Full wwPDB EM Validation Report (i)

Feb 27, 2024 – 09:13 AM EST

PDB ID	:	6V1Y
EMDB ID	:	EMD-21019
Title	:	Cryo-EM Structure of the Hyperpolarization-Activated Potassium Channel KAT1: Octamer
Authors	:	Clark, M.D.; Contreras, G.F.; Shen, R.; Perozo, E.
Deposited on	:	2019-11-21
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

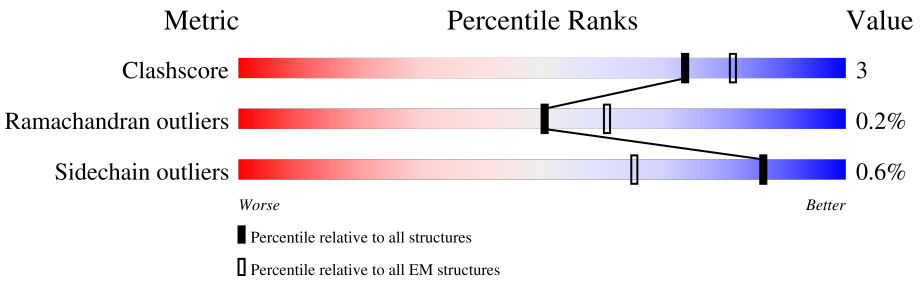
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	512	9% 79% 8% 13%
1	B	512	9% 79% 8% 13%
1	C	512	9% 79% 8% 13%
1	D	512	9% 79% 8% 13%
1	M	512	7% 79% 8% 13%
1	N	512	8% 79% 8% 13%
1	O	512	8% 78% 9% 13%
1	P	512	8% 79% 8% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27896 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 Potassium channel KAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	446	3424	2262	569	578	15	0	0
1	B	446	3424	2262	569	578	15	0	0
1	C	446	3424	2262	569	578	15	0	0
1	D	446	3424	2262	569	578	15	0	0
1	M	446	3424	2262	569	578	15	0	0
1	N	446	3424	2262	569	578	15	0	0
1	O	446	3424	2262	569	578	15	0	0
1	P	446	3424	2262	569	578	15	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	SER	-	expression tag	UNP Q39128
A	504	ARG	-	expression tag	UNP Q39128
A	505	GLY	-	expression tag	UNP Q39128
A	506	SER	-	expression tag	UNP Q39128
A	507	LEU	-	expression tag	UNP Q39128
A	508	GLU	-	expression tag	UNP Q39128
A	509	VAL	-	expression tag	UNP Q39128
A	510	LEU	-	expression tag	UNP Q39128
A	511	PHE	-	expression tag	UNP Q39128
A	512	GLN	-	expression tag	UNP Q39128
B	503	SER	-	expression tag	UNP Q39128
B	504	ARG	-	expression tag	UNP Q39128
B	505	GLY	-	expression tag	UNP Q39128
B	506	SER	-	expression tag	UNP Q39128

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	LEU	-	expression tag	UNP Q39128
B	508	GLU	-	expression tag	UNP Q39128
B	509	VAL	-	expression tag	UNP Q39128
B	510	LEU	-	expression tag	UNP Q39128
B	511	PHE	-	expression tag	UNP Q39128
B	512	GLN	-	expression tag	UNP Q39128
C	503	SER	-	expression tag	UNP Q39128
C	504	ARG	-	expression tag	UNP Q39128
C	505	GLY	-	expression tag	UNP Q39128
C	506	SER	-	expression tag	UNP Q39128
C	507	LEU	-	expression tag	UNP Q39128
C	508	GLU	-	expression tag	UNP Q39128
C	509	VAL	-	expression tag	UNP Q39128
C	510	LEU	-	expression tag	UNP Q39128
C	511	PHE	-	expression tag	UNP Q39128
C	512	GLN	-	expression tag	UNP Q39128
D	503	SER	-	expression tag	UNP Q39128
D	504	ARG	-	expression tag	UNP Q39128
D	505	GLY	-	expression tag	UNP Q39128
D	506	SER	-	expression tag	UNP Q39128
D	507	LEU	-	expression tag	UNP Q39128
D	508	GLU	-	expression tag	UNP Q39128
D	509	VAL	-	expression tag	UNP Q39128
D	510	LEU	-	expression tag	UNP Q39128
D	511	PHE	-	expression tag	UNP Q39128
D	512	GLN	-	expression tag	UNP Q39128
M	503	SER	-	expression tag	UNP Q39128
M	504	ARG	-	expression tag	UNP Q39128
M	505	GLY	-	expression tag	UNP Q39128
M	506	SER	-	expression tag	UNP Q39128
M	507	LEU	-	expression tag	UNP Q39128
M	508	GLU	-	expression tag	UNP Q39128
M	509	VAL	-	expression tag	UNP Q39128
M	510	LEU	-	expression tag	UNP Q39128
M	511	PHE	-	expression tag	UNP Q39128
M	512	GLN	-	expression tag	UNP Q39128
N	503	SER	-	expression tag	UNP Q39128
N	504	ARG	-	expression tag	UNP Q39128
N	505	GLY	-	expression tag	UNP Q39128
N	506	SER	-	expression tag	UNP Q39128
N	507	LEU	-	expression tag	UNP Q39128
N	508	GLU	-	expression tag	UNP Q39128

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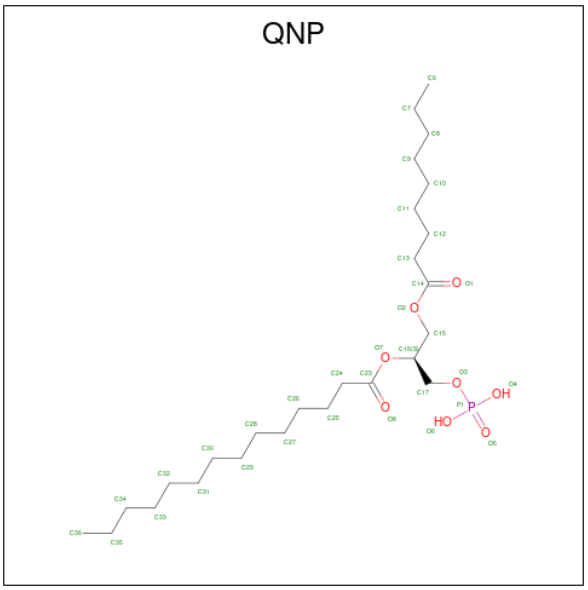
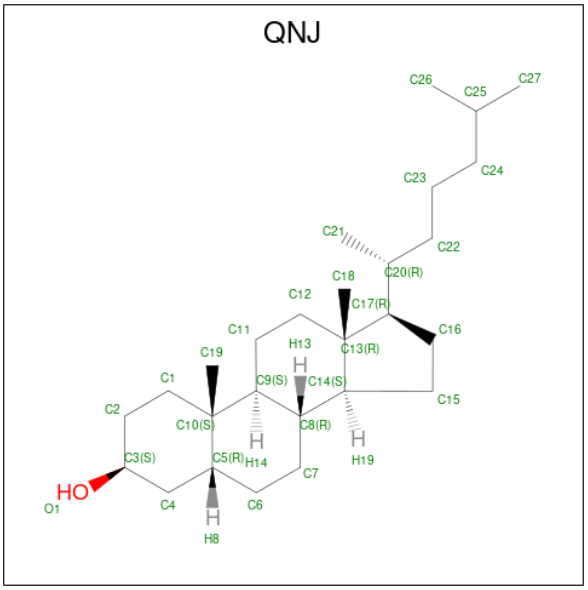
Chain	Residue	Modelled	Actual	Comment	Reference
N	509	VAL	-	expression tag	UNP Q39128
N	510	LEU	-	expression tag	UNP Q39128
N	511	PHE	-	expression tag	UNP Q39128
N	512	GLN	-	expression tag	UNP Q39128
O	503	SER	-	expression tag	UNP Q39128
O	504	ARG	-	expression tag	UNP Q39128
O	505	GLY	-	expression tag	UNP Q39128
O	506	SER	-	expression tag	UNP Q39128
O	507	LEU	-	expression tag	UNP Q39128
O	508	GLU	-	expression tag	UNP Q39128
O	509	VAL	-	expression tag	UNP Q39128
O	510	LEU	-	expression tag	UNP Q39128
O	511	PHE	-	expression tag	UNP Q39128
O	512	GLN	-	expression tag	UNP Q39128
P	503	SER	-	expression tag	UNP Q39128
P	504	ARG	-	expression tag	UNP Q39128
P	505	GLY	-	expression tag	UNP Q39128
P	506	SER	-	expression tag	UNP Q39128
P	507	LEU	-	expression tag	UNP Q39128
P	508	GLU	-	expression tag	UNP Q39128
P	509	VAL	-	expression tag	UNP Q39128
P	510	LEU	-	expression tag	UNP Q39128
P	511	PHE	-	expression tag	UNP Q39128
P	512	GLN	-	expression tag	UNP Q39128

- Molecule 2 is (2S)-1-(nonanoyloxy)-3-(phosphonooxy)propan-2-yl tetradecanoate (three-letter code: QNP) (formula: $C_{26}H_{51}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	35	26	8	1	0
2	B	1	35	26	8	1	0
2	C	1	35	26	8	1	0
2	D	1	35	26	8	1	0
2	M	1	35	26	8	1	0
2	N	1	35	26	8	1	0
2	O	1	35	26	8	1	0
2	P	1	35	26	8	1	0

- Molecule 3 is (3beta,5beta,14beta,17alpha)-cholestan-3-ol (three-letter code: QNJ) (formula: $C_{27}H_{48}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	28	27	1	0
3	B	1	28	27	1	0
3	C	1	28	27	1	0

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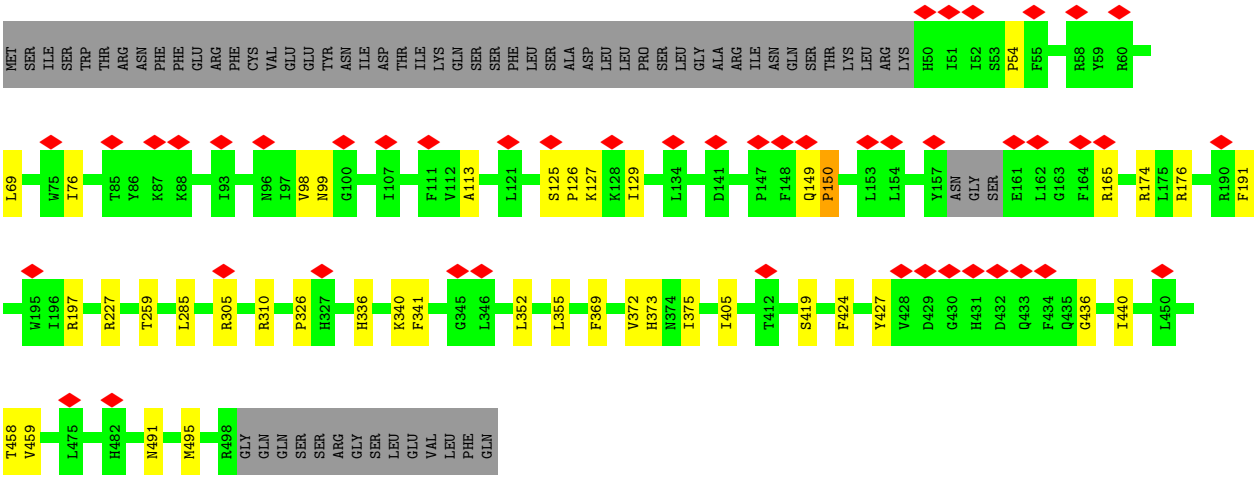
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	D	1	28	27	1	0
3	M	1	28	27	1	0
3	N	1	28	27	1	0
3	O	1	28	27	1	0
3	P	1	28	27	1	0

3 Residue-property plots (i)

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

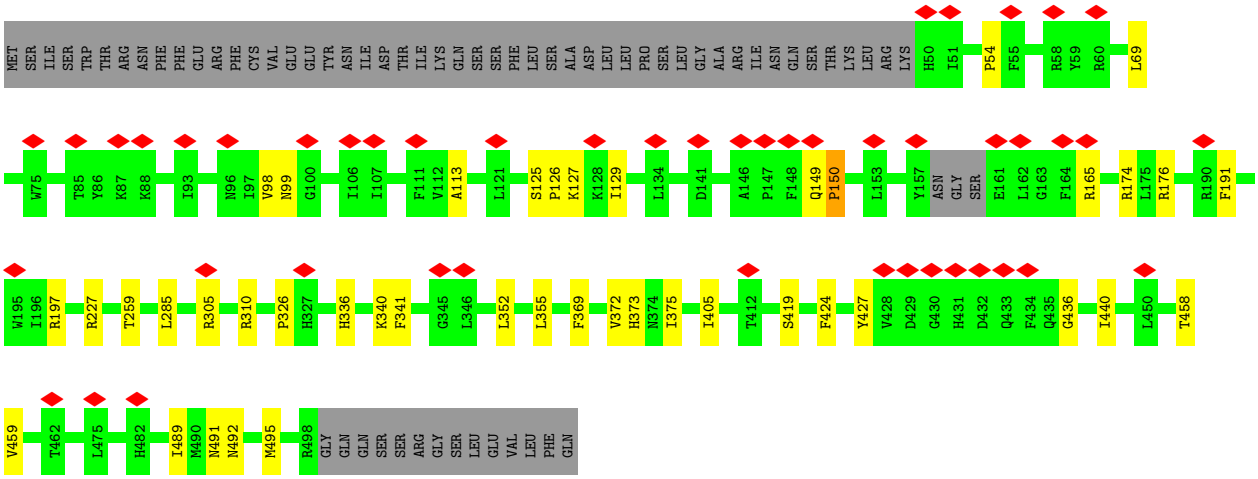
- Molecule 1: Potassium channel KAT1

Chain A:



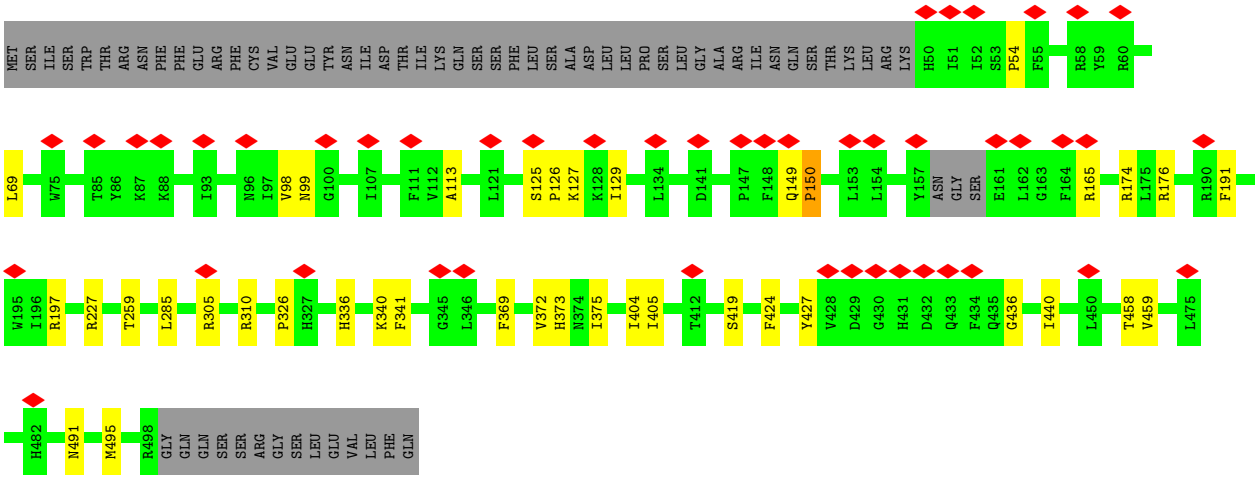
- Molecule 1: Potassium channel KAT1

Chain B:



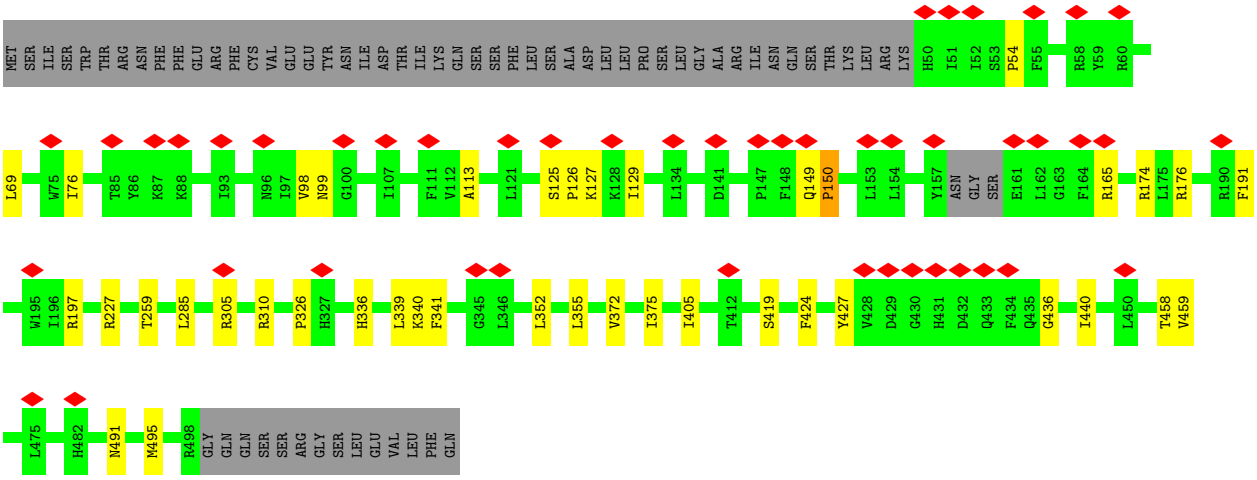
- Molecule 1: Potassium channel KAT1

Chain C:



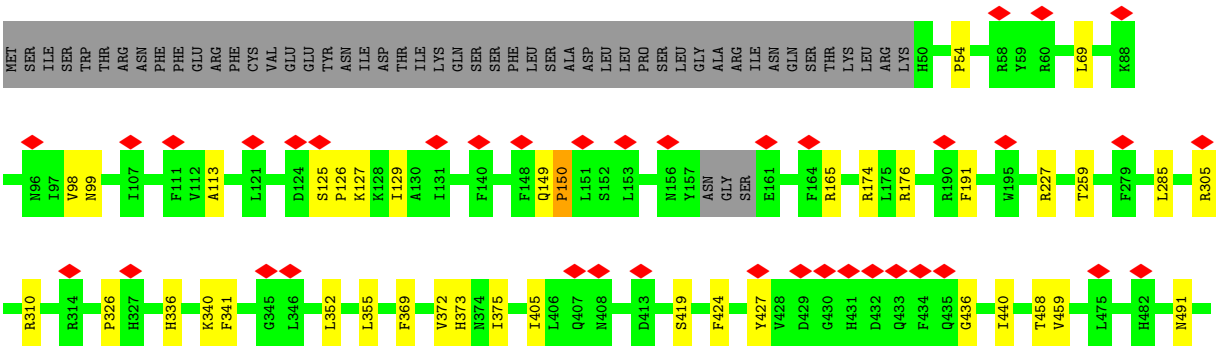
• Molecule 1: Potassium channel KAT1

Chain D:



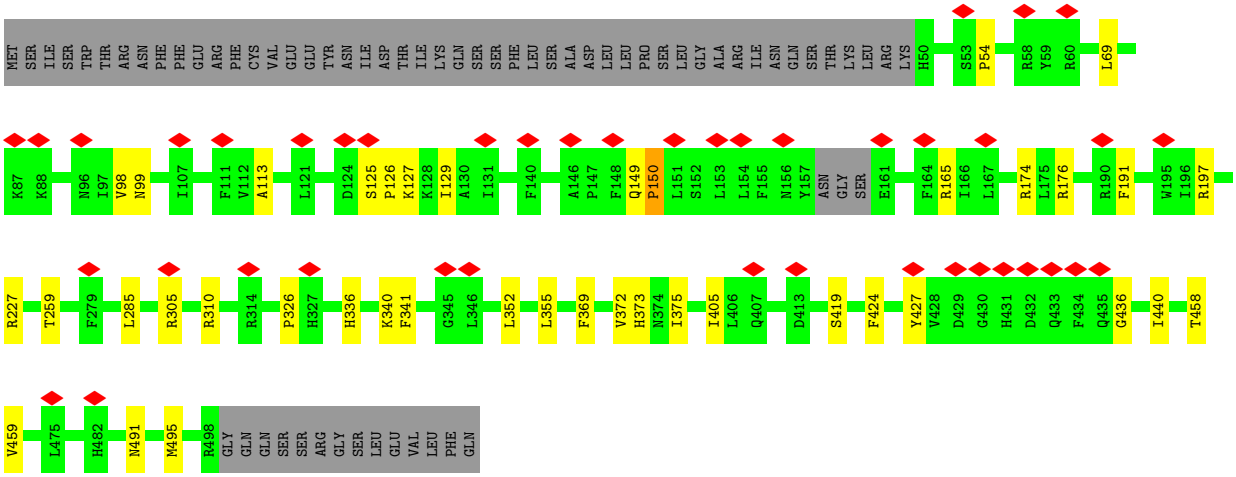
• Molecule 1: Potassium channel KAT1

Chain M:



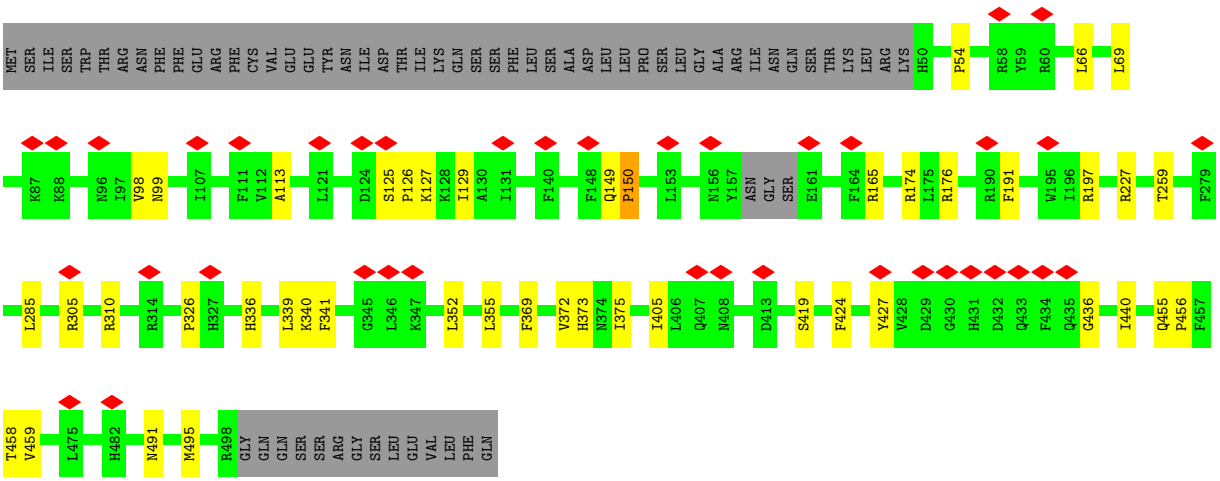
• Molecule 1: Potassium channel KAT1

Chain N:



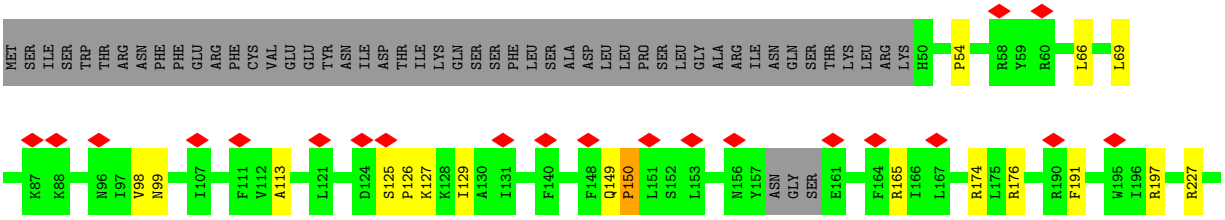
• Molecule 1: Potassium channel KAT1

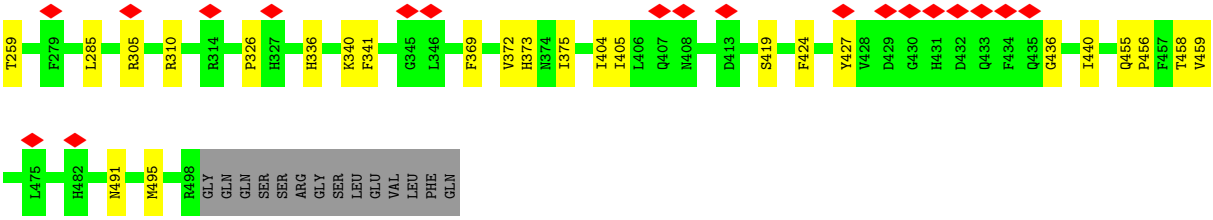
Chain O:



• Molecule 1: Potassium channel KAT1

Chain P:




T259
F279
L285
R305
R310
R314
P326
H327
H336
K340
F341
G345
L346
F369
V372
H373
N374
I375
I404
I405
L406
Q407
N408
D413
S419
F424
Y427
V428
D429
G430
H431
D432
Q433
F434
Q435
G436
I440
Q455
P456
F457
T458
V459

L475
H482
N491
N495
R498
GLY
GLN
GLN
SER
SER
ARG
GLY
SER
LEU
GLU
VAL
LEU
PHE
GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	91689	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0366	Depositor
Map size (Å)	361.76, 361.76, 361.76	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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: QNJ, QNP

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	0.50	1/3524 (0.0%)	0.62	0/4821
1	B	0.50	1/3524 (0.0%)	0.62	0/4821
1	C	0.50	1/3524 (0.0%)	0.62	0/4821
1	D	0.50	1/3524 (0.0%)	0.62	0/4821
1	M	0.50	1/3524 (0.0%)	0.62	0/4821
1	N	0.50	1/3524 (0.0%)	0.62	0/4821
1	O	0.50	1/3524 (0.0%)	0.62	0/4821
1	P	0.50	1/3524 (0.0%)	0.62	0/4821
All	All	0.50	8/28192 (0.0%)	0.62	0/38568

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	PRO	C-N	7.00	1.50	1.34
1	C	150	PRO	C-N	7.00	1.50	1.34
1	D	150	PRO	C-N	7.00	1.50	1.34
1	M	150	PRO	C-N	7.00	1.50	1.34
1	P	150	PRO	C-N	7.00	1.50	1.34
1	O	150	PRO	C-N	6.99	1.50	1.34
1	B	150	PRO	C-N	6.97	1.50	1.34
1	N	150	PRO	C-N	6.97	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3223	24	0
1	B	3424	0	3223	24	0
1	C	3424	0	3223	23	0
1	D	3424	0	3223	25	0
1	M	3424	0	3223	22	0
1	N	3424	0	3223	23	0
1	O	3424	0	3223	26	0
1	P	3424	0	3223	26	0
2	A	35	0	0	1	0
2	B	35	0	0	1	0
2	C	35	0	0	1	0
2	D	35	0	0	1	0
2	M	35	0	0	0	0
2	N	35	0	0	1	0
2	O	35	0	0	1	0
2	P	35	0	0	1	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
3	M	28	0	0	0	0
3	N	28	0	0	0	0
3	O	28	0	0	0	0
3	P	28	0	0	0	0
All	All	27896	0	25784	177	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 3.

All (177) 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:C:424:PHE:CB	1:C:436:GLY:HA3	2.24	0.68
1:O:424:PHE:CB	1:O:436:GLY:HA3	2.24	0.68
1:B:424:PHE:CB	1:B:436:GLY:HA3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PHE:CB	1:A:436:GLY:HA3	2.24	0.67
1:M:424:PHE:CB	1:M:436:GLY:HA3	2.24	0.67
1:P:424:PHE:CB	1:P:436:GLY:HA3	2.24	0.67
1:D:424:PHE:CB	1:D:436:GLY:HA3	2.24	0.67
1:N:424:PHE:CB	1:N:436:GLY:HA3	2.24	0.67
1:A:191:PHE:O	1:B:310:ARG:NH1	2.31	0.64
1:M:191:PHE:O	1:N:310:ARG:NH1	2.31	0.63
1:P:336:HIS:HE1	1:P:340:LYS:HE3	1.72	0.55
1:A:419:SER:HA	1:A:440:ILE:HG12	1.89	0.55
1:M:419:SER:HA	1:M:440:ILE:HG12	1.89	0.55
1:D:336:HIS:HE1	1:D:340:LYS:HE3	1.72	0.55
1:M:336:HIS:HE1	1:M:340:LYS:HE3	1.72	0.55
1:N:336:HIS:HE1	1:N:340:LYS:HE3	1.72	0.55
1:C:336:HIS:HE1	1:C:340:LYS:HE3	1.72	0.55
1:A:310:ARG:NH1	1:D:191:PHE:O	2.40	0.55
1:B:419:SER:HA	1:B:440:ILE:HG12	1.89	0.55
1:C:191:PHE:O	1:D:310:ARG:NH1	2.40	0.54
1:C:419:SER:HA	1:C:440:ILE:HG12	1.89	0.54
1:N:419:SER:HA	1:N:440:ILE:HG12	1.89	0.54
1:O:191:PHE:O	1:P:310:ARG:NH1	2.41	0.54
1:M:310:ARG:NH1	1:P:191:PHE:O	2.40	0.54
1:P:419:SER:HA	1:P:440:ILE:HG12	1.89	0.54
1:O:419:SER:HA	1:O:440:ILE:HG12	1.89	0.54
1:A:336:HIS:HE1	1:A:340:LYS:HE3	1.72	0.54
1:B:491:ASN:O	1:B:495:MET:CB	2.56	0.54
1:B:405:ILE:H	1:B:459:VAL:HB	1.73	0.54
1:D:405:ILE:H	1:D:459:VAL:HB	1.73	0.54
1:O:405:ILE:H	1:O:459:VAL:HB	1.73	0.54
1:A:491:ASN:O	1:A:495:MET:CB	2.56	0.53
1:C:405:ILE:H	1:C:459:VAL:HB	1.73	0.53
1:N:405:ILE:H	1:N:459:VAL:HB	1.73	0.53
1:O:491:ASN:O	1:O:495:MET:CB	2.56	0.53
1:D:491:ASN:O	1:D:495:MET:CB	2.56	0.53
1:B:336:HIS:HE1	1:B:340:LYS:HE3	1.72	0.53
1:M:491:ASN:O	1:M:495:MET:CB	2.56	0.53
1:A:405:ILE:H	1:A:459:VAL:HB	1.73	0.53
1:B:191:PHE:O	1:C:310:ARG:NH1	2.42	0.53
1:C:491:ASN:O	1:C:495:MET:CB	2.56	0.53
1:O:336:HIS:HE1	1:O:340:LYS:HE3	1.72	0.53
1:D:419:SER:HA	1:D:440:ILE:HG12	1.89	0.53
1:P:491:ASN:O	1:P:495:MET:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:PHE:O	1:O:310:ARG:NH1	2.42	0.53
1:M:99:ASN:OD1	1:M:174:ARG:NH2	2.37	0.53
1:N:491:ASN:O	1:N:495:MET:CB	2.56	0.53
1:P:405:ILE:H	1:P:459:VAL:HB	1.73	0.53
1:A:99:ASN:OD1	1:A:174:ARG:NH2	2.37	0.53
1:M:405:ILE:H	1:M:459:VAL:HB	1.73	0.52
1:D:99:ASN:OD1	1:D:174:ARG:NH2	2.37	0.52
1:N:99:ASN:OD1	1:N:174:ARG:NH2	2.37	0.51
1:B:99:ASN:OD1	1:B:174:ARG:NH2	2.37	0.51
1:N:336:HIS:CE1	1:N:340:LYS:HE3	2.46	0.51
1:M:336:HIS:CE1	1:M:340:LYS:HE3	2.46	0.51
1:A:336:HIS:CE1	1:A:340:LYS:HE3	2.46	0.50
1:C:336:HIS:CE1	1:C:340:LYS:HE3	2.46	0.50
1:P:336:HIS:CE1	1:P:340:LYS:HE3	2.46	0.50
1:B:336:HIS:CE1	1:B:340:LYS:HE3	2.46	0.50
1:D:336:HIS:CE1	1:D:340:LYS:HE3	2.46	0.50
1:O:336:HIS:CE1	1:O:340:LYS:HE3	2.46	0.50
1:B:69:LEU:HD11	1:B:98:VAL:HG22	1.95	0.49
1:O:99:ASN:OD1	1:O:174:ARG:NH2	2.37	0.49
1:M:69:LEU:HD11	1:M:98:VAL:HG22	1.95	0.49
1:N:69:LEU:HD11	1:N:98:VAL:HG22	1.95	0.49
1:A:69:LEU:HD11	1:A:98:VAL:HG22	1.95	0.49
1:P:69:LEU:HD11	1:P:98:VAL:HG22	1.95	0.48
1:O:69:LEU:HD11	1:O:98:VAL:HG22	1.95	0.48
1:C:69:LEU:HD11	1:C:98:VAL:HG22	1.95	0.48
1:D:69:LEU:HD11	1:D:98:VAL:HG22	1.95	0.48
1:O:149:GLN:HE21	1:O:165:ARG:HA	1.80	0.47
1:C:99:ASN:OD1	1:C:174:ARG:NH2	2.37	0.46
1:N:149:GLN:HE21	1:N:165:ARG:HA	1.81	0.46
1:B:149:GLN:HE21	1:B:165:ARG:HA	1.81	0.46
1:C:149:GLN:HE21	1:C:165:ARG:HA	1.81	0.46
1:A:259:THR:HG22	1:D:285:LEU:HD22	1.98	0.46
1:C:285:LEU:HD22	1:D:259:THR:HG22	1.98	0.46
1:M:149:GLN:HE21	1:M:165:ARG:HA	1.81	0.45
1:O:285:LEU:HD22	1:P:259:THR:HG22	1.98	0.45
1:D:149:GLN:HE21	1:D:165:ARG:HA	1.81	0.45
1:M:285:LEU:HD22	1:N:259:THR:HG22	1.98	0.45
1:P:149:GLN:HE21	1:P:165:ARG:HA	1.80	0.45
1:M:259:THR:HG22	1:P:285:LEU:HD22	1.98	0.45
1:A:285:LEU:HD22	1:B:259:THR:HG22	1.98	0.45
1:A:149:GLN:HE21	1:A:165:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:427:TYR:CB	1:O:458:THR:OG1	2.65	0.45
1:B:427:TYR:CB	1:B:458:THR:OG1	2.65	0.44
1:C:427:TYR:CB	1:C:458:THR:OG1	2.65	0.44
1:D:126:PRO:HA	1:D:129:ILE:HD12	1.99	0.44
1:D:427:TYR:CB	1:D:458:THR:OG1	2.65	0.44
1:A:126:PRO:HA	1:A:129:ILE:HD12	1.99	0.44
1:N:427:TYR:CB	1:N:458:THR:OG1	2.65	0.44
1:P:427:TYR:CB	1:P:458:THR:OG1	2.65	0.44
1:C:126:PRO:HA	1:C:129:ILE:HD12	1.99	0.44
1:A:427:TYR:CB	1:A:458:THR:OG1	2.65	0.44
1:B:372:VAL:HA	1:B:375:ILE:HD11	2.00	0.44
1:M:427:TYR:CB	1:M:458:THR:OG1	2.65	0.44
1:N:372:VAL:HA	1:N:375:ILE:HD11	2.00	0.43
1:O:126:PRO:HA	1:O:129:ILE:HD12	1.99	0.43
1:C:372:VAL:HA	1:C:375:ILE:HD11	2.00	0.43
1:P:197:ARG:NH1	2:P:602:QNP:O4	2.51	0.43
1:B:126:PRO:HA	1:B:129:ILE:HD12	1.99	0.43
1:P:126:PRO:HA	1:P:129:ILE:HD12	1.99	0.43
1:C:197:ARG:NH1	2:C:602:QNP:O4	2.51	0.43
1:B:197:ARG:NH1	2:B:601:QNP:O4	2.52	0.43
1:D:197:ARG:NH1	2:D:602:QNP:O4	2.51	0.43
1:N:125:SER:O	1:N:127:LYS:N	2.52	0.43
1:N:126:PRO:HA	1:N:129:ILE:HD12	1.99	0.43
1:O:372:VAL:HA	1:O:375:ILE:HD11	2.00	0.43
1:P:99:ASN:OD1	1:P:174:ARG:NH2	2.37	0.43
1:M:372:VAL:HA	1:M:375:ILE:HD11	2.00	0.43
1:N:285:LEU:HD22	1:O:259:THR:HG22	2.01	0.43
1:A:54:PRO:HD3	1:A:113:ALA:HB3	2.01	0.43
1:A:125:SER:O	1:A:127:LYS:N	2.52	0.43
1:B:125:SER:O	1:B:127:LYS:N	2.52	0.43
1:D:372:VAL:HA	1:D:375:ILE:HD11	2.00	0.43
1:M:54:PRO:HD3	1:M:113:ALA:HB3	2.01	0.43
1:C:54:PRO:HD3	1:C:113:ALA:HB3	2.01	0.43
1:M:126:PRO:HA	1:M:129:ILE:HD12	1.99	0.43
1:N:54:PRO:HD3	1:N:113:ALA:HB3	2.01	0.43
1:N:149:GLN:N	1:N:150:PRO:CD	2.82	0.43
1:O:149:GLN:N	1:O:150:PRO:CD	2.82	0.43
1:P:54:PRO:HD3	1:P:113:ALA:HB3	2.01	0.43
1:B:54:PRO:HD3	1:B:113:ALA:HB3	2.01	0.42
1:P:125:SER:O	1:P:127:LYS:N	2.52	0.42
1:A:197:ARG:NH1	2:A:601:QNP:O4	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLN:N	1:C:150:PRO:CD	2.82	0.42
1:B:285:LEU:HD22	1:C:259:THR:HG22	2.01	0.42
1:O:54:PRO:HD3	1:O:113:ALA:HB3	2.01	0.42
1:A:372:VAL:HA	1:A:375:ILE:HD11	2.00	0.42
1:C:125:SER:O	1:C:127:LYS:N	2.52	0.42
1:D:54:PRO:HD3	1:D:113:ALA:HB3	2.01	0.42
1:D:125:SER:O	1:D:127:LYS:N	2.52	0.42
1:A:149:GLN:N	1:A:150:PRO:CD	2.82	0.42
1:B:149:GLN:N	1:B:150:PRO:CD	2.82	0.42
1:P:404:ILE:N	1:P:459:VAL:O	2.45	0.42
1:M:125:SER:O	1:M:127:LYS:N	2.52	0.42
1:M:149:GLN:N	1:M:150:PRO:CD	2.82	0.42
1:O:125:SER:O	1:O:127:LYS:N	2.52	0.42
1:A:305:ARG:HG2	1:A:341:PHE:HE1	1.85	0.42
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.90	0.42
1:P:372:VAL:HA	1:P:375:ILE:HD11	2.00	0.42
1:O:197:ARG:NH1	2:O:602:QNP:O4	2.51	0.42
1:O:339:LEU:HD23	1:O:339:LEU:HA	1.90	0.42
1:P:455:GLN:HA	1:P:456:PRO:HD3	1.93	0.42
1:B:305:ARG:HG2	1:B:341:PHE:HE1	1.85	0.42
1:N:305:ARG:HG2	1:N:341:PHE:HE1	1.85	0.42
1:D:149:GLN:N	1:D:150:PRO:CD	2.82	0.41
1:D:305:ARG:HG2	1:D:341:PHE:HE1	1.85	0.41
1:O:305:ARG:HG2	1:O:341:PHE:HE1	1.85	0.41
1:O:455:GLN:HA	1:O:456:PRO:HD3	1.93	0.41
1:P:149:GLN:N	1:P:150:PRO:CD	2.82	0.41
1:P:66:LEU:HD23	1:P:66:LEU:HA	1.91	0.41
1:M:305:ARG:HG2	1:M:341:PHE:HE1	1.85	0.41
1:N:197:ARG:NH1	2:N:601:QNP:O4	2.52	0.41
1:C:369:PHE:O	1:C:373:HIS:HB2	2.21	0.41
1:P:369:PHE:O	1:P:373:HIS:HB2	2.21	0.41
1:B:369:PHE:O	1:B:373:HIS:HB2	2.21	0.41
1:C:305:ARG:HG2	1:C:341:PHE:HE1	1.85	0.41
1:M:369:PHE:O	1:M:373:HIS:HB2	2.21	0.41
1:P:375:ILE:HD13	1:P:375:ILE:HG21	1.89	0.41
1:B:352:LEU:HD23	1:B:355:LEU:HD12	2.03	0.41
1:M:352:LEU:HD23	1:M:355:LEU:HD12	2.03	0.41
1:N:352:LEU:HD23	1:N:355:LEU:HD12	2.03	0.41
1:N:369:PHE:O	1:N:373:HIS:HB2	2.21	0.41
1:D:76:ILE:HD13	1:D:76:ILE:HA	1.92	0.40
1:D:339:LEU:HD23	1:D:339:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ILE:HA	1:B:492:ASN:HD22	1.87	0.40
1:C:404:ILE:N	1:C:459:VAL:O	2.45	0.40
1:O:66:LEU:HD23	1:O:66:LEU:HA	1.91	0.40
1:P:305:ARG:HG2	1:P:341:PHE:HE1	1.85	0.40
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.92	0.40
1:A:352:LEU:HD23	1:A:355:LEU:HD12	2.03	0.40
1:A:369:PHE:O	1:A:373:HIS:HB2	2.21	0.40
1:D:352:LEU:HD23	1:D:355:LEU:HD12	2.03	0.40
1:O:352:LEU:HD23	1:O:355:LEU:HD12	2.03	0.40
1:O:369:PHE:O	1:O:373:HIS:HB2	2.21	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	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	B	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	C	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	D	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	M	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	N	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	O	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
1	P	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	47	79
All	All	3536/4096 (86%)	3192 (90%)	336 (10%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	B	326	PRO
1	C	326	PRO
1	D	326	PRO
1	M	326	PRO
1	N	326	PRO
1	O	326	PRO
1	P	326	PRO

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	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	B	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	C	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	D	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	M	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	N	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	O	331/459 (72%)	329 (99%)	2 (1%)	86 92
1	P	331/459 (72%)	329 (99%)	2 (1%)	86 92
All	All	2648/3672 (72%)	2632 (99%)	16 (1%)	86 92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	227	ARG
1	B	176	ARG
1	B	227	ARG
1	C	176	ARG
1	C	227	ARG
1	D	176	ARG
1	D	227	ARG

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Mol	Chain	Res	Type
1	M	176	ARG
1	M	227	ARG
1	N	176	ARG
1	N	227	ARG
1	O	176	ARG
1	O	227	ARG
1	P	176	ARG
1	P	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	A	492	ASN
1	B	336	HIS
1	B	492	ASN
1	C	336	HIS
1	C	492	ASN
1	D	336	HIS
1	D	492	ASN
1	M	336	HIS
1	M	492	ASN
1	N	336	HIS
1	N	492	ASN
1	O	336	HIS
1	O	492	ASN
1	P	336	HIS
1	P	492	ASN

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)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	QNJ	O	601	-	31,31,31	1.79	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	P	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
2	QNP	C	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	C	601	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
3	QNJ	N	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	M	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
2	QNP	B	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	P	601	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	D	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
2	QNP	A	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	D	601	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
3	QNJ	M	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	N	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	B	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	O	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	A	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QNJ	O	601	-	-	5/10/68/68	0/4/4/4
2	QNP	P	602	-	-	19/36/36/36	-
2	QNP	C	602	-	-	19/36/36/36	-
3	QNJ	C	601	-	-	5/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QNJ	N	602	-	-	5/10/68/68	0/4/4/4
2	QNP	M	601	-	-	19/36/36/36	-
2	QNP	B	601	-	-	19/36/36/36	-
3	QNJ	P	601	-	-	5/10/68/68	0/4/4/4
2	QNP	D	602	-	-	19/36/36/36	-
2	QNP	A	601	-	-	19/36/36/36	-
3	QNJ	D	601	-	-	5/10/68/68	0/4/4/4
3	QNJ	M	602	-	-	5/10/68/68	0/4/4/4
2	QNP	N	601	-	-	19/36/36/36	-
3	QNJ	B	602	-	-	5/10/68/68	0/4/4/4
2	QNP	O	602	-	-	19/36/36/36	-
3	QNJ	A	602	-	-	5/10/68/68	0/4/4/4

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	QNJ	C19-C10	-4.43	1.46	1.54
3	N	602	QNJ	C19-C10	-4.43	1.46	1.54
3	A	602	QNJ	C19-C10	-4.43	1.46	1.54
3	B	602	QNJ	C19-C10	-4.43	1.46	1.54
3	C	601	QNJ	C19-C10	-4.43	1.46	1.54
3	D	601	QNJ	C19-C10	-4.43	1.46	1.54
3	P	601	QNJ	C19-C10	-4.42	1.46	1.54
3	M	602	QNJ	C19-C10	-4.42	1.46	1.54
3	P	601	QNJ	C12-C11	-3.61	1.45	1.53
3	M	602	QNJ	C12-C11	-3.60	1.45	1.53
3	A	602	QNJ	C12-C11	-3.59	1.45	1.53
3	B	602	QNJ	C12-C11	-3.59	1.45	1.53
3	C	601	QNJ	C12-C11	-3.59	1.45	1.53
3	D	601	QNJ	C12-C11	-3.59	1.45	1.53
3	N	602	QNJ	C12-C11	-3.58	1.45	1.53
3	O	601	QNJ	C12-C11	-3.56	1.45	1.53
3	P	601	QNJ	C20-C17	3.24	1.60	1.54
3	A	602	QNJ	C20-C17	3.22	1.60	1.54
3	B	602	QNJ	C20-C17	3.22	1.60	1.54
3	C	601	QNJ	C20-C17	3.22	1.60	1.54
3	D	601	QNJ	C20-C17	3.22	1.60	1.54
3	N	602	QNJ	C20-C17	3.22	1.60	1.54
3	M	602	QNJ	C20-C17	3.20	1.60	1.54
3	O	601	QNJ	C20-C17	3.18	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	QNJ	O1-C3	-3.14	1.34	1.43
3	P	601	QNJ	O1-C3	-3.12	1.34	1.43
3	A	602	QNJ	O1-C3	-3.12	1.34	1.43
3	B	602	QNJ	O1-C3	-3.12	1.34	1.43
3	C	601	QNJ	O1-C3	-3.12	1.34	1.43
3	D	601	QNJ	O1-C3	-3.12	1.34	1.43
3	N	602	QNJ	O1-C3	-3.11	1.34	1.43
3	M	602	QNJ	O1-C3	-3.10	1.34	1.43
3	M	602	QNJ	C22-C20	-3.06	1.46	1.54
3	N	602	QNJ	C22-C20	-3.04	1.46	1.54
3	P	601	QNJ	C22-C20	-3.03	1.46	1.54
3	A	602	QNJ	C22-C20	-3.03	1.46	1.54
3	B	602	QNJ	C22-C20	-3.03	1.46	1.54
3	C	601	QNJ	C22-C20	-3.03	1.46	1.54
3	D	601	QNJ	C22-C20	-3.03	1.46	1.54
3	O	601	QNJ	C22-C20	-2.99	1.46	1.54
3	M	602	QNJ	C10-C9	-2.98	1.50	1.56
3	P	601	QNJ	C10-C9	-2.97	1.50	1.56
3	A	602	QNJ	C10-C9	-2.95	1.50	1.56
3	B	602	QNJ	C10-C9	-2.95	1.50	1.56
3	C	601	QNJ	C10-C9	-2.95	1.50	1.56
3	D	601	QNJ	C10-C9	-2.95	1.50	1.56
3	N	602	QNJ	C10-C9	-2.94	1.50	1.56
3	O	601	QNJ	C10-C9	-2.93	1.50	1.56
2	M	601	QNP	O7-C16	-2.75	1.39	1.46
2	A	601	QNP	O7-C16	-2.71	1.39	1.46
2	O	602	QNP	O7-C16	-2.71	1.39	1.46
2	C	602	QNP	O7-C16	-2.71	1.39	1.46
2	D	602	QNP	O7-C16	-2.71	1.39	1.46
2	P	602	QNP	O7-C16	-2.71	1.39	1.46
2	B	601	QNP	O7-C16	-2.70	1.39	1.46
2	N	601	QNP	O7-C16	-2.70	1.39	1.46
2	M	601	QNP	O2-C14	2.43	1.40	1.33
2	A	601	QNP	O2-C14	2.40	1.40	1.33
2	D	602	QNP	O2-C14	2.40	1.40	1.33
2	C	602	QNP	O2-C14	2.39	1.40	1.33
2	P	602	QNP	O2-C14	2.38	1.40	1.33
2	B	601	QNP	O2-C14	2.38	1.40	1.33
2	N	601	QNP	O2-C14	2.38	1.40	1.33
2	O	602	QNP	O2-C14	2.37	1.40	1.33
3	N	602	QNJ	C11-C9	-2.32	1.49	1.53
3	A	602	QNJ	C11-C9	-2.29	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	QNJ	C11-C9	-2.29	1.49	1.53
3	C	601	QNJ	C11-C9	-2.29	1.49	1.53
3	D	601	QNJ	C11-C9	-2.29	1.49	1.53
2	P	602	QNP	O2-C15	-2.28	1.40	1.45
3	M	602	QNJ	C11-C9	-2.28	1.49	1.53
3	O	601	QNJ	C11-C9	-2.28	1.50	1.53
2	D	602	QNP	O2-C15	-2.26	1.40	1.45
2	C	602	QNP	O2-C15	-2.25	1.40	1.45
2	O	602	QNP	O2-C15	-2.24	1.40	1.45
2	M	601	QNP	O2-C15	-2.23	1.40	1.45
3	P	601	QNJ	C11-C9	-2.23	1.50	1.53
2	A	601	QNP	O2-C15	-2.23	1.40	1.45
2	B	601	QNP	O2-C15	-2.22	1.40	1.45
2	N	601	QNP	O2-C15	-2.21	1.40	1.45
3	M	602	QNJ	C1-C2	-2.18	1.48	1.53
3	P	601	QNJ	C1-C2	-2.18	1.48	1.53
3	A	602	QNJ	C1-C2	-2.17	1.48	1.53
3	B	602	QNJ	C1-C2	-2.17	1.48	1.53
3	C	601	QNJ	C1-C2	-2.17	1.48	1.53
3	D	601	QNJ	C1-C2	-2.17	1.48	1.53
2	P	602	QNP	O7-C23	2.17	1.40	1.34
2	D	602	QNP	O7-C23	2.17	1.40	1.34
3	N	602	QNJ	C1-C2	-2.16	1.48	1.53
2	B	601	QNP	O7-C23	2.16	1.40	1.34
3	O	601	QNJ	C1-C2	-2.16	1.48	1.53
2	N	601	QNP	O7-C23	2.15	1.40	1.34
2	C	602	QNP	O7-C23	2.15	1.40	1.34
2	O	602	QNP	O7-C23	2.13	1.40	1.34
2	M	601	QNP	O7-C23	2.12	1.40	1.34
2	A	601	QNP	O7-C23	2.12	1.40	1.34
2	P	602	QNP	O1-C14	-2.11	1.16	1.22
2	O	602	QNP	O1-C14	-2.11	1.16	1.22
2	C	602	QNP	O1-C14	-2.11	1.16	1.22
2	D	602	QNP	O1-C14	-2.11	1.16	1.22
2	B	601	QNP	O1-C14	-2.09	1.16	1.22
2	M	601	QNP	O1-C14	-2.08	1.16	1.22
2	N	601	QNP	O1-C14	-2.07	1.16	1.22
2	A	601	QNP	O1-C14	-2.07	1.16	1.22

All (136) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	602	QNJ	C21-C20-C22	-6.12	100.77	110.36
3	O	601	QNJ	C21-C20-C22	-6.11	100.78	110.36
3	A	602	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	B	602	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	C	601	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	D	601	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	N	602	QNJ	C21-C20-C22	-6.10	100.81	110.36
3	P	601	QNJ	C21-C20-C22	-6.10	100.81	110.36
3	M	602	QNJ	C4-C5-C10	4.95	117.92	112.66
3	N	602	QNJ	C4-C5-C10	4.93	117.89	112.66
3	A	602	QNJ	C4-C5-C10	4.90	117.87	112.66
3	B	602	QNJ	C4-C5-C10	4.90	117.87	112.66
3	C	601	QNJ	C4-C5-C10	4.90	117.87	112.66
3	D	601	QNJ	C4-C5-C10	4.90	117.87	112.66
3	O	601	QNJ	C4-C5-C10	4.90	117.86	112.66
3	P	601	QNJ	C4-C5-C10	4.88	117.84	112.66
3	P	601	QNJ	C5-C4-C3	4.00	118.63	112.76
3	O	601	QNJ	C5-C4-C3	4.00	118.63	112.76
3	A	602	QNJ	C5-C4-C3	3.98	118.61	112.76
3	B	602	QNJ	C5-C4-C3	3.98	118.61	112.76
3	C	601	QNJ	C5-C4-C3	3.98	118.61	112.76
3	D	601	QNJ	C5-C4-C3	3.98	118.61	112.76
3	N	602	QNJ	C5-C4-C3	3.96	118.57	112.76
3	O	601	QNJ	C21-C20-C17	3.95	118.97	112.92
3	P	601	QNJ	C21-C20-C17	3.94	118.95	112.92
3	M	602	QNJ	C5-C4-C3	3.94	118.54	112.76
3	A	602	QNJ	C21-C20-C17	3.93	118.93	112.92
3	B	602	QNJ	C21-C20-C17	3.93	118.93	112.92
3	C	601	QNJ	C21-C20-C17	3.93	118.93	112.92
3	D	601	QNJ	C21-C20-C17	3.93	118.93	112.92
3	N	602	QNJ	C21-C20-C17	3.92	118.93	112.92
3	M	602	QNJ	C21-C20-C17	3.91	118.90	112.92
3	P	601	QNJ	C11-C9-C10	-3.79	109.55	113.91
3	M	602	QNJ	C11-C9-C10	-3.77	109.57	113.91
3	A	602	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	B	602	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	C	601	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	D	601	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	O	601	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	N	602	QNJ	C11-C9-C10	-3.74	109.60	113.91
2	M	601	QNP	O7-C23-C24	3.52	119.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	602	QNP	O7-C23-C24	3.52	119.08	111.50
2	A	601	QNP	O7-C23-C24	3.52	119.08	111.50
2	C	602	QNP	O7-C23-C24	3.51	119.07	111.50
2	B	601	QNP	O7-C23-C24	3.49	119.02	111.50
2	P	602	QNP	O7-C23-C24	3.49	119.02	111.50
2	N	601	QNP	O7-C23-C24	3.48	119.01	111.50
2	D	602	QNP	O7-C23-C24	3.48	119.00	111.50
2	N	601	QNP	C17-C16-C15	-3.39	103.78	111.79
2	A	601	QNP	C17-C16-C15	-3.38	103.79	111.79
2	B	601	QNP	C17-C16-C15	-3.38	103.80	111.79
2	M	601	QNP	C17-C16-C15	-3.38	103.80	111.79
2	O	602	QNP	C17-C16-C15	-3.37	103.82	111.79
2	C	602	QNP	C17-C16-C15	-3.36	103.83	111.79
2	D	602	QNP	C17-C16-C15	-3.36	103.84	111.79
2	P	602	QNP	C17-C16-C15	-3.36	103.85	111.79
2	N	601	QNP	O2-C14-C13	3.26	122.14	111.91
2	D	602	QNP	O2-C14-C13	3.26	122.14	111.91
2	A	601	QNP	O2-C14-C13	3.26	122.14	111.91
2	B	601	QNP	O2-C14-C13	3.26	122.14	111.91
2	P	602	QNP	O2-C14-C13	3.26	122.13	111.91
2	M	601	QNP	O2-C14-C13	3.25	122.11	111.91
2	O	602	QNP	O2-C14-C13	3.24	122.09	111.91
2	C	602	QNP	O2-C14-C13	3.24	122.09	111.91
3	M	602	QNJ	C16-C17-C20	-3.12	107.31	112.15
3	O	601	QNJ	C1-C10-C5	3.11	112.37	107.77
3	N	602	QNJ	C1-C10-C5	3.10	112.35	107.77
3	N	602	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	A	602	QNJ	C1-C10-C5	3.09	112.34	107.77
3	B	602	QNJ	C1-C10-C5	3.09	112.34	107.77
3	C	601	QNJ	C1-C10-C5	3.09	112.34	107.77
3	D	601	QNJ	C1-C10-C5	3.09	112.34	107.77
3	A	602	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	B	602	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	C	601	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	D	601	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	P	601	QNJ	C1-C10-C5	3.09	112.33	107.77
3	P	601	QNJ	C16-C17-C20	-3.08	107.38	112.15
3	O	601	QNJ	C16-C17-C20	-3.06	107.41	112.15
3	M	602	QNJ	C1-C10-C5	3.06	112.29	107.77
3	O	601	QNJ	C13-C14-C8	-3.01	109.92	114.38
3	N	602	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	A	602	QNJ	C13-C14-C8	-2.98	109.96	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	C	601	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	D	601	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	P	601	QNJ	C13-C14-C8	-2.98	109.97	114.38
3	M	602	QNJ	C13-C14-C8	-2.97	109.98	114.38
2	M	601	QNP	O3-P1-O5	2.86	114.48	106.47
2	O	602	QNP	O3-P1-O5	2.84	114.44	106.47
2	A	601	QNP	O3-P1-O5	2.84	114.43	106.47
2	P	602	QNP	O3-P1-O5	2.84	114.43	106.47
2	D	602	QNP	O3-P1-O5	2.83	114.42	106.47
2	C	602	QNP	O3-P1-O5	2.83	114.41	106.47
2	N	601	QNP	O3-P1-O5	2.83	114.40	106.47
2	B	601	QNP	O3-P1-O5	2.82	114.38	106.47
3	M	602	QNJ	C19-C10-C5	-2.78	105.65	110.36
3	P	601	QNJ	C19-C10-C5	-2.78	105.66	110.36
3	A	602	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	B	602	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	C	601	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	D	601	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	O	601	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	N	602	QNJ	C19-C10-C5	-2.75	105.69	110.36
3	N	602	QNJ	C9-C10-C5	2.54	112.14	108.58
3	O	601	QNJ	C9-C10-C5	2.53	112.13	108.58
3	A	602	QNJ	C9-C10-C5	2.53	112.13	108.58
3	B	602	QNJ	C9-C10-C5	2.53	112.13	108.58
3	C	601	QNJ	C9-C10-C5	2.53	112.13	108.58
3	D	601	QNJ	C9-C10-C5	2.53	112.13	108.58
3	M	602	QNJ	C9-C10-C5	2.53	112.13	108.58
3	P	601	QNJ	C9-C10-C5	2.51	112.11	108.58
3	P	601	QNJ	C6-C7-C8	2.20	115.76	112.14
3	M	602	QNJ	C6-C7-C8	2.19	115.75	112.14
3	A	602	QNJ	C6-C7-C8	2.19	115.74	112.14
3	B	602	QNJ	C6-C7-C8	2.19	115.74	112.14
3	C	601	QNJ	C6-C7-C8	2.19	115.74	112.14
3	D	601	QNJ	C6-C7-C8	2.19	115.74	112.14
3	N	602	QNJ	C6-C7-C8	2.17	115.71	112.14
3	O	601	QNJ	C6-C7-C8	2.16	115.70	112.14
3	O	601	QNJ	C16-C17-C13	-2.10	101.31	103.84
3	N	602	QNJ	C16-C17-C13	-2.09	101.32	103.84
3	A	602	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	B	602	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	C	601	QNJ	C16-C17-C13	-2.09	101.33	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	601	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	P	601	QNJ	C16-C17-C13	-2.06	101.36	103.84
3	M	602	QNJ	C16-C17-C13	-2.06	101.36	103.84
2	O	602	QNP	O1-C14-C13	-2.02	115.83	123.73
2	P	602	QNP	O1-C14-C13	-2.02	115.85	123.73
2	C	602	QNP	O1-C14-C13	-2.02	115.86	123.73
2	A	601	QNP	O1-C14-C13	-2.02	115.86	123.73
2	N	601	QNP	O1-C14-C13	-2.02	115.87	123.73
2	D	602	QNP	O1-C14-C13	-2.02	115.87	123.73
2	B	601	QNP	O1-C14-C13	-2.01	115.88	123.73
2	M	601	QNP	O1-C14-C13	-2.01	115.90	123.73

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	QNP	C24-C23-O7-C16
2	A	601	QNP	C17-O3-P1-O4
2	A	601	QNP	C17-O3-P1-O5
2	A	601	QNP	C17-O3-P1-O6
2	B	601	QNP	C24-C23-O7-C16
2	B	601	QNP	C17-O3-P1-O4
2	B	601	QNP	C17-O3-P1-O5
2	B	601	QNP	C17-O3-P1-O6
2	C	602	QNP	C24-C23-O7-C16
2	C	602	QNP	C17-O3-P1-O4
2	C	602	QNP	C17-O3-P1-O5
2	C	602	QNP	C17-O3-P1-O6
2	D	602	QNP	C24-C23-O7-C16
2	D	602	QNP	C17-O3-P1-O4
2	D	602	QNP	C17-O3-P1-O5
2	D	602	QNP	C17-O3-P1-O6
2	M	601	QNP	C24-C23-O7-C16
2	M	601	QNP	C17-O3-P1-O4
2	M	601	QNP	C17-O3-P1-O5
2	M	601	QNP	C17-O3-P1-O6
2	N	601	QNP	C24-C23-O7-C16
2	N	601	QNP	C17-O3-P1-O4
2	N	601	QNP	C17-O3-P1-O5
2	N	601	QNP	C17-O3-P1-O6
2	O	602	QNP	C24-C23-O7-C16
2	O	602	QNP	C17-O3-P1-O4

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Mol	Chain	Res	Type	Atoms
2	O	602	QNP	C17-O3-P1-O5
2	O	602	QNP	C17-O3-P1-O6
2	P	602	QNP	C24-C23-O7-C16
2	P	602	QNP	C17-O3-P1-O4
2	P	602	QNP	C17-O3-P1-O5
2	P	602	QNP	C17-O3-P1-O6
2	A	601	QNP	O8-C23-O7-C16
2	B	601	QNP	O8-C23-O7-C16
2	C	602	QNP	O8-C23-O7-C16
2	D	602	QNP	O8-C23-O7-C16
2	M	601	QNP	O8-C23-O7-C16
2	N	601	QNP	O8-C23-O7-C16
2	O	602	QNP	O8-C23-O7-C16
2	P	602	QNP	O8-C23-O7-C16
2	A	601	QNP	C13-C14-O2-C15
2	B	601	QNP	C13-C14-O2-C15
2	C	602	QNP	C13-C14-O2-C15
2	D	602	QNP	C13-C14-O2-C15
2	M	601	QNP	C13-C14-O2-C15
2	N	601	QNP	C13-C14-O2-C15
2	O	602	QNP	C13-C14-O2-C15
2	P	602	QNP	C13-C14-O2-C15
2	A	601	QNP	O1-C14-O2-C15
2	B	601	QNP	O1-C14-O2-C15
2	C	602	QNP	O1-C14-O2-C15
2	D	602	QNP	O1-C14-O2-C15
2	M	601	QNP	O1-C14-O2-C15
2	N	601	QNP	O1-C14-O2-C15
2	O	602	QNP	O1-C14-O2-C15
2	P	602	QNP	O1-C14-O2-C15
3	A	602	QNJ	C17-C20-C22-C23
3	B	602	QNJ	C17-C20-C22-C23
3	C	601	QNJ	C17-C20-C22-C23
3	D	601	QNJ	C17-C20-C22-C23
3	M	602	QNJ	C17-C20-C22-C23
3	N	602	QNJ	C17-C20-C22-C23
3	O	601	QNJ	C17-C20-C22-C23
3	P	601	QNJ	C17-C20-C22-C23
3	A	602	QNJ	C21-C20-C22-C23
3	B	602	QNJ	C21-C20-C22-C23
3	C	601	QNJ	C21-C20-C22-C23
3	D	601	QNJ	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	M	602	QNJ	C21-C20-C22-C23
3	N	602	QNJ	C21-C20-C22-C23
3	O	601	QNJ	C21-C20-C22-C23
3	P	601	QNJ	C21-C20-C22-C23
2	A	601	QNP	C23-C24-C25-C26
2	B	601	QNP	C23-C24-C25-C26
2	C	602	QNP	C23-C24-C25-C26
2	D	602	QNP	C23-C24-C25-C26
2	M	601	QNP	C23-C24-C25-C26
2	N	601	QNP	C23-C24-C25-C26
2	O	602	QNP	C23-C24-C25-C26
2	P	602	QNP	C23-C24-C25-C26
3	A	602	QNJ	C16-C17-C20-C22
3	B	602	QNJ	C16-C17-C20-C22
3	C	601	QNJ	C16-C17-C20-C22
3	D	601	QNJ	C16-C17-C20-C22
3	M	602	QNJ	C16-C17-C20-C22
3	N	602	QNJ	C16-C17-C20-C22
3	O	601	QNJ	C16-C17-C20-C22
3	P	601	QNJ	C16-C17-C20-C22
2	A	601	QNP	C9-C10-C11-C12
2	B	601	QNP	C9-C10-C11-C12
2	C	602	QNP	C9-C10-C11-C12
2	D	602	QNP	C9-C10-C11-C12
2	M	601	QNP	C9-C10-C11-C12
2	N	601	QNP	C9-C10-C11-C12
2	O	602	QNP	C9-C10-C11-C12
2	P	602	QNP	C9-C10-C11-C12
2	A	601	QNP	C7-C8-C9-C10
2	B	601	QNP	C7-C8-C9-C10
2	C	602	QNP	C7-C8-C9-C10
2	D	602	QNP	C7-C8-C9-C10
2	M	601	QNP	C7-C8-C9-C10
2	N	601	QNP	C7-C8-C9-C10
2	O	602	QNP	C7-C8-C9-C10
2	P	602	QNP	C7-C8-C9-C10
2	A	601	QNP	C24-C25-C26-C27
2	B	601	QNP	C24-C25-C26-C27
2	C	602	QNP	C24-C25-C26-C27
2	D	602	QNP	C24-C25-C26-C27
2	M	601	QNP	C24-C25-C26-C27
2	N	601	QNP	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	O	602	QNP	C24-C25-C26-C27
2	P	602	QNP	C24-C25-C26-C27
2	A	601	QNP	C31-C32-C33-C34
2	B	601	QNP	C31-C32-C33-C34
2	C	602	QNP	C31-C32-C33-C34
2	D	602	QNP	C31-C32-C33-C34
2	M	601	QNP	C31-C32-C33-C34
2	N	601	QNP	C31-C32-C33-C34
2	O	602	QNP	C31-C32-C33-C34
2	P	602	QNP	C31-C32-C33-C34
2	O	602	QNP	C30-C31-C32-C33
2	P	602	QNP	C30-C31-C32-C33
2	A	601	QNP	C30-C31-C32-C33
2	B	601	QNP	C30-C31-C32-C33
2	C	602	QNP	C30-C31-C32-C33
2	D	602	QNP	C30-C31-C32-C33
2	M	601	QNP	C30-C31-C32-C33
2	N	601	QNP	C30-C31-C32-C33
2	A	601	QNP	C11-C10-C9-C8
2	B	601	QNP	C11-C10-C9-C8
2	C	602	QNP	C11-C10-C9-C8
2	D	602	QNP	C11-C10-C9-C8
2	M	601	QNP	C11-C10-C9-C8
2	N	601	QNP	C11-C10-C9-C8
2	O	602	QNP	C11-C10-C9-C8
2	P	602	QNP	C11-C10-C9-C8
2	A	601	QNP	C29-C30-C31-C32
2	C	602	QNP	C28-C29-C30-C31
2	M	601	QNP	C29-C30-C31-C32
2	O	602	QNP	C28-C29-C30-C31
2	P	602	QNP	C28-C29-C30-C31
2	A	601	QNP	C28-C29-C30-C31
2	B	601	QNP	C28-C29-C30-C31
2	B	601	QNP	C29-C30-C31-C32
2	C	602	QNP	C29-C30-C31-C32
2	D	602	QNP	C28-C29-C30-C31
2	D	602	QNP	C29-C30-C31-C32
2	M	601	QNP	C28-C29-C30-C31
2	N	601	QNP	C28-C29-C30-C31
2	N	601	QNP	C29-C30-C31-C32
2	O	602	QNP	C29-C30-C31-C32
2	P	602	QNP	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
2	A	601	QNP	C6-C7-C8-C9
2	C	602	QNP	C6-C7-C8-C9
2	O	602	QNP	C6-C7-C8-C9
2	B	601	QNP	C6-C7-C8-C9
2	D	602	QNP	C6-C7-C8-C9
2	M	601	QNP	C6-C7-C8-C9
2	N	601	QNP	C6-C7-C8-C9
2	P	602	QNP	C6-C7-C8-C9
2	A	601	QNP	C17-C16-O7-C23
2	B	601	QNP	C17-C16-O7-C23
2	C	602	QNP	C17-C16-O7-C23
2	D	602	QNP	C17-C16-O7-C23
2	M	601	QNP	C17-C16-O7-C23
2	N	601	QNP	C17-C16-O7-C23
2	O	602	QNP	C17-C16-O7-C23
2	P	602	QNP	C17-C16-O7-C23
3	M	602	QNJ	C22-C23-C24-C25
3	O	601	QNJ	C22-C23-C24-C25
3	A	602	QNJ	C22-C23-C24-C25
3	B	602	QNJ	C22-C23-C24-C25
3	C	601	QNJ	C22-C23-C24-C25
3	D	601	QNJ	C22-C23-C24-C25
3	P	601	QNJ	C22-C23-C24-C25
2	A	601	QNP	C15-C16-C17-O3
2	B	601	QNP	C15-C16-C17-O3
2	C	602	QNP	C15-C16-C17-O3
2	D	602	QNP	C15-C16-C17-O3
2	M	601	QNP	C15-C16-C17-O3
2	N	601	QNP	C15-C16-C17-O3
2	O	602	QNP	C15-C16-C17-O3
2	P	602	QNP	C15-C16-C17-O3
3	N	602	QNJ	C22-C23-C24-C25
3	P	601	QNJ	C23-C24-C25-C27
3	A	602	QNJ	C23-C24-C25-C27
3	B	602	QNJ	C23-C24-C25-C27
3	C	601	QNJ	C23-C24-C25-C27
3	D	601	QNJ	C23-C24-C25-C27
3	O	601	QNJ	C23-C24-C25-C27
3	M	602	QNJ	C23-C24-C25-C27
3	N	602	QNJ	C23-C24-C25-C27

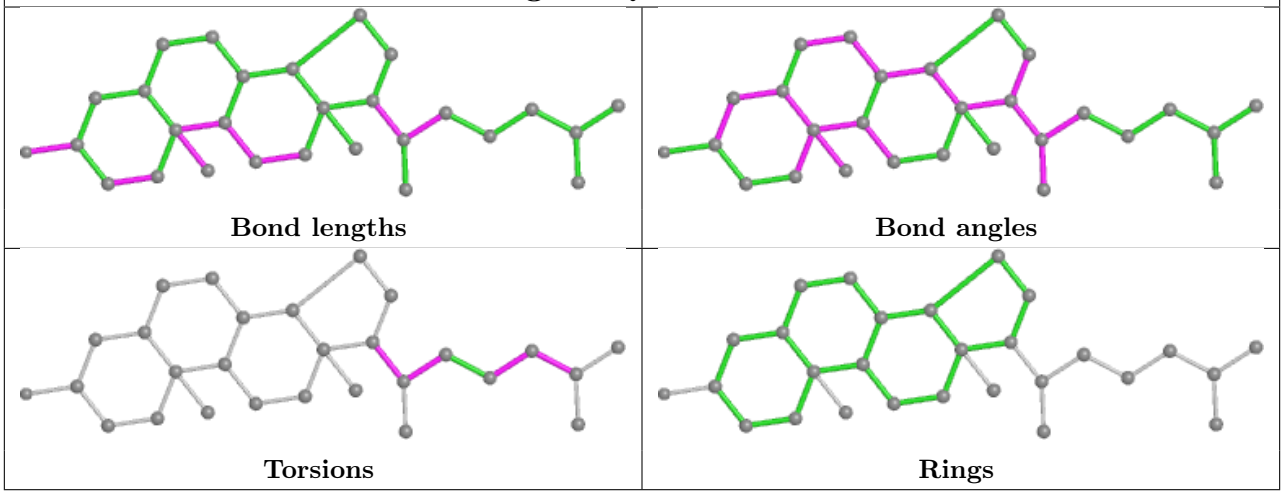
There are no ring outliers.

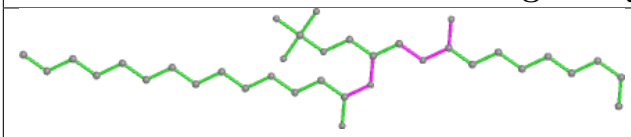
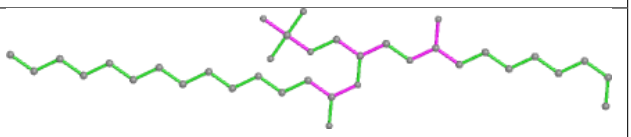
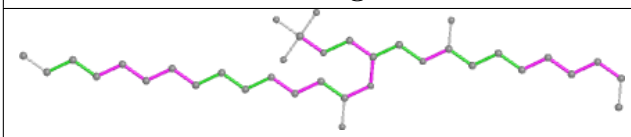
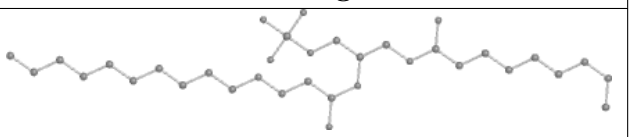
7 monomers are involved in 7 short contacts:

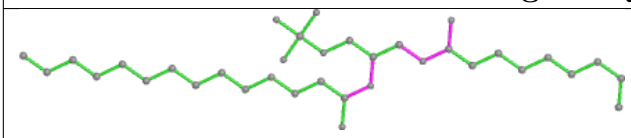
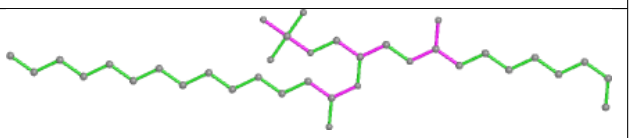
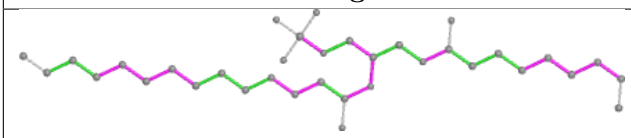
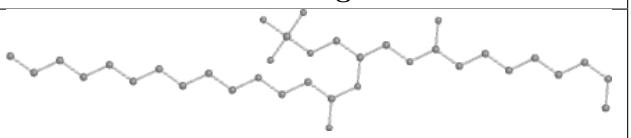
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	602	QNP	1	0
2	C	602	QNP	1	0
2	B	601	QNP	1	0
2	D	602	QNP	1	0
2	A	601	QNP	1	0
2	N	601	QNP	1	0
2	O	602	QNP	1	0

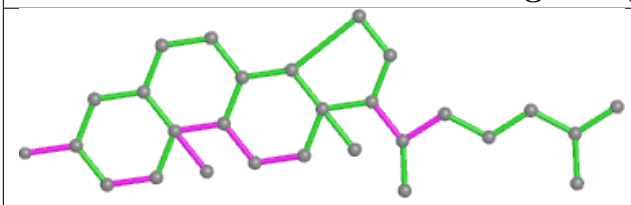
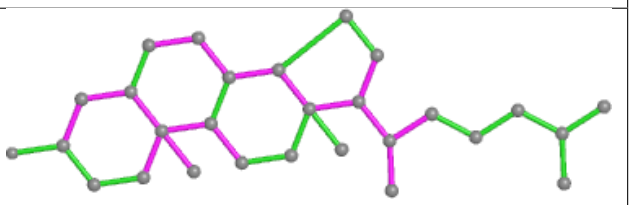
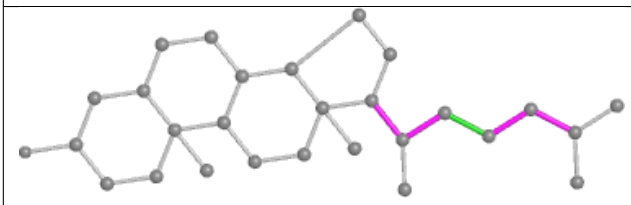
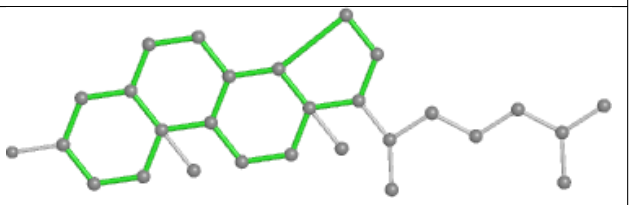
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

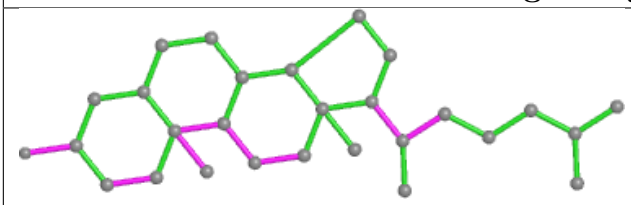
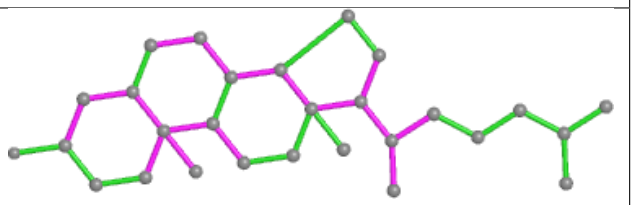
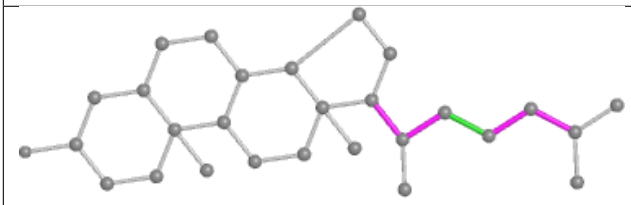
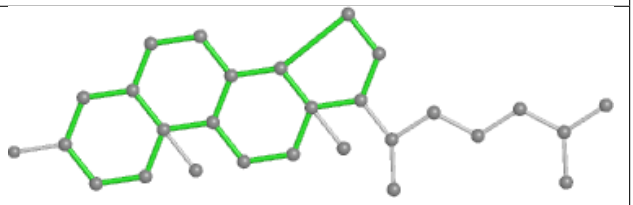
Ligand QNJ O 601

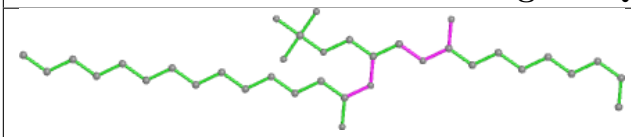
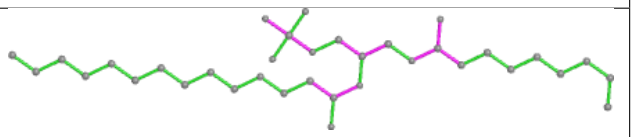
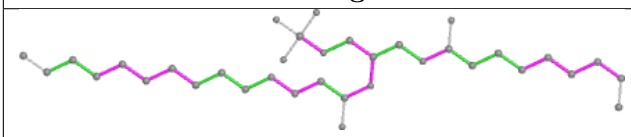
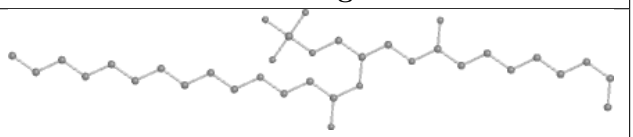


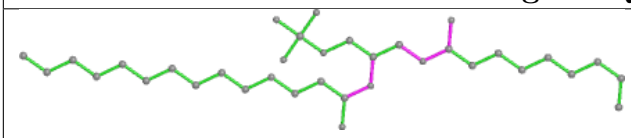
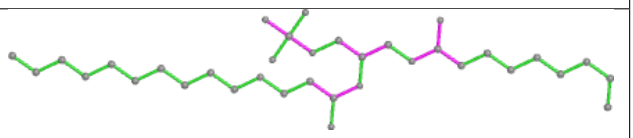
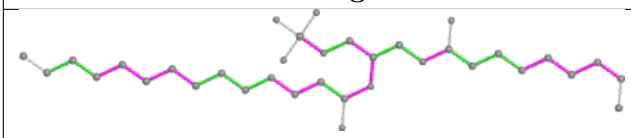
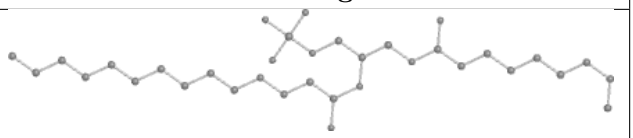
Ligand QNP P 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand QNP C 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

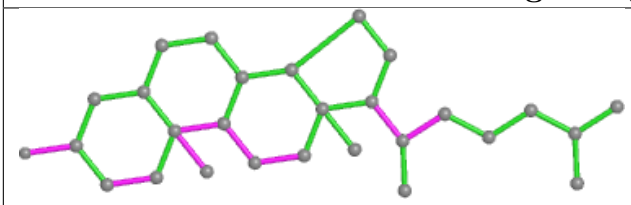
Ligand QNJ C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand QNJ N 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

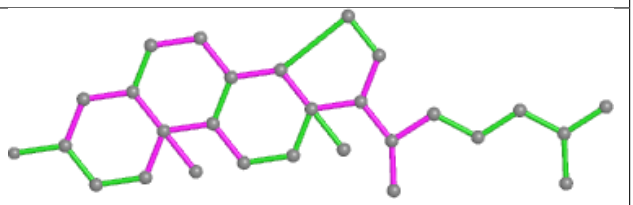
Ligand QNP M 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand QNP B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

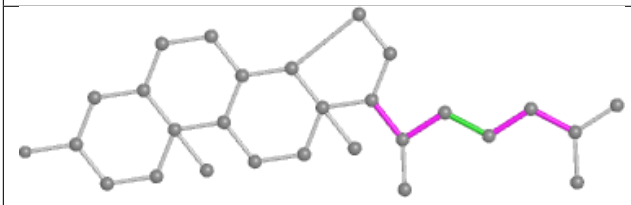
Ligand QNJ P 601



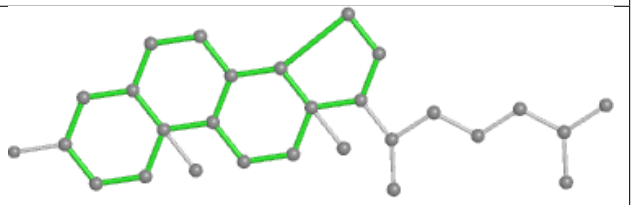
Bond lengths



Bond angles

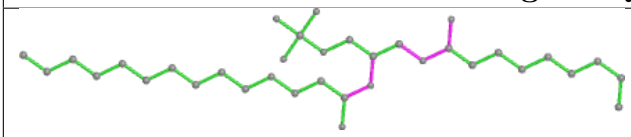


Torsions

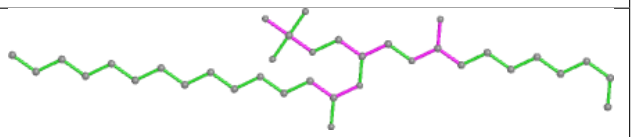


Rings

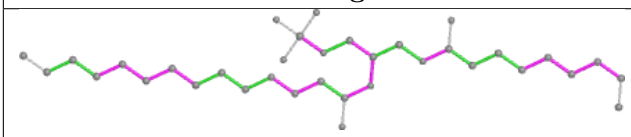
Ligand QNP D 602



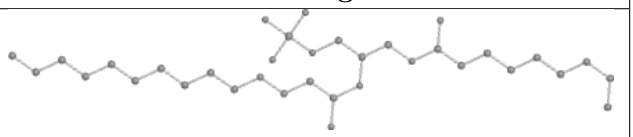
Bond lengths



Bond angles

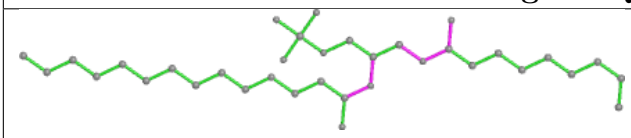


Torsions

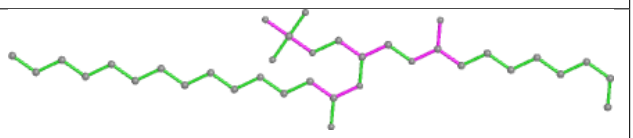


Rings

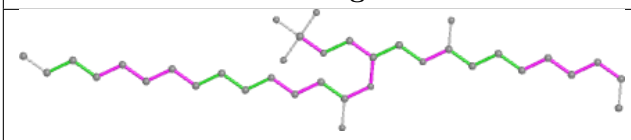
Ligand QNP A 601



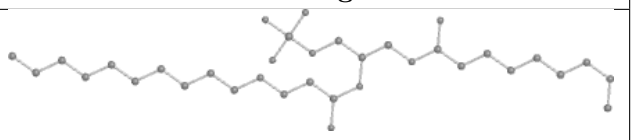
Bond lengths



Bond angles

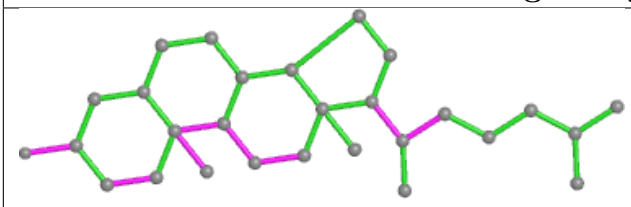


Torsions

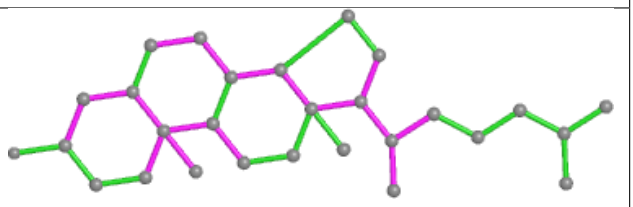


Rings

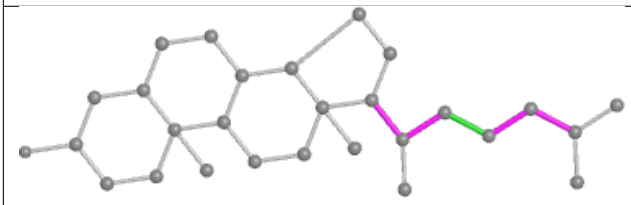
Ligand QNJ D 601



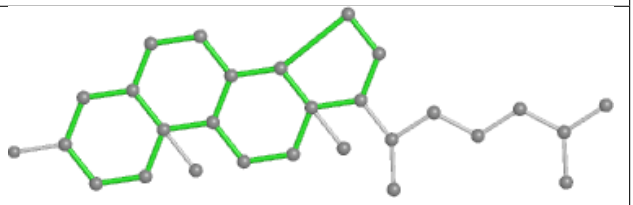
Bond lengths



Bond angles

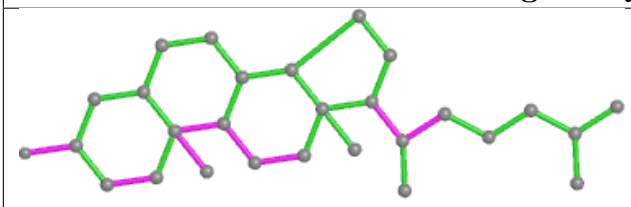


Torsions

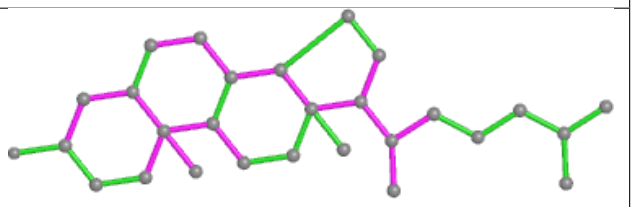


Rings

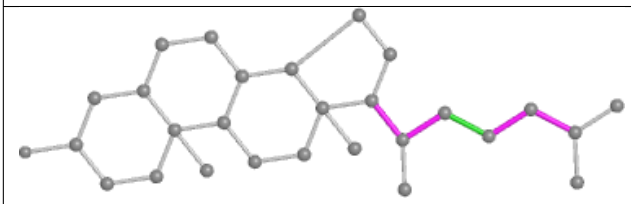
Ligand QNJ M 602



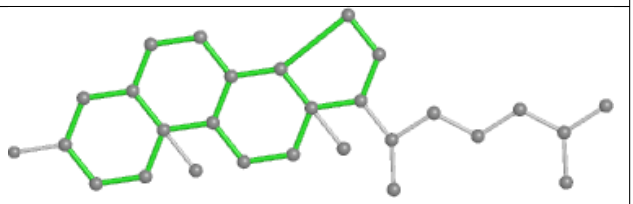
Bond lengths



Bond angles

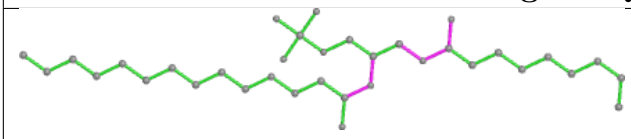


Torsions

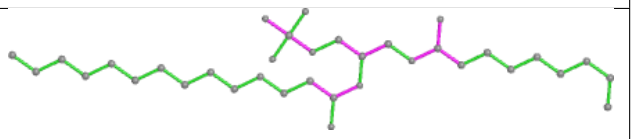


Rings

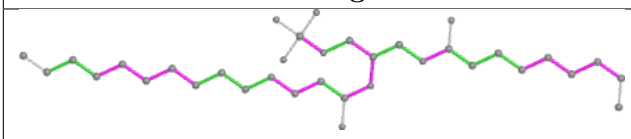
Ligand QNP N 601



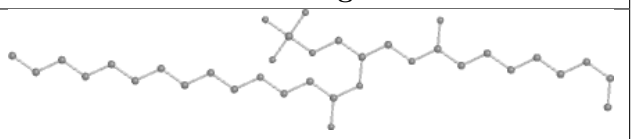
Bond lengths



Bond angles

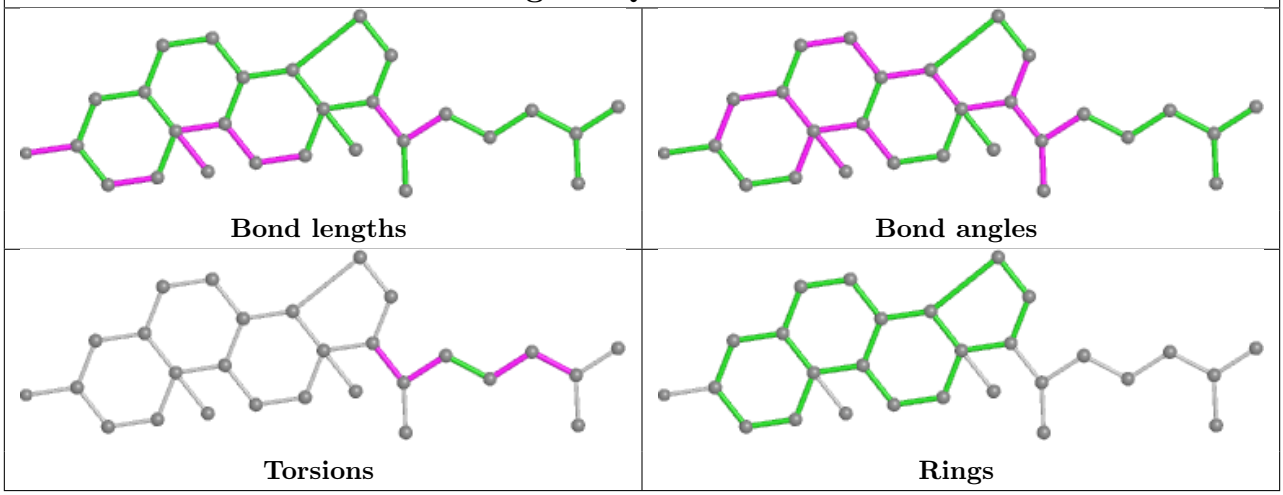


Torsions

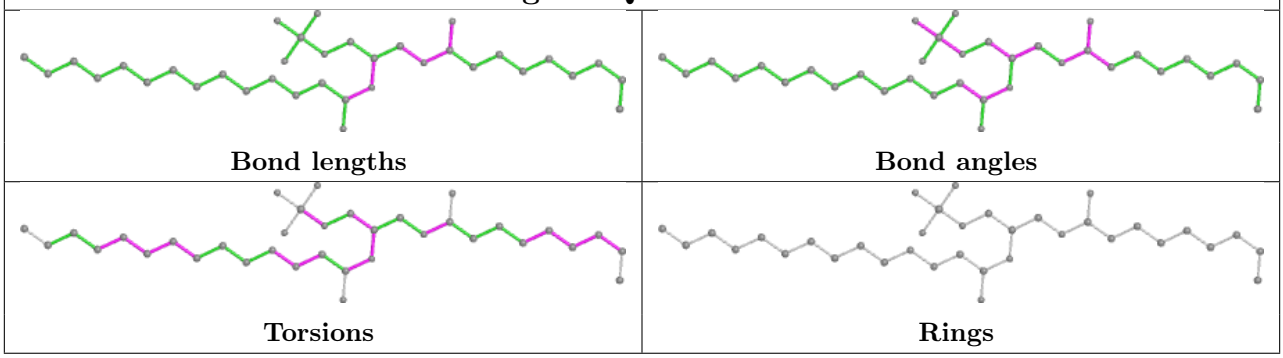


Rings

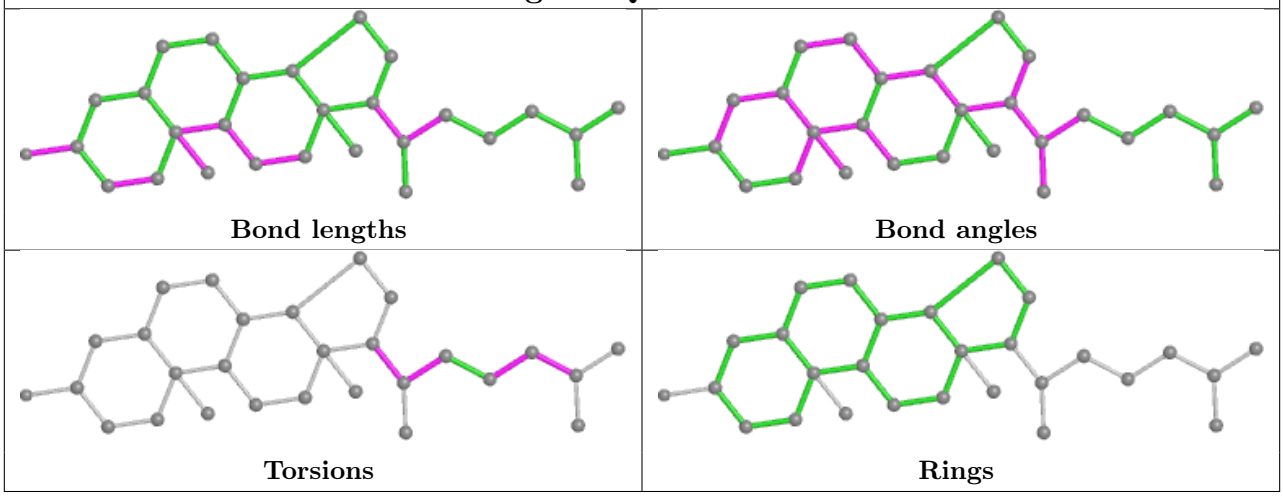
Ligand QNJ B 602



Ligand QNP O 602



Ligand QNJ A 602



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.

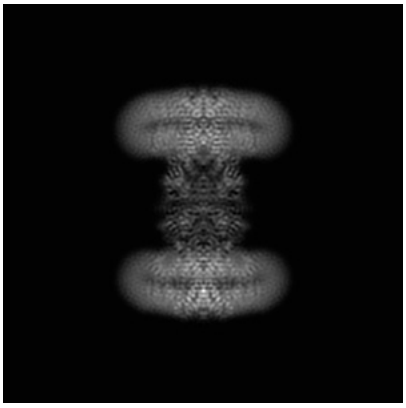
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21019. These allow visual inspection of the internal detail of the map and identification of artifacts.

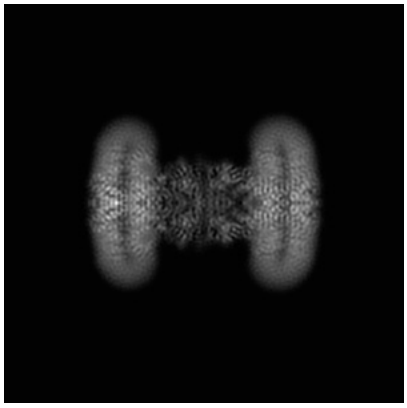
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

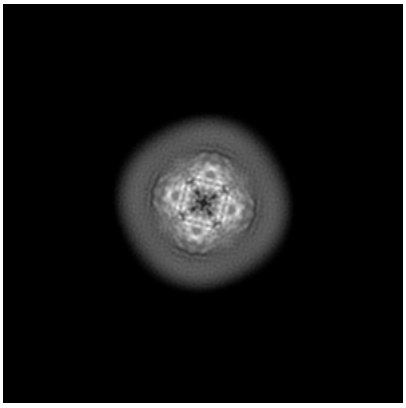
6.1.1 Primary map



X



Y

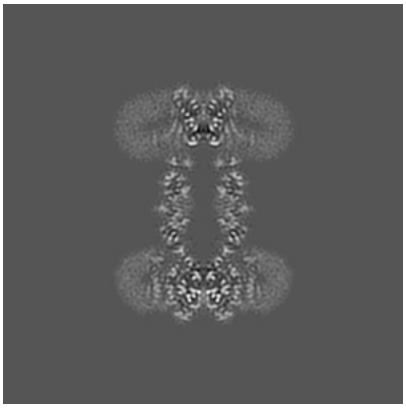


Z

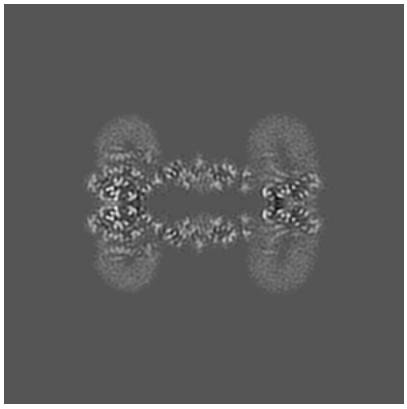
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

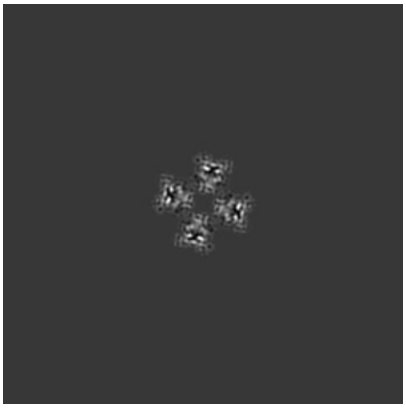
6.2.1 Primary map



X Index: 170



Y Index: 170

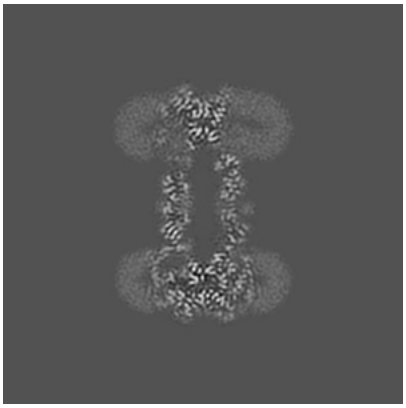


Z Index: 170

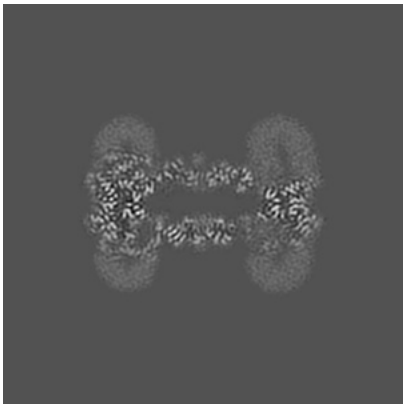
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

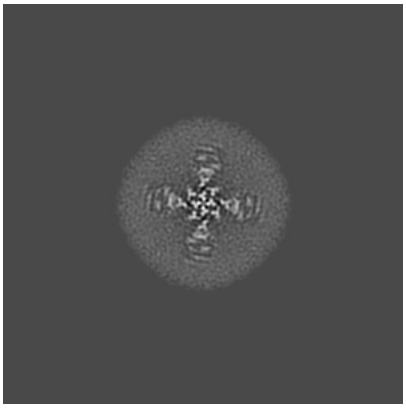
6.3.1 Primary map



X Index: 167



Y Index: 173

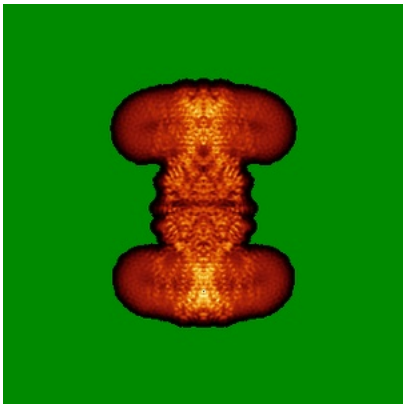


Z Index: 95

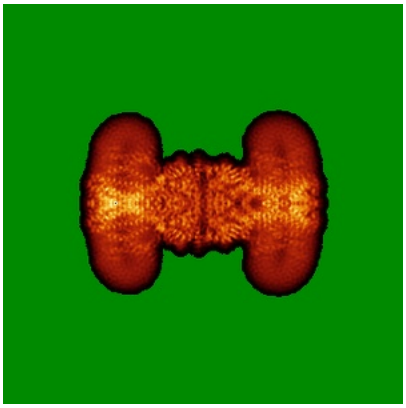
The images above show the largest variance slices of the map in three orthogonal directions.

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

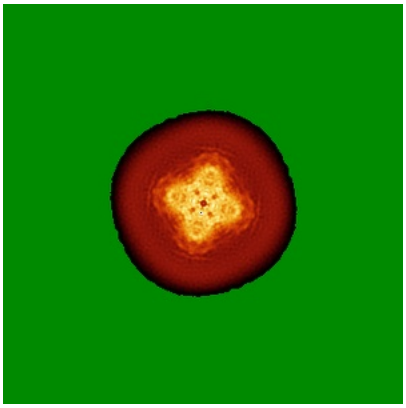
6.4.1 Primary map



X



Y

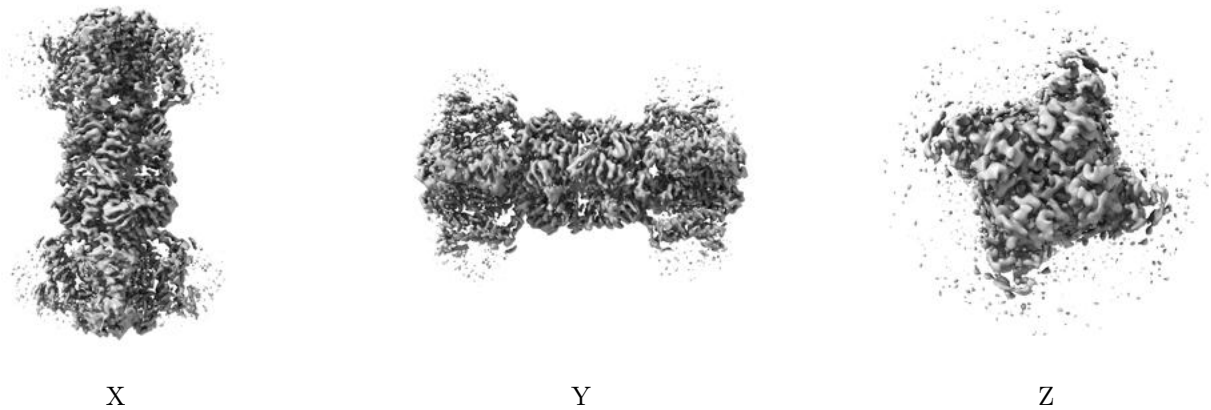


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0366. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

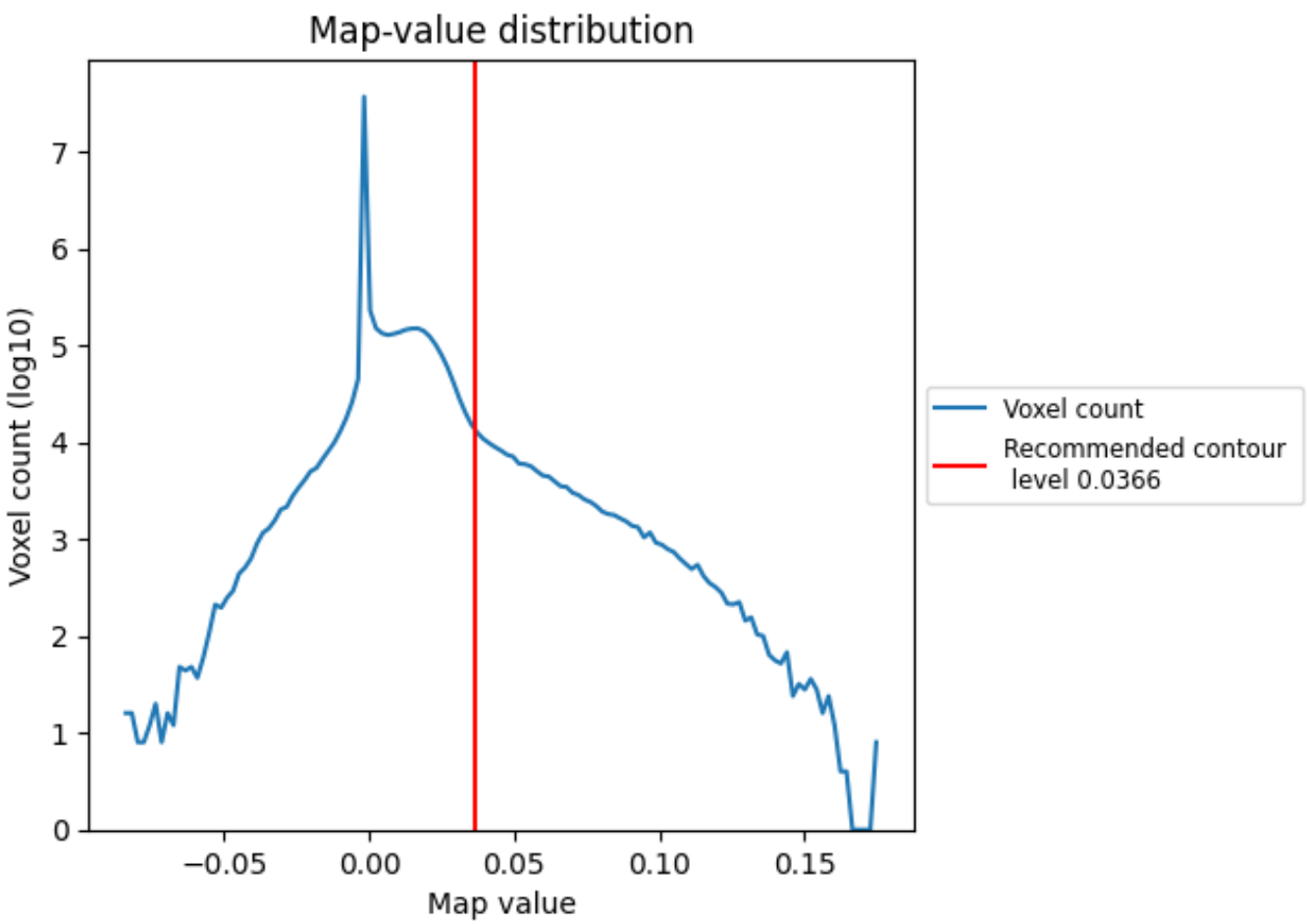
6.6 Mask visualisation (i)

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

7 Map analysis (i)

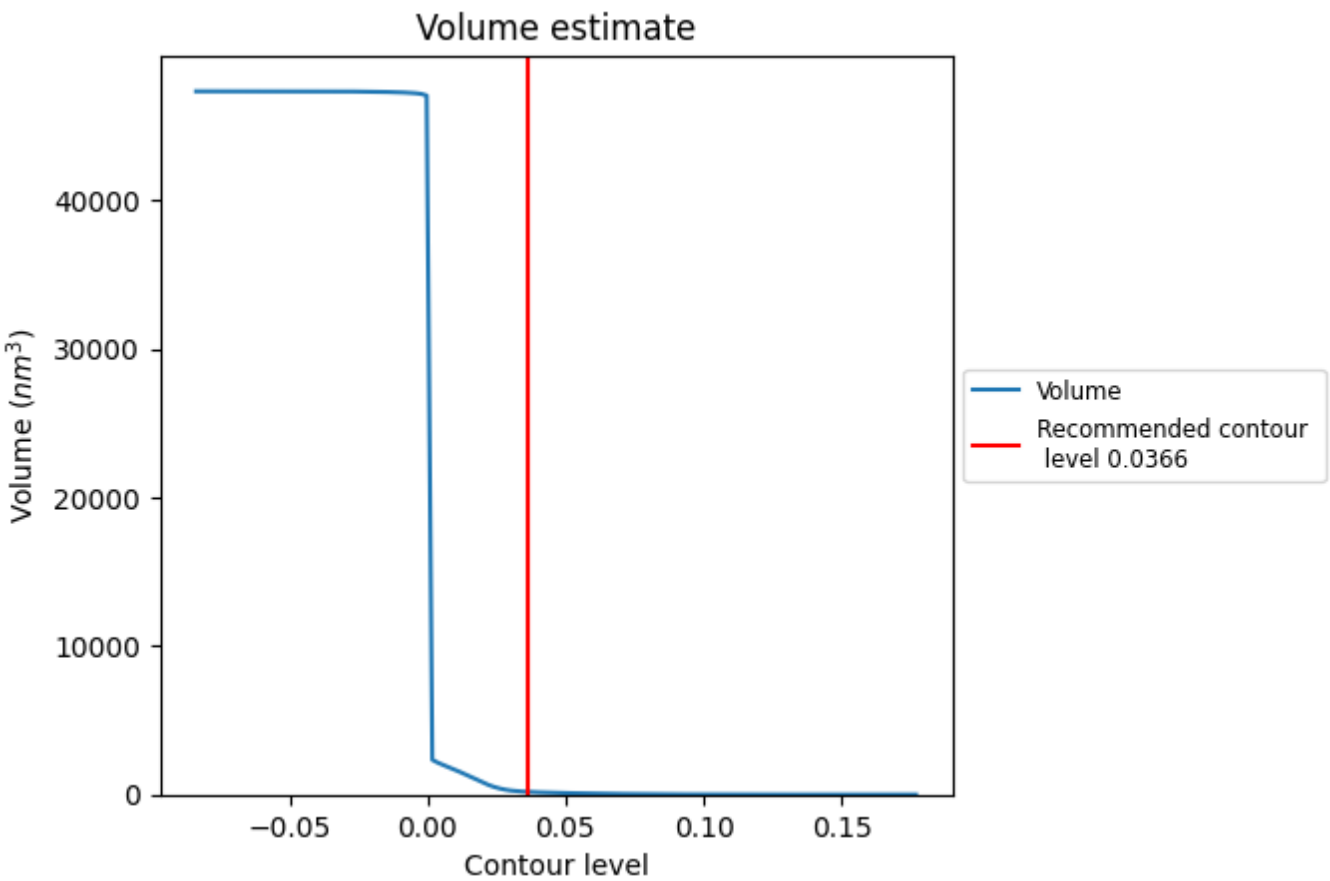
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

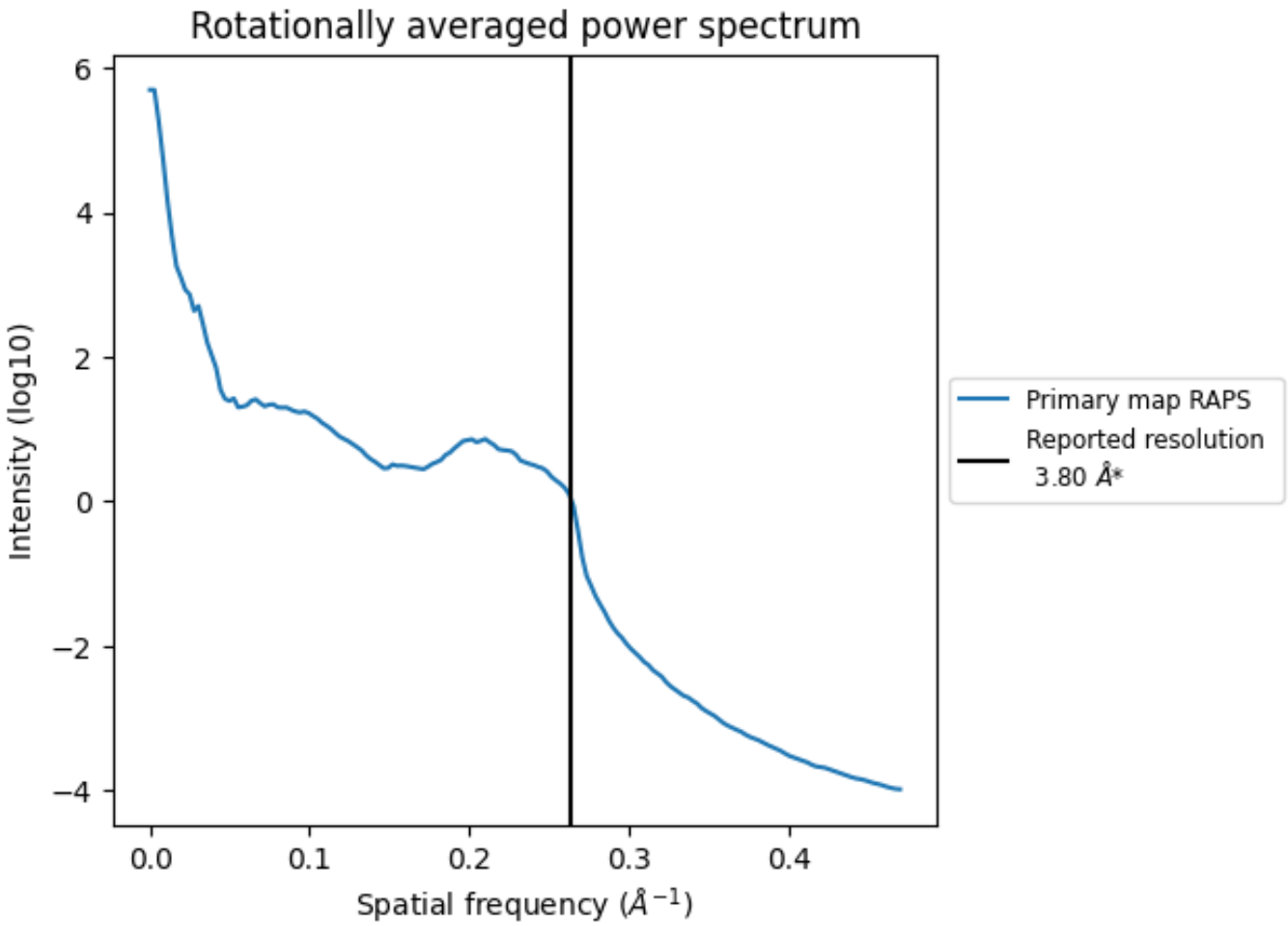
7.2 Volume estimate (i)



The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 161 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)

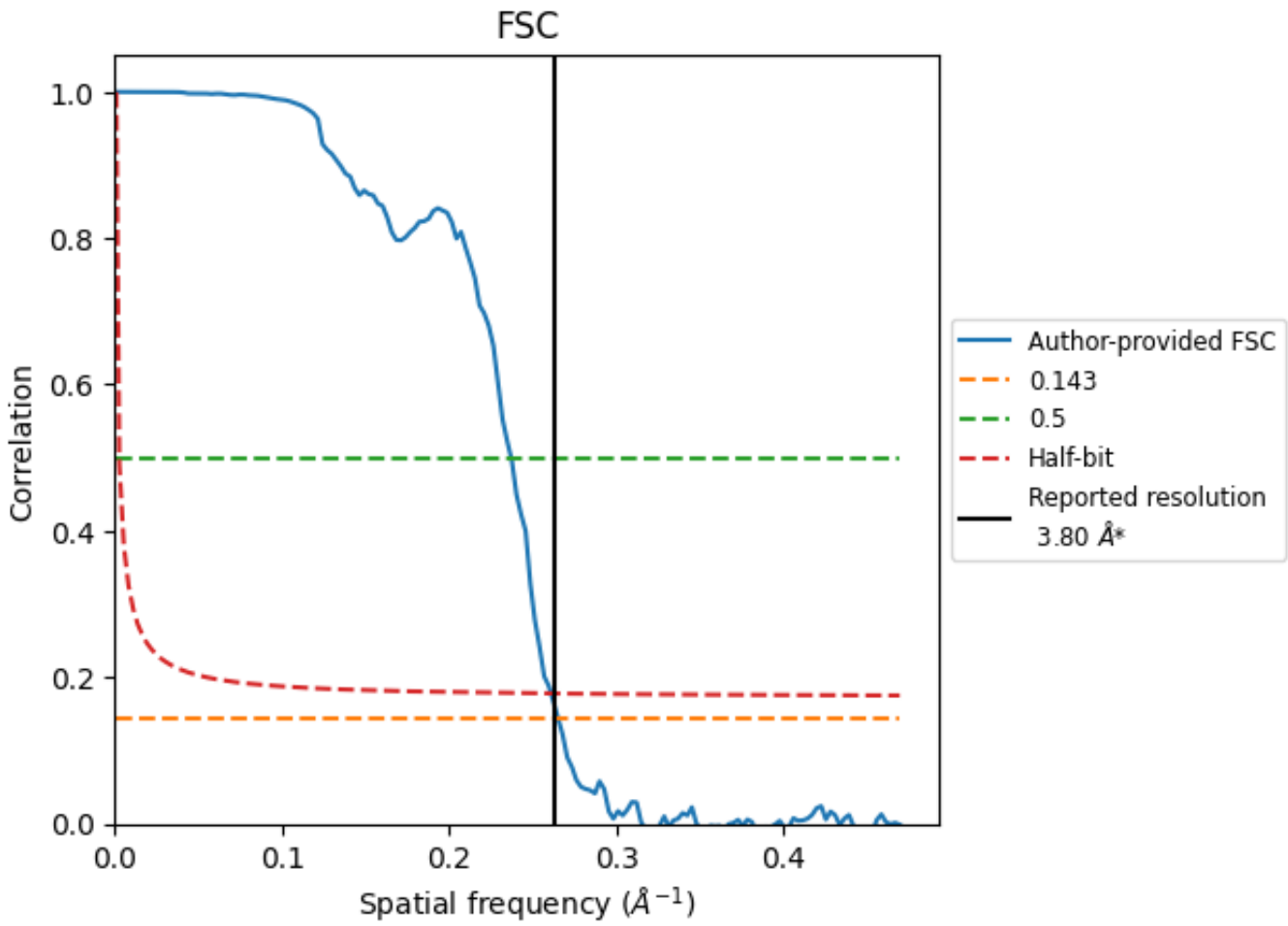


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

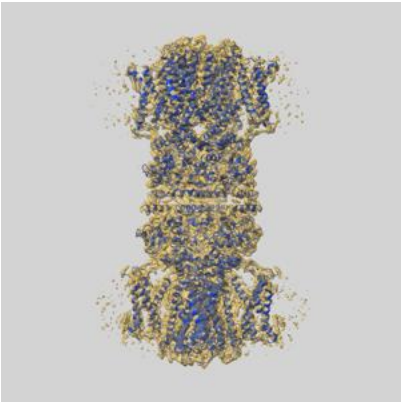
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.21	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

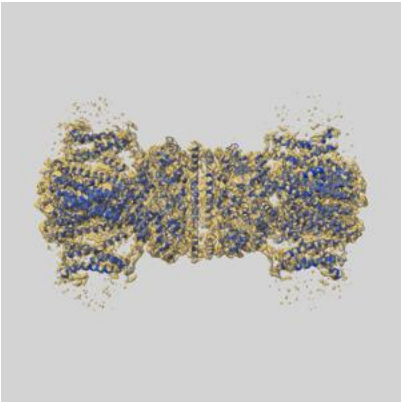
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21019 and PDB model 6V1Y. Per-residue inclusion information can be found in section 3 on page 8.

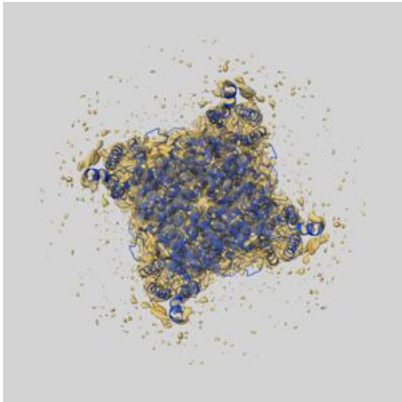
9.1 Map-model overlay (i)



X



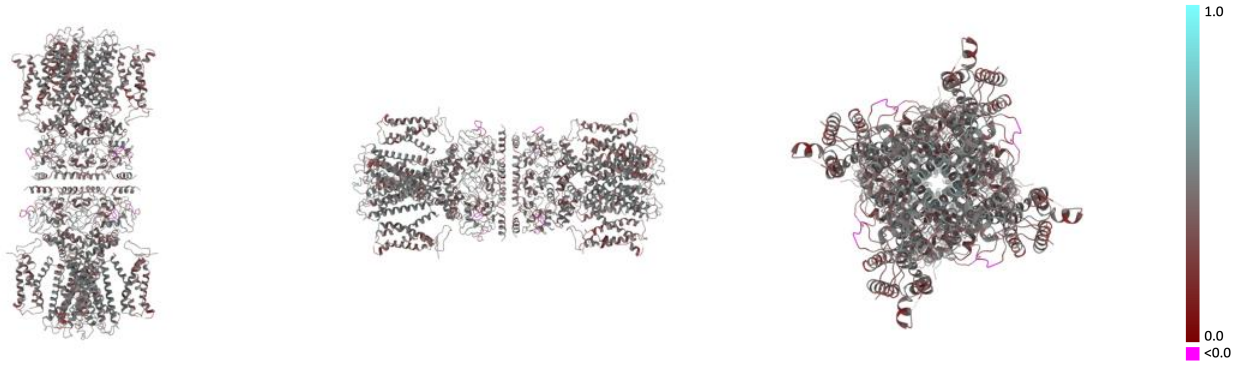
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0366 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

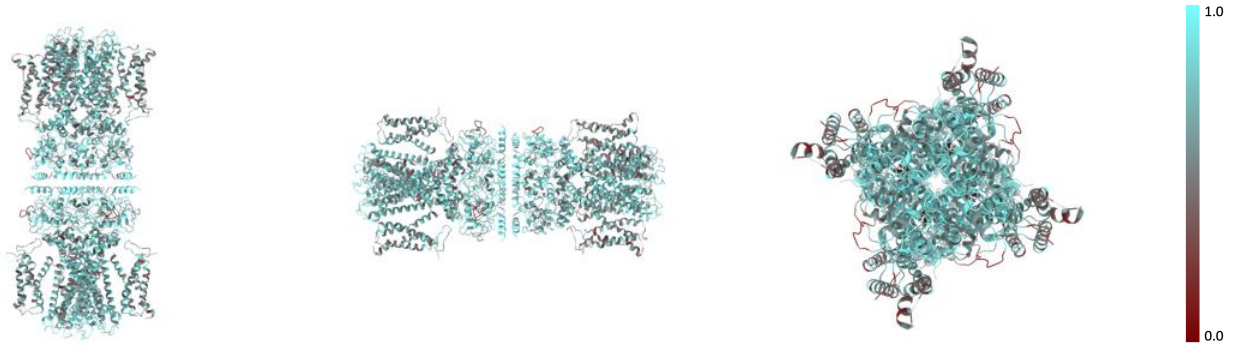
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

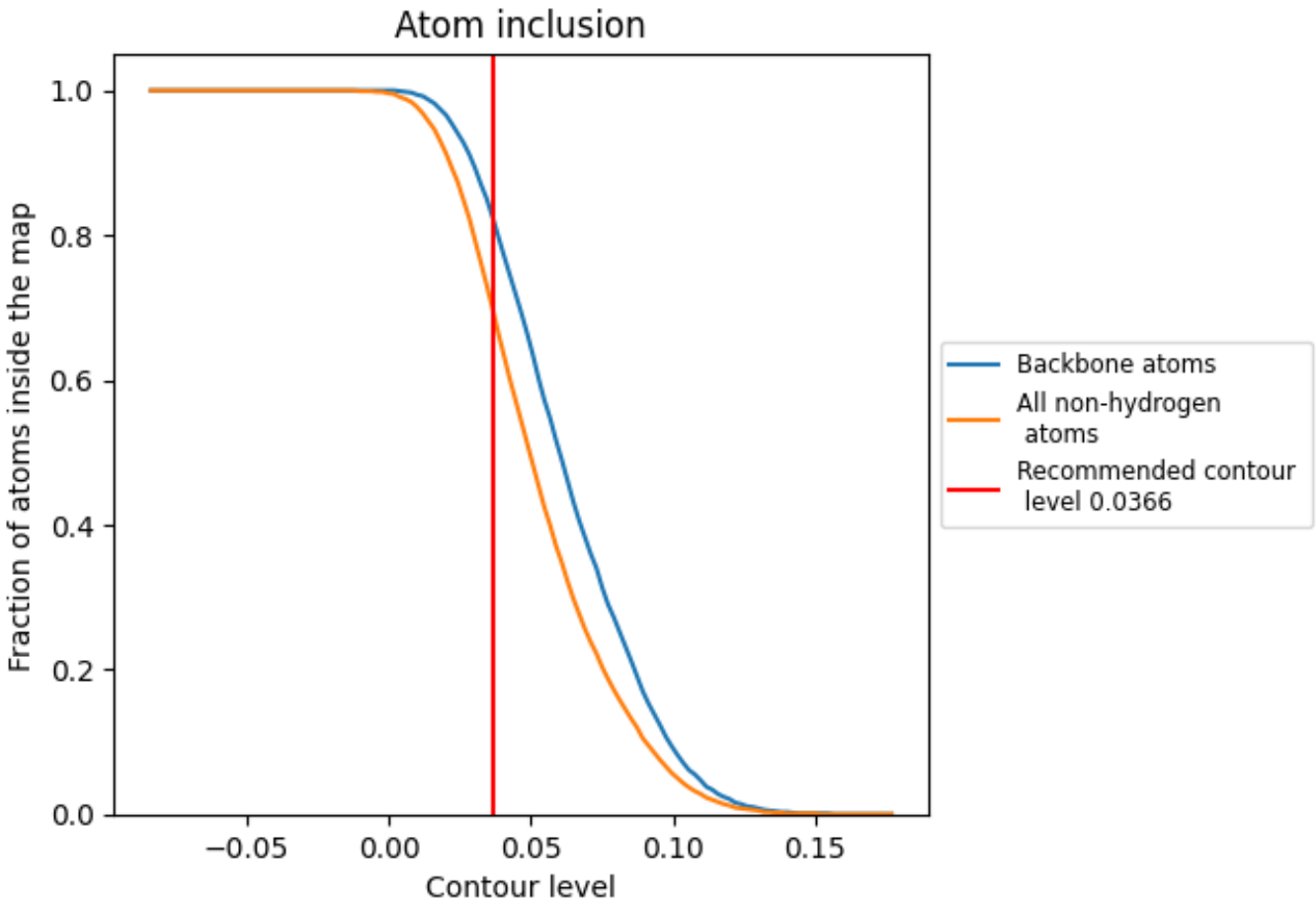
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0366).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.0366) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.4310
A	0.6850	0.4240
B	0.6890	0.4230
C	0.6850	0.4240
D	0.6850	0.4240
M	0.7070	0.4380
N	0.7060	0.4390
O	0.7070	0.4380
P	0.7070	0.4370