



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 04:07 AM JST

PDB ID : 7FDV  
EMDB ID : EMD-31547  
Title : Cryo-EM structure of the human cholesterol transporter ABCG1 in complex with cholesterol  
Authors : Xu, D.; Li, Y.Y.; Yang, F.R.; Sun, C.R.; Pan, J.H.; Wang, L.; Chen, Z.P.; Fang, S.C.; Yao, X.B.; Hou, W.T.; Zhou, C.Z.; Chen, Y.  
Deposited on : 2021-07-18  
Resolution : 3.26 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](mailto: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>.

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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) : 2.31.3

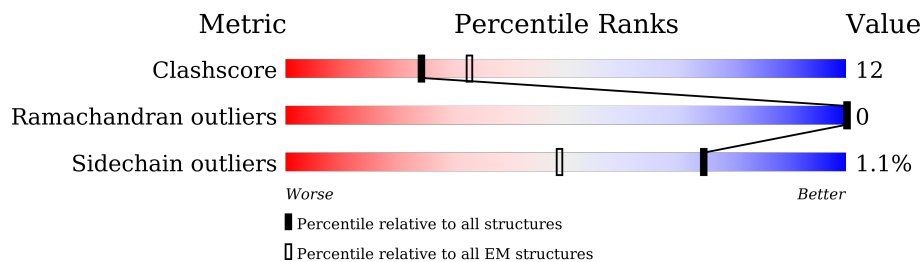
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.26 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  $\geq 3$ , 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	678	
1	D	678	

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
2	ATP	A	701	-	-	X	-
2	ATP	D	702	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8508 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.

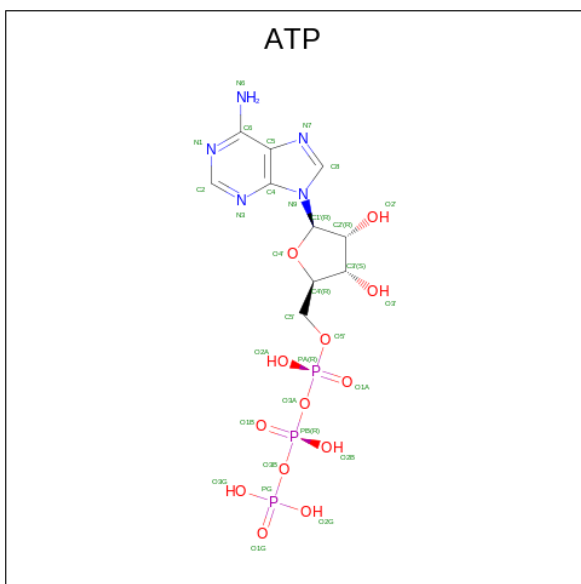
- Molecule 1 is a protein called ATP-binding cassette sub-family G member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	529	4147	2702	678	733	34	0	0
1	D	529	4147	2702	678	733	34	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLN	GLU	conflict	UNP P45844
D	242	GLN	GLU	conflict	UNP P45844

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



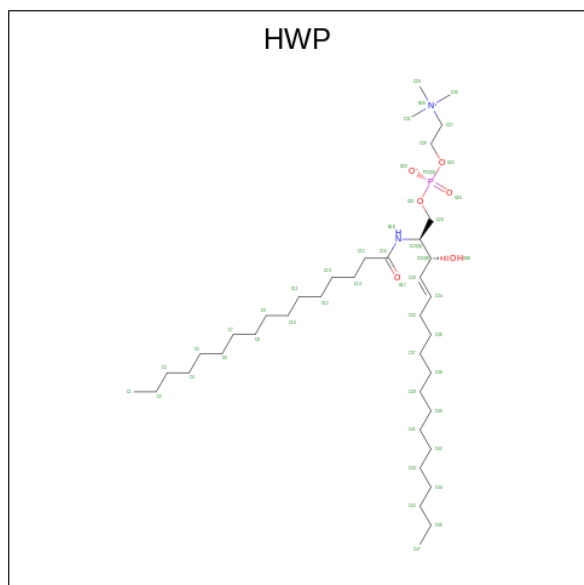
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

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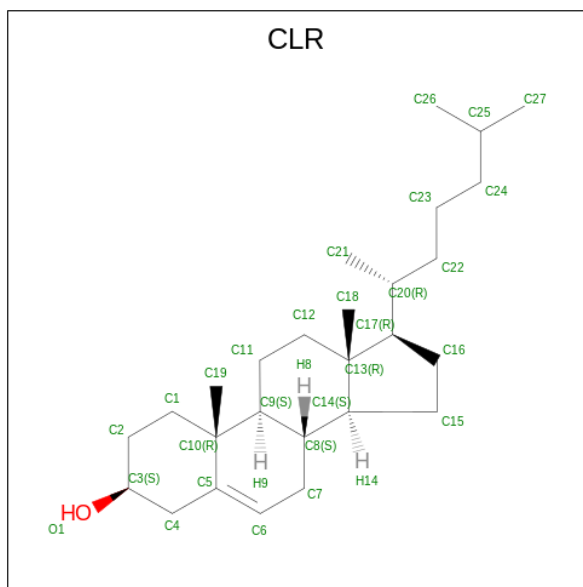
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	D	1	31	10	5	13	3	0

- Molecule 3 is [(E,2S,3R)-2-(hexadecanoylamino)-3-oxidanyl-octadec-4-enyl] 2-(trimethyl azaniumyl)ethyl phosphate (three-letter code: HWP) (formula: C<sub>39</sub>H<sub>79</sub>N<sub>2</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



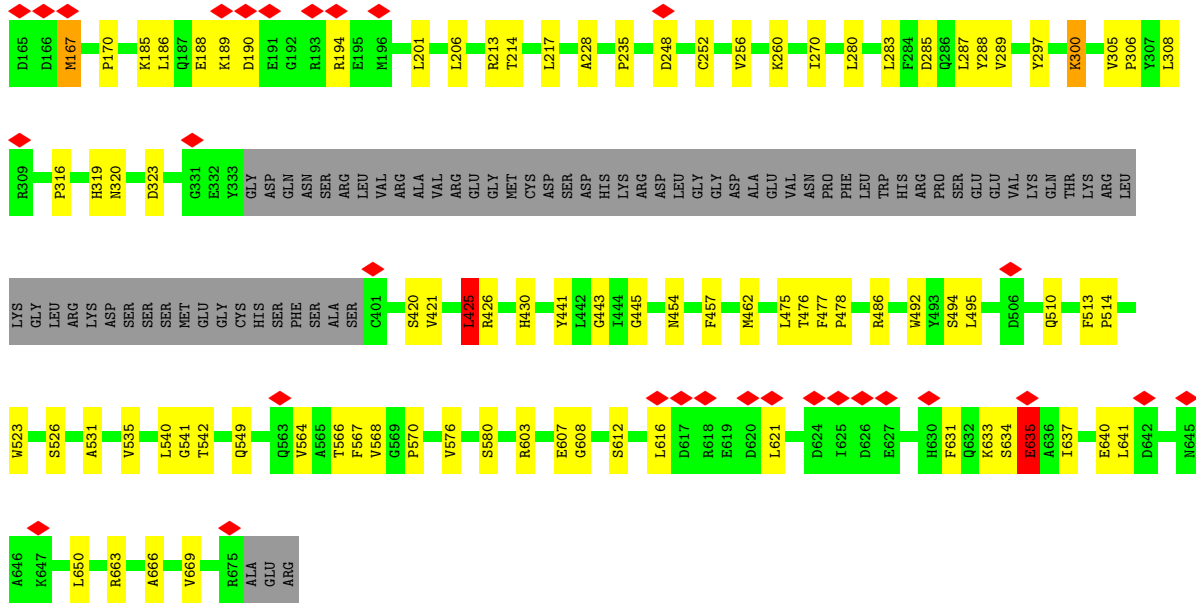
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	48	39	2	6	1	0
3	D	1	48	39	2	6	1	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	D	1	Total	C	O	0
			28	27	1	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151593	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 ( $e^-/\text{\AA}^2$ )	57.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.104	Depositor
Minimum map value	-1.230	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	242.4, 242.4, 242.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	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: HWP, CLR, ATP

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	0.34	0/4236	0.51	2/5729 (0.0%)
1	D	0.34	0/4236	0.51	2/5729 (0.0%)
All	All	0.34	0/8472	0.51	4/11458 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	635	GLU	CB-CA-C	-8.69	93.03	110.40
1	A	635	GLU	CB-CA-C	-8.20	94.00	110.40
1	A	425	LEU	CB-CG-CD1	-7.15	98.85	111.00
1	D	425	LEU	CB-CG-CD1	-7.14	98.87	111.00

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	4147	0	4238	88	0
1	D	4147	0	4238	89	0
2	A	31	0	12	22	0
2	D	31	0	12	21	0
3	A	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	48	0	0	1	0
4	A	28	0	46	19	0
4	D	28	0	46	16	0
All	All	8508	0	8592	204	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 12.

All (204) 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:A:634:SER:O	1:A:635:GLU:HB3	1.35	1.13
1:D:123:GLY:HA2	2:D:702:ATP:H5'1	1.15	1.11
1:A:123:GLY:CA	2:A:701:ATP:H5'1	1.81	1.10
1:D:634:SER:O	1:D:635:GLU:HB3	1.35	1.10
1:D:635:GLU:CG	1:D:635:GLU:O	2.00	1.09
1:A:100:LEU:HD23	2:A:701:ATP:H2	1.10	1.09
1:D:123:GLY:CA	2:D:702:ATP:H5'1	1.81	1.08
1:D:100:LEU:HD23	2:D:702:ATP:H2	1.10	1.07
1:A:123:GLY:HA2	2:A:701:ATP:H5'1	1.15	1.06
1:A:635:GLU:O	1:A:635:GLU:HG2	1.29	1.06
1:D:100:LEU:HD23	2:D:702:ATP:C2	1.91	1.06
1:A:100:LEU:HD23	2:A:701:ATP:C2	1.91	1.04
1:D:635:GLU:O	1:D:635:GLU:HG2	1.22	1.04
1:A:635:GLU:O	1:A:635:GLU:CG	2.06	1.02
1:A:126:THR:HB	2:A:701:ATP:O3'	1.62	0.98
1:D:126:THR:HB	2:D:702:ATP:O3'	1.62	0.98
1:A:124:LYS:HG2	2:A:701:ATP:O2A	1.66	0.95
1:D:124:LYS:HG2	2:D:702:ATP:O2A	1.66	0.94
1:D:100:LEU:CD2	2:D:702:ATP:C2	2.52	0.93
1:A:100:LEU:CD2	2:A:701:ATP:C2	2.52	0.90
1:A:87:PRO:HA	1:A:97:TYR:H	1.47	0.80
1:D:124:LYS:CG	2:D:702:ATP:O2A	2.31	0.79
4:D:701:CLR:H212	4:D:701:CLR:H121	1.64	0.79
1:D:87:PRO:HA	1:D:97:TYR:H	1.47	0.79
1:A:124:LYS:CG	2:A:701:ATP:O2A	2.31	0.78
1:D:123:GLY:CA	2:D:702:ATP:C5'	2.62	0.78
4:A:703:CLR:H212	4:A:703:CLR:H121	1.64	0.77
1:A:123:GLY:CA	2:A:701:ATP:C5'	2.62	0.76
1:D:126:THR:CB	2:D:702:ATP:O3'	2.34	0.76
1:A:126:THR:CB	2:A:701:ATP:O3'	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:H	1:D:194:ARG:HD3	1.52	0.74
1:A:190:ASP:H	1:A:194:ARG:HD3	1.52	0.74
1:A:123:GLY:H	2:A:701:ATP:C5'	2.03	0.71
1:D:123:GLY:H	2:D:702:ATP:C5'	2.03	0.69
1:D:443:GLY:HA2	1:D:526:SER:HB3	1.74	0.69
1:D:421:VAL:HG11	1:D:476:THR:HG21	1.74	0.69
1:D:123:GLY:N	2:D:702:ATP:C5'	2.56	0.69
1:A:443:GLY:HA2	1:A:526:SER:HB3	1.74	0.68
1:A:634:SER:O	1:A:635:GLU:CB	2.23	0.68
1:A:421:VAL:HG11	1:A:476:THR:HG21	1.74	0.68
1:A:123:GLY:N	2:A:701:ATP:C5'	2.56	0.68
1:D:126:THR:N	2:D:702:ATP:O3'	2.27	0.67
1:A:126:THR:N	2:A:701:ATP:O3'	2.27	0.67
1:A:84:TYR:HD2	1:A:100:LEU:HD12	1.63	0.64
1:A:549:GLN:OE1	1:A:663:ARG:NH1	2.32	0.63
1:D:84:TYR:HD2	1:D:100:LEU:HD12	1.63	0.63
1:D:549:GLN:OE1	1:D:663:ARG:NH1	2.32	0.62
1:A:123:GLY:HA2	2:A:701:ATP:C5'	2.09	0.61
4:A:703:CLR:H242	4:A:703:CLR:H213	1.83	0.61
4:A:703:CLR:H212	4:A:703:CLR:C12	2.31	0.60
4:D:701:CLR:H212	4:D:701:CLR:C12	2.31	0.60
1:D:123:GLY:HA2	2:D:702:ATP:C5'	2.09	0.60
4:D:701:CLR:H213	4:D:701:CLR:H242	1.83	0.60
1:A:188:GLU:O	1:A:194:ARG:NH1	2.35	0.60
1:D:188:GLU:O	1:D:194:ARG:NH1	2.35	0.59
1:A:621:LEU:HD22	1:A:633:LYS:HG2	1.86	0.58
1:A:125:SER:HB2	2:A:701:ATP:O1B	2.03	0.58
1:D:125:SER:HB2	2:D:702:ATP:O1B	2.03	0.58
1:D:621:LEU:HD22	1:D:633:LYS:HG2	1.86	0.57
1:A:167:MET:HG2	1:A:486:ARG:HE	1.70	0.56
1:D:631:PHE:HE1	1:D:640:GLU:HG3	1.71	0.56
1:A:631:PHE:HE1	1:A:640:GLU:HG3	1.71	0.56
1:D:634:SER:O	1:D:635:GLU:CB	2.23	0.56
1:A:120:SER:OG	2:A:701:ATP:O3G	2.20	0.55
4:A:703:CLR:C27	4:A:703:CLR:C22	2.84	0.55
1:A:206:LEU:HD22	1:A:228:ALA:HB2	1.89	0.55
1:D:167:MET:HG2	1:D:486:ARG:HE	1.70	0.55
1:D:316:PRO:HG2	1:D:319:HIS:CG	2.41	0.55
4:D:701:CLR:C27	4:D:701:CLR:C22	2.84	0.55
1:A:316:PRO:HG2	1:A:319:HIS:CG	2.41	0.55
1:A:540:LEU:HD21	1:A:608:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:HD22	1:D:228:ALA:HB2	1.89	0.54
1:D:540:LEU:HD21	1:D:608:GLY:HA3	1.89	0.54
4:A:703:CLR:C27	4:A:703:CLR:H221	2.39	0.53
4:D:701:CLR:H213	4:D:701:CLR:C24	2.38	0.53
4:D:701:CLR:C27	4:D:701:CLR:H221	2.39	0.53
1:A:631:PHE:CE1	1:A:640:GLU:HG3	2.44	0.53
4:A:703:CLR:H213	4:A:703:CLR:C24	2.38	0.53
1:D:631:PHE:CE1	1:D:640:GLU:HG3	2.44	0.53
4:D:701:CLR:C24	4:D:701:CLR:C21	2.85	0.53
1:A:567:PHE:CD1	4:A:703:CLR:H152	2.44	0.52
1:D:567:PHE:CD1	4:D:701:CLR:H152	2.44	0.52
4:A:703:CLR:C24	4:A:703:CLR:C21	2.85	0.52
1:A:612:SER:HA	1:A:616:LEU:HB2	1.92	0.52
1:D:426:ARG:NH1	1:D:510:GLN:OE1	2.43	0.52
1:D:120:SER:OG	2:D:702:ATP:O3G	2.20	0.51
1:D:190:ASP:H	1:D:194:ARG:CD	2.23	0.51
1:D:84:TYR:HD2	1:D:100:LEU:CD1	2.23	0.51
1:A:426:ARG:NH1	1:A:510:GLN:OE1	2.43	0.51
1:D:612:SER:HA	1:D:616:LEU:HB2	1.92	0.51
4:D:701:CLR:C22	4:D:701:CLR:H273	2.41	0.51
1:A:84:TYR:HD2	1:A:100:LEU:CD1	2.23	0.51
1:A:320:ASN:ND2	1:A:323:ASP:OD2	2.35	0.50
1:A:526:SER:O	1:A:526:SER:OG	2.29	0.50
1:A:603:ARG:NH1	1:A:607:GLU:OE1	2.44	0.50
1:D:603:ARG:NH1	1:D:607:GLU:OE1	2.44	0.50
1:A:190:ASP:H	1:A:194:ARG:CD	2.23	0.50
1:D:420:SER:OG	3:D:703:HWP:O25	2.30	0.49
1:A:420:SER:OG	3:A:702:HWP:O25	2.30	0.49
4:D:701:CLR:H221	4:D:701:CLR:H272	1.95	0.49
4:A:703:CLR:C22	4:A:703:CLR:H273	2.41	0.49
4:A:703:CLR:H221	4:A:703:CLR:H272	1.95	0.48
1:D:125:SER:HB3	2:D:702:ATP:H4'	1.96	0.48
1:D:287:LEU:HD22	1:D:297:TYR:HD2	1.79	0.48
1:A:170:PRO:HA	1:A:214:THR:HB	1.96	0.48
1:A:125:SER:HB3	2:A:701:ATP:H4'	1.96	0.48
1:A:152:LEU:HD12	1:A:156:ARG:HH21	1.79	0.47
1:A:564:VAL:O	1:A:568:VAL:HG23	2.14	0.47
1:D:125:SER:HB2	2:D:702:ATP:O3A	2.15	0.47
1:D:170:PRO:HA	1:D:214:THR:HB	1.96	0.47
4:D:701:CLR:H183	4:D:701:CLR:H20	1.64	0.47
1:A:287:LEU:HD22	1:A:297:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:PHE:HD1	4:A:703:CLR:H152	1.78	0.47
1:D:564:VAL:O	1:D:568:VAL:HG23	2.14	0.47
1:A:260:LYS:NZ	1:A:285:ASP:OD1	2.45	0.46
1:D:152:LEU:HD12	1:D:156:ARG:HH21	1.79	0.46
1:A:475:LEU:HD12	1:A:476:THR:HG23	1.98	0.46
1:A:425:LEU:HD22	1:A:425:LEU:HA	1.54	0.46
1:D:256:VAL:HG12	1:D:283:LEU:HD11	1.98	0.46
1:A:125:SER:HB2	2:A:701:ATP:O3A	2.15	0.46
1:D:567:PHE:HD1	4:D:701:CLR:H152	1.78	0.46
1:D:666:ALA:HA	1:D:669:VAL:HG12	1.98	0.46
1:A:256:VAL:HG21	1:A:280:LEU:HD11	1.98	0.45
1:D:260:LYS:NZ	1:D:285:ASP:OD1	2.45	0.45
4:A:703:CLR:H213	1:D:566:THR:HG21	1.98	0.45
1:D:185:LYS:HE2	1:D:492:TRP:NE1	2.31	0.45
1:D:248:ASP:O	1:D:252:CYS:HB2	2.17	0.45
1:D:256:VAL:HG21	1:D:280:LEU:HD11	1.98	0.45
1:D:475:LEU:HD12	1:D:476:THR:HG23	1.98	0.45
1:A:666:ALA:HA	1:A:669:VAL:HG12	1.98	0.45
1:A:126:THR:CA	2:A:701:ATP:O3'	2.64	0.45
1:A:185:LYS:HE2	1:A:492:TRP:NE1	2.31	0.45
1:A:566:THR:HG21	4:D:701:CLR:H213	1.98	0.45
1:A:248:ASP:O	1:A:252:CYS:HB2	2.17	0.45
1:D:126:THR:CA	2:D:702:ATP:O3'	2.64	0.45
1:A:189:LYS:HA	1:A:194:ARG:HH11	1.82	0.45
1:D:189:LYS:HA	1:D:194:ARG:HH11	1.82	0.45
1:D:300:LYS:HB2	1:D:300:LYS:HE2	1.81	0.45
1:D:462:MET:HE1	1:D:541:GLY:HA2	1.99	0.45
1:D:425:LEU:HD22	1:D:425:LEU:HA	1.54	0.44
1:A:125:SER:HB2	2:A:701:ATP:PB	2.57	0.44
1:D:125:SER:HB2	2:D:702:ATP:PB	2.57	0.44
1:D:576:VAL:O	1:D:580:SER:OG	2.25	0.44
1:A:256:VAL:HG12	1:A:283:LEU:HD11	1.98	0.44
1:A:531:ALA:O	1:A:535:VAL:HG22	2.18	0.44
1:D:84:TYR:CD2	1:D:100:LEU:CD1	3.01	0.44
1:D:320:ASN:ND2	1:D:323:ASP:OD2	2.35	0.44
4:D:701:CLR:H22	4:D:701:CLR:H192	1.60	0.44
2:A:701:ATP:N3	2:A:701:ATP:H2'	2.33	0.44
1:D:494:SER:OG	1:D:495:LEU:N	2.51	0.43
1:A:189:LYS:HA	1:A:194:ARG:HD3	2.00	0.43
1:A:655:LEU:HD23	1:A:655:LEU:HA	1.86	0.43
1:D:637:ILE:HG13	1:D:641:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:702:ATP:N3	2:D:702:ATP:H2'	2.33	0.43
1:A:494:SER:OG	1:A:495:LEU:N	2.51	0.43
1:D:84:TYR:CD2	1:D:100:LEU:HD12	2.49	0.43
1:D:289:VAL:CG1	1:D:297:TYR:HB3	2.49	0.43
1:A:213:ARG:O	1:A:217:LEU:HD13	2.19	0.43
1:A:445:GLY:HA2	1:A:454:ASN:ND2	2.34	0.43
1:D:531:ALA:O	1:D:535:VAL:HG22	2.18	0.43
1:A:289:VAL:CG1	1:A:297:TYR:HB3	2.49	0.43
1:A:637:ILE:HG13	1:A:641:LEU:HD23	2.00	0.43
1:A:84:TYR:CD2	1:A:100:LEU:CD1	3.01	0.42
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.90	0.42
1:A:425:LEU:HA	1:A:425:LEU:HD13	1.80	0.42
4:A:703:CLR:H262	4:A:703:CLR:H231	1.87	0.42
1:D:189:LYS:HA	1:D:194:ARG:HD3	2.00	0.42
1:D:477:PHE:N	1:D:478:PRO:HD2	2.35	0.42
1:D:441:TYR:CZ	1:D:457:PHE:HB2	2.55	0.42
1:D:305:VAL:HG23	1:D:306:PRO:HD3	2.01	0.42
4:A:703:CLR:H192	4:A:703:CLR:H22	1.60	0.42
1:D:445:GLY:HA2	1:D:454:ASN:ND2	2.34	0.42
1:D:650:LEU:HD12	1:D:650:LEU:HA	1.87	0.42
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.80	0.42
1:A:441:TYR:CZ	1:A:457:PHE:HB2	2.55	0.42
1:A:125:SER:CB	2:A:701:ATP:O1B	2.68	0.42
1:A:477:PHE:N	1:A:478:PRO:HD2	2.35	0.42
1:D:213:ARG:O	1:D:217:LEU:HD13	2.19	0.42
1:A:506:ASP:N	1:A:506:ASP:OD1	2.53	0.42
1:D:160:CYS:SG	1:D:235:PRO:HG3	2.60	0.41
1:D:186:LEU:HD12	1:D:186:LEU:O	2.20	0.41
1:D:270:ILE:H	1:D:270:ILE:HG13	1.64	0.41
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.88	0.41
1:A:186:LEU:HD12	1:A:186:LEU:O	2.20	0.41
1:A:514:PRO:HG2	1:A:542:THR:HG22	2.03	0.41
1:D:570:PRO:HB2	4:D:701:CLR:C19	2.50	0.41
1:A:116:ILE:HD13	1:A:127:LEU:HD23	2.02	0.41
4:A:703:CLR:H211	4:D:701:CLR:H211	2.02	0.41
1:D:116:ILE:HD13	1:D:127:LEU:HD23	2.02	0.41
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.80	0.41
1:D:430:HIS:HD1	1:D:513:PHE:HB3	1.86	0.41
1:A:462:MET:HE1	1:A:541:GLY:HA2	2.02	0.41
4:A:703:CLR:H8	4:A:703:CLR:H182	1.65	0.41
1:D:105:SER:O	1:D:288:TYR:OH	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:PRO:HG2	1:D:542:THR:HG22	2.03	0.41
1:D:540:LEU:HD12	1:D:540:LEU:HA	1.88	0.41
1:A:160:CYS:SG	1:A:235:PRO:HG3	2.60	0.41
1:A:305:VAL:HG23	1:A:306:PRO:HD3	2.01	0.41
1:A:527:GLN:HB3	1:A:528:PRO:HD2	2.03	0.41
1:A:570:PRO:HB2	4:A:703:CLR:C19	2.50	0.40
4:A:703:CLR:H183	4:A:703:CLR:H20	1.64	0.40
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.90	0.40
1:A:563:GLN:OE1	4:A:703:CLR:H262	2.22	0.40
1:D:189:LYS:HA	1:D:194:ARG:NH1	2.37	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	523/678 (77%)	475 (91%)	48 (9%)	0	100	100
1	D	523/678 (77%)	475 (91%)	48 (9%)	0	100	100
All	All	1046/1356 (77%)	950 (91%)	96 (9%)	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	454/582 (78%)	449 (99%)	5 (1%)	73	84
1	D	454/582 (78%)	449 (99%)	5 (1%)	73	84
All	All	908/1164 (78%)	898 (99%)	10 (1%)	74	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	MET
1	A	300	LYS
1	A	425	LEU
1	A	523	TRP
1	A	635	GLU
1	D	167	MET
1	D	300	LYS
1	D	425	LEU
1	D	523	TRP
1	D	635	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	630	HIS
1	D	630	HIS

### 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](#)

6 ligands are modelled in this entry.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	D	702	-	26,33,33	0.94	1 (3%)	31,52,52	1.60	5 (16%)
4	CLR	D	701	-	31,31,31	1.95	12 (38%)	48,48,48	2.46	20 (41%)
2	ATP	A	701	-	26,33,33	0.94	1 (3%)	31,52,52	1.60	5 (16%)
3	HWP	D	703	-	46,47,47	1.59	6 (13%)	52,55,55	0.83	2 (3%)
3	HWP	A	702	-	46,47,47	1.59	6 (13%)	52,55,55	0.83	2 (3%)
4	CLR	A	703	-	31,31,31	1.95	12 (38%)	48,48,48	2.46	20 (41%)

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	ATP	D	702	-	-	2/18/38/38	0/3/3/3
4	CLR	D	701	-	-	6/10/68/68	0/4/4/4
2	ATP	A	701	-	-	2/18/38/38	0/3/3/3
3	HWP	D	703	-	-	27/52/52/52	-
3	HWP	A	702	-	-	27/52/52/52	-
4	CLR	A	703	-	-	6/10/68/68	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	HWP	C16-N18	6.84	1.48	1.34
3	D	703	HWP	C16-N18	6.84	1.48	1.34
4	A	703	CLR	C20-C17	-4.07	1.47	1.54
4	D	701	CLR	C20-C17	-4.07	1.47	1.54
4	A	703	CLR	C13-C17	-3.77	1.47	1.55
4	D	701	CLR	C13-C17	-3.77	1.47	1.55
4	A	703	CLR	C13-C14	-3.63	1.48	1.55
4	D	701	CLR	C13-C14	-3.63	1.48	1.55
3	A	702	HWP	C20-C19	3.25	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	HWP	C20-C19	3.25	1.58	1.51
4	A	703	CLR	C18-C13	-3.23	1.48	1.54
4	D	701	CLR	C18-C13	-3.23	1.48	1.54
3	A	702	HWP	C32-C33	3.03	1.55	1.50
3	D	703	HWP	C32-C33	3.03	1.55	1.50
4	A	703	CLR	C10-C9	-3.02	1.51	1.56
4	D	701	CLR	C10-C9	-3.02	1.51	1.56
3	A	702	HWP	O17-C16	-2.79	1.17	1.23
3	D	703	HWP	O17-C16	-2.79	1.17	1.23
4	A	703	CLR	C8-C14	-2.69	1.48	1.53
4	D	701	CLR	C8-C14	-2.69	1.48	1.53
3	A	702	HWP	C15-C16	2.55	1.56	1.51
3	D	703	HWP	C15-C16	2.55	1.56	1.51
3	A	702	HWP	O48-C32	-2.52	1.38	1.43
3	D	703	HWP	O48-C32	-2.52	1.38	1.43
2	A	701	ATP	C5-C4	2.50	1.47	1.40
2	D	702	ATP	C5-C4	2.50	1.47	1.40
4	A	703	CLR	C19-C10	-2.49	1.50	1.54
4	D	701	CLR	C19-C10	-2.49	1.50	1.54
4	A	703	CLR	C10-C5	-2.32	1.48	1.52
4	D	701	CLR	C10-C5	-2.32	1.48	1.52
4	A	703	CLR	C7-C8	-2.30	1.49	1.53
4	D	701	CLR	C7-C8	-2.30	1.49	1.53
4	A	703	CLR	C8-C9	-2.26	1.49	1.53
4	D	701	CLR	C8-C9	-2.26	1.49	1.53
4	A	703	CLR	C1-C10	-2.23	1.50	1.54
4	D	701	CLR	C1-C10	-2.23	1.50	1.54
4	A	703	CLR	C12-C13	-2.14	1.50	1.54
4	D	701	CLR	C12-C13	-2.14	1.50	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CLR	C8-C7-C6	-7.42	102.07	112.73
4	D	701	CLR	C8-C7-C6	-7.42	102.07	112.73
4	A	703	CLR	C13-C17-C20	-6.97	108.57	119.49
4	D	701	CLR	C13-C17-C20	-6.97	108.57	119.49
4	A	703	CLR	C13-C14-C8	-5.37	106.42	114.38
4	D	701	CLR	C13-C14-C8	-5.37	106.42	114.38
4	A	703	CLR	C21-C20-C17	-4.37	106.23	112.92
4	D	701	CLR	C21-C20-C17	-4.37	106.23	112.92
4	A	703	CLR	C1-C10-C9	3.94	114.23	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	CLR	C1-C10-C9	3.94	114.23	108.73
4	A	703	CLR	C7-C6-C5	-3.75	118.15	125.06
4	D	701	CLR	C7-C6-C5	-3.75	118.15	125.06
2	A	701	ATP	PB-O3B-PG	-3.60	120.47	132.83
2	D	702	ATP	PB-O3B-PG	-3.60	120.47	132.83
2	A	701	ATP	PA-O3A-PB	-3.56	120.62	132.83
2	D	702	ATP	PA-O3A-PB	-3.56	120.62	132.83
2	A	701	ATP	C3'-C2'-C1'	3.39	106.09	100.98
2	D	702	ATP	C3'-C2'-C1'	3.39	106.09	100.98
3	A	702	HWP	C15-C16-N18	3.18	121.34	115.83
3	D	703	HWP	C15-C16-N18	3.18	121.34	115.83
2	A	701	ATP	N3-C2-N1	-3.14	123.77	128.68
2	D	702	ATP	N3-C2-N1	-3.14	123.77	128.68
4	A	703	CLR	C1-C10-C5	-3.11	103.07	108.75
4	D	701	CLR	C1-C10-C5	-3.11	103.07	108.75
4	A	703	CLR	C15-C14-C8	-2.92	114.26	119.08
4	D	701	CLR	C15-C14-C8	-2.92	114.26	119.08
4	A	703	CLR	C11-C12-C13	-2.80	107.98	112.78
4	D	701	CLR	C11-C12-C13	-2.80	107.98	112.78
4	A	703	CLR	C2-C1-C10	-2.76	106.75	112.74
4	D	701	CLR	C2-C1-C10	-2.76	106.75	112.74
4	A	703	CLR	C23-C24-C25	-2.66	103.42	115.98
4	D	701	CLR	C23-C24-C25	-2.66	103.42	115.98
2	A	701	ATP	C4-C5-N7	-2.66	106.63	109.40
2	D	702	ATP	C4-C5-N7	-2.66	106.63	109.40
4	A	703	CLR	C9-C10-C5	2.60	113.73	109.65
4	D	701	CLR	C9-C10-C5	2.60	113.73	109.65
4	A	703	CLR	C12-C13-C14	2.54	111.22	107.27
4	D	701	CLR	C12-C13-C14	2.54	111.22	107.27
4	A	703	CLR	C7-C8-C9	-2.49	106.69	109.71
4	D	701	CLR	C7-C8-C9	-2.49	106.69	109.71
4	A	703	CLR	C3-C4-C5	-2.40	107.96	112.03
4	D	701	CLR	C3-C4-C5	-2.40	107.96	112.03
4	A	703	CLR	C18-C13-C17	-2.24	107.54	111.71
4	D	701	CLR	C18-C13-C17	-2.24	107.54	111.71
3	A	702	HWP	O17-C16-N18	-2.23	119.19	122.95
3	D	703	HWP	O17-C16-N18	-2.23	119.19	122.95
4	A	703	CLR	C10-C9-C8	-2.15	109.50	112.73
4	D	701	CLR	C10-C9-C8	-2.15	109.50	112.73
4	A	703	CLR	C19-C10-C1	-2.14	106.05	109.43
4	D	701	CLR	C19-C10-C1	-2.14	106.05	109.43
4	A	703	CLR	C7-C8-C14	-2.06	107.92	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	CLR	C7-C8-C14	-2.06	107.92	110.91
4	A	703	CLR	C18-C13-C14	-2.06	107.87	111.71
4	D	701	CLR	C18-C13-C14	-2.06	107.87	111.71

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C4'-C5'-O5'-PA
2	D	702	ATP	C4'-C5'-O5'-PA
3	A	702	HWP	N18-C19-C20-O21
3	A	702	HWP	C32-C19-C20-O21
3	A	702	HWP	O25-C26-C27-N28
3	A	702	HWP	C20-O21-P22-O25
3	A	702	HWP	C26-O25-P22-O23
3	A	702	HWP	C26-O25-P22-O24
3	A	702	HWP	C20-C19-C32-C33
3	A	702	HWP	C20-C19-C32-O48
3	D	703	HWP	N18-C19-C20-O21
3	D	703	HWP	C32-C19-C20-O21
3	D	703	HWP	O25-C26-C27-N28
3	D	703	HWP	C20-O21-P22-O25
3	D	703	HWP	C26-O25-P22-O23
3	D	703	HWP	C26-O25-P22-O24
3	D	703	HWP	C20-C19-C32-C33
3	D	703	HWP	C20-C19-C32-O48
4	A	703	CLR	C21-C20-C22-C23
4	D	701	CLR	C21-C20-C22-C23
3	A	702	HWP	C13-C14-C15-C16
3	D	703	HWP	C13-C14-C15-C16
3	A	702	HWP	C26-O25-P22-O21
3	D	703	HWP	C26-O25-P22-O21
3	A	702	HWP	C14-C15-C16-N18
3	D	703	HWP	C14-C15-C16-N18
3	A	702	HWP	C14-C15-C16-O17
3	D	703	HWP	C14-C15-C16-O17
3	A	702	HWP	C37-C38-C39-C40
3	D	703	HWP	C37-C38-C39-C40
3	A	702	HWP	C12-C13-C14-C15
3	D	703	HWP	C12-C13-C14-C15
4	A	703	CLR	C22-C23-C24-C25
4	D	701	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	A	702	HWP	C10-C11-C12-C13
3	D	703	HWP	C10-C11-C12-C13
3	A	702	HWP	C34-C35-C36-C37
3	D	703	HWP	C34-C35-C36-C37
3	A	702	HWP	C39-C40-C41-C42
3	D	703	HWP	C39-C40-C41-C42
3	A	702	HWP	C2-C3-C4-C5
3	D	703	HWP	C2-C3-C4-C5
3	A	702	HWP	C35-C36-C37-C38
3	D	703	HWP	C35-C36-C37-C38
3	A	702	HWP	C1-C2-C3-C4
3	D	703	HWP	C1-C2-C3-C4
3	A	702	HWP	C11-C12-C13-C14
3	D	703	HWP	C11-C12-C13-C14
4	A	703	CLR	C13-C17-C20-C21
4	D	701	CLR	C13-C17-C20-C21
3	A	702	HWP	C40-C41-C42-C43
3	D	703	HWP	C40-C41-C42-C43
3	A	702	HWP	C5-C6-C7-C8
3	D	703	HWP	C5-C6-C7-C8
4	A	703	CLR	C20-C22-C23-C24
4	D	701	CLR	C20-C22-C23-C24
3	A	702	HWP	C4-C5-C6-C7
3	D	703	HWP	C4-C5-C6-C7
3	A	702	HWP	N18-C19-C32-C33
3	D	703	HWP	N18-C19-C32-C33
3	A	702	HWP	N18-C19-C32-O48
3	D	703	HWP	N18-C19-C32-O48
4	A	703	CLR	C13-C17-C20-C22
4	D	701	CLR	C13-C17-C20-C22
4	A	703	CLR	C17-C20-C22-C23
4	D	701	CLR	C17-C20-C22-C23
3	A	702	HWP	C3-C4-C5-C6
3	D	703	HWP	C3-C4-C5-C6
2	A	701	ATP	PG-O3B-PB-O2B
2	D	702	ATP	PG-O3B-PB-O2B

There are no ring outliers.

6 monomers are involved in 79 short contacts:

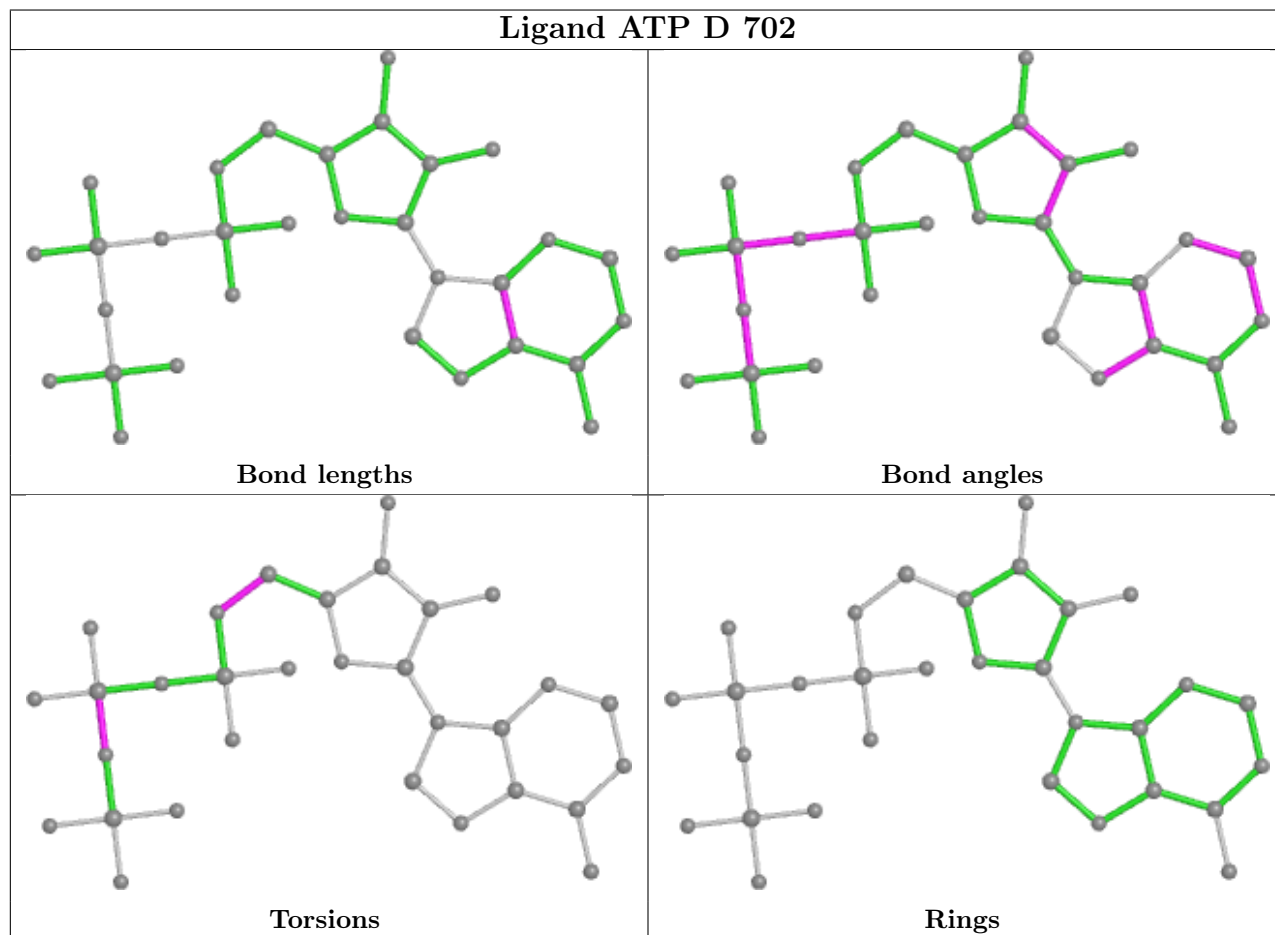
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	ATP	21	0

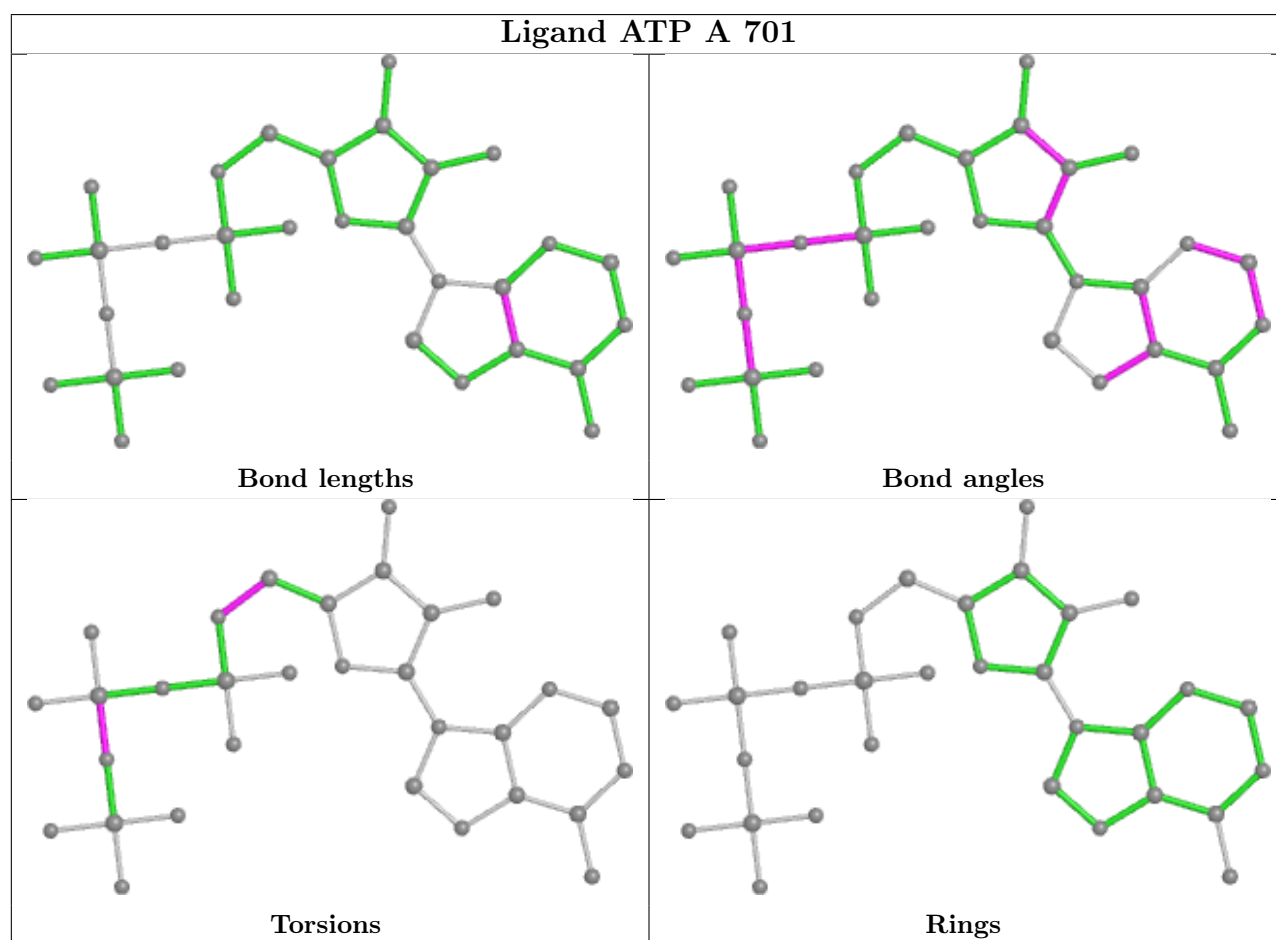
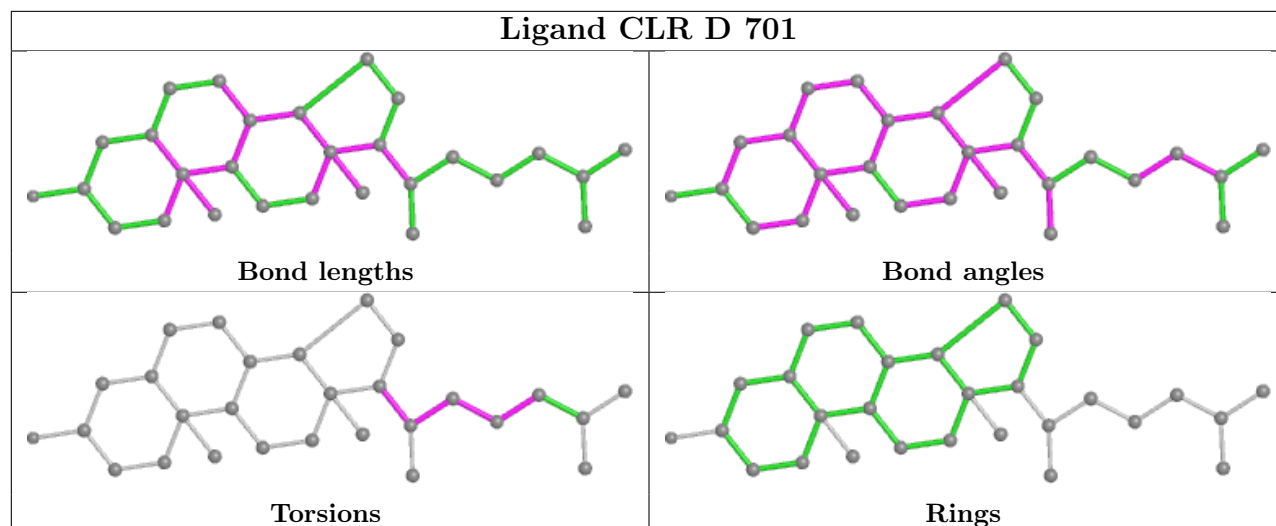
*Continued on next page...*

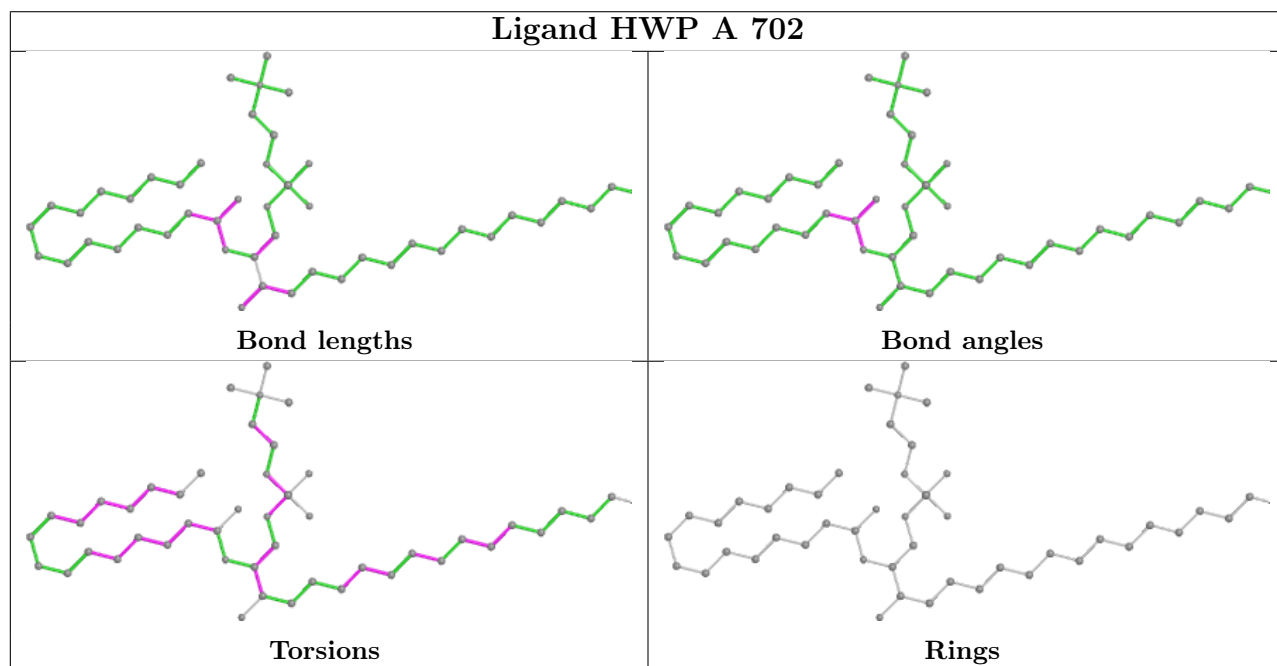
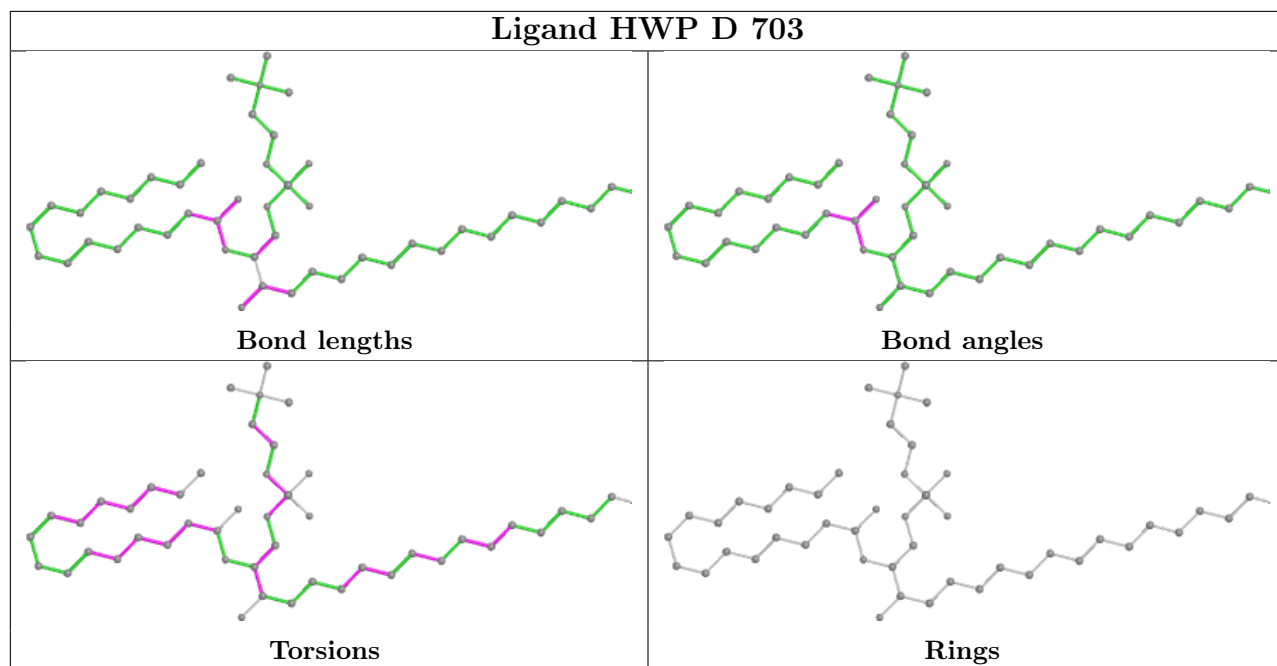
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	CLR	16	0
2	A	701	ATP	22	0
3	D	703	HWP	1	0
3	A	702	HWP	1	0
4	A	703	CLR	19	0

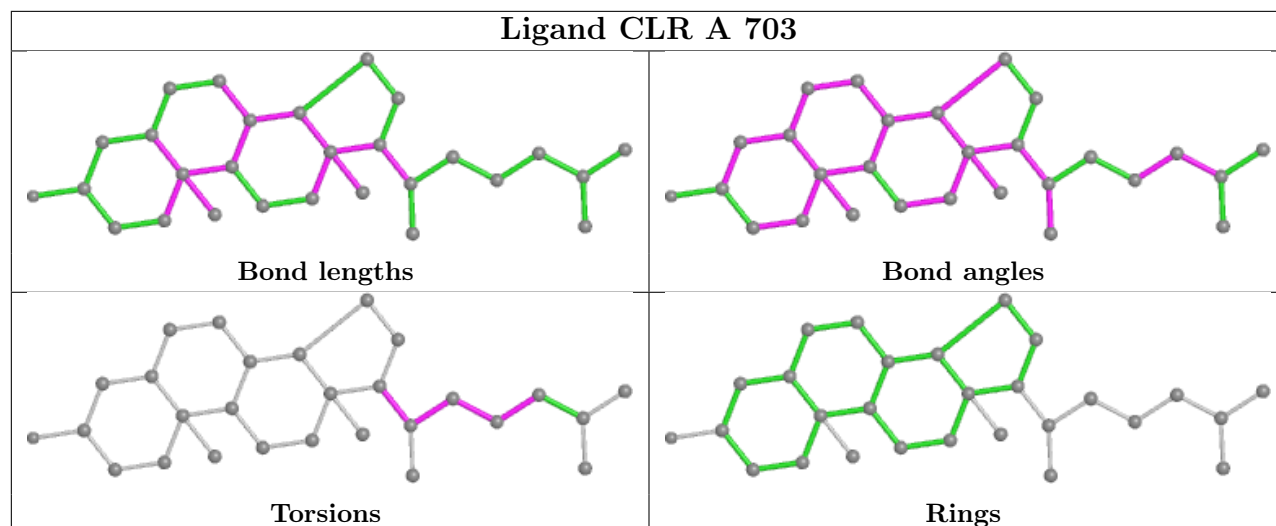
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

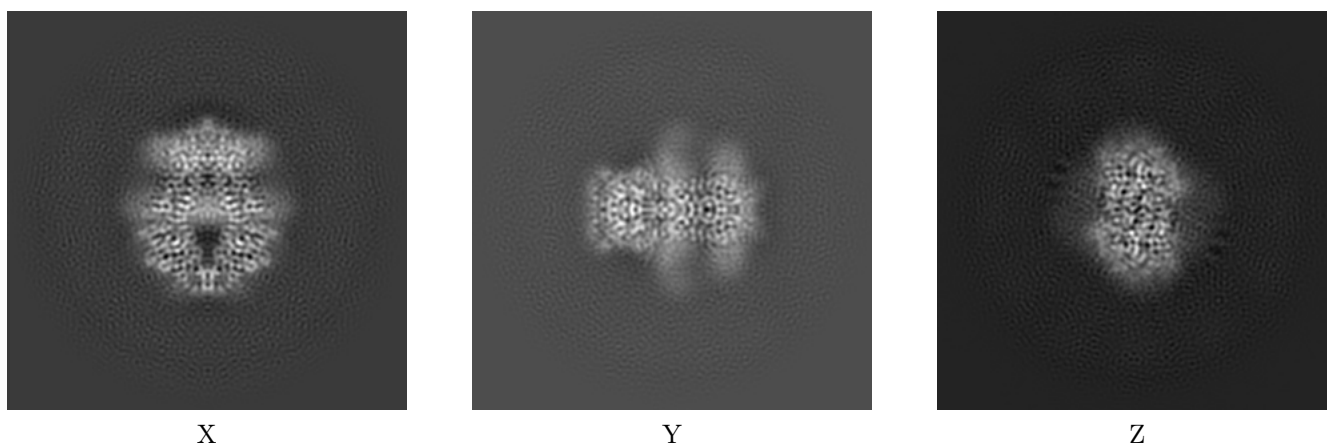
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31547. 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](#)

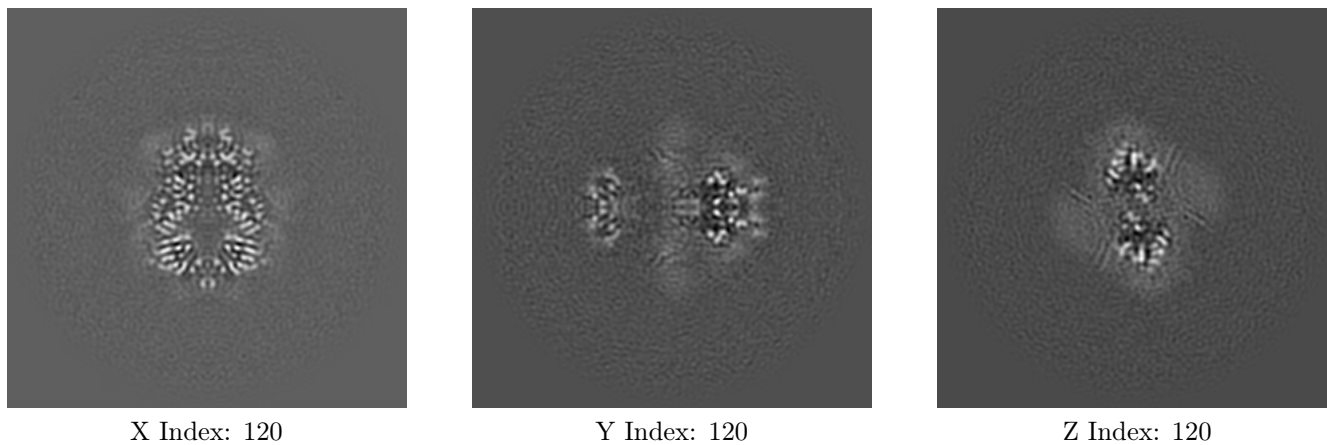
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

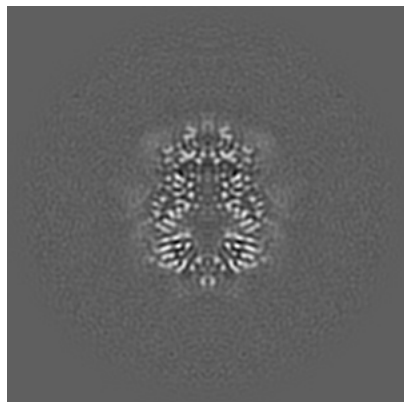
#### 6.2.1 Primary map



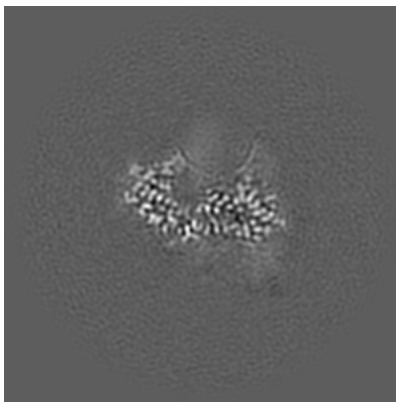
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

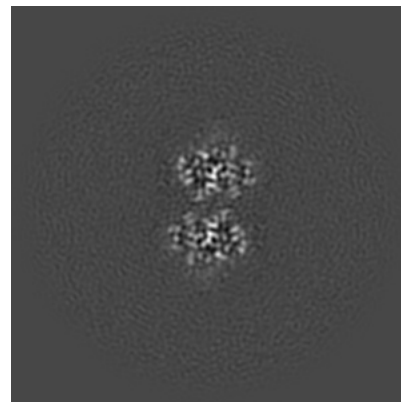
### 6.3.1 Primary map



X Index: 120



Y Index: 134

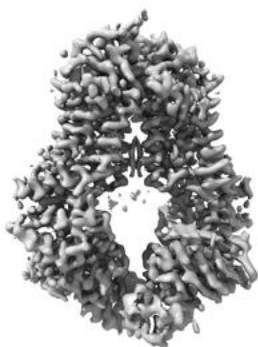


Z Index: 96

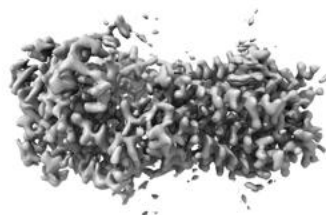
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

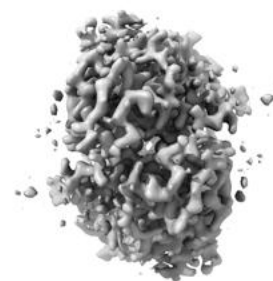
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

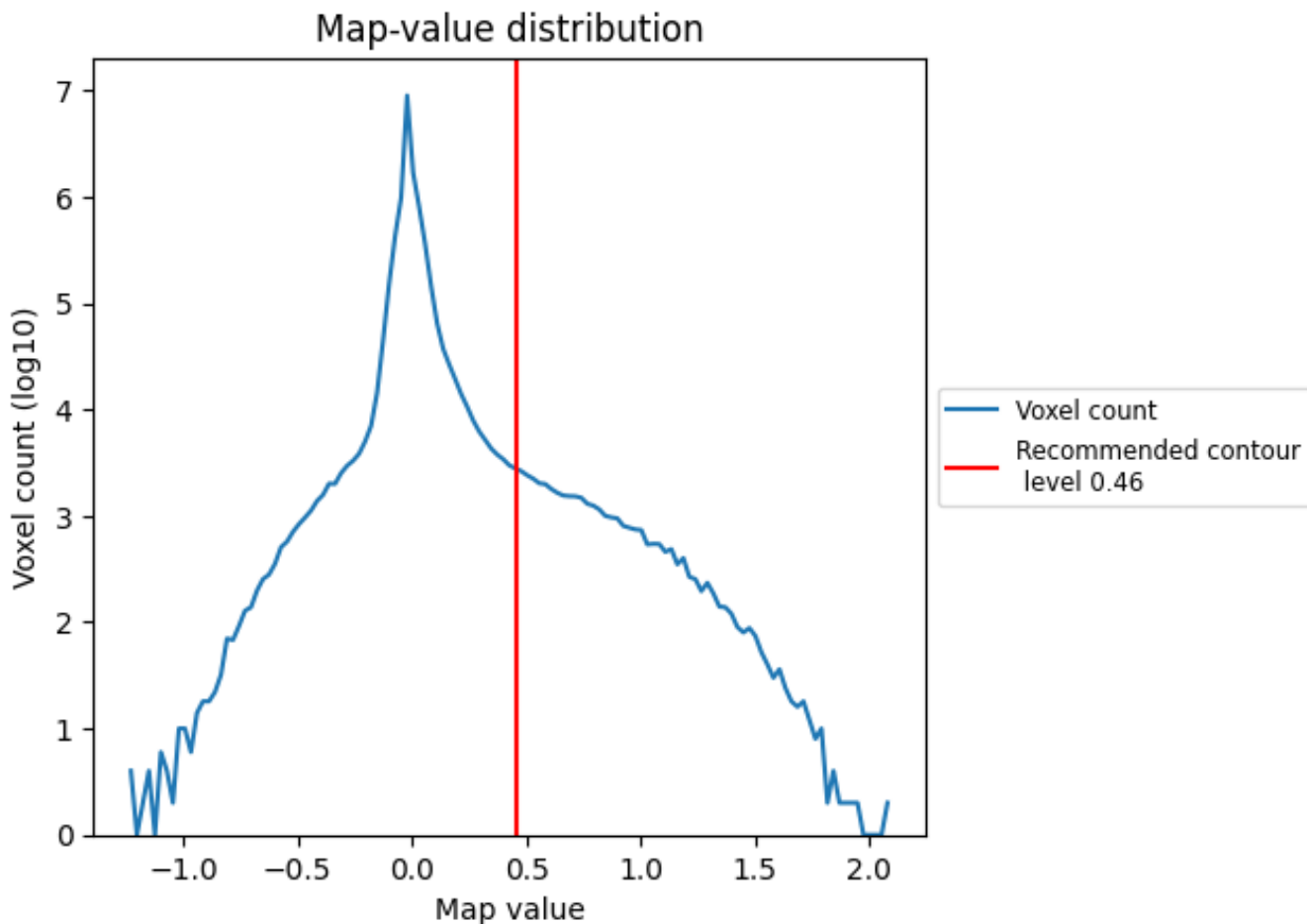
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

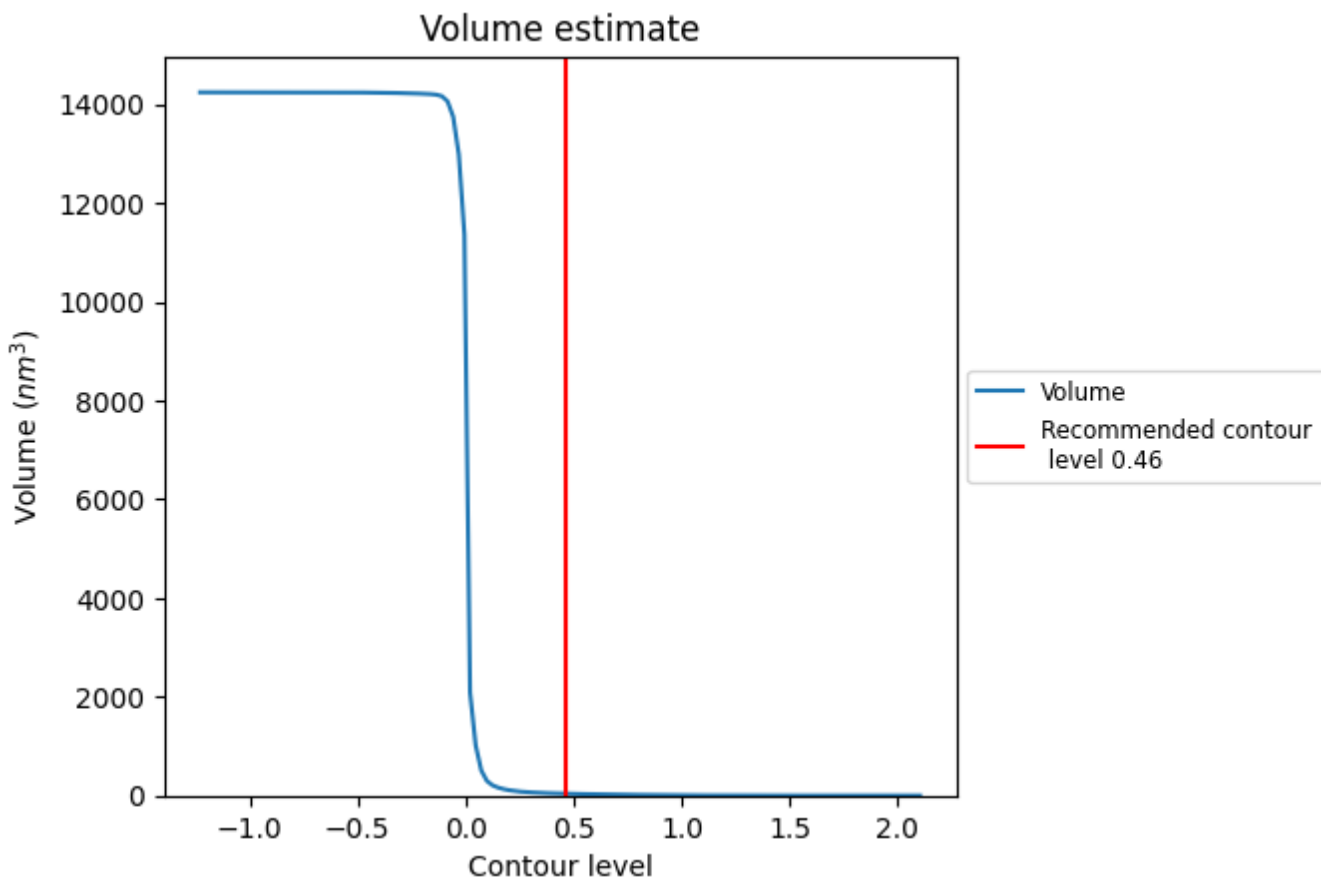
This section contains the results of statistical analysis of the map.

### 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.

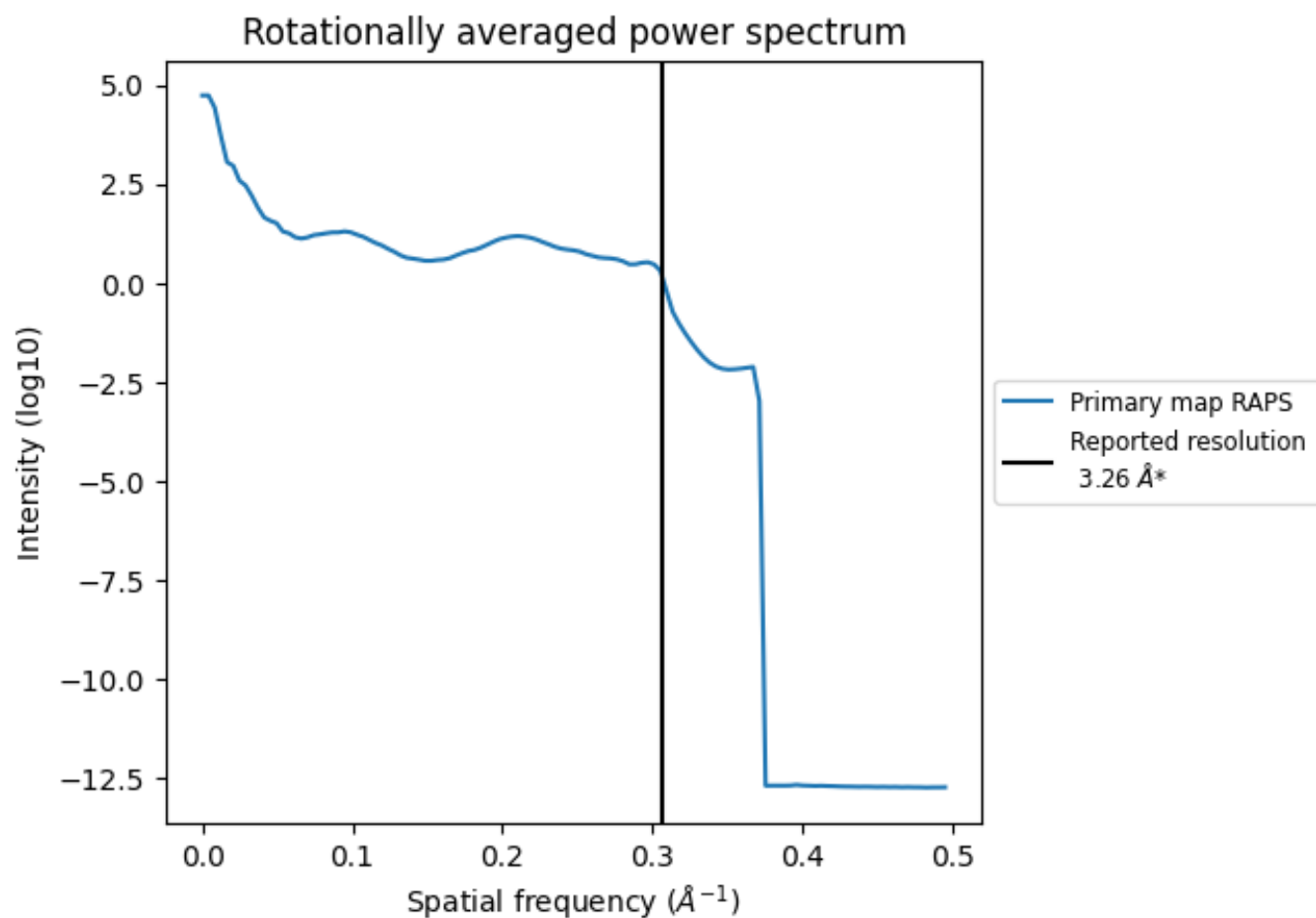
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39  $\text{nm}^3$ ; this corresponds to an approximate mass of 35 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 0.307 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

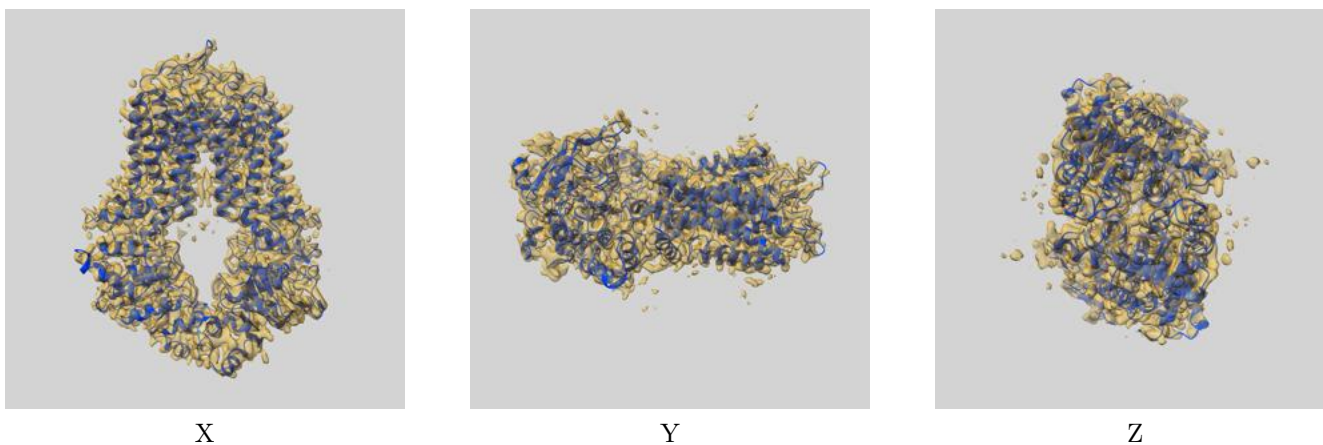
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

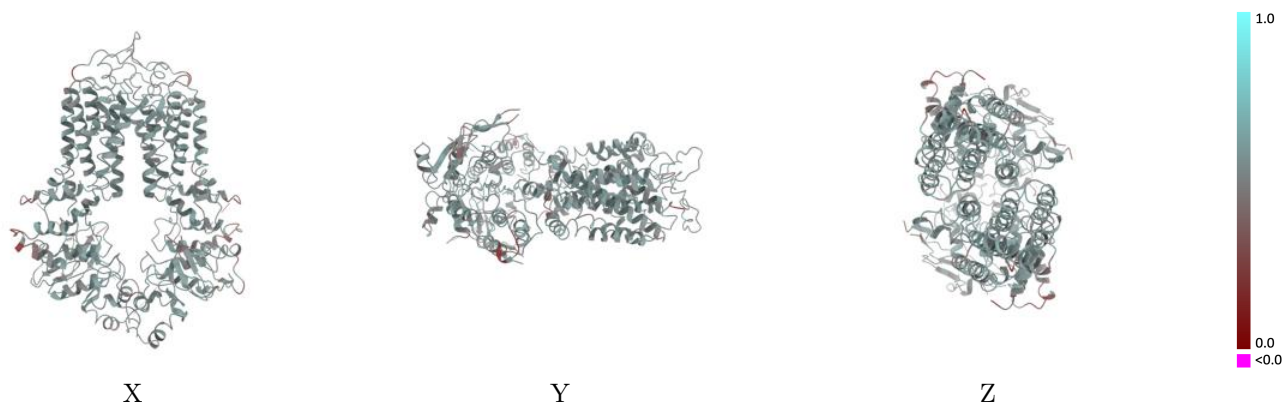
This section contains information regarding the fit between EMDB map EMD-31547 and PDB model 7FDV. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



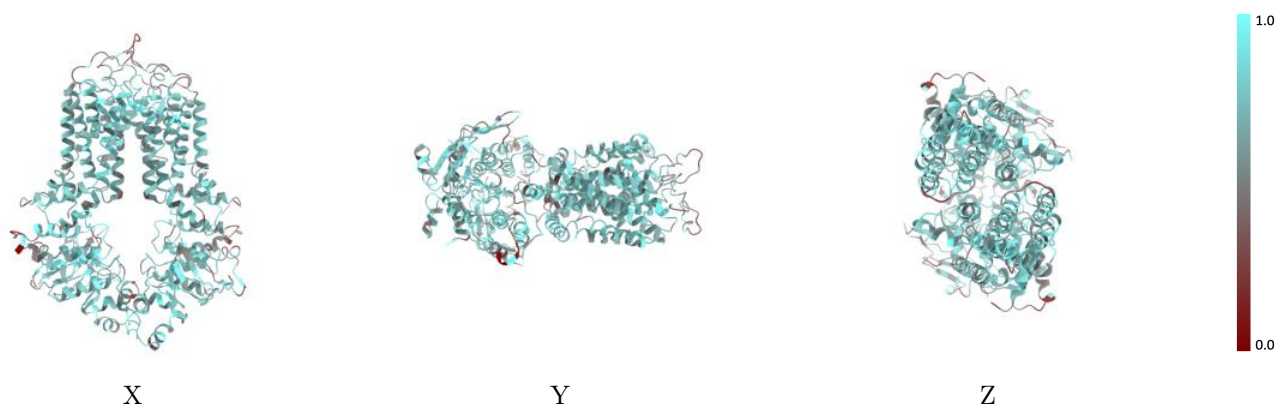
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



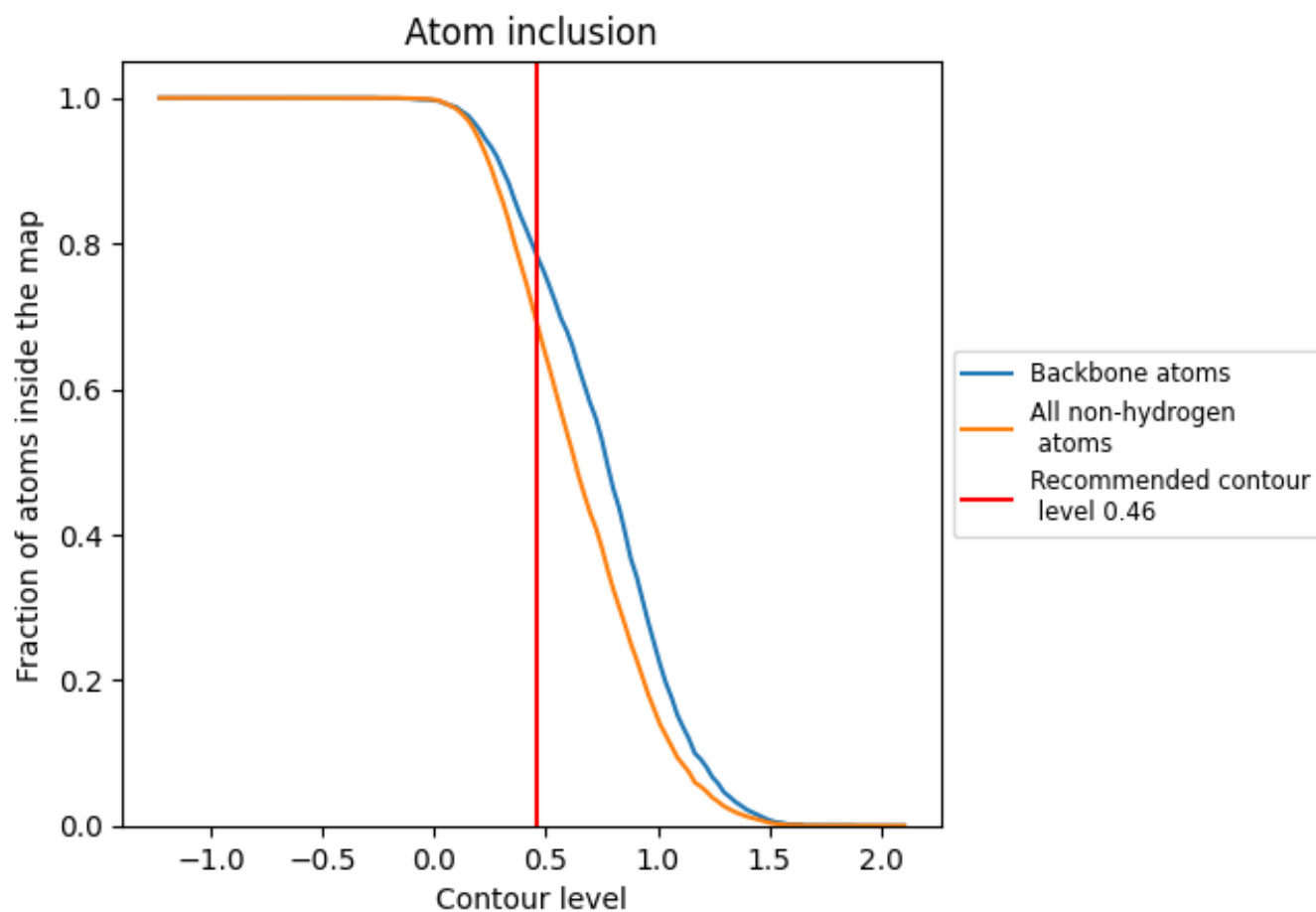
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).




## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6895	 0.5280
A	 0.6895	 0.5270
D	 0.6895	 0.5280

