



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 08:03 PM JST

PDB ID : 9LRM / pdb_00009lrm
EMDB ID : EMD-63339
Title : Cryo-EM structure of collagenase H (E416Q mutant) from *Hathewayia histolytica* in complex with collagen model peptide (Pro-Hyp-Gly)₁₀
Authors : Oki, H.; Kawahara, K.
Deposited on : 2025-01-31
Resolution : 3.40 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 : 1.8.5 (274361), CSD as541be (2020)
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

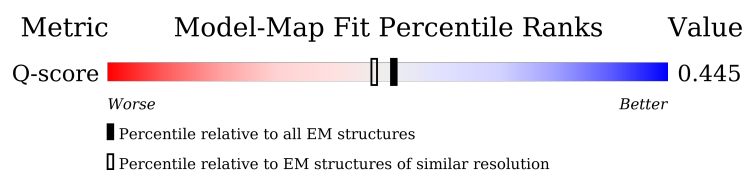
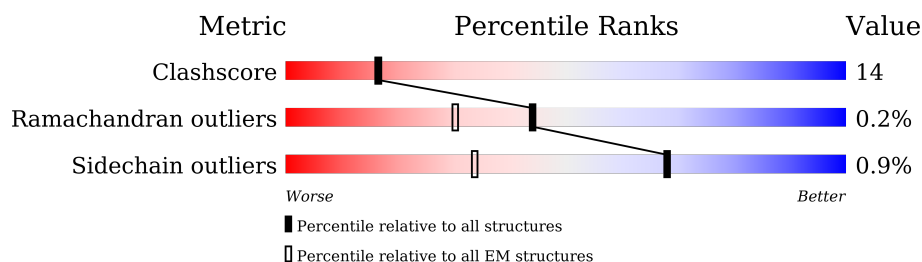
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	983	6% 54% 24% 22%
1	G	983	5% 51% 26% 22%
2	B	30	20% 53% 43% .
2	C	30	10% 63% 33% .

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Mol	Chain	Length	Quality of chain
2	D	30	57% 33% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13062 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 Collagenase ColH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	769	Total	C	N	O	S	0	0
			6256	3976	1034	1231	15		
1	G	766	Total	C	N	O	S	0	0
			6230	3962	1029	1224	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q46085
A	0	SER	-	expression tag	UNP Q46085
A	416	GLN	GLU	engineered mutation	UNP Q46085
G	-1	GLY	-	expression tag	UNP Q46085
G	0	SER	-	expression tag	UNP Q46085
G	416	GLN	GLU	engineered mutation	UNP Q46085

- Molecule 2 is a protein called (Pro-Hyp-Gly)₁₀.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	30	Total	C	N	O	0	0
			190	120	30	40		
2	D	30	Total	C	N	O	0	0
			190	120	30	40		
2	C	30	Total	C	N	O	0	0
			190	120	30	40		

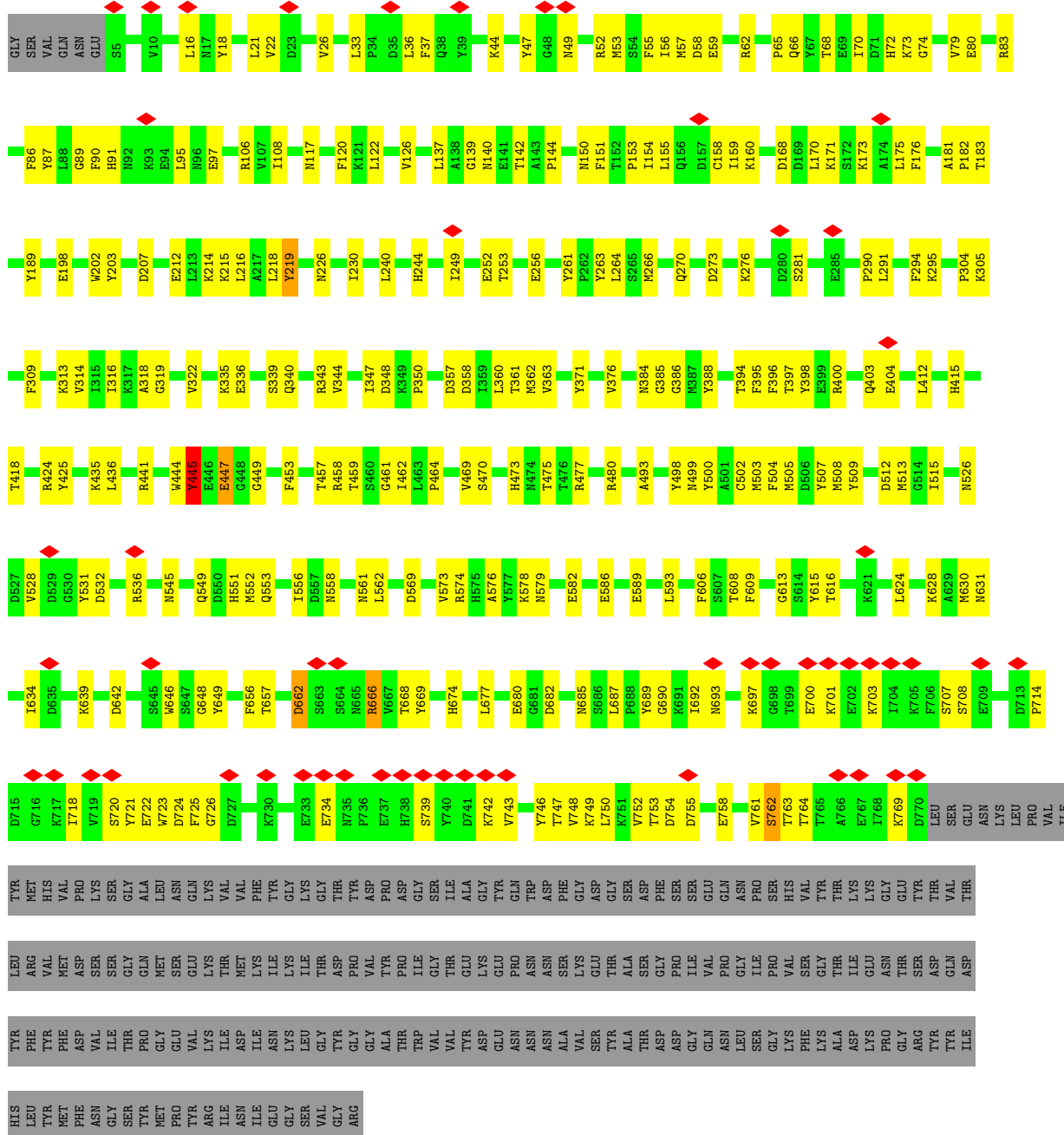
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	G	2	Total	Ca	0
			2	2	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

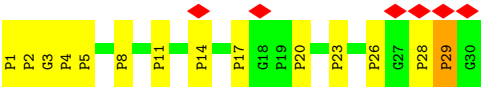
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0

- Molecule 1: Collagenase ColH



- Molecule 2: (Pro-Hyp-Gly)₁₀

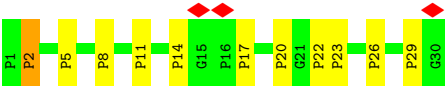




● Molecule 2: (Pro-Hyp-Gly)10



● Molecule 2: (Pro-Hyp-Gly)10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58438	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.584	Depositor
Minimum map value	-0.330	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	261.0, 261.0, 261.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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: CA, ZN, HYP

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	0.17	0/6400	0.30	0/8648
1	G	0.15	0/6374	0.36	1/8613 (0.0%)
2	B	0.14	0/109	0.32	0/136
2	C	0.15	0/109	0.38	0/136
2	D	0.18	0/109	0.35	0/136
All	All	0.16	0/13101	0.33	1/17669 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	445	TYR	N-CA-C	-6.10	105.50	113.12

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	A	6256	0	6063	162	0
1	G	6230	0	6043	200	0
2	B	190	0	172	9	0
2	C	190	0	172	2	0
2	D	190	0	172	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	G	2	0	0	0	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
All	All	13062	0	12622	363	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (363) 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:G:219:TYR:HD2	1:G:230:ILE:HD11	1.28	0.98
1:G:616:THR:CG2	1:G:666:ARG:HD2	1.95	0.95
1:G:219:TYR:CD2	1:G:230:ILE:HD11	2.02	0.95
1:A:314:VAL:HG13	1:A:362:MET:HE1	1.57	0.85
1:A:196:LYS:HD3	1:A:197:PRO:HD2	1.64	0.79
1:G:219:TYR:HD2	1:G:230:ILE:CD1	1.96	0.78
1:G:616:THR:HG23	1:G:666:ARG:HD2	1.61	0.78
1:A:345:TYR:CE1	1:A:520:ASN:OD1	2.35	0.78
1:A:79:VAL:HG11	1:A:133:ALA:HB1	1.64	0.77
1:G:505:MET:HA	1:G:508:MET:HG3	1.66	0.77
1:G:447:GLU:HG3	1:G:498:TYR:CE1	2.21	0.76
1:A:67:TYR:HA	1:A:73:LYS:HE2	1.68	0.76
1:A:493:ALA:HB3	2:B:28:PRO:HD2	1.70	0.73
1:G:122:LEU:HD11	1:G:154:ILE:HG23	1.69	0.73
2:B:1:PRO:HD3	1:G:90:PHE:CE1	2.24	0.73
1:A:304:PRO:HD2	1:A:319:GLY:HA2	1.70	0.72
1:A:482:LYS:HG2	1:A:545:ASN:HD21	1.53	0.72
1:A:44:LYS:HE2	1:A:94:GLU:HG3	1.72	0.70
1:A:99:ASN:OD1	1:A:104:LYS:NZ	2.23	0.70
1:A:63:ARG:HD2	1:A:73:LYS:HB2	1.74	0.70
1:A:720:SER:HB3	1:A:753:THR:HB	1.74	0.69
1:G:579:ASN:HB3	1:G:582:GLU:HG3	1.73	0.69
1:G:447:GLU:HG3	1:G:498:TYR:CD1	2.28	0.69
1:G:697:LYS:HE2	1:G:769:LYS:HB2	1.75	0.69
1:G:304:PRO:HD2	1:G:319:GLY:HA2	1.74	0.68
1:G:86:PHE:HB3	1:G:140:ASN:HD22	1.60	0.66
1:G:666:ARG:HB3	1:G:666:ARG:NH1	2.09	0.66
1:G:574:ARG:HE	1:G:687:LEU:HG	1.61	0.66
1:A:79:VAL:HG23	1:A:137:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HD2	1:A:251:ILE:HD12	1.77	0.65
1:G:725:PHE:HA	1:G:748:VAL:HG13	1.79	0.65
1:A:22:VAL:HG21	1:A:59:GLU:HG3	1.79	0.65
1:A:152:THR:O	1:A:155:LEU:N	2.30	0.64
1:A:422:GLN:HE22	1:A:449:GLY:HA3	1.62	0.64
1:A:473:HIS:HA	1:A:556:ILE:HD12	1.79	0.64
1:G:57:MET:HE1	1:G:106:ARG:HG3	1.79	0.64
1:G:662:ASP:CG	1:G:668:THR:HG1	2.05	0.64
1:G:477:ARG:NH2	1:G:553:GLN:OE1	2.31	0.63
1:A:430:GLN:HB2	1:A:433:ARG:HE	1.63	0.63
1:G:616:THR:CG2	1:G:666:ARG:CD	2.73	0.63
1:G:576:ALA:O	1:G:646:TRP:NE1	2.32	0.63
1:G:313:LYS:HD3	1:G:314:VAL:HG23	1.81	0.62
1:A:173:LYS:HD2	2:B:29:HYP:HB2	1.80	0.62
1:G:358:ASP:OD1	1:G:424:ARG:NH2	2.33	0.62
1:G:726:GLY:HA3	1:G:746:TYR:HB3	1.81	0.62
1:G:513:MET:HB3	1:G:624:LEU:HD22	1.80	0.62
1:G:361:THR:C	1:G:362:MET:HE2	2.25	0.62
1:A:573:VAL:HG22	1:A:689:TYR:HB2	1.82	0.62
1:A:533:ASN:OD1	1:A:536:ARG:NH2	2.33	0.62
1:A:277:ARG:HH21	2:C:22:PRO:HB3	1.66	0.61
1:G:22:VAL:HG11	1:G:59:GLU:HG2	1.81	0.61
1:G:120:PHE:HE1	1:G:154:ILE:HD11	1.65	0.61
1:A:94:GLU:OE2	1:A:94:GLU:N	2.26	0.61
1:A:451:GLU:OE1	1:A:465:ARG:NH1	2.31	0.61
1:G:549:GLN:HA	1:G:552:MET:HE3	1.82	0.61
1:G:158:CYS:HB2	1:G:175:LEU:HD21	1.82	0.60
1:G:693:ASN:ND2	1:G:707:SER:O	2.34	0.60
1:G:624:LEU:O	1:G:628:LYS:HG3	2.02	0.60
1:A:642:ASP:O	1:A:650:LYS:NZ	2.33	0.60
1:A:574:ARG:HE	1:A:687:LEU:HD12	1.66	0.59
1:G:718:ILE:HA	1:G:754:ASP:HA	1.83	0.59
1:G:755:ASP:OD1	1:G:755:ASP:N	2.34	0.59
1:G:266:MET:HE1	1:G:270:GLN:NE2	2.17	0.59
1:A:574:ARG:HB3	1:A:687:LEU:HB2	1.84	0.59
1:A:255:THR:O	1:A:259:LYS:HG2	2.03	0.59
1:G:700:GLU:HG2	1:G:701:LYS:HG2	1.84	0.58
1:G:159:ILE:HD11	1:G:216:LEU:HG	1.84	0.58
1:A:574:ARG:NH1	1:A:575:HIS:O	2.36	0.58
1:G:72:HIS:HB3	1:G:126:VAL:HG13	1.86	0.58
1:G:218:LEU:O	1:G:218:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ILE:HG12	1:G:144:PRO:HG2	1.85	0.58
1:A:599:GLU:HG3	1:A:610:THR:HB	1.86	0.57
1:A:579:ASN:HB3	1:A:582:GLU:HB2	1.86	0.57
1:G:168:ASP:OD1	1:G:170:LEU:N	2.37	0.57
1:G:207:ASP:OD1	1:G:244:HIS:NE2	2.37	0.57
1:G:58:ASP:OD2	1:G:62:ARG:NH1	2.37	0.57
1:G:218:LEU:HD12	1:G:256:GLU:HB3	1.86	0.57
1:G:89:GLY:HA2	1:G:95:LEU:HB3	1.86	0.57
1:G:388:TYR:HD1	1:G:395:PHE:HB3	1.69	0.57
1:A:388:TYR:HD1	1:A:395:PHE:HB3	1.69	0.56
1:A:362:MET:HG2	1:A:395:PHE:CZ	2.41	0.56
1:A:371:TYR:HB2	1:A:398:TYR:HB3	1.85	0.56
1:G:336:GLU:O	1:G:339:SER:OG	2.20	0.56
1:A:111:ILE:HG22	1:A:115:GLN:NE2	2.21	0.56
1:G:436:LEU:HD11	1:G:526:ASN:HA	1.87	0.56
1:A:574:ARG:HH21	1:A:687:LEU:HG	1.70	0.56
1:G:361:THR:HB	1:G:394:THR:HG23	1.87	0.56
1:G:578:LYS:NZ	1:G:586:GLU:OE1	2.38	0.56
1:G:609:PHE:HB3	1:G:677:LEU:HD13	1.88	0.55
1:A:10:VAL:HG22	1:A:36:LEU:HD23	1.87	0.55
1:A:89:GLY:HA2	1:A:95:LEU:HB3	1.89	0.55
1:G:469:VAL:HG11	1:G:562:LEU:HD12	1.89	0.55
1:G:593:LEU:HD23	1:G:613:GLY:HA3	1.89	0.55
1:A:269:LEU:HB3	1:A:376:VAL:HG11	1.88	0.55
1:A:498:TYR:CE2	2:D:28:PRO:HD3	2.41	0.55
1:G:344:VAL:HG11	1:G:453:PHE:CZ	2.42	0.55
1:A:334:SER:HB3	1:A:413:PHE:HE1	1.72	0.54
1:G:666:ARG:CB	1:G:666:ARG:CZ	2.85	0.54
1:A:273:ASP:HB2	1:A:376:VAL:HG13	1.88	0.54
1:A:222:ILE:HD13	1:A:230:ILE:HD12	1.89	0.54
1:G:343:ARG:HG2	1:G:656:PHE:CD1	2.42	0.54
1:G:473:HIS:HA	1:G:556:ILE:HD12	1.89	0.54
1:A:699:THR:HB	1:A:702:GLU:HB2	1.88	0.54
1:G:558:ASN:OD1	1:G:561:ASN:ND2	2.40	0.54
1:A:7:ARG:NH2	1:A:31:GLU:O	2.41	0.54
1:A:647:SER:HB3	1:A:714:PRO:HB2	1.89	0.54
1:G:66:GLN:O	1:G:73:LYS:NZ	2.41	0.54
2:B:1:PRO:HD3	1:G:90:PHE:CD1	2.43	0.54
1:G:475:THR:O	1:G:480:ARG:NH2	2.40	0.54
1:G:718:ILE:HD13	1:G:752:VAL:HB	1.90	0.53
1:A:476:THR:OG1	1:A:478:ASN:OD1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:VAL:HG23	1:G:74:GLY:HA3	1.90	0.53
1:A:156:GLN:O	1:A:160:LYS:HG3	2.08	0.53
1:G:457:THR:OG1	1:G:461:GLY:O	2.25	0.53
1:G:662:ASP:OD2	1:G:662:ASP:N	2.40	0.53
1:G:183:THR:HA	1:G:240:LEU:HD11	1.91	0.53
1:G:458:ARG:NH2	1:G:642:ASP:OD1	2.41	0.53
1:G:615:TYR:HB3	1:G:669:TYR:HB2	1.91	0.53
1:A:75:ILE:O	1:A:79:VAL:HG12	2.09	0.53
1:G:216:LEU:O	1:G:219:TYR:HB3	2.09	0.53
1:A:131:VAL:HG12	1:A:174:ALA:HB1	1.90	0.53
1:G:445:TYR:C	1:G:445:TYR:CD1	2.86	0.53
1:G:512:ASP:HB3	1:G:515:ILE:HD12	1.89	0.53
1:G:80:GLU:HA	1:G:83:ARG:HG2	1.90	0.53
1:G:662:ASP:OD1	1:G:668:THR:OG1	2.26	0.52
1:G:340:GLN:O	1:G:344:VAL:HG12	2.10	0.52
2:B:4:PRO:HB3	1:G:37:PHE:CG	2.44	0.52
1:G:263:TYR:CE1	1:G:264:LEU:HD23	2.45	0.52
1:A:251:ILE:HG13	1:A:279:TYR:CD2	2.44	0.52
1:G:343:ARG:NH1	1:G:631:ASN:OD1	2.42	0.52
1:G:586:GLU:HA	1:G:589:GLU:HG2	1.92	0.52
1:G:357:ASP:OD1	1:G:424:ARG:NH2	2.43	0.51
1:G:441:ARG:HB3	1:G:531:TYR:HE2	1.75	0.51
1:G:499:ASN:O	1:G:502:CYS:HB3	2.10	0.51
1:A:324:GLU:OE2	1:A:324:GLU:N	2.32	0.51
1:A:41:SER:O	1:A:44:LYS:HB3	2.10	0.51
1:G:459:THR:HG21	1:G:639:LYS:HD3	1.92	0.51
1:G:507:TYR:HB2	1:G:551:HIS:HD2	1.75	0.51
1:A:139:GLY:HA2	1:A:181:ALA:HA	1.92	0.51
1:G:52:ARG:O	1:G:56:ILE:HG13	2.10	0.50
1:G:276:LYS:HA	1:G:281:SER:HA	1.93	0.50
1:G:33:LEU:HB3	1:G:36:LEU:HD23	1.92	0.50
1:G:403:GLN:NE2	1:G:404:GLU:OE2	2.43	0.50
1:G:358:ASP:HA	1:G:424:ARG:HH22	1.76	0.50
1:A:412:LEU:O	1:A:416:GLN:HG2	2.12	0.50
1:G:386:GLY:HA3	1:G:412:LEU:HD21	1.94	0.50
1:G:447:GLU:HA	1:G:447:GLU:OE1	2.08	0.50
1:A:491:TYR:CE1	2:D:26:HYP:HD22	2.47	0.50
1:G:435:LYS:HB2	1:G:528:VAL:HG21	1.94	0.50
1:G:470:SER:O	1:G:473:HIS:ND1	2.42	0.50
1:A:358:ASP:OD1	1:A:424:ARG:NH1	2.39	0.49
1:G:363:VAL:HB	1:G:396:PHE:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:HG3	1:A:52:ARG:HH12	1.76	0.49
1:G:316:ILE:HG12	1:G:362:MET:HG2	1.94	0.49
1:A:198:GLU:OE2	1:A:247:ASN:ND2	2.46	0.49
1:A:458:ARG:NH2	1:A:642:ASP:OD2	2.45	0.49
1:A:751:LYS:HD2	1:A:761:VAL:HG22	1.93	0.49
1:G:400:ARG:HH22	1:G:412:LEU:HD13	1.78	0.49
1:G:606:PHE:HE1	1:G:608:THR:HG22	1.77	0.49
1:G:68:THR:HG23	1:G:70:ILE:H	1.77	0.49
1:G:273:ASP:HB2	1:G:376:VAL:HB	1.95	0.49
1:A:500:TYR:HD1	1:A:552:MET:HE2	1.77	0.49
1:G:266:MET:HE1	1:G:270:GLN:HE21	1.76	0.49
1:A:400:ARG:HH22	1:A:412:LEU:HG	1.78	0.49
1:A:595:ASP:OD1	1:A:595:ASP:N	2.46	0.49
1:G:720:SER:HB3	1:G:753:THR:HB	1.95	0.49
1:A:56:ILE:O	1:A:60:ILE:HG13	2.12	0.49
1:A:322:VAL:HG21	1:A:364:ILE:HG22	1.94	0.49
1:A:548:TYR:CZ	1:A:552:MET:HE3	2.47	0.49
1:G:137:LEU:O	1:G:142:THR:OG1	2.25	0.48
1:G:219:TYR:HE2	1:G:226:ASN:HD22	1.60	0.48
1:G:66:GLN:HG3	1:G:73:LYS:HZ3	1.78	0.48
1:G:708:SER:OG	1:G:734:GLU:O	2.30	0.48
1:A:326:LYS:O	1:A:330:LEU:HG	2.13	0.48
1:A:699:THR:HG22	1:A:701:LYS:H	1.78	0.48
1:A:26:VAL:HA	1:A:74:GLY:HA3	1.96	0.48
1:A:101:ARG:O	1:A:105:GLU:HG2	2.13	0.48
1:A:721:TYR:CE1	1:A:734:GLU:HG3	2.49	0.48
1:A:594:LYS:HA	1:A:594:LYS:HD3	1.52	0.48
1:G:318:ALA:HB1	1:G:322:VAL:HG11	1.95	0.48
1:A:315:ILE:HD11	1:A:359:ILE:HD11	1.95	0.48
1:A:362:MET:HG2	1:A:395:PHE:CE2	2.48	0.48
1:A:569:ASP:HB3	1:A:689:TYR:CE2	2.49	0.48
1:A:332:TRP:CD1	1:A:571:TYR:HB3	2.49	0.48
2:B:3:GLY:HA2	1:G:87:TYR:CE2	2.49	0.48
1:G:291:LEU:HG	1:G:295:LYS:HD2	1.95	0.47
1:G:703:LYS:HD2	1:G:739:SER:HB2	1.95	0.47
1:G:198:GLU:HG3	1:G:203:TYR:CZ	2.49	0.47
1:G:189:TYR:CD2	1:G:202:TRP:HZ3	2.32	0.47
1:A:83:ARG:NE	1:A:136:LEU:HD11	2.29	0.47
1:A:482:LYS:HG2	1:A:545:ASN:ND2	2.23	0.47
1:A:66:GLN:HG3	1:A:73:LYS:HE3	1.96	0.47
1:G:459:THR:O	1:G:459:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:O	1:A:96:ASN:ND2	2.48	0.47
1:A:697:LYS:HZ2	1:A:767:GLU:HB3	1.80	0.47
1:G:397:THR:HG22	1:G:398:TYR:H	1.80	0.47
1:A:58:ASP:O	1:A:62:ARG:HG2	2.14	0.47
1:A:360:LEU:HG	1:A:362:MET:HE2	1.97	0.47
1:A:554:GLU:O	1:A:558:ASN:ND2	2.48	0.47
1:G:723:TRP:NE1	1:G:750:LEU:HD13	2.30	0.47
1:A:755:ASP:OD1	1:A:755:ASP:N	2.46	0.47
2:C:2:HYP:HD22	1:G:176:PHE:HZ	1.79	0.47
1:G:666:ARG:HB3	1:G:666:ARG:CZ	2.44	0.47
1:G:347:ILE:HD11	1:G:425:TYR:HB3	1.97	0.47
1:G:480:ARG:HG2	1:G:500:TYR:HE1	1.79	0.47
1:A:236:HIS:O	1:A:240:LEU:HB2	2.15	0.46
1:A:558:ASN:HB3	1:A:561:ASN:HD21	1.80	0.46
1:G:79:VAL:HG22	1:G:137:LEU:HD22	1.96	0.46
1:G:462:ILE:HB	1:G:509:TYR:CE2	2.50	0.46
1:A:237:ILE:HG12	1:A:253:THR:HG21	1.96	0.46
1:A:104:LYS:NZ	1:A:141:GLU:HB2	2.31	0.46
1:G:18:TYR:HB3	1:G:55:PHE:CD2	2.50	0.46
1:G:44:LYS:O	1:G:44:LYS:NZ	2.38	0.46
1:G:350:PRO:HB3	1:G:424:ARG:HG3	1.96	0.46
1:G:86:PHE:HB3	1:G:140:ASN:ND2	2.28	0.46
1:G:371:TYR:HB2	1:G:398:TYR:HB3	1.97	0.46
1:G:16:LEU:HD23	1:G:21:LEU:HA	1.97	0.46
1:G:708:SER:HB3	1:G:723:TRP:HZ2	1.80	0.46
1:A:578:LYS:HD2	1:A:646:TRP:HB2	1.97	0.46
1:G:18:TYR:HB3	1:G:55:PHE:CE2	2.51	0.46
1:A:442:LEU:O	1:A:446:GLU:HG2	2.15	0.46
1:A:569:ASP:OD1	1:A:569:ASP:N	2.49	0.46
1:G:160:LYS:HD2	1:G:160:LYS:N	2.30	0.46
1:G:173:LYS:HB2	1:G:173:LYS:HE2	1.72	0.46
1:G:219:TYR:CD2	1:G:230:ILE:CD1	2.80	0.46
1:A:657:THR:HG22	1:A:658:ASN:OD1	2.16	0.46
1:A:703:LYS:HG2	1:A:737:GLU:HB3	1.98	0.45
1:G:500:TYR:HA	1:G:503:MET:HE2	1.97	0.45
1:A:262:PRO:O	1:A:265:SER:OG	2.25	0.45
1:A:621:LYS:HE3	1:A:621:LYS:HB2	1.77	0.45
1:A:127:GLN:O	1:A:130:ILE:HG22	2.17	0.45
1:G:290:PRO:HD2	1:G:294:PHE:HE1	1.81	0.45
2:D:25:PRO:HA	2:D:26:HYP:HD23	1.81	0.45
1:G:139:GLY:HA2	1:G:181:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:LYS:HE3	1:G:253:THR:HB	1.99	0.45
1:A:179:LEU:HB3	1:A:236:HIS:CD2	2.51	0.45
1:A:498:TYR:CD2	2:D:28:PRO:HD3	2.51	0.45
1:G:444:TRP:CE3	1:G:444:TRP:O	2.69	0.45
1:G:549:GLN:HA	1:G:552:MET:CE	2.46	0.45
1:A:323:GLU:OE2	1:A:323:GLU:HA	2.16	0.45
1:G:360:LEU:HG	1:G:362:MET:HE1	1.99	0.45
1:G:680:GLU:OE2	1:G:680:GLU:N	2.49	0.45
1:A:183:THR:HA	1:A:240:LEU:HD11	1.99	0.45
1:G:536:ARG:HG3	1:G:536:ARG:HH11	1.81	0.45
1:G:335:LYS:HG3	1:G:674:HIS:CE1	2.52	0.45
1:A:53:MET:HE1	1:A:82:VAL:HA	1.98	0.45
1:A:14:LYS:HB3	1:A:14:LYS:HE3	1.89	0.44
1:A:462:ILE:HB	1:A:509:TYR:CE2	2.51	0.44
1:G:215:LYS:O	1:G:219:TYR:HB2	2.17	0.44
1:A:418:THR:HG21	1:A:453:PHE:HB2	1.99	0.44
1:G:305:LYS:HB3	1:G:305:LYS:HE3	1.86	0.44
1:A:22:VAL:HG11	1:A:59:GLU:OE1	2.17	0.44
1:A:173:LYS:HE2	1:A:173:LYS:HB2	1.65	0.44
1:G:724:ASP:OD1	1:G:749:LYS:HB3	2.17	0.44
1:A:40:SER:H	1:A:43:ALA:HB3	1.82	0.44
1:A:86:PHE:HB3	1:A:140:ASN:ND2	2.32	0.44
1:A:148:VAL:HB	1:A:206:ILE:HG21	1.98	0.44
1:G:545:ASN:O	1:G:549:GLN:HG2	2.18	0.44
1:G:749:LYS:HG3	1:G:761:VAL:HG13	1.99	0.44
1:A:317:LYS:HE2	1:A:317:LYS:HB3	1.75	0.44
1:A:448:GLY:C	1:A:505:MET:HG3	2.42	0.44
1:A:483:LEU:O	1:A:487:VAL:HG13	2.18	0.44
1:G:397:THR:HG22	1:G:398:TYR:N	2.32	0.44
1:G:692:ILE:HG21	1:G:764:THR:HG21	1.99	0.44
1:A:524:LYS:HB3	1:A:524:LYS:HE3	1.64	0.44
1:G:49:ASN:HB2	1:G:52:ARG:HH21	1.82	0.44
1:G:150:ASN:O	1:G:153:PRO:HD2	2.18	0.44
1:A:414:ARG:HB3	1:A:454:ALA:HA	2.00	0.44
2:B:1:PRO:HB2	1:G:87:TYR:CD2	2.52	0.44
1:G:721:TYR:CD2	1:G:734:GLU:HA	2.53	0.44
1:G:384:ASN:OD1	1:G:384:ASN:N	2.51	0.44
1:A:531:TYR:O	1:A:535:ILE:HG12	2.18	0.43
1:G:335:LYS:HA	1:G:335:LYS:HD3	1.74	0.43
1:A:100:LYS:HD2	1:A:100:LYS:HA	1.74	0.43
1:G:108:ILE:HD12	1:G:108:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:CE2	2:D:29:HYP:HD23	2.53	0.43
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.84	0.43
1:G:646:TRP:HB3	1:G:649:TYR:CE2	2.53	0.43
1:A:13:LEU:HA	1:A:16:LEU:HD12	2.01	0.43
1:A:80:GLU:O	1:A:83:ARG:HG2	2.17	0.43
1:A:700:GLU:HG2	1:A:701:LYS:HG2	2.00	0.43
1:G:685:ASN:ND2	1:G:758:GLU:OE2	2.50	0.43
1:G:532:ASP:O	1:G:536:ARG:HG2	2.17	0.43
1:G:722:GLU:OE1	1:G:723:TRP:N	2.52	0.43
1:A:697:LYS:HD2	1:A:767:GLU:HB3	2.01	0.43
1:G:151:PHE:HA	1:G:154:ILE:HD13	2.01	0.43
1:A:469:VAL:HG13	1:A:556:ILE:HD13	2.01	0.42
1:G:266:MET:CE	1:G:270:GLN:HE21	2.32	0.42
1:G:504:PHE:O	1:G:507:TYR:HB3	2.19	0.42
1:G:569:ASP:HB3	1:G:689:TYR:CE2	2.55	0.42
1:A:431:TRP:CE2	2:D:25:PRO:HD3	2.54	0.42
1:A:18:TYR:HB3	1:A:55:PHE:CD1	2.54	0.42
1:A:179:LEU:HD22	1:A:213:LEU:HD21	2.01	0.42
1:A:193:THR:OG1	1:A:195:GLU:HG2	2.20	0.42
1:A:368:PRO:HG3	1:A:398:TYR:CE2	2.55	0.42
1:G:441:ARG:HB3	1:G:531:TYR:CE2	2.54	0.42
1:A:150:ASN:O	1:A:153:PRO:HD2	2.20	0.42
1:A:307:TYR:CE2	1:A:327:VAL:HG21	2.54	0.42
1:A:315:ILE:O	1:A:362:MET:HE3	2.20	0.42
1:A:447:GLU:OE1	1:A:447:GLU:HA	2.13	0.42
1:G:385:GLY:C	1:G:412:LEU:HD11	2.44	0.42
1:A:614:SER:OG	1:A:615:TYR:N	2.53	0.42
1:A:624:LEU:O	1:A:628:LYS:HG2	2.20	0.42
1:G:97:GLU:H	1:G:97:GLU:CD	2.27	0.42
1:G:181:ALA:HB3	1:G:182:PRO:HD3	2.01	0.42
1:G:336:GLU:OE2	1:G:458:ARG:N	2.53	0.41
1:G:65:PRO:HA	1:G:117:ASN:HD21	1.84	0.41
1:A:458:ARG:HD3	1:A:571:TYR:OH	2.20	0.41
1:G:47:TYR:HD1	1:G:53:MET:HE1	1.84	0.41
1:G:573:VAL:HG11	1:G:714:PRO:HG3	2.02	0.41
1:G:630:MET:HG2	1:G:669:TYR:CE2	2.55	0.41
1:A:283:ASP:OD1	1:A:284:ALA:N	2.53	0.41
1:G:309:PHE:HB2	1:G:314:VAL:HB	2.02	0.41
1:G:574:ARG:HH12	1:G:682:ASP:HB3	1.85	0.41
1:G:616:THR:HG22	1:G:666:ARG:CD	2.50	0.41
1:A:687:LEU:HD23	1:A:758:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:HD12	1:G:212:GLU:OE2	2.20	0.41
1:A:552:MET:O	1:A:556:ILE:HG12	2.20	0.41
1:G:168:ASP:OD1	1:G:168:ASP:C	2.63	0.41
1:G:634:ILE:HD13	1:G:634:ILE:HA	1.92	0.41
1:A:135:GLY:HA2	1:A:151:PHE:CZ	2.56	0.41
1:A:660:LYS:HE3	1:A:660:LYS:HB2	1.84	0.41
1:G:155:LEU:HB3	1:G:212:GLU:HG2	2.03	0.41
1:G:219:TYR:O	1:G:261:TYR:OH	2.36	0.41
1:A:14:LYS:HE2	1:A:42:ASP:HA	2.01	0.41
1:A:452:LEU:HD22	1:A:505:MET:HB3	2.02	0.41
1:A:609:PHE:HB3	1:A:677:LEU:HD22	2.02	0.41
1:G:444:TRP:CE3	1:G:444:TRP:C	2.99	0.41
1:A:210:ILE:HB	1:A:244:HIS:CD2	2.56	0.41
1:A:210:ILE:HB	1:A:244:HIS:HD2	1.85	0.41
1:A:513:MET:HB3	1:A:624:LEU:HD22	2.02	0.41
2:B:1:PRO:HD2	1:G:91:HIS:HE1	1.85	0.41
1:G:57:MET:HE1	1:G:106:ARG:CG	2.49	0.41
1:G:449:GLY:N	1:G:505:MET:SD	2.94	0.41
1:G:690:GLY:O	1:G:762:SER:OG	2.28	0.41
1:A:3:ASN:HD22	1:A:475:THR:HG22	1.86	0.41
1:A:198:GLU:HA	1:A:203:TYR:CD2	2.56	0.41
1:A:316:ILE:HG12	1:A:362:MET:SD	2.62	0.41
1:A:431:TRP:CE3	2:D:24:GLY:HA2	2.56	0.41
1:A:436:LEU:HD23	1:A:442:LEU:HD11	2.02	0.41
1:A:586:GLU:O	1:A:589:GLU:HG3	2.21	0.41
2:B:1:PRO:CD	1:G:90:PHE:CD1	3.04	0.41
2:D:2:HYP:HD23	1:G:493:ALA:HB1	2.03	0.41
1:G:415:HIS:O	1:G:418:THR:OG1	2.29	0.41
1:A:121:LYS:HE2	1:A:121:LYS:HB3	1.81	0.40
1:A:175:LEU:HB3	1:A:228:TRP:HH2	1.85	0.40
1:G:348:ASP:CG	1:G:657:THR:HG21	2.46	0.40
1:G:444:TRP:C	1:G:444:TRP:CD2	2.98	0.40
1:G:747:THR:HG23	1:G:763:THR:HG23	2.03	0.40
1:G:418:THR:HG21	1:G:453:PHE:HB2	2.03	0.40
1:A:548:TYR:CE1	1:A:552:MET:HE3	2.56	0.40
1:G:168:ASP:HB3	1:G:171:LYS:HD2	2.02	0.40
1:G:708:SER:HB3	1:G:723:TRP:CZ2	2.55	0.40
1:G:742:LYS:HG3	1:G:746:TYR:OH	2.22	0.40
1:A:495:PHE:CD2	2:D:29:HYP:HD23	2.56	0.40
1:G:249:ILE:HA	1:G:252:GLU:OE2	2.21	0.40
1:G:344:VAL:HG11	1:G:453:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:569:ASP:HB3	1:G:689:TYR:CZ	2.57	0.40
1:A:5:SER:O	1:A:7:ARG:N	2.54	0.40
1:A:141:GLU:HA	1:A:185:ASP:OD1	2.22	0.40
1:A:251:ILE:N	1:A:279:TYR:HE2	2.19	0.40
1:G:464:PRO:HB2	1:G:562:LEU:HD13	2.03	0.40
1:G:646:TRP:CH2	1:G:648:GLY:HA3	2.56	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	767/983 (78%)	751 (98%)	14 (2%)	2 (0%)	36	65
1	G	764/983 (78%)	746 (98%)	17 (2%)	1 (0%)	48	78
2	B	18/30 (60%)	18 (100%)	0	0	100	100
2	C	18/30 (60%)	17 (94%)	1 (6%)	0	100	100
2	D	18/30 (60%)	18 (100%)	0	0	100	100
All	All	1585/2056 (77%)	1550 (98%)	32 (2%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	4	GLU
1	G	219	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	684/867 (79%)	677 (99%)	7 (1%)	68	75
1	G	681/867 (78%)	675 (99%)	6 (1%)	70	76
2	B	10/10 (100%)	10 (100%)	0	100	100
2	C	10/10 (100%)	10 (100%)	0	100	100
2	D	10/10 (100%)	10 (100%)	0	100	100
All	All	1395/1764 (79%)	1382 (99%)	13 (1%)	68	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	156	GLN
1	A	199	ASN
1	A	221	LYS
1	A	222	ILE
1	A	370	GLU
1	A	682	ASP
1	G	445	TYR
1	G	447	GLU
1	G	662	ASP
1	G	666	ARG
1	G	743	VAL
1	G	762	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	91	HIS
1	A	92	ASN
1	A	156	GLN
1	A	177	ASN

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Mol	Chain	Res	Type
1	A	232	ASN
1	A	267	GLN
1	A	274	GLN
1	A	278	HIS
1	A	340	GLN
1	A	374	ASN
1	A	422	GLN
1	A	473	HIS
1	A	545	ASN
1	A	558	ASN
1	A	674	HIS
1	G	66	GLN
1	G	161	ASN
1	G	177	ASN
1	G	225	ASN
1	G	510	ASN
1	G	551	HIS
1	G	561	ASN
1	G	735	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

30 non-standard protein/DNA/RNA residues 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	HYP	C	8	2	6,8,9	0.95	0	5,10,12	1.63	1 (20%)
2	HYP	C	2	2	6,8,9	0.94	0	5,10,12	1.67	1 (20%)
2	HYP	B	26	2	6,8,9	0.88	0	5,10,12	1.62	1 (20%)
2	HYP	C	26	2	6,8,9	0.88	0	5,10,12	1.61	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HYP	D	26	2,4	6,8,9	0.84	0	5,10,12	1.87	2 (40%)
2	HYP	B	5	2	6,8,9	0.89	0	5,10,12	1.68	1 (20%)
2	HYP	C	23	2	6,8,9	0.85	0	5,10,12	1.74	2 (40%)
2	HYP	C	29	2	6,8,9	0.86	0	5,10,12	1.71	1 (20%)
2	HYP	C	5	2	6,8,9	0.95	0	5,10,12	2.04	2 (40%)
2	HYP	B	17	2	6,8,9	0.87	0	5,10,12	1.71	1 (20%)
2	HYP	B	20	2	6,8,9	0.92	0	5,10,12	1.63	1 (20%)
2	HYP	D	17	2	6,8,9	0.87	0	5,10,12	1.85	2 (40%)
2	HYP	B	8	2	6,8,9	0.87	0	5,10,12	1.75	2 (40%)
2	HYP	B	2	2	6,8,9	0.88	0	5,10,12	1.67	1 (20%)
2	HYP	B	23	2	6,8,9	0.87	0	5,10,12	1.86	2 (40%)
2	HYP	D	2	2	6,8,9	0.89	0	5,10,12	1.80	2 (40%)
2	HYP	D	23	2	6,8,9	0.82	0	5,10,12	1.65	1 (20%)
2	HYP	D	20	2	6,8,9	0.87	0	5,10,12	1.82	2 (40%)
2	HYP	C	11	2	6,8,9	0.90	0	5,10,12	1.69	1 (20%)
2	HYP	D	8	2	6,8,9	0.86	0	5,10,12	1.67	1 (20%)
2	HYP	B	11	2	6,8,9	0.87	0	5,10,12	1.79	2 (40%)
2	HYP	B	29	2	6,8,9	0.89	0	5,10,12	1.78	2 (40%)
2	HYP	D	5	2	6,8,9	0.88	0	5,10,12	1.64	1 (20%)
2	HYP	B	14	2	6,8,9	0.89	0	5,10,12	1.79	2 (40%)
2	HYP	D	11	2	6,8,9	0.89	0	5,10,12	1.63	1 (20%)
2	HYP	D	29	2	6,8,9	0.95	0	5,10,12	1.78	2 (40%)
2	HYP	C	14	2	6,8,9	0.93	0	5,10,12	1.88	2 (40%)
2	HYP	C	17	2	6,8,9	0.89	0	5,10,12	1.65	1 (20%)
2	HYP	C	20	2	6,8,9	0.91	0	5,10,12	1.58	1 (20%)
2	HYP	D	14	2	6,8,9	0.87	0	5,10,12	1.73	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	C	8	2	-	0/0/11/13	0/1/1/1
2	HYP	C	2	2	-	0/0/11/13	0/1/1/1
2	HYP	B	26	2	-	0/0/11/13	0/1/1/1
2	HYP	C	26	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	D	26	2,4	-	0/0/11/13	0/1/1/1
2	HYP	B	5	2	-	0/0/11/13	0/1/1/1
2	HYP	C	23	2	-	0/0/11/13	0/1/1/1
2	HYP	C	29	2	-	0/0/11/13	0/1/1/1
2	HYP	C	5	2	-	0/0/11/13	0/1/1/1
2	HYP	B	17	2	-	0/0/11/13	0/1/1/1
2	HYP	B	20	2	-	0/0/11/13	0/1/1/1
2	HYP	D	17	2	-	0/0/11/13	0/1/1/1
2	HYP	B	8	2	-	0/0/11/13	0/1/1/1
2	HYP	B	2	2	-	0/0/11/13	0/1/1/1
2	HYP	B	23	2	-	0/0/11/13	0/1/1/1
2	HYP	D	2	2	-	0/0/11/13	0/1/1/1
2	HYP	D	23	2	-	0/0/11/13	0/1/1/1
2	HYP	D	20	2	-	0/0/11/13	0/1/1/1
2	HYP	C	11	2	-	0/0/11/13	0/1/1/1
2	HYP	D	8	2	-	0/0/11/13	0/1/1/1
2	HYP	B	11	2	-	0/0/11/13	0/1/1/1
2	HYP	B	29	2	-	0/0/11/13	0/1/1/1
2	HYP	D	5	2	-	0/0/11/13	0/1/1/1
2	HYP	B	14	2	-	0/0/11/13	0/1/1/1
2	HYP	D	11	2	-	0/0/11/13	0/1/1/1
2	HYP	D	29	2	-	0/0/11/13	0/1/1/1
2	HYP	C	14	2	-	0/0/11/13	0/1/1/1
2	HYP	C	17	2	-	0/0/11/13	0/1/1/1
2	HYP	C	20	2	-	0/0/11/13	0/1/1/1
2	HYP	D	14	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	HYP	CG-CB-CA	3.14	107.92	103.96
2	D	26	HYP	CG-CB-CA	2.83	107.53	103.96
2	C	14	HYP	CG-CB-CA	2.64	107.29	103.96
2	B	23	HYP	CG-CB-CA	2.62	107.27	103.96
2	D	17	HYP	CG-CB-CA	2.46	107.06	103.96
2	D	20	HYP	CG-CB-CA	2.42	107.01	103.96
2	D	29	HYP	CG-CB-CA	2.38	106.96	103.96
2	C	2	HYP	OD1-CG-CB	2.31	115.75	110.03
2	B	11	HYP	OD1-CG-CB	2.29	115.70	110.03
2	C	29	HYP	OD1-CG-CB	2.28	115.66	110.03
2	D	11	HYP	OD1-CG-CB	2.25	115.59	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	HYP	CG-CB-CA	2.25	106.80	103.96
2	B	26	HYP	OD1-CG-CB	2.24	115.58	110.03
2	C	26	HYP	OD1-CG-CB	2.24	115.58	110.03
2	B	5	HYP	OD1-CG-CB	2.24	115.56	110.03
2	B	8	HYP	OD1-CG-CB	2.23	115.55	110.03
2	B	29	HYP	OD1-CG-CB	2.23	115.55	110.03
2	B	14	HYP	OD1-CG-CB	2.23	115.54	110.03
2	D	17	HYP	OD1-CG-CB	2.23	115.54	110.03
2	C	20	HYP	OD1-CG-CB	2.23	115.54	110.03
2	B	2	HYP	OD1-CG-CB	2.23	115.54	110.03
2	D	2	HYP	OD1-CG-CB	2.22	115.53	110.03
2	C	14	HYP	OD1-CG-CB	2.22	115.53	110.03
2	D	29	HYP	OD1-CG-CB	2.22	115.53	110.03
2	C	11	HYP	OD1-CG-CB	2.22	115.53	110.03
2	B	17	HYP	OD1-CG-CB	2.22	115.52	110.03
2	D	14	HYP	OD1-CG-CB	2.21	115.50	110.03
2	B	14	HYP	CG-CB-CA	2.21	106.75	103.96
2	D	8	HYP	OD1-CG-CB	2.21	115.50	110.03
2	B	20	HYP	OD1-CG-CB	2.21	115.50	110.03
2	B	23	HYP	OD1-CG-CB	2.21	115.49	110.03
2	D	5	HYP	OD1-CG-CB	2.20	115.48	110.03
2	C	8	HYP	OD1-CG-CB	2.20	115.48	110.03
2	D	20	HYP	OD1-CG-CB	2.20	115.47	110.03
2	C	17	HYP	OD1-CG-CB	2.20	115.47	110.03
2	D	26	HYP	OD1-CG-CB	2.18	115.43	110.03
2	D	23	HYP	OD1-CG-CB	2.17	115.39	110.03
2	C	23	HYP	OD1-CG-CB	2.16	115.38	110.03
2	C	5	HYP	OD1-CG-CB	2.16	115.37	110.03
2	B	29	HYP	CG-CB-CA	2.13	106.66	103.96
2	C	23	HYP	CG-CB-CA	2.12	106.63	103.96
2	B	11	HYP	CG-CB-CA	2.10	106.62	103.96
2	B	8	HYP	CG-CB-CA	2.00	106.49	103.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	HYP	1	0
2	D	26	HYP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	HYP	1	0
2	B	29	HYP	1	0
2	D	29	HYP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

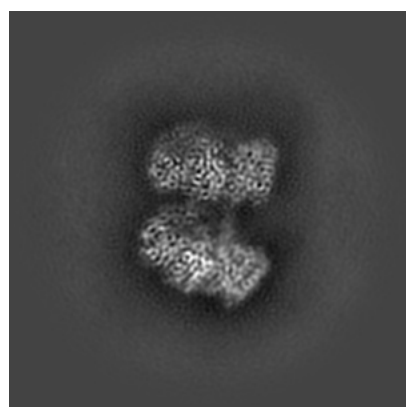
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63339. These allow visual inspection of the internal detail of the map and identification of artifacts.

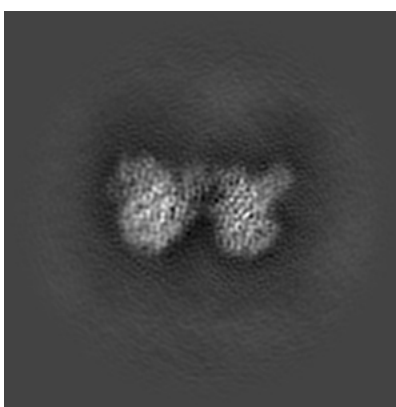
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

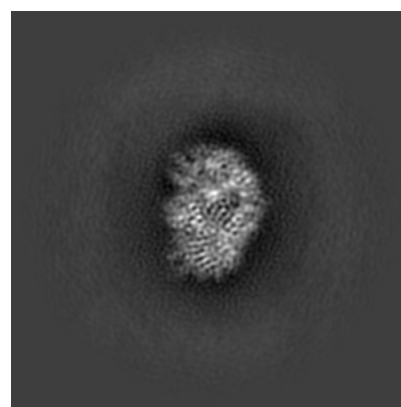
6.1.1 Primary map



X



Y

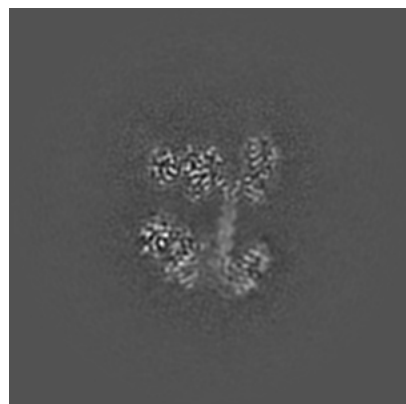


Z

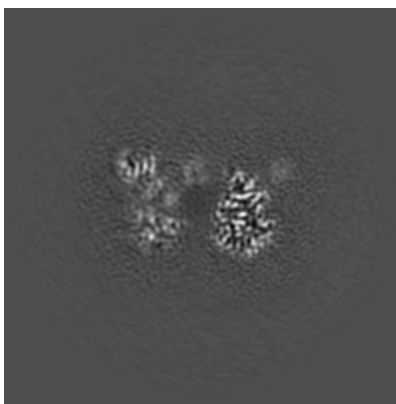
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

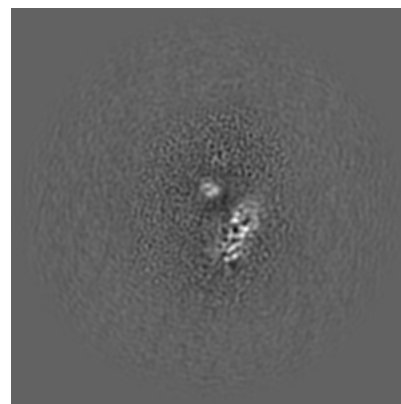
6.2.1 Primary map



X Index: 150



Y Index: 150

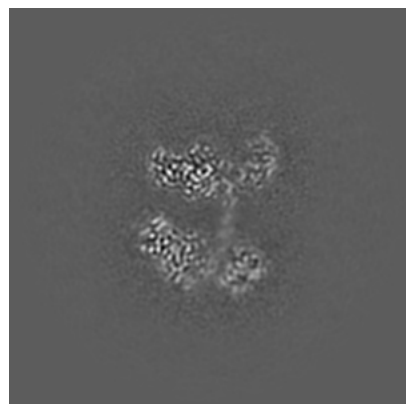


Z Index: 150

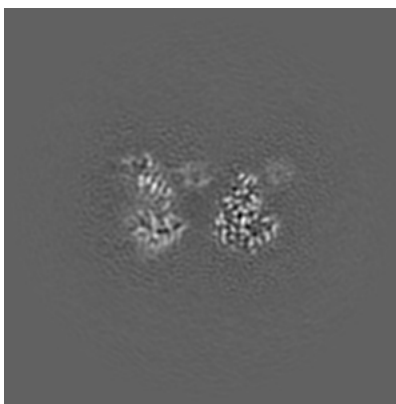
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

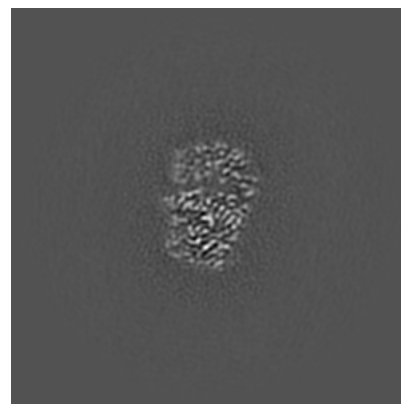
6.3.1 Primary map



X Index: 145



Y Index: 145

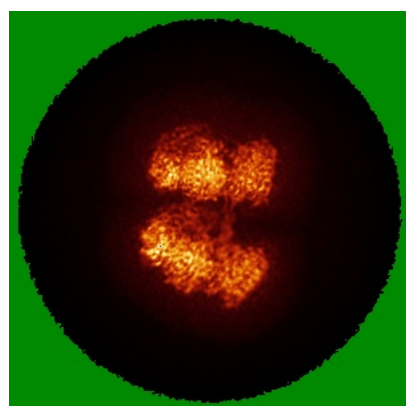


Z Index: 176

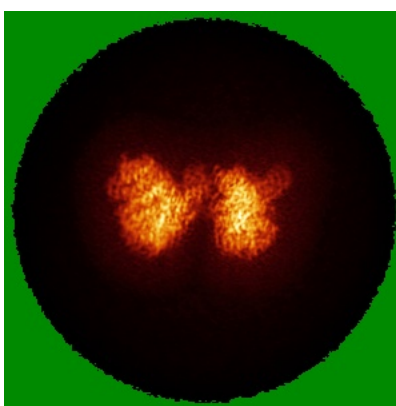
The images above show the largest variance slices of the map in three orthogonal directions.

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

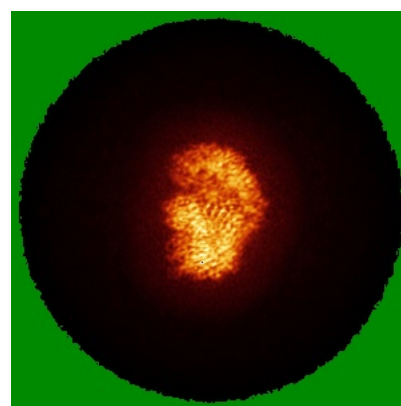
6.4.1 Primary map



X



Y

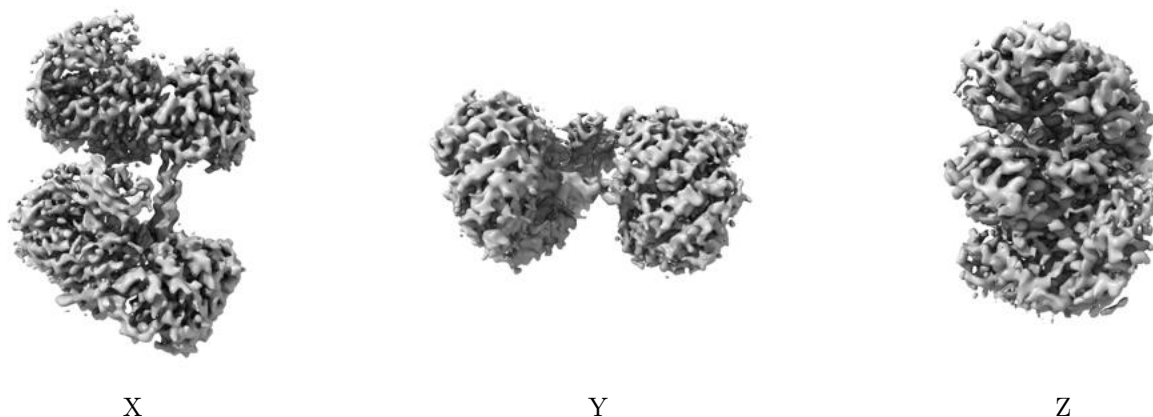


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

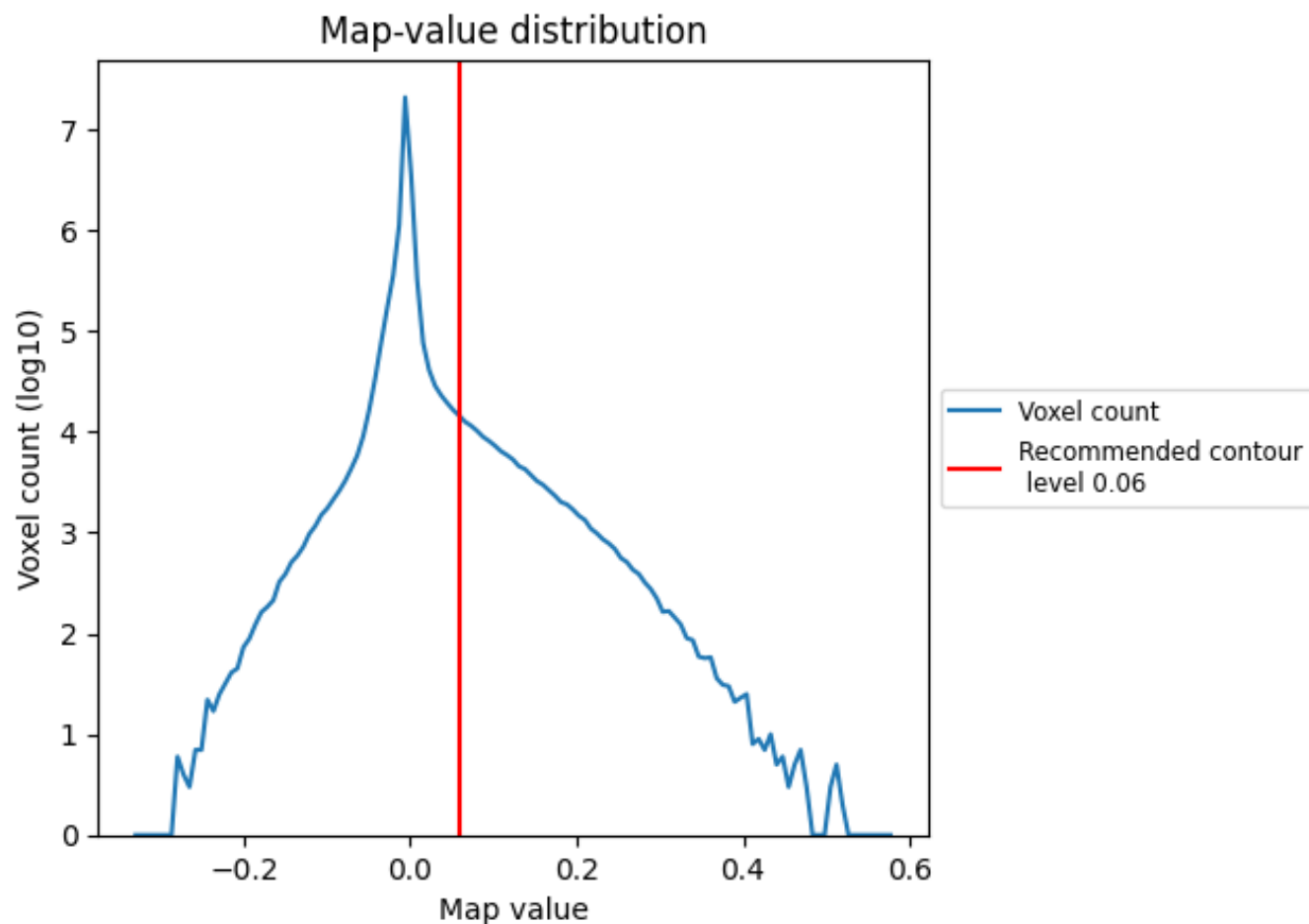
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

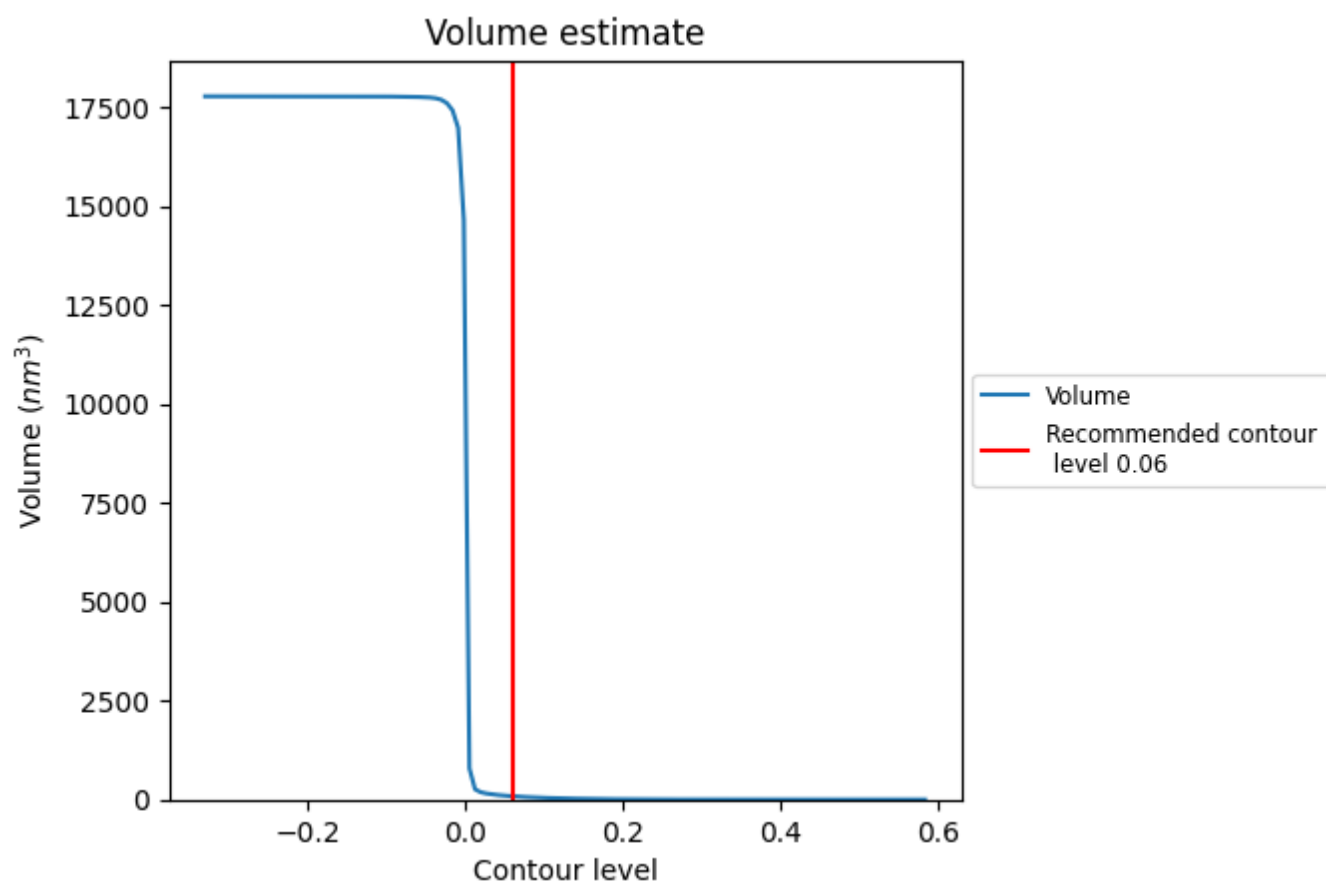
This section contains the results of statistical analysis of the map.

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.

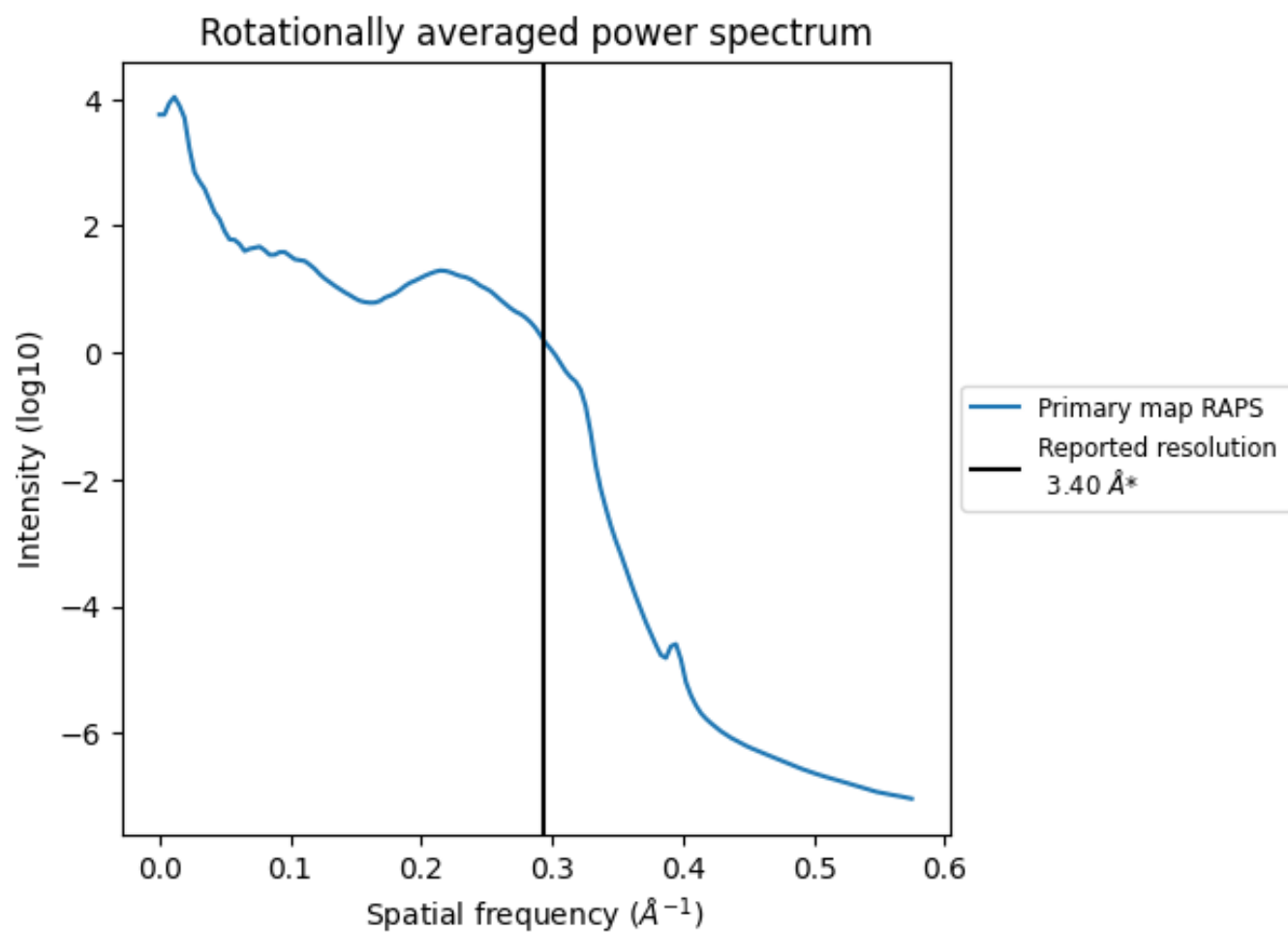
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 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 0.294 Å⁻¹

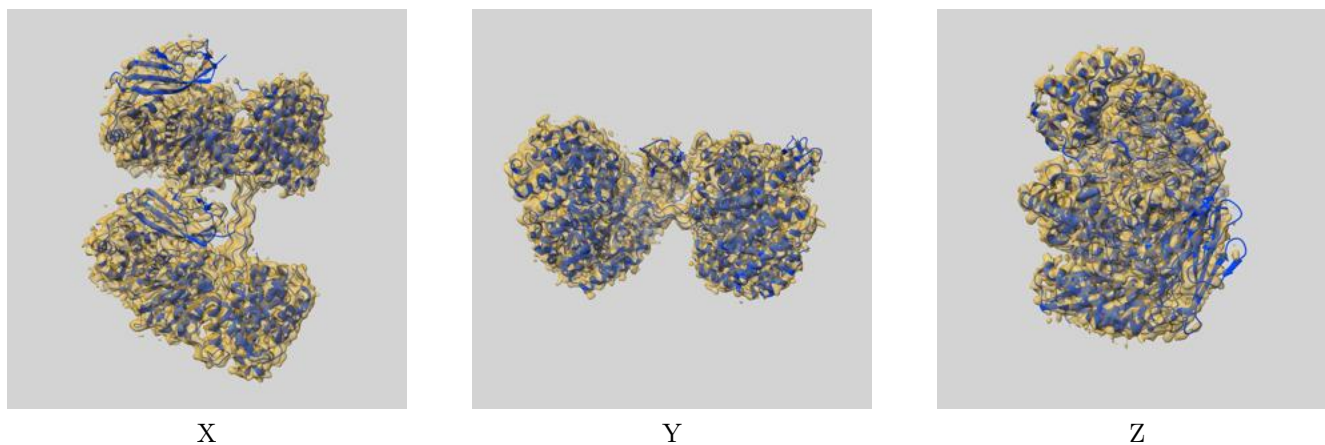
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

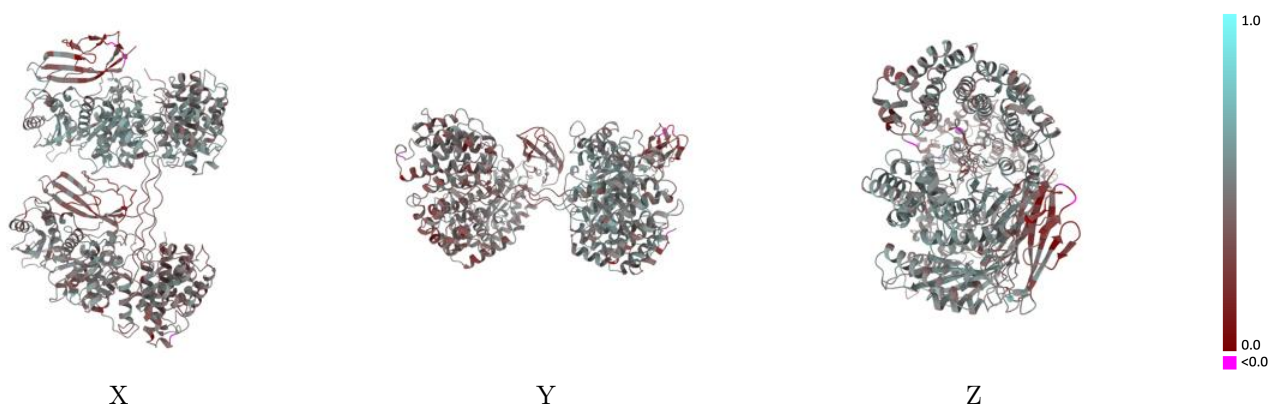
This section contains information regarding the fit between EMDB map EMD-63339 and PDB model 9LRM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



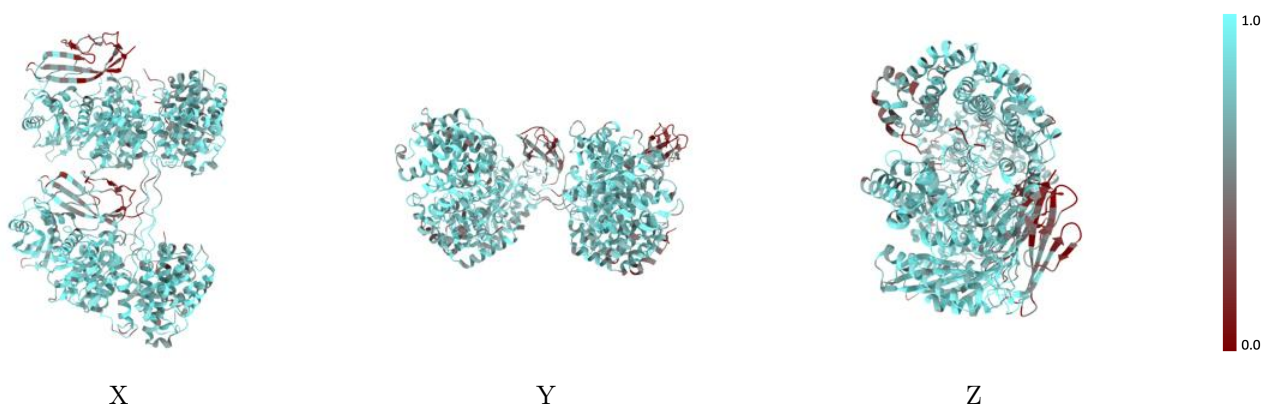
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



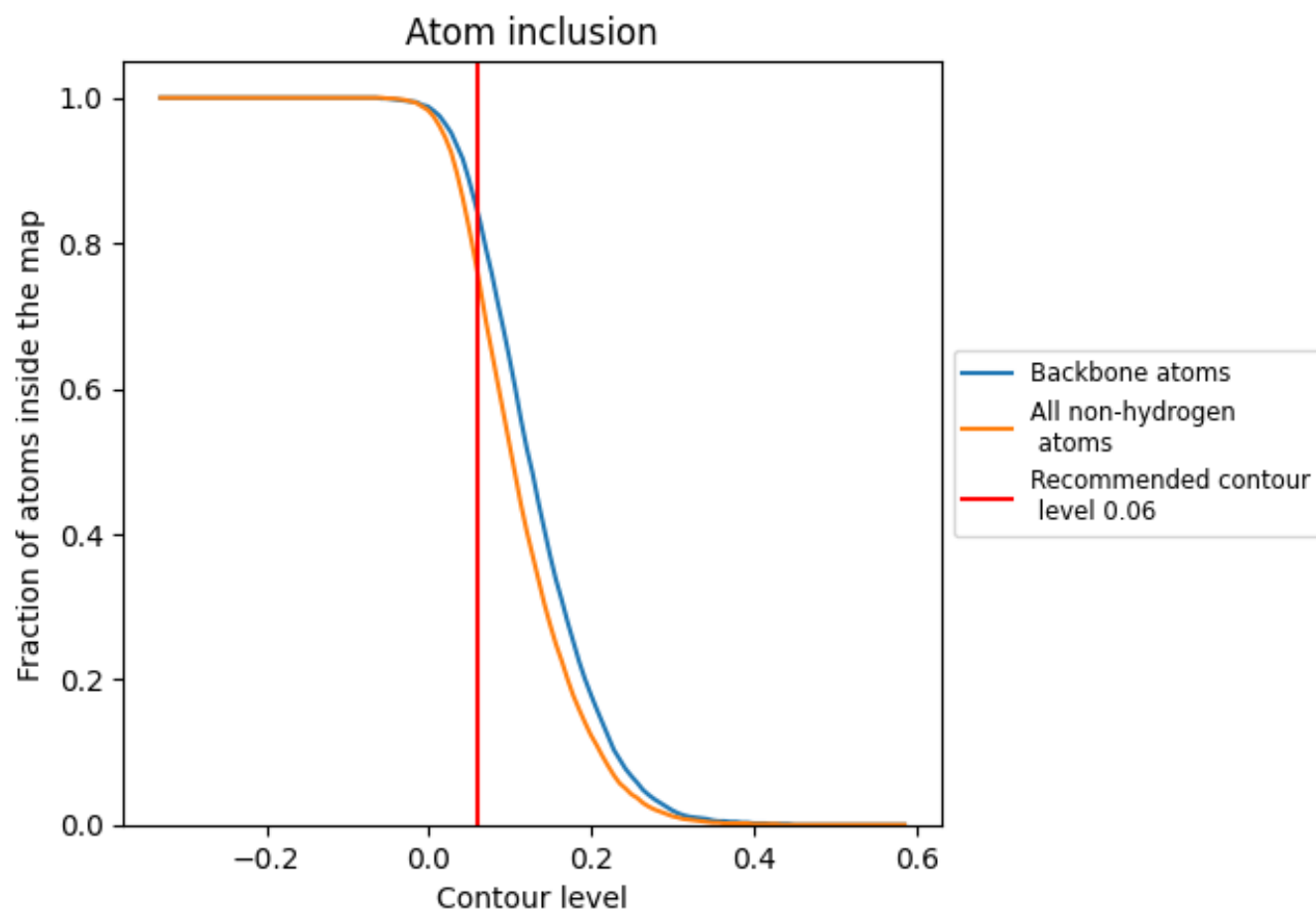
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.4450
A	0.7520	0.4840
B	0.6740	0.3300
C	0.7950	0.4070
D	0.8000	0.4030
G	0.7640	0.4130

