Full wwPDB EM Validation Report (i)

May 27, 2024 – 10:11 AM JST

PDB ID	:	7DNZ
EMDB ID	:	EMD-30791
Title	:	Cryo-EM structure of the human ABCB6 (Hemin and GSH-bound)
Authors	:	Kim, S.; Lee, S.S.; Park, J.G.; Kim, J.W.; Kim, S.; Kim, N.J.; Hong, S.; Kang, J.Y.; Jin, M.S.
Deposited on	:	2020-12-11
Resolution	:	3.60 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 (i) 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 (1)) were used in the production of this report:

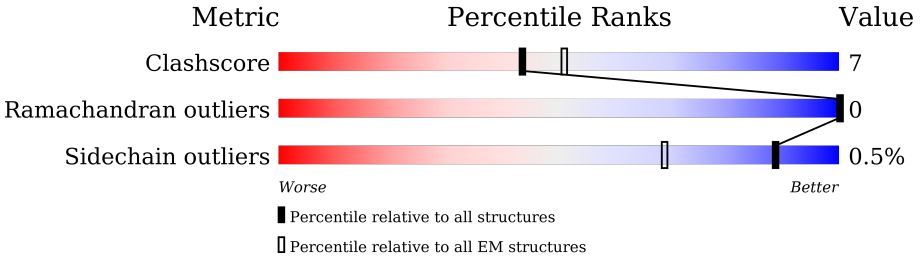
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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 <=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	842	19% 57% 13% 30%
1	B	842	19% 59% 11% 30%

2 Entry composition (i)

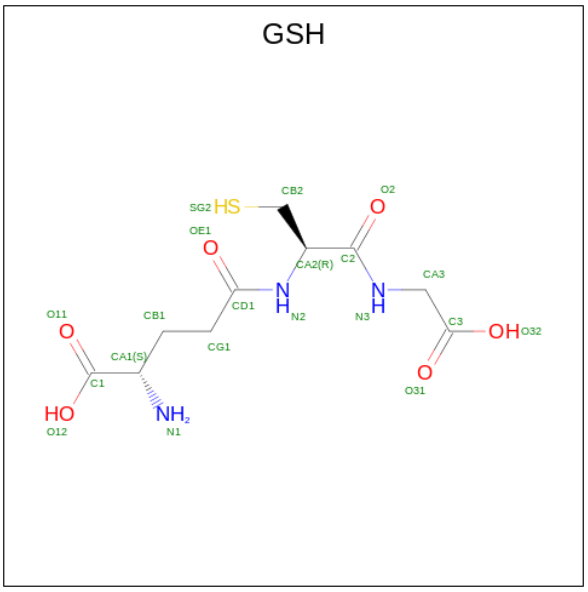
There are 4 unique types of molecules in this entry. The entry contains 9671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-binding cassette sub-family B member 6, mitochondrial.

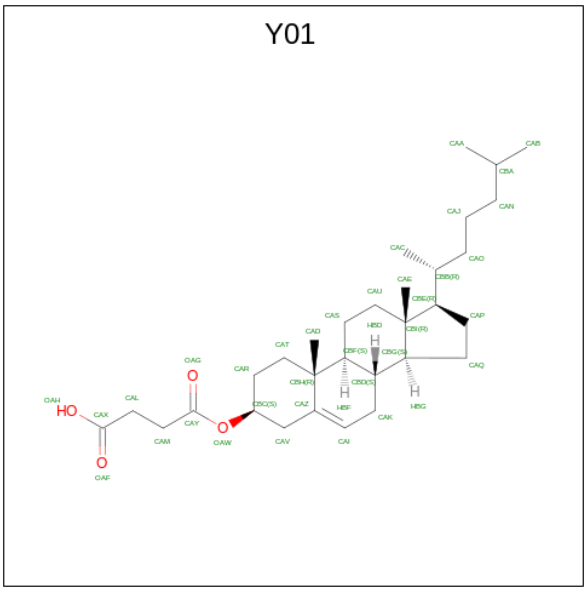
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	591	4669	2998	809	845	17	0	0
1	B	591	4669	2998	809	845	17	0	0

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



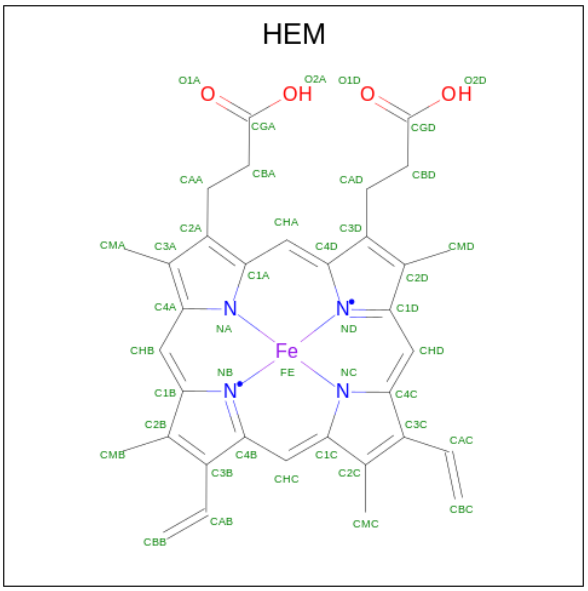
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	20	10	3	6	1	0
2	A	1	20	10	3	6	1	0
2	B	1	20	10	3	6	1	0
2	B	1	20	10	3	6	1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	35	31	4	0
			Total	C	O	
3	A	1	35	31	4	0
			Total	C	O	
3	A	1	35	31	4	0
			Total	C	O	
3	B	1	35	31	4	0
			Total	C	O	
3	B	1	35	31	4	0
			Total	C	O	
3	B	1	35	31	4	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



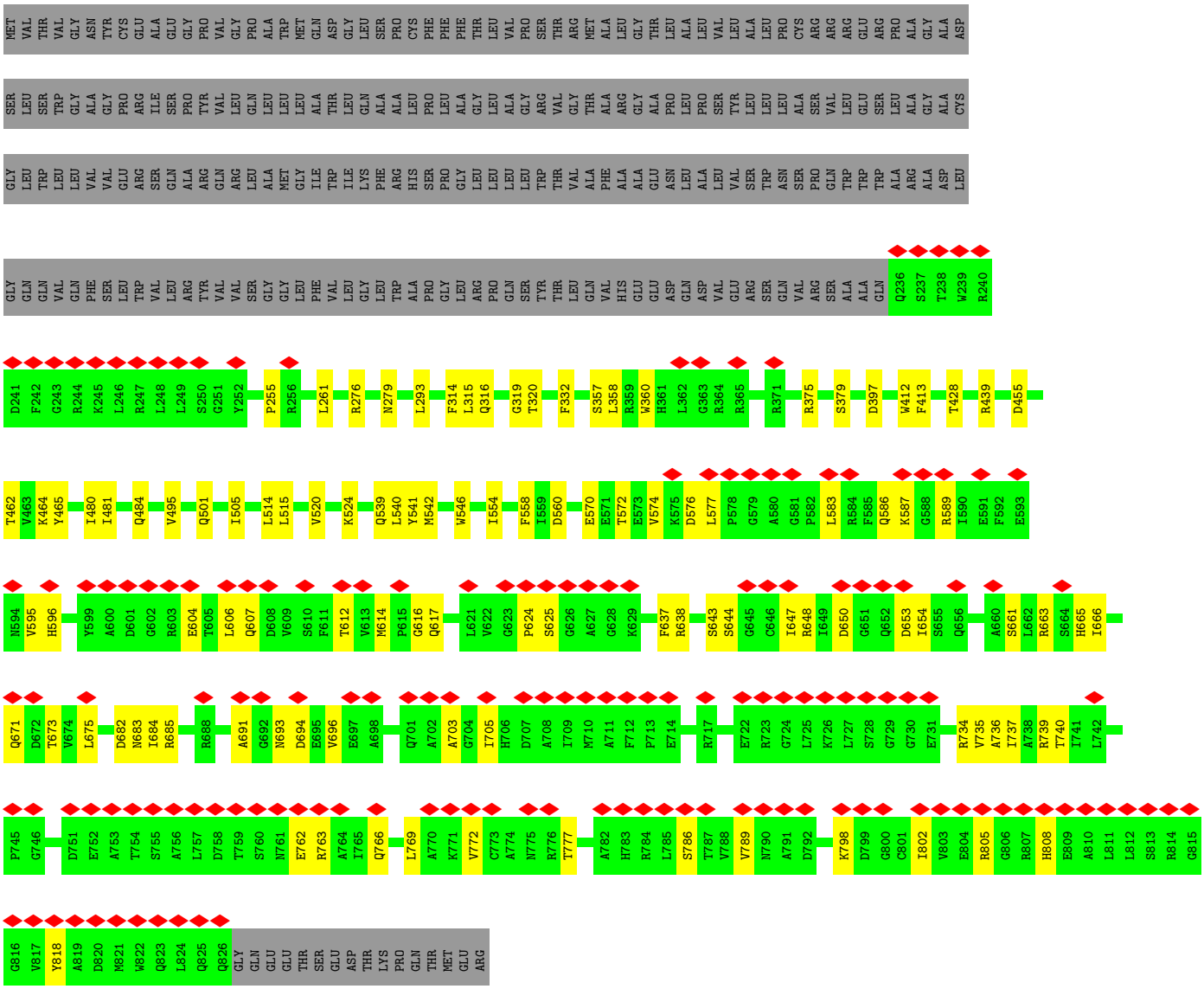
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
4	B	1	43	34	1	4	4	0

3 Residue-property plots (i)

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

- Molecule 1: ATP-binding cassette sub-family B member 6, mitochondrial

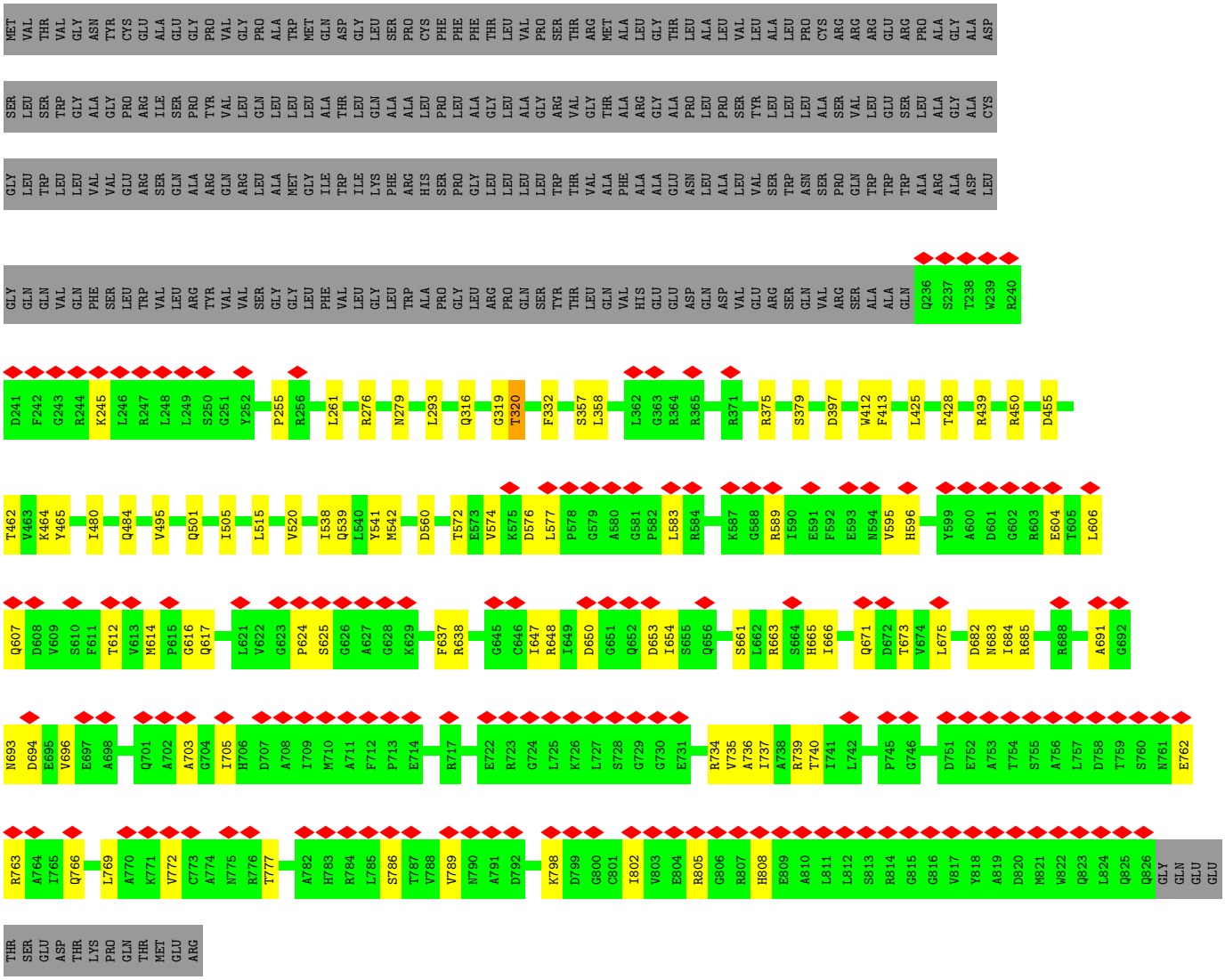
Chain A:



- Molecule 1: ATP-binding cassette sub-family B member 6, mitochondrial

Chain B:

19%
59%
11%
30%


MET VAL THR VAL GLY ASN TYR CYS GLU ALA GLU GLY PRO VAL GLY PRO ALA TRP MET GLN ASP GLY LEU SER PRO CYS PHE PHE PHE THR LEU VAL PRO SER THR ARG MET ALA LEU GLY THR LEU ALA LEU VAL LEU ALA LEU PRO CYS ARG ARG ARG GLU ARG PRO ALA GLY ALA ASP
SER LEU SER TRP GLY ALA GLY PRO ARG ILE SER PRO TYR VAL LEU GLN LEU LEU LEU ALA THR LEU GLN ALA ALA LEU PRO LEU ALA GLY LEU ALA GLY ARG VAL GLY THR ALA ARG GLY ALA PRO LEU PRO SER TYR LEU LEU LEU ALA SER VAL LEU GLU SER LEU ALA GLY ALA CYS
GLY LEU TRP LEU LEU VAL VAL GLU ARG SER SER GLN ALA ARG GLN ARG LEU ALA MET GLY ILE TRP ILE LYS PHE ARG HIS SER PRO GLY LEU LEU LEU LEU TRP THR VAL ALA PHE ALA ALA GLU ASN LEU ALA LEU VAL SER TRP ASN SER PRO GLN TRP TRP TRP ALA ARG ALA ASP LEU
GLY GLN GLN VAL GLN PHE SER LEU TRP VAL LEU ARG TYR VAL VAL SER GLY GLY LEU PHE VAL LEU GLY LEU TRP ALA PRO GLY LEU ARG PRO GLN SER TYR THR LEU GLN VAL HIS GLU GLU ASP GLN ASP VAL GLU ARG SER GLN VAL ARG SER ALA ALA GLN Q236 S237 T238 W239 R240
D241 F242 G243 R244 K245 L246 R247 L248 L249 S250 G251 Y252 P255 R256 L261 R276 N279 L293 Q316 G319 T320 F332 S357 L358 L362 G363 R364 R365 R371 R375 S379 D397 W412 F413 L425 T428 R439 R450 D455
T462 V463 K464 Y465 I480 Q484 V495 Q501 I505 L515 V520 I538 Q539 L540 Y541 M542 D560 T572 E573 V574 K575 D576 L577 P578 G579 A580 G581 P582 L583 R584 K587 G588 R589 I590 E591 F592 E593 N594 V595 H596 Y599 A600 D601 G602 R603 E604 T605 L606
Q607 D608 V609 S610 F611 T612 V613 M614 P615 G616 Q617 L621 V622 G623 P624 S625 G626 A627 G628 K629 F637 R638 G645 C646 I647 R648 I649 D650 G651 Q652 D653 I654 S655 Q656 S661 L662 R663 S664 H665 I666 Q671 D672 T673 V674 L675 D682 N683 I684 R685 R688 A691 G692
N693 D694 E695 V696 E697 A698 Q701 A702 A703 G704 I705 H706 D707 A708 I709 M710 A711 F712 P713 E714 R717 E722 R723 G724 L725 K726 L727 S728 G729 G730 E731 R734 V735 A736 I737 A738 R739 T740 I741 L742 P745 G746 D751 E752 A753 T754 S755 A756 L757 D758 T759 S760 N761 E762
R763 A764 I765 Q766 L769 A770 K771 V772 C773 A774 N775 R776 T777 A782 H783 R784 L785 S786 T787 V788 V789 N790 A791 D792 K798 D799 G800 C801 I802 V803 E804 R805 G806 R807 H808 E809 A810 L811 L812 S813 R814 G815 G816 V817 Y818 A819 D820 M821 W822 Q823 L824 Q825 Q826 GLY GLN GLU GLU
THR SER GLU ASP THR LYS PRO GLN THR MET GLU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283866	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.223	Depositor
Minimum map value	-0.849	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.306	Depositor
Map size (Å)	232.4, 232.4, 232.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: Y01, GSH, HEM

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	0.47	0/4760	0.62	0/6456
1	B	0.47	0/4760	0.61	0/6456
All	All	0.47	0/9520	0.61	0/12912

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	A	4669	0	4726	77	0
1	B	4669	0	4726	71	0
2	A	40	0	30	1	0
2	B	40	0	30	0	0
3	A	105	0	147	2	0
3	B	105	0	147	2	0
4	B	43	0	30	0	0
All	All	9671	0	9836	137	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 7.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:HH21	1:B:279:ASN:HD22	1.40	0.69
1:A:276:ARG:HH21	1:A:279:ASN:HD22	1.40	0.69
1:A:638:ARG:NH1	1:A:654:ILE:O	2.30	0.64
1:B:638:ARG:NH1	1:B:654:ILE:O	2.30	0.64
1:A:542:MET:CE	1:B:319:GLY:HA3	2.29	0.63
1:A:542:MET:HE1	1:B:319:GLY:HA3	1.82	0.61
1:B:428:THR:OG1	1:B:501:GLN:NE2	2.36	0.58
1:A:428:THR:OG1	1:A:501:GLN:NE2	2.36	0.58
1:A:703:ALA:O	1:A:734:ARG:NH1	2.37	0.58
1:B:703:ALA:O	1:B:734:ARG:NH1	2.37	0.57
1:A:589:ARG:NH2	1:A:612:THR:OG1	2.38	0.57
1:B:589:ARG:NH2	1:B:612:THR:OG1	2.38	0.56
1:B:683:ASN:O	1:B:739:ARG:NH2	2.38	0.56
1:A:673:THR:HG21	1:A:736:ALA:HB2	1.88	0.56
1:B:673:THR:HG21	1:B:736:ALA:HB2	1.88	0.56
1:A:320:THR:HG23	1:A:542:MET:HB3	1.88	0.55
1:A:319:GLY:HA3	1:B:542:MET:CE	2.36	0.55
1:B:763:ARG:HA	1:B:766:GLN:HB2	1.89	0.55
1:A:683:ASN:O	1:A:739:ARG:NH2	2.38	0.55
1:A:625:SER:O	1:A:798:LYS:NZ	2.40	0.54
1:B:625:SER:O	1:B:798:LYS:NZ	2.40	0.54
1:B:648:ARG:HG2	1:B:653:ASP:HA	1.90	0.54
1:A:682:ASP:HA	1:A:685:ARG:HB2	1.90	0.54
1:A:648:ARG:HG2	1:A:653:ASP:HA	1.90	0.53
1:A:763:ARG:HA	1:A:766:GLN:HB2	1.89	0.53
1:A:684:ILE:HG22	1:A:735:VAL:HG13	1.91	0.53
1:B:279:ASN:OD1	1:B:539:GLN:NE2	2.42	0.52
1:A:279:ASN:OD1	1:A:539:GLN:NE2	2.43	0.52
1:B:595:VAL:HG21	1:B:647:ILE:HG13	1.91	0.52
1:A:693:ASN:OD1	1:A:694:ASP:N	2.42	0.52
1:B:682:ASP:HA	1:B:685:ARG:HB2	1.90	0.52
1:A:595:VAL:HG21	1:A:647:ILE:HG13	1.91	0.52
1:B:693:ASN:OD1	1:B:694:ASP:N	2.42	0.52
1:B:684:ILE:HG22	1:B:735:VAL:HG13	1.91	0.52
1:A:332:PHE:HB2	1:B:495:VAL:HG21	1.92	0.51
1:A:495:VAL:HG21	1:B:332:PHE:HB2	1.94	0.50
1:A:808:HIS:ND1	1:A:818:TYR:OH	2.30	0.50
1:B:675:LEU:HD11	1:B:683:ASN:HB3	1.94	0.50
1:B:576:ASP:N	1:B:576:ASP:OD1	2.45	0.50
1:A:576:ASP:N	1:A:576:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:SER:HA	1:B:789:VAL:HG22	1.94	0.49
1:A:675:LEU:HD11	1:A:683:ASN:HB3	1.94	0.49
1:A:786:SER:HA	1:A:789:VAL:HG22	1.95	0.49
1:B:357:SER:OG	1:B:358:LEU:N	2.46	0.48
1:A:357:SER:OG	1:A:358:LEU:N	2.46	0.48
1:A:319:GLY:HA3	1:B:542:MET:HE1	1.97	0.47
1:A:589:ARG:N	1:A:650:ASP:OD1	2.39	0.47
1:B:663:ARG:HA	1:B:666:ILE:HG22	1.96	0.47
1:A:314:PHE:HD2	1:A:315:LEU:HD12	1.80	0.47
1:A:546:TRP:HH2	1:B:320:THR:HG21	1.80	0.47
1:B:589:ARG:N	1:B:650:ASP:OD1	2.39	0.47
3:A:904:Y01:HAO1	3:A:904:Y01:HAP1	1.58	0.46
1:A:375:ARG:HB3	1:A:560:ASP:OD2	2.15	0.46
1:B:375:ARG:HB3	1:B:560:ASP:OD2	2.15	0.46
1:A:663:ARG:HA	1:A:666:ILE:HG22	1.97	0.46
1:A:694:ASP:N	1:A:694:ASP:OD1	2.49	0.46
1:A:293:LEU:HD11	1:B:520:VAL:HG13	1.98	0.45
1:A:685:ARG:NH1	1:A:691:ALA:O	2.49	0.45
1:B:694:ASP:N	1:B:694:ASP:OD1	2.49	0.45
1:A:375:ARG:O	1:A:379:SER:HB3	2.16	0.45
1:B:685:ARG:NH1	1:B:691:ALA:O	2.49	0.45
1:A:480:ILE:O	1:A:484:GLN:HG2	2.17	0.45
1:A:520:VAL:HG13	1:B:293:LEU:HD11	1.99	0.45
3:B:905:Y01:HAO1	3:B:905:Y01:HAP1	1.60	0.45
1:A:614:MET:H	1:A:617:GLN:HG3	1.82	0.44
1:A:505:ILE:HG13	1:A:541:TYR:CD1	2.53	0.44
1:A:637:PHE:CE2	1:A:663:ARG:HG3	2.52	0.44
1:B:375:ARG:O	1:B:379:SER:HB3	2.17	0.44
1:B:505:ILE:HG13	1:B:541:TYR:CD1	2.53	0.44
1:B:637:PHE:CE2	1:B:663:ARG:HG3	2.53	0.44
1:B:413:PHE:HE1	1:B:515:LEU:HD22	1.83	0.44
1:B:604:GLU:OE2	1:B:607:GLN:NE2	2.51	0.44
1:B:614:MET:H	1:B:617:GLN:HG3	1.82	0.44
1:A:413:PHE:HE1	1:A:515:LEU:HD22	1.83	0.44
1:B:480:ILE:O	1:B:484:GLN:HG2	2.17	0.44
1:A:439:ARG:HE	1:A:439:ARG:HB2	1.64	0.44
1:A:737:ILE:HA	1:A:740:THR:HG22	2.00	0.44
1:A:572:THR:HG22	1:A:574:VAL:HG13	2.00	0.43
1:A:604:GLU:OE2	1:A:607:GLN:NE2	2.51	0.43
1:A:624:PRO:HB2	1:A:798:LYS:HD3	1.99	0.43
1:A:661:SER:O	1:A:665:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:HD13	1:A:481:ILE:HA	1.90	0.43
1:A:542:MET:HE3	1:B:319:GLY:HA3	1.98	0.43
1:B:769:LEU:HA	1:B:772:VAL:HG12	1.99	0.43
1:A:464:LYS:HD2	1:A:464:LYS:HA	1.89	0.43
1:A:769:LEU:HA	1:A:772:VAL:HG12	2.00	0.43
1:B:624:PRO:HB2	1:B:798:LYS:HD3	1.99	0.43
1:B:671:GLN:NE2	1:B:671:GLN:HA	2.34	0.43
1:B:737:ILE:HA	1:B:740:THR:HG22	2.00	0.43
1:A:671:GLN:NE2	1:A:671:GLN:HA	2.34	0.42
1:B:245:LYS:H	1:B:245:LYS:HG3	1.68	0.42
1:A:293:LEU:HD21	1:B:520:VAL:HG11	2.01	0.42
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.84	0.42
1:A:413:PHE:CE1	1:A:515:LEU:HD22	2.54	0.42
1:A:520:VAL:HG11	1:B:293:LEU:HD21	2.01	0.42
1:B:538:ILE:HD13	1:B:538:ILE:HA	1.91	0.42
1:B:577:LEU:HD23	1:B:577:LEU:HA	1.95	0.42
1:B:661:SER:O	1:B:665:HIS:ND1	2.51	0.42
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.92	0.42
1:A:540:LEU:HA	1:A:540:LEU:HD23	1.82	0.41
1:B:413:PHE:CE1	1:B:515:LEU:HD22	2.54	0.41
1:B:762:GLU:OE1	1:B:763:ARG:NH2	2.54	0.41
1:A:524:LYS:HE2	1:A:524:LYS:HB3	1.92	0.41
1:B:693:ASN:HA	1:B:696:VAL:HG12	2.02	0.41
1:B:439:ARG:HE	1:B:439:ARG:HB2	1.64	0.41
1:B:572:THR:HG22	1:B:574:VAL:HG13	2.00	0.41
1:A:279:ASN:ND2	1:A:397:ASP:OD1	2.53	0.41
1:A:319:GLY:HA3	1:B:542:MET:HE3	2.03	0.41
1:B:255:PRO:HG2	1:B:261:LEU:HB3	2.02	0.41
1:B:462:THR:HA	1:B:465:TYR:HD1	1.86	0.41
1:A:762:GLU:OE1	1:A:763:ARG:NH2	2.54	0.41
1:B:412:TRP:CD2	3:B:905:Y01:HAI	2.55	0.41
1:B:705:ILE:HG13	1:B:734:ARG:HD3	2.02	0.41
1:A:586:GLN:HG2	1:A:587:LYS:HD3	2.03	0.41
2:A:902:GSH:HN2	1:B:450:ARG:HG3	1.85	0.41
1:B:616:GLY:H	1:B:777:THR:HG22	1.86	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.95	0.41
1:A:596:HIS:HA	1:A:606:LEU:HB3	2.03	0.41
1:B:450:ARG:HD3	1:B:450:ARG:HA	1.87	0.41
1:B:464:LYS:HA	1:B:464:LYS:HD2	1.89	0.41
1:B:596:HIS:HA	1:B:606:LEU:HB3	2.03	0.41
1:B:789:VAL:HG12	1:B:808:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TRP:NE1	1:A:570:GLU:OE2	2.44	0.41
1:A:462:THR:HA	1:A:465:TYR:HD1	1.86	0.41
1:B:279:ASN:ND2	1:B:397:ASP:OD1	2.53	0.41
1:B:425:LEU:HA	1:B:425:LEU:HD23	1.88	0.41
1:B:583:LEU:HD22	1:B:665:HIS:CG	2.56	0.41
1:B:802:ILE:HD11	1:B:805:ARG:HD2	2.03	0.41
1:A:693:ASN:HA	1:A:696:VAL:HG12	2.02	0.40
1:A:643:SER:OG	1:A:644:SER:N	2.54	0.40
1:A:583:LEU:HD22	1:A:665:HIS:CG	2.56	0.40
1:A:255:PRO:HG2	1:A:261:LEU:HB3	2.02	0.40
1:A:412:TRP:CE2	3:A:904:Y01:HAI	2.57	0.40
1:A:554:ILE:O	1:A:558:PHE:HB2	2.22	0.40
1:A:616:GLY:H	1:A:777:THR:HG22	1.86	0.40
1:A:705:ILE:HG13	1:A:734:ARG:HD3	2.02	0.40
1:A:802:ILE:HD11	1:A:805:ARG:HD2	2.03	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	589/842 (70%)	563 (96%)	26 (4%)	0	100	100
1	B	589/842 (70%)	561 (95%)	28 (5%)	0	100	100
All	All	1178/1684 (70%)	1124 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/701 (71%)	496 (100%)	2 (0%)	91 97
1	B	498/701 (71%)	495 (99%)	3 (1%)	86 94
All	All	996/1402 (71%)	991 (100%)	5 (0%)	89 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	455	ASP
1	B	316	GLN
1	B	320	THR
1	B	455	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	316	GLN
1	A	328	ASN
1	A	539	GLN
1	B	279	ASN
1	B	328	ASN
1	B	539	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)

11 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	$\#\|Z\| > 2$
3	Y01	A	905	-	38,38,38	0.44	0	57,57,57	0.64	1 (1%)
3	Y01	A	903	-	38,38,38	0.47	0	57,57,57	0.66	0
2	GSH	A	901	-	18,19,19	0.69	0	23,24,24	0.71	0
3	Y01	B	906	-	38,38,38	0.47	0	57,57,57	0.67	0
3	Y01	B	904	-	38,38,38	0.46	0	57,57,57	0.66	0
2	GSH	B	903	-	18,19,19	0.69	0	23,24,24	0.69	0
3	Y01	B	905	-	38,38,38	0.49	0	57,57,57	0.68	1 (1%)
4	HEM	B	901	-	41,50,50	1.34	7 (17%)	45,82,82	1.83	8 (17%)
3	Y01	A	904	-	38,38,38	0.49	0	57,57,57	0.66	1 (1%)
2	GSH	B	902	-	18,19,19	0.70	0	23,24,24	0.72	0
2	GSH	A	902	-	18,19,19	0.70	0	23,24,24	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
3	Y01	A	905	-	-	10/19/77/77	0/4/4/4
3	Y01	A	903	-	-	4/19/77/77	0/4/4/4
2	GSH	A	901	-	-	13/24/24/24	-
3	Y01	B	906	-	-	2/19/77/77	0/4/4/4
3	Y01	B	904	-	-	8/19/77/77	0/4/4/4
2	GSH	B	903	-	-	4/24/24/24	-
3	Y01	B	905	-	-	6/19/77/77	0/4/4/4
4	HEM	B	901	-	-	2/12/54/54	-
3	Y01	A	904	-	-	6/19/77/77	0/4/4/4
2	GSH	B	902	-	-	15/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	A	902	-	-	3/24/24/24	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	HEM	C4D-ND	-3.59	1.34	1.40
4	B	901	HEM	C1B-NB	-3.46	1.34	1.40
4	B	901	HEM	FE-NB	2.79	2.10	1.96
4	B	901	HEM	CHB-C1B	2.30	1.40	1.35
4	B	901	HEM	C1D-ND	-2.13	1.34	1.38
4	B	901	HEM	FE-ND	-2.09	1.86	1.96
4	B	901	HEM	C4B-NB	-2.04	1.34	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	HEM	CHC-C4B-NB	5.37	130.27	124.43
4	B	901	HEM	C1B-NB-C4B	4.42	109.64	105.07
4	B	901	HEM	CHD-C1D-ND	4.13	128.92	124.43
4	B	901	HEM	CHA-C4D-ND	3.40	128.59	124.38
4	B	901	HEM	CHB-C1B-NB	3.02	128.11	124.38
4	B	901	HEM	C4D-ND-C1D	2.86	108.03	105.07
4	B	901	HEM	CHD-C1D-C2D	-2.34	121.33	124.98
3	A	904	Y01	CAP-CAQ-CBG	-2.09	100.98	105.13
3	B	905	Y01	CAP-CAQ-CBG	-2.09	100.99	105.13
4	B	901	HEM	CMA-C3A-C4A	-2.07	125.29	128.46
3	A	905	Y01	OAW-CBC-CAR	2.01	113.19	108.33

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GSH	O11-C1-CA1-N1
2	A	901	GSH	CG1-CD1-N2-CA2
2	A	902	GSH	O11-C1-CA1-N1
2	B	902	GSH	O11-C1-CA1-N1
2	B	903	GSH	O11-C1-CA1-N1
3	A	903	Y01	OAG-CAY-OAW-CBC
3	A	903	Y01	CAM-CAY-OAW-CBC
3	A	905	Y01	CAV-CBC-OAW-CAY
3	B	904	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	B	904	Y01	CAM-CAY-OAW-CBC
4	B	901	HEM	C2B-C3B-CAB-CBB
3	B	904	Y01	CAC-CBB-CBE-CAP
3	B	904	Y01	CAC-CBB-CBE-CBI
2	A	901	GSH	OE1-CD1-N2-CA2
3	B	904	Y01	CAO-CBB-CBE-CBI
3	B	904	Y01	CAO-CBB-CBE-CAP
2	B	902	GSH	OE1-CD1-N2-CA2
2	B	902	GSH	CG1-CD1-N2-CA2
2	B	902	GSH	O12-C1-CA1-N1
2	A	901	GSH	O12-C1-CA1-N1
2	B	903	GSH	O31-C3-CA3-N3
2	B	903	GSH	O32-C3-CA3-N3
2	B	903	GSH	O12-C1-CA1-N1
3	A	905	Y01	CAM-CAY-OAW-CBC
2	A	902	GSH	O12-C1-CA1-N1
3	B	905	Y01	CAO-CBB-CBE-CBI
3	A	905	Y01	OAG-CAY-OAW-CBC
3	B	905	Y01	CAC-CBB-CBE-CAP
3	A	904	Y01	CAO-CBB-CBE-CBI
4	B	901	HEM	C4B-C3B-CAB-CBB
3	B	905	Y01	CAO-CBB-CBE-CAP
3	A	904	Y01	CAO-CBB-CBE-CAP
3	A	904	Y01	CAC-CBB-CBE-CAP
2	A	901	GSH	O2-C2-CA2-N2
3	A	904	Y01	CAL-CAM-CAY-OAW
3	A	904	Y01	CAC-CBB-CBE-CBI
3	B	905	Y01	CAC-CBB-CBE-CBI
2	A	901	GSH	N3-C2-CA2-N2
3	B	905	Y01	CAL-CAM-CAY-OAW
2	B	902	GSH	O2-C2-CA2-N2
2	B	902	GSH	N3-C2-CA2-N2
3	A	905	Y01	CAL-CAM-CAY-OAW
2	A	901	GSH	N2-CD1-CG1-CB1
2	A	901	GSH	OE1-CD1-CG1-CB1
2	B	902	GSH	OE1-CD1-CG1-CB1
2	A	901	GSH	O11-C1-CA1-CB1
2	A	901	GSH	O12-C1-CA1-CB1
2	B	902	GSH	O11-C1-CA1-CB1
2	B	902	GSH	N1-CA1-CB1-CG1
2	B	902	GSH	O12-C1-CA1-CB1
2	B	902	GSH	N2-CD1-CG1-CB1

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Mol	Chain	Res	Type	Atoms
2	B	902	GSH	O2-C2-N3-CA3
3	B	904	Y01	CAM-CAL-CAX-OAF
3	A	905	Y01	CAC-CBB-CBE-CBI
3	A	903	Y01	CAM-CAL-CAX-OAF
2	A	901	GSH	C2-CA2-CB2-SG2
2	B	902	GSH	C2-CA2-CB2-SG2
3	A	903	Y01	CAM-CAL-CAX-OAH
3	B	904	Y01	CAM-CAL-CAX-OAH
3	A	904	Y01	CAL-CAM-CAY-OAG
3	A	905	Y01	CAO-CBB-CBE-CBI
3	A	905	Y01	CAM-CAL-CAX-OAH
2	A	902	GSH	O2-C2-CA2-N2
3	B	905	Y01	CAL-CAM-CAY-OAG
3	B	906	Y01	CAM-CAL-CAX-OAH
3	A	905	Y01	CAM-CAL-CAX-OAF
3	A	905	Y01	CAL-CAM-CAY-OAG
3	B	906	Y01	CAM-CAL-CAX-OAF
2	A	901	GSH	C1-CA1-CB1-CG1
2	B	902	GSH	C1-CA1-CB1-CG1
3	A	905	Y01	CAO-CBB-CBE-CAP
2	B	902	GSH	CA2-C2-N3-CA3
2	A	901	GSH	N1-CA1-CB1-CG1

There are no ring outliers.

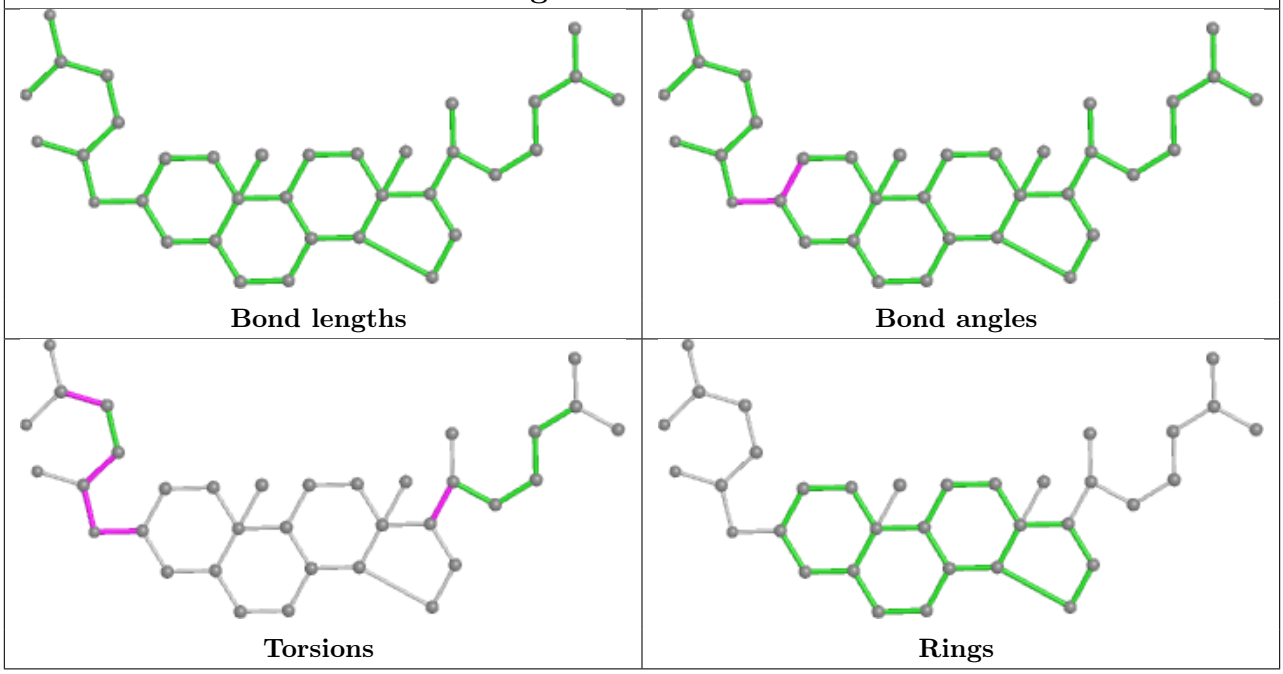
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	905	Y01	2	0
3	A	904	Y01	2	0
2	A	902	GSH	1	0

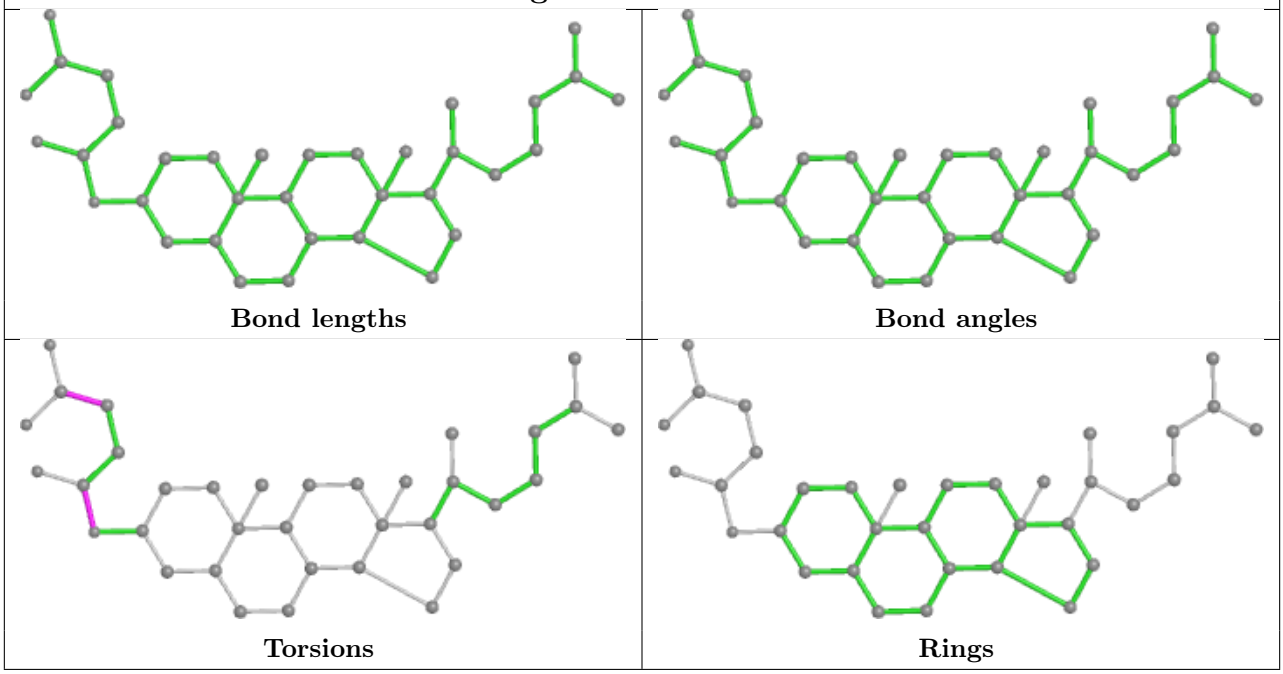
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

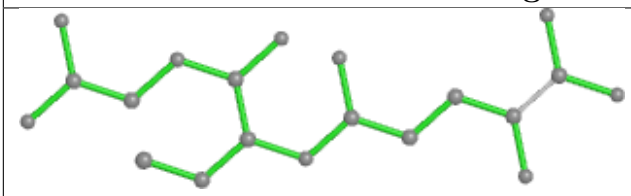
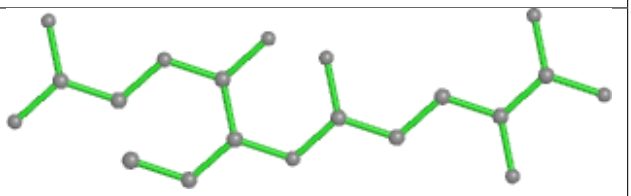
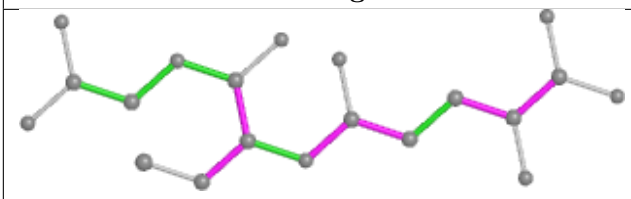
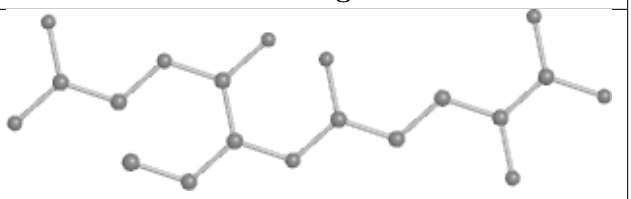
equivalents in the CSD to analyse the geometry.

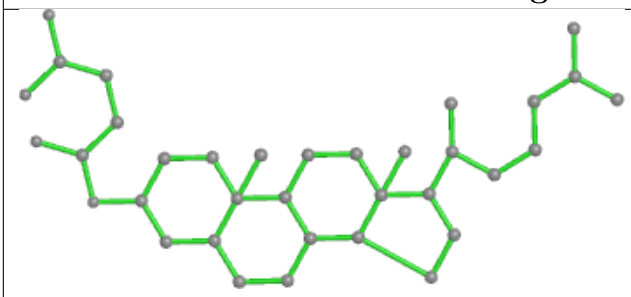
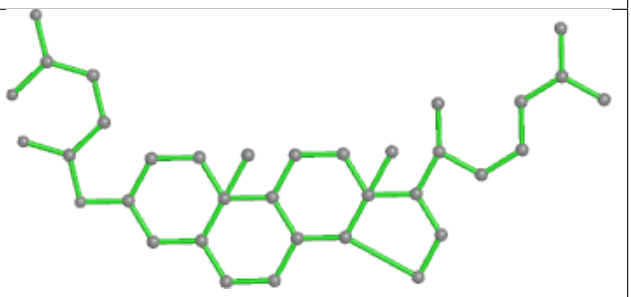
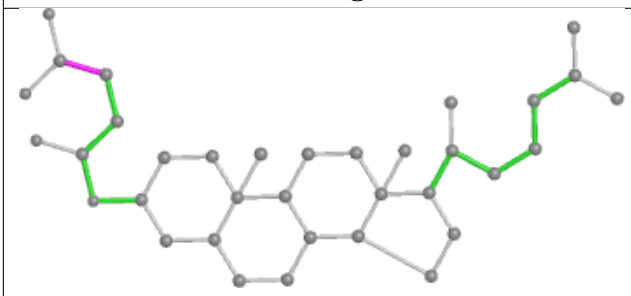
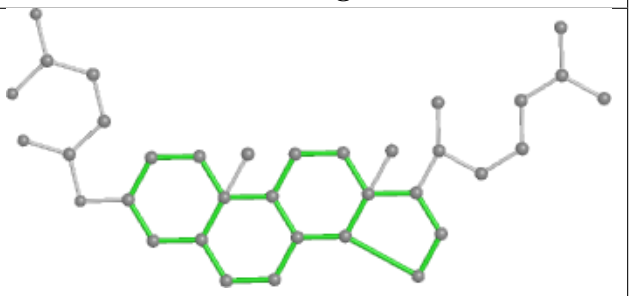
Ligand Y01 A 905



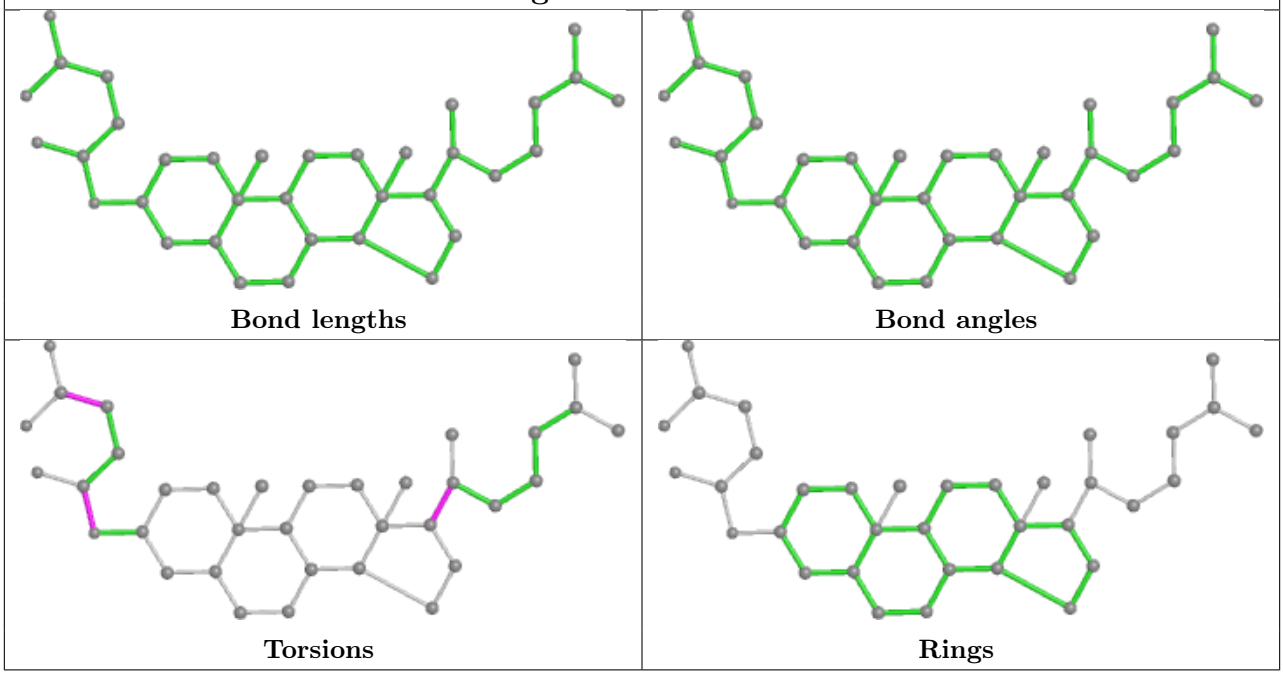
Ligand Y01 A 903



Ligand GSH A 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

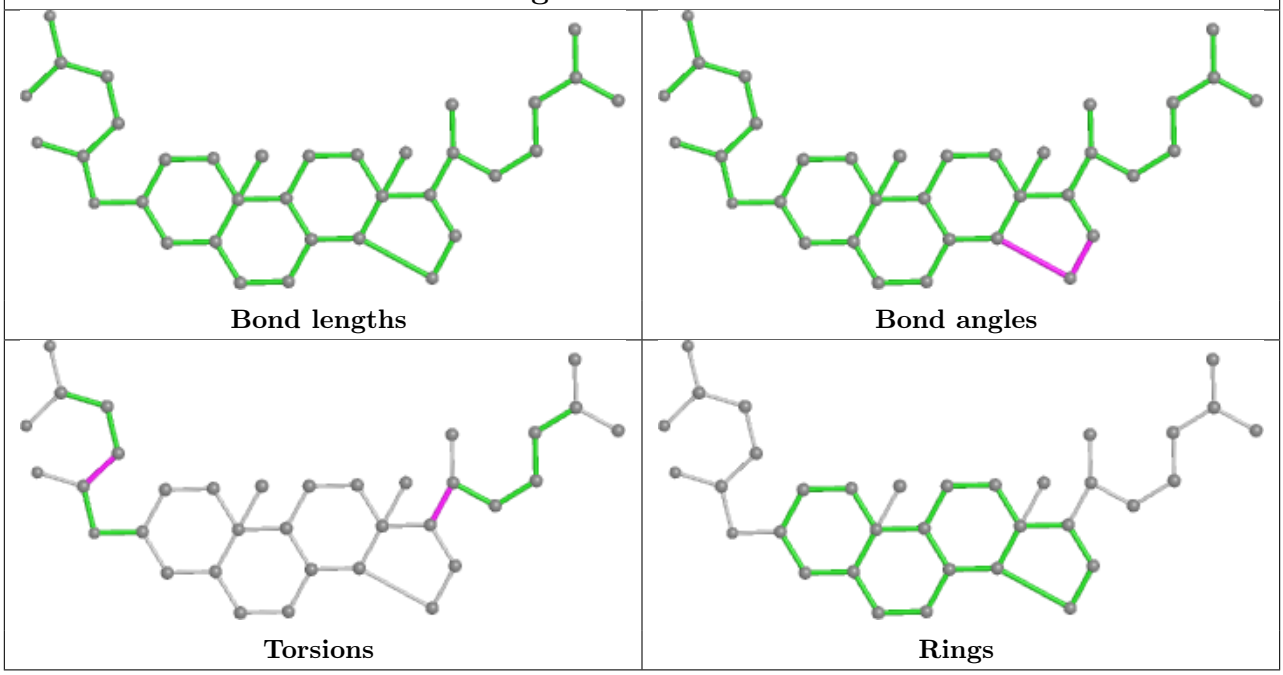
Ligand Y01 B 906	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 B 904

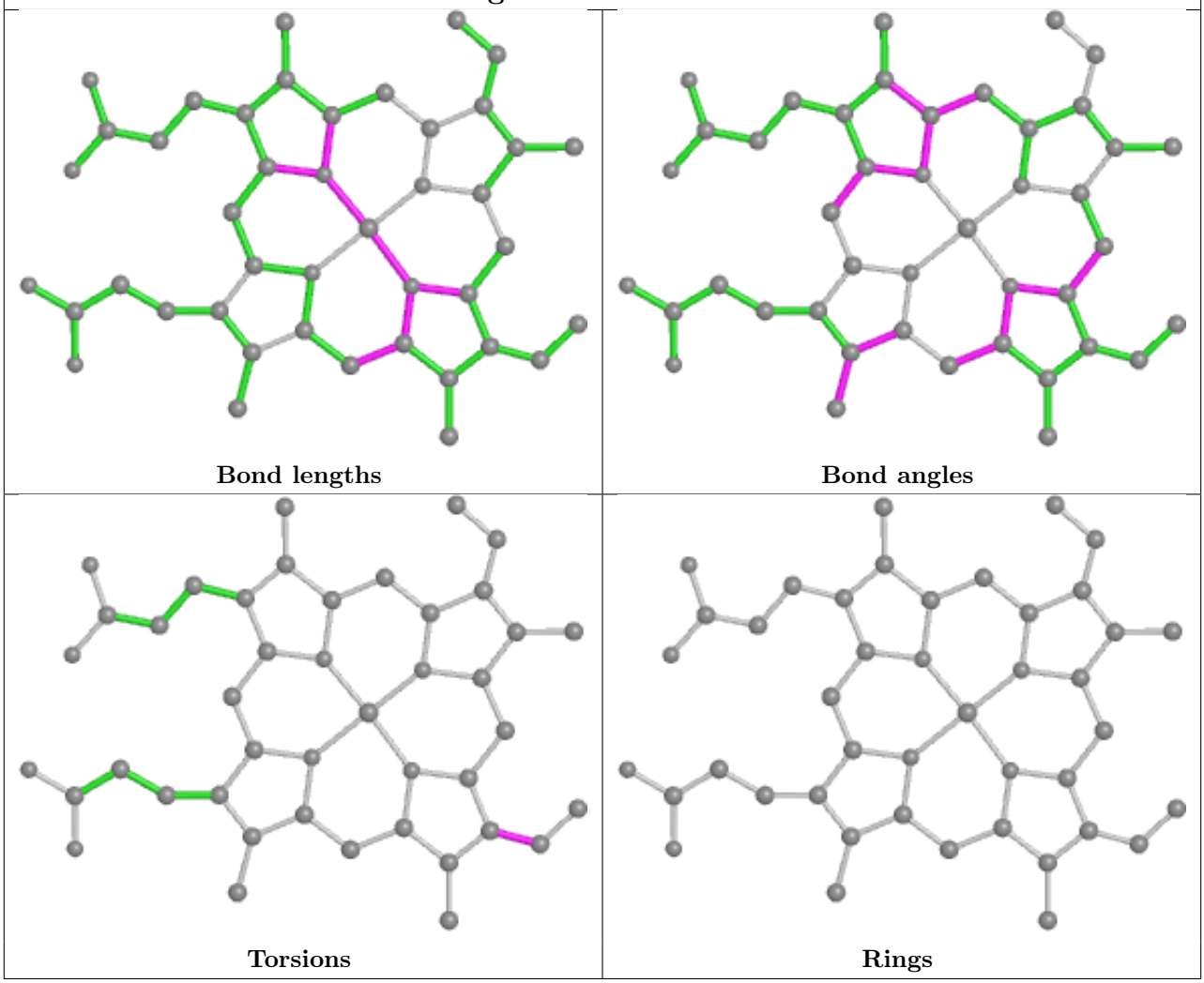


Ligand GSH B 903

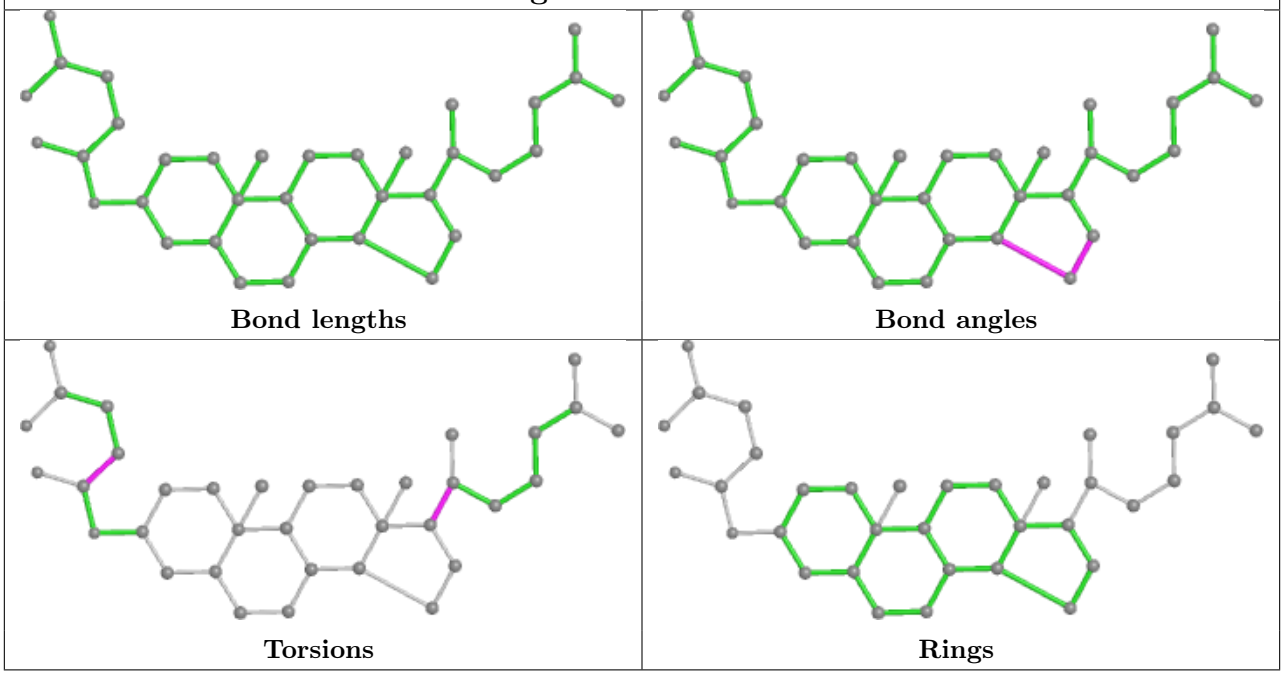
Ligand Y01 B 905



Ligand HEM B 901



Ligand Y01 A 904



Ligand GSH B 902

Ligand GSH A 902

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.

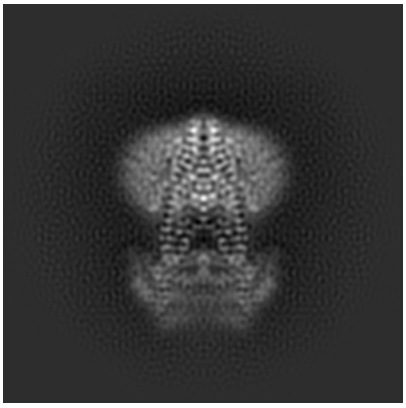
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30791. 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



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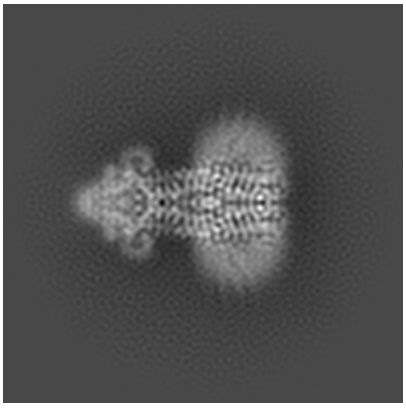
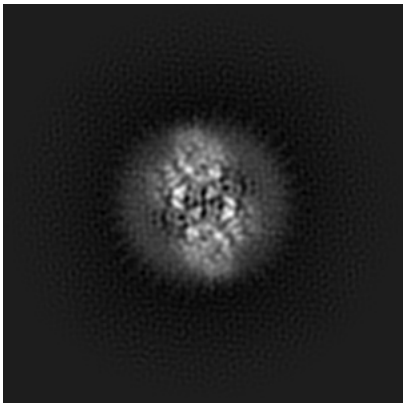


Y

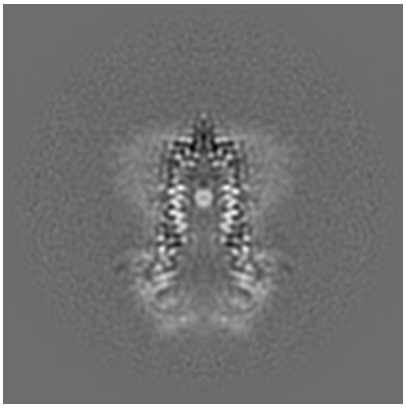


Z

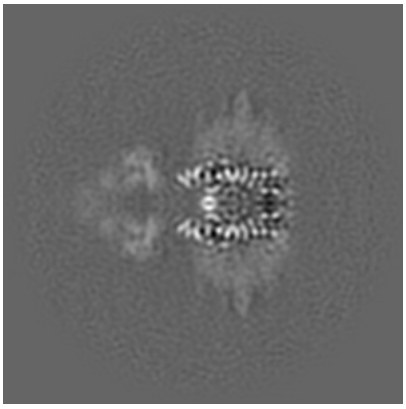
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

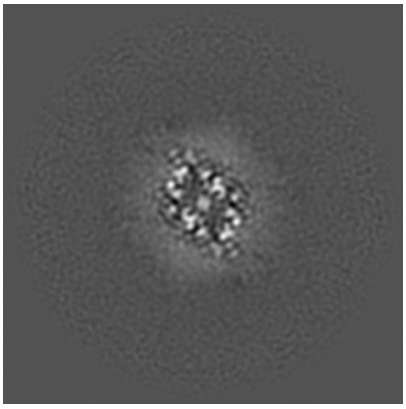
6.2.1 Primary map



X Index: 140



Y Index: 140

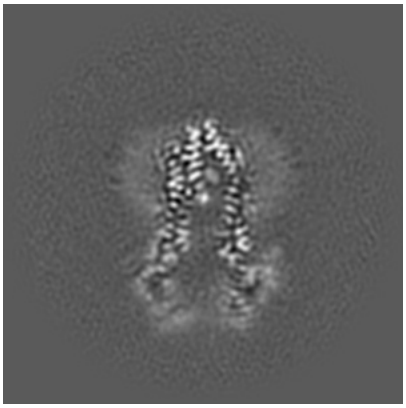


Z Index: 140

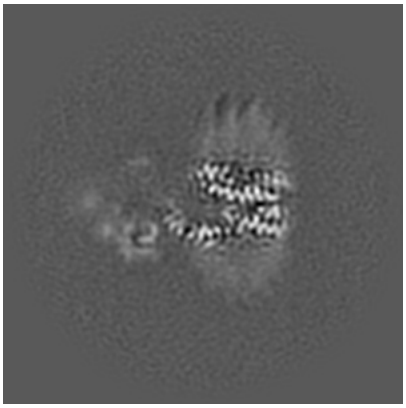
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

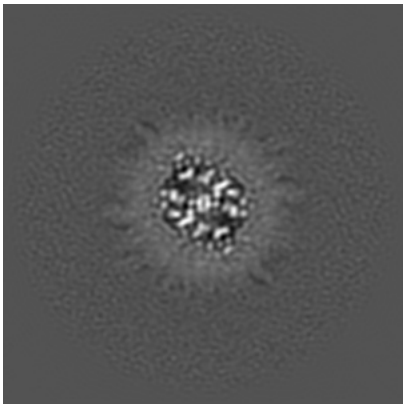
6.3.1 Primary map



X Index: 136



Y Index: 147

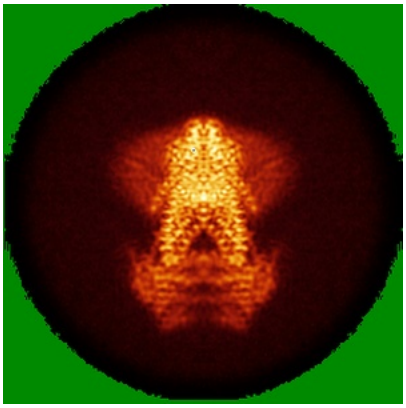


Z Index: 145

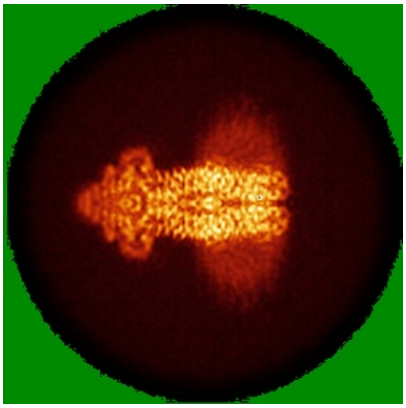
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

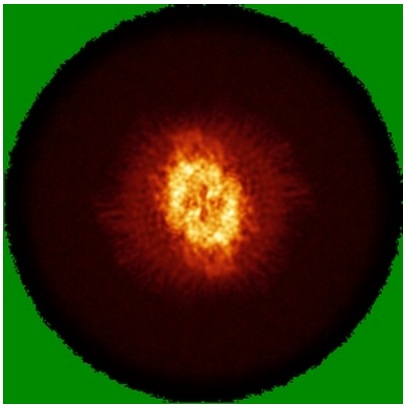
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.306. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

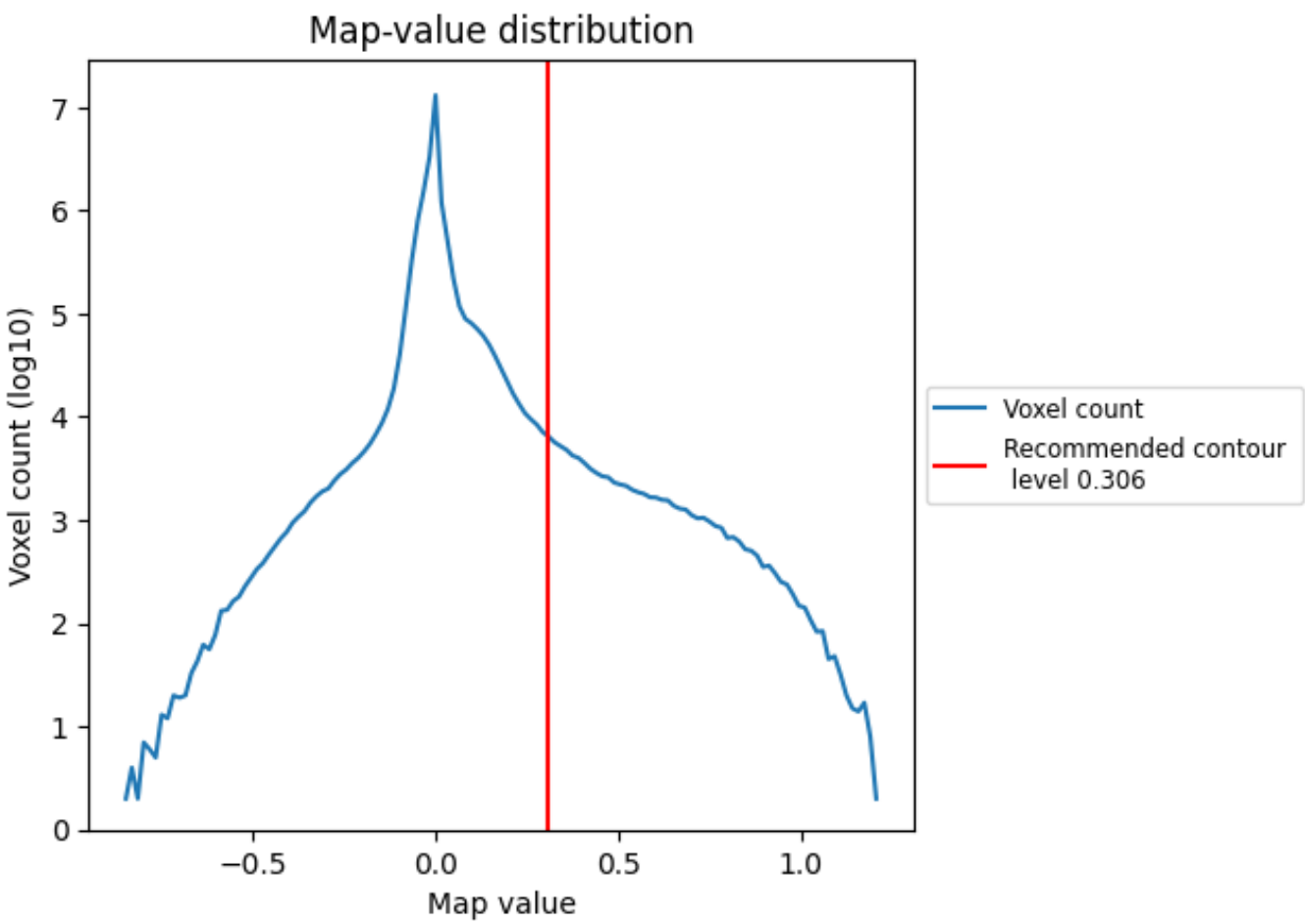
6.6 Mask visualisation (i)

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

7 Map analysis (i)

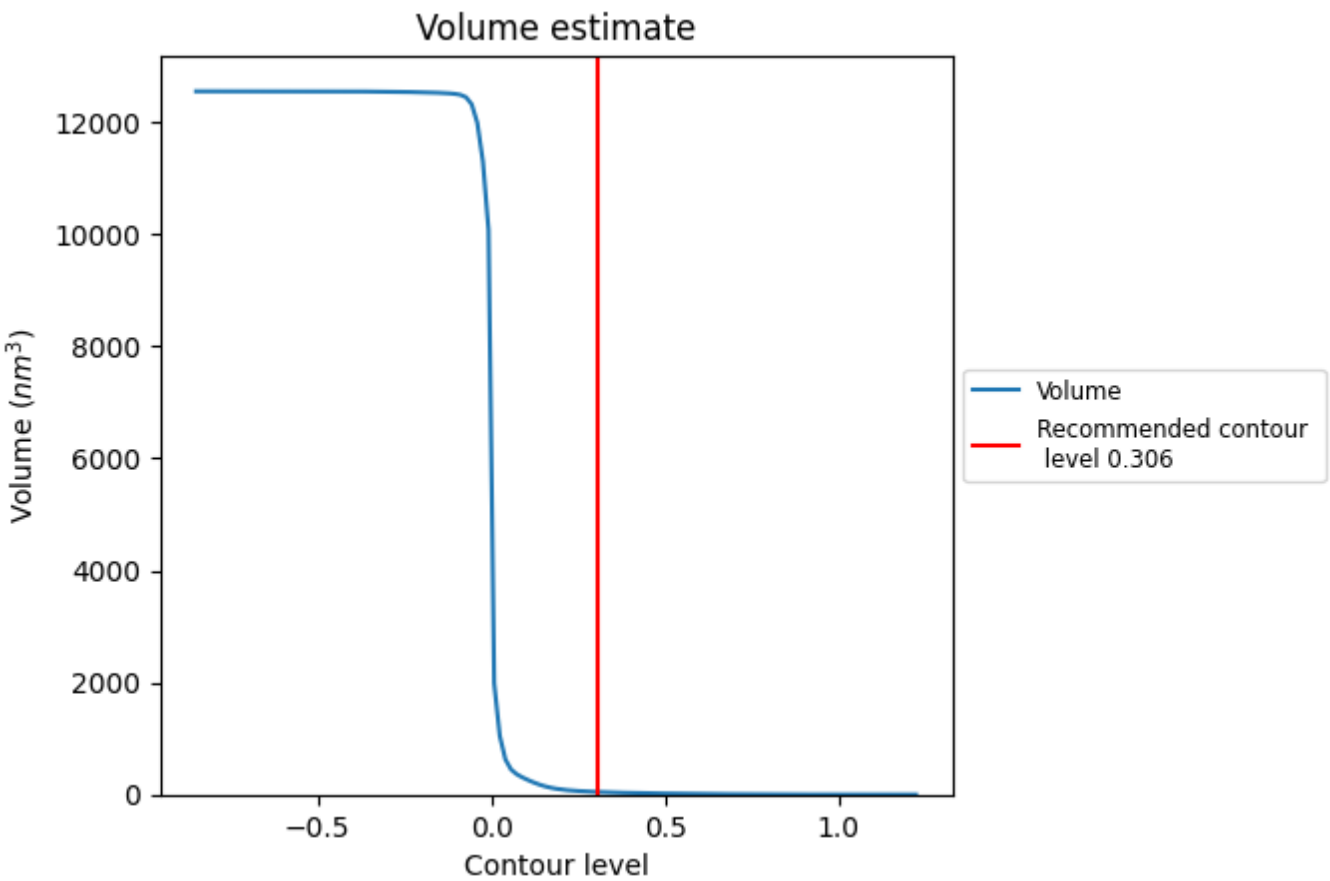
This section contains the results of statistical analysis of the map.

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.

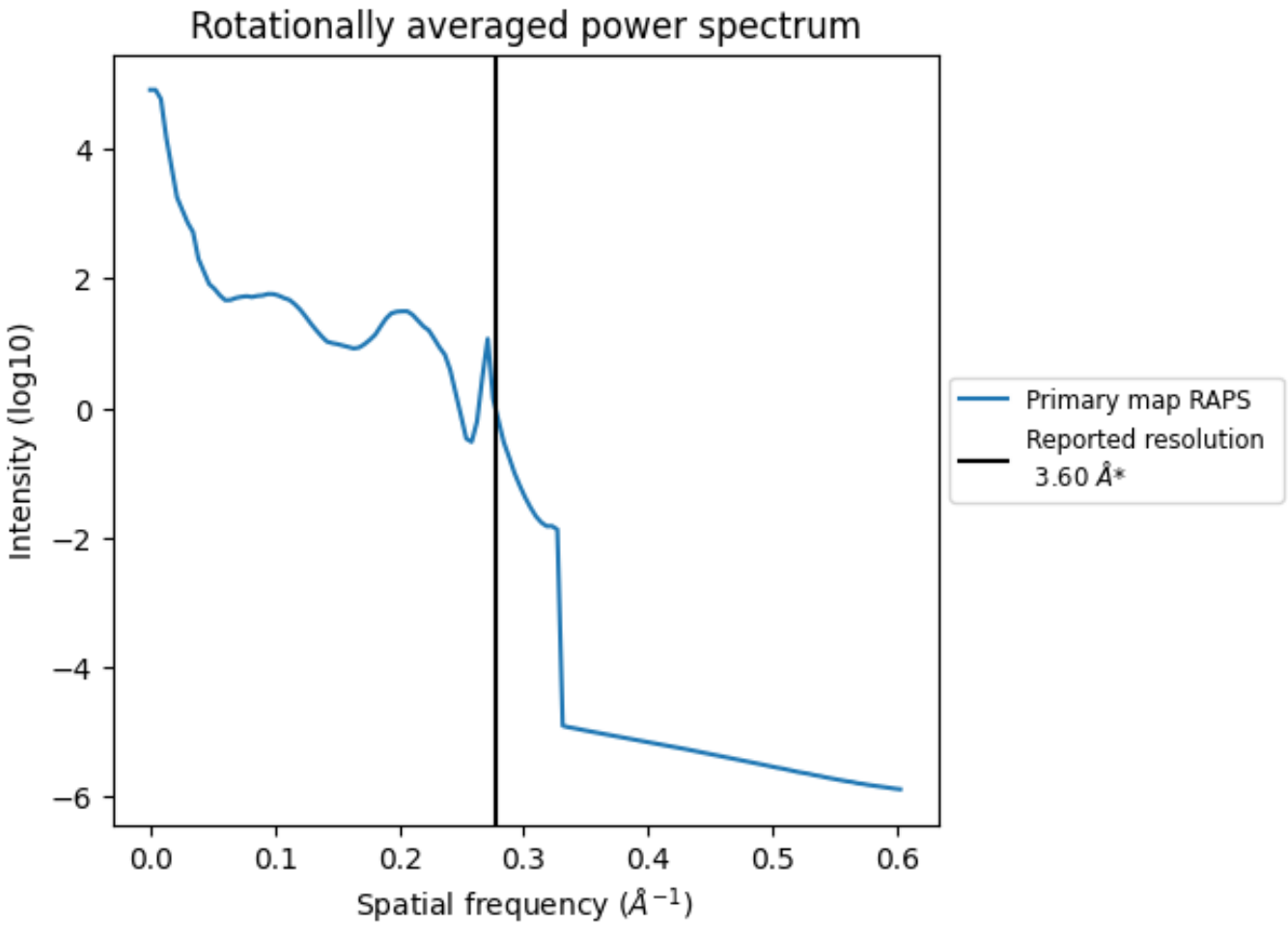
7.2 Volume estimate (i)



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 42 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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

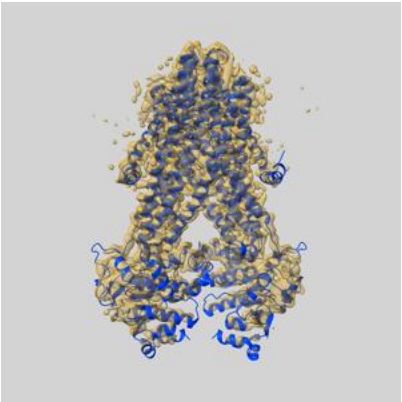
8 Fourier-Shell correlation (i)

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

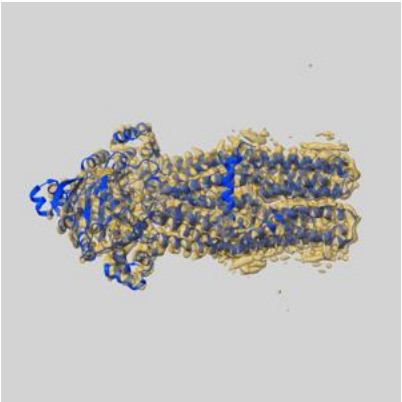
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30791 and PDB model 7DNZ. Per-residue inclusion information can be found in section 3 on page 6.

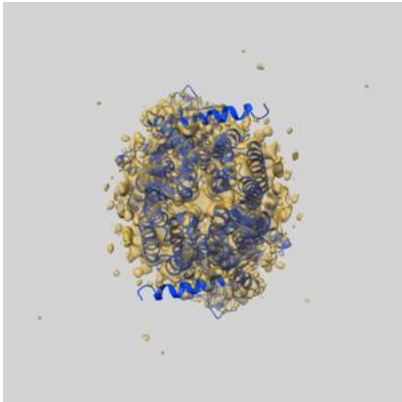
9.1 Map-model overlay (i)



X



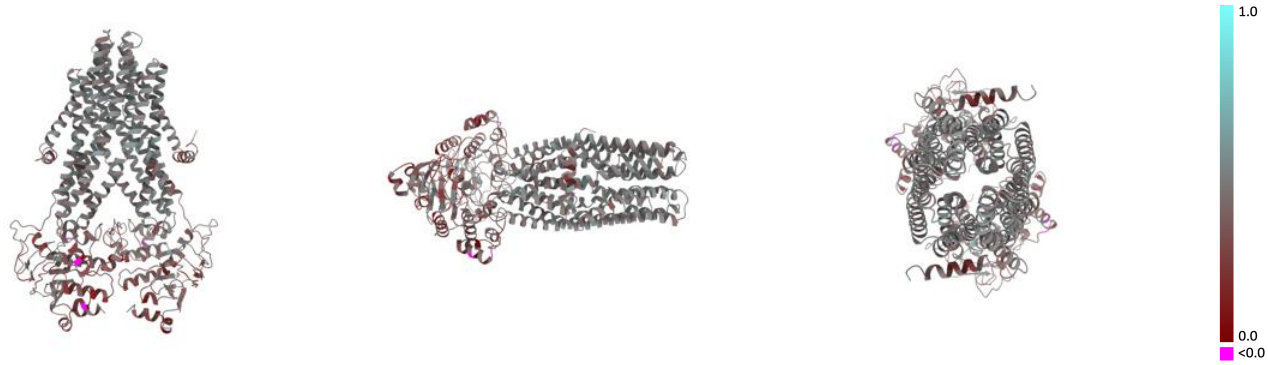
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.306 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.

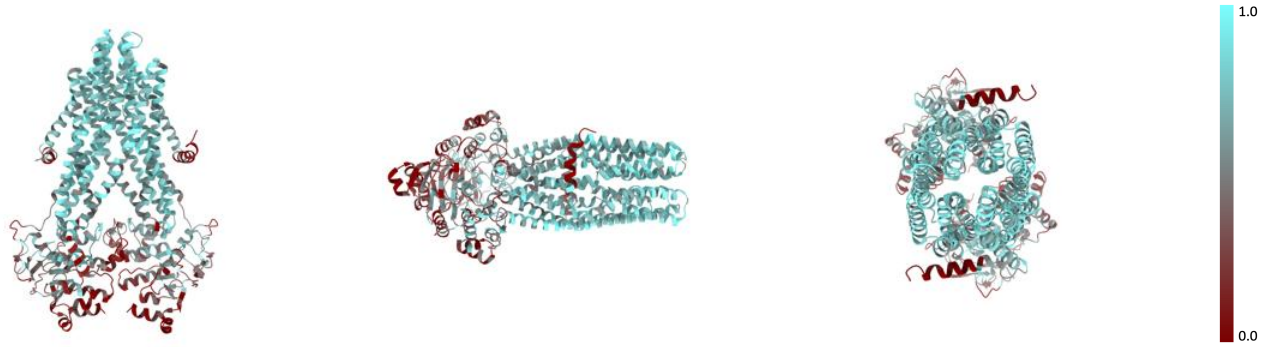
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

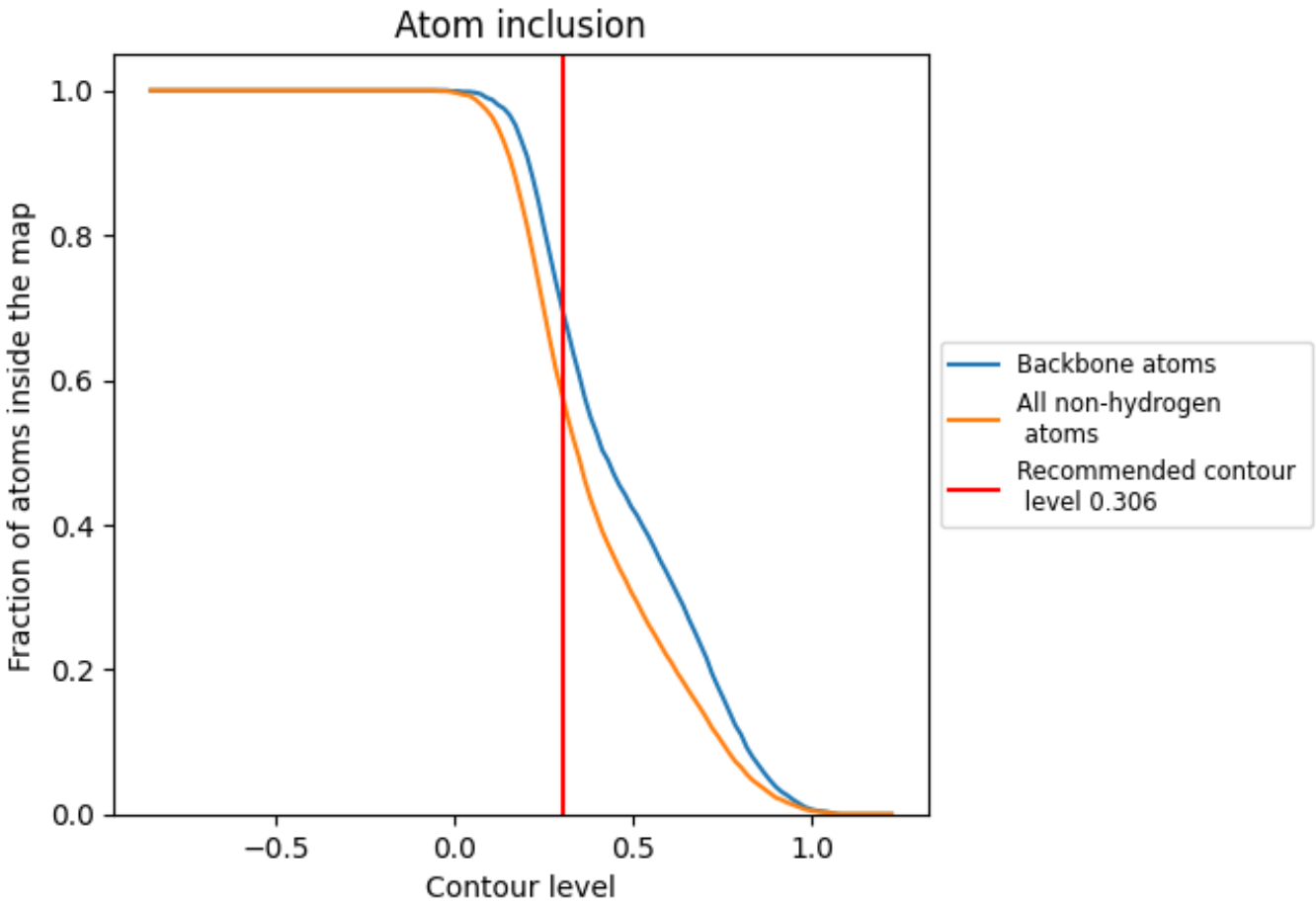
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.306).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.4150
A	0.5670	0.4170
B	0.5700	0.4140