



Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 11:18 AM EST

PDB ID : 8HA0
EMDB ID : EMD-34585
Title : Molecular recognition of two endogenous hormones by the human parathyroid hormone receptor-1
Authors : Zhao, L.; Xu, H.E.; Yuan, Q.
Deposited on : 2022-10-26
Resolution : 2.62 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

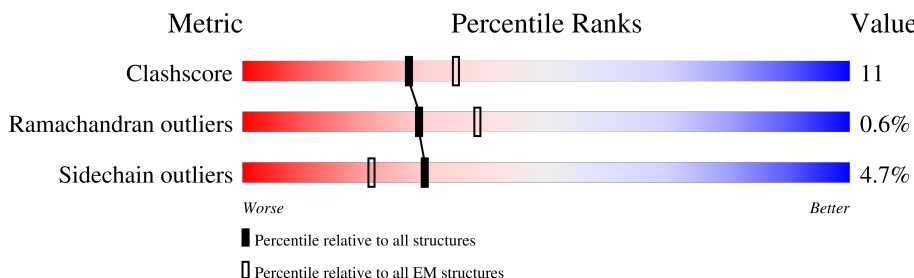
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	361	
2	B	400	
3	G	71	
4	N	140	
5	P	34	
6	R	476	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLR	R	1501	-	-	X	-
7	CLR	R	1502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9385 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 Guanine nucleotide-binding protein g(s) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1950	1232	350	360	8		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total	C	N	O	S	0	0
			2614	1612	470	511	21		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	expression tag	UNP P54311
B	-32	HIS	-	expression tag	UNP P54311
B	-31	HIS	-	expression tag	UNP P54311
B	-30	HIS	-	expression tag	UNP P54311
B	-29	HIS	-	expression tag	UNP P54311
B	-28	HIS	-	expression tag	UNP P54311
B	-27	HIS	-	expression tag	UNP P54311
B	-26	SER	-	expression tag	UNP P54311
B	-25	SER	-	expression tag	UNP P54311
B	-24	GLY	-	expression tag	UNP P54311
B	-23	LEU	-	expression tag	UNP P54311
B	-22	VAL	-	expression tag	UNP P54311
B	-21	PRO	-	expression tag	UNP P54311
B	-20	ARG	-	expression tag	UNP P54311
B	-19	GLY	-	expression tag	UNP P54311
B	-18	SER	-	expression tag	UNP P54311
B	-17	HIS	-	expression tag	UNP P54311
B	-16	MET	-	expression tag	UNP P54311
B	-15	ALA	-	expression tag	UNP P54311
B	-14	SER	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P54311
B	-12	HIS	-	expression tag	UNP P54311
B	-11	HIS	-	expression tag	UNP P54311
B	-10	HIS	-	expression tag	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit

gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	129	Total	C	N	O	S	0	0
			983	611	173	193	6		

- Molecule 5 is a protein called Parathyroid hormone.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	34	Total	C	N	O	S	0	0
			289	181	55	51	2		

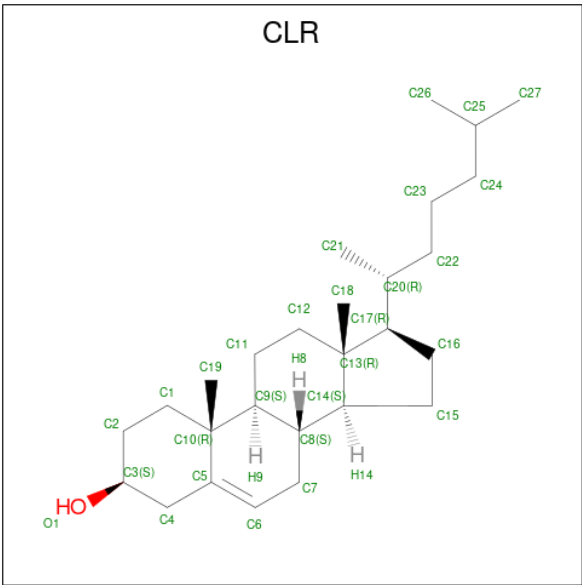
- Molecule 6 is a protein called Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	359	Total	C	N	O	S	0	0
			2947	1948	491	488	20		

There are 2 discrepancies between the modelled and reference sequences:

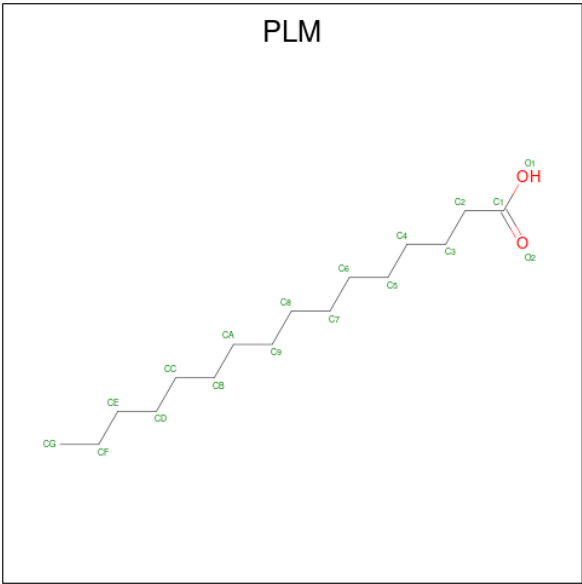
Chain	Residue	Modelled	Actual	Comment	Reference
R	188	ALA	GLY	conflict	UNP Q03431
R	484	ARG	LYS	conflict	UNP Q03431

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			112	108	4	
7	R	1	Total	C	O	0
			112	108	4	
7	R	1	Total	C	O	0
			112	108	4	
7	R	1	Total	C	O	0
			112	108	4	

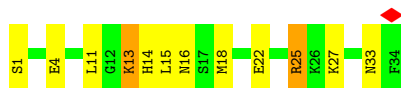
- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



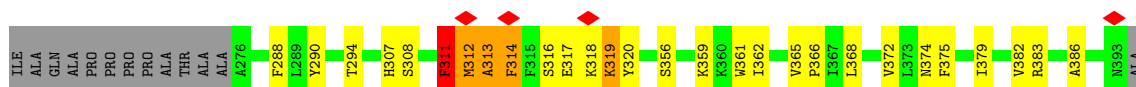
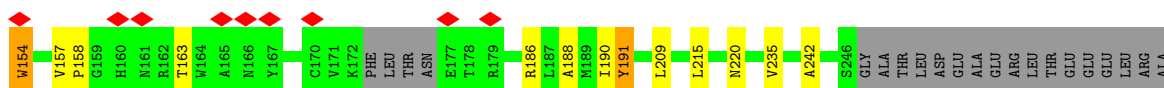
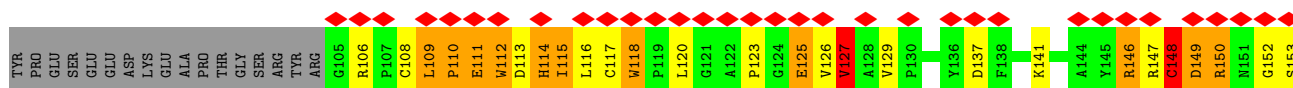
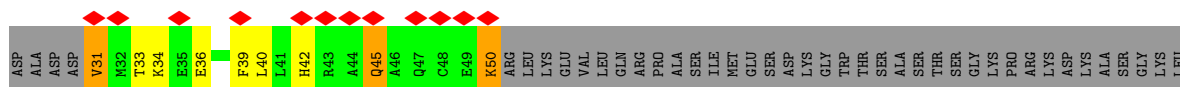
Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			54	48	6	
8	R	1	Total	C	O	0
			54	48	6	
8	R	1	Total	C	O	0
			54	48	6	



• Molecule 5: Parathyroid hormone



• Molecule 6: Parathyroid hormone/parathyroid hormone-related peptide receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	407467	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.713	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	247.2, 247.2, 247.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/1989	0.37	0/2677
2	B	0.24	0/2661	0.43	0/3607
3	G	0.25	0/442	0.37	0/597
4	N	0.25	0/1004	0.43	0/1360
5	P	0.62	0/294	0.71	0/391
6	R	0.39	2/3035 (0.1%)	0.56	3/4123 (0.1%)
All	All	0.31	2/9425 (0.0%)	0.47	3/12755 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	R	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	148	CYS	CB-SG	5.84	1.92	1.82
6	R	149	ASP	N-CA	5.00	1.56	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	320	TYR	N-CA-C	-8.41	88.28	111.00
6	R	313	ALA	N-CA-C	-5.99	94.83	111.00
6	R	148	CYS	CA-CB-SG	5.78	124.40	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	R	114	HIS	Mainchain
6	R	311	PHE	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1950	0	1925	30	0
2	B	2614	0	2518	15	0
3	G	436	0	448	0	0
4	N	983	0	949	9	0
5	P	289	0	292	7	0
6	R	2947	0	2928	166	0
7	R	112	0	180	91	0
8	R	54	0	93	11	0
All	All	9385	0	9333	202	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 11.

All (202) 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)
6:R:361:TRP:CH2	7:R:1502:CLR:C19	1.78	1.64
6:R:372:VAL:HG21	7:R:1502:CLR:C27	1.30	1.60
6:R:110:PRO:O	6:R:154:TRP:CZ3	1.69	1.44
6:R:386:ALA:CB	7:R:1503:CLR:H22	1.46	1.43
6:R:110:PRO:O	6:R:154:TRP:CH2	1.75	1.39
1:A:380:ARG:HG3	6:R:314:PHE:CE2	1.59	1.37
6:R:50:LYS:HD2	6:R:50:LYS:C	1.17	1.33
6:R:365:VAL:HG12	7:R:1501:CLR:C27	1.61	1.30
6:R:368:LEU:HD13	7:R:1502:CLR:C18	1.63	1.27
6:R:361:TRP:CZ2	7:R:1502:CLR:C19	2.19	1.25
6:R:366:PRO:CD	7:R:1501:CLR:H271	1.67	1.24
6:R:386:ALA:CB	7:R:1503:CLR:C2	2.17	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:382:VAL:CG1	7:R:1503:CLR:H111	1.69	1.20
6:R:372:VAL:CG2	7:R:1502:CLR:H271	1.71	1.20
6:R:372:VAL:CG2	7:R:1502:CLR:C27	2.22	1.18
6:R:382:VAL:HG11	7:R:1503:CLR:H111	1.19	1.15
6:R:365:VAL:HG12	7:R:1501:CLR:H272	1.20	1.15
6:R:50:LYS:C	6:R:50:LYS:CD	2.10	1.14
1:A:380:ARG:HA	6:R:314:PHE:HZ	1.04	1.14
6:R:372:VAL:HG21	7:R:1502:CLR:H273	1.22	1.14
6:R:382:VAL:HG12	7:R:1503:CLR:H193	1.19	1.13
1:A:380:ARG:HA	6:R:314:PHE:CZ	1.85	1.11
6:R:368:LEU:HD13	7:R:1502:CLR:H181	1.33	1.10
6:R:372:VAL:HG21	7:R:1502:CLR:H271	1.09	1.08
6:R:50:LYS:HD2	6:R:50:LYS:O	1.53	1.06
6:R:368:LEU:CD1	7:R:1502:CLR:C18	2.33	1.05
1:A:380:ARG:HG3	6:R:314:PHE:CZ	1.92	1.04
6:R:386:ALA:HB2	7:R:1503:CLR:H22	1.37	1.04
6:R:361:TRP:CH2	7:R:1502:CLR:H192	1.92	1.03
6:R:386:ALA:HB1	7:R:1503:CLR:C2	1.85	1.03
6:R:362:ILE:CG1	7:R:1501:CLR:H193	1.88	1.03
6:R:362:ILE:HG12	7:R:1501:CLR:H111	1.36	1.03
6:R:361:TRP:CZ2	7:R:1502:CLR:H192	1.92	1.02
1:A:380:ARG:CA	6:R:314:PHE:HZ	1.73	0.99
1:A:383:ILE:HB	6:R:314:PHE:HE1	1.24	0.99
6:R:365:VAL:CG1	7:R:1501:CLR:H273	1.93	0.99
1:A:383:ILE:HB	6:R:314:PHE:CE1	1.98	0.98
6:R:368:LEU:CD1	7:R:1502:CLR:H183	1.94	0.97
6:R:365:VAL:HG12	7:R:1501:CLR:H273	1.43	0.96
6:R:365:VAL:CG1	7:R:1501:CLR:C27	2.44	0.94
6:R:362:ILE:CD1	7:R:1501:CLR:H193	1.97	0.93
6:R:366:PRO:HD3	7:R:1501:CLR:H271	1.46	0.93
6:R:362:ILE:HD11	7:R:1501:CLR:H193	1.48	0.93
1:A:380:ARG:HG3	6:R:314:PHE:HE2	1.20	0.93
6:R:366:PRO:CG	7:R:1501:CLR:H271	1.97	0.93
6:R:450:PHE:CZ	7:R:1504:CLR:H221	2.03	0.92
6:R:361:TRP:CH2	7:R:1502:CLR:H191	2.05	0.92
6:R:386:ALA:HB3	7:R:1503:CLR:H22	1.49	0.91
6:R:382:VAL:HG11	7:R:1503:CLR:C11	2.00	0.91
6:R:110:PRO:O	6:R:154:TRP:HZ3	1.54	0.90
1:A:380:ARG:CG	6:R:314:PHE:CE2	2.53	0.88
6:R:386:ALA:HB1	7:R:1503:CLR:H21	1.56	0.88
6:R:366:PRO:N	7:R:1501:CLR:H271	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:386:ALA:HB2	7:R:1503:CLR:C2	1.97	0.86
6:R:382:VAL:HG12	7:R:1503:CLR:C19	2.05	0.86
6:R:450:PHE:HZ	7:R:1504:CLR:H213	1.38	0.86
6:R:368:LEU:HD13	7:R:1502:CLR:H183	1.48	0.86
6:R:361:TRP:HH2	7:R:1502:CLR:C19	1.52	0.85
6:R:382:VAL:CG1	7:R:1503:CLR:C11	2.56	0.79
6:R:359:LYS:HA	7:R:1501:CLR:H192	1.64	0.79
6:R:361:TRP:HH2	7:R:1502:CLR:H191	1.43	0.79
6:R:50:LYS:CD	6:R:50:LYS:O	2.23	0.78
6:R:366:PRO:CD	7:R:1501:CLR:C27	2.58	0.78
6:R:362:ILE:HG13	7:R:1501:CLR:H193	1.65	0.77
6:R:372:VAL:HG21	7:R:1502:CLR:C25	2.14	0.76
1:A:383:ILE:CG2	6:R:314:PHE:HD1	1.99	0.76
1:A:380:ARG:CG	6:R:314:PHE:HE2	1.98	0.75
6:R:382:VAL:CG1	7:R:1503:CLR:H193	2.11	0.75
6:R:450:PHE:HZ	7:R:1504:CLR:C21	2.00	0.75
6:R:382:VAL:HG12	7:R:1503:CLR:H111	1.66	0.75
6:R:447:PHE:CE1	8:R:1505:PLM:HG1	2.21	0.74
6:R:386:ALA:CB	7:R:1503:CLR:H21	2.13	0.74
1:A:383:ILE:CG2	6:R:314:PHE:CD1	2.70	0.74
6:R:366:PRO:N	7:R:1501:CLR:C27	2.51	0.74
6:R:446:LEU:HD23	8:R:1505:PLM:CG	2.18	0.73
1:A:344:GLU:OE1	1:A:347:ARG:NH2	2.22	0.73
6:R:450:PHE:CZ	7:R:1504:CLR:C22	2.71	0.73
1:A:380:ARG:CG	6:R:314:PHE:CZ	2.72	0.72
6:R:235:VAL:HG11	8:R:1506:PLM:HC2	1.70	0.72
6:R:110:PRO:O	6:R:154:TRP:HH2	1.65	0.71
6:R:372:VAL:CG2	7:R:1502:CLR:H273	2.03	0.71
6:R:215:LEU:O	6:R:220:ASN:ND2	2.24	0.71
6:R:362:ILE:HG13	7:R:1501:CLR:C19	2.20	0.71
6:R:356:SER:O	6:R:359:LYS:NZ	2.23	0.71
6:R:366:PRO:HG3	7:R:1501:CLR:H271	1.70	0.70
1:A:380:ARG:CA	6:R:314:PHE:CZ	2.60	0.70
4:N:29:PHE:O	4:N:72:ARG:NH2	2.25	0.69
6:R:50:LYS:O	6:R:50:LYS:CE	2.42	0.68
6:R:450:PHE:CE2	7:R:1504:CLR:H221	2.29	0.68
6:R:366:PRO:HD3	7:R:1501:CLR:C27	2.21	0.67
6:R:109:LEU:O	6:R:154:TRP:HH2	1.77	0.67
6:R:450:PHE:CZ	7:R:1504:CLR:H213	2.28	0.67
1:A:383:ILE:CB	6:R:314:PHE:HE1	2.05	0.66
6:R:362:ILE:CG1	7:R:1501:CLR:C19	2.71	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:368:LEU:HD12	7:R:1502:CLR:H183	1.76	0.66
6:R:113:ASP:HB2	6:R:118:TRP:HZ2	1.61	0.65
6:R:362:ILE:HA	7:R:1501:CLR:C18	2.26	0.65
1:A:380:ARG:CB	6:R:314:PHE:HZ	2.11	0.64
6:R:362:ILE:HD11	7:R:1501:CLR:C19	2.27	0.64
6:R:366:PRO:HG3	7:R:1501:CLR:H261	1.80	0.63
1:A:383:ILE:HG21	6:R:314:PHE:HD1	1.61	0.63
1:A:383:ILE:HG21	6:R:314:PHE:CD1	2.34	0.63
1:A:383:ILE:CB	6:R:314:PHE:CE1	2.79	0.62
6:R:372:VAL:HG11	7:R:1502:CLR:H273	1.81	0.61
6:R:359:LYS:HA	7:R:1501:CLR:C19	2.30	0.61
4:N:7:SER:N	4:N:21:SER:O	2.34	0.61
4:N:67:ARG:NH2	4:N:90:ASP:OD2	2.33	0.61
6:R:446:LEU:HD23	8:R:1505:PLM:HG1	1.85	0.59
6:R:125:GLU:HG2	6:R:127:VAL:HG22	1.85	0.59
6:R:362:ILE:HA	7:R:1501:CLR:H182	1.85	0.58
6:R:290:TYR:O	6:R:294:THR:HG23	2.03	0.58
6:R:450:PHE:CZ	7:R:1504:CLR:C21	2.85	0.57
2:B:153:ASP:OD1	2:B:156:GLN:N	2.38	0.57
6:R:314:PHE:C	6:R:316:SER:H	2.09	0.56
6:R:361:TRP:HZ2	7:R:1502:CLR:H192	1.63	0.55
1:A:383:ILE:HG22	6:R:314:PHE:CD1	2.41	0.55
1:A:383:ILE:HG22	6:R:314:PHE:HD1	1.71	0.55
1:A:380:ARG:CB	6:R:314:PHE:CZ	2.90	0.54
6:R:109:LEU:O	6:R:154:TRP:CH2	2.60	0.54
6:R:113:ASP:C	6:R:115:ILE:H	2.10	0.54
1:A:36:LEU:N	1:A:220:HIS:O	2.38	0.54
2:B:147:SER:OG	2:B:188:MET:O	2.16	0.54
6:R:242:ALA:CB	8:R:1506:PLM:H42	2.38	0.53
6:R:446:LEU:CD2	8:R:1505:PLM:CG	2.87	0.53
6:R:446:LEU:HD23	8:R:1505:PLM:HG3	1.91	0.53
6:R:42:HIS:CE1	6:R:45:GLN:HE22	2.27	0.52
6:R:314:PHE:C	6:R:316:SER:N	2.60	0.52
6:R:375:PHE:CE2	6:R:379:ILE:HD11	2.44	0.52
6:R:235:VAL:CG1	8:R:1506:PLM:HC2	2.37	0.52
6:R:111:GLU:OE1	6:R:163:THR:HG21	2.10	0.51
6:R:157:VAL:N	6:R:158:PRO:CD	2.74	0.51
6:R:209:LEU:HG	6:R:460:CYS:SG	2.52	0.51
4:N:52:SER:HG	4:N:57:SER:HG	1.59	0.50
5:P:14:HIS:HD2	5:P:15:LEU:HD23	1.77	0.50
6:R:366:PRO:CB	7:R:1501:CLR:H261	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:308:SER:O	6:R:313:ALA:HB3	2.11	0.49
6:R:148:CYS:HB3	6:R:152:GLY:HA2	1.94	0.49
6:R:374:ASN:ND2	6:R:417:PHE:O	2.46	0.49
1:A:364:THR:HG22	1:A:366:SER:H	1.77	0.49
6:R:186:ARG:HG3	7:R:1504:CLR:H3	1.94	0.49
4:N:6:GLU:OE1	4:N:6:GLU:N	2.45	0.48
6:R:50:LYS:O	6:R:50:LYS:HE2	2.13	0.48
6:R:383:ARG:HA	7:R:1503:CLR:H192	1.94	0.48
6:R:190:ILE:HG22	7:R:1504:CLR:H9	1.95	0.48
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.94	0.48
6:R:372:VAL:CB	7:R:1502:CLR:C27	2.89	0.48
6:R:372:VAL:CG1	7:R:1502:CLR:H273	2.44	0.48
2:B:295:ASN:OD1	2:B:304:ARG:NH2	2.45	0.48
4:N:50:ASP:OD1	4:N:59:SER:OG	2.28	0.48
6:R:362:ILE:CG1	7:R:1501:CLR:H111	2.26	0.47
6:R:127:VAL:HB	6:R:146:ARG:HG3	1.96	0.47
6:R:365:VAL:C	7:R:1501:CLR:H272	2.34	0.47
6:R:366:PRO:HG3	7:R:1501:CLR:C27	2.44	0.47
6:R:209:LEU:HD21	6:R:460:CYS:SG	2.55	0.47
6:R:365:VAL:HG11	7:R:1501:CLR:H232	1.97	0.47
6:R:431:GLU:OE1	6:R:431:GLU:N	2.44	0.47
4:N:91:THR:HG23	4:N:91:THR:O	2.15	0.47
5:P:13:LYS:O	5:P:14:HIS:C	2.50	0.47
4:N:61:THR:HG22	4:N:64:VAL:HG22	1.97	0.46
6:R:112:TRP:NE1	6:R:117:CYS:HA	2.30	0.46
6:R:447:PHE:CE1	8:R:1505:PLM:CG	2.97	0.46
5:P:16:ASN:HD21	6:R:33:THR:HB	1.80	0.46
1:A:383:ILE:CG2	6:R:314:PHE:CE1	2.99	0.46
6:R:365:VAL:CB	7:R:1501:CLR:H273	2.44	0.46
6:R:406:LEU:HD21	7:R:1503:CLR:H11	1.98	0.46
6:R:366:PRO:CG	7:R:1501:CLR:H261	2.44	0.46
2:B:123:ILE:CD1	2:B:171:ILE:HD12	2.47	0.45
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.40	0.45
6:R:311:PHE:HB3	6:R:312:MET:HG3	1.99	0.45
1:A:368:ASP:N	1:A:368:ASP:OD1	2.50	0.45
2:B:289:TYR:HH	2:B:297:TRP:HE1	1.63	0.45
6:R:461:PHE:O	6:R:467:GLN:NE2	2.44	0.44
7:R:1503:CLR:H183	7:R:1503:CLR:H212	2.00	0.44
6:R:365:VAL:C	7:R:1501:CLR:C27	2.85	0.44
6:R:362:ILE:HG12	7:R:1501:CLR:H193	1.91	0.44
1:A:283:ARG:O	1:A:357:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:447:PHE:CE1	8:R:1505:PLM:CF	3.00	0.44
2:B:136:SER:O	2:B:137:ARG:NH1	2.52	0.43
6:R:366:PRO:HB3	7:R:1501:CLR:H261	1.99	0.43
6:R:372:VAL:CB	7:R:1502:CLR:H273	2.48	0.43
1:A:42:ASP:OD1	1:A:43:ASN:N	2.52	0.42
5:P:1:SER:N	6:R:425:MET:O	2.48	0.42
5:P:25:ARG:HA	5:P:25:ARG:HD3	1.80	0.42
6:R:109:LEU:HD12	6:R:109:LEU:HA	1.69	0.42
6:R:447:PHE:HE1	8:R:1505:PLM:CF	2.33	0.42
2:B:170:ASP:O	2:B:174:GLY:N	2.46	0.42
2:B:51:LEU:HD23	2:B:87:THR:HG23	2.01	0.42
1:A:26:ASP:OD2	2:B:78:LYS:NZ	2.47	0.42
7:R:1504:CLR:H212	7:R:1504:CLR:H183	2.02	0.42
2:B:55:LEU:HD12	2:B:76:ASP:OD2	2.20	0.41
5:P:22:GLU:HA	5:P:22:GLU:OE1	2.20	0.41
2:B:51:LEU:CD2	2:B:87:THR:HG23	2.51	0.41
6:R:317:GLU:HB3	6:R:319:LYS:H	1.85	0.41
6:R:419:VAL:O	6:R:422:ILE:HG22	2.20	0.41
6:R:150:ARG:H	6:R:150:ARG:HG3	1.62	0.41
4:N:52:SER:OG	4:N:57:SER:OG	2.33	0.41
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.49	0.41
6:R:109:LEU:HA	6:R:110:PRO:HD2	1.82	0.41
6:R:372:VAL:HG23	7:R:1502:CLR:H271	1.83	0.40
2:B:291:ASP:OD1	2:B:291:ASP:N	2.55	0.40
5:P:13:LYS:NZ	6:R:31:VAL:HG23	2.36	0.40
6:R:188:ALA:HA	6:R:191:TYR:CE2	2.57	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	231/361 (64%)	229 (99%)	2 (1%)	0	100	100
2	B	339/400 (85%)	339 (100%)	0	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	127/140 (91%)	124 (98%)	3 (2%)	0	100	100
5	P	32/34 (94%)	32 (100%)	0	0	100	100
6	R	349/476 (73%)	322 (92%)	20 (6%)	7 (2%)	7	13
All	All	1133/1482 (76%)	1101 (97%)	25 (2%)	7 (1%)	29	45

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	110	PRO
6	R	127	VAL
6	R	149	ASP
6	R	111	GLU
6	R	114	HIS
6	R	116	LEU
6	R	123	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/315 (67%)	212 (100%)	0	100	100
2	B	282/328 (86%)	278 (99%)	4 (1%)	67	84
3	G	46/58 (79%)	46 (100%)	0	100	100
4	N	107/116 (92%)	106 (99%)	1 (1%)	78	90
5	P	33/33 (100%)	26 (79%)	7 (21%)	1	1
6	R	313/407 (77%)	278 (89%)	35 (11%)	6	10
All	All	993/1257 (79%)	946 (95%)	47 (5%)	30	49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	TYR
2	B	78	LYS
2	B	197	ARG
2	B	234	PHE
4	N	108	PHE
5	P	4	GLU
5	P	11	LEU
5	P	13	LYS
5	P	18	MET
5	P	25	ARG
5	P	27	LYS
5	P	33	ASN
6	R	31	VAL
6	R	34	LYS
6	R	36	GLU
6	R	39	PHE
6	R	40	LEU
6	R	45	GLN
6	R	50	LYS
6	R	106	ARG
6	R	108	CYS
6	R	109	LEU
6	R	112	TRP
6	R	115	ILE
6	R	118	TRP
6	R	120	LEU
6	R	125	GLU
6	R	126	VAL
6	R	127	VAL
6	R	129	VAL
6	R	137	ASP
6	R	141	LYS
6	R	146	ARG
6	R	147	ARG
6	R	148	CYS
6	R	150	ARG
6	R	153	SER
6	R	154	TRP
6	R	191	TYR
6	R	288	PHE
6	R	307	HIS
6	R	311	PHE
6	R	312	MET

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Mol	Chain	Res	Type
6	R	314	PHE
6	R	318	LYS
6	R	319	LYS
6	R	460	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	GLN
2	B	268	ASN
2	B	293	ASN
5	P	6	GLN
5	P	14	HIS
6	R	45	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PLM	R	1507	-	17,17,17	0.53	0	17,17,17	0.71	0
7	CLR	R	1504	-	31,31,31	0.30	0	48,48,48	0.40	0
7	CLR	R	1502	-	31,31,31	0.33	0	48,48,48	0.37	0
7	CLR	R	1503	-	31,31,31	0.30	0	48,48,48	0.36	0
7	CLR	R	1501	-	31,31,31	0.31	0	48,48,48	0.38	0
8	PLM	R	1505	-	17,17,17	0.53	0	17,17,17	0.49	0
8	PLM	R	1506	-	17,17,17	0.54	0	17,17,17	0.71	0

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
8	PLM	R	1507	-	-	8/15/15/15	-
7	CLR	R	1504	-	-	3/10/68/68	0/4/4/4
7	CLR	R	1502	-	-	1/10/68/68	0/4/4/4
7	CLR	R	1503	-	-	3/10/68/68	0/4/4/4
7	CLR	R	1501	-	-	3/10/68/68	0/4/4/4
8	PLM	R	1505	-	-	10/15/15/15	-
8	PLM	R	1506	-	-	8/15/15/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	1505	PLM	C7-C8-C9-CA
7	R	1503	CLR	C17-C20-C22-C23
7	R	1503	CLR	C21-C20-C22-C23
7	R	1504	CLR	C17-C20-C22-C23
7	R	1501	CLR	C17-C20-C22-C23
7	R	1504	CLR	C21-C20-C22-C23
7	R	1501	CLR	C21-C20-C22-C23
7	R	1504	CLR	C20-C22-C23-C24
8	R	1505	PLM	C3-C4-C5-C6
8	R	1505	PLM	CB-CC-CD-CE
8	R	1505	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	R	1505	PLM	CA-CB-CC-CD
8	R	1505	PLM	C5-C6-C7-C8
8	R	1506	PLM	CA-CB-CC-CD
8	R	1507	PLM	CA-CB-CC-CD
8	R	1505	PLM	C9-CA-CB-CC
7	R	1501	CLR	C20-C22-C23-C24
8	R	1507	PLM	CD-CE-CF-CG
8	R	1506	PLM	CD-CE-CF-CG
8	R	1506	PLM	C8-C9-CA-CB
8	R	1507	PLM	C8-C9-CA-CB
8	R	1506	PLM	CC-CD-CE-CF
8	R	1507	PLM	CC-CD-CE-CF
8	R	1506	PLM	C9-CA-CB-CC
8	R	1507	PLM	C9-CA-CB-CC
7	R	1503	CLR	C22-C23-C24-C25
8	R	1505	PLM	O2-C1-C2-C3
8	R	1505	PLM	O1-C1-C2-C3
8	R	1506	PLM	O2-C1-C2-C3
8	R	1507	PLM	O2-C1-C2-C3
8	R	1506	PLM	O1-C1-C2-C3
8	R	1507	PLM	O1-C1-C2-C3
7	R	1502	CLR	C20-C22-C23-C24
8	R	1505	PLM	C1-C2-C3-C4
8	R	1506	PLM	C4-C5-C6-C7
8	R	1507	PLM	C4-C5-C6-C7

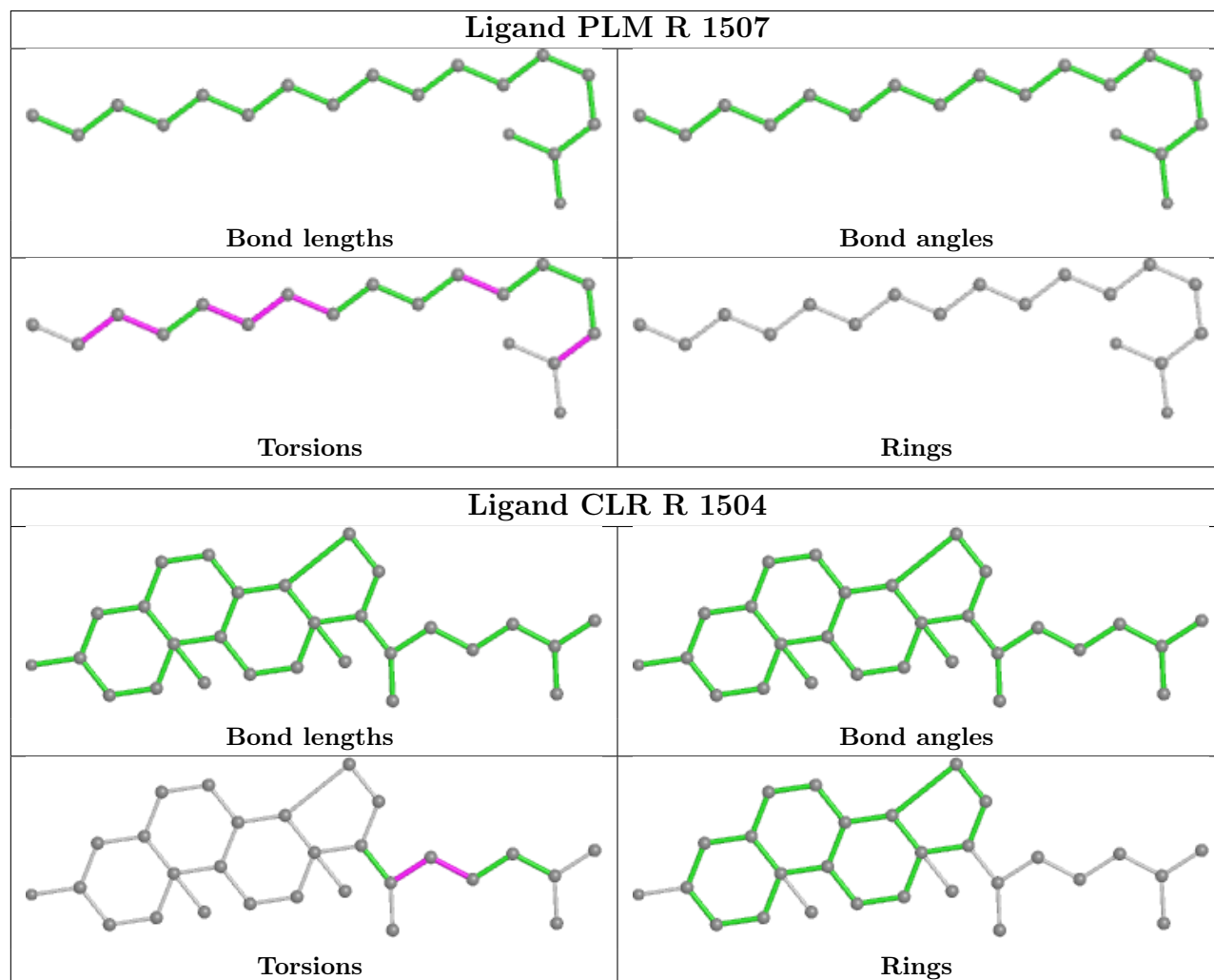
There are no ring outliers.

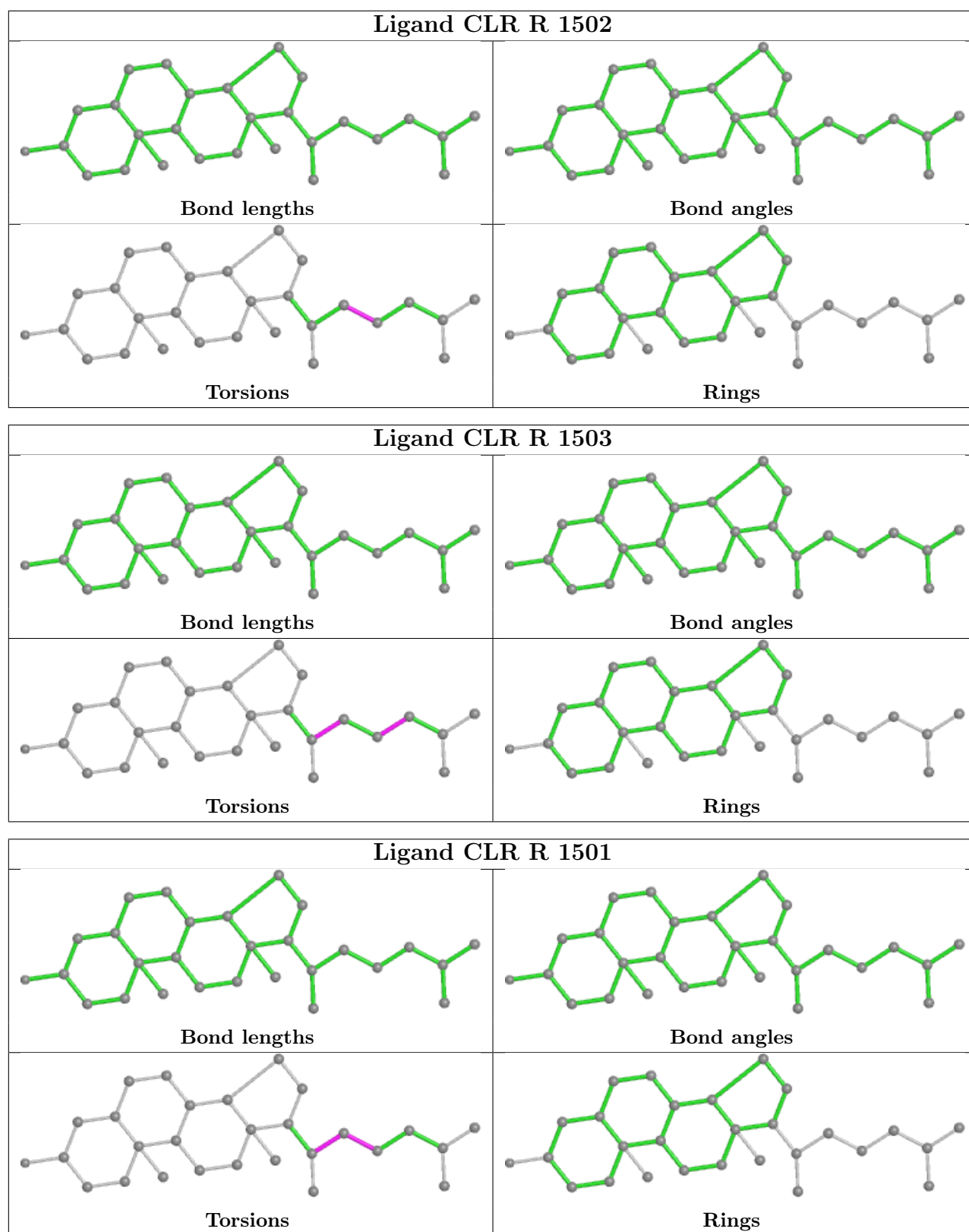
6 monomers are involved in 102 short contacts:

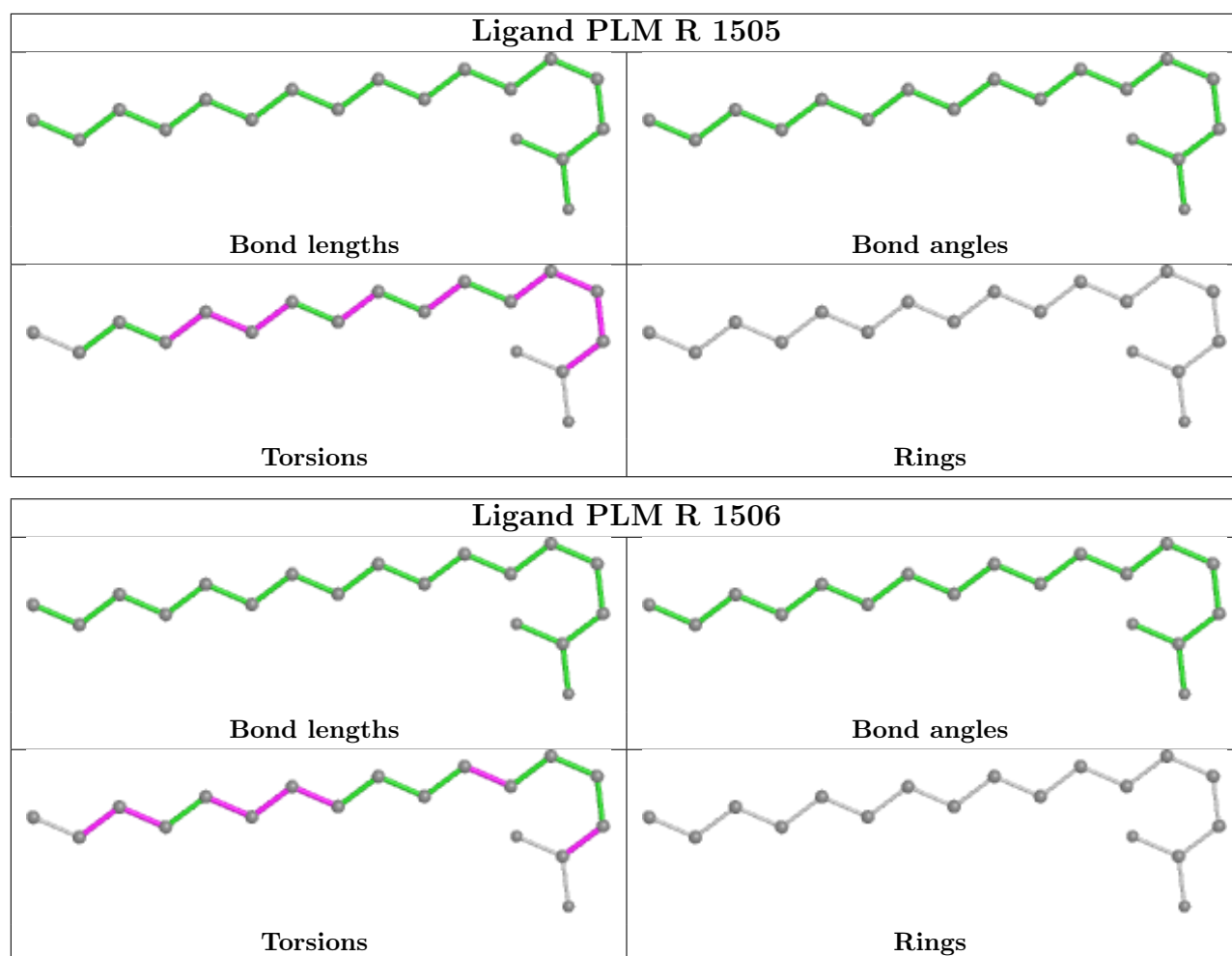
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1504	CLR	10	0
7	R	1502	CLR	26	0
7	R	1503	CLR	19	0
7	R	1501	CLR	36	0
8	R	1505	PLM	8	0
8	R	1506	PLM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

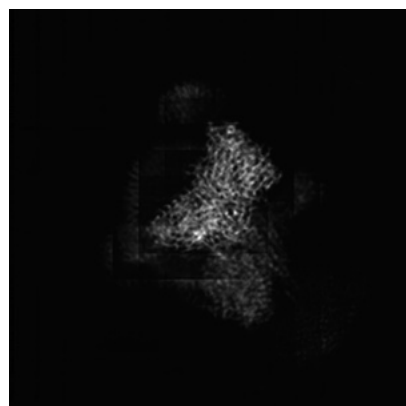
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34585. These allow visual inspection of the internal detail of the map and identification of artifacts.

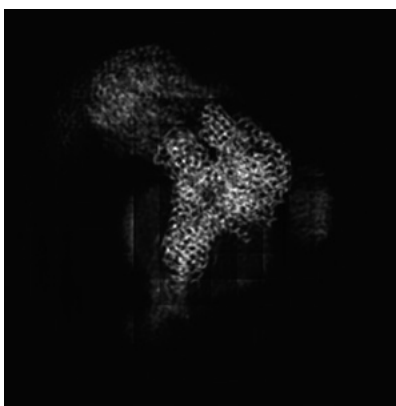
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

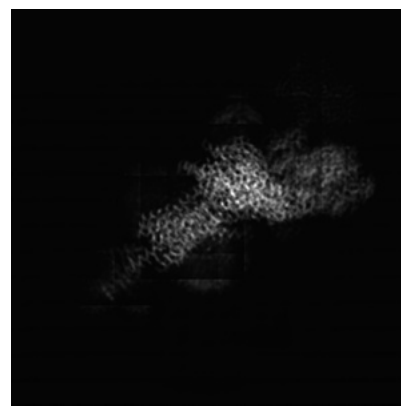
6.1.1 Primary map



X

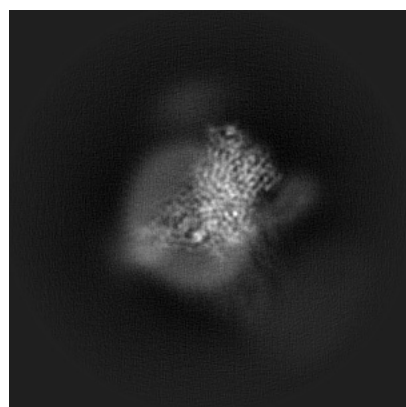


Y

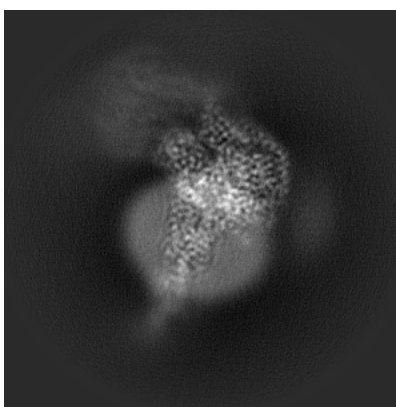


Z

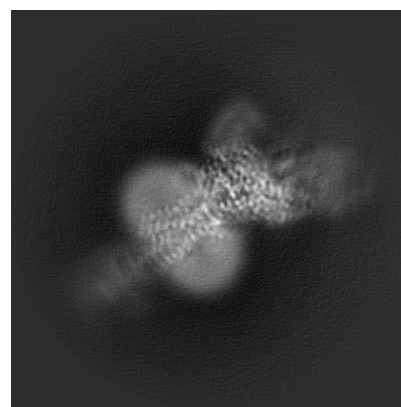
6.1.2 Raw map



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: 150

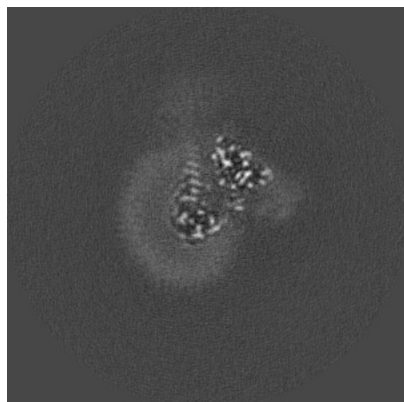


Y Index: 150

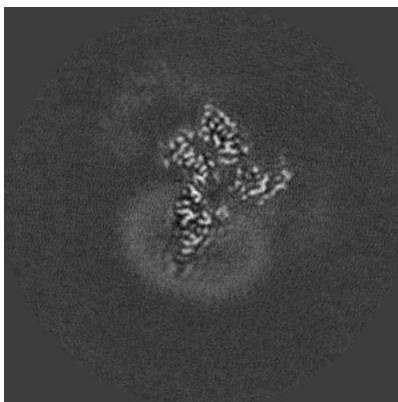


Z Index: 150

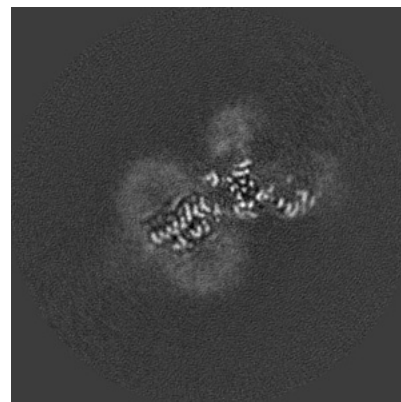
6.2.2 Raw map



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: 177

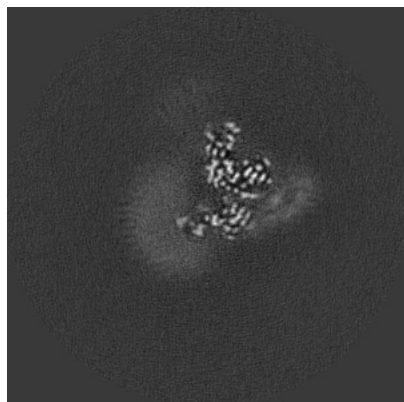


Y Index: 166

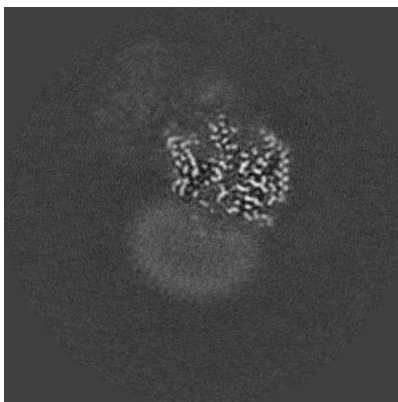


Z Index: 135

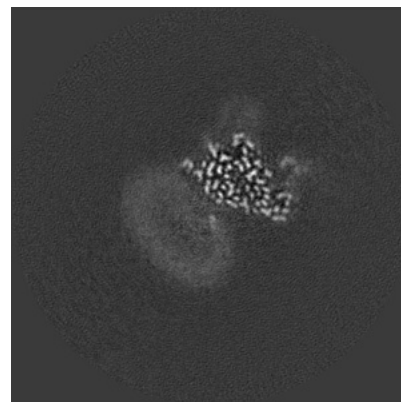
6.3.2 Raw map



X Index: 163



Y Index: 166



Z Index: 175

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

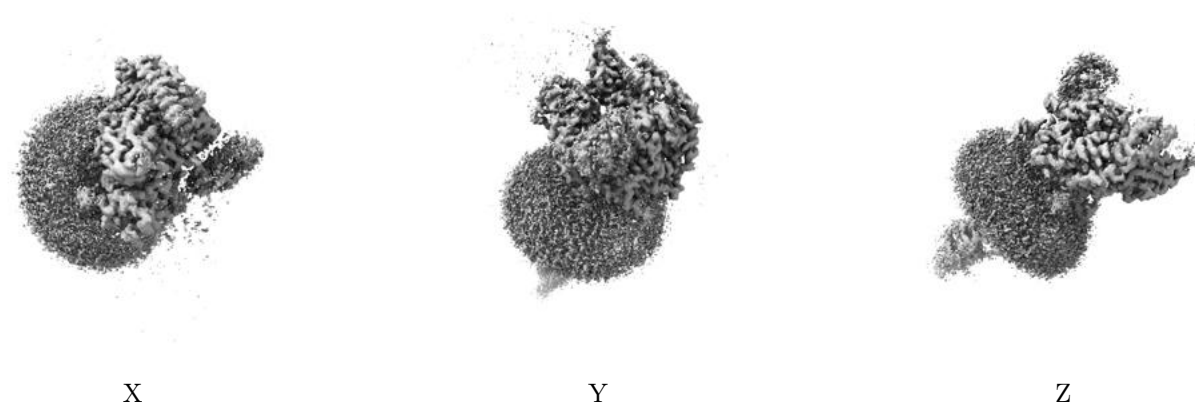
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

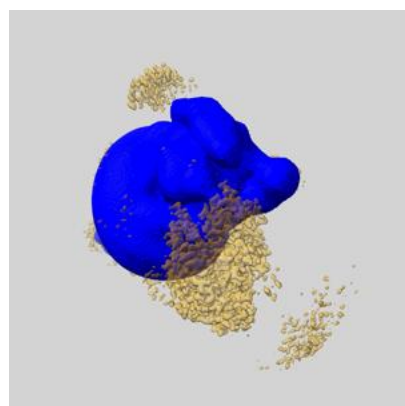
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

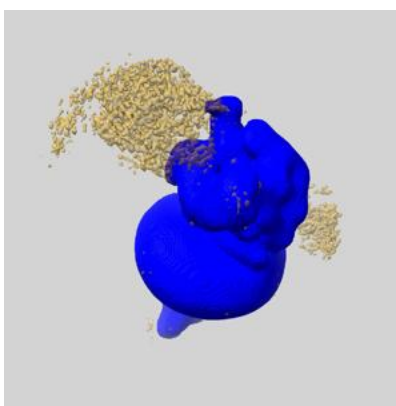
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

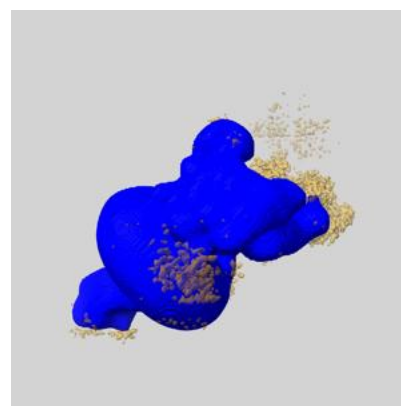
6.5.1 emd_34585_msk_1.map [i](#)



X



Y

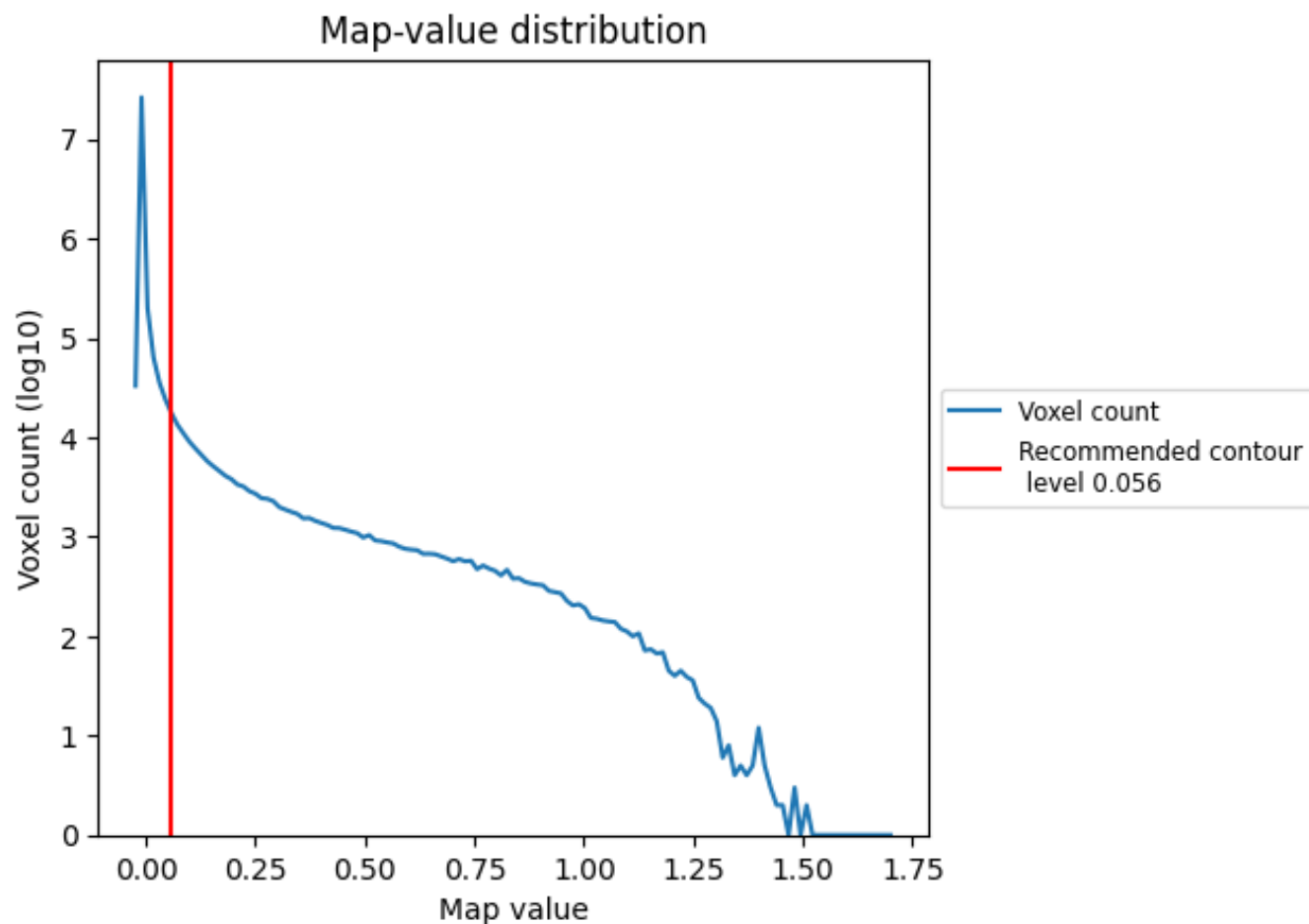


Z

7 Map analysis [i](#)

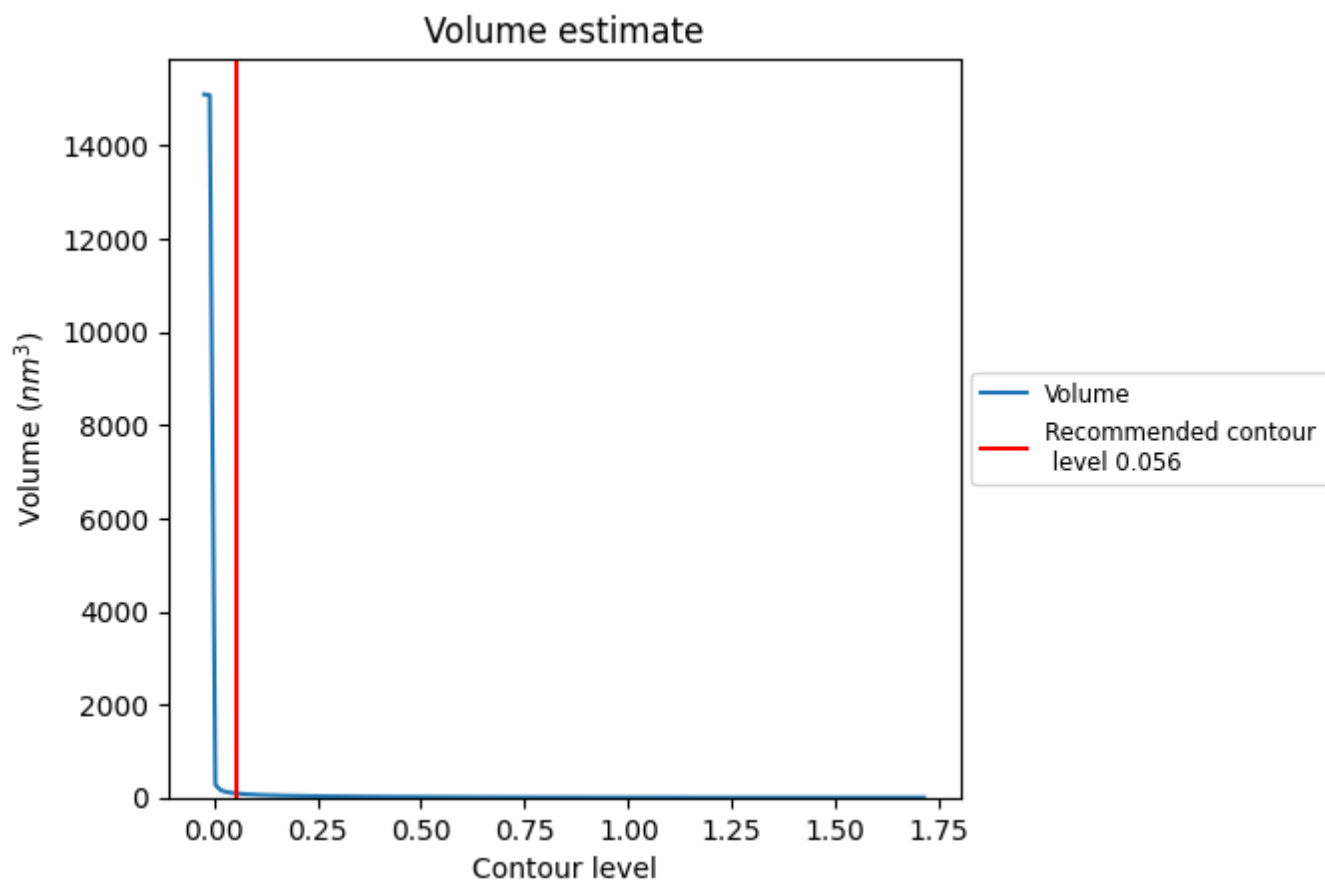
This section contains the results of statistical analysis of the map.

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.

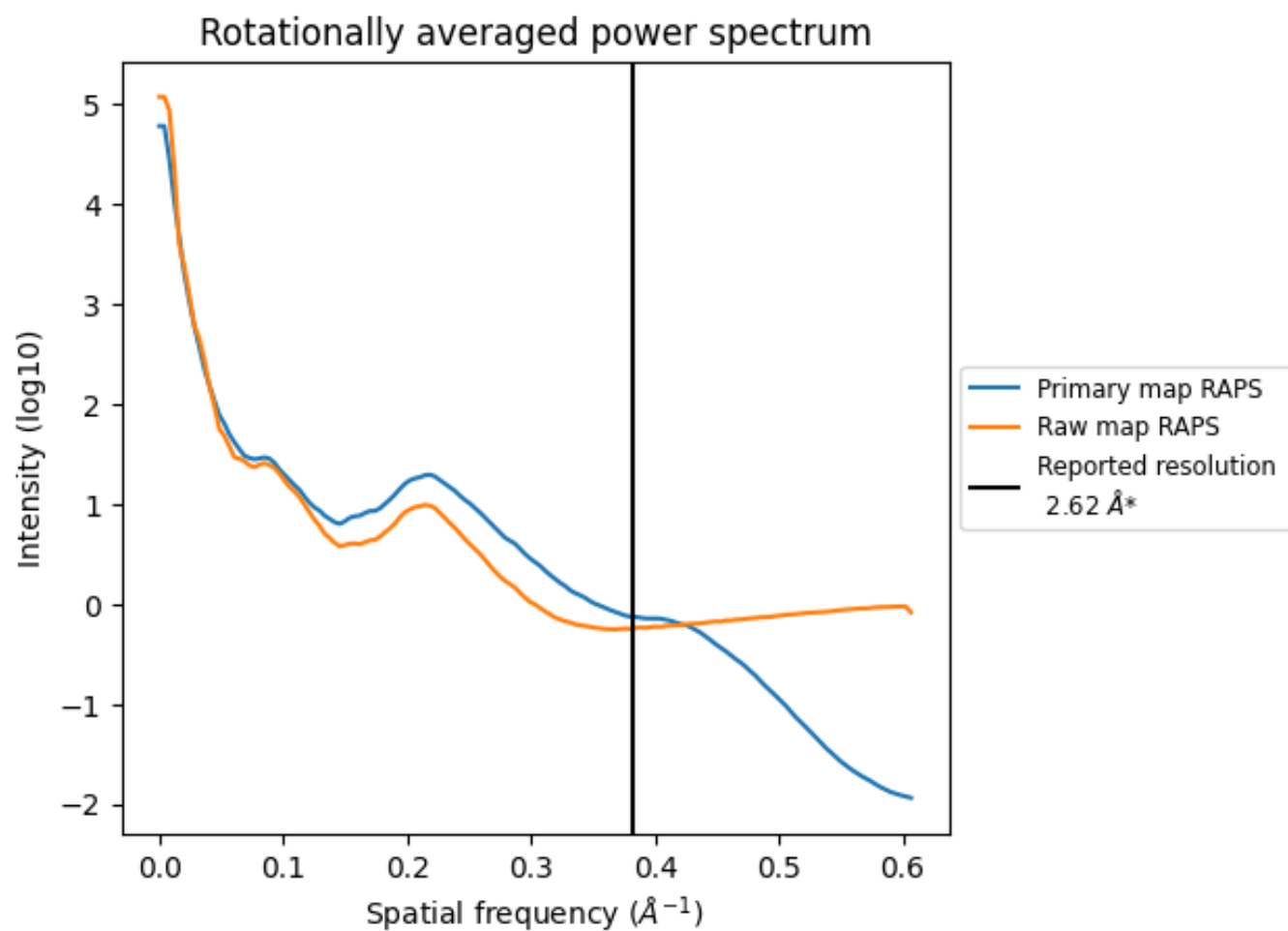
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm^3 ; this corresponds to an approximate mass of 79 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 ⓘ

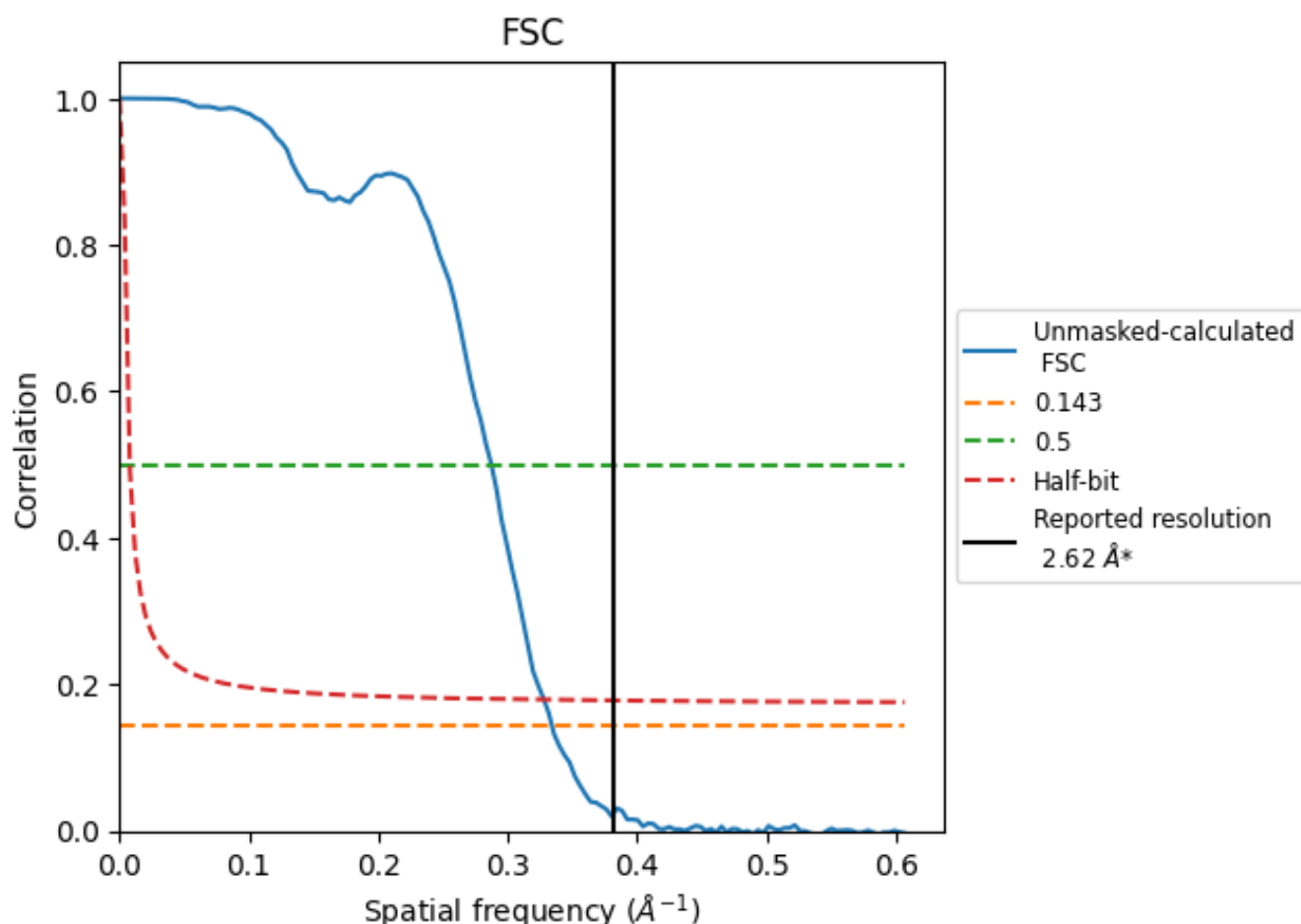


*Reported resolution corresponds to spatial frequency of 0.382 \AA^{-1}

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 0.382 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.48	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

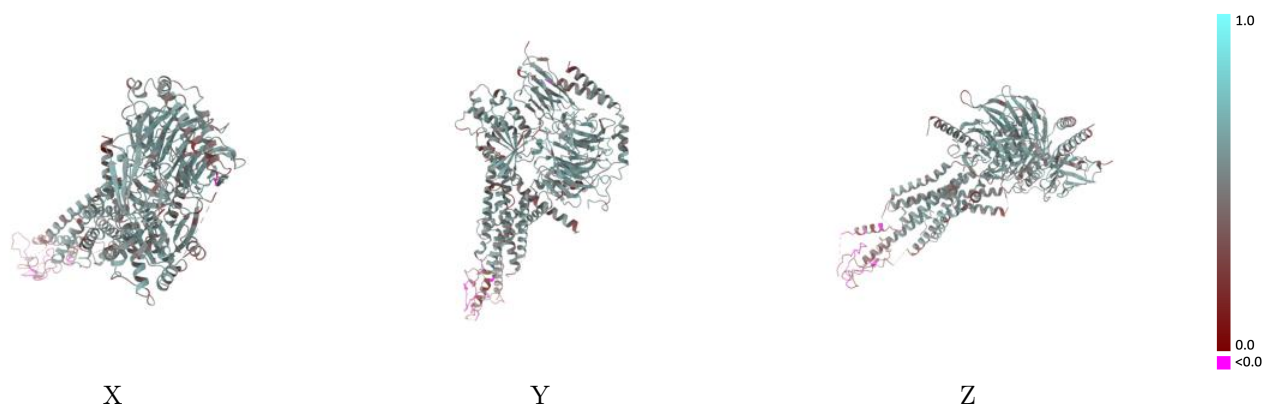
This section contains information regarding the fit between EMDB map EMD-34585 and PDB model 8HA0. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



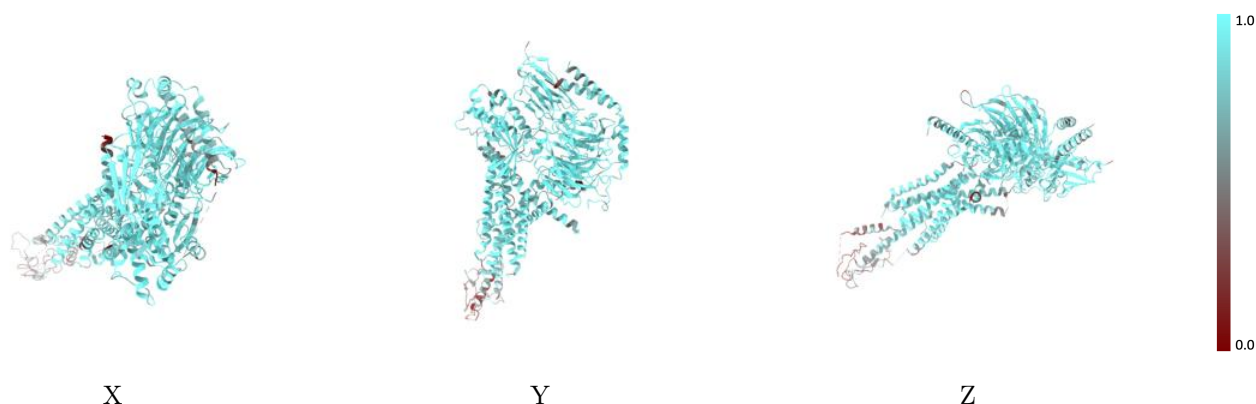
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



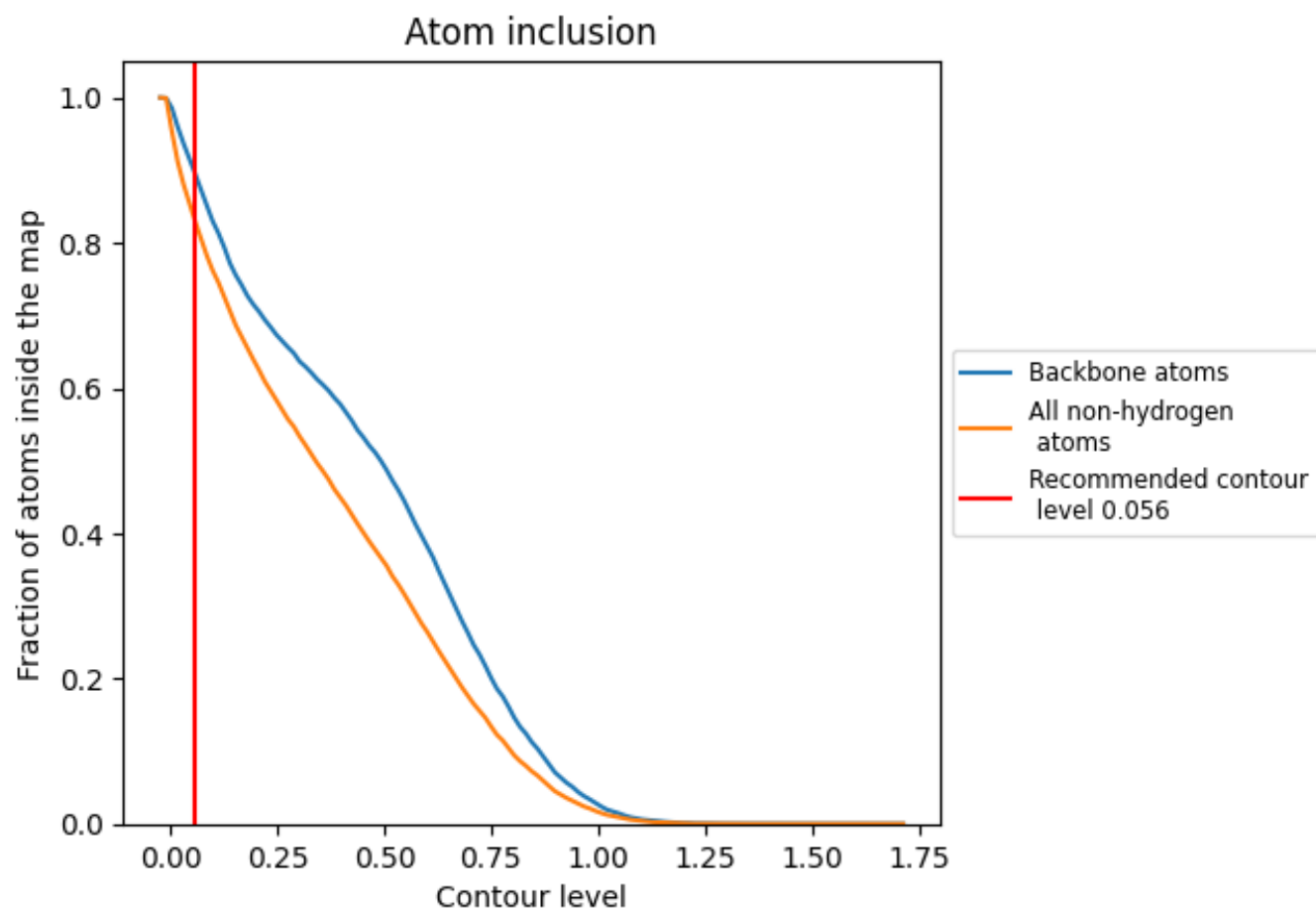
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.056).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8334	<div><div></div></div> 0.4850
A	<div><div></div></div> 0.8877	<div><div></div></div> 0.5180
B	<div><div></div></div> 0.9060	<div><div></div></div> 0.5510
G	<div><div></div></div> 0.8182	<div><div></div></div> 0.5000
N	<div><div></div></div> 0.9021	<div><div></div></div> 0.5300
P	<div><div></div></div> 0.7923	<div><div></div></div> 0.4740
R	<div><div></div></div> 0.7227	<div><div></div></div> 0.3920

1.0

0.0

<0.0