Full wwPDB EM Validation Report ⓘ

Feb 13, 2023 – 12:16 AM JST

PDB ID	:	7YTJ
EMDB ID	:	EMD-34090
Title	:	Cryo-EM structure of VTC complex
Authors	:	Guan, Z.Y.; Chen, J.; Liu, R.W.; Chen, Y.K.; Xing, Q.; Du, Z.M.; Liu, Z.
Deposited on	:	2022-08-15
Resolution	:	3.00 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:

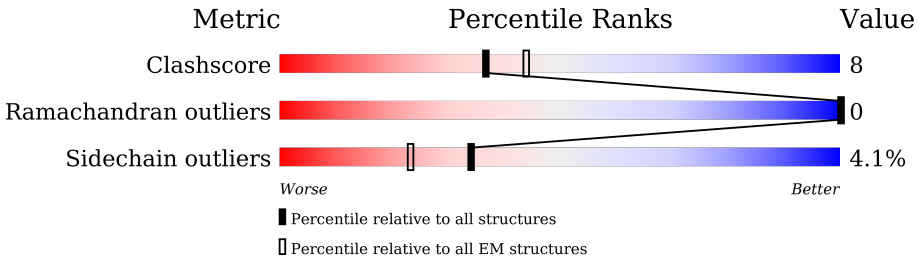
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.00 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	D	754	66% 14% 20%
2	A	143	6% 64% 18% 17%
2	B	143	6% 55% 15% 29%
2	C	143	6% 54% 16% 29%
3	E	864	15% 56% 18% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13137 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 Vacuolar transporter chaperone 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	601	4940	3189	836	901	14	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP P47075
D	2	ALA	-	expression tag	UNP P47075
D	265	ALA	ARG	conflict	UNP P47075
D	267	ALA	ARG	conflict	UNP P47075
D	427	ASN	GLU	conflict	UNP P47075
D	723	LEU	-	expression tag	UNP P47075
D	724	GLU	-	expression tag	UNP P47075
D	725	SER	-	expression tag	UNP P47075
D	726	ALA	-	expression tag	UNP P47075
D	727	TRP	-	expression tag	UNP P47075
D	728	SER	-	expression tag	UNP P47075
D	729	HIS	-	expression tag	UNP P47075
D	730	PRO	-	expression tag	UNP P47075
D	731	GLN	-	expression tag	UNP P47075
D	732	PHE	-	expression tag	UNP P47075
D	733	GLU	-	expression tag	UNP P47075
D	734	LYS	-	expression tag	UNP P47075
D	735	GLY	-	expression tag	UNP P47075
D	736	GLY	-	expression tag	UNP P47075
D	737	GLY	-	expression tag	UNP P47075
D	738	SER	-	expression tag	UNP P47075
D	739	GLY	-	expression tag	UNP P47075
D	740	GLY	-	expression tag	UNP P47075
D	741	GLY	-	expression tag	UNP P47075
D	742	SER	-	expression tag	UNP P47075
D	743	GLY	-	expression tag	UNP P47075
D	744	GLY	-	expression tag	UNP P47075
D	745	SER	-	expression tag	UNP P47075

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Chain	Residue	Modelled	Actual	Comment	Reference
D	746	ALA	-	expression tag	UNP P47075
D	747	TRP	-	expression tag	UNP P47075
D	748	SER	-	expression tag	UNP P47075
D	749	HIS	-	expression tag	UNP P47075
D	750	PRO	-	expression tag	UNP P47075
D	751	GLN	-	expression tag	UNP P47075
D	752	PHE	-	expression tag	UNP P47075
D	753	GLU	-	expression tag	UNP P47075
D	754	LYS	-	expression tag	UNP P47075

- Molecule 2 is a protein called Vacuolar transporter chaperone 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	119	Total	C	N	O	S	0	0
			941	625	163	149	4		
2	B	102	Total	C	N	O	S	0	0
			811	541	137	129	4		
2	C	102	Total	C	N	O	S	0	0
			811	541	137	129	4		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	initiating methionine	UNP P40046
A	35	ALA	-	expression tag	UNP P40046
A	164	LEU	-	expression tag	UNP P40046
A	165	GLU	-	expression tag	UNP P40046
A	166	SER	-	expression tag	UNP P40046
A	167	ALA	-	expression tag	UNP P40046
A	168	TYR	-	expression tag	UNP P40046
A	169	PRO	-	expression tag	UNP P40046
A	170	TYR	-	expression tag	UNP P40046
A	171	ASP	-	expression tag	UNP P40046
A	172	VAL	-	expression tag	UNP P40046
A	173	PRO	-	expression tag	UNP P40046
A	174	ASP	-	expression tag	UNP P40046
A	175	TYR	-	expression tag	UNP P40046
A	176	ALA	-	expression tag	UNP P40046
B	34	MET	-	initiating methionine	UNP P40046
B	35	ALA	-	expression tag	UNP P40046
B	164	LEU	-	expression tag	UNP P40046
B	165	GLU	-	expression tag	UNP P40046

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Chain	Residue	Modelled	Actual	Comment	Reference
B	166	SER	-	expression tag	UNP P40046
B	167	ALA	-	expression tag	UNP P40046
B	168	TYR	-	expression tag	UNP P40046
B	169	PRO	-	expression tag	UNP P40046
B	170	TYR	-	expression tag	UNP P40046
B	171	ASP	-	expression tag	UNP P40046
B	172	VAL	-	expression tag	UNP P40046
B	173	PRO	-	expression tag	UNP P40046
B	174	ASP	-	expression tag	UNP P40046
B	175	TYR	-	expression tag	UNP P40046
B	176	ALA	-	expression tag	UNP P40046
C	34	MET	-	initiating methionine	UNP P40046
C	35	ALA	-	expression tag	UNP P40046
C	164	LEU	-	expression tag	UNP P40046
C	165	GLU	-	expression tag	UNP P40046
C	166	SER	-	expression tag	UNP P40046
C	167	ALA	-	expression tag	UNP P40046
C	168	TYR	-	expression tag	UNP P40046
C	169	PRO	-	expression tag	UNP P40046
C	170	TYR	-	expression tag	UNP P40046
C	171	ASP	-	expression tag	UNP P40046
C	172	VAL	-	expression tag	UNP P40046
C	173	PRO	-	expression tag	UNP P40046
C	174	ASP	-	expression tag	UNP P40046
C	175	TYR	-	expression tag	UNP P40046
C	176	ALA	-	expression tag	UNP P40046

- Molecule 3 is a protein called Vacuolar transporter chaperone 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	650	Total	C	N	O	S	0	0
			5408	3472	919	1009	8		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP Q02725
E	2	ASP	-	expression tag	UNP Q02725
E	3	TYR	-	expression tag	UNP Q02725
E	4	LYS	-	expression tag	UNP Q02725
E	5	ASP	-	expression tag	UNP Q02725
E	6	ASP	-	expression tag	UNP Q02725

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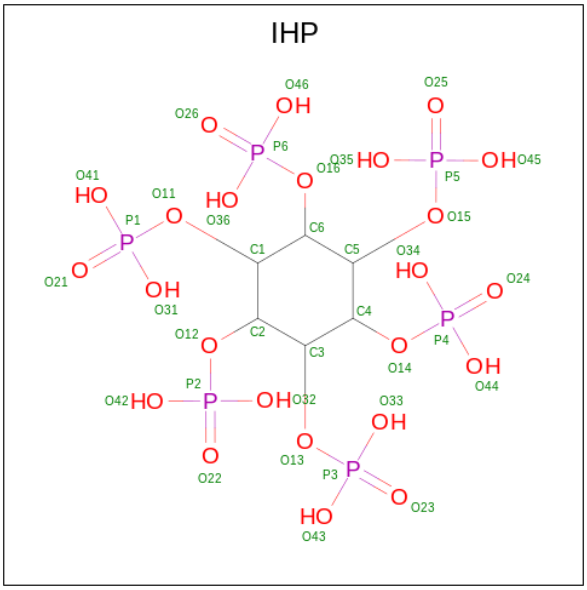
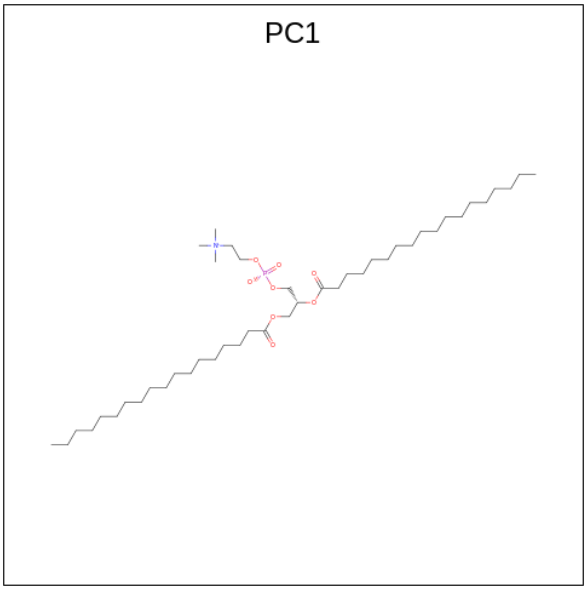
Chain	Residue	Modelled	Actual	Comment	Reference
E	7	ASP	-	expression tag	UNP Q02725
E	8	ASP	-	expression tag	UNP Q02725
E	9	LYS	-	expression tag	UNP Q02725
E	10	GLY	-	expression tag	UNP Q02725
E	11	ASP	-	expression tag	UNP Q02725
E	12	TYR	-	expression tag	UNP Q02725
E	13	LYS	-	expression tag	UNP Q02725
E	14	ASP	-	expression tag	UNP Q02725
E	15	ASP	-	expression tag	UNP Q02725
E	16	ASP	-	expression tag	UNP Q02725
E	17	ASP	-	expression tag	UNP Q02725
E	18	LYS	-	expression tag	UNP Q02725
E	19	ILE	-	expression tag	UNP Q02725
E	20	ASP	-	expression tag	UNP Q02725
E	21	TYR	-	expression tag	UNP Q02725
E	22	LYS	-	expression tag	UNP Q02725
E	23	ASP	-	expression tag	UNP Q02725
E	24	ASP	-	expression tag	UNP Q02725
E	25	ASP	-	expression tag	UNP Q02725
E	26	ASP	-	expression tag	UNP Q02725
E	27	LYS	-	expression tag	UNP Q02725
E	28	GLY	-	expression tag	UNP Q02725
E	29	SER	-	expression tag	UNP Q02725

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



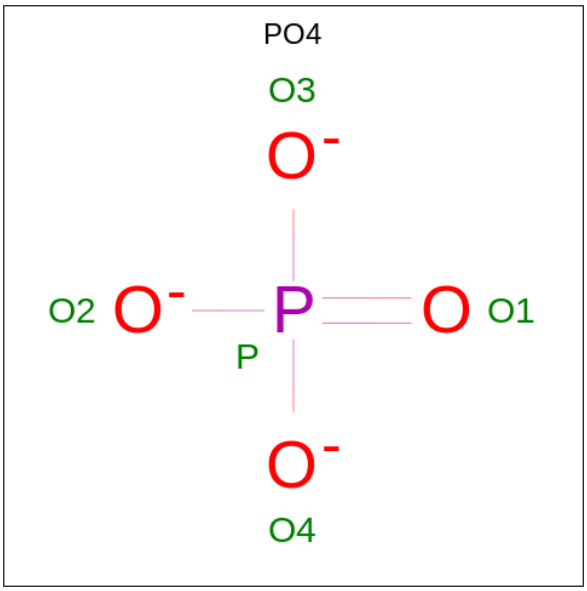
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	O	P	0
			36	6	24	6	
4	D	1	Total	C	O	P	0
			36	6	24	6	
4	D	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	E	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

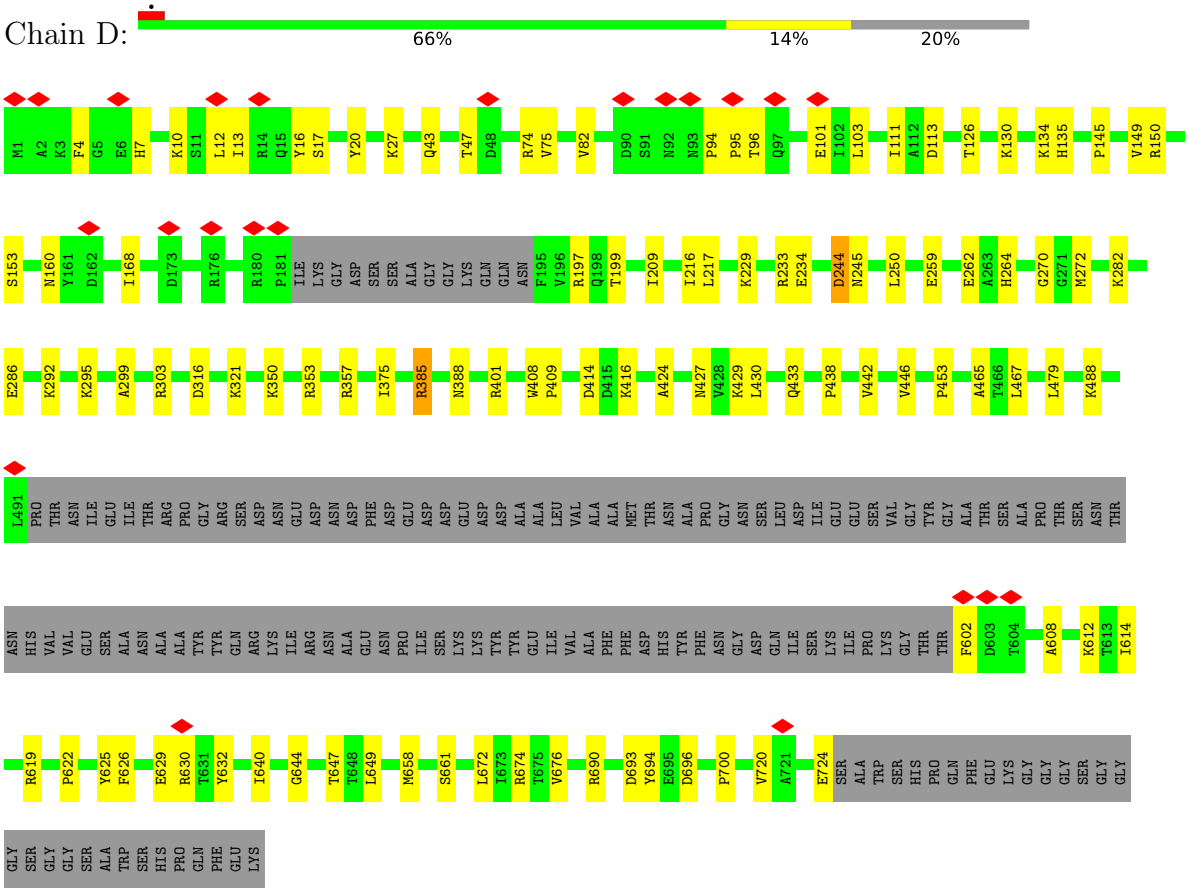


Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

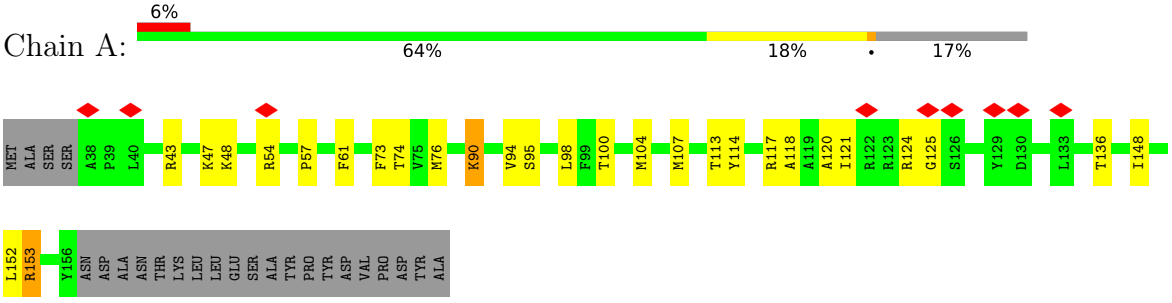
3 Residue-property plots (i)

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: Vacuolar transporter chaperone 4

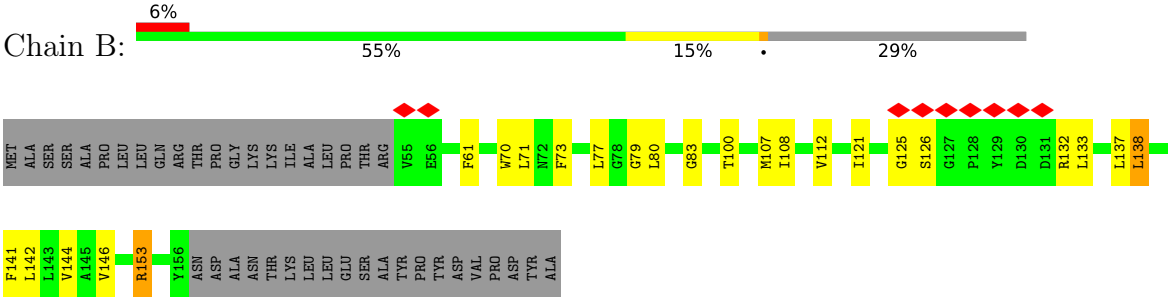


• Molecule 2: Vacuolar transporter chaperone 1



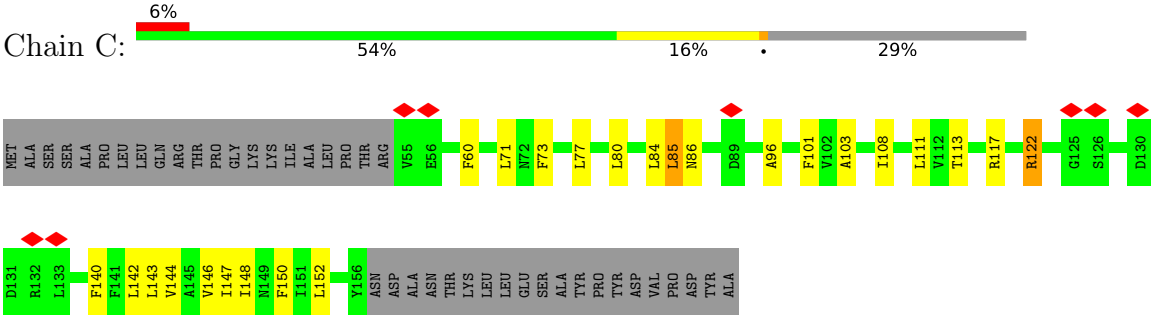
• Molecule 2: Vacuolar transporter chaperone 1

Chain B:



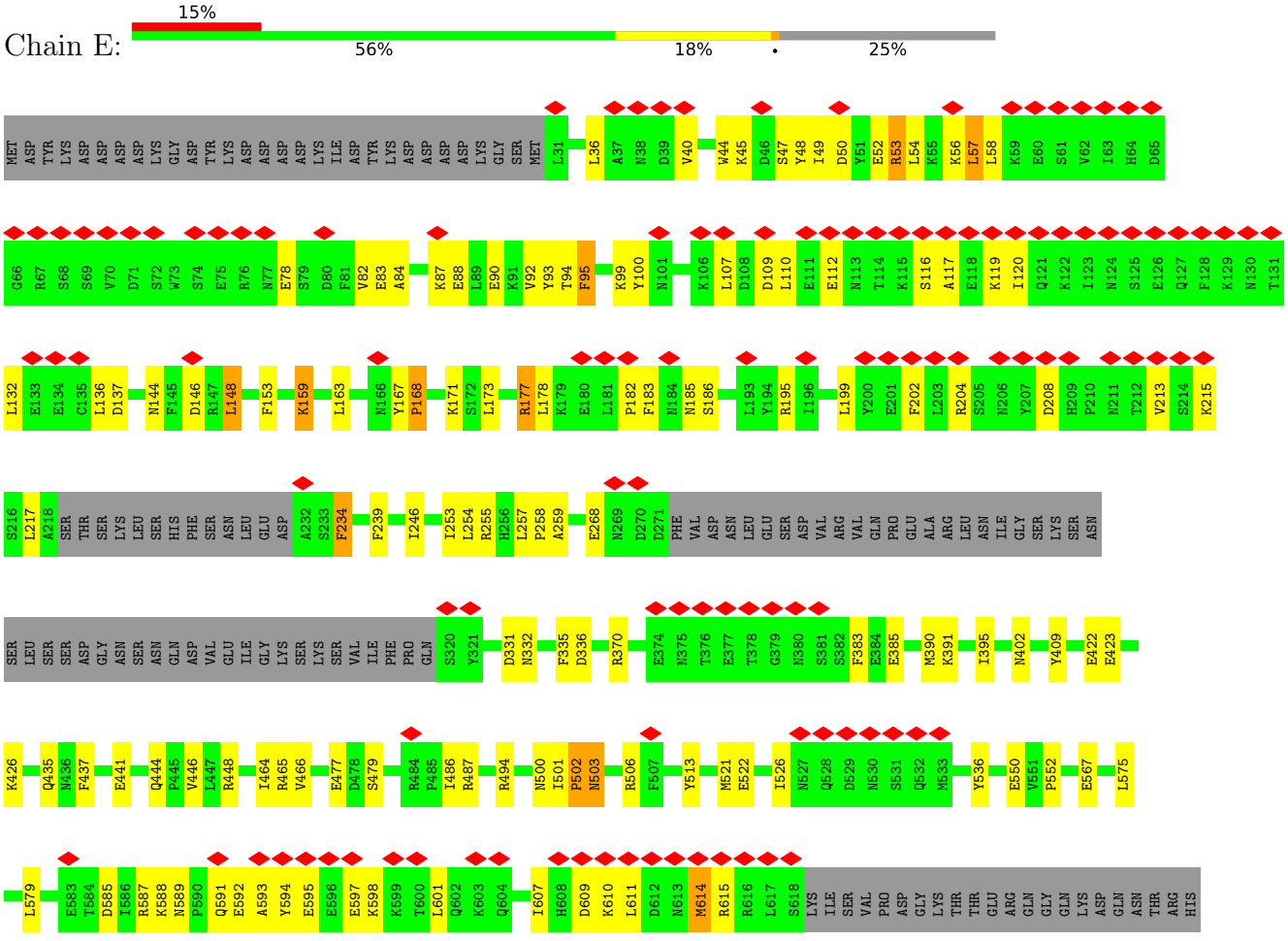
• Molecule 2: Vacuolar transporter chaperone 1

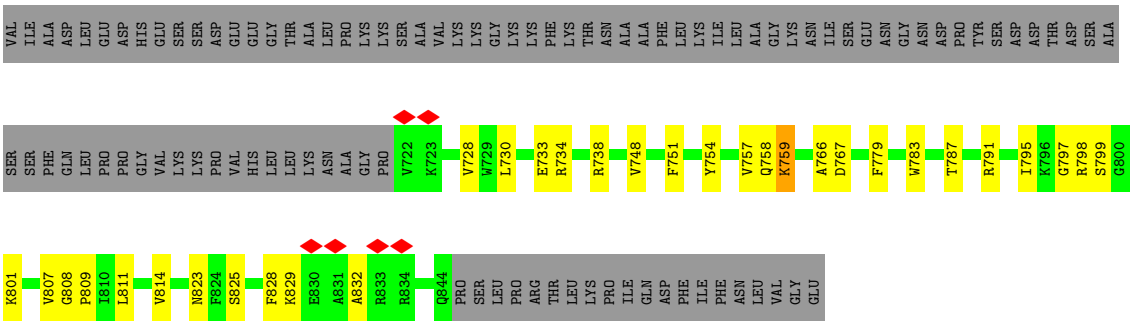
Chain C:



• Molecule 3: Vacuolar transporter chaperone 3

Chain E:




VAL ILE ALA ASP LEU GLU ASP HIS GLU SER SER ASP GLU GLU GLY THR ALA LEU PRO LYS LYS SER ALA VAL LYS LYS GLY LYS LYS PHE LYS THR ASN ALA ALA PHE LEU LYS ILE LEU ALA GLY LYS ASN ILE SER GLU ASN GLY ASN ASP PRO TYR SER ASP ASP THR ASP SER ALA
SER SER PHE GLN LEU PRO PRO GLY VAL LYS LYS PRO VAL HIS LEU LEU LYS ASN ALA GLY PRO V722 K723 V728 W729 L730 E733 R734 R738 V748 F751 Y754 V757 Q758 K759 A766 D767 F779 W783 T787 R791 I795 K796 G797 R798 S799 G800
K801 V807 G808 P809 I810 L811 V814 N823 F824 S825 F828 K829 E830 A831 A832 R833 R834 Q844 PRO SER LEU PRO ARG THR LEU LYS PRO ILE GLN ASP PHE ILE PHE ASN LEU VAL GLY GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	734934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.565	Depositor
Minimum map value	-3.078	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, PO4, IHP

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	D	0.27	0/5052	0.48	0/6831
2	A	0.26	0/965	0.51	0/1307
2	B	0.27	0/832	0.48	0/1126
2	C	0.26	0/832	0.49	0/1126
3	E	0.27	0/5529	0.53	4/7479 (0.1%)
All	All	0.27	0/13210	0.50	4/17869 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	PRO	CA-N-CD	-9.30	98.48	111.50
3	E	168	PRO	CA-N-CD	-7.73	100.68	111.50
3	E	57	LEU	CA-CB-CG	6.70	130.72	115.30
3	E	148	LEU	CA-CB-CG	6.42	130.07	115.30

There are no chirality outliers.

There are no planarity outliers.

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	D	4940	0	4991	66	0
2	A	941	0	990	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	811	0	838	21	0
2	C	811	0	838	21	0
3	E	5408	0	5387	113	0
4	D	108	0	18	6	0
5	D	54	0	88	7	0
5	E	54	0	88	11	0
6	D	10	0	0	0	0
All	All	13137	0	13238	219	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 8.

All (219) 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:D:145:PRO:HG3	3:E:594:TYR:HB2	1.60	0.84
3:E:589:ASN:HB3	3:E:592:GLU:HB2	1.58	0.83
3:E:594:TYR:HA	3:E:598:LYS:HB3	1.61	0.82
3:E:593:ALA:HA	3:E:597:GLU:HB2	1.62	0.82
2:C:113:THR:HG22	2:C:117:ARG:HD2	1.61	0.81
3:E:40:VAL:HA	3:E:48:TYR:HE2	1.45	0.81
2:C:60:PHE:HB2	2:C:122:ARG:HH12	1.55	0.72
3:E:791:ARG:O	3:E:795:ILE:HG12	1.89	0.71
3:E:95:PHE:HE1	3:E:99:LYS:HD2	1.54	0.70
1:D:286:GLU:OE2	1:D:619:ARG:NH1	2.29	0.66
2:B:79:GLY:HA2	5:E:901:PC1:H3C1	1.79	0.64
2:C:84:LEU:HB3	2:C:96:ALA:HB2	1.79	0.64
5:D:1003:PC1:H3A1	5:D:1003:PC1:H3F1	1.80	0.64
3:E:592:GLU:HA	3:E:595:GLU:HB2	1.80	0.64
1:D:229:LYS:O	3:E:465:ARG:NH2	2.32	0.63
3:E:53:ARG:O	3:E:57:LEU:HD12	1.98	0.63
2:C:80:LEU:HB3	5:E:901:PC1:H3B2	1.80	0.63
3:E:734:ARG:O	3:E:738:ARG:HG3	1.98	0.63
3:E:178:LEU:HD22	3:E:185:ASN:HD21	1.63	0.62
2:A:100:THR:O	2:A:104:MET:HG2	2.00	0.62
2:B:121:ILE:HD12	2:B:125:GLY:HA2	1.83	0.61
1:D:12:LEU:HD13	1:D:17:SER:HB3	1.83	0.61
2:C:140:PHE:O	2:C:144:VAL:HG23	2.00	0.60
3:E:173:LEU:H	3:E:173:LEU:HD12	1.66	0.60
1:D:282:LYS:NZ	4:D:1002:IHP:O22	2.30	0.59
1:D:74:ARG:NH2	1:D:113:ASP:OD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ASN:HD21	1:D:350:LYS:HB3	1.68	0.59
1:D:321:LYS:NZ	4:D:1004:IHP:O11	2.35	0.58
3:E:331:ASP:HB3	3:E:446:VAL:HG21	1.84	0.58
1:D:75:VAL:HG22	1:D:168:ILE:HD11	1.84	0.58
3:E:83:GLU:O	3:E:87:LYS:HG2	2.03	0.58
1:D:353:ARG:NH1	1:D:388:ASN:OD1	2.35	0.58
3:E:502:PRO:HD2	3:E:503:ASN:N	2.19	0.57
1:D:126:THR:HG23	3:E:255:ARG:HD2	1.86	0.56
2:A:148:ILE:O	2:A:152:LEU:HD12	2.05	0.56
2:B:153:ARG:HH21	3:E:758:GLN:HE22	1.52	0.56
3:E:168:PRO:HD2	3:E:168:PRO:O	2.04	0.56
1:D:442:VAL:O	1:D:446:VAL:HG22	2.05	0.56
3:E:78:GLU:O	3:E:82:VAL:HG23	2.04	0.56
5:D:1003:PC1:H3D1	5:E:901:PC1:H2B1	1.86	0.56
3:E:54:LEU:HD21	3:E:88:GLU:HG3	1.89	0.56
3:E:757:VAL:HG23	3:E:766:ALA:HB3	1.88	0.56
4:D:1004:IHP:O45	3:E:409:TYR:OH	2.20	0.55
3:E:90:GLU:OE2	3:E:94:THR:OG1	2.24	0.55
2:C:80:LEU:HD21	5:E:901:PC1:H2C2	1.88	0.55
3:E:52:GLU:O	3:E:56:LYS:HD2	2.07	0.55
2:A:136:THR:HG23	2:C:111:LEU:HD21	1.87	0.55
2:B:133:LEU:O	2:B:137:LEU:HG	2.07	0.55
3:E:448:ARG:NE	3:E:477:GLU:OE2	2.38	0.55
3:E:797:GLY:O	3:E:799:SER:N	2.39	0.55
2:C:77:LEU:HB3	2:C:103:ALA:HB2	1.90	0.54
1:D:217:LEU:HD22	3:E:258:PRO:HG3	1.90	0.54
3:E:477:GLU:HG2	3:E:494:ARG:HD3	1.90	0.54
5:D:1003:PC1:H221	5:E:901:PC1:H321	1.90	0.53
3:E:116:SER:O	3:E:119:LYS:N	2.41	0.53
3:E:204:ARG:O	3:E:208:ASP:HB2	2.09	0.53
3:E:614:MET:SD	3:E:615:ARG:N	2.81	0.53
3:E:95:PHE:CE1	3:E:99:LYS:HD2	2.41	0.53
1:D:488:LYS:HG2	2:A:48:LYS:HE3	1.91	0.52
2:C:143:LEU:O	2:C:147:ILE:HG12	2.09	0.52
3:E:502:PRO:HD2	3:E:503:ASN:H	1.74	0.52
2:A:153:ARG:HG2	2:C:85:LEU:HD22	1.92	0.52
1:D:453:PRO:HD2	2:A:47:LYS:HD3	1.91	0.52
2:B:70:TRP:HZ3	2:B:138:LEU:HD13	1.73	0.52
1:D:672:LEU:O	1:D:676:VAL:HG23	2.10	0.51
1:D:209:ILE:HD11	1:D:424:ALA:HB3	1.92	0.51
2:A:153:ARG:NH2	2:C:86:ASN:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:HG21	3:E:591:GLN:HB2	1.92	0.51
1:D:199:THR:HG23	1:D:429:LYS:HG2	1.93	0.51
3:E:234:PHE:HB2	3:E:526:ILE:HD13	1.91	0.51
3:E:730:LEU:O	3:E:734:ARG:HG2	2.11	0.51
3:E:829:LYS:O	3:E:832:ALA:N	2.37	0.51
2:B:70:TRP:CZ3	2:B:138:LEU:HD13	2.46	0.50
3:E:748:VAL:HG11	5:E:901:PC1:H2B2	1.93	0.50
3:E:49:ILE:HB	3:E:153:PHE:HE2	1.77	0.50
3:E:95:PHE:HD1	3:E:95:PHE:O	1.94	0.50
1:D:82:VAL:HG22	1:D:103:LEU:HD13	1.94	0.50
2:B:71:LEU:HD13	2:C:73:PHE:CE1	2.47	0.50
3:E:607:ILE:O	3:E:610:LYS:HG2	2.12	0.50
1:D:632:TYR:CE2	3:E:809:PRO:HB3	2.47	0.50
1:D:430:LEU:HD21	1:D:442:VAL:HG11	1.94	0.49
3:E:783:TRP:CZ2	3:E:787:THR:HG21	2.47	0.49
3:E:109:ASP:O	3:E:112:GLU:HG3	2.13	0.49
1:D:27:LYS:HG3	1:D:134:LYS:HE3	1.93	0.49
5:D:1003:PC1:H372	5:D:1003:PC1:H2E2	1.95	0.49
3:E:422:GLU:HG2	3:E:423:GLU:N	2.26	0.49
2:C:142:LEU:O	2:C:146:VAL:HG23	2.13	0.49
3:E:486:ILE:HG22	3:E:494:ARG:HD2	1.94	0.48
3:E:44:TRP:N	3:E:44:TRP:CD1	2.81	0.48
3:E:117:ALA:HA	3:E:120:ILE:HD12	1.93	0.48
3:E:47:SER:HG	3:E:95:PHE:HE2	1.59	0.48
3:E:159:LYS:O	3:E:163:LEU:HG	2.13	0.48
1:D:12:LEU:HB3	1:D:20:TYR:HE2	1.78	0.48
2:B:153:ARG:NH2	3:E:758:GLN:HE22	2.11	0.48
3:E:254:LEU:HD21	3:E:259:ALA:HB2	1.96	0.48
3:E:331:ASP:OD2	3:E:335:PHE:HA	2.14	0.48
1:D:95:PRO:O	1:D:96:THR:OG1	2.25	0.48
1:D:640:ILE:O	1:D:644:GLY:N	2.40	0.48
1:D:720:VAL:HG13	1:D:724:GLU:HG3	1.96	0.48
2:A:73:PHE:CE2	2:C:71:LEU:HD23	2.49	0.47
5:E:901:PC1:H2C2	5:E:901:PC1:H2F1	1.62	0.47
1:D:250:LEU:HD21	1:D:264:HIS:HD2	1.80	0.47
1:D:465:ALA:HB1	1:D:479:LEU:HD22	1.96	0.47
1:D:647:THR:HA	3:E:823:ASN:HD21	1.80	0.47
2:A:121:ILE:HA	2:A:125:GLY:HA2	1.97	0.47
1:D:216:ILE:HD13	1:D:375:ILE:HG21	1.97	0.47
1:D:626:PHE:HE2	3:E:728:VAL:HG13	1.80	0.47
2:B:80:LEU:HD22	3:E:748:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:167:TYR:HB3	3:E:168:PRO:HD3	1.98	0.46
3:E:779:PHE:CZ	3:E:811:LEU:HD23	2.50	0.46
1:D:12:LEU:HD22	1:D:17:SER:HA	1.97	0.46
1:D:295:LYS:NZ	4:D:1002:IHP:O41	2.40	0.46
3:E:487:ARG:HB3	3:E:494:ARG:HG2	1.97	0.46
3:E:53:ARG:HH12	3:E:84:ALA:HB1	1.80	0.46
1:D:234:GLU:O	1:D:270:GLY:HA2	2.16	0.46
1:D:622:PRO:O	1:D:625:TYR:HB2	2.16	0.46
3:E:49:ILE:HB	3:E:153:PHE:CE2	2.51	0.46
3:E:585:ASP:OD1	3:E:587:ARG:NH1	2.48	0.46
1:D:244:ASP:OD2	1:D:250:LEU:HB2	2.16	0.45
1:D:250:LEU:HD23	1:D:262:GLU:O	2.17	0.45
2:B:83:GLY:HA3	5:E:901:PC1:H262	1.98	0.45
2:B:141:PHE:HA	2:B:144:VAL:HG12	1.98	0.45
3:E:100:TYR:CE2	3:E:182:PRO:HG2	2.50	0.45
2:B:71:LEU:HD23	2:B:71:LEU:HA	1.82	0.45
2:A:76:MET:HG2	5:E:901:PC1:H2G1	1.99	0.45
1:D:13:ILE:HD11	1:D:16:TYR:HE1	1.81	0.44
1:D:303:ARG:NH2	4:D:1004:IHP:O46	2.50	0.44
1:D:608:ALA:HB1	1:D:612:LYS:O	2.17	0.44
2:B:121:ILE:HD13	2:B:126:SER:H	1.81	0.44
3:E:136:LEU:HD12	3:E:137:ASP:N	2.32	0.44
3:E:332:ASN:HD21	3:E:336:ASP:HB2	1.82	0.44
3:E:239:PHE:CE1	3:E:550:GLU:HG3	2.53	0.44
3:E:257:LEU:HD11	3:E:464:ILE:HG22	2.00	0.44
1:D:245:ASN:ND2	1:D:350:LYS:HB3	2.33	0.44
2:B:146:VAL:HG22	3:E:751:PHE:HE2	1.83	0.44
3:E:213:VAL:HG13	3:E:215:LYS:H	1.82	0.44
3:E:464:ILE:HD11	3:E:536:TYR:CD1	2.53	0.44
1:D:626:PHE:O	1:D:630:ARG:HG3	2.17	0.44
1:D:694:TYR:CD2	2:A:57:PRO:HB3	2.53	0.44
2:A:90:LYS:O	2:A:94:VAL:HG23	2.18	0.44
1:D:357:ARG:NH2	1:D:401:ARG:O	2.50	0.44
3:E:594:TYR:HB3	3:E:598:LYS:HE3	2.00	0.44
1:D:4:PHE:HB2	1:D:130:LYS:HE2	2.00	0.43
1:D:649:LEU:HB2	1:D:661:SER:HB2	1.99	0.43
2:C:148:ILE:O	2:C:152:LEU:HG	2.18	0.43
2:A:120:ALA:O	2:A:125:GLY:N	2.39	0.43
5:D:1003:PC1:H2F2	5:D:1003:PC1:H2C2	1.74	0.43
3:E:783:TRP:CH2	3:E:787:THR:HG21	2.53	0.43
1:D:43:GLN:O	1:D:47:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:93:TYR:HD1	3:E:177:ARG:HG3	1.84	0.43
3:E:100:TYR:CD2	3:E:182:PRO:HG2	2.53	0.43
3:E:107:LEU:HD13	3:E:195:ARG:HD2	2.00	0.43
3:E:444:GLN:OE1	3:E:479:SER:OG	2.35	0.43
5:D:1003:PC1:H3D1	5:E:901:PC1:H2D1	2.01	0.43
3:E:437:PHE:CE1	3:E:441:GLU:HG3	2.53	0.42
1:D:674:ARG:NH2	1:D:696:ASP:OD1	2.46	0.42
2:B:108:ILE:O	2:B:112:VAL:HG23	2.19	0.42
2:A:74:THR:HG21	2:A:107:MET:HB2	2.01	0.42
2:B:61:PHE:HE1	2:C:117:ARG:HH21	1.67	0.42
3:E:110:LEU:HD23	3:E:199:LEU:HD12	2.00	0.42
1:D:94:PRO:O	1:D:96:THR:HG23	2.20	0.42
1:D:299:ALA:HB3	3:E:268:GLU:HA	2.01	0.42
1:D:385:ARG:HD3	1:D:467:LEU:HB3	2.02	0.42
3:E:53:ARG:NH1	3:E:84:ALA:HB1	2.35	0.42
3:E:575:LEU:HB3	3:E:579:LEU:HD12	2.00	0.42
2:C:122:ARG:N	2:C:122:ARG:HD2	2.34	0.42
3:E:370:ARG:HB3	3:E:383:PHE:CE1	2.55	0.42
3:E:597:GLU:OE1	3:E:597:GLU:N	2.52	0.42
2:A:153:ARG:HE	2:A:153:ARG:HB2	1.68	0.42
3:E:50:ASP:HB3	3:E:53:ARG:HG2	2.01	0.42
2:B:100:THR:HG21	2:C:150:PHE:CE2	2.55	0.42
3:E:144:ASN:O	3:E:148:LEU:HD12	2.19	0.42
3:E:186:SER:HB2	3:E:552:PRO:HD2	2.01	0.42
3:E:402:ASN:HA	3:E:435:GLN:NE2	2.35	0.42
3:E:607:ILE:O	3:E:611:LEU:HG	2.20	0.42
2:C:108:ILE:HD13	2:C:108:ILE:HA	1.90	0.41
3:E:132:LEU:HD21	3:E:199:LEU:HB2	2.02	0.41
3:E:598:LYS:HA	3:E:601:LEU:HB3	2.01	0.41
3:E:50:ASP:O	3:E:53:ARG:HG2	2.20	0.41
3:E:811:LEU:HA	3:E:814:VAL:HG22	2.02	0.41
3:E:783:TRP:CE2	3:E:808:GLY:HA3	2.55	0.41
2:A:113:THR:HG22	2:A:117:ARG:HE	1.85	0.41
3:E:370:ARG:HG2	3:E:385:GLU:HG3	2.03	0.41
1:D:408:TRP:CG	1:D:409:PRO:HA	2.56	0.41
1:D:430:LEU:HD22	1:D:438:PRO:HB3	2.02	0.41
3:E:88:GLU:O	3:E:92:VAL:HG23	2.20	0.41
3:E:795:ILE:O	3:E:798:ARG:HG2	2.21	0.41
1:D:693:ASP:OD1	1:D:693:ASP:N	2.38	0.41
2:A:118:ALA:HA	2:A:121:ILE:HG12	2.01	0.41
2:B:77:LEU:HD11	2:B:142:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:MET:HB3	3:E:828:PHE:CZ	2.56	0.41
3:E:783:TRP:CH2	3:E:809:PRO:HD3	2.55	0.41
1:D:111:ILE:HG13	1:D:168:ILE:HG21	2.03	0.41
1:D:135:HIS:CD2	1:D:135:HIS:C	2.95	0.41
1:D:629:GLU:O	1:D:632:TYR:HB3	2.21	0.41
2:A:73:PHE:CZ	2:C:71:LEU:HB3	2.56	0.41
2:B:70:TRP:HA	2:B:73:PHE:HD2	1.85	0.41
3:E:36:LEU:O	3:E:40:VAL:HG23	2.20	0.41
3:E:253:ILE:HD11	3:E:521:MET:HE1	2.02	0.41
3:E:390:MET:HE2	3:E:395:ILE:HG12	2.03	0.41
3:E:501:ILE:HG13	3:E:502:PRO:HD3	2.03	0.41
3:E:588:LYS:HB3	3:E:597:GLU:OE2	2.21	0.41
1:D:488:LYS:HE3	2:A:47:LYS:NZ	2.36	0.41
5:D:1003:PC1:H221	5:D:1003:PC1:H252	1.89	0.41
3:E:391:LYS:O	3:E:395:ILE:HG13	2.21	0.41
3:E:95:PHE:CD1	3:E:95:PHE:C	2.94	0.40
1:D:658:MET:HB3	3:E:828:PHE:HZ	1.85	0.40
1:D:199:THR:HG21	4:D:1002:IHP:O44	2.22	0.40
2:A:57:PRO:HB2	2:A:61:PHE:CE2	2.57	0.40
2:B:100:THR:HG21	2:C:150:PHE:CZ	2.56	0.40
3:E:253:ILE:HD13	3:E:466:VAL:HG11	2.03	0.40
1:D:602:PHE:N	2:A:43:ARG:O	2.55	0.40
3:E:759:LYS:HE3	5:E:901:PC1:H11	2.03	0.40
1:D:608:ALA:HB2	1:D:614:ILE:HG13	2.03	0.40
1:D:626:PHE:CE2	3:E:728:VAL:HG13	2.57	0.40
1:D:700:PRO:HG2	2:A:114:TYR:CE2	2.57	0.40
2:B:153:ARG:HB3	3:E:754:TYR:CE2	2.57	0.40
3:E:58:LEU:HD23	3:E:58:LEU:HA	1.95	0.40
3:E:246:ILE:HD13	3:E:246:ILE:HA	1.85	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	D	595/754 (79%)	580 (98%)	15 (2%)	0	100	100
2	A	117/143 (82%)	111 (95%)	6 (5%)	0	100	100
2	B	100/143 (70%)	96 (96%)	4 (4%)	0	100	100
2	C	100/143 (70%)	97 (97%)	3 (3%)	0	100	100
3	E	642/864 (74%)	619 (96%)	23 (4%)	0	100	100
All	All	1554/2047 (76%)	1503 (97%)	51 (3%)	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	D	550/671 (82%)	531 (96%)	19 (4%)	36	71
2	A	97/117 (83%)	91 (94%)	6 (6%)	18	52
2	B	83/117 (71%)	79 (95%)	4 (5%)	25	62
2	C	83/117 (71%)	80 (96%)	3 (4%)	35	70
3	E	606/797 (76%)	580 (96%)	26 (4%)	29	66
All	All	1419/1819 (78%)	1361 (96%)	58 (4%)	34	67

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	7	HIS
1	D	10	LYS
1	D	101	GLU
1	D	150	ARG
1	D	153	SER
1	D	160	ASN
1	D	197	ARG
1	D	233	ARG
1	D	244	ASP
1	D	259	GLU

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Mol	Chain	Res	Type
1	D	272	MET
1	D	292	LYS
1	D	316	ASP
1	D	385	ARG
1	D	414	ASP
1	D	416	LYS
1	D	427	ASN
1	D	433	GLN
1	D	690	ARG
2	A	54	ARG
2	A	90	LYS
2	A	95	SER
2	A	98	LEU
2	A	124	ARG
2	A	153	ARG
2	B	107	MET
2	B	132	ARG
2	B	138	LEU
2	B	153	ARG
2	C	85	LEU
2	C	101	PHE
2	C	122	ARG
3	E	45	LYS
3	E	53	ARG
3	E	95	PHE
3	E	146	ASP
3	E	159	LYS
3	E	171	LYS
3	E	177	ARG
3	E	183	PHE
3	E	202	PHE
3	E	217	LEU
3	E	234	PHE
3	E	426	LYS
3	E	500	ASN
3	E	503	ASN
3	E	506	ARG
3	E	513	TYR
3	E	522	GLU
3	E	567	GLU
3	E	609	ASP
3	E	614	MET

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Mol	Chain	Res	Type
3	E	733	GLU
3	E	759	LYS
3	E	767	ASP
3	E	801	LYS
3	E	807	VAL
3	E	825	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	15	GLN
1	D	160	ASN
1	D	198	GLN
1	D	264	HIS
1	D	335	ASN
1	D	427	ASN
1	D	605	GLN
3	E	101	ASN
3	E	185	ASN
3	E	433	ASN
3	E	462	GLN
3	E	527	ASN
3	E	602	GLN
3	E	758	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
6	PO4	D	1006	-	4,4,4	0.93	0	6,6,6	0.44	0
5	PC1	D	1003	-	53,53,53	0.93	4 (7%)	59,61,61	1.03	2 (3%)
4	IHP	D	1004	-	36,36,36	1.51	6 (16%)	54,60,60	0.84	3 (5%)
5	PC1	E	901	-	53,53,53	0.94	4 (7%)	59,61,61	1.05	2 (3%)
4	IHP	D	1002	-	36,36,36	1.54	6 (16%)	54,60,60	1.06	6 (11%)
4	IHP	D	1001	-	36,36,36	1.48	6 (16%)	54,60,60	1.06	5 (9%)
6	PO4	D	1005	-	4,4,4	0.93	0	6,6,6	0.44	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
5	PC1	D	1003	-	-	24/57/57/57	-
4	IHP	D	1004	-	-	7/30/54/54	0/1/1/1
5	PC1	E	901	-	-	25/57/57/57	-
4	IHP	D	1002	-	-	12/30/54/54	0/1/1/1
4	IHP	D	1001	-	-	7/30/54/54	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	IHP	P4-O14	3.57	1.66	1.59
4	D	1004	IHP	P1-O11	3.54	1.66	1.59
4	D	1002	IHP	P3-O13	3.46	1.65	1.59
4	D	1002	IHP	P6-O16	3.34	1.65	1.59
4	D	1002	IHP	P1-O11	3.31	1.65	1.59
4	D	1002	IHP	P5-O15	3.24	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	IHP	P2-O12	3.23	1.65	1.59
4	D	1001	IHP	P1-O11	3.22	1.65	1.59
4	D	1004	IHP	P4-O14	3.22	1.65	1.59
4	D	1004	IHP	P3-O13	3.17	1.65	1.59
4	D	1001	IHP	P6-O16	3.16	1.65	1.59
4	D	1001	IHP	P4-O14	3.16	1.65	1.59
4	D	1001	IHP	P2-O12	3.16	1.65	1.59
4	D	1001	IHP	P3-O13	3.15	1.65	1.59
4	D	1004	IHP	P5-O15	3.14	1.65	1.59
4	D	1001	IHP	P5-O15	3.13	1.65	1.59
4	D	1004	IHP	P2-O12	3.13	1.65	1.59
4	D	1004	IHP	P6-O16	3.10	1.65	1.59
5	D	1003	PC1	O21-C2	-2.62	1.40	1.46
5	E	901	PC1	O21-C2	-2.44	1.40	1.46
5	E	901	PC1	O31-C31	2.40	1.40	1.33
5	D	1003	PC1	O31-C31	2.34	1.40	1.33
5	E	901	PC1	O21-C21	2.18	1.40	1.34
5	E	901	PC1	O31-C3	-2.17	1.40	1.45
5	D	1003	PC1	O31-C3	-2.12	1.40	1.45
5	D	1003	PC1	O21-C21	2.03	1.40	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	901	PC1	O21-C21-C22	4.10	120.34	111.50
5	D	1003	PC1	O21-C21-C22	3.88	119.86	111.50
4	D	1001	IHP	C5-C4-C3	3.58	118.24	110.41
4	D	1001	IHP	C4-C3-C2	3.37	117.79	110.41
4	D	1001	IHP	C6-C5-C4	3.14	117.28	110.41
4	D	1004	IHP	C6-C1-C2	2.80	116.55	110.41
4	D	1001	IHP	C3-C2-C1	2.65	116.21	110.41
5	E	901	PC1	O31-C31-C32	2.62	120.14	111.91
4	D	1002	IHP	O12-C2-C3	2.60	114.82	108.69
4	D	1002	IHP	O13-C3-C2	2.51	114.61	108.69
5	D	1003	PC1	O31-C31-C32	2.46	119.63	111.91
4	D	1002	IHP	O16-C6-C5	2.34	114.20	108.69
4	D	1001	IHP	C5-C6-C1	2.29	115.43	110.41
4	D	1004	IHP	C5-C6-C1	2.20	115.23	110.41
4	D	1002	IHP	C6-C1-C2	-2.12	105.78	110.41
4	D	1002	IHP	O15-C5-C6	2.04	113.49	108.69
4	D	1004	IHP	O11-C1-C2	2.04	113.48	108.69
4	D	1002	IHP	C4-C3-C2	-2.02	105.99	110.41

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1001	IHP	C2-C1-O11-P1
4	D	1001	IHP	C2-O12-P2-O22
4	D	1001	IHP	C5-O15-P5-O25
4	D	1002	IHP	C2-C3-O13-P3
4	D	1002	IHP	C3-C4-O14-P4
4	D	1002	IHP	C5-C4-O14-P4
4	D	1002	IHP	C6-O16-P6-O46
4	D	1004	IHP	C2-C1-O11-P1
4	D	1004	IHP	C2-O12-P2-O22
5	D	1003	PC1	O21-C2-C3-O31
5	E	901	PC1	C1-O11-P-O12
5	E	901	PC1	C1-O11-P-O14
5	E	901	PC1	C1-O11-P-O13
5	E	901	PC1	C22-C21-O21-C2
5	E	901	PC1	O22-C21-O21-C2
5	E	901	PC1	O32-C31-O31-C3
5	E	901	PC1	C32-C31-O31-C3
5	E	901	PC1	C31-C32-C33-C34
5	E	901	PC1	C21-C22-C23-C24
5	E	901	PC1	C39-C3A-C3B-C3C
4	D	1001	IHP	C6-C1-O11-P1
4	D	1002	IHP	C2-C1-O11-P1
4	D	1002	IHP	C4-C3-O13-P3
5	D	1003	PC1	C39-C3A-C3B-C3C
5	E	901	PC1	C32-C33-C34-C35
5	D	1003	PC1	C27-C28-C29-C2A
5	E	901	PC1	C3D-C3E-C3F-C3G
5	D	1003	PC1	C23-C24-C25-C26
5	D	1003	PC1	C24-C25-C26-C27
5	D	1003	PC1	C25-C26-C27-C28
5	E	901	PC1	C29-C2A-C2B-C2C
5	D	1003	PC1	C22-C21-O21-C2
5	D	1003	PC1	O22-C21-O21-C2
5	D	1003	PC1	O21-C21-C22-C23
5	D	1003	PC1	C3B-C3C-C3D-C3E
5	D	1003	PC1	C3D-C3E-C3F-C3G
5	E	901	PC1	O21-C2-C3-O31
5	D	1003	PC1	C35-C36-C37-C38
4	D	1002	IHP	C2-O12-P2-O22
5	D	1003	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	D	1003	PC1	C22-C23-C24-C25
5	D	1003	PC1	C1-C2-C3-O31
4	D	1001	IHP	C3-C2-O12-P2
4	D	1001	IHP	C5-O15-P5-O45
4	D	1002	IHP	C1-O11-P1-O31
4	D	1002	IHP	C5-O15-P5-O35
5	E	901	PC1	O11-C1-C2-C3
5	E	901	PC1	O11-C1-C2-O21
5	E	901	PC1	C2B-C2C-C2D-C2E
5	D	1003	PC1	C11-O13-P-O11
5	E	901	PC1	C11-O13-P-O11
4	D	1004	IHP	C6-C1-O11-P1
5	D	1003	PC1	O22-C21-C22-C23
5	D	1003	PC1	C29-C2A-C2B-C2C
5	E	901	PC1	C2C-C2D-C2E-C2F
5	D	1003	PC1	C34-C35-C36-C37
5	D	1003	PC1	C32-C33-C34-C35
4	D	1002	IHP	C6-C1-O11-P1
4	D	1004	IHP	C4-C5-O15-P5
5	D	1003	PC1	O11-C1-C2-O21
4	D	1001	IHP	C4-O14-P4-O24
4	D	1004	IHP	C6-O16-P6-O26
5	E	901	PC1	O31-C31-C32-C33
5	E	901	PC1	C23-C24-C25-C26
5	E	901	PC1	C3C-C3D-C3E-C3F
4	D	1002	IHP	C2-O12-P2-O42
4	D	1002	IHP	C5-O15-P5-O45
4	D	1004	IHP	C1-O11-P1-O41
4	D	1004	IHP	C2-O12-P2-O32
5	E	901	PC1	O32-C31-C32-C33
5	E	901	PC1	C1-C2-C3-O31
5	D	1003	PC1	C11-O13-P-O14
5	D	1003	PC1	C1-O11-P-O14
5	E	901	PC1	C11-O13-P-O14
5	D	1003	PC1	C2B-C2C-C2D-C2E

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1003	PC1	7	0
4	D	1004	IHP	3	0

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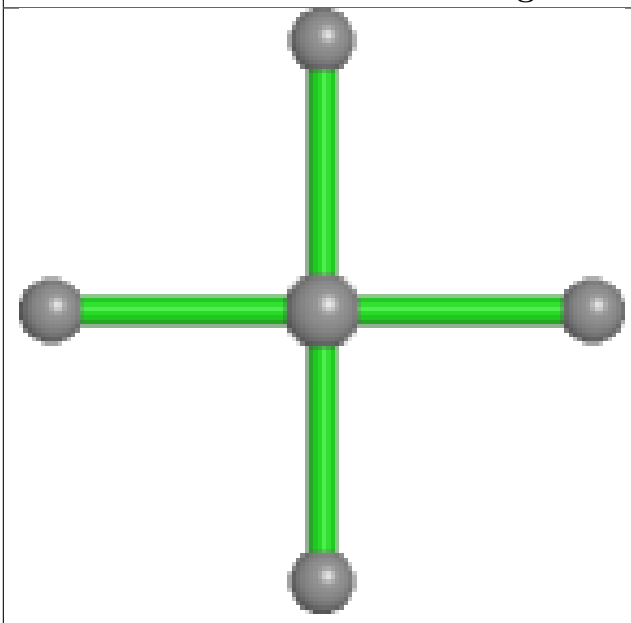
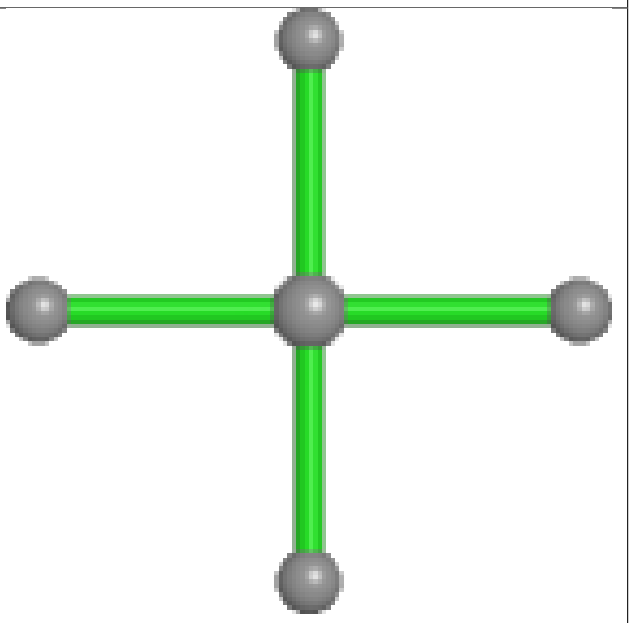
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	901	PC1	11	0
4	D	1002	IHP	3	0

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 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.

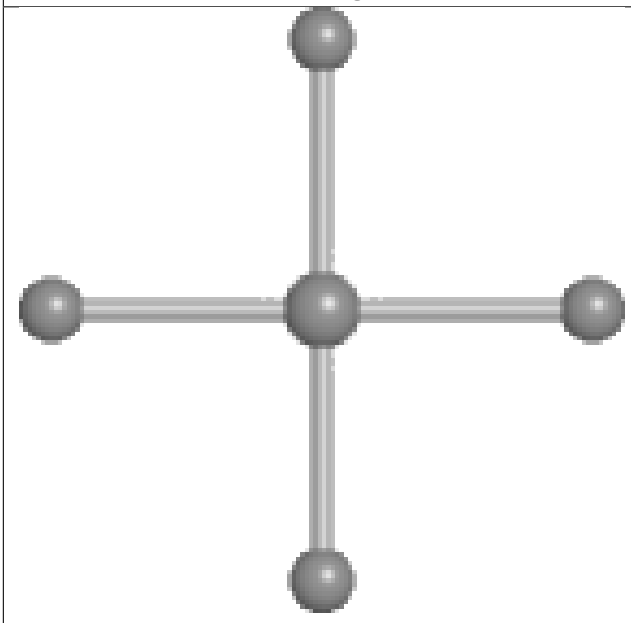
Ligand PO4 D 1006



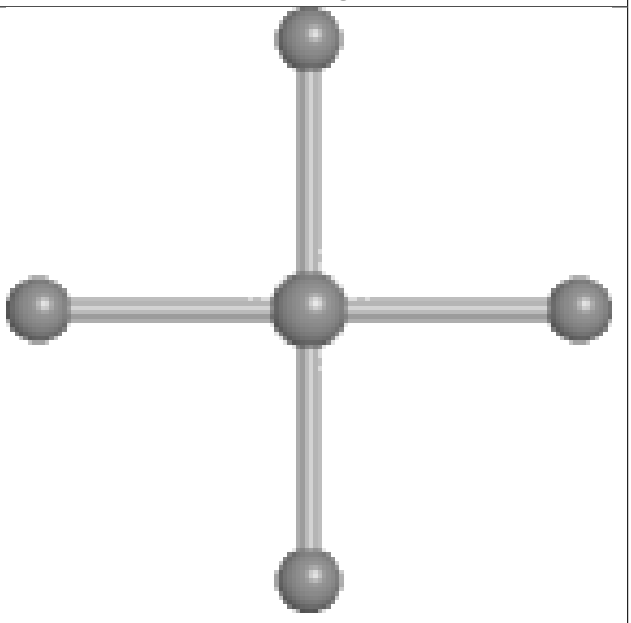
Bond lengths



Bond angles

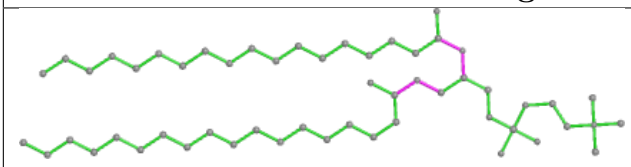


Torsions

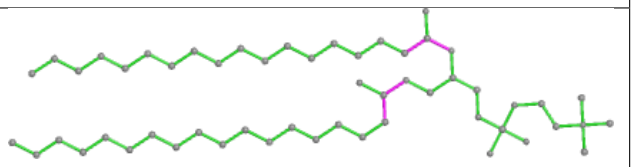


Rings

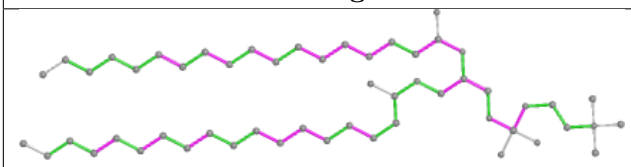
Ligand PC1 D 1003



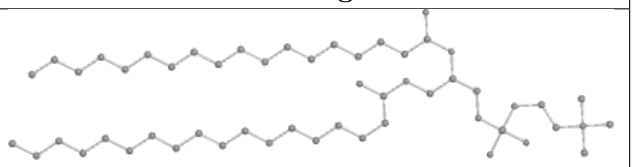
Bond lengths



Bond angles

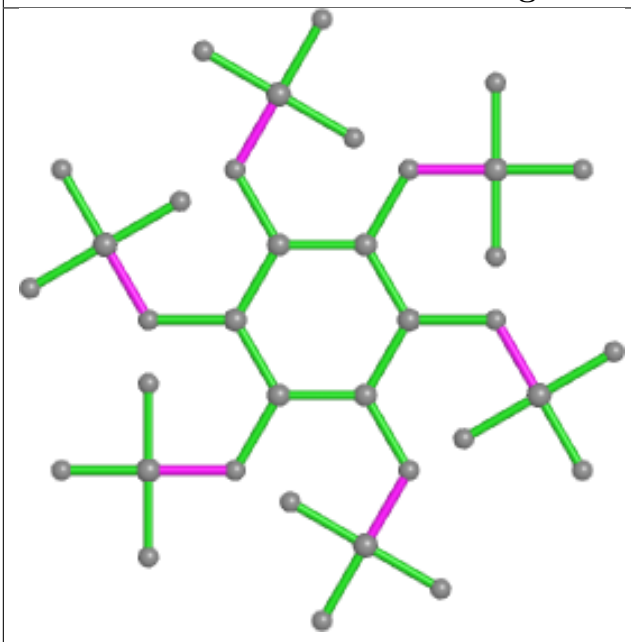


Torsions

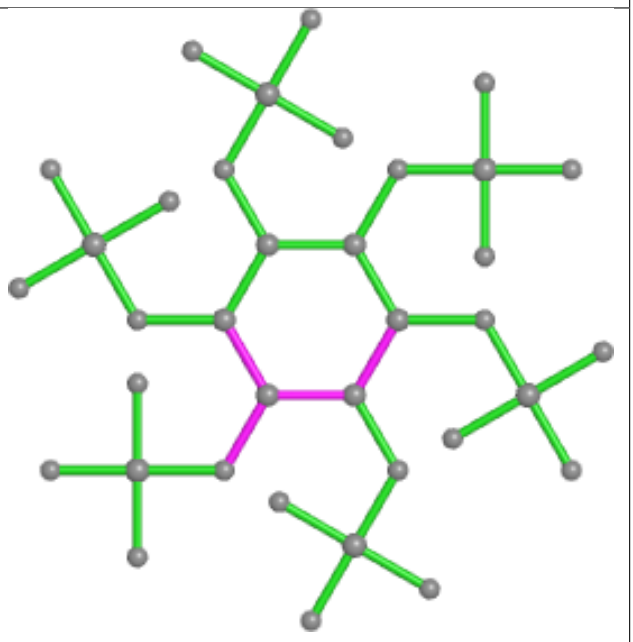


Rings

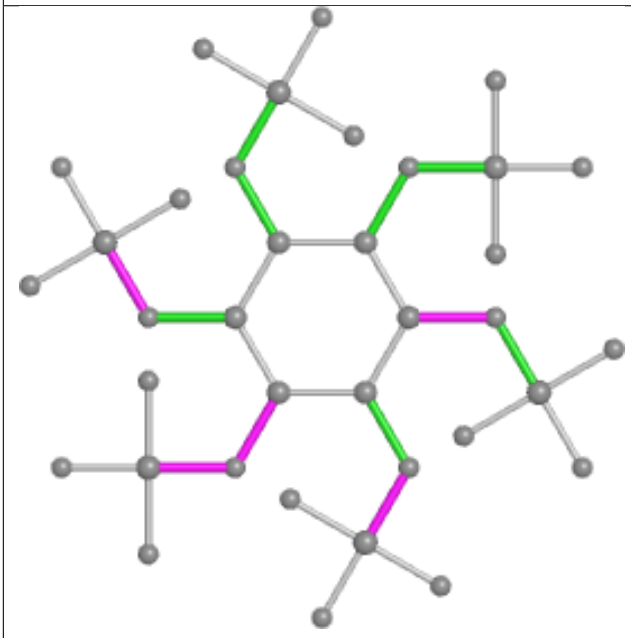
Ligand IHP D 1004



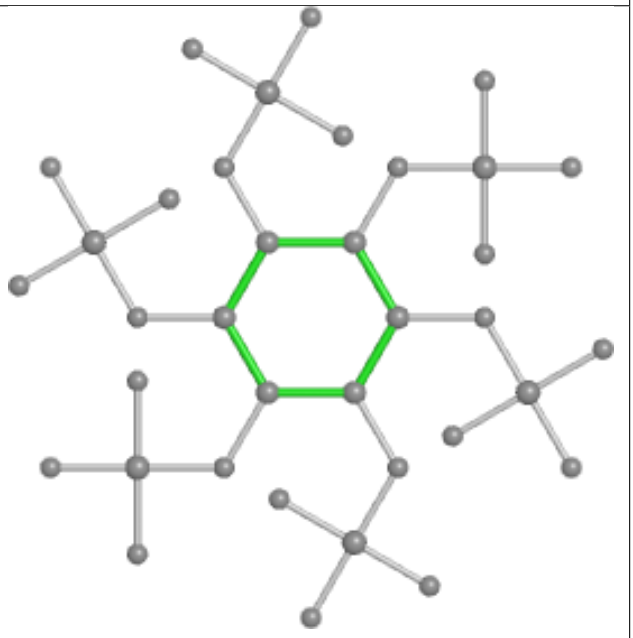
Bond lengths



Bond angles

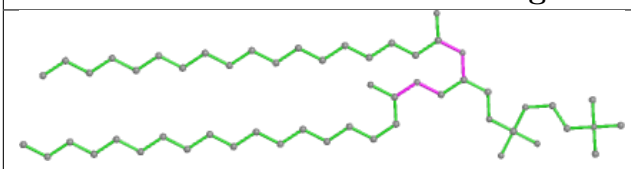


Torsions

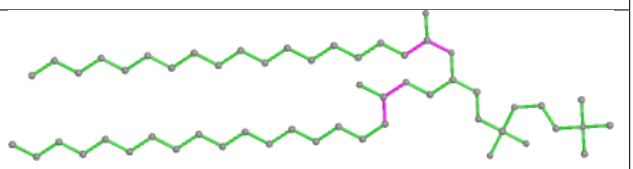


Rings

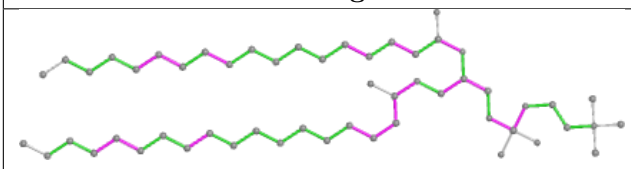
Ligand PC1 E 901



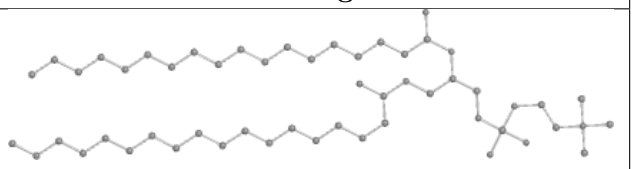
Bond lengths



Bond angles

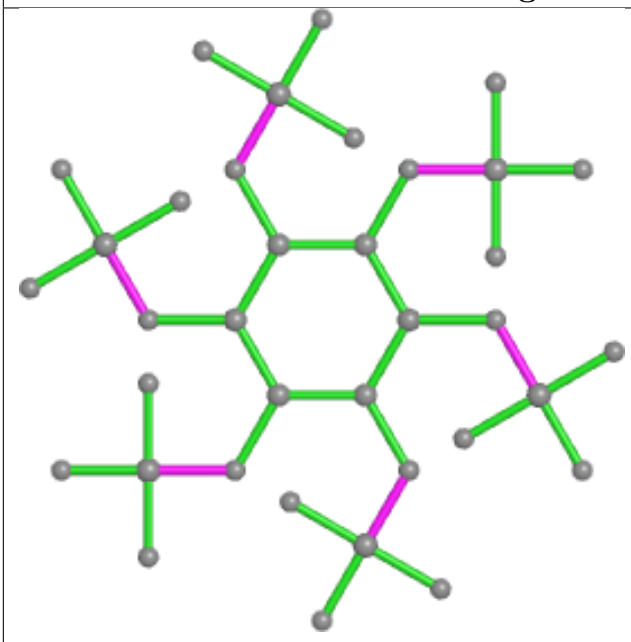


Torsions

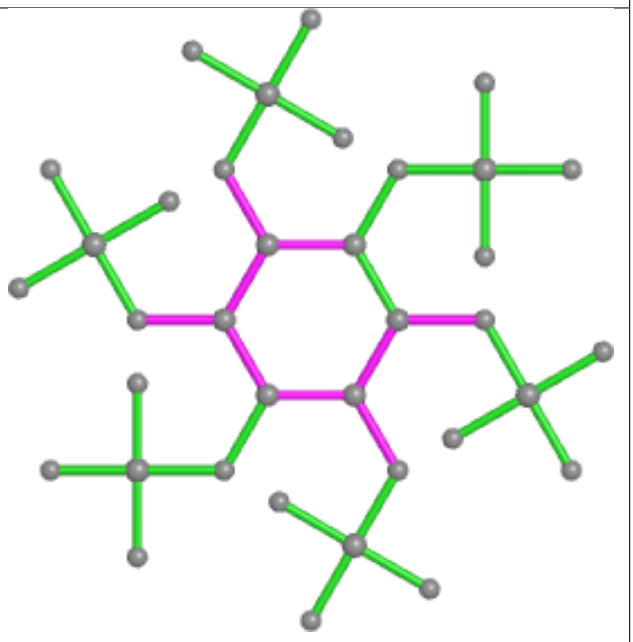


Rings

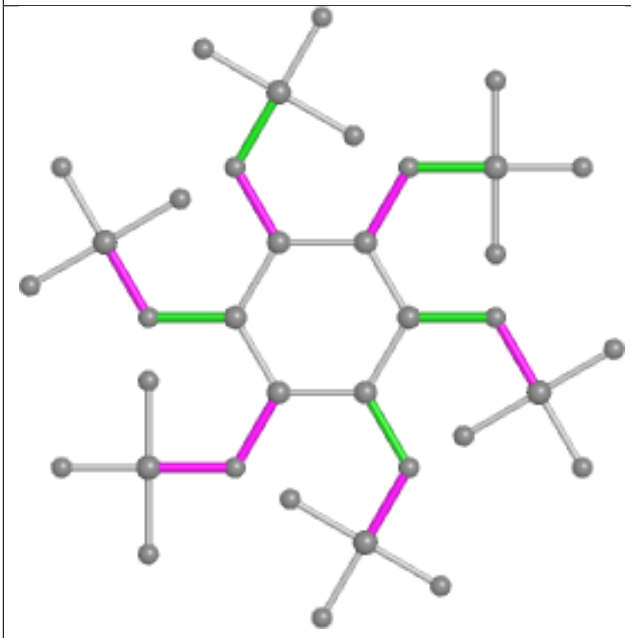
Ligand IHP D 1002



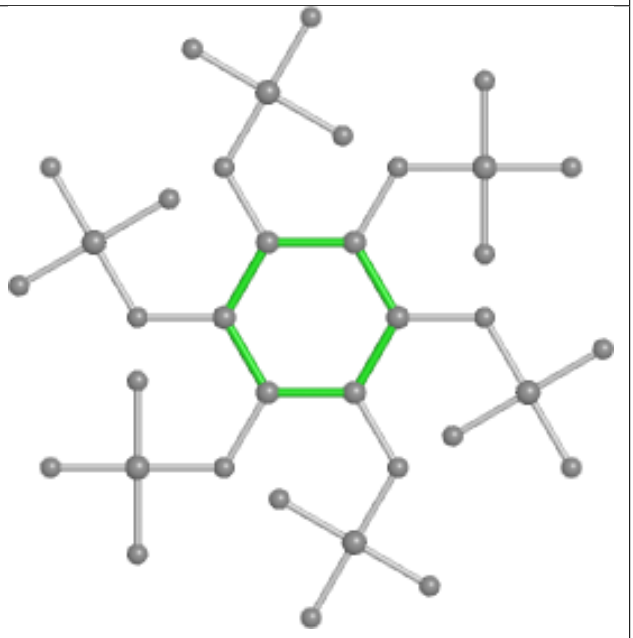
Bond lengths



Bond angles

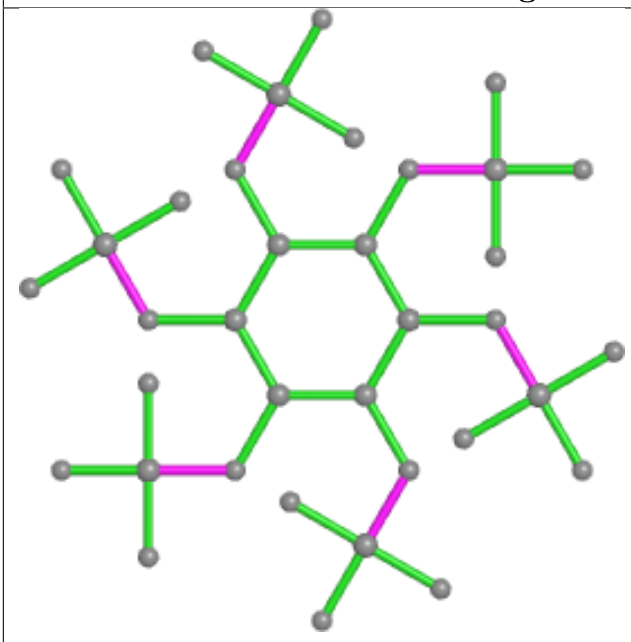


Torsions

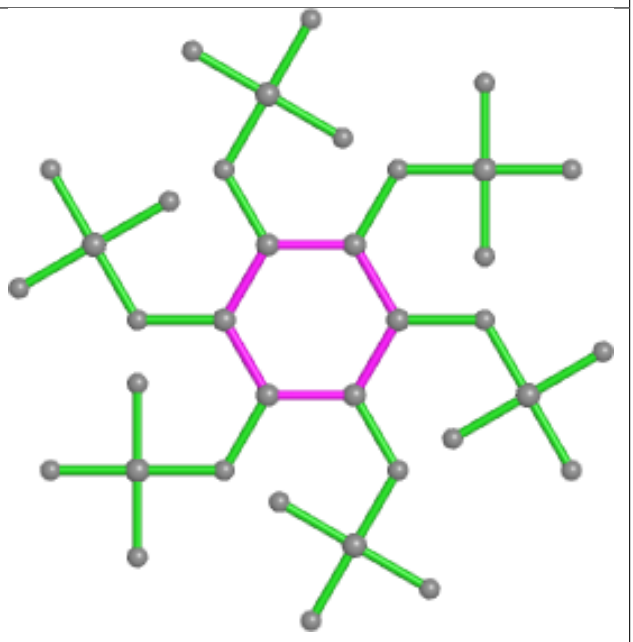


Rings

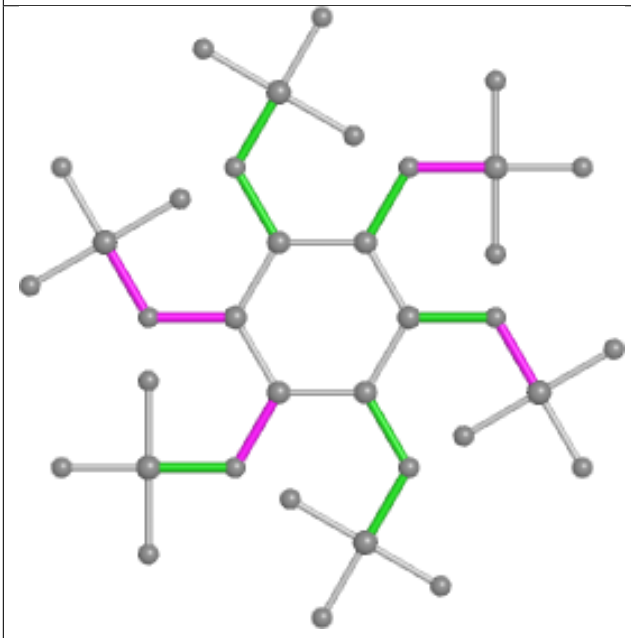
Ligand IHP D 1001



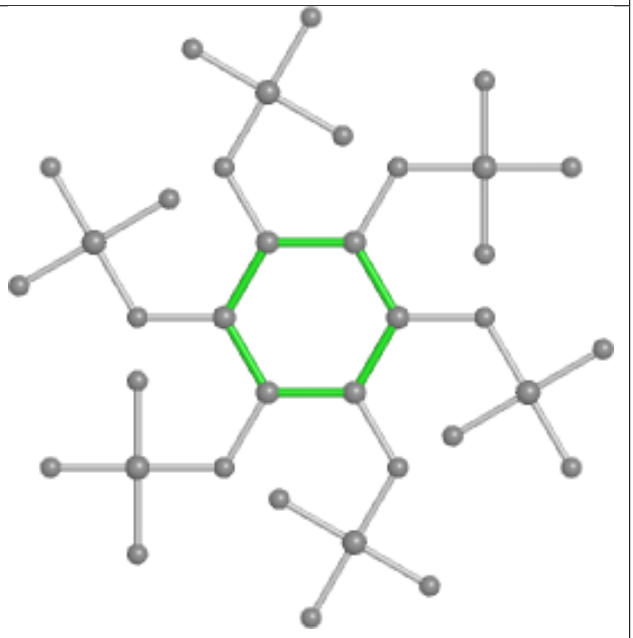
Bond lengths



Bond angles

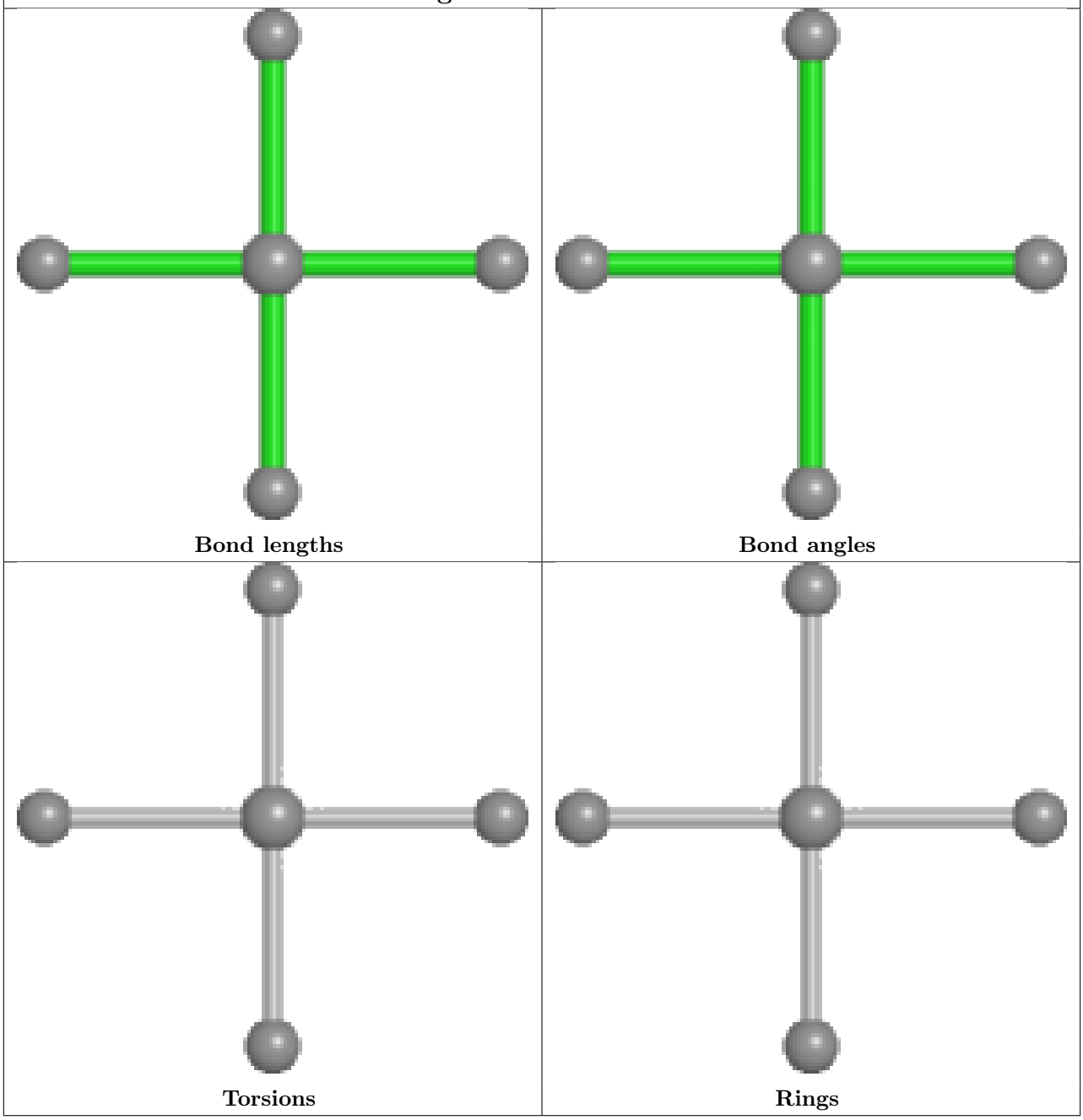


Torsions



Rings

Ligand PO4 D 1005



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.

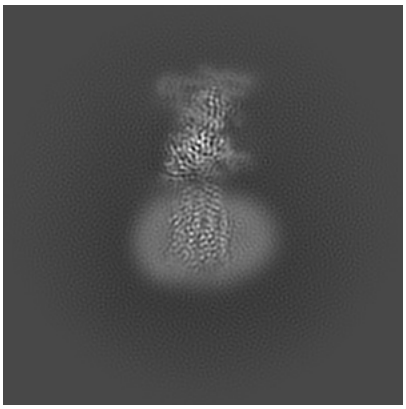
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34090. These allow visual inspection of the internal detail of the map and identification of artifacts.

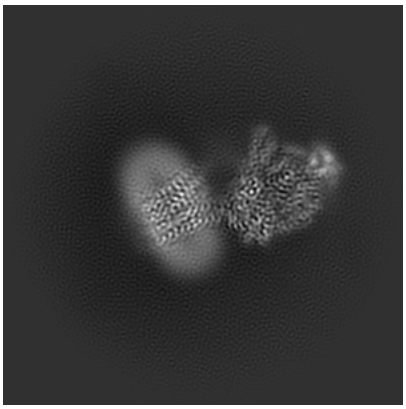
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

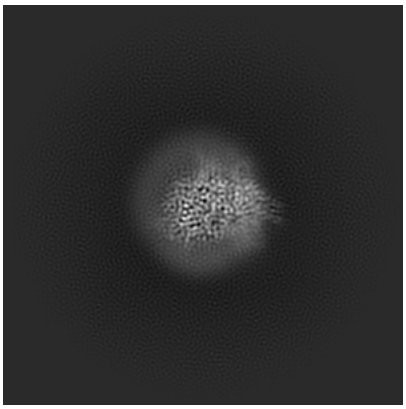
6.1.1 Primary map



X

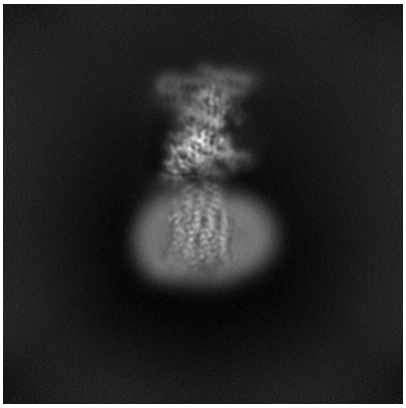


Y



Z

6.1.2 Raw map



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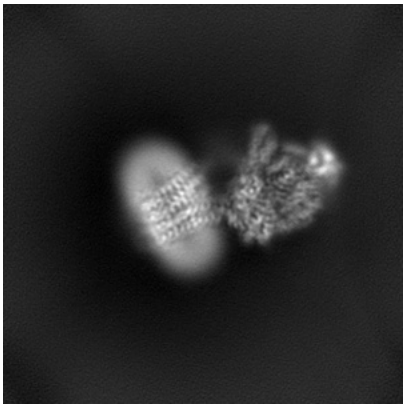
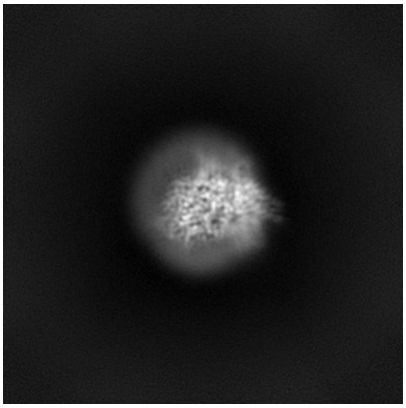


Y

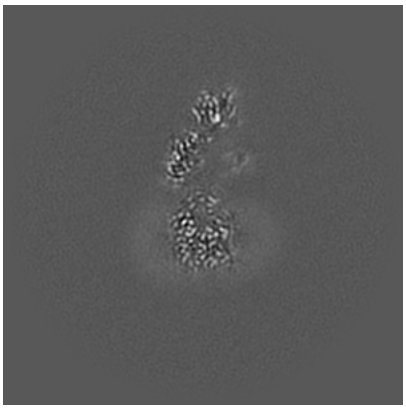


Z

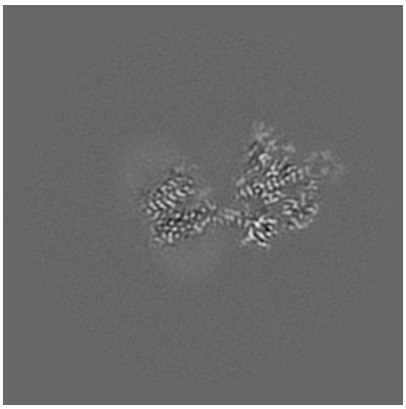
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

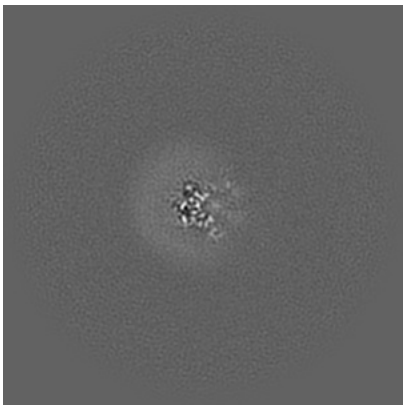
6.2.1 Primary map



X Index: 140

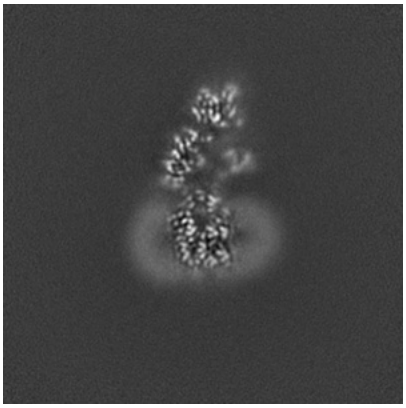


Y Index: 140

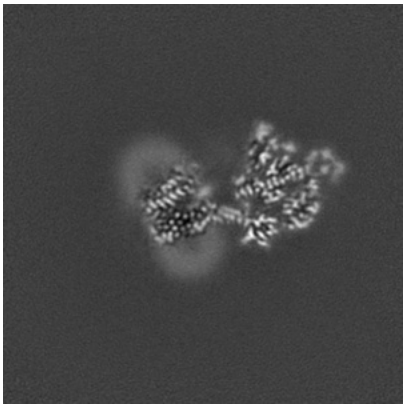


Z Index: 140

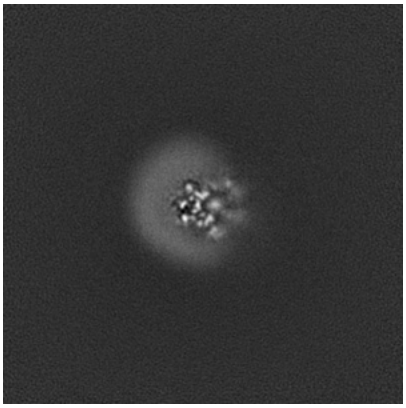
6.2.2 Raw map



X Index: 140



Y Index: 140

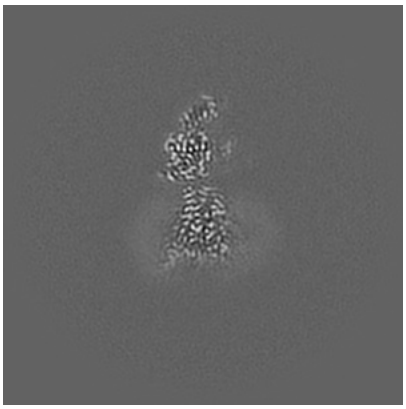


Z Index: 140

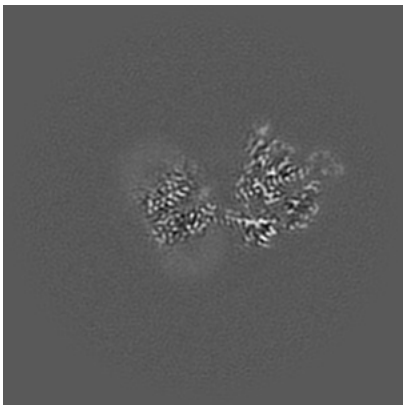
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

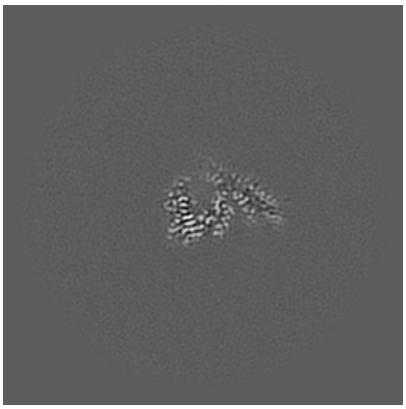
6.3.1 Primary map



X Index: 129

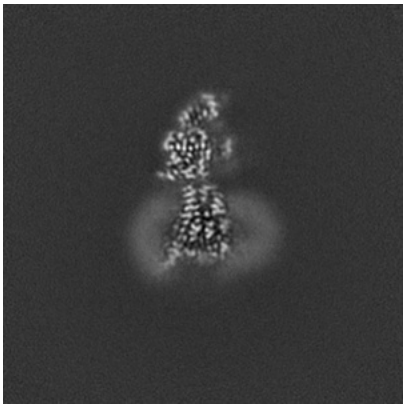


Y Index: 139

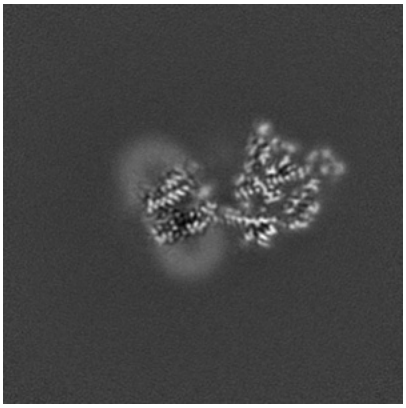


Z Index: 178

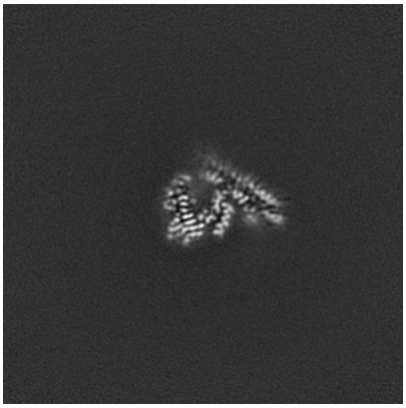
6.3.2 Raw map



X Index: 129



Y Index: 139

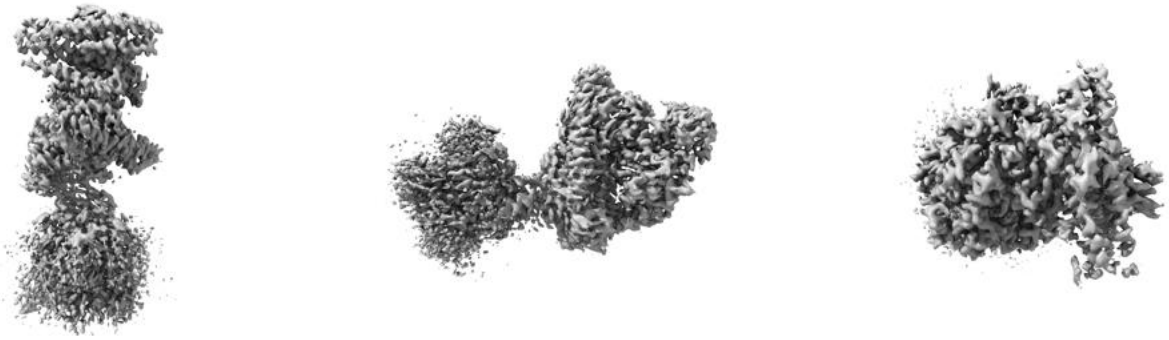


Z Index: 178

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

6.4 Orthogonal surface views (i)

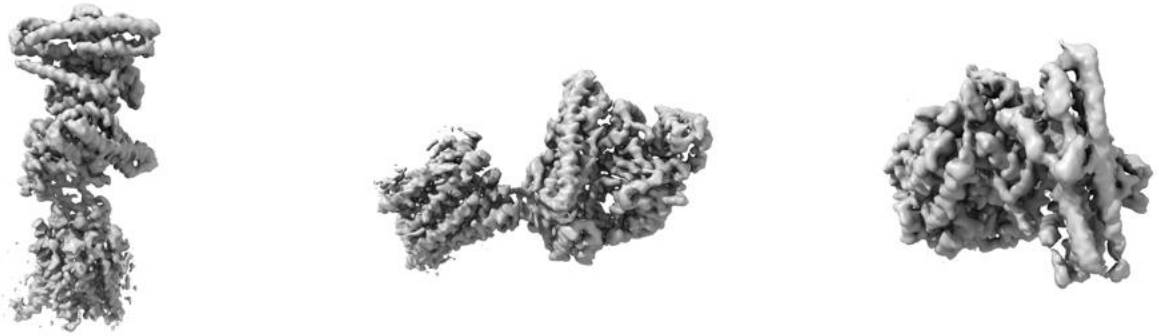
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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



X Y Z

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.

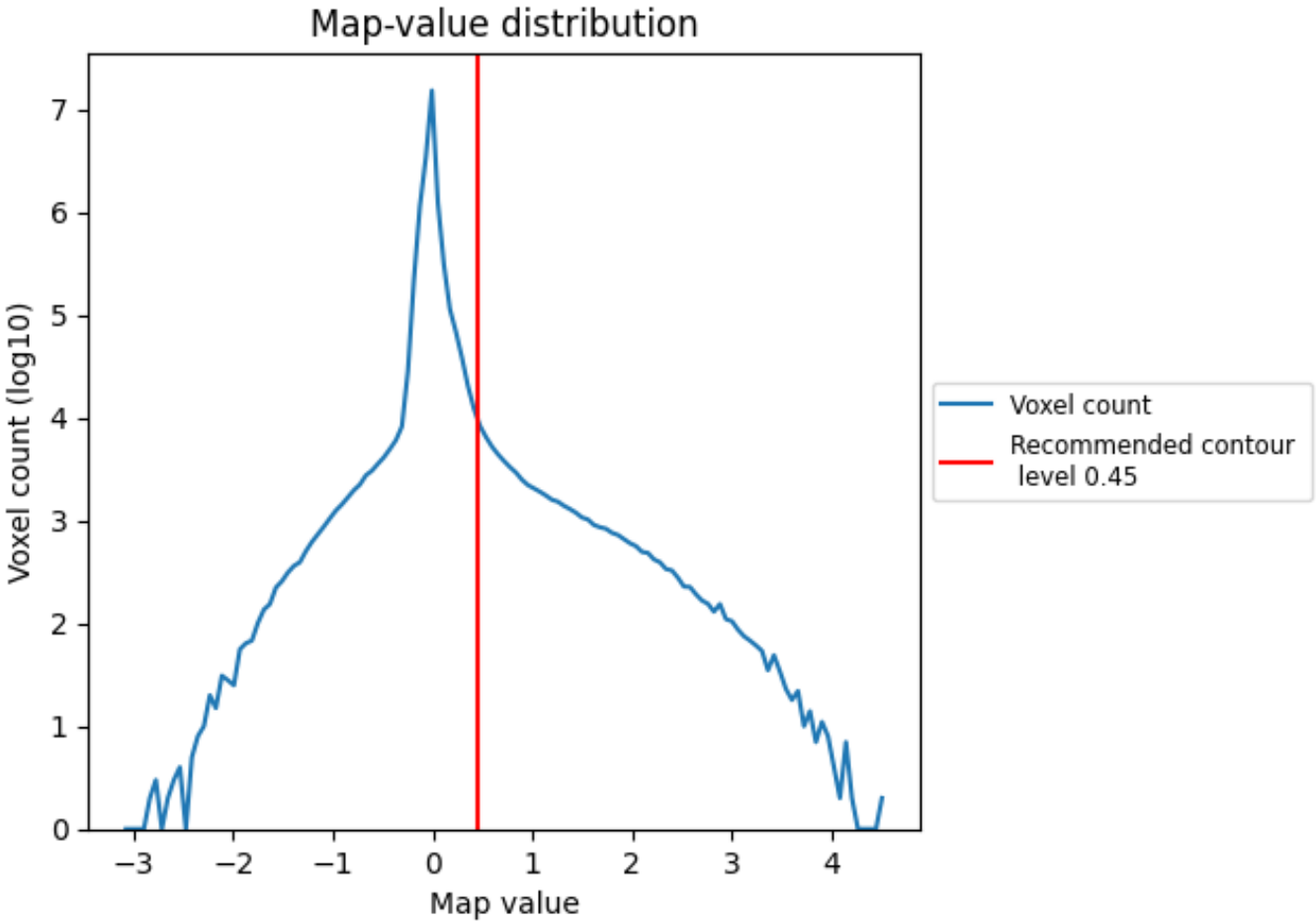
6.5 Mask visualisation (i)

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

7 Map analysis

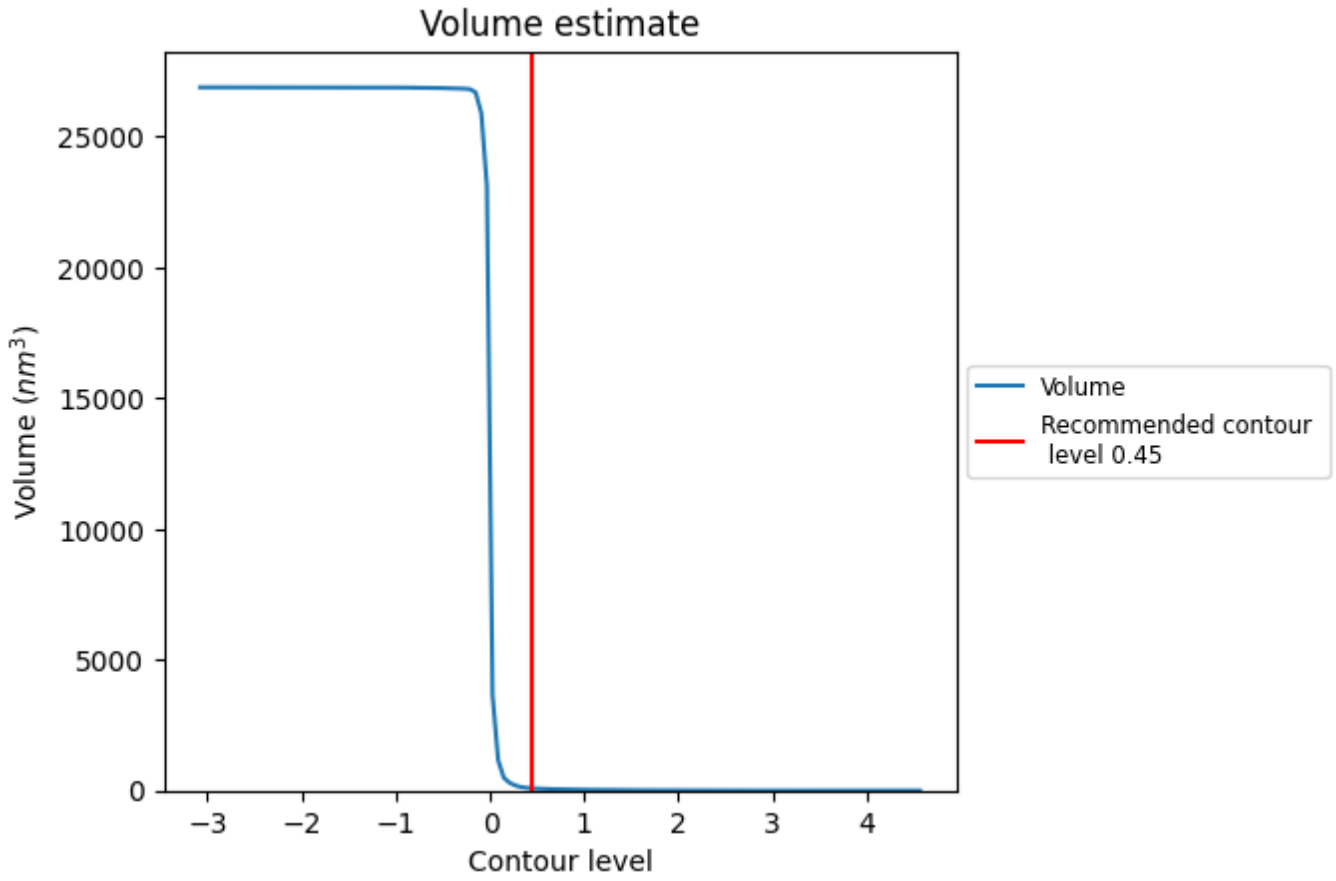
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

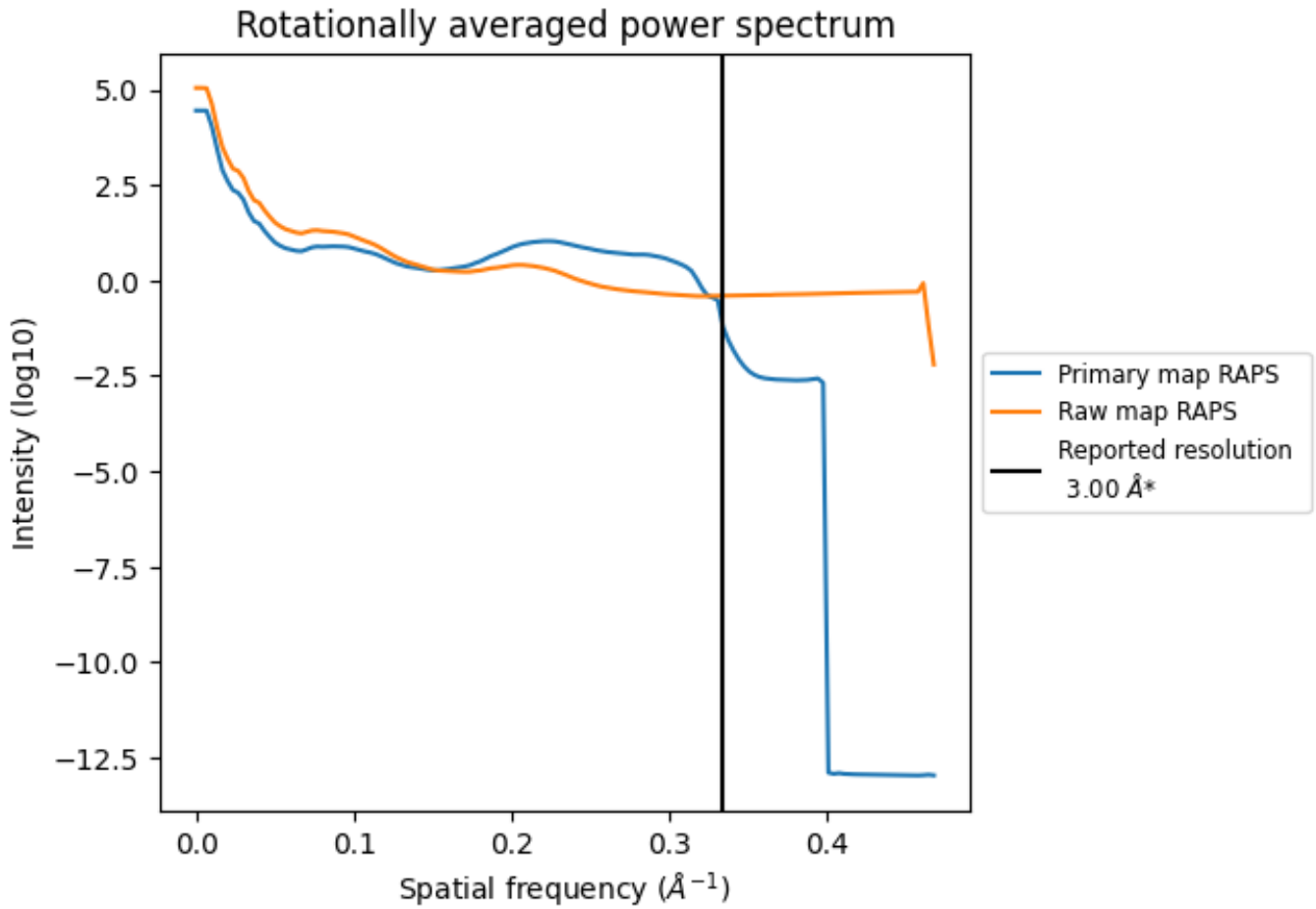
7.2 Volume estimate



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 76 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)

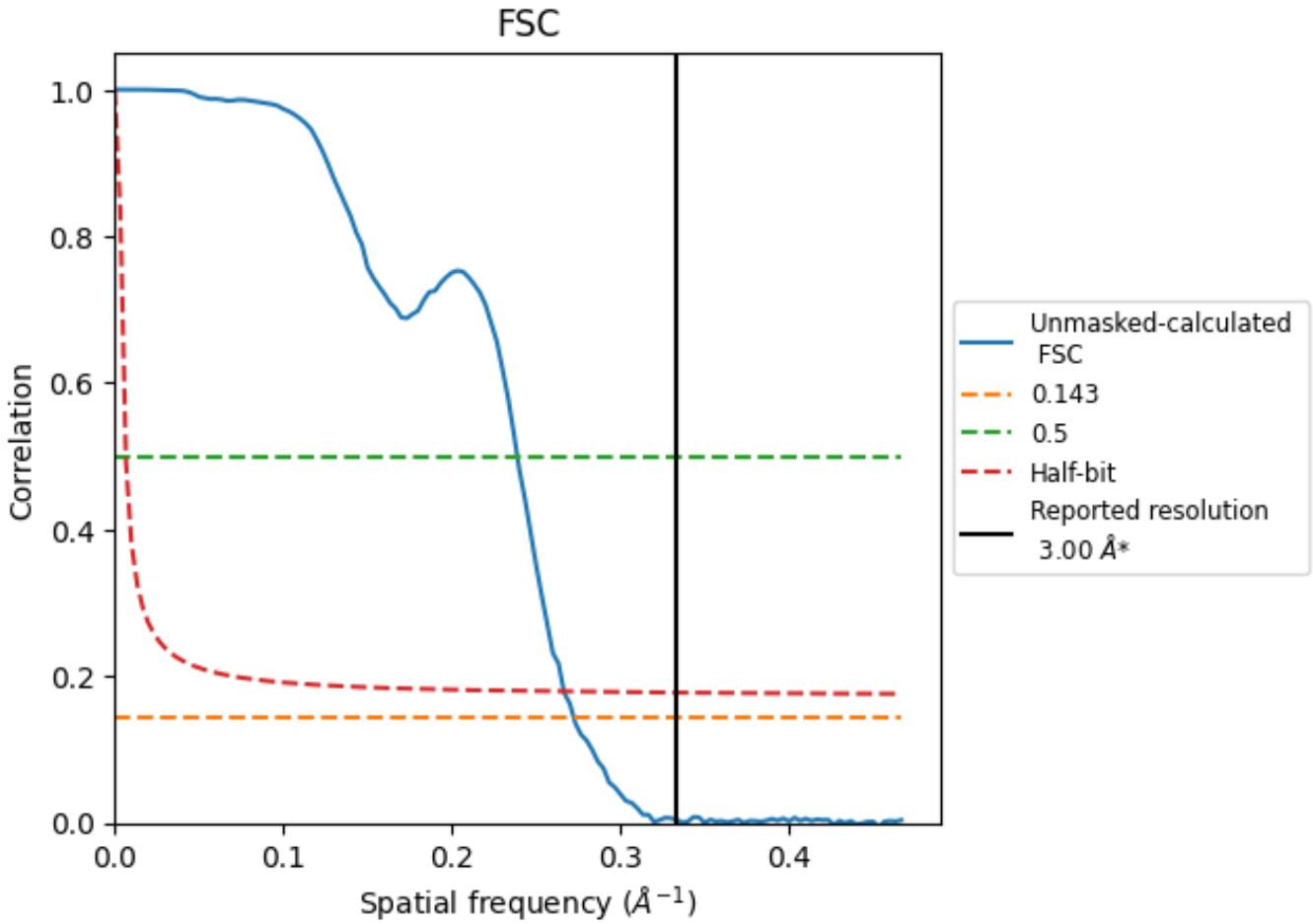


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

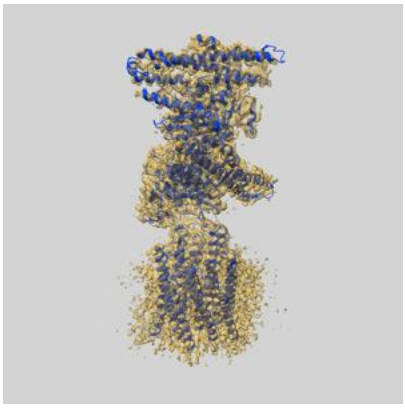
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.18	3.75

*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 3.67 differs from the reported value 3.0 by more than 10 %

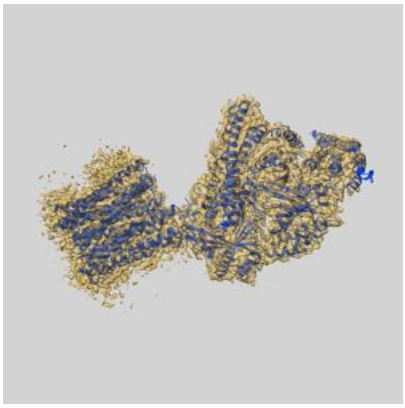
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34090 and PDB model 7YTJ. Per-residue inclusion information can be found in section 3 on page 9.

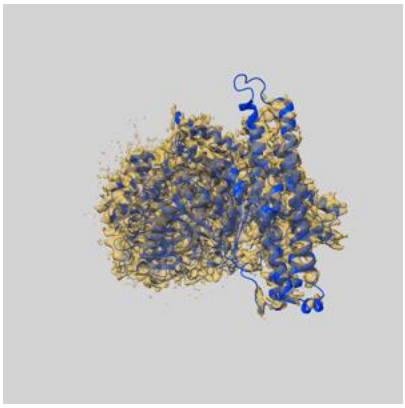
9.1 Map-model overlay



X



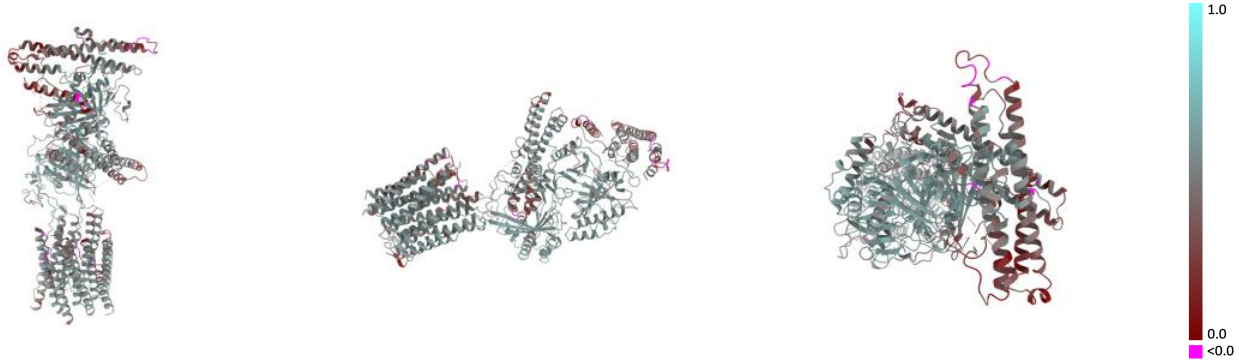
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

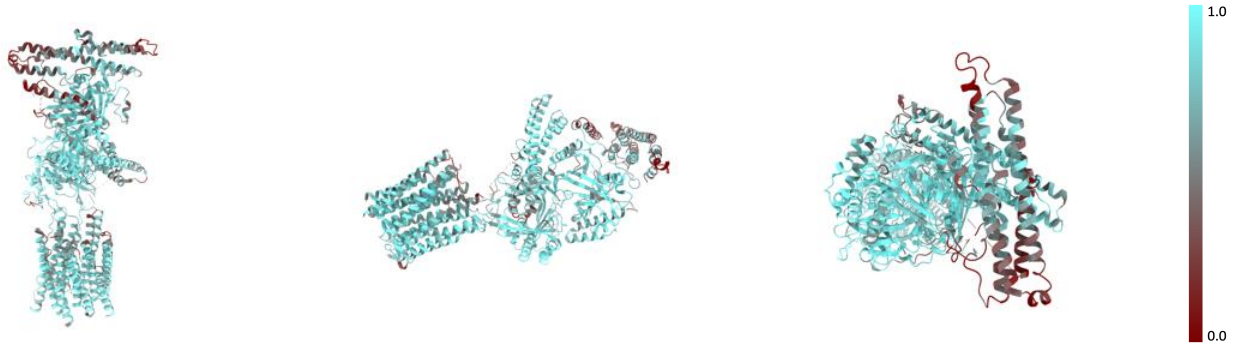
9.2 Q-score mapped to coordinate model



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.

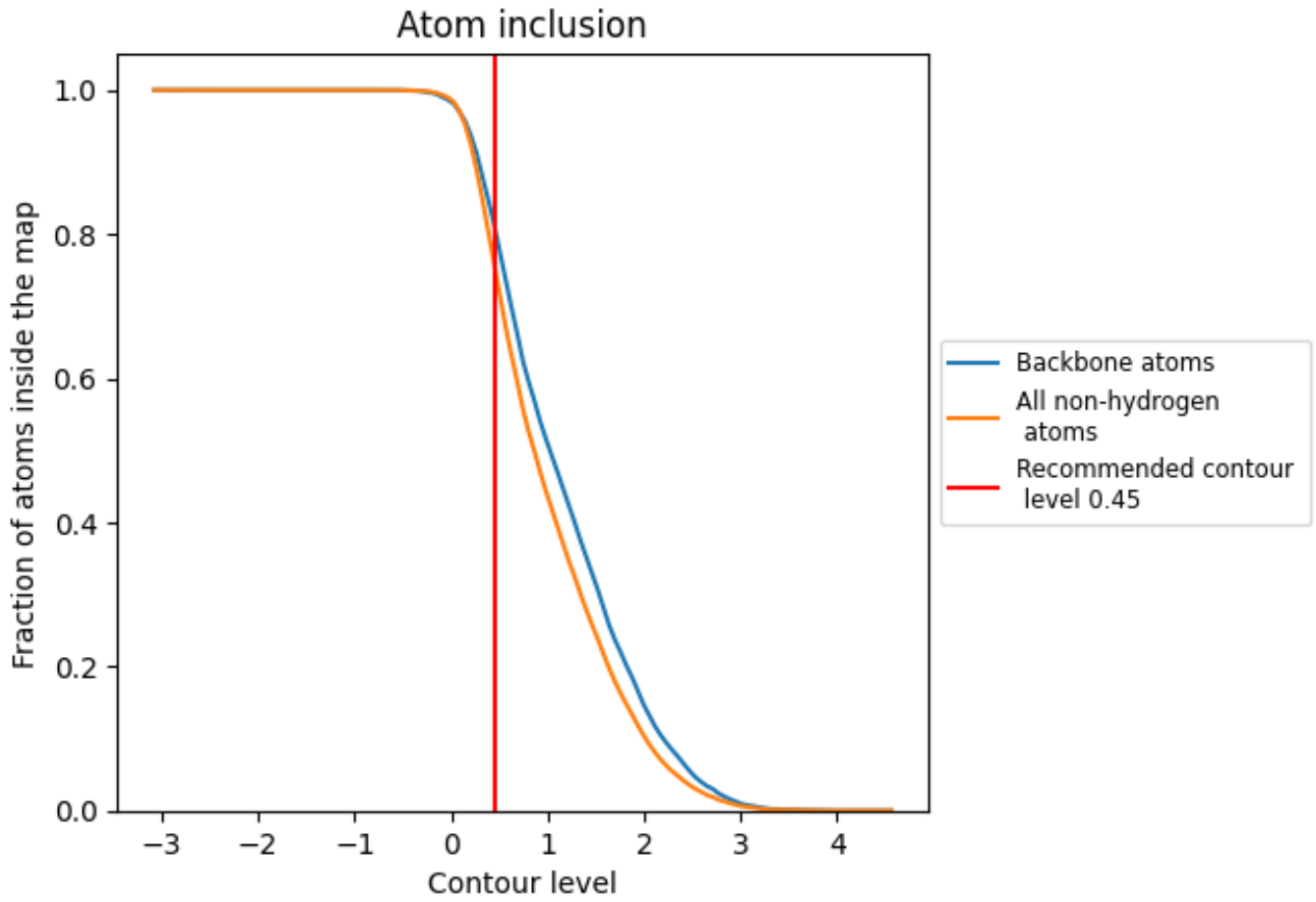
9.3 Atom inclusion mapped to coordinate model



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7567	0.4850
A	0.7749	0.4760
B	0.7719	0.4740
C	0.7643	0.4610
D	0.8226	0.5190
E	0.6884	0.4610