:HB2	1.98	0.46
2:A:3539:ASP:O	2:A:3542:TRP:N	2.35	0.46
2:A:3638:ARG:HG3	2:A:3643:SER:HA	1.97	0.46
6:R:116:CYS:SG	6:R:138:SER:OG	2.74	0.46
2:A:2908:ASN:OD1	2:A:2909:GLU:N	2.48	0.46
4:B:458:GLU:O	4:B:461:LYS:CB	2.64	0.46
4:B:483:TYR:HE2	4:B:485:LEU:HD23	1.80	0.46
6:R:310:ILE:HG13	6:R:310:ILE:O	2.13	0.46
2:A:2769:PHE:HA	2:A:2799:SER:HA	1.97	0.46
2:A:2927:GLY:O	2:A:2942:HIS:N	2.49	0.46
2:A:3338:THR:HG23	2:A:3355:GLU:HG3	1.97	0.46
3:L:89:LEU:HB2	3:L:110:GLU:C	2.41	0.46
2:A:1876:ALA:HB3	2:A:2726:LEU:HD13	1.97	0.46
3:L:6:GLN:HA	3:L:23:CYS:HB3	1.98	0.46
3:L:24:LYS:HA	3:L:75:THR:O	2.15	0.46
6:R:240:GLU:HA	6:R:250:HIS:HA	1.98	0.46
6:R:344:PHE:HB3	6:R:354:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1889:SER:HA	2:A:1916:LYS:HB2	1.98	0.46
2:A:2000:ASN:HA	2:A:2005:ILE:HG22	1.97	0.46
2:A:3176:GLN:HB2	2:A:3338:THR:HB	1.98	0.46
2:A:3407:GLU:HB2	2:A:3430:LYS:HB3	1.98	0.46
2:A:3603:HIS:ND1	2:A:3615:ASP:OD1	2.47	0.46
4:B:502:ASP:OD1	4:B:502:ASP:N	2.49	0.46
1:H:52:SER:OG	1:H:53:SER:N	2.49	0.46
2:A:3375:ASP:OD1	2:A:3375:ASP:N	2.49	0.46
4:B:448:ASP:O	4:B:452:SER:N	2.49	0.46
1:H:84:ASN:HB3	4:B:441:PHE:HE1	1.81	0.46
2:A:1838:HIS:ND1	2:A:1854:ASP:O	2.49	0.46
2:A:2862:THR:HG22	2:A:2863:GLU:N	2.27	0.46
2:A:2940:GLY:H	2:A:2965:SER:HA	1.81	0.46
2:A:3433:ILE:HD13	2:A:3436:LEU:HD22	1.97	0.46
3:L:41:TRP:CD1	3:L:54:ILE:HD11	2.50	0.46
3:L:89:LEU:HD12	3:L:89:LEU:O	2.16	0.46
4:B:92:PRO:HA	4:B:95:TRP:CZ3	2.51	0.46
2:A:1875:LEU:HD23	2:A:1875:LEU:H	1.81	0.45
2:A:2446:VAL:O	2:A:2450:LEU:N	2.48	0.45
4:B:281:LEU:HD13	4:B:285:LEU:HD13	1.98	0.45
4:B:443:GLN:O	4:B:447:ASP:HB2	2.16	0.45
6:R:94:ASP:OD1	6:R:95:CYS:N	2.46	0.45
3:L:141:LEU:HB2	3:L:180:LEU:O	2.15	0.45
6:R:243:CYS:SG	6:R:265:SER:OG	2.74	0.45
1:H:129:PRO:HG3	1:H:210:HIS:HB2	1.99	0.45
2:A:2455:GLN:HE22	2:A:2459:LEU:HD21	1.81	0.45
3:L:41:TRP:CH2	3:L:94:CYS:HB3	2.52	0.45
6:R:290:ILE:O	6:R:291:THR:OG1	2.32	0.45
2:A:1914:ASN:HB3	2:A:1926:GLN:HA	1.99	0.45
2:A:2839:HIS:ND1	2:A:2855:ASN:O	2.49	0.45
4:B:146:SER:N	4:B:222:GLU:O	2.50	0.45
4:B:287:THR:N	4:B:305:LEU:HD21	2.32	0.45
4:B:462:LEU:O	4:B:466:GLN:N	2.49	0.45
2:A:2060:TYR:HD1	2:A:2758:LEU:HA	1.81	0.45
2:A:3442:GLN:HE22	2:A:3444:LEU:HB2	1.80	0.45
4:B:259:PHE:CD1	4:B:331:MET:HE1	2.52	0.45
1:H:6:GLU:OE2	1:H:116:GLY:N	2.49	0.45
2:A:3440:PHE:CZ	2:A:3442:GLN:HB2	2.52	0.45
2:A:3365:HIS:HA	2:A:3383:GLY:O	2.16	0.45
4:B:310:GLU:OE1	4:B:310:GLU:N	2.46	0.45
5:N:99:ALA:HB3	5:N:105:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1937:PRO:O	2:A:1938:LEU:HG	2.17	0.45
3:L:19:VAL:HG21	3:L:109:LEU:HD11	1.99	0.45
6:R:202:PHE:HB2	6:R:212:SER:HB3	1.97	0.45
4:B:165:ASP:HA	4:B:254:GLN:HG2	1.98	0.45
6:R:302:CYS:HB2	6:R:307:ASP:HB2	1.98	0.45
1:H:2:VAL:HA	1:H:25:SER:O	2.17	0.45
1:H:209:ASN:HB2	1:H:216:LYS:HZ1	1.82	0.45
2:A:1895:VAL:O	2:A:1910:HIS:N	2.50	0.45
2:A:3166:LYS:NZ	6:R:160:CYS:O	2.49	0.45
2:A:3547:LYS:HB2	2:A:3566:SER:HB2	1.98	0.45
4:B:119:ASN:HD22	4:B:122:LEU:HD13	1.82	0.45
4:B:129:THR:C	4:B:249:PRO:HB2	2.42	0.45
6:R:296:CYS:H	6:R:308:GLU:HA	1.82	0.45
2:A:1939:ALA:HB1	2:A:2738:ILE:HG13	1.99	0.44
2:A:2981:LEU:HD23	2:A:2981:LEU:H	1.82	0.44
2:A:2970:VAL:HG12	2:A:2992:VAL:HG13	1.99	0.44
4:B:90:LEU:HB2	4:B:95:TRP:NE1	2.32	0.44
1:H:157:PRO:HD2	1:H:210:HIS:CE1	2.52	0.44
2:A:1883:THR:N	2:A:1894:ASN:OD1	2.43	0.44
2:A:3073:ASN:HB2	2:A:3088:GLN:HB2	1.99	0.44
2:A:3361:ASP:O	2:A:3362:ILE:HD13	2.18	0.44
2:A:3654:GLN:HE22	2:A:3714:PRO:HA	1.81	0.44
4:B:130:TRP:N	4:B:249:PRO:HB2	2.31	0.44
4:B:130:TRP:CE2	4:B:161:LEU:HD22	2.53	0.44
1:H:76:LYS:NZ	1:H:78:THR:HG21	2.32	0.44
2:A:2979:GLY:HA3	2:A:2982:ASN:HB3	1.99	0.44
4:B:73:GLN:H	4:B:73:GLN:CD	2.25	0.44
6:R:320:ASP:N	6:R:320:ASP:OD1	2.50	0.44
2:A:1887:SER:N	2:A:1890:LEU:O	2.49	0.44
2:A:3174:LYS:HB3	2:A:3176:GLN:HE22	1.82	0.44
4:B:17:GLY:HA2	4:B:297:ASP:HB3	1.99	0.44
1:H:103:ASP:OD1	1:H:103:ASP:N	2.50	0.44
2:A:3509:TYR:CD1	2:A:3538:ILE:HB	2.52	0.44
6:R:148:CYS:HB3	6:R:160:CYS:HB3	1.71	0.44
1:H:17:SER:HA	1:H:83:MET:O	2.18	0.44
2:A:2947:SER:HB2	5:N:101:SER:HB3	2.00	0.44
2:A:3062:LEU:HD23	2:A:3062:LEU:O	2.17	0.44
2:A:3356:LEU:HA	2:A:3363:VAL:O	2.18	0.44
4:B:256:SER:O	4:B:257:LYS:HE2	2.17	0.44
4:B:424:PHE:HA	4:B:427:ILE:HG12	2.00	0.44
2:A:1973:THR:HG23	2:A:1976:GLU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3042:GLN:HB3	2:A:3045:GLU:HB3	1.99	0.43
2:A:3345:SER:N	2:A:3348:ILE:O	2.51	0.43
4:B:90:LEU:HD13	4:B:108:PRO:HB2	1.99	0.43
4:B:282:GLU:HA	4:B:286:LEU:HB2	2.00	0.43
4:B:514:ALA:O	4:B:518:GLY:N	2.50	0.43
3:L:91:VAL:HA	3:L:108:LYS:HA	2.00	0.43
5:N:36:TRP:CG	5:N:81:LEU:HD22	2.53	0.43
2:A:3567:THR:O	2:A:3582:GLU:HA	2.18	0.43
2:A:2968:LEU:C	2:A:2969:ARG:HD3	2.43	0.43
2:A:3095:GLN:HB2	2:A:3122:ASN:ND2	2.32	0.43
3:L:96:GLN:NE2	3:L:102:THR:HB	2.34	0.43
4:B:230:PRO:HA	4:B:233:TRP:CG	2.54	0.43
6:R:117:HIS:HD1	6:R:138:SER:HG	1.61	0.43
1:H:35:HIS:CD2	1:H:99:ARG:HB2	2.54	0.43
5:N:7:SER:N	5:N:21:SER:O	2.50	0.43
2:A:2884:ASP:OD1	2:A:2885:SER:N	2.52	0.43
2:A:3046:ILE:O	2:A:3078:LEU:N	2.51	0.43
4:B:248:LEU:HD21	4:B:258:PRO:HB3	2.01	0.43
4:B:366:GLN:HA	4:B:369:ILE:HD12	1.99	0.43
6:R:163:GLN:HA	6:R:166:ALA:HB3	2.00	0.43
6:R:196:PRO:HB2	6:R:197:CYS:H	1.61	0.43
1:H:100:PRO:HG2	1:H:108:TYR:HB3	2.01	0.43
2:A:2971:ASN:O	2:A:2990:SER:HA	2.18	0.43
3:L:41:TRP:HD1	3:L:54:ILE:HD11	1.84	0.43
3:L:165:GLN:O	3:L:182:SER:OG	2.32	0.43
5:N:33:ASN:HB3	5:N:101:SER:HA	2.01	0.43
6:R:260:ASP:OD1	6:R:260:ASP:N	2.52	0.43
2:A:1905:MET:N	2:A:1905:MET:HE2	2.34	0.43
1:H:71:SER:OG	1:H:72:ARG:N	2.52	0.42
1:H:156:PHE:HB3	1:H:157:PRO:HD3	2.00	0.42
2:A:1891:HIS:HB2	2:A:1914:ASN:OD1	2.19	0.42
2:A:1926:GLN:N	2:A:1949:SER:O	2.38	0.42
4:B:507:GLU:HG2	4:B:532:PHE:CE2	2.53	0.42
2:A:2832:SER:N	2:A:2835:LEU:O	2.51	0.42
2:A:3460:PHE:CZ	2:A:3462:TYR:HB3	2.53	0.42
3:L:60:ARG:HH21	3:L:69:THR:HG22	1.84	0.42
2:A:2937:SER:O	2:A:2937:SER:OG	2.35	0.42
2:A:3359:GLN:N	7:A:4601:NAG:O6	2.51	0.42
2:A:3405:PHE:HB2	2:A:3432:GLN:O	2.18	0.42
2:A:3561:SER:O	2:A:3588:THR:OG1	2.17	0.42
2:A:3601:GLN:N	2:A:3601:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3630:LYS:HE2	2:A:3630:LYS:HB3	1.87	0.42
4:B:247:VAL:HG23	4:B:324:ASN:ND2	2.33	0.42
2:A:1895:VAL:HB	2:A:1910:HIS:HB3	2.02	0.42
2:A:1917:LEU:HD12	2:A:1917:LEU:HA	1.88	0.42
2:A:2453:GLU:O	2:A:2457:LEU:N	2.51	0.42
2:A:3634:LYS:HA	2:A:3647:GLN:HB2	2.00	0.42
4:B:230:PRO:HD3	4:B:321:THR:HG21	2.01	0.42
6:R:319:LEU:HD23	6:R:319:LEU:O	2.19	0.42
1:H:158:GLU:O	1:H:160:VAL:N	2.53	0.42
1:H:178:ALA:HB2	1:H:188:LEU:HD23	2.00	0.42
2:A:3425:VAL:O	2:A:3444:LEU:N	2.46	0.42
4:B:154:GLU:OE1	4:B:156:TYR:HB3	2.19	0.42
2:A:1869:ASN:HB3	2:A:1880:ASP:HB2	2.02	0.42
4:B:331:MET:HE2	4:B:331:MET:HA	2.01	0.42
2:A:1899:VAL:O	2:A:1906:THR:OG1	2.31	0.42
2:A:2803:VAL:HG12	2:A:2833:LYS:HD2	2.00	0.42
2:A:2920:ALA:HB2	2:A:2949:THR:HG23	2.00	0.42
2:A:2929:TRP:N	2:A:2939:GLU:OE2	2.52	0.42
6:R:216:CYS:N	6:R:227:ASP:O	2.51	0.42
6:R:316:ASN:HA	6:R:331:ASP:HB3	2.00	0.42
1:H:30:SER:O	1:H:53:SER:HB2	2.19	0.42
2:A:3657:ALA:HB2	2:A:3712:LYS:NZ	2.34	0.42
4:B:65:HIS:CE1	4:B:331:MET:HB2	2.55	0.42
2:A:3126:LEU:HD22	2:A:3153:TRP:HA	2.02	0.42
6:R:347:VAL:HG13	6:R:347:VAL:O	2.20	0.42
3:L:75:THR:HG23	3:L:76:ASP:OD2	2.19	0.41
1:H:39:GLN:OE1	1:H:45:LEU:HD22	2.20	0.41
1:H:165:ASN:O	1:H:207:ASN:ND2	2.53	0.41
1:H:181:GLN:HE22	1:H:187:SER:N	2.17	0.41
2:A:2891:HIS:CD2	2:A:2904:ALA:HB3	2.55	0.41
2:A:3399:LEU:HD23	2:A:3409:SER:HA	2.02	0.41
4:B:50:GLN:N	4:B:50:GLN:OE1	2.52	0.41
6:R:83:ILE:HB	6:R:87:TRP:CD1	2.55	0.41
2:A:1924:THR:OG1	2:A:1926:GLN:NE2	2.53	0.41
2:A:3117:ILE:HB	2:A:3171:LEU:HD13	2.01	0.41
2:A:3460:PHE:CD2	2:A:3477:VAL:HG12	2.56	0.41
4:B:219:ASN:HA	4:B:239:SER:HB3	2.02	0.41
4:B:461:LYS:HA	4:B:464:GLU:CD	2.44	0.41
6:R:337:GLU:HG3	6:R:339:LEU:HG	2.01	0.41
2:A:2860:LEU:O	2:A:2867:LEU:N	2.37	0.41
4:B:109:ILE:HD11	4:B:265:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:ILE:HG12	4:B:245:VAL:CG1	2.47	0.41
4:B:146:SER:O	4:B:223:THR:HA	2.20	0.41
1:H:5:VAL:HG23	1:H:23:ALA:HB3	2.02	0.41
1:H:109:PRO:HG3	3:L:40:ALA:HB2	2.03	0.41
2:A:1934:LYS:HB2	2:A:1941:THR:HB	2.01	0.41
4:B:215:GLU:O	4:B:219:ASN:ND2	2.53	0.41
4:B:483:TYR:CE2	4:B:485:LEU:HD23	2.56	0.41
6:R:332:LEU:O	6:R:335:GLY:N	2.53	0.41
2:A:3666:GLU:HA	2:A:3701:HIS:HA	2.01	0.41
5:N:91:THR:HG22	5:N:120:THR:HA	2.02	0.41
2:A:2441:ASP:N	2:A:2441:ASP:OD1	2.53	0.41
2:A:2923:SER:O	2:A:2945:GLN:HG2	2.21	0.41
2:A:3394:LYS:HD3	6:R:213:SER:HB2	2.01	0.41
2:A:3649:GLU:N	2:A:3660:ASP:O	2.53	0.41
6:R:285:HIS:HB2	6:R:306:SER:HB3	2.02	0.41
1:H:39:GLN:HB2	1:H:45:LEU:HD13	2.03	0.41
2:A:3083:GLN:N	2:A:3106:ASN:OD1	2.54	0.41
2:A:3396:ALA:HB1	7:A:4604:NAG:H82	2.03	0.41
4:B:20:GLY:HA3	4:B:293:ALA:O	2.20	0.41
4:B:210:ASP:O	4:B:214:ALA:N	2.50	0.41
5:N:39:GLN:O	5:N:92:ALA:HB1	2.19	0.41
2:A:2835:LEU:HD13	2:A:2860:LEU:HB2	2.02	0.41
2:A:3021:HIS:HB3	2:A:3035:ASN:HB3	2.03	0.41
2:A:3042:GLN:HG2	2:A:3043:PRO:HD2	2.03	0.41
2:A:3120:GLU:HG3	2:A:3168:SER:CB	2.50	0.41
2:A:3465:ASN:OD1	7:A:4605:NAG:H2	2.21	0.41
2:A:3656:LYS:HB2	2:A:3658:HIS:NE2	2.36	0.41
4:B:93:PHE:CE1	4:B:326:GLN:HA	2.56	0.41
6:R:99:SER:O	6:R:99:SER:OG	2.35	0.41
1:H:84:ASN:HB3	4:B:441:PHE:CE1	2.56	0.41
1:H:91:THR:HG23	1:H:120:THR:HA	2.02	0.41
2:A:2921:TRP:HB3	2:A:2948:PHE:HB3	2.03	0.41
2:A:3098:TYR:CE1	2:A:3100:GLN:HB2	2.56	0.41
2:A:3172:SER:HB3	2:A:3174:LYS:NZ	2.36	0.41
5:N:83:MET:HE1	5:N:119:VAL:HG21	2.03	0.41
6:R:170:ASP:OD1	6:R:170:ASP:N	2.54	0.41
1:H:45:LEU:HB3	3:L:103:PHE:CD2	2.55	0.40
2:A:2945:GLN:HE21	2:A:2945:GLN:HB3	1.73	0.40
2:A:3107:ASN:C	2:A:3109:ASN:H	2.28	0.40
2:A:3355:GLU:N	2:A:3355:GLU:OE1	2.54	0.40
2:A:3527:ARG:NH1	6:R:309:PRO:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:LEU:N	4:B:246:THR:O	2.54	0.40
4:B:162:ILE:O	4:B:192:GLY:HA3	2.20	0.40
5:N:33:ASN:O	5:N:98:ALA:HA	2.21	0.40
2:A:3038:PHE:O	2:A:3048:ALA:HA	2.22	0.40
2:A:3084:GLN:HG2	2:A:3104:ALA:O	2.20	0.40
2:A:1992:TYR:HD1	2:A:2013:THR:HG22	1.86	0.40
2:A:3535:THR:OG1	2:A:3536:SER:N	2.55	0.40
2:A:1898:SER:OG	2:A:1907:ILE:HG13	2.22	0.40
2:A:3454:VAL:HB	2:A:3483:LEU:HB3	2.03	0.40
4:B:101:ASN:O	4:B:101:ASN:ND2	2.54	0.40
6:R:346:LEU:HB3	6:R:353:GLU:H	1.85	0.40
2:A:2001:THR:OG1	2:A:2004:LYS:O	2.39	0.40
2:A:2403:LYS:HD2	2:A:2404:LEU:HD22	2.04	0.40
2:A:3404:LYS:HG2	2:A:3405:PHE:HD1	1.85	0.40
3:L:20:THR:OG1	3:L:78:THR:OG1	2.29	0.40
4:B:199:LEU:O	4:B:204:HIS:N	2.47	0.40
4:B:247:VAL:HB	4:B:323:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	167/234 (71%)	160 (96%)	7 (4%)	0	100	100
2	A	1099/4563 (24%)	1019 (93%)	80 (7%)	0	100	100
3	L	170/219 (78%)	161 (95%)	9 (5%)	0	100	100
4	B	452/545 (83%)	438 (97%)	14 (3%)	0	100	100
5	N	122/131 (93%)	109 (89%)	13 (11%)	0	100	100
6	R	262/860 (30%)	232 (88%)	30 (12%)	0	100	100
All	All	2272/6552 (35%)	2119 (93%)	153 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	135/199 (68%)	135 (100%)	0	100	100
2	A	902/4080 (22%)	902 (100%)	0	100	100
3	L	124/192 (65%)	124 (100%)	0	100	100
4	B	323/433 (75%)	323 (100%)	0	100	100
5	N	75/103 (73%)	75 (100%)	0	100	100
6	R	202/755 (27%)	202 (100%)	0	100	100
All	All	1761/5762 (31%)	1761 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	174	HIS
1	H	207	ASN
2	A	2064	GLN
2	A	2861	HIS
2	A	2865	ASN
2	A	3073	ASN
2	A	3167	GLN
2	A	3176	GLN
2	A	3353	ASN
2	A	3358	ASN
2	A	3518	ASN
2	A	3533	GLN
2	A	3583	HIS
2	A	3606	GLN
2	A	3652	ASN
2	A	3654	GLN
4	B	151	ASN

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Mol	Chain	Res	Type
4	B	420	GLN
4	B	515	ASN
4	B	517	ASN
6	R	92	GLN
6	R	247	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](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
7	NAG	A	4602	2	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
7	NAG	A	4601	2	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
7	NAG	A	4604	2	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
7	NAG	A	4605	2	14,14,15	0.84	0	17,19,21	1.84	2 (11%)
7	NAG	A	4603	2	14,14,15	0.74	0	17,19,21	2.31	3 (17%)

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
7	NAG	A	4602	2	-	2/6/23/26	0/1/1/1
7	NAG	A	4601	2	-	1/6/23/26	0/1/1/1
7	NAG	A	4604	2	-	1/6/23/26	0/1/1/1
7	NAG	A	4605	2	-	1/6/23/26	0/1/1/1
7	NAG	A	4603	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4603	NAG	C2-N2-C7	8.23	133.94	122.90
7	A	4605	NAG	C1-O5-C5	6.44	120.81	112.19
7	A	4601	NAG	C2-N2-C7	3.05	126.99	122.90
7	A	4603	NAG	C8-C7-N2	2.62	120.47	116.12
7	A	4604	NAG	O5-C1-C2	-2.19	107.91	111.29
7	A	4605	NAG	C3-C4-C5	-2.17	106.31	110.23
7	A	4602	NAG	C2-N2-C7	2.05	125.65	122.90
7	A	4603	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4602	NAG	C8-C7-N2-C2
7	A	4602	NAG	O7-C7-N2-C2
7	A	4603	NAG	C8-C7-N2-C2
7	A	4603	NAG	O7-C7-N2-C2
7	A	4604	NAG	O5-C5-C6-O6
7	A	4605	NAG	O5-C5-C6-O6
7	A	4603	NAG	C1-C2-N2-C7
7	A	4601	NAG	C3-C2-N2-C7
7	A	4603	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4601	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4604	NAG	1	0
7	A	4605	NAG	2	0

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.

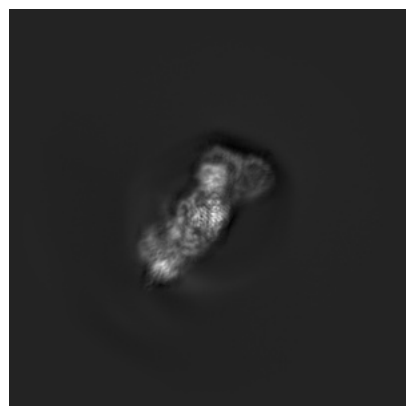
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44450. These allow visual inspection of the internal detail of the map and identification of artifacts.

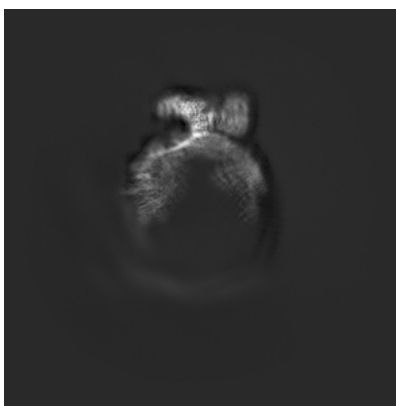
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

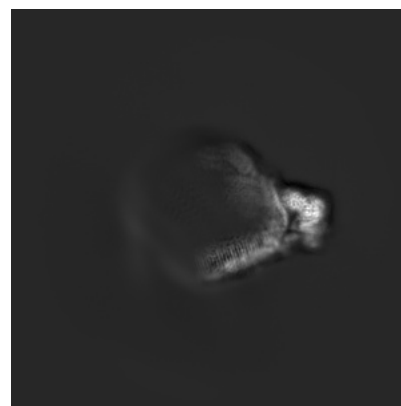
6.1.1 Primary map



X

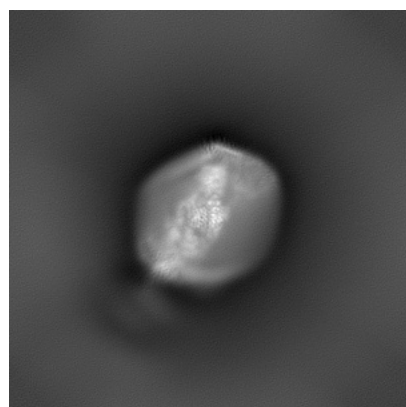


Y

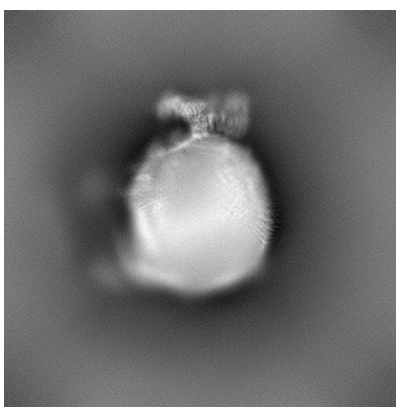


Z

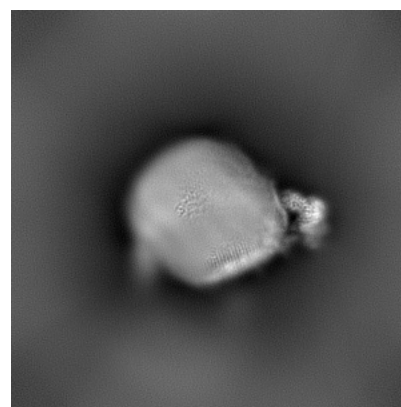
6.1.2 Raw map



X



Y

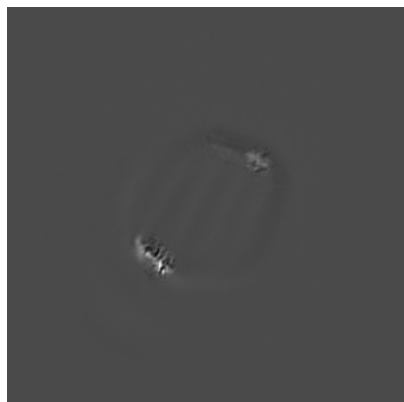


Z

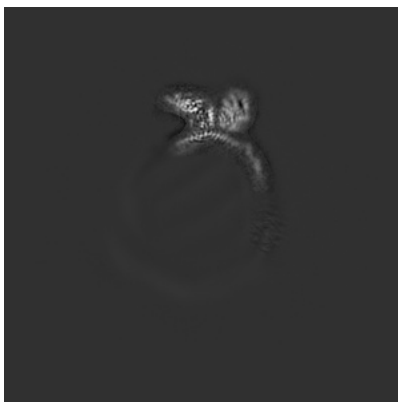
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

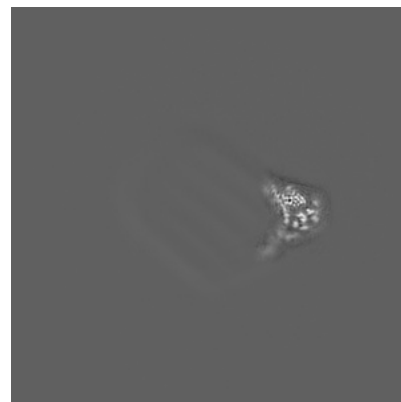
6.2.1 Primary map



X Index: 168

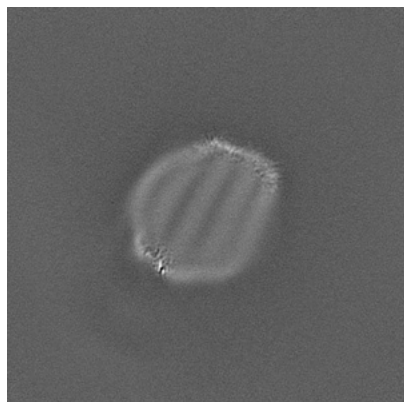


Y Index: 168

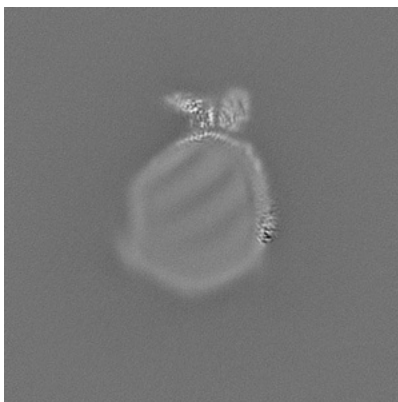


Z Index: 168

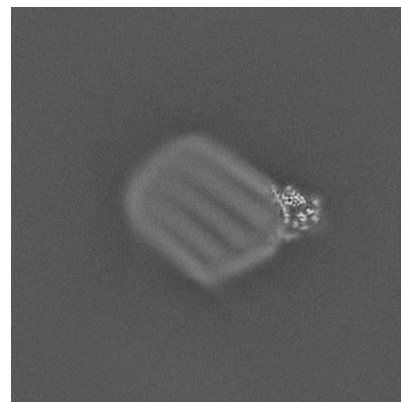
6.2.2 Raw map



X Index: 168



Y Index: 168

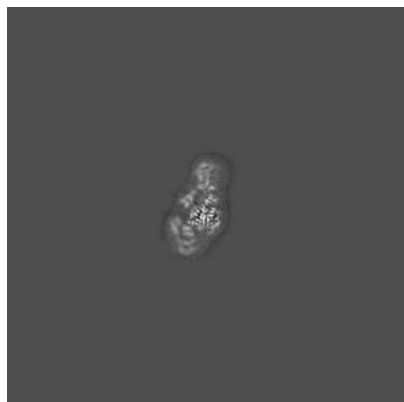


Z Index: 168

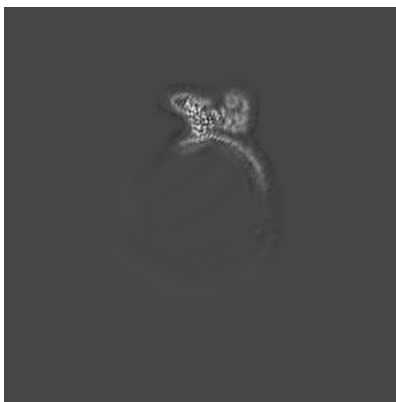
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

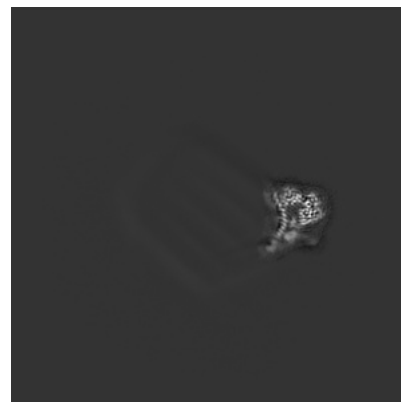
6.3.1 Primary map



X Index: 248

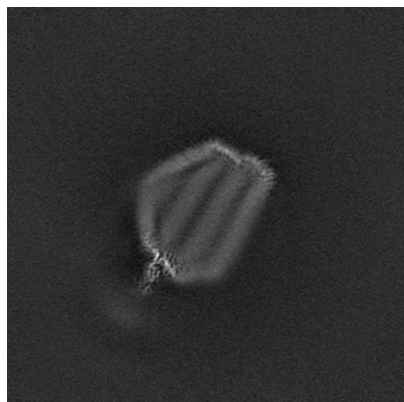


Y Index: 171

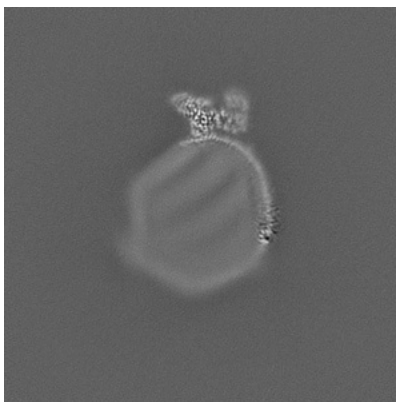


Z Index: 160

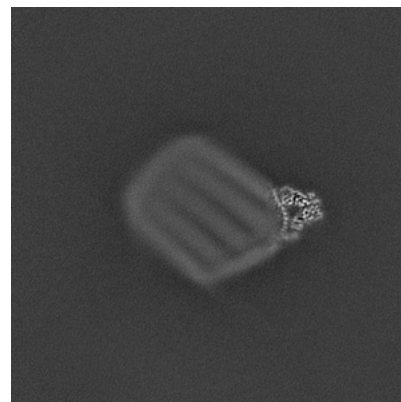
6.3.2 Raw map



X Index: 184



Y Index: 172

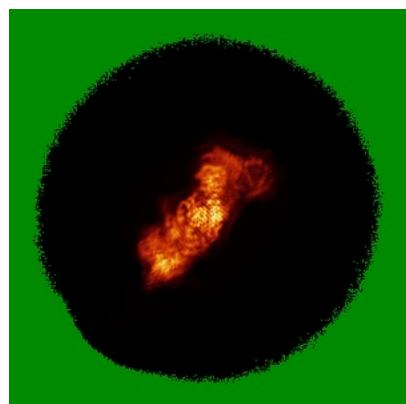


Z Index: 163

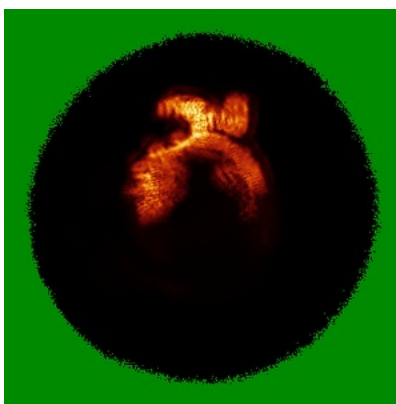
The images above show the largest variance slices of the map in three orthogonal directions.

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

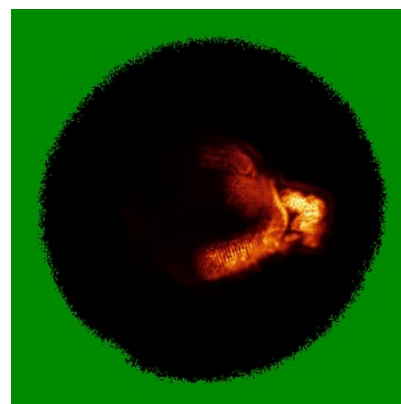
6.4.1 Primary map



X

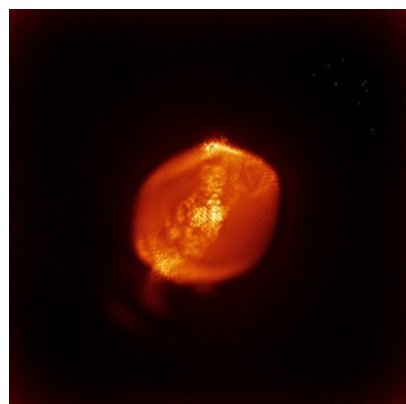


Y

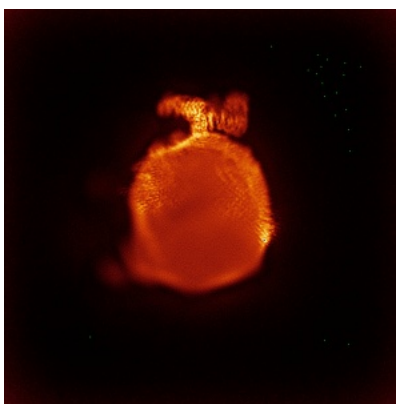


Z

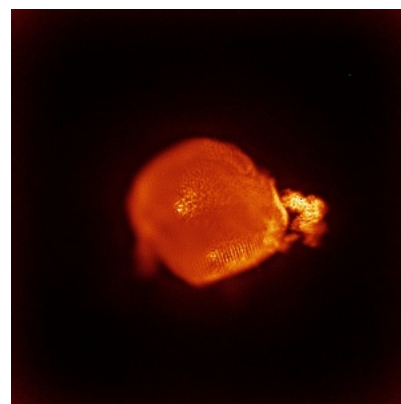
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

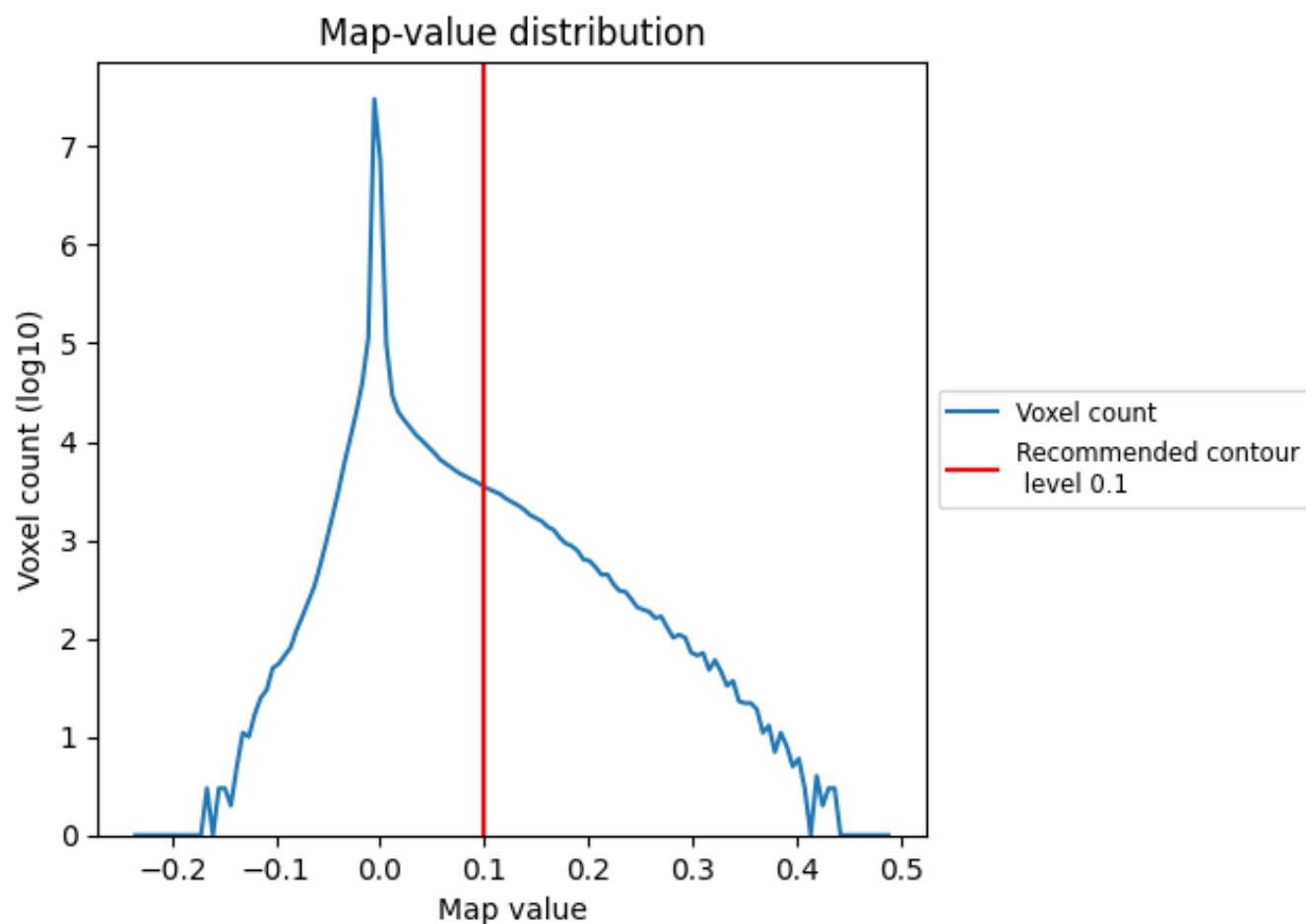
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

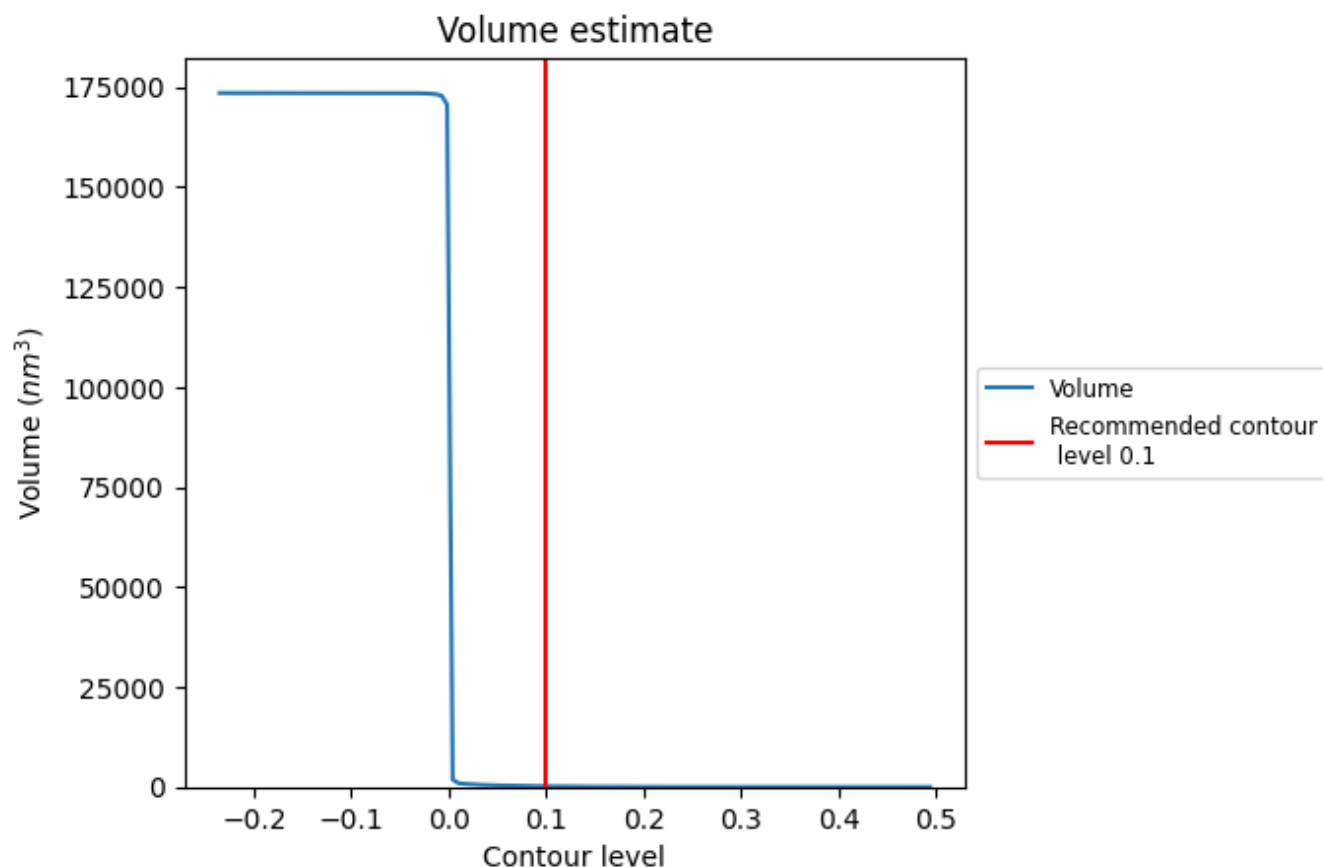
This section contains the results of statistical analysis of the map.

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.

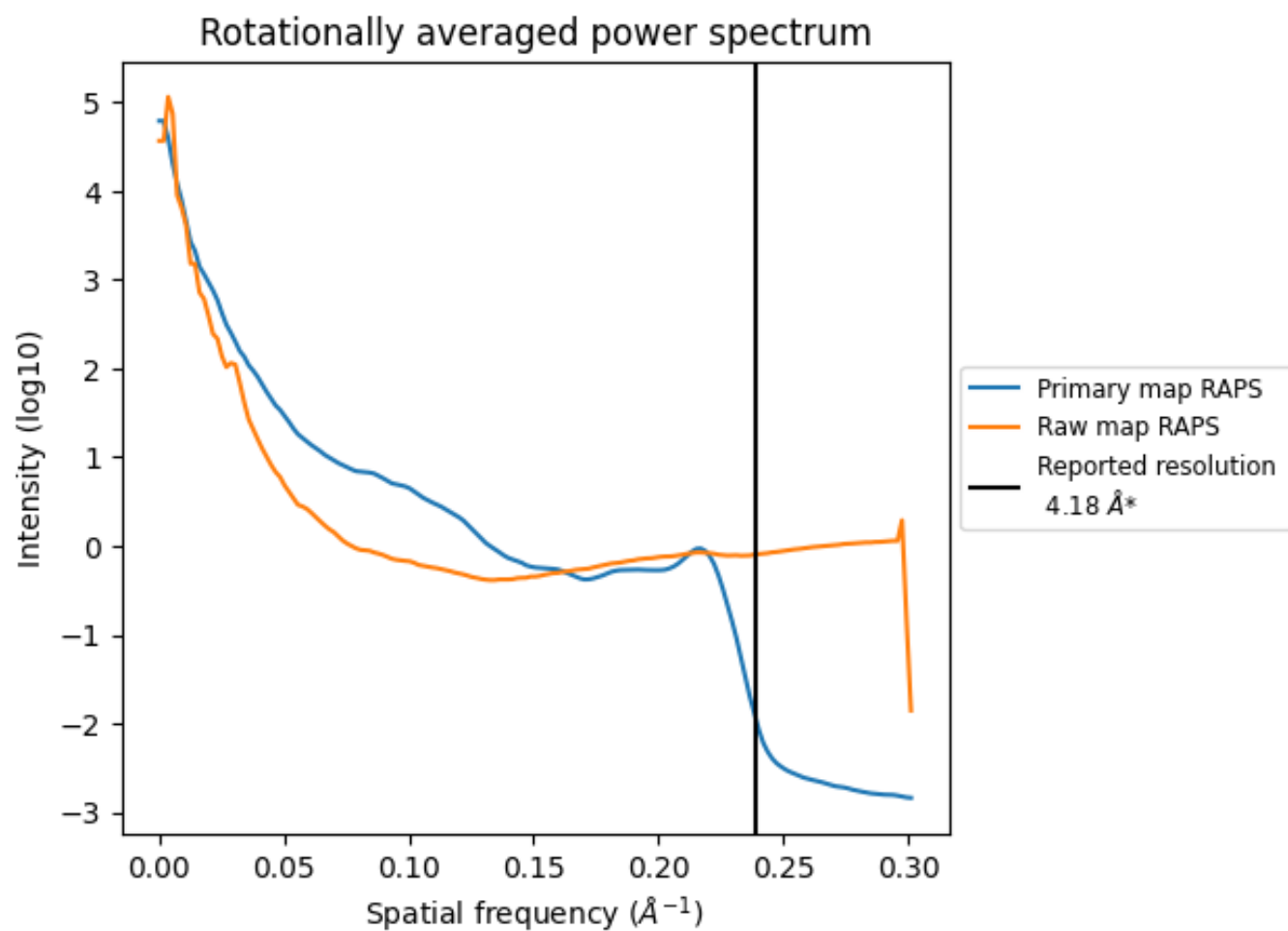
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 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 ⓘ

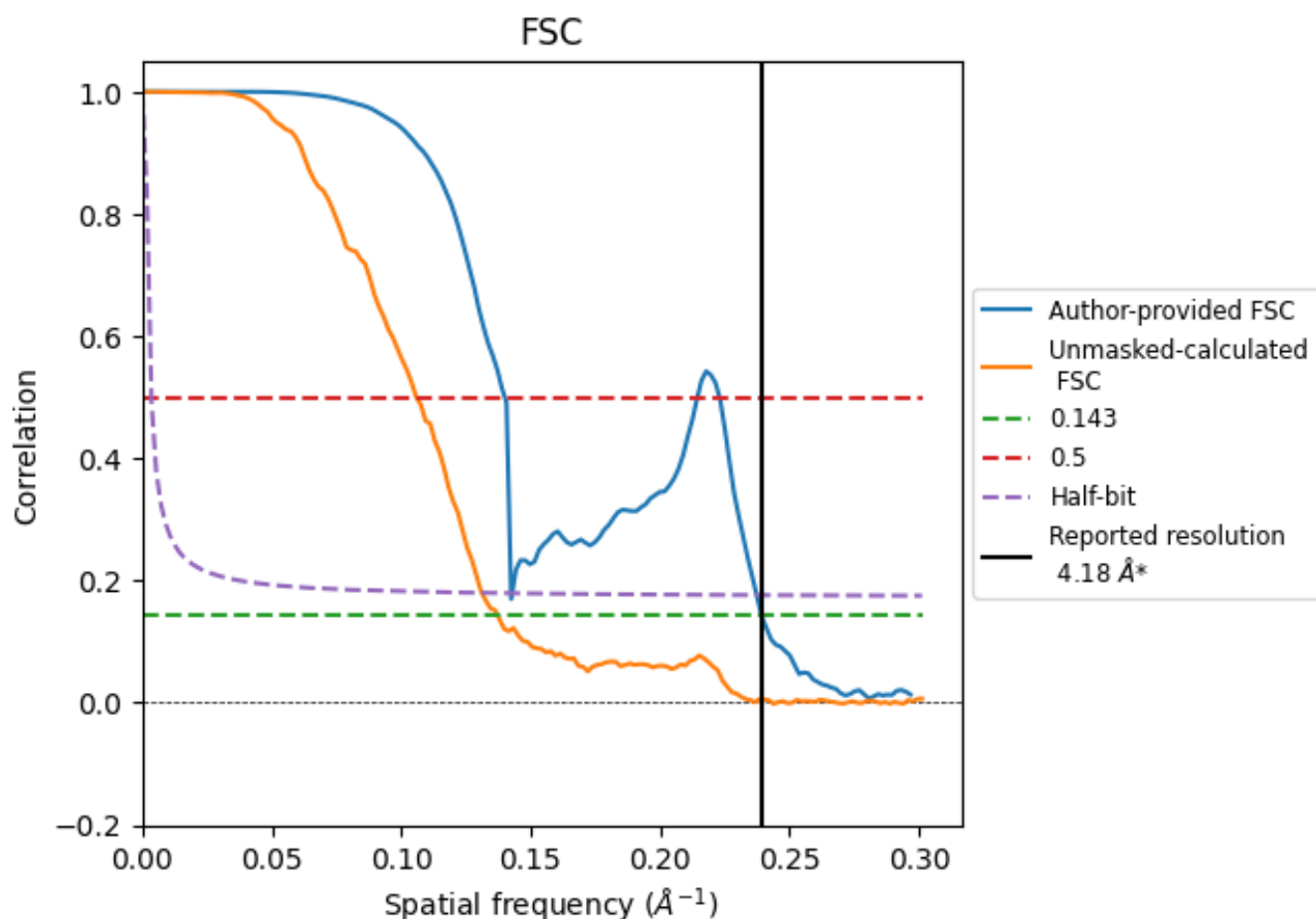


*Reported resolution corresponds to spatial frequency of 0.239 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.239 $\text{\AA}^{-1}$

8.2 Resolution estimates

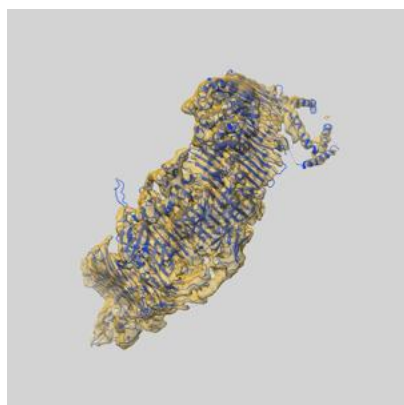
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.18	-	-
Author-provided FSC curve	4.18	7.14	7.02
Unmasked-calculated*	7.29	9.45	7.63

*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 7.29 differs from the reported value 4.18 by more than 10 %

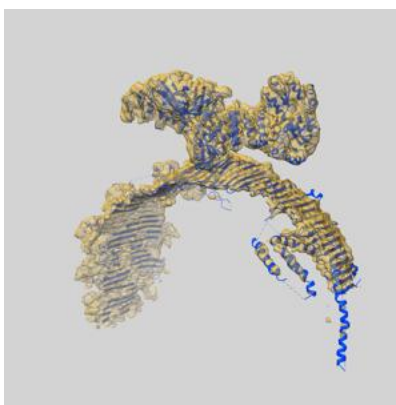
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44450 and PDB model 9BDE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

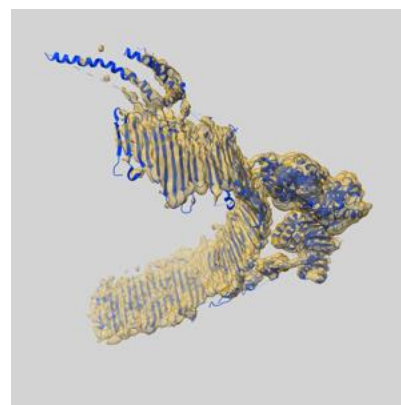
9.1 Map-model overlay [i](#)



X



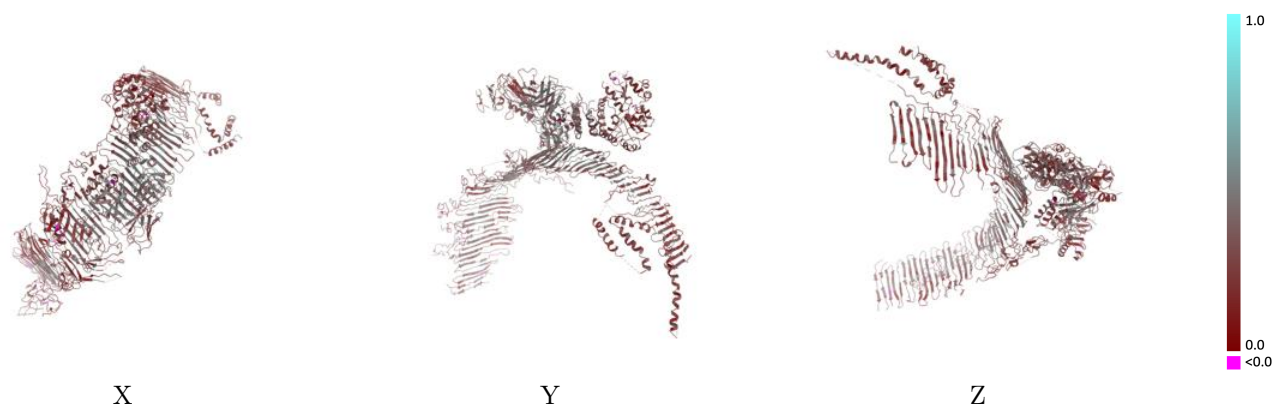
Y



Z

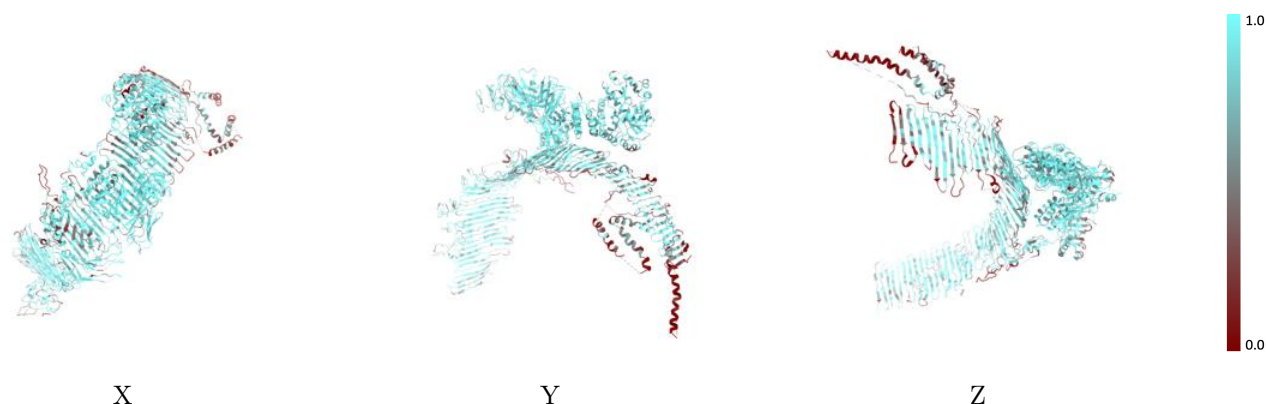
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



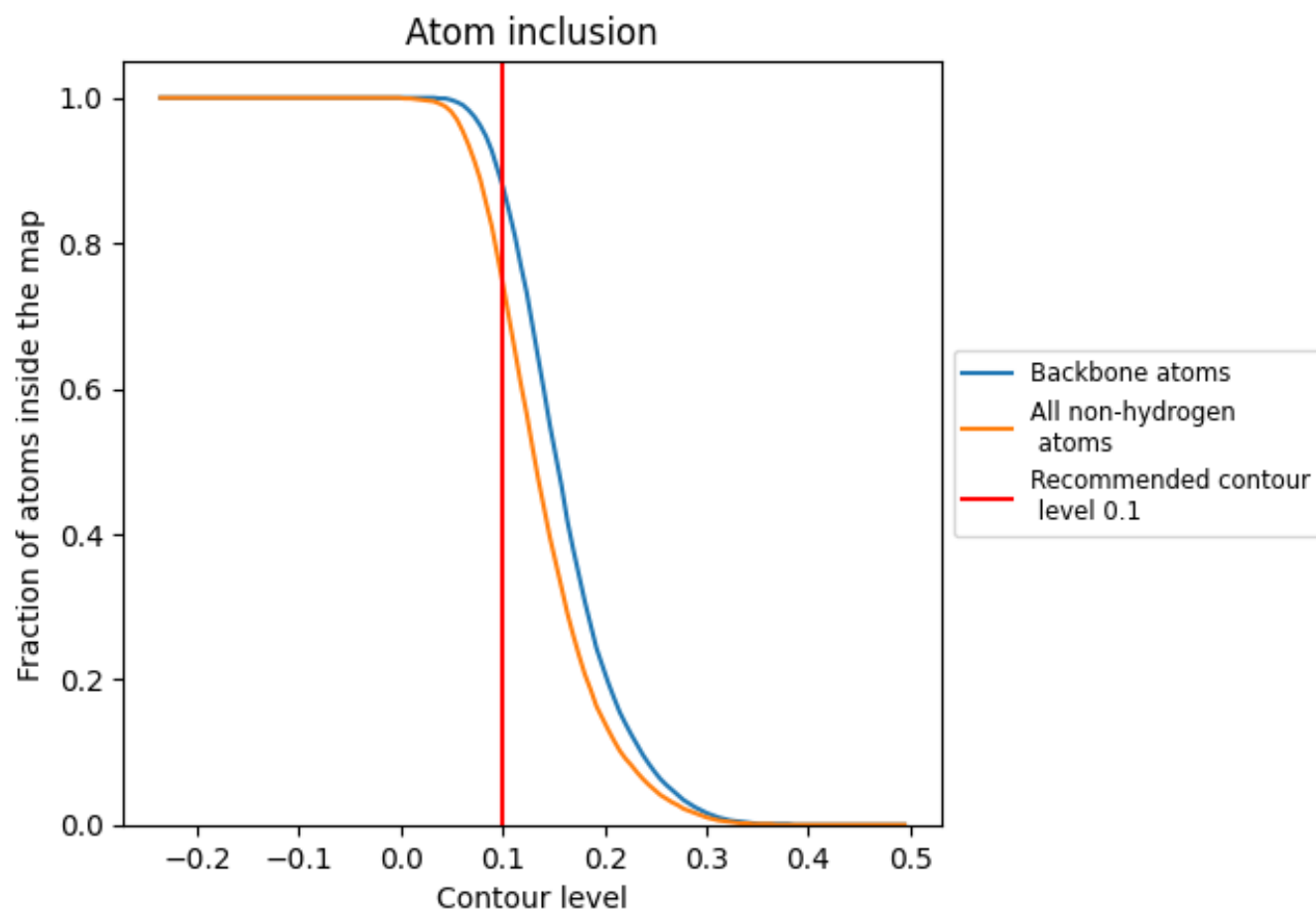
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.3110
A	0.6640	0.3150
B	0.8210	0.2770
H	0.8730	0.3790
L	0.8660	0.3440
N	0.9450	0.4300
R	0.7410	0.2350

1.0

0.0

<0.0