Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 10:14 AM JST

PDB ID	:	9LJ1 / pdb_00009lj1
EMDB ID	:	EMD-63130
Title	:	Human KCNQ5-CaM-PIP2-HN37 complex in a closed conformation.
Authors	:	Yang, Z.; Guo, J.
Deposited on	:	2025-01-14
Resolution	:	3.20 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:

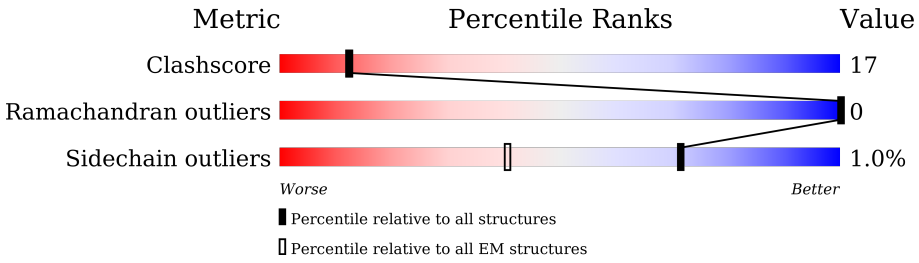
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	626	36% 18% 45%
1	B	626	36% 18% 45%
1	D	626	37% 18% 45%
1	G	626	36% 18% 45%
2	C	177	61% 66% 16% 19%
2	E	177	62% 66% 16% 19%
2	F	177	60% 66% 16% 19%
2	H	177	61% 66% 16% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31832 atoms, of which 15948 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 voltage-gated channel subfamily KQT member 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	0
			5691	1832	2900	491	455	13		
1	B	344	Total	C	H	N	O	S	0	0
			5691	1832	2900	491	455	13		
1	D	344	Total	C	H	N	O	S	0	0
			5691	1832	2900	491	455	13		
1	G	344	Total	C	H	N	O	S	0	0
			5691	1832	2900	491	455	13		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	initiating methionine	UNP Q9NR82
A	699	LEU	-	expression tag	UNP Q9NR82
A	700	GLU	-	expression tag	UNP Q9NR82
A	701	GLY	-	expression tag	UNP Q9NR82
A	702	GLY	-	expression tag	UNP Q9NR82
A	703	SER	-	expression tag	UNP Q9NR82
A	704	SER	-	expression tag	UNP Q9NR82
A	705	GLY	-	expression tag	UNP Q9NR82
A	706	GLY	-	expression tag	UNP Q9NR82
A	707	TRP	-	expression tag	UNP Q9NR82
A	708	SER	-	expression tag	UNP Q9NR82
A	709	HIS	-	expression tag	UNP Q9NR82
A	710	PRO	-	expression tag	UNP Q9NR82
A	711	GLN	-	expression tag	UNP Q9NR82
A	712	PHE	-	expression tag	UNP Q9NR82
A	713	GLU	-	expression tag	UNP Q9NR82
A	714	LYS	-	expression tag	UNP Q9NR82
B	89	MET	-	initiating methionine	UNP Q9NR82
B	699	LEU	-	expression tag	UNP Q9NR82
B	700	GLU	-	expression tag	UNP Q9NR82
B	701	GLY	-	expression tag	UNP Q9NR82
B	702	GLY	-	expression tag	UNP Q9NR82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	703	SER	-	expression tag	UNP Q9NR82
B	704	SER	-	expression tag	UNP Q9NR82
B	705	GLY	-	expression tag	UNP Q9NR82
B	706	GLY	-	expression tag	UNP Q9NR82
B	707	TRP	-	expression tag	UNP Q9NR82
B	708	SER	-	expression tag	UNP Q9NR82
B	709	HIS	-	expression tag	UNP Q9NR82
B	710	PRO	-	expression tag	UNP Q9NR82
B	711	GLN	-	expression tag	UNP Q9NR82
B	712	PHE	-	expression tag	UNP Q9NR82
B	713	GLU	-	expression tag	UNP Q9NR82
B	714	LYS	-	expression tag	UNP Q9NR82
D	89	MET	-	initiating methionine	UNP Q9NR82
D	699	LEU	-	expression tag	UNP Q9NR82
D	700	GLU	-	expression tag	UNP Q9NR82
D	701	GLY	-	expression tag	UNP Q9NR82
D	702	GLY	-	expression tag	UNP Q9NR82
D	703	SER	-	expression tag	UNP Q9NR82
D	704	SER	-	expression tag	UNP Q9NR82
D	705	GLY	-	expression tag	UNP Q9NR82
D	706	GLY	-	expression tag	UNP Q9NR82
D	707	TRP	-	expression tag	UNP Q9NR82
D	708	SER	-	expression tag	UNP Q9NR82
D	709	HIS	-	expression tag	UNP Q9NR82
D	710	PRO	-	expression tag	UNP Q9NR82
D	711	GLN	-	expression tag	UNP Q9NR82
D	712	PHE	-	expression tag	UNP Q9NR82
D	713	GLU	-	expression tag	UNP Q9NR82
D	714	LYS	-	expression tag	UNP Q9NR82
G	89	MET	-	initiating methionine	UNP Q9NR82
G	699	LEU	-	expression tag	UNP Q9NR82
G	700	GLU	-	expression tag	UNP Q9NR82
G	701	GLY	-	expression tag	UNP Q9NR82
G	702	GLY	-	expression tag	UNP Q9NR82
G	703	SER	-	expression tag	UNP Q9NR82
G	704	SER	-	expression tag	UNP Q9NR82
G	705	GLY	-	expression tag	UNP Q9NR82
G	706	GLY	-	expression tag	UNP Q9NR82
G	707	TRP	-	expression tag	UNP Q9NR82
G	708	SER	-	expression tag	UNP Q9NR82
G	709	HIS	-	expression tag	UNP Q9NR82
G	710	PRO	-	expression tag	UNP Q9NR82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	711	GLN	-	expression tag	UNP Q9NR82
G	712	PHE	-	expression tag	UNP Q9NR82
G	713	GLU	-	expression tag	UNP Q9NR82
G	714	LYS	-	expression tag	UNP Q9NR82

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	C	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	F	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		
2	H	144	Total	C	H	N	O	S	0	0
			2130	682	1022	180	237	9		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	150	LEU	-	expression tag	UNP P0DP25
E	151	GLU	-	expression tag	UNP P0DP25
E	152	GLY	-	expression tag	UNP P0DP25
E	153	GLY	-	expression tag	UNP P0DP25
E	154	SER	-	expression tag	UNP P0DP25
E	155	SER	-	expression tag	UNP P0DP25
E	156	GLY	-	expression tag	UNP P0DP25
E	157	GLY	-	expression tag	UNP P0DP25
E	158	LEU	-	expression tag	UNP P0DP25
E	159	VAL	-	expression tag	UNP P0DP25
E	160	PRO	-	expression tag	UNP P0DP25
E	161	ARG	-	expression tag	UNP P0DP25
E	162	GLY	-	expression tag	UNP P0DP25
E	163	SER	-	expression tag	UNP P0DP25
E	164	GLY	-	expression tag	UNP P0DP25
E	165	GLY	-	expression tag	UNP P0DP25
E	166	SER	-	expression tag	UNP P0DP25
E	167	SER	-	expression tag	UNP P0DP25
E	168	GLY	-	expression tag	UNP P0DP25
E	169	GLY	-	expression tag	UNP P0DP25
E	170	HIS	-	expression tag	UNP P0DP25
E	171	HIS	-	expression tag	UNP P0DP25

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	172	HIS	-	expression tag	UNP P0DP25
E	173	HIS	-	expression tag	UNP P0DP25
E	174	HIS	-	expression tag	UNP P0DP25
E	175	HIS	-	expression tag	UNP P0DP25
E	176	HIS	-	expression tag	UNP P0DP25
E	177	HIS	-	expression tag	UNP P0DP25
C	150	LEU	-	expression tag	UNP P0DP25
C	151	GLU	-	expression tag	UNP P0DP25
C	152	GLY	-	expression tag	UNP P0DP25
C	153	GLY	-	expression tag	UNP P0DP25
C	154	SER	-	expression tag	UNP P0DP25
C	155	SER	-	expression tag	UNP P0DP25
C	156	GLY	-	expression tag	UNP P0DP25
C	157	GLY	-	expression tag	UNP P0DP25
C	158	LEU	-	expression tag	UNP P0DP25
C	159	VAL	-	expression tag	UNP P0DP25
C	160	PRO	-	expression tag	UNP P0DP25
C	161	ARG	-	expression tag	UNP P0DP25
C	162	GLY	-	expression tag	UNP P0DP25
C	163	SER	-	expression tag	UNP P0DP25
C	164	GLY	-	expression tag	UNP P0DP25
C	165	GLY	-	expression tag	UNP P0DP25
C	166	SER	-	expression tag	UNP P0DP25
C	167	SER	-	expression tag	UNP P0DP25
C	168	GLY	-	expression tag	UNP P0DP25
C	169	GLY	-	expression tag	UNP P0DP25
C	170	HIS	-	expression tag	UNP P0DP25
C	171	HIS	-	expression tag	UNP P0DP25
C	172	HIS	-	expression tag	UNP P0DP25
C	173	HIS	-	expression tag	UNP P0DP25
C	174	HIS	-	expression tag	UNP P0DP25
C	175	HIS	-	expression tag	UNP P0DP25
C	176	HIS	-	expression tag	UNP P0DP25
C	177	HIS	-	expression tag	UNP P0DP25
F	150	LEU	-	expression tag	UNP P0DP25
F	151	GLU	-	expression tag	UNP P0DP25
F	152	GLY	-	expression tag	UNP P0DP25
F	153	GLY	-	expression tag	UNP P0DP25
F	154	SER	-	expression tag	UNP P0DP25
F	155	SER	-	expression tag	UNP P0DP25
F	156	GLY	-	expression tag	UNP P0DP25
F	157	GLY	-	expression tag	UNP P0DP25

Continued on next page...

Continued from previous page...

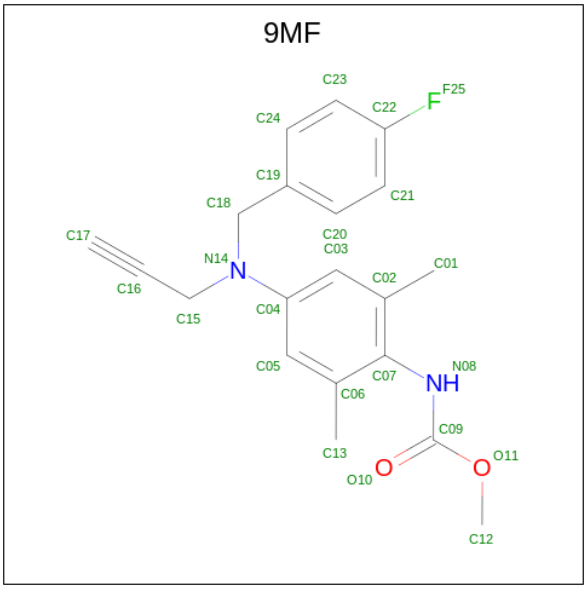
Chain	Residue	Modelled	Actual	Comment	Reference
F	158	LEU	-	expression tag	UNP P0DP25
F	159	VAL	-	expression tag	UNP P0DP25
F	160	PRO	-	expression tag	UNP P0DP25
F	161	ARG	-	expression tag	UNP P0DP25
F	162	GLY	-	expression tag	UNP P0DP25
F	163	SER	-	expression tag	UNP P0DP25
F	164	GLY	-	expression tag	UNP P0DP25
F	165	GLY	-	expression tag	UNP P0DP25
F	166	SER	-	expression tag	UNP P0DP25
F	167	SER	-	expression tag	UNP P0DP25
F	168	GLY	-	expression tag	UNP P0DP25
F	169	GLY	-	expression tag	UNP P0DP25
F	170	HIS	-	expression tag	UNP P0DP25
F	171	HIS	-	expression tag	UNP P0DP25
F	172	HIS	-	expression tag	UNP P0DP25
F	173	HIS	-	expression tag	UNP P0DP25
F	174	HIS	-	expression tag	UNP P0DP25
F	175	HIS	-	expression tag	UNP P0DP25
F	176	HIS	-	expression tag	UNP P0DP25
F	177	HIS	-	expression tag	UNP P0DP25
H	150	LEU	-	expression tag	UNP P0DP25
H	151	GLU	-	expression tag	UNP P0DP25
H	152	GLY	-	expression tag	UNP P0DP25
H	153	GLY	-	expression tag	UNP P0DP25
H	154	SER	-	expression tag	UNP P0DP25
H	155	SER	-	expression tag	UNP P0DP25
H	156	GLY	-	expression tag	UNP P0DP25
H	157	GLY	-	expression tag	UNP P0DP25
H	158	LEU	-	expression tag	UNP P0DP25
H	159	VAL	-	expression tag	UNP P0DP25
H	160	PRO	-	expression tag	UNP P0DP25
H	161	ARG	-	expression tag	UNP P0DP25
H	162	GLY	-	expression tag	UNP P0DP25
H	163	SER	-	expression tag	UNP P0DP25
H	164	GLY	-	expression tag	UNP P0DP25
H	165	GLY	-	expression tag	UNP P0DP25
H	166	SER	-	expression tag	UNP P0DP25
H	167	SER	-	expression tag	UNP P0DP25
H	168	GLY	-	expression tag	UNP P0DP25
H	169	GLY	-	expression tag	UNP P0DP25
H	170	HIS	-	expression tag	UNP P0DP25
H	171	HIS	-	expression tag	UNP P0DP25

Continued on next page...

Continued from previous page...

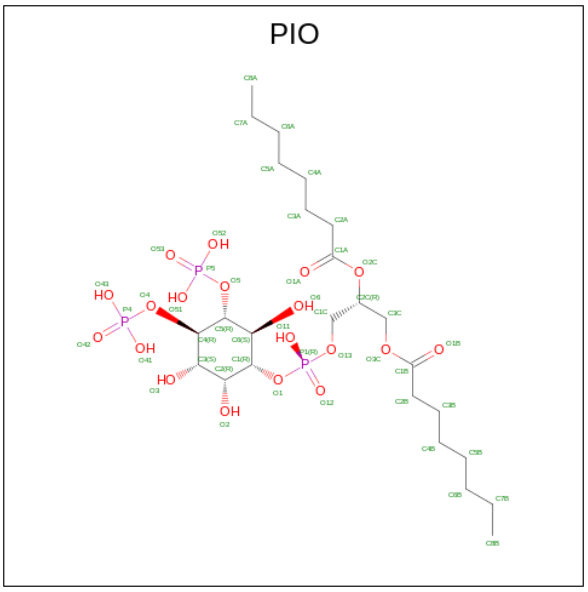
Chain	Residue	Modelled	Actual	Comment	Reference
H	172	HIS	-	expression tag	UNP P0DP25
H	173	HIS	-	expression tag	UNP P0DP25
H	174	HIS	-	expression tag	UNP P0DP25
H	175	HIS	-	expression tag	UNP P0DP25
H	176	HIS	-	expression tag	UNP P0DP25
H	177	HIS	-	expression tag	UNP P0DP25

- Molecule 3 is methyl N-[4-[(4-fluorophenyl)methyl-prop-2-ynyl-amino]-2,6-dimethyl-phenyl]carbamate (CCD ID: 9MF) (formula: $C_{20}H_{21}FN_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	H	N	O	0
			46	20	1	21	2	2	
3	A	1	Total	C	F	H	N	O	0
			46	20	1	21	2	2	
3	B	1	Total	C	F	H	N	O	0
			46	20	1	21	2	2	
3	D	1	Total	C	F	H	N	O	0
			46	20	1	21	2	2	

- Molecule 4 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: $C_{25}H_{49}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



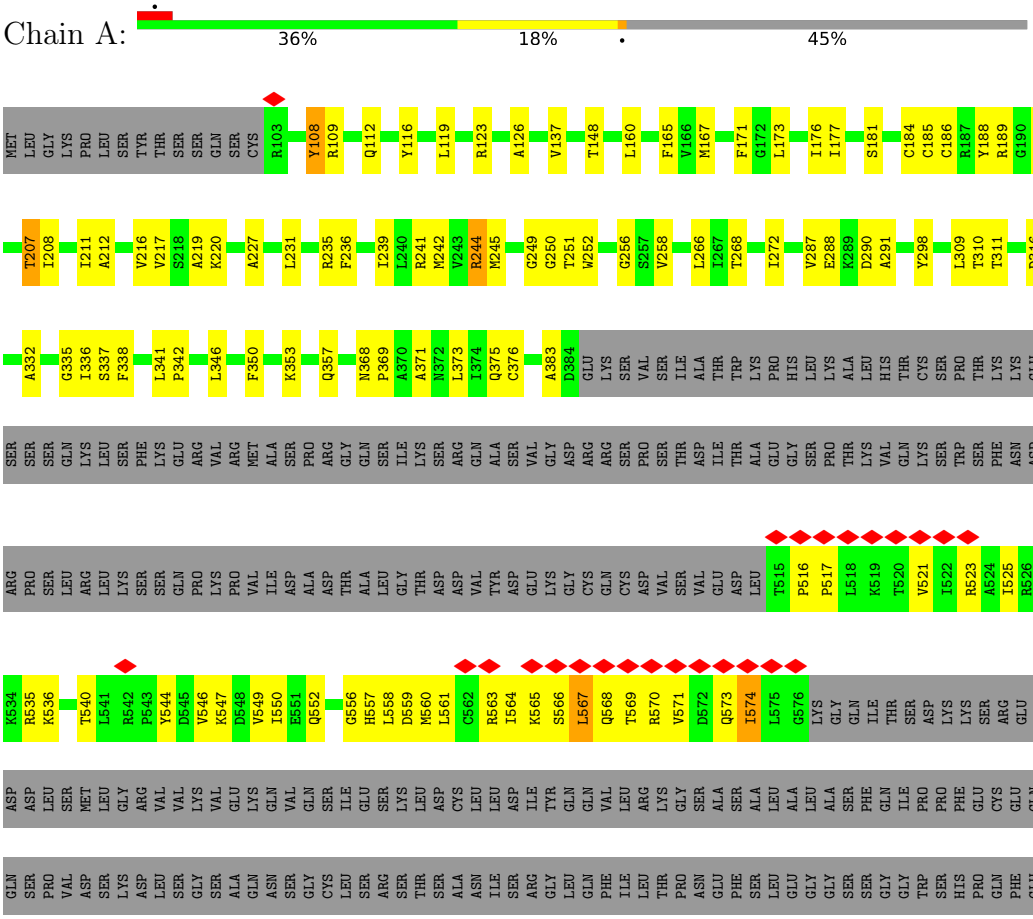
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	O	P	0
			91	25	44	19	3	
4	B	1	Total	C	H	O	P	0
			91	25	44	19	3	
4	D	1	Total	C	H	O	P	0
			91	25	44	19	3	
4	G	1	Total	C	H	O	P	0
			91	25	44	19	3	

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.

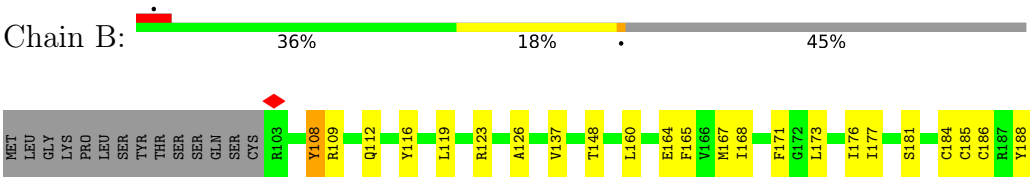
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

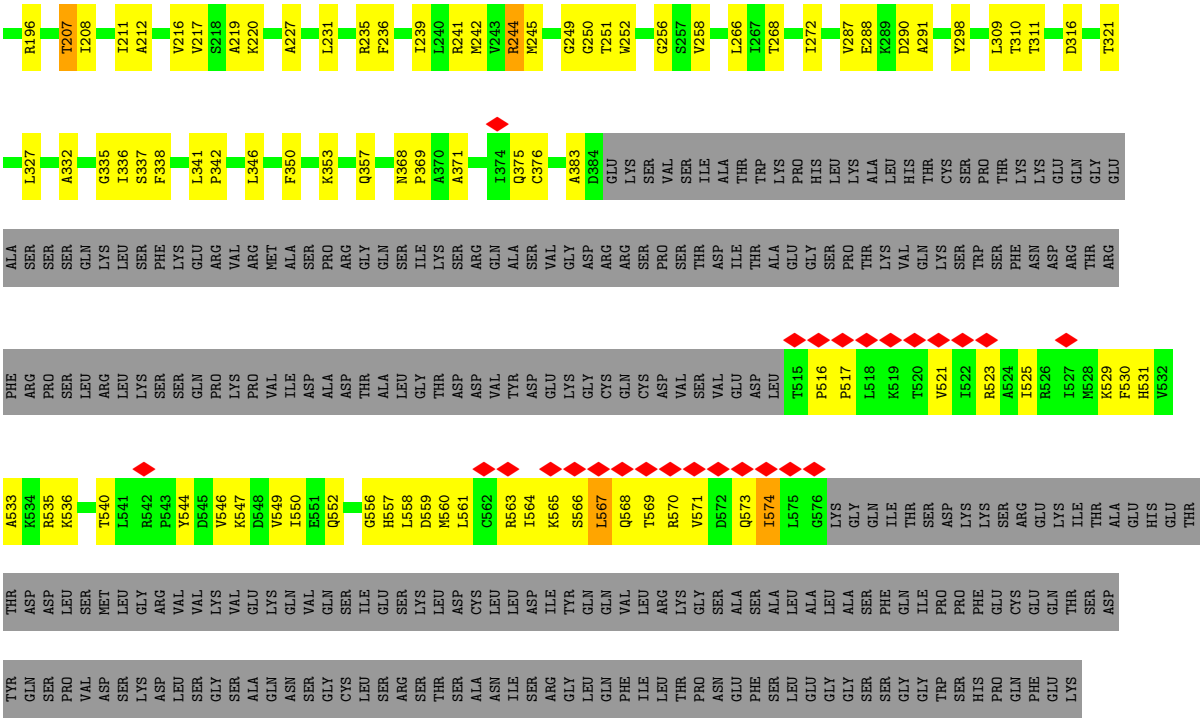
Chain A:



• Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

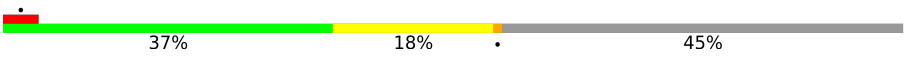
Chain B:

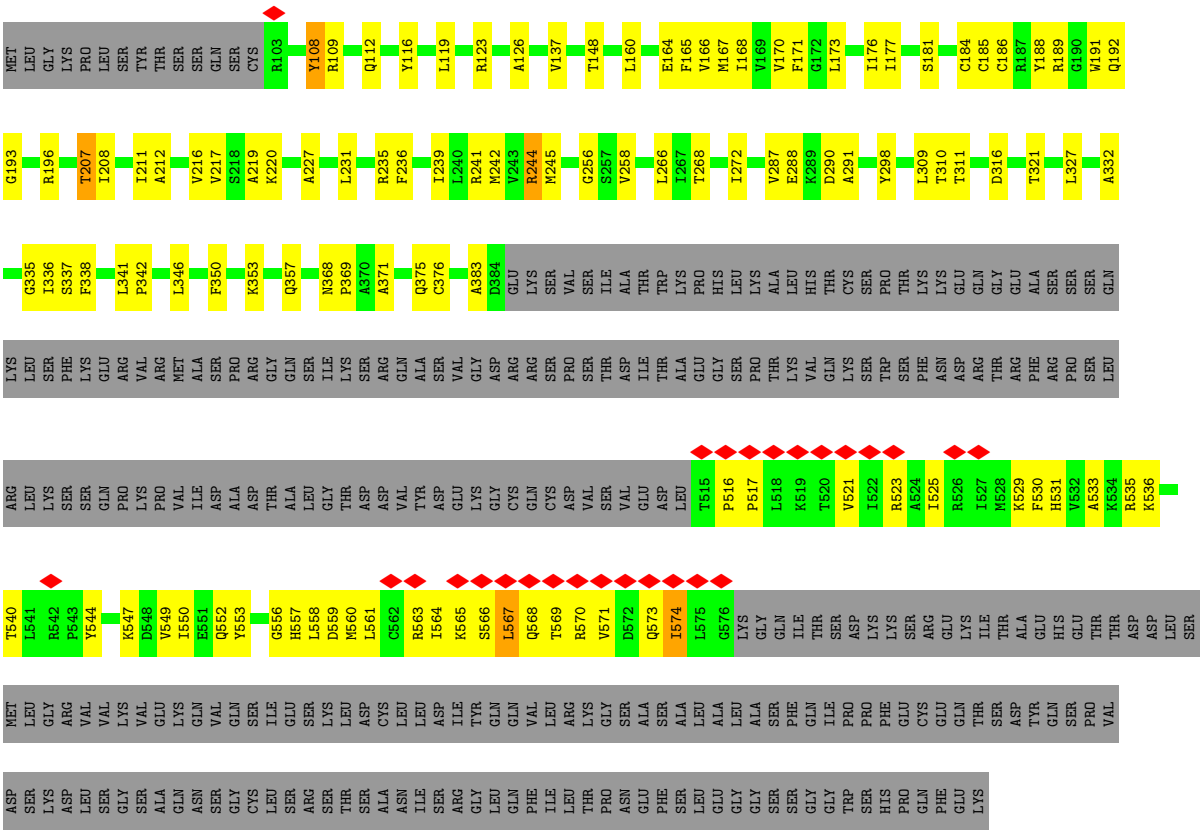




• Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

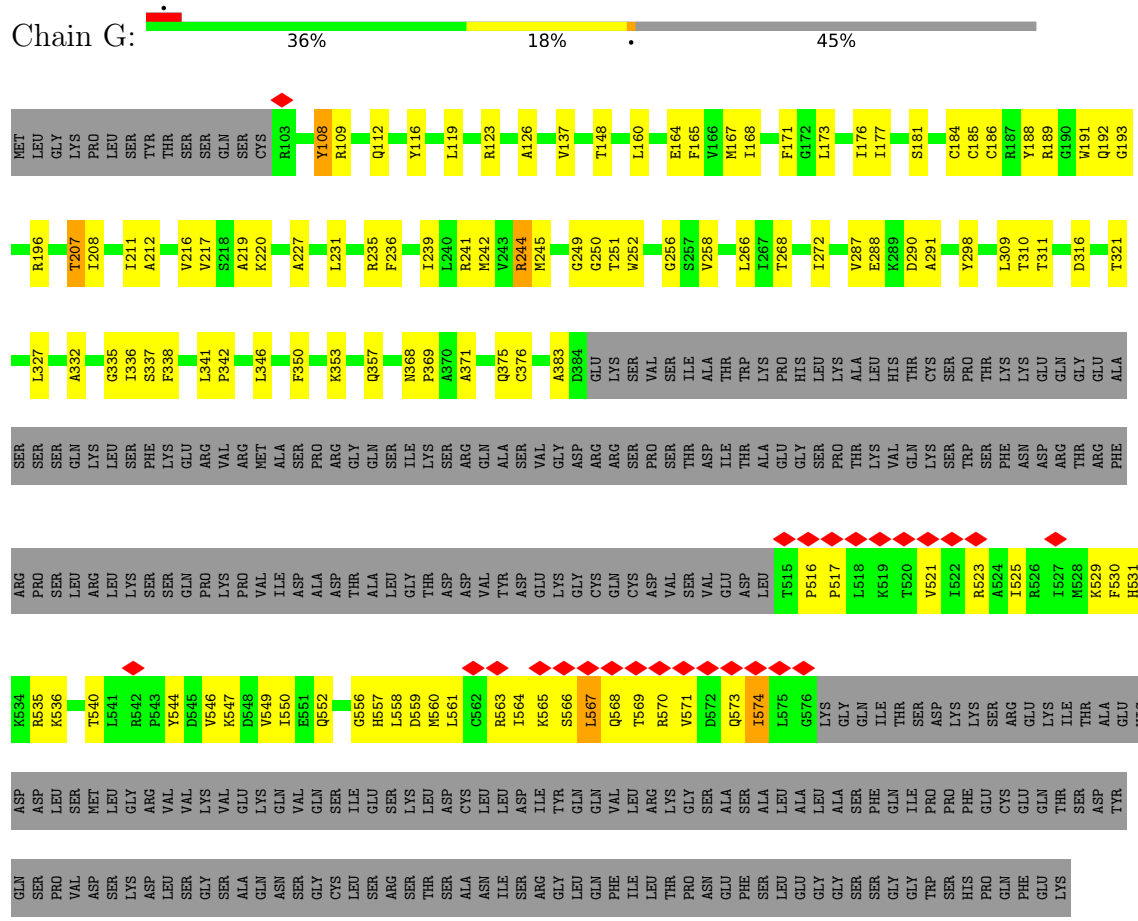
Chain D:





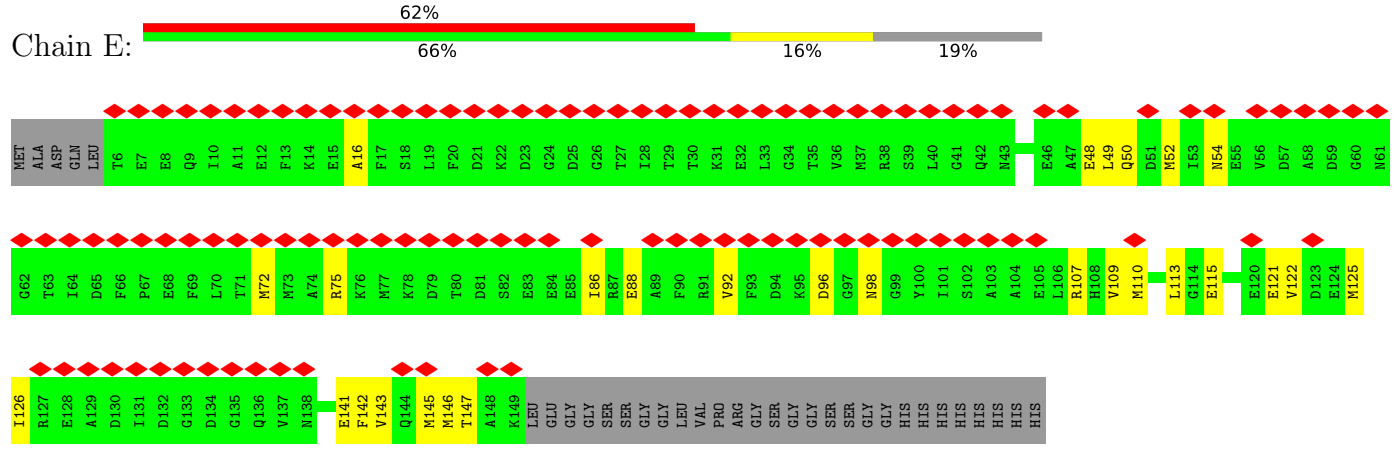
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

Chain G:



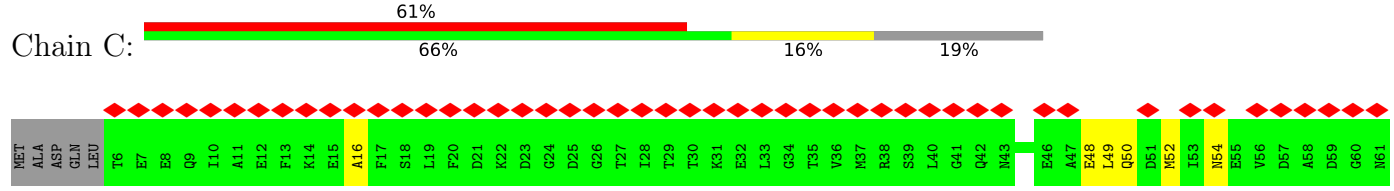
• Molecule 2: Calmodulin-3

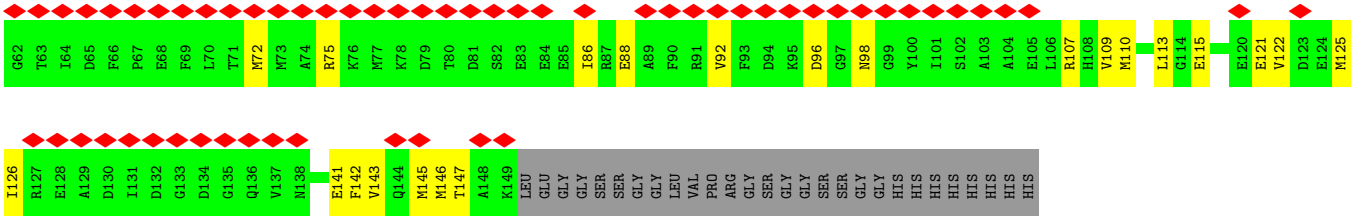
Chain E:



• Molecule 2: Calmodulin-3

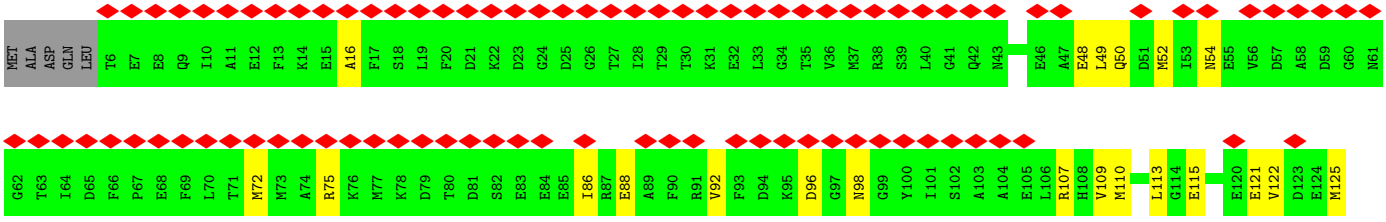
Chain C:





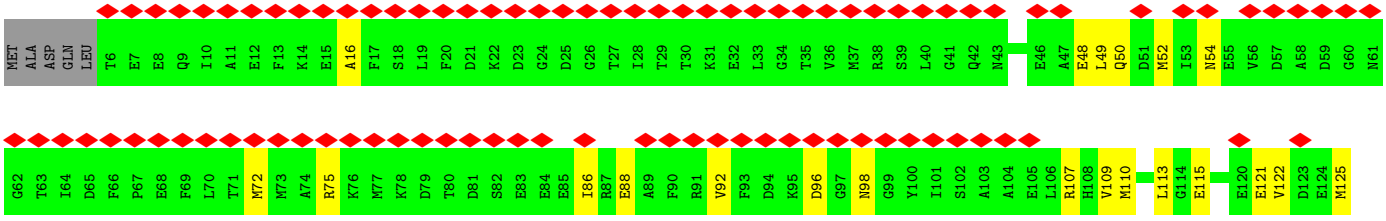
• Molecule 2: Calmodulin-3

Chain F:



• Molecule 2: Calmodulin-3

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	223.2, 223.2, 223.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9MF, PIO

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	0.35	0/2859	0.47	1/3865 (0.0%)
1	B	0.35	0/2859	0.47	1/3865 (0.0%)
1	D	0.35	0/2859	0.47	1/3865 (0.0%)
1	G	0.35	0/2859	0.47	1/3865 (0.0%)
2	C	0.10	0/1120	0.26	0/1507
2	E	0.10	0/1120	0.26	0/1507
2	F	0.10	0/1120	0.26	0/1507
2	H	0.10	0/1120	0.26	0/1507
All	All	0.30	0/15916	0.42	4/21488 (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})
1	A	574	ILE	CB-CA-C	-5.57	104.84	111.97
1	B	574	ILE	CB-CA-C	-5.57	104.84	111.97
1	D	574	ILE	CB-CA-C	-5.57	104.84	111.97
1	G	574	ILE	CB-CA-C	-5.57	104.84	111.97

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	A	2791	2900	2900	117	0
1	B	2791	2900	2900	119	0
1	D	2791	2900	2900	115	0
1	G	2791	2900	2900	115	0
2	C	1108	1022	1022	31	0
2	E	1108	1022	1022	31	0
2	F	1108	1022	1022	31	0
2	H	1108	1022	1022	31	0
3	A	50	42	0	0	0
3	B	25	21	0	0	0
3	D	25	21	0	0	0
4	A	47	44	44	2	0
4	B	47	44	44	2	0
4	D	47	44	44	2	0
4	G	47	44	44	2	0
All	All	15884	15948	15864	529	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 17.

All (529) 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:567:LEU:HD21	1:G:567:LEU:HD22	1.56	0.88
1:A:567:LEU:HD21	1:B:567:LEU:HD22	1.56	0.88
1:A:567:LEU:HD22	1:G:567:LEU:HD21	1.56	0.88
1:B:567:LEU:HD21	1:D:567:LEU:HD22	1.56	0.87
1:B:186:CYS:SG	1:B:189:ARG:NH2	2.48	0.87
1:A:186:CYS:SG	1:A:189:ARG:NH2	2.48	0.87
1:G:186:CYS:SG	1:G:189:ARG:NH2	2.48	0.86
1:D:186:CYS:SG	1:D:189:ARG:NH2	2.48	0.86
1:A:567:LEU:HD13	1:G:567:LEU:HD11	1.66	0.77
1:A:567:LEU:HD11	1:B:567:LEU:HD13	1.66	0.77
1:D:567:LEU:HD11	1:G:567:LEU:HD13	1.66	0.75
1:B:567:LEU:HD11	1:D:567:LEU:HD13	1.66	0.75
1:G:525:ILE:HG22	1:G:529:LYS:HE3	1.69	0.74
1:D:525:ILE:HG22	1:D:529:LYS:HE3	1.69	0.74
1:A:525:ILE:HG22	1:A:529:LYS:HE3	1.69	0.74
1:B:525:ILE:HG22	1:B:529:LYS:HE3	1.69	0.72
1:G:119:LEU:HD11	1:G:177:ILE:HG22	1.72	0.72
1:B:119:LEU:HD11	1:B:177:ILE:HG22	1.72	0.71
1:A:119:LEU:HD11	1:A:177:ILE:HG22	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LEU:CD2	1:B:567:LEU:HD22	2.21	0.71
1:D:119:LEU:HD11	1:D:177:ILE:HG22	1.72	0.71
1:A:567:LEU:HD22	1:G:567:LEU:CD2	2.21	0.71
2:F:142:PHE:HA	2:F:145:MET:HE3	1.73	0.70
2:E:142:PHE:HA	2:E:145:MET:HE3	1.73	0.70
1:B:567:LEU:CD2	1:D:567:LEU:HD22	2.21	0.70
2:H:142:PHE:HA	2:H:145:MET:HE3	1.73	0.70
2:E:72:MET:SD	2:E:75:ARG:NH2	2.66	0.69
2:F:72:MET:SD	2:F:75:ARG:NH2	2.66	0.69
2:C:72:MET:SD	2:C:75:ARG:NH2	2.66	0.69
1:D:567:LEU:CD2	1:G:567:LEU:HD22	2.21	0.69
2:C:142:PHE:HA	2:C:145:MET:HE3	1.73	0.69
2:H:72:MET:SD	2:H:75:ARG:NH2	2.66	0.68
1:B:564:ILE:HD12	1:B:567:LEU:HD23	1.78	0.66
1:A:564:ILE:HD12	1:A:567:LEU:HD23	1.78	0.66
1:G:564:ILE:HD12	1:G:567:LEU:HD23	1.78	0.65
2:C:122:VAL:HA	2:C:125:MET:HE3	1.80	0.64
1:D:564:ILE:HD12	1:D:567:LEU:HD23	1.78	0.64
2:E:122:VAL:HA	2:E:125:MET:HE3	1.80	0.64
2:F:122:VAL:HA	2:F:125:MET:HE3	1.80	0.64
1:A:309:LEU:HD22	1:A:335:GLY:HA3	1.80	0.64
1:D:332:ALA:O	1:D:336:ILE:HG23	1.98	0.63
1:D:341:LEU:HB2	1:D:342:PRO:HD3	1.80	0.63
1:A:341:LEU:HB2	1:A:342:PRO:HD3	1.80	0.63
1:B:332:ALA:O	1:B:336:ILE:HG23	1.98	0.63
1:G:332:ALA:O	1:G:336:ILE:HG23	1.98	0.63
1:B:341:LEU:HB2	1:B:342:PRO:HD3	1.80	0.63
2:C:141:GLU:C	2:C:145:MET:HE3	2.24	0.63
1:A:332:ALA:O	1:A:336:ILE:HG23	1.98	0.62
1:D:309:LEU:HD22	1:D:335:GLY:HA3	1.80	0.62
1:G:341:LEU:HB2	1:G:342:PRO:HD3	1.80	0.62
2:F:141:GLU:C	2:F:145:MET:HE3	2.24	0.62
1:B:309:LEU:HD22	1:B:335:GLY:HA3	1.80	0.62
2:H:122:VAL:HA	2:H:125:MET:HE3	1.80	0.62
2:E:141:GLU:C	2:E:145:MET:HE3	2.24	0.62
1:G:309:LEU:HD22	1:G:335:GLY:HA3	1.80	0.62
1:D:369:PRO:HB3	1:D:536:LYS:HG3	1.83	0.61
2:H:141:GLU:C	2:H:145:MET:HE3	2.24	0.61
1:A:369:PRO:HB3	1:A:536:LYS:HG3	1.83	0.61
1:G:369:PRO:HB3	1:G:536:LYS:HG3	1.83	0.61
1:B:369:PRO:HB3	1:B:536:LYS:HG3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ILE:HG12	1:G:549:VAL:HG11	1.84	0.60
1:D:288:GLU:OE2	1:D:321:THR:N	2.36	0.59
1:A:549:VAL:HG11	1:G:550:ILE:HG12	1.84	0.59
1:B:160:LEU:CD2	1:B:235:ARG:NH1	2.66	0.59
1:B:550:ILE:HG12	1:D:549:VAL:HG11	1.84	0.59
1:A:160:LEU:CD2	1:A:235:ARG:NH1	2.66	0.59
1:G:160:LEU:CD2	1:G:235:ARG:NH1	2.66	0.59
1:B:290:ASP:OD1	1:B:291:ALA:N	2.36	0.58
1:A:550:ILE:HG12	1:B:549:VAL:HG11	1.84	0.58
1:B:288:GLU:OE2	1:B:321:THR:N	2.36	0.58
1:D:137:VAL:HG12	1:D:242:MET:HE3	1.85	0.58
1:D:160:LEU:CD2	1:D:235:ARG:NH1	2.66	0.58
2:F:96:ASP:OD2	2:F:98:ASN:ND2	2.37	0.58
1:G:288:GLU:OE2	1:G:321:THR:N	2.36	0.58
1:A:288:GLU:OE2	1:A:321:THR:N	2.36	0.58
1:B:547:LYS:HA	1:B:550:ILE:HD12	1.86	0.58
2:C:96:ASP:OD2	2:C:98:ASN:ND2	2.37	0.58
1:D:290:ASP:OD1	1:D:291:ALA:N	2.36	0.58
1:G:290:ASP:OD1	1:G:291:ALA:N	2.36	0.58
1:G:137:VAL:HG12	1:G:242:MET:HE3	1.85	0.58
1:G:547:LYS:HA	1:G:550:ILE:HD12	1.86	0.58
1:D:547:LYS:HA	1:D:550:ILE:HD12	1.86	0.57
2:C:142:PHE:CA	2:C:145:MET:HE3	2.35	0.57
2:F:142:PHE:CA	2:F:145:MET:HE3	2.35	0.57
1:A:137:VAL:HG12	1:A:242:MET:HE3	1.85	0.57
1:B:137:VAL:HG12	1:B:242:MET:HE3	1.85	0.57
2:H:96:ASP:OD2	2:H:98:ASN:ND2	2.37	0.57
1:A:547:LYS:HA	1:A:550:ILE:HD12	1.86	0.57
1:B:310:THR:O	1:B:311:THR:OG1	2.19	0.57
2:C:141:GLU:OE1	2:C:145:MET:HE1	2.05	0.56
2:F:141:GLU:OE1	2:F:145:MET:HE1	2.05	0.56
2:E:142:PHE:CA	2:E:145:MET:HE3	2.35	0.56
1:A:290:ASP:OD1	1:A:291:ALA:N	2.36	0.56
2:H:141:GLU:OE1	2:H:145:MET:HE1	2.05	0.56
2:H:142:PHE:CA	2:H:145:MET:HE3	2.35	0.56
2:E:96:ASP:OD2	2:E:98:ASN:ND2	2.37	0.56
1:B:560:MET:HA	1:B:563:ARG:NE	2.21	0.56
1:D:560:MET:HA	1:D:563:ARG:NE	2.21	0.56
2:E:141:GLU:OE1	2:E:145:MET:HE1	2.05	0.56
1:A:560:MET:HA	1:A:563:ARG:NE	2.21	0.55
1:G:560:MET:HA	1:G:563:ARG:NE	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:SD	1:A:171:PHE:CE1	3.00	0.54
1:B:189:ARG:O	1:B:192:GLN:NE2	2.40	0.54
1:D:160:LEU:HD23	1:D:235:ARG:NH1	2.23	0.54
1:D:167:MET:SD	1:D:171:PHE:CE1	3.00	0.54
1:G:189:ARG:O	1:G:192:GLN:NE2	2.40	0.54
1:A:189:ARG:O	1:A:192:GLN:NE2	2.40	0.54
2:E:142:PHE:O	2:E:146:MET:HG3	2.08	0.54
1:B:160:LEU:HD23	1:B:235:ARG:NH1	2.23	0.54
1:B:167:MET:SD	1:B:171:PHE:CE1	3.00	0.54
1:G:167:MET:SD	1:G:171:PHE:CE1	3.00	0.54
1:D:189:ARG:O	1:D:192:GLN:NE2	2.40	0.54
2:F:142:PHE:O	2:F:146:MET:HG3	2.08	0.54
2:H:142:PHE:O	2:H:146:MET:HG3	2.08	0.54
1:G:310:THR:O	1:G:311:THR:OG1	2.19	0.54
1:D:119:LEU:CD1	1:D:177:ILE:HG22	2.38	0.53
1:G:160:LEU:HD23	1:G:235:ARG:NH1	2.23	0.53
2:C:142:PHE:O	2:C:146:MET:HG3	2.08	0.53
1:G:119:LEU:CD1	1:G:177:ILE:HG22	2.38	0.53
1:B:266:LEU:HD11	1:B:346:LEU:HD21	1.90	0.53
1:B:559:ASP:O	1:B:563:ARG:HG3	2.09	0.53
1:B:561:LEU:HD11	1:B:565:LYS:HE3	1.91	0.53
1:D:561:LEU:HD11	1:D:565:LYS:HE3	1.91	0.53
1:A:160:LEU:HD23	1:A:235:ARG:NH1	2.23	0.53
1:G:559:ASP:O	1:G:563:ARG:HG3	2.09	0.53
1:A:561:LEU:HD11	1:A:565:LYS:HE3	1.91	0.53
1:G:561:LEU:HD11	1:G:565:LYS:HE3	1.91	0.53
1:A:266:LEU:HD11	1:A:346:LEU:HD21	1.90	0.52
1:D:369:PRO:HG2	1:D:540:THR:HG21	1.91	0.52
1:G:266:LEU:HD11	1:G:346:LEU:HD21	1.90	0.52
1:A:559:ASP:O	1:A:563:ARG:HG3	2.09	0.52
1:B:369:PRO:HG2	1:B:540:THR:HG21	1.91	0.52
1:A:119:LEU:CD1	1:A:177:ILE:HG22	2.38	0.52
1:D:559:ASP:O	1:D:563:ARG:HG3	2.09	0.52
2:H:142:PHE:O	2:H:145:MET:HG2	2.10	0.52
1:B:191:TRP:CD2	1:B:192:GLN:N	2.78	0.51
2:F:142:PHE:O	2:F:145:MET:HG2	2.10	0.51
1:G:369:PRO:HG2	1:G:540:THR:HG21	1.91	0.51
2:C:147:THR:HG22	2:C:147:THR:O	2.11	0.51
1:D:191:TRP:CD2	1:D:192:GLN:N	2.78	0.51
1:D:266:LEU:HD11	1:D:346:LEU:HD21	1.90	0.51
1:A:369:PRO:HG2	1:A:540:THR:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:THR:O	2:E:147:THR:HG22	2.11	0.51
2:H:147:THR:HG22	2:H:147:THR:O	2.11	0.51
1:A:171:PHE:CE2	1:A:241:ARG:HD2	2.46	0.51
1:A:338:PHE:CD1	1:A:341:LEU:HD11	2.46	0.51
2:E:142:PHE:O	2:E:145:MET:HG2	2.10	0.51
1:B:171:PHE:CE2	1:B:241:ARG:HD2	2.46	0.51
2:C:142:PHE:O	2:C:145:MET:HG2	2.10	0.51
1:G:191:TRP:CD2	1:G:192:GLN:N	2.78	0.51
1:A:191:TRP:CD2	1:A:192:GLN:N	2.78	0.51
1:B:119:LEU:CD1	1:B:177:ILE:HG22	2.38	0.51
1:B:216:VAL:HG13	1:B:231:LEU:HD22	1.93	0.50
2:F:147:THR:HG22	2:F:147:THR:O	2.11	0.50
1:G:216:VAL:HG13	1:G:231:LEU:HD22	1.93	0.50
1:G:219:ALA:HB1	1:G:227:ALA:HB1	1.94	0.50
1:B:316:ASP:OD1	1:B:316:ASP:N	2.44	0.50
1:D:171:PHE:CE2	1:D:241:ARG:HD2	2.46	0.50
2:E:141:GLU:O	2:E:145:MET:HE3	2.12	0.50
1:D:216:VAL:HG13	1:D:231:LEU:HD22	1.93	0.50
1:G:171:PHE:CE2	1:G:241:ARG:HD2	2.46	0.50
1:B:338:PHE:CD1	1:B:341:LEU:HD11	2.46	0.50
1:B:525:ILE:HG23	2:C:52:MET:CE	2.42	0.50
1:D:310:THR:O	1:D:311:THR:OG1	2.19	0.50
1:G:338:PHE:CD1	1:G:341:LEU:HD11	2.46	0.50
1:B:558:LEU:HD12	1:B:559:ASP:N	2.27	0.50
2:C:142:PHE:N	2:C:145:MET:HE3	2.27	0.50
2:H:141:GLU:O	2:H:145:MET:HE3	2.12	0.50
1:A:566:SER:O	1:A:570:ARG:HG2	2.12	0.49
2:H:142:PHE:N	2:H:145:MET:HE3	2.27	0.49
2:C:141:GLU:O	2:C:145:MET:HE3	2.12	0.49
1:A:525:ILE:HG23	2:E:52:MET:CE	2.42	0.49
1:A:558:LEU:HD12	1:A:559:ASP:N	2.27	0.49
1:B:137:VAL:HG22	1:B:167:MET:HE1	1.95	0.49
2:F:141:GLU:O	2:F:145:MET:HE3	2.12	0.49
1:B:566:SER:O	1:B:570:ARG:HG2	2.12	0.49
1:D:338:PHE:CD1	1:D:341:LEU:HD11	2.46	0.49
1:A:137:VAL:HG22	1:A:167:MET:HE1	1.95	0.49
1:A:216:VAL:HG13	1:A:231:LEU:HD22	1.93	0.49
1:A:567:LEU:HA	1:A:570:ARG:CZ	2.43	0.49
1:B:112:GLN:HG2	1:B:184:CYS:HB2	1.94	0.49
1:D:219:ALA:HB1	1:D:227:ALA:HB1	1.94	0.49
1:D:525:ILE:HG23	2:F:52:MET:CE	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:PHE:N	2:F:145:MET:HE3	2.27	0.49
1:G:558:LEU:HD12	1:G:559:ASP:N	2.27	0.49
1:G:566:SER:O	1:G:570:ARG:HG2	2.12	0.49
1:G:567:LEU:HA	1:G:570:ARG:CZ	2.43	0.49
2:E:142:PHE:N	2:E:145:MET:HE3	2.27	0.49
1:G:137:VAL:HG22	1:G:167:MET:HE1	1.95	0.49
1:A:112:GLN:HG2	1:A:184:CYS:HB2	1.94	0.49
1:A:310:THR:O	1:A:311:THR:OG1	2.19	0.49
1:D:137:VAL:HG22	1:D:167:MET:HE1	1.95	0.49
1:D:566:SER:O	1:D:570:ARG:HG2	2.12	0.49
1:G:525:ILE:HG23	2:H:52:MET:CE	2.42	0.49
1:A:219:ALA:HB1	1:A:227:ALA:HB1	1.94	0.48
1:B:219:ALA:HB1	1:B:227:ALA:HB1	1.94	0.48
1:D:567:LEU:HA	1:D:570:ARG:CZ	2.43	0.48
1:D:316:ASP:OD1	1:D:316:ASP:N	2.44	0.48
1:D:558:LEU:HD12	1:D:559:ASP:N	2.27	0.48
1:G:112:GLN:HG2	1:G:184:CYS:HB2	1.94	0.48
1:B:567:LEU:HA	1:B:570:ARG:CZ	2.43	0.48
1:B:108:TYR:CD1	1:B:109:ARG:N	2.82	0.48
1:D:112:GLN:HG2	1:D:184:CYS:HB2	1.94	0.48
1:G:316:ASP:OD1	1:G:316:ASP:N	2.44	0.48
1:A:338:PHE:HD1	1:A:341:LEU:CD1	2.27	0.48
1:B:338:PHE:HD1	1:B:341:LEU:CD1	2.27	0.47
1:G:108:TYR:CD1	1:G:109:ARG:N	2.82	0.47
1:A:316:ASP:N	1:A:316:ASP:OD1	2.44	0.47
1:B:212:ALA:O	1:B:216:VAL:HG23	2.14	0.47
1:D:212:ALA:O	1:D:216:VAL:HG23	2.14	0.47
1:A:567:LEU:HD21	1:B:567:LEU:CD2	2.38	0.47
1:D:108:TYR:CD1	1:D:109:ARG:N	2.82	0.47
1:A:557:HIS:HA	1:A:560:MET:HE2	1.96	0.47
1:D:338:PHE:HD1	1:D:341:LEU:CD1	2.27	0.47
1:A:212:ALA:O	1:A:216:VAL:HG23	2.14	0.47
1:D:557:HIS:HA	1:D:560:MET:HE2	1.96	0.47
2:F:86:ILE:HG21	2:F:146:MET:HE1	1.97	0.47
1:G:338:PHE:HD1	1:G:341:LEU:CD1	2.27	0.47
1:G:212:ALA:O	1:G:216:VAL:HG23	2.14	0.47
1:A:108:TYR:CD1	1:A:109:ARG:N	2.82	0.47
1:D:567:LEU:HD21	1:G:567:LEU:CD2	2.38	0.47
1:G:557:HIS:HA	1:G:560:MET:HE2	1.96	0.47
1:B:220:LYS:HE3	1:B:235:ARG:NH1	2.30	0.47
1:B:557:HIS:HA	1:B:560:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LYS:HE3	1:D:235:ARG:NH1	2.30	0.46
1:G:220:LYS:HE3	1:G:235:ARG:NH1	2.30	0.46
1:G:337:SER:O	1:G:341:LEU:HG	2.15	0.46
1:D:337:SER:O	1:D:341:LEU:HG	2.15	0.46
2:C:86:ILE:HG21	2:C:146:MET:HE1	1.97	0.46
1:B:160:LEU:HD21	1:B:235:ARG:CZ	2.46	0.46
1:B:207:THR:HG22	1:B:208:ILE:N	2.30	0.46
1:B:337:SER:O	1:B:341:LEU:HG	2.15	0.46
1:A:207:THR:HG22	1:A:208:ILE:N	2.30	0.46
1:A:220:LYS:HE3	1:A:235:ARG:NH1	2.30	0.46
1:A:236:PHE:O	1:A:239:ILE:HG22	2.16	0.46
1:A:375:GLN:OE1	2:E:115:GLU:N	2.49	0.46
1:B:338:PHE:HA	1:B:341:LEU:CD1	2.46	0.46
1:D:160:LEU:HD21	1:D:235:ARG:CZ	2.46	0.46
1:G:338:PHE:HA	1:G:341:LEU:CD1	2.46	0.46
1:A:571:VAL:HA	1:A:574:ILE:HG12	1.98	0.46
1:B:571:VAL:HA	1:B:574:ILE:HG12	1.98	0.46
1:D:207:THR:HG22	1:D:208:ILE:N	2.30	0.46
1:G:207:THR:HG22	1:G:208:ILE:N	2.30	0.46
1:G:375:GLN:OE1	2:H:115:GLU:N	2.49	0.46
1:G:531:HIS:O	1:G:535:ARG:NH1	2.49	0.46
1:A:123:ARG:H	1:A:126:ALA:HB3	1.81	0.46
1:A:557:HIS:HA	1:A:560:MET:HG2	1.98	0.46
2:E:86:ILE:HG21	2:E:146:MET:HE1	1.97	0.46
1:B:236:PHE:O	1:B:239:ILE:HG22	2.16	0.46
1:B:521:VAL:HB	2:C:16:ALA:HB1	1.98	0.46
2:C:50:GLN:NE2	2:C:54:ASN:OD1	2.49	0.46
1:G:236:PHE:O	1:G:239:ILE:HG22	2.16	0.46
1:G:376:CYS:SG	1:G:533:ALA:HB3	2.56	0.46
1:G:557:HIS:HA	1:G:560:MET:HG2	1.98	0.46
1:B:123:ARG:H	1:B:126:ALA:HB3	1.81	0.46
1:B:375:GLN:OE1	2:C:115:GLU:N	2.49	0.46
1:D:123:ARG:H	1:D:126:ALA:HB3	1.81	0.46
1:D:375:GLN:OE1	2:F:115:GLU:N	2.49	0.46
1:D:376:CYS:SG	1:D:533:ALA:HB3	2.56	0.46
1:G:571:VAL:HA	1:G:574:ILE:HG12	1.98	0.46
1:A:567:LEU:HD21	1:B:567:LEU:HB2	1.97	0.46
1:D:236:PHE:O	1:D:239:ILE:HG22	2.16	0.46
1:D:338:PHE:CD1	1:D:341:LEU:CD1	2.99	0.46
1:D:567:LEU:HD21	1:G:567:LEU:HB2	1.97	0.46
1:G:338:PHE:CD1	1:G:341:LEU:CD1	2.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:521:VAL:HB	2:H:16:ALA:HB1	1.98	0.46
1:A:337:SER:O	1:A:341:LEU:HG	2.15	0.45
1:A:338:PHE:HA	1:A:341:LEU:CD1	2.46	0.45
1:A:568:GLN:NE2	1:A:569:THR:HG23	2.31	0.45
1:B:338:PHE:CD1	1:B:341:LEU:CD1	2.99	0.45
2:H:141:GLU:O	2:H:145:MET:CE	2.65	0.45
1:A:571:VAL:HG11	1:B:570:ARG:HG3	1.98	0.45
1:D:338:PHE:HA	1:D:341:LEU:CD1	2.46	0.45
1:D:531:HIS:O	1:D:535:ARG:NH1	2.49	0.45
2:F:109:VAL:HG13	2:F:113:LEU:HD12	1.99	0.45
1:D:571:VAL:HA	1:D:574:ILE:HG12	1.98	0.45
1:A:531:HIS:O	1:A:535:ARG:NH1	2.49	0.45
2:C:109:VAL:HG13	2:C:113:LEU:HD12	1.99	0.45
1:G:568:GLN:NE2	1:G:569:THR:HG23	2.31	0.45
2:H:109:VAL:HG13	2:H:113:LEU:HD12	1.99	0.45
1:A:371:ALA:CB	2:E:113:LEU:HB3	2.47	0.45
1:A:567:LEU:HB2	1:G:567:LEU:HD21	1.97	0.45
1:B:376:CYS:SG	1:B:533:ALA:HB3	2.56	0.45
1:B:531:HIS:O	1:B:535:ARG:NH1	2.49	0.45
1:B:567:LEU:HD21	1:D:567:LEU:HB2	1.97	0.45
2:H:86:ILE:HG21	2:H:146:MET:HE1	1.97	0.45
1:A:376:CYS:SG	1:A:533:ALA:HB3	2.56	0.45
1:D:571:VAL:HG11	1:G:570:ARG:HG3	1.98	0.45
1:A:525:ILE:HG23	2:E:52:MET:HE1	1.99	0.45
1:A:570:ARG:HG3	1:G:571:VAL:HG11	1.98	0.45
4:A:802:PIO:H4AA	1:G:256:GLY:HA3	1.99	0.45
2:E:109:VAL:HG13	2:E:113:LEU:HD12	1.99	0.45
1:D:207:THR:O	1:D:211:ILE:HG12	2.17	0.45
1:D:568:GLN:NE2	1:D:569:THR:HG23	2.31	0.45
1:G:368:ASN:HB2	1:G:369:PRO:HD3	1.98	0.45
1:G:371:ALA:CB	2:H:113:LEU:HB3	2.47	0.45
1:A:160:LEU:HD21	1:A:235:ARG:CZ	2.46	0.45
2:E:50:GLN:NE2	2:E:54:ASN:OD1	2.49	0.45
1:B:371:ALA:CB	2:C:113:LEU:HB3	2.47	0.45
1:D:521:VAL:HB	2:F:16:ALA:HB1	1.98	0.45
2:F:141:GLU:O	2:F:145:MET:CE	2.65	0.45
1:G:160:LEU:HD21	1:G:235:ARG:CZ	2.46	0.45
1:A:188:TYR:C	1:A:193:GLY:HA3	2.42	0.45
1:A:338:PHE:CD1	1:A:341:LEU:CD1	2.99	0.45
2:E:141:GLU:O	2:E:145:MET:CE	2.65	0.45
1:B:525:ILE:HG23	2:C:52:MET:HE1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ARG:H	1:G:126:ALA:HB3	1.81	0.45
1:G:561:LEU:O	1:G:564:ILE:HG22	2.17	0.45
1:A:521:VAL:HB	2:E:16:ALA:HB1	1.98	0.45
1:A:561:LEU:O	1:A:564:ILE:HG22	2.17	0.45
1:B:368:ASN:HB2	1:B:369:PRO:HD3	1.98	0.45
1:B:557:HIS:HA	1:B:560:MET:HG2	1.98	0.45
1:B:568:GLN:NE2	1:B:569:THR:HG23	2.31	0.45
1:D:557:HIS:HA	1:D:560:MET:HG2	1.98	0.45
1:A:256:GLY:HA3	4:B:801:PIO:H4AA	1.99	0.44
1:B:567:LEU:HD21	1:D:567:LEU:CD2	2.38	0.44
1:D:188:TYR:C	1:D:193:GLY:HA3	2.42	0.44
1:G:188:TYR:C	1:G:193:GLY:HA3	2.42	0.44
1:A:560:MET:HE1	1:B:556:GLY:HA2	2.00	0.44
2:E:48:GLU:OE1	2:E:49:LEU:HD22	2.17	0.44
1:B:561:LEU:O	1:B:564:ILE:HG22	2.17	0.44
2:C:141:GLU:O	2:C:145:MET:CE	2.65	0.44
1:D:371:ALA:CB	2:F:113:LEU:HB3	2.47	0.44
1:B:207:THR:O	1:B:211:ILE:HG12	2.17	0.44
2:C:122:VAL:CA	2:C:125:MET:HE3	2.46	0.44
1:D:368:ASN:HB2	1:D:369:PRO:HD3	1.98	0.44
1:G:336:ILE:HG13	1:G:337:SER:N	2.32	0.44
1:A:207:THR:O	1:A:211:ILE:HG12	2.17	0.44
1:B:256:GLY:HA3	4:D:801:PIO:H4AA	1.99	0.44
2:F:107:ARG:HD2	2:F:122:VAL:HG11	2.00	0.44
1:G:207:THR:O	1:G:211:ILE:HG12	2.17	0.44
2:H:48:GLU:OE1	2:H:49:LEU:HD22	2.17	0.44
1:A:556:GLY:HA2	1:G:560:MET:HE1	2.00	0.44
1:B:188:TYR:C	1:B:193:GLY:HA3	2.42	0.44
2:C:48:GLU:OE1	2:C:49:LEU:HD22	2.17	0.44
2:F:50:GLN:NE2	2:F:54:ASN:OD1	2.49	0.44
1:G:160:LEU:CD2	1:G:235:ARG:CZ	2.96	0.44
1:G:525:ILE:HG23	2:H:52:MET:HE1	1.99	0.44
2:H:107:ARG:HD2	2:H:122:VAL:HG11	2.00	0.44
1:A:116:TYR:N	1:A:181:SER:HB3	2.33	0.44
1:A:137:VAL:CG1	1:A:242:MET:HE3	2.48	0.44
1:B:560:MET:HE1	1:D:556:GLY:HA2	2.00	0.44
1:D:256:GLY:HA3	4:G:1000:PIO:H4AA	1.99	0.44
1:D:268:THR:O	1:D:272:ILE:HG12	2.18	0.44
1:G:191:TRP:CE3	1:G:192:GLN:N	2.86	0.44
1:G:383:ALA:O	1:G:523:ARG:NH1	2.51	0.44
1:A:160:LEU:CD2	1:A:235:ARG:CZ	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:O	1:A:272:ILE:HG12	2.18	0.44
1:A:567:LEU:HA	1:A:570:ARG:NE	2.33	0.44
1:D:561:LEU:O	1:D:564:ILE:HG22	2.17	0.44
1:D:567:LEU:HA	1:D:570:ARG:NE	2.33	0.44
2:H:50:GLN:NE2	2:H:54:ASN:OD1	2.49	0.44
1:A:368:ASN:HB2	1:A:369:PRO:HD3	1.98	0.44
2:E:107:ARG:HD2	2:E:122:VAL:HG11	2.00	0.44
1:B:336:ILE:HG13	1:B:337:SER:N	2.32	0.44
1:A:191:TRP:CE3	1:A:192:GLN:N	2.86	0.43
1:B:571:VAL:HG11	1:D:570:ARG:HG3	1.98	0.43
1:D:336:ILE:HG13	1:D:337:SER:N	2.32	0.43
1:D:525:ILE:HG23	2:F:52:MET:HE1	1.99	0.43
2:F:48:GLU:OE1	2:F:49:LEU:HD22	2.17	0.43
2:E:88:GLU:O	2:E:92:VAL:HG23	2.19	0.43
1:B:116:TYR:N	1:B:181:SER:HB3	2.33	0.43
1:B:137:VAL:CG1	1:B:242:MET:HE3	2.48	0.43
1:D:191:TRP:CE3	1:D:192:GLN:N	2.86	0.43
1:G:116:TYR:N	1:G:181:SER:HB3	2.33	0.43
1:A:336:ILE:HG13	1:A:337:SER:N	2.32	0.43
1:A:376:CYS:SG	1:A:530:PHE:HA	2.59	0.43
2:E:122:VAL:CA	2:E:125:MET:HE3	2.46	0.43
1:B:108:TYR:CD1	1:B:108:TYR:C	2.95	0.43
1:B:268:THR:O	1:B:272:ILE:HG12	2.18	0.43
2:C:88:GLU:O	2:C:92:VAL:HG23	2.19	0.43
1:D:560:MET:HE1	1:G:556:GLY:HA2	2.00	0.43
1:G:567:LEU:HA	1:G:570:ARG:NE	2.33	0.43
1:A:550:ILE:HD11	1:B:544:TYR:OH	2.18	0.43
1:B:191:TRP:CE3	1:B:192:GLN:N	2.86	0.43
1:D:383:ALA:O	1:D:523:ARG:NH1	2.51	0.43
1:A:383:ALA:O	1:A:523:ARG:NH1	2.51	0.43
1:B:160:LEU:CD2	1:B:235:ARG:CZ	2.96	0.43
1:B:567:LEU:HA	1:B:570:ARG:NE	2.33	0.43
2:C:107:ARG:HD2	2:C:122:VAL:HG11	2.00	0.43
1:D:116:TYR:N	1:D:181:SER:HB3	2.33	0.43
2:H:88:GLU:O	2:H:92:VAL:HG23	2.19	0.43
1:D:160:LEU:CD2	1:D:235:ARG:CZ	2.96	0.43
1:A:544:TYR:OH	1:G:550:ILE:HD11	2.18	0.43
1:B:287:VAL:HG21	1:B:327:LEU:HD12	2.01	0.43
1:B:516:PRO:N	1:B:517:PRO:HD2	2.34	0.43
1:D:516:PRO:N	1:D:517:PRO:HD2	2.34	0.43
2:F:88:GLU:O	2:F:92:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:VAL:CA	2:F:125:MET:HE3	2.46	0.43
1:G:376:CYS:SG	1:G:530:PHE:HA	2.59	0.43
1:D:244:ARG:HG2	1:D:245:MET:N	2.34	0.43
1:D:338:PHE:HA	1:D:341:LEU:HG	2.01	0.43
1:A:287:VAL:HG21	1:A:327:LEU:HD12	2.01	0.43
1:B:376:CYS:SG	1:B:530:PHE:HA	2.59	0.43
1:G:137:VAL:CG1	1:G:242:MET:HE3	2.48	0.43
1:G:268:THR:O	1:G:272:ILE:HG12	2.18	0.43
1:A:185:CYS:O	1:A:186:CYS:HB2	2.19	0.42
1:A:570:ARG:HA	1:A:573:GLN:CD	2.44	0.42
1:B:570:ARG:HA	1:B:573:GLN:CD	2.44	0.42
2:H:110:MET:HE3	2:H:122:VAL:HG13	2.01	0.42
1:A:338:PHE:HA	1:A:341:LEU:HG	2.01	0.42
1:A:516:PRO:N	1:A:517:PRO:HD2	2.34	0.42
1:A:549:VAL:HA	1:A:552:GLN:HB2	2.01	0.42
1:B:550:ILE:HD11	1:D:544:TYR:OH	2.18	0.42
1:D:258:VAL:HG21	1:D:350:PHE:CE1	2.54	0.42
1:D:550:ILE:HD11	1:G:544:TYR:OH	2.18	0.42
1:G:185:CYS:O	1:G:186:CYS:HB2	2.19	0.42
1:G:516:PRO:N	1:G:517:PRO:HD2	2.34	0.42
1:A:108:TYR:CD1	1:A:108:TYR:C	2.95	0.42
2:C:110:MET:HE3	2:C:122:VAL:HG13	2.01	0.42
1:G:549:VAL:HA	1:G:552:GLN:HB2	2.01	0.42
1:A:258:VAL:HG21	1:A:350:PHE:CE1	2.54	0.42
1:B:383:ALA:O	1:B:523:ARG:NH1	2.51	0.42
1:D:137:VAL:CG1	1:D:242:MET:HE3	2.48	0.42
1:D:570:ARG:HA	1:D:573:GLN:CD	2.44	0.42
2:F:110:MET:HE3	2:F:122:VAL:HG13	2.01	0.42
1:G:137:VAL:CG2	1:G:167:MET:HE1	2.50	0.42
1:A:148:THR:HG21	1:G:298:TYR:H	1.85	0.42
1:G:160:LEU:HG	1:G:235:ARG:NH1	2.35	0.42
1:G:173:LEU:O	1:G:176:ILE:HG13	2.20	0.42
1:A:137:VAL:CG2	1:A:167:MET:HE1	2.50	0.42
1:B:244:ARG:HG2	1:B:245:MET:N	2.34	0.42
1:B:258:VAL:HG21	1:B:350:PHE:CE1	2.54	0.42
1:B:549:VAL:HA	1:B:552:GLN:HB2	2.01	0.42
1:D:165:PHE:CE1	1:D:217:VAL:HG11	2.55	0.42
1:D:549:VAL:HA	1:D:552:GLN:HB2	2.01	0.42
4:G:1000:PIO:C5B	4:G:1000:PIO:H8AA	2.50	0.42
1:A:167:MET:SD	1:A:171:PHE:HE1	2.43	0.42
1:A:298:TYR:H	1:B:148:THR:HG21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:PIO:C5B	4:A:802:PIO:H8AA	2.50	0.42
1:B:160:LEU:HG	1:B:235:ARG:NH1	2.35	0.42
1:B:165:PHE:CE1	1:B:217:VAL:HG11	2.55	0.42
4:B:801:PIO:C5B	4:B:801:PIO:H8AA	2.50	0.42
1:D:137:VAL:CG2	1:D:167:MET:HE1	2.50	0.42
1:D:298:TYR:H	1:G:148:THR:HG21	1.85	0.42
1:D:376:CYS:SG	1:D:530:PHE:HA	2.59	0.42
1:A:567:LEU:CD2	1:G:567:LEU:HD21	2.38	0.42
2:C:122:VAL:O	2:C:126:ILE:HG12	2.20	0.42
1:D:160:LEU:HG	1:D:235:ARG:NH1	2.35	0.42
1:D:287:VAL:HG21	1:D:327:LEU:HD12	2.01	0.42
1:G:165:PHE:CE1	1:G:217:VAL:HG11	2.55	0.42
1:G:353:LYS:O	1:G:357:GLN:HG2	2.20	0.42
1:A:173:LEU:O	1:A:176:ILE:HG13	2.20	0.42
1:A:353:LYS:O	1:A:357:GLN:HG2	2.20	0.42
1:B:185:CYS:O	1:B:186:CYS:HB2	2.19	0.42
2:C:107:ARG:NH1	2:C:122:VAL:HG11	2.35	0.42
4:D:801:PIO:C5B	4:D:801:PIO:H8AA	2.50	0.42
1:G:258:VAL:HG21	1:G:350:PHE:CE1	2.54	0.42
2:F:107:ARG:NH1	2:F:122:VAL:HG11	2.35	0.42
1:G:338:PHE:HA	1:G:341:LEU:HG	2.01	0.42
1:B:137:VAL:CG2	1:B:167:MET:HE1	2.50	0.41
2:H:122:VAL:CA	2:H:125:MET:HE3	2.46	0.41
1:A:112:GLN:HG2	1:A:181:SER:HA	2.03	0.41
1:A:165:PHE:CE1	1:A:217:VAL:HG11	2.55	0.41
1:B:196:ARG:NE	1:B:196:ARG:HA	2.36	0.41
1:D:196:ARG:HA	1:D:196:ARG:NE	2.36	0.41
1:G:287:VAL:HG21	1:G:327:LEU:HD12	2.01	0.41
1:D:108:TYR:CD1	1:D:108:TYR:C	2.95	0.41
2:E:122:VAL:O	2:E:126:ILE:HG12	2.20	0.41
1:B:167:MET:SD	1:B:171:PHE:HE1	2.43	0.41
1:B:249:GLY:O	1:B:250:GLY:C	2.64	0.41
1:G:570:ARG:HA	1:G:573:GLN:CD	2.44	0.41
2:H:107:ARG:NH1	2:H:122:VAL:HG11	2.35	0.41
1:A:244:ARG:HG2	1:A:245:MET:N	2.34	0.41
1:A:546:VAL:O	1:A:550:ILE:HG13	2.21	0.41
2:E:107:ARG:NH1	2:E:122:VAL:HG11	2.35	0.41
1:B:173:LEU:O	1:B:176:ILE:HG13	2.20	0.41
1:B:353:LYS:O	1:B:357:GLN:HG2	2.20	0.41
1:A:196:ARG:HA	1:A:196:ARG:NE	2.36	0.41
1:B:338:PHE:HA	1:B:341:LEU:HG	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:VAL:O	1:B:550:ILE:HG13	2.21	0.41
1:G:244:ARG:HG2	1:G:245:MET:N	2.34	0.41
1:G:546:VAL:O	1:G:550:ILE:HG13	2.21	0.41
1:A:568:GLN:HB3	1:B:570:ARG:CZ	2.51	0.41
1:A:570:ARG:CZ	1:G:568:GLN:HB3	2.51	0.41
1:B:231:LEU:O	1:B:235:ARG:HG2	2.21	0.41
1:D:185:CYS:O	1:D:186:CYS:HB2	2.19	0.41
1:D:231:LEU:O	1:D:235:ARG:HG2	2.21	0.41
2:E:86:ILE:HG21	2:E:146:MET:CE	2.51	0.41
1:B:112:GLN:HG2	1:B:181:SER:HA	2.03	0.41
1:B:298:TYR:H	1:D:148:THR:HG21	1.85	0.41
2:C:121:GLU:C	2:C:125:MET:HE3	2.46	0.41
1:D:568:GLN:HB3	1:G:570:ARG:CZ	2.51	0.41
1:G:108:TYR:CD1	1:G:108:TYR:C	2.95	0.41
1:A:160:LEU:HG	1:A:235:ARG:NH1	2.35	0.41
1:A:231:LEU:O	1:A:235:ARG:HG2	2.21	0.41
1:A:338:PHE:HD1	1:A:341:LEU:HD12	1.85	0.41
2:E:110:MET:HE3	2:E:122:VAL:HG13	2.01	0.41
2:E:121:GLU:C	2:E:125:MET:HE3	2.46	0.41
2:E:143:VAL:HA	2:E:146:MET:SD	2.61	0.41
1:B:164:GLU:O	1:B:168:ILE:HG22	2.21	0.41
1:B:207:THR:CG2	1:B:208:ILE:N	2.84	0.41
1:B:251:THR:O	1:B:252:TRP:C	2.63	0.41
2:C:86:ILE:HG21	2:C:146:MET:CE	2.51	0.41
2:C:143:VAL:HA	2:C:146:MET:SD	2.61	0.41
1:D:173:LEU:O	1:D:176:ILE:HG13	2.20	0.41
1:D:353:LYS:O	1:D:357:GLN:HG2	2.20	0.41
2:F:121:GLU:C	2:F:125:MET:HE3	2.46	0.41
2:F:143:VAL:HA	2:F:146:MET:SD	2.61	0.41
2:H:86:ILE:HG21	2:H:146:MET:CE	2.51	0.41
2:H:122:VAL:O	2:H:126:ILE:HG12	2.20	0.41
1:B:570:ARG:O	1:B:574:ILE:HG12	2.21	0.41
1:D:112:GLN:HG2	1:D:181:SER:HA	2.03	0.41
1:D:164:GLU:O	1:D:168:ILE:HG22	2.21	0.41
1:G:207:THR:CG2	1:G:208:ILE:N	2.84	0.41
1:A:570:ARG:O	1:A:574:ILE:HG12	2.21	0.40
1:B:564:ILE:HD13	1:D:563:ARG:HB3	2.03	0.40
1:G:196:ARG:NE	1:G:196:ARG:HA	2.36	0.40
1:G:251:THR:O	1:G:252:TRP:C	2.63	0.40
1:G:338:PHE:HD1	1:G:341:LEU:HD12	1.85	0.40
1:A:249:GLY:O	1:A:250:GLY:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:PHE:HD1	1:B:341:LEU:HD12	1.85	0.40
1:D:338:PHE:HD1	1:D:341:LEU:HD12	1.85	0.40
2:F:122:VAL:O	2:F:126:ILE:HG12	2.20	0.40
1:G:231:LEU:O	1:G:235:ARG:HG2	2.21	0.40
1:G:249:GLY:O	1:G:250:GLY:C	2.64	0.40
2:H:121:GLU:C	2:H:125:MET:HE3	2.46	0.40
2:F:86:ILE:HG21	2:F:146:MET:CE	2.51	0.40
1:A:373:LEU:HA	1:A:376:CYS:SG	2.62	0.40
1:D:220:LYS:CE	1:D:235:ARG:NH1	2.85	0.40
1:G:164:GLU:O	1:G:168:ILE:HG22	2.21	0.40
1:G:570:ARG:O	1:G:574:ILE:HG12	2.21	0.40
2:H:143:VAL:HA	2:H:146:MET:SD	2.61	0.40
1:A:251:THR:O	1:A:252:TRP:C	2.63	0.40
1:A:564:ILE:HD13	1:B:563:ARG:HB3	2.03	0.40
1:B:220:LYS:CE	1:B:235:ARG:NH1	2.85	0.40
1:D:166:VAL:O	1:D:170:VAL:HG12	2.22	0.40
1:D:550:ILE:HA	1:D:553:TYR:CD2	2.57	0.40
1:D:570:ARG:O	1:D:574:ILE:HG12	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	340/626 (54%)	332 (98%)	8 (2%)	0	100	100
1	B	340/626 (54%)	332 (98%)	8 (2%)	0	100	100
1	D	340/626 (54%)	332 (98%)	8 (2%)	0	100	100
1	G	340/626 (54%)	332 (98%)	8 (2%)	0	100	100
2	C	142/177 (80%)	139 (98%)	3 (2%)	0	100	100
2	E	142/177 (80%)	139 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	142/177 (80%)	139 (98%)	3 (2%)	0	100	100
2	H	142/177 (80%)	139 (98%)	3 (2%)	0	100	100
All	All	1928/3212 (60%)	1884 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/545 (54%)	291 (99%)	4 (1%)	62	82
1	B	295/545 (54%)	291 (99%)	4 (1%)	62	82
1	D	295/545 (54%)	291 (99%)	4 (1%)	62	82
1	G	295/545 (54%)	291 (99%)	4 (1%)	62	82
2	C	115/146 (79%)	115 (100%)	0	100	100
2	E	115/146 (79%)	115 (100%)	0	100	100
2	F	115/146 (79%)	115 (100%)	0	100	100
2	H	115/146 (79%)	115 (100%)	0	100	100
All	All	1640/2764 (59%)	1624 (99%)	16 (1%)	71	87

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

Mol	Chain	Res	Type
1	A	108	TYR
1	A	207	THR
1	A	244	ARG
1	A	567	LEU
1	B	108	TYR
1	B	207	THR
1	B	244	ARG
1	B	567	LEU
1	D	108	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	207	THR
1	D	244	ARG
1	D	567	LEU
1	G	108	TYR
1	G	207	THR
1	G	244	ARG
1	G	567	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	238	GLN
1	B	130	HIS
1	B	238	GLN
2	C	50	GLN
2	C	54	ASN
1	D	238	GLN
2	F	50	GLN
2	F	54	ASN
1	G	238	GLN
2	H	50	GLN
2	H	54	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
4	PIO	A	802	-	47,47,47	1.46	10 (21%)	61,65,65	1.58	9 (14%)
3	9MF	A	801	-	26,26,26	1.69	5 (19%)	34,35,35	1.99	6 (17%)
3	9MF	D	802	-	26,26,26	1.69	5 (19%)	34,35,35	1.99	6 (17%)
4	PIO	G	1000	-	47,47,47	1.46	10 (21%)	61,65,65	1.58	9 (14%)
3	9MF	A	803	-	26,26,26	1.69	5 (19%)	34,35,35	1.99	6 (17%)
4	PIO	D	801	-	47,47,47	1.46	10 (21%)	61,65,65	1.58	9 (14%)
4	PIO	B	801	-	47,47,47	1.46	10 (21%)	61,65,65	1.58	9 (14%)
3	9MF	B	802	-	26,26,26	1.69	5 (19%)	34,35,35	1.99	6 (17%)

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
4	PIO	A	802	-	-	22/44/68/68	0/1/1/1
3	9MF	A	801	-	-	0/16/17/17	0/2/2/2
3	9MF	D	802	-	-	0/16/17/17	0/2/2/2
4	PIO	G	1000	-	-	22/44/68/68	0/1/1/1
3	9MF	A	803	-	-	0/16/17/17	0/2/2/2
4	PIO	D	801	-	-	22/44/68/68	0/1/1/1
4	PIO	B	801	-	-	22/44/68/68	0/1/1/1
3	9MF	B	802	-	-	0/16/17/17	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	9MF	C09-N08	4.39	1.45	1.36
3	A	803	9MF	C09-N08	4.39	1.45	1.36
3	B	802	9MF	C09-N08	4.39	1.45	1.36
3	D	802	9MF	C09-N08	4.39	1.45	1.36
3	A	801	9MF	C15-C16	4.29	1.52	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	9MF	C15-C16	4.29	1.52	1.47
3	B	802	9MF	C15-C16	4.29	1.52	1.47
3	D	802	9MF	C15-C16	4.29	1.52	1.47
4	A	802	PIO	P4-O4	3.31	1.65	1.59
4	B	801	PIO	P4-O4	3.31	1.65	1.59
4	D	801	PIO	P4-O4	3.31	1.65	1.59
4	G	1000	PIO	P4-O4	3.31	1.65	1.59
3	A	801	9MF	O11-C09	3.19	1.39	1.34
3	A	803	9MF	O11-C09	3.19	1.39	1.34
3	B	802	9MF	O11-C09	3.19	1.39	1.34
3	D	802	9MF	O11-C09	3.19	1.39	1.34
4	A	802	PIO	P5-O5	3.09	1.65	1.59
4	B	801	PIO	P5-O5	3.09	1.65	1.59
4	D	801	PIO	P5-O5	3.09	1.65	1.59
4	G	1000	PIO	P5-O5	3.09	1.65	1.59
4	A	802	PIO	O3C-C1B	2.68	1.41	1.33
4	B	801	PIO	O3C-C1B	2.68	1.41	1.33
4	D	801	PIO	O3C-C1B	2.68	1.41	1.33
4	G	1000	PIO	O3C-C1B	2.68	1.41	1.33
4	A	802	PIO	C2-C1	-2.58	1.45	1.52
4	B	801	PIO	C2-C1	-2.58	1.45	1.52
4	D	801	PIO	C2-C1	-2.58	1.45	1.52
4	G	1000	PIO	C2-C1	-2.58	1.45	1.52
4	A	802	PIO	O2C-C2C	-2.57	1.40	1.46
4	B	801	PIO	O2C-C2C	-2.57	1.40	1.46
4	D	801	PIO	O2C-C2C	-2.57	1.40	1.46
4	G	1000	PIO	O2C-C2C	-2.57	1.40	1.46
4	A	802	PIO	C6-C1	-2.36	1.46	1.52
4	B	801	PIO	C6-C1	-2.36	1.46	1.52
4	D	801	PIO	C6-C1	-2.36	1.46	1.52
4	G	1000	PIO	C6-C1	-2.36	1.46	1.52
3	A	801	9MF	O11-C12	-2.20	1.40	1.45
3	A	803	9MF	O11-C12	-2.20	1.40	1.45
3	B	802	9MF	O11-C12	-2.20	1.40	1.45
3	D	802	9MF	O11-C12	-2.20	1.40	1.45
4	A	802	PIO	P5-O51	-2.19	1.46	1.54
4	B	801	PIO	P5-O51	-2.19	1.46	1.54
4	D	801	PIO	P5-O51	-2.19	1.46	1.54
4	G	1000	PIO	P5-O51	-2.19	1.46	1.54
4	A	802	PIO	P4-O41	-2.17	1.46	1.54
4	B	801	PIO	P4-O41	-2.17	1.46	1.54
4	D	801	PIO	P4-O41	-2.17	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1000	PIO	P4-O41	-2.17	1.46	1.54
3	A	801	9MF	C04-N14	2.17	1.44	1.38
3	A	803	9MF	C04-N14	2.17	1.44	1.38
3	B	802	9MF	C04-N14	2.17	1.44	1.38
3	D	802	9MF	C04-N14	2.17	1.44	1.38
4	A	802	PIO	P5-O52	-2.16	1.46	1.54
4	B	801	PIO	P5-O52	-2.16	1.46	1.54
4	D	801	PIO	P5-O52	-2.16	1.46	1.54
4	G	1000	PIO	P5-O52	-2.16	1.46	1.54
4	A	802	PIO	P4-O43	-2.13	1.46	1.54
4	B	801	PIO	P4-O43	-2.13	1.46	1.54
4	D	801	PIO	P4-O43	-2.13	1.46	1.54
4	G	1000	PIO	P4-O43	-2.13	1.46	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	9MF	O11-C09-N08	8.25	120.79	109.25
3	A	803	9MF	O11-C09-N08	8.25	120.79	109.25
3	B	802	9MF	O11-C09-N08	8.25	120.79	109.25
3	D	802	9MF	O11-C09-N08	8.25	120.79	109.25
4	A	802	PIO	C5-C6-C1	4.59	118.49	108.96
4	B	801	PIO	C5-C6-C1	4.59	118.49	108.96
4	D	801	PIO	C5-C6-C1	4.59	118.49	108.96
4	G	1000	PIO	C5-C6-C1	4.59	118.49	108.96
4	A	802	PIO	O2C-C1A-C2A	4.27	120.70	111.50
4	B	801	PIO	O2C-C1A-C2A	4.27	120.70	111.50
4	D	801	PIO	O2C-C1A-C2A	4.27	120.70	111.50
4	G	1000	PIO	O2C-C1A-C2A	4.27	120.70	111.50
4	A	802	PIO	C3-C2-C1	3.85	118.48	109.68
4	B	801	PIO	C3-C2-C1	3.85	118.48	109.68
4	D	801	PIO	C3-C2-C1	3.85	118.48	109.68
4	G	1000	PIO	C3-C2-C1	3.85	118.48	109.68
4	A	802	PIO	C6-C1-C2	3.61	116.06	110.85
4	B	801	PIO	C6-C1-C2	3.61	116.06	110.85
4	D	801	PIO	C6-C1-C2	3.61	116.06	110.85
4	G	1000	PIO	C6-C1-C2	3.61	116.06	110.85
3	A	801	9MF	O11-C09-O10	-3.28	119.75	124.58
3	A	803	9MF	O11-C09-O10	-3.28	119.75	124.58
3	B	802	9MF	O11-C09-O10	-3.28	119.75	124.58
3	D	802	9MF	O11-C09-O10	-3.28	119.75	124.58
3	A	801	9MF	O10-C09-N08	-3.06	119.45	126.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	9MF	O10-C09-N08	-3.06	119.45	126.11
3	B	802	9MF	O10-C09-N08	-3.06	119.45	126.11
3	D	802	9MF	O10-C09-N08	-3.06	119.45	126.11
4	A	802	PIO	O2-C2-C3	-2.85	103.76	110.35
4	B	801	PIO	O2-C2-C3	-2.85	103.76	110.35
4	D	801	PIO	O2-C2-C3	-2.85	103.76	110.35
4	G	1000	PIO	O2-C2-C3	-2.85	103.76	110.35
3	A	801	9MF	C19-C18-N14	-2.78	109.71	114.18
3	A	803	9MF	C19-C18-N14	-2.78	109.71	114.18
3	B	802	9MF	C19-C18-N14	-2.78	109.71	114.18
3	D	802	9MF	C19-C18-N14	-2.78	109.71	114.18
4	A	802	PIO	O3C-C1B-C2B	2.70	120.37	111.91
4	B	801	PIO	O3C-C1B-C2B	2.70	120.37	111.91
4	D	801	PIO	O3C-C1B-C2B	2.70	120.37	111.91
4	G	1000	PIO	O3C-C1B-C2B	2.70	120.37	111.91
4	A	802	PIO	O11-P1-O12	-2.31	100.84	112.24
4	B	801	PIO	O11-P1-O12	-2.31	100.84	112.24
4	D	801	PIO	O11-P1-O12	-2.31	100.84	112.24
4	G	1000	PIO	O11-P1-O12	-2.31	100.84	112.24
4	A	802	PIO	O1-C1-C6	-2.24	103.45	108.66
4	B	801	PIO	O1-C1-C6	-2.24	103.45	108.66
4	D	801	PIO	O1-C1-C6	-2.24	103.45	108.66
4	G	1000	PIO	O1-C1-C6	-2.24	103.45	108.66
4	A	802	PIO	O43-P4-O4	2.14	115.57	105.99
4	B	801	PIO	O43-P4-O4	2.14	115.57	105.99
4	D	801	PIO	O43-P4-O4	2.14	115.57	105.99
4	G	1000	PIO	O43-P4-O4	2.14	115.57	105.99
3	A	801	9MF	C07-N08-C09	-2.09	118.97	123.42
3	A	803	9MF	C07-N08-C09	-2.09	118.97	123.42
3	B	802	9MF	C07-N08-C09	-2.09	118.97	123.42
3	D	802	9MF	C07-N08-C09	-2.09	118.97	123.42
3	A	801	9MF	C12-O11-C09	-2.06	113.23	115.66
3	A	803	9MF	C12-O11-C09	-2.06	113.23	115.66
3	B	802	9MF	C12-O11-C09	-2.06	113.23	115.66
3	D	802	9MF	C12-O11-C09	-2.06	113.23	115.66

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	PIO	C1C-O13-P1-O11
4	A	802	PIO	C1C-O13-P1-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	802	PIO	C4-O4-P4-O42
4	A	802	PIO	C5-O5-P5-O52
4	A	802	PIO	C2A-C1A-O2C-C2C
4	B	801	PIO	C1C-O13-P1-O11
4	B	801	PIO	C1C-O13-P1-O12
4	B	801	PIO	C4-O4-P4-O42
4	B	801	PIO	C5-O5-P5-O52
4	B	801	PIO	C2A-C1A-O2C-C2C
4	D	801	PIO	C1C-O13-P1-O11
4	D	801	PIO	C1C-O13-P1-O12
4	D	801	PIO	C4-O4-P4-O42
4	D	801	PIO	C5-O5-P5-O52
4	D	801	PIO	C2A-C1A-O2C-C2C
4	G	1000	PIO	C1C-O13-P1-O11
4	G	1000	PIO	C1C-O13-P1-O12
4	G	1000	PIO	C4-O4-P4-O42
4	G	1000	PIO	C5-O5-P5-O52
4	G	1000	PIO	C2A-C1A-O2C-C2C
4	A	802	PIO	O1A-C1A-O2C-C2C
4	B	801	PIO	O1A-C1A-O2C-C2C
4	D	801	PIO	O1A-C1A-O2C-C2C
4	G	1000	PIO	O1A-C1A-O2C-C2C
4	A	802	PIO	C1-O1-P1-O13
4	B	801	PIO	C1-O1-P1-O13
4	D	801	PIO	C1-O1-P1-O13
4	G	1000	PIO	C1-O1-P1-O13
4	A	802	PIO	C1B-C2B-C3B-C4B
4	B	801	PIO	C1B-C2B-C3B-C4B
4	D	801	PIO	C1B-C2B-C3B-C4B
4	G	1000	PIO	C1B-C2B-C3B-C4B
4	A	802	PIO	C2B-C3B-C4B-C5B
4	B	801	PIO	C2B-C3B-C4B-C5B
4	D	801	PIO	C2B-C3B-C4B-C5B
4	G	1000	PIO	C2B-C3B-C4B-C5B
4	A	802	PIO	C1C-O13-P1-O1
4	B	801	PIO	C1C-O13-P1-O1
4	D	801	PIO	C1C-O13-P1-O1
4	G	1000	PIO	C1C-O13-P1-O1
4	A	802	PIO	O13-C1C-C2C-C3C
4	B	801	PIO	O13-C1C-C2C-C3C
4	D	801	PIO	O13-C1C-C2C-C3C
4	G	1000	PIO	O13-C1C-C2C-C3C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	802	PIO	C3A-C4A-C5A-C6A
4	B	801	PIO	C3A-C4A-C5A-C6A
4	D	801	PIO	C3A-C4A-C5A-C6A
4	G	1000	PIO	C3A-C4A-C5A-C6A
4	A	802	PIO	C2C-C1C-O13-P1
4	B	801	PIO	C2C-C1C-O13-P1
4	D	801	PIO	C2C-C1C-O13-P1
4	G	1000	PIO	C2C-C1C-O13-P1
4	A	802	PIO	C5-O5-P5-O53
4	B	801	PIO	C5-O5-P5-O53
4	D	801	PIO	C5-O5-P5-O53
4	G	1000	PIO	C5-O5-P5-O53
4	A	802	PIO	O13-C1C-C2C-O2C
4	B	801	PIO	O13-C1C-C2C-O2C
4	D	801	PIO	O13-C1C-C2C-O2C
4	G	1000	PIO	O13-C1C-C2C-O2C
4	A	802	PIO	C5B-C6B-C7B-C8B
4	B	801	PIO	C5B-C6B-C7B-C8B
4	D	801	PIO	C5B-C6B-C7B-C8B
4	G	1000	PIO	C5B-C6B-C7B-C8B
4	A	802	PIO	C3B-C4B-C5B-C6B
4	B	801	PIO	C3B-C4B-C5B-C6B
4	D	801	PIO	C3B-C4B-C5B-C6B
4	G	1000	PIO	C3B-C4B-C5B-C6B
4	A	802	PIO	O1B-C1B-O3C-C3C
4	B	801	PIO	O1B-C1B-O3C-C3C
4	D	801	PIO	O1B-C1B-O3C-C3C
4	G	1000	PIO	O1B-C1B-O3C-C3C
4	A	802	PIO	C2B-C1B-O3C-C3C
4	B	801	PIO	C2B-C1B-O3C-C3C
4	D	801	PIO	C2B-C1B-O3C-C3C
4	G	1000	PIO	C2B-C1B-O3C-C3C
4	A	802	PIO	C4A-C5A-C6A-C7A
4	B	801	PIO	C4A-C5A-C6A-C7A
4	D	801	PIO	C4A-C5A-C6A-C7A
4	G	1000	PIO	C4A-C5A-C6A-C7A
4	A	802	PIO	C1C-C2C-O2C-C1A
4	B	801	PIO	C1C-C2C-O2C-C1A
4	D	801	PIO	C1C-C2C-O2C-C1A
4	G	1000	PIO	C1C-C2C-O2C-C1A
4	A	802	PIO	C3C-C2C-O2C-C1A
4	B	801	PIO	C3C-C2C-O2C-C1A

Continued on next page...

Continued from previous page...

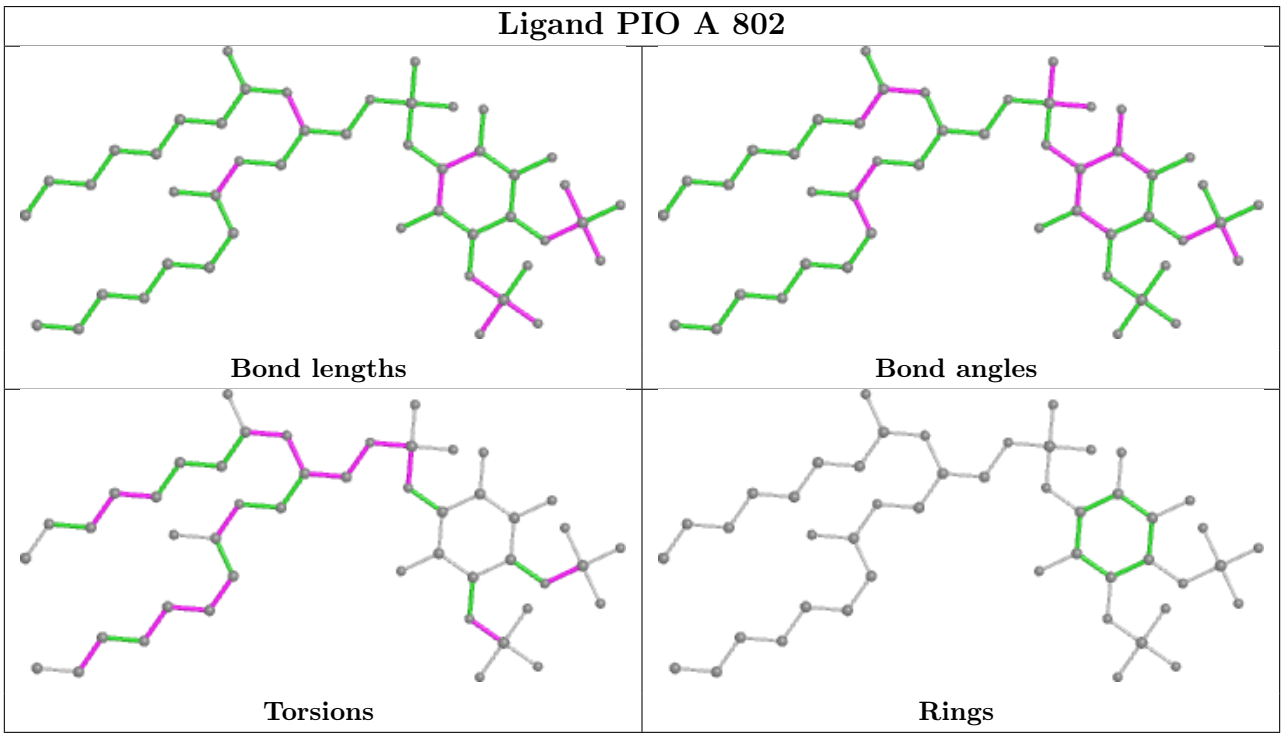
Mol	Chain	Res	Type	Atoms
4	D	801	PIO	C3C-C2C-O2C-C1A
4	G	1000	PIO	C3C-C2C-O2C-C1A

There are no ring outliers.

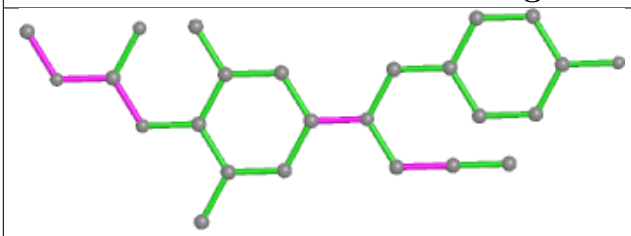
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	PIO	2	0
4	G	1000	PIO	2	0
4	D	801	PIO	2	0
4	B	801	PIO	2	0

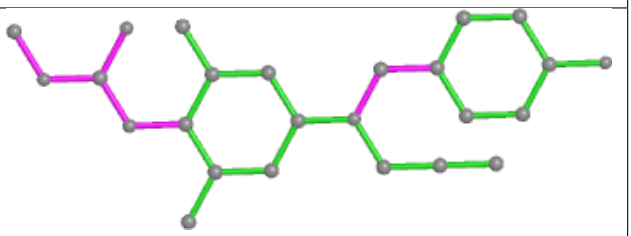
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



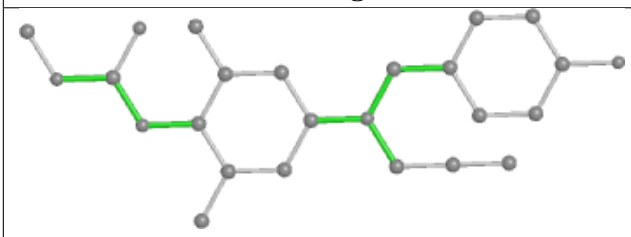
Ligand 9MF A 801



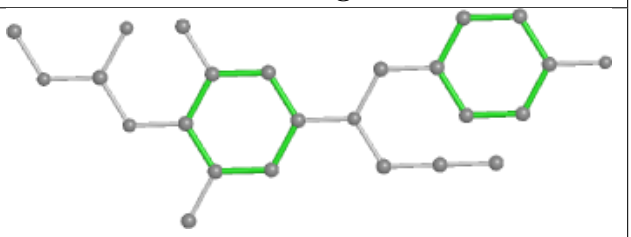
Bond lengths



Bond angles

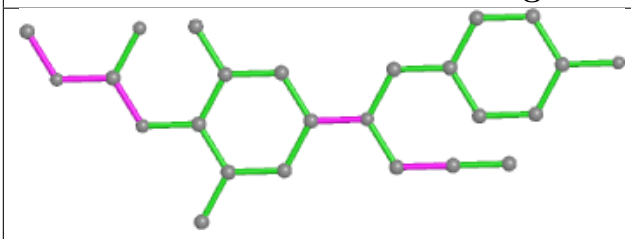


Torsions

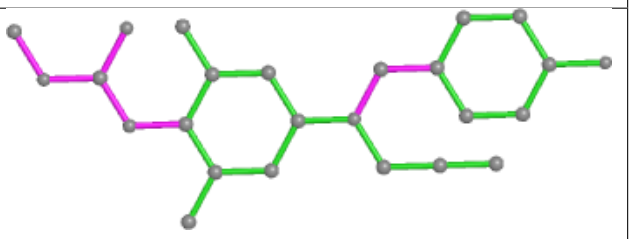


Rings

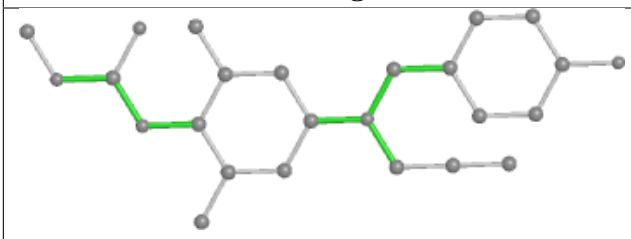
Ligand 9MF D 802



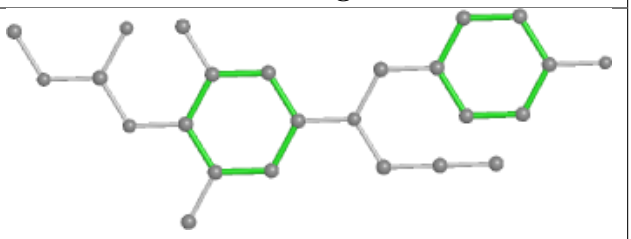
Bond lengths



Bond angles

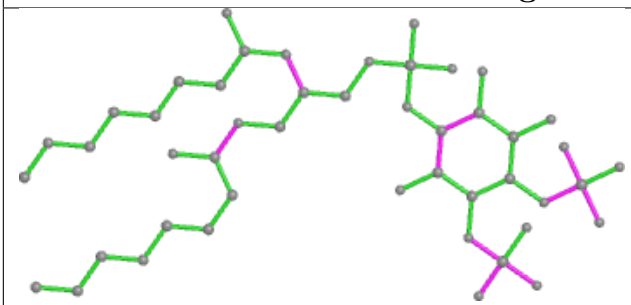


Torsions

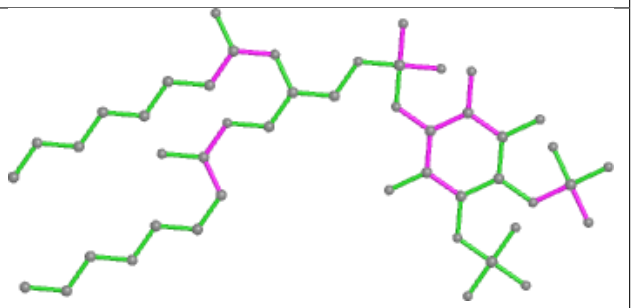


Rings

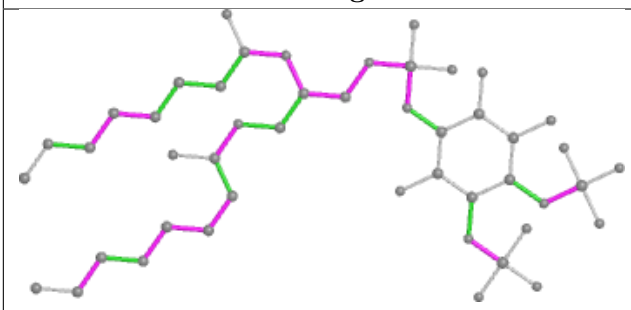
Ligand PIO G 1000



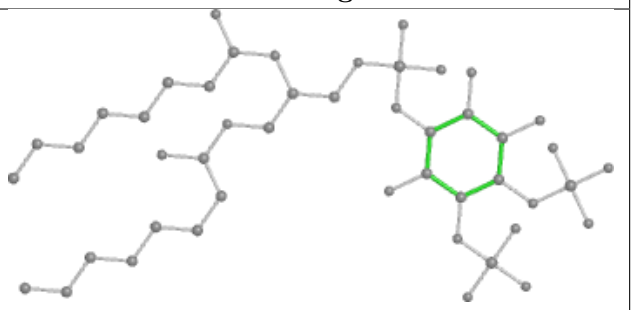
Bond lengths



Bond angles

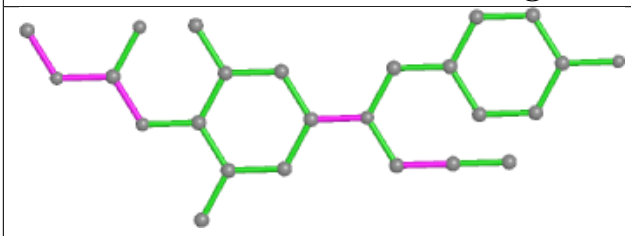


Torsions

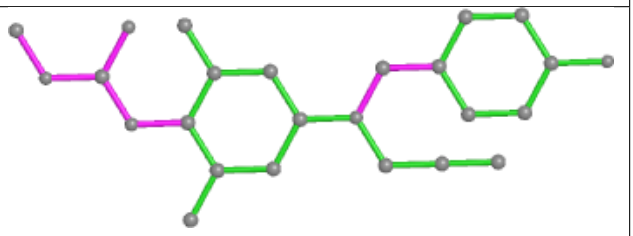


Rings

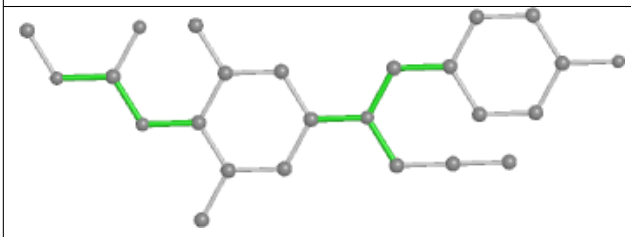
Ligand 9MF A 803



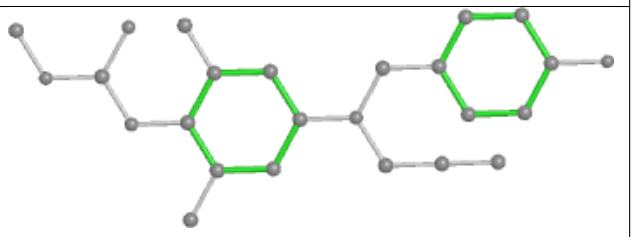
Bond lengths



Bond angles

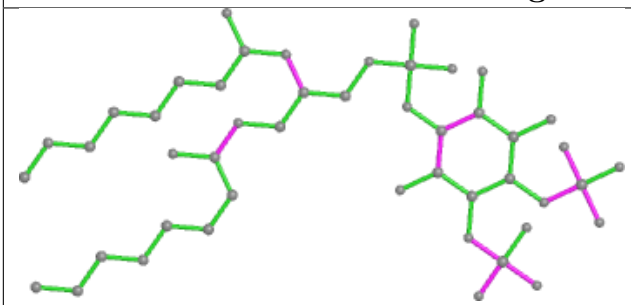


Torsions

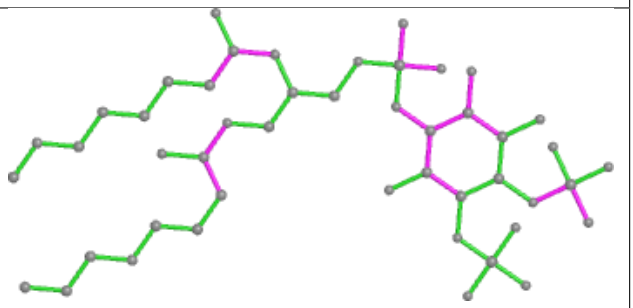


Rings

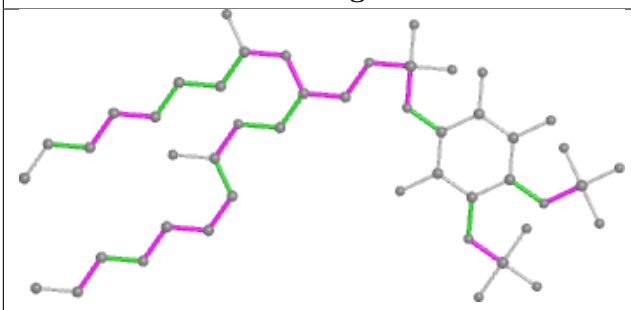
Ligand PIO D 801



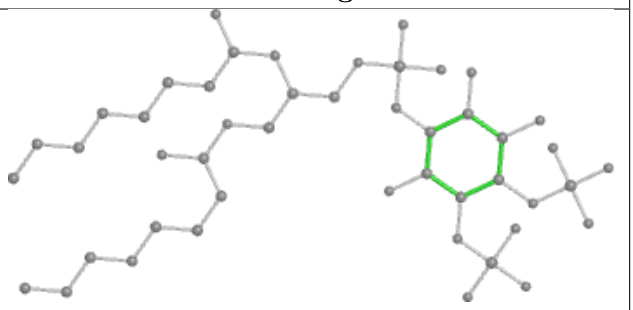
Bond lengths



Bond angles

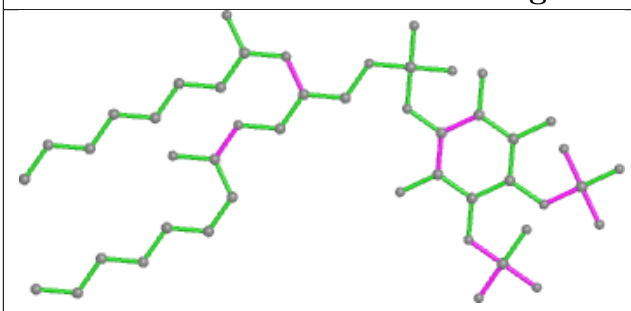


Torsions

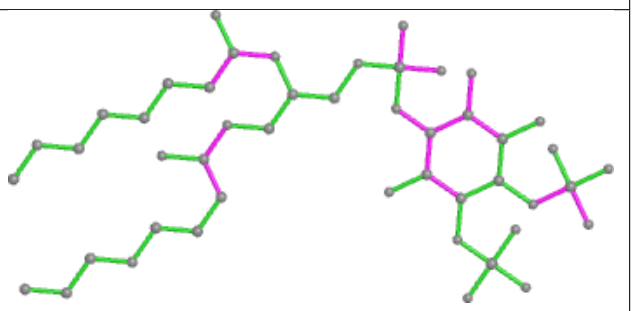


Rings

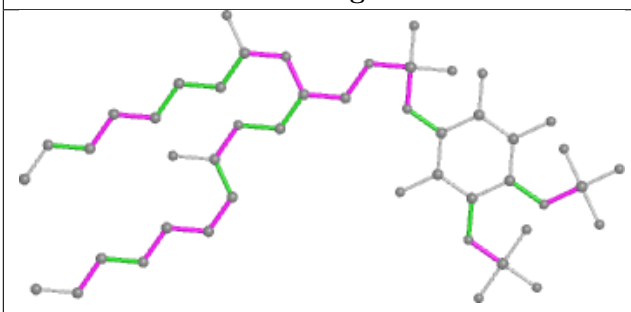
Ligand PIO B 801



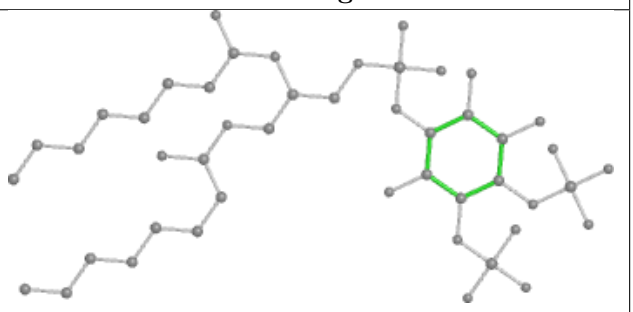
Bond lengths



Bond angles

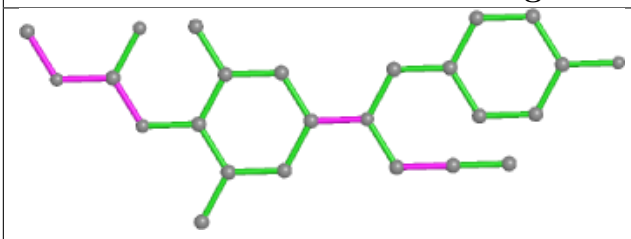


Torsions

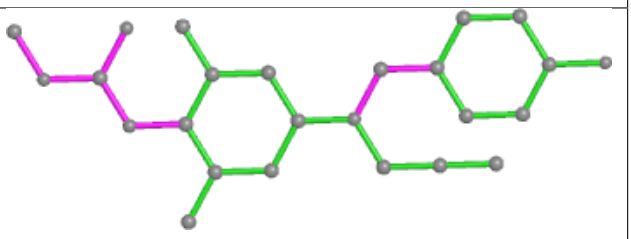


Rings

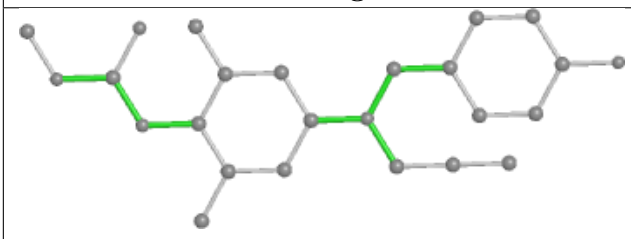
Ligand 9MF B 802



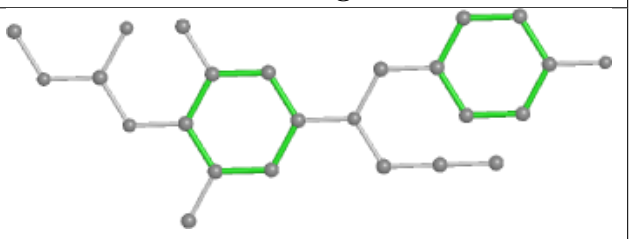
Bond lengths



Bond angles



Torsions



Rings

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.

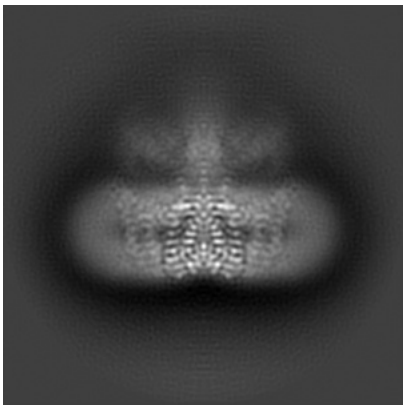
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63130. These allow visual inspection of the internal detail of the map and identification of artifacts.

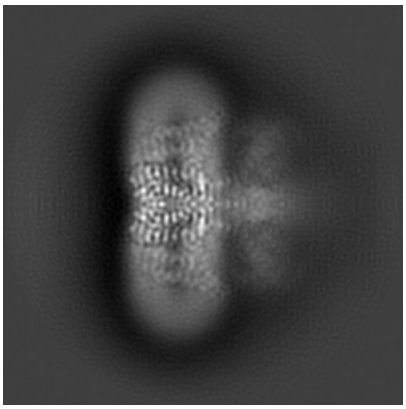
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

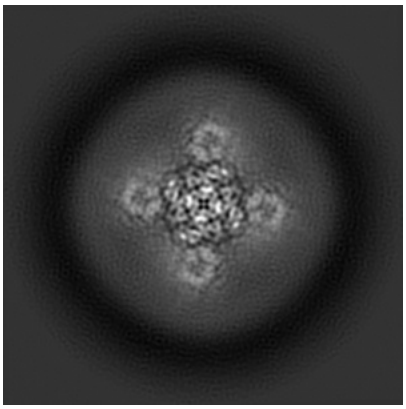
6.1.1 Primary map



X

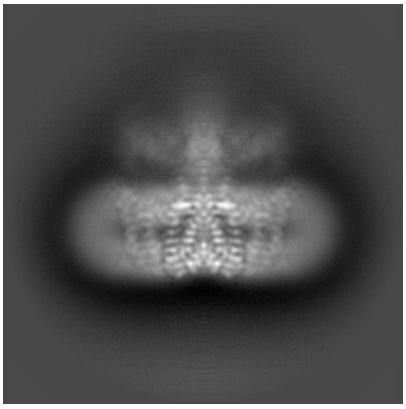


Y

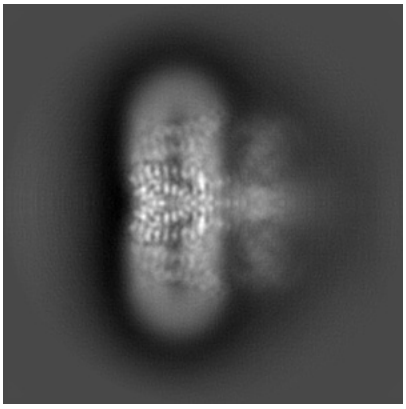


Z

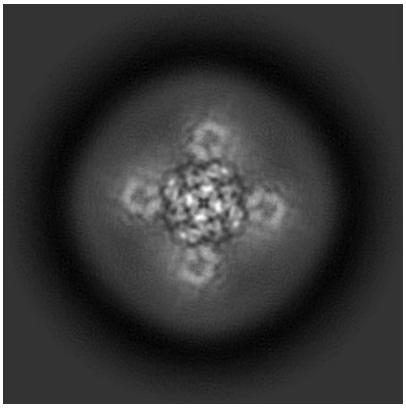
6.1.2 Raw map



X



Y

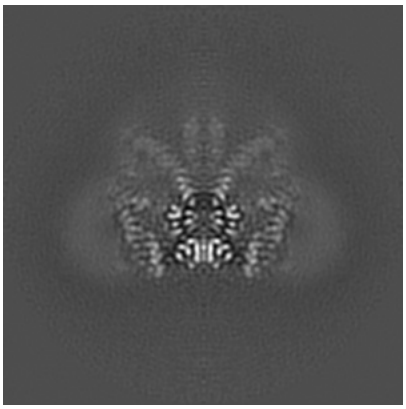


Z

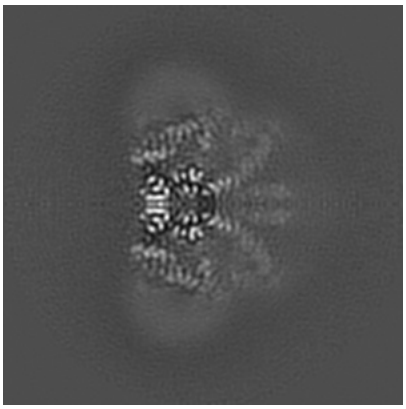
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

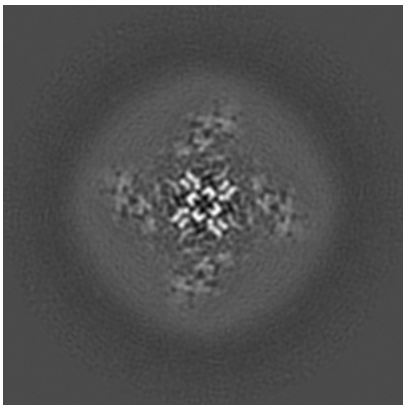
6.2.1 Primary map



X Index: 120

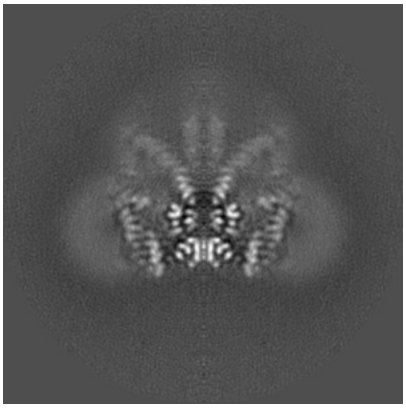


Y Index: 120

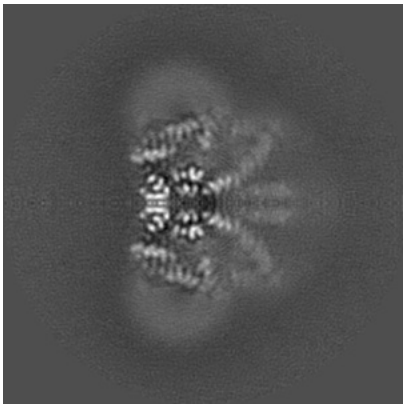


Z Index: 120

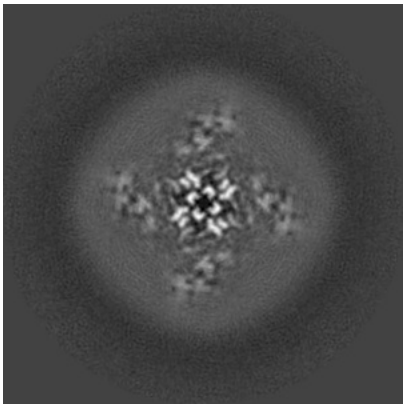
6.2.2 Raw map



X Index: 120



Y Index: 120

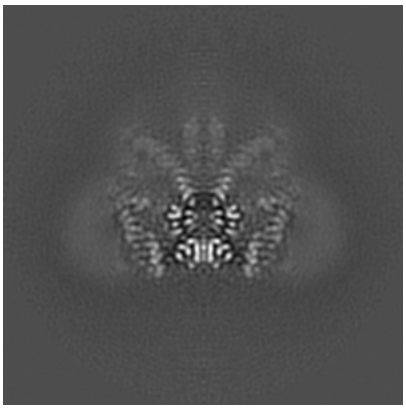


Z Index: 120

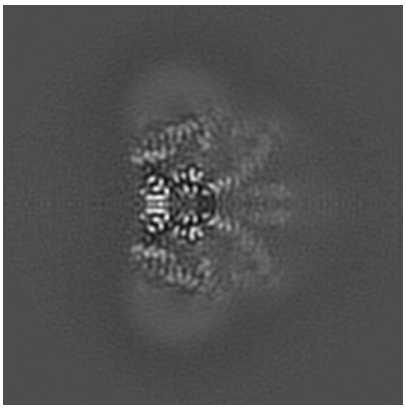
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

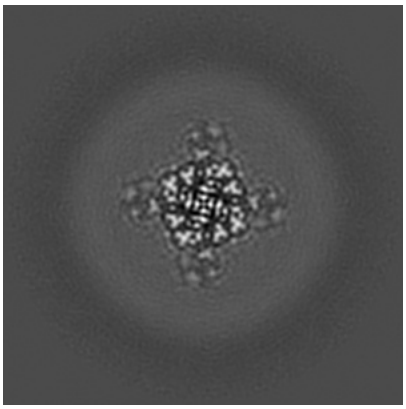
6.3.1 Primary map



X Index: 120

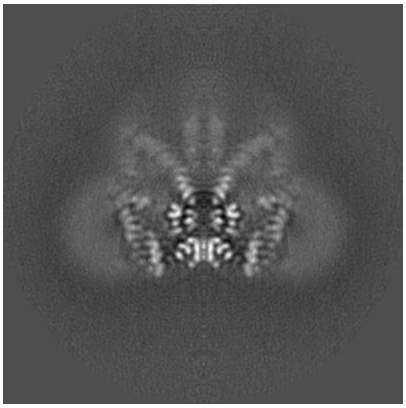


Y Index: 120

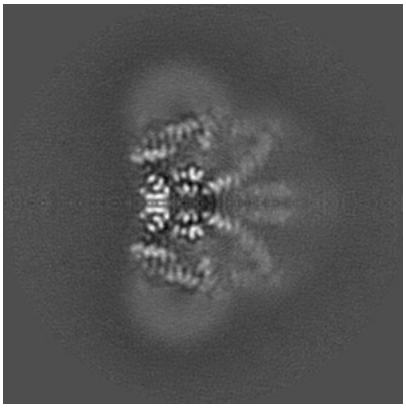


Z Index: 92

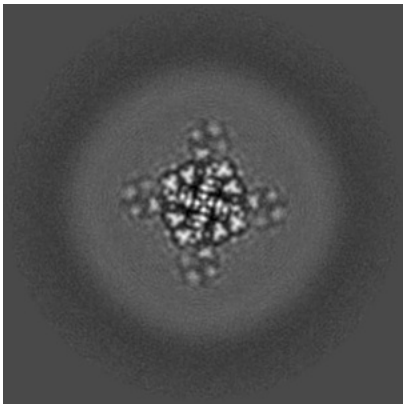
6.3.2 Raw map



X Index: 120



Y Index: 120

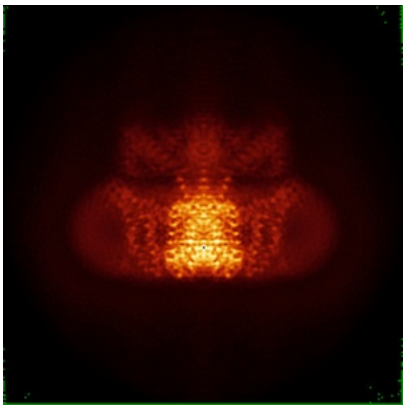


Z Index: 92

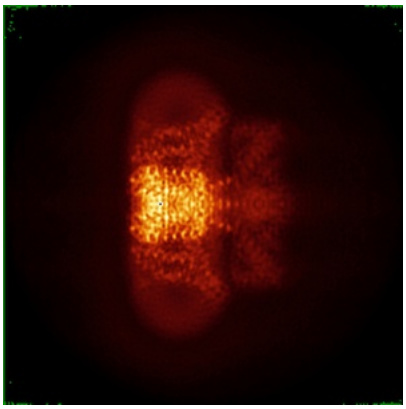
The images above show the largest variance slices of the map in three orthogonal directions.

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

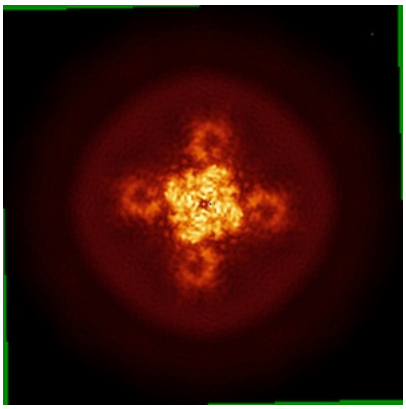
6.4.1 Primary map



X

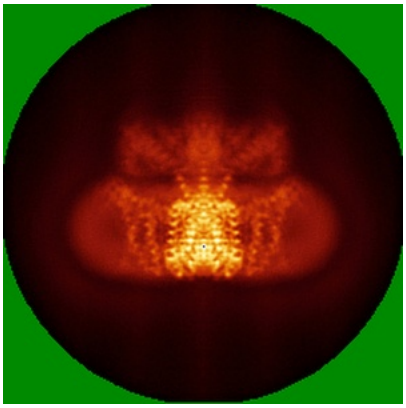


Y

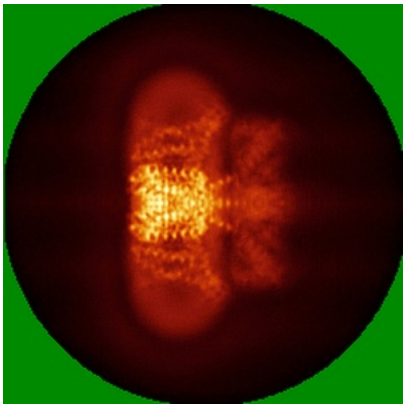


Z

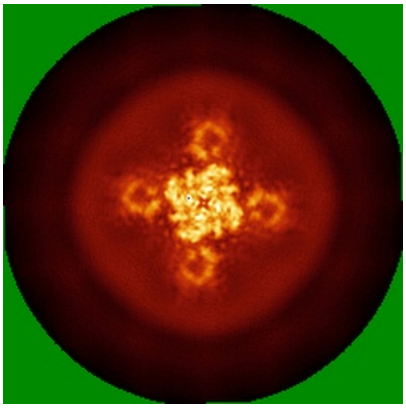
6.4.2 Raw map



X



Y

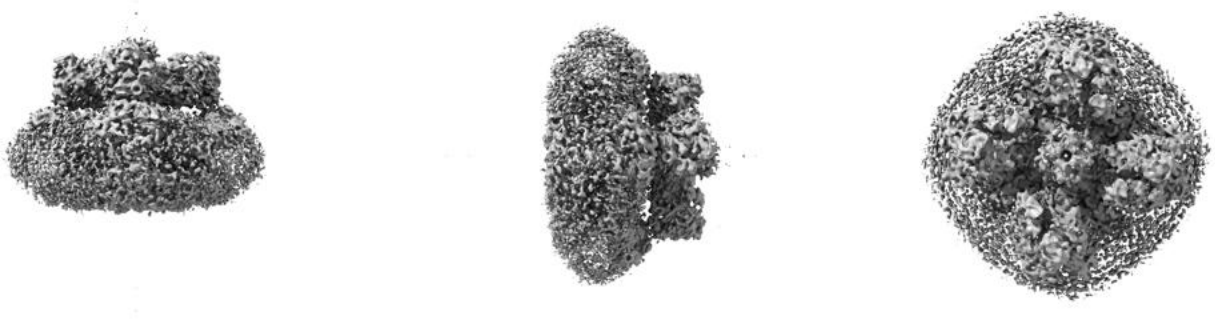


Z

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

6.5 Orthogonal surface views (i)

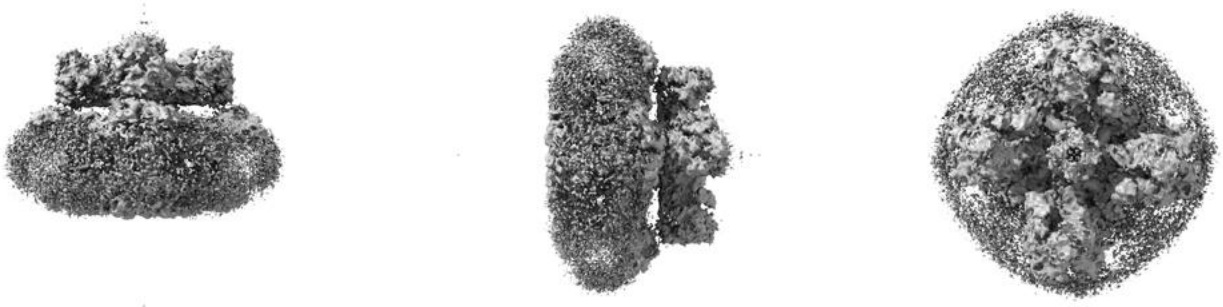
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

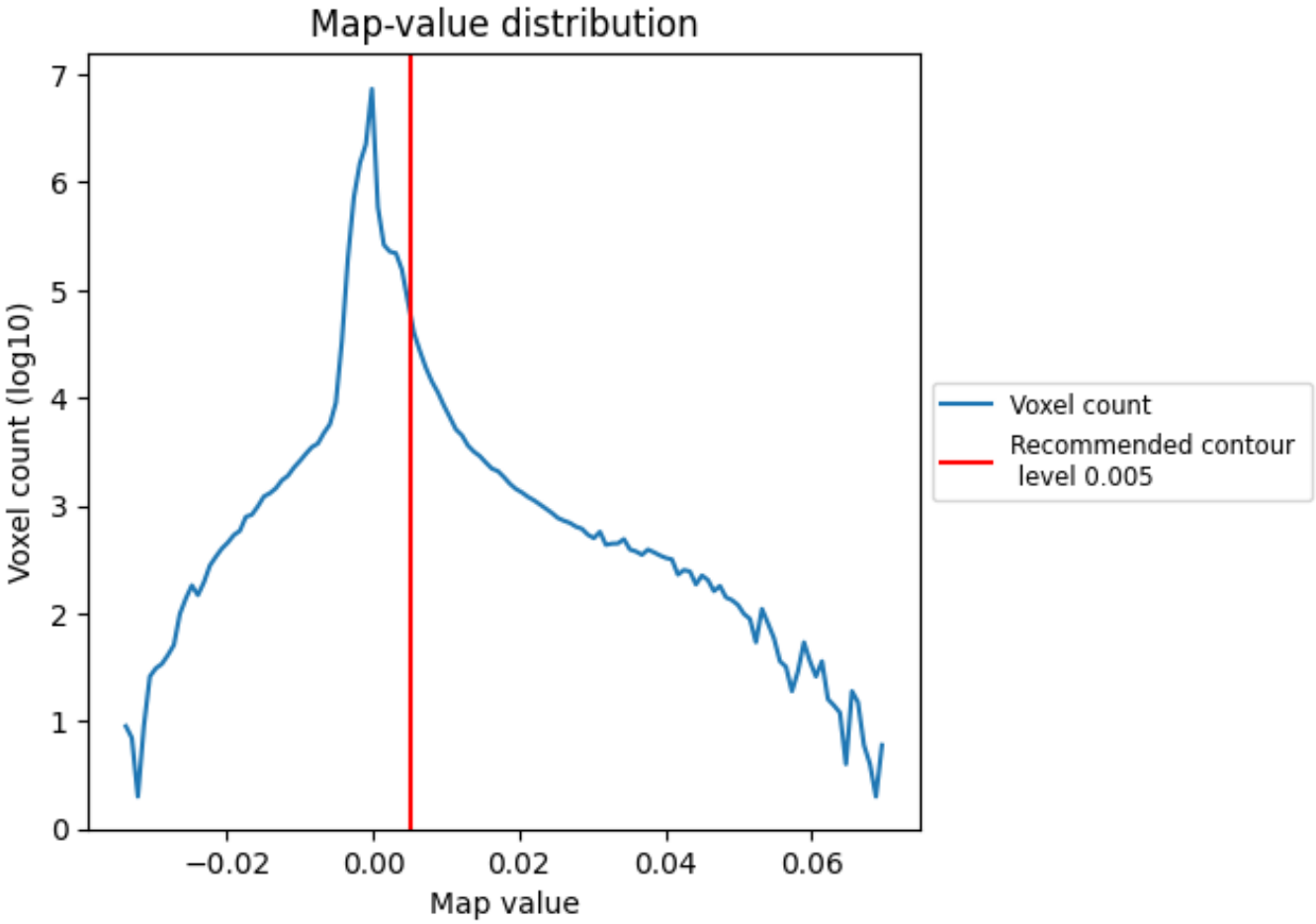
6.6 Mask visualisation (i)

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

7 Map analysis

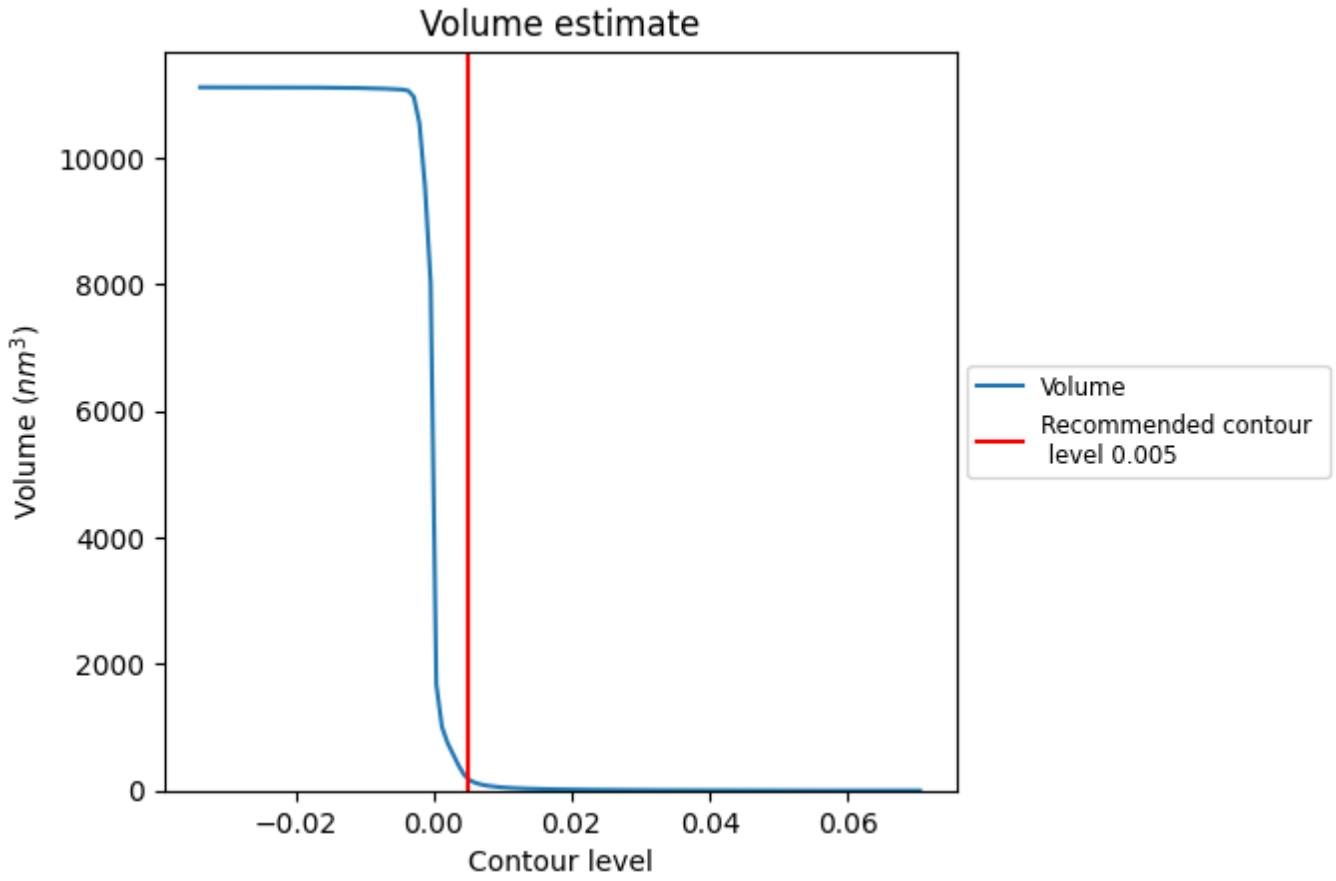
This section contains the results of statistical analysis of the map.

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.

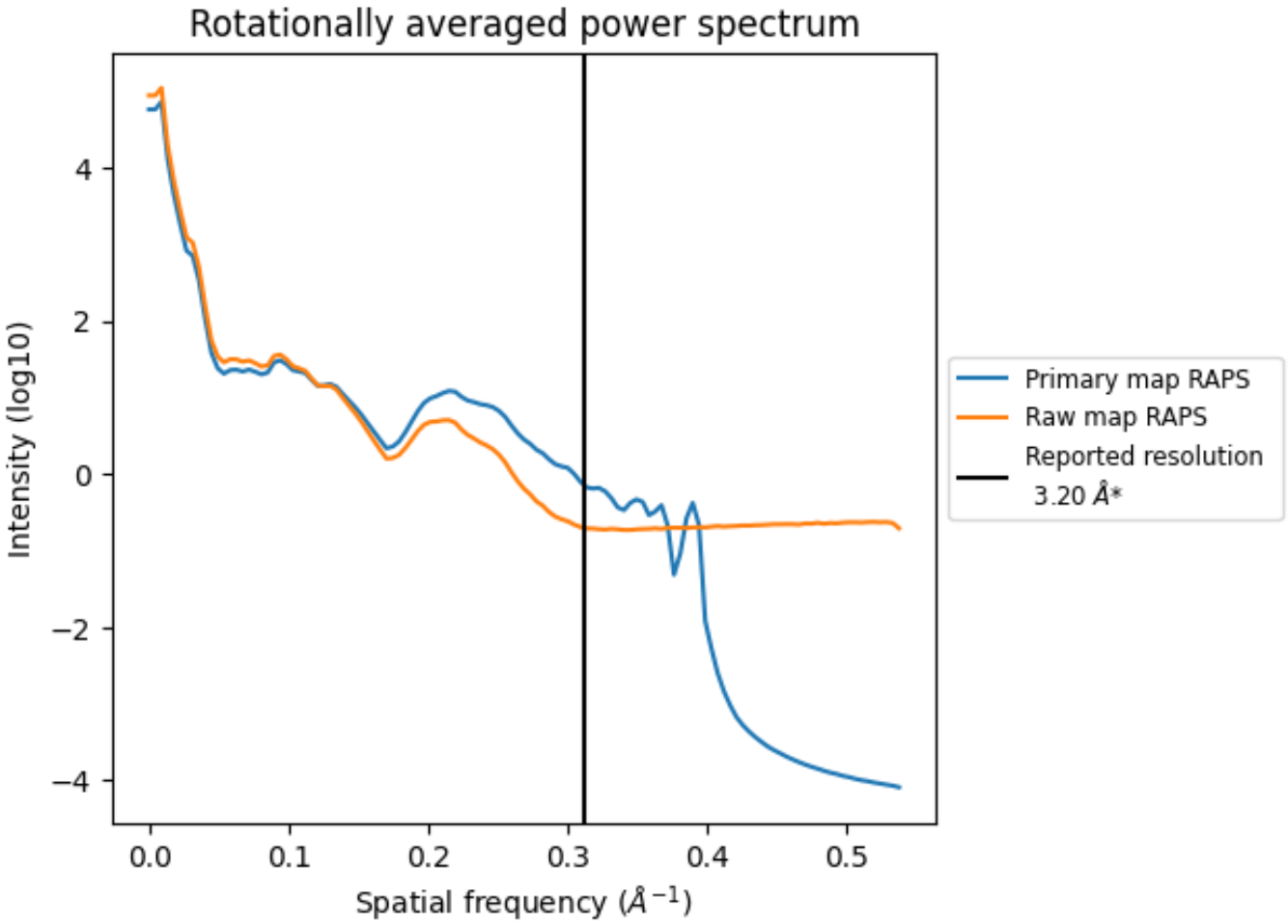
7.2 Volume estimate



The volume at the recommended contour level is 190 nm^3; this corresponds to an approximate mass of 172 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)

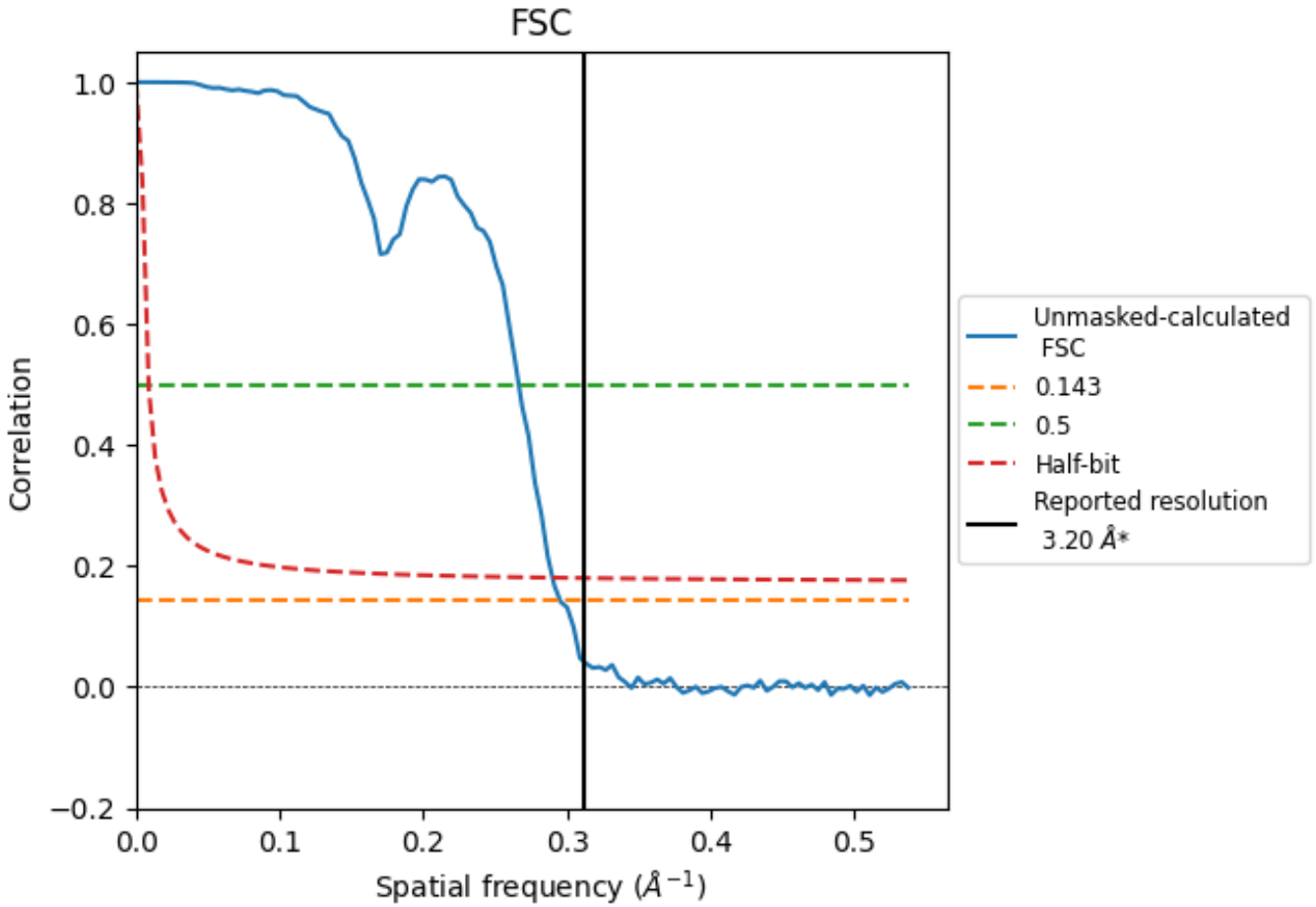


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

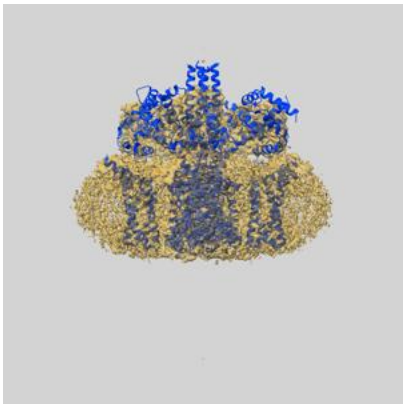
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	3.75	3.45

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

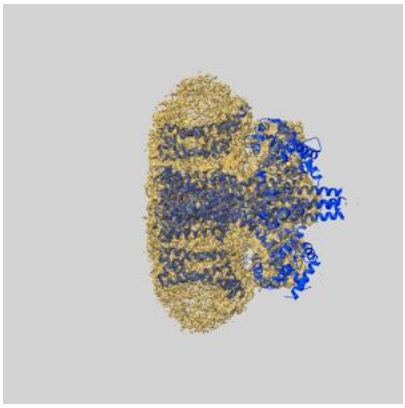
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63130 and PDB model 9LJ1. Per-residue inclusion information can be found in section 3 on page 10.

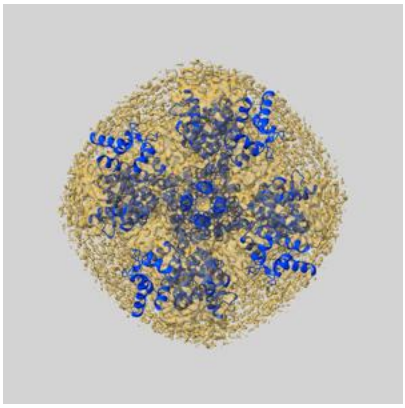
9.1 Map-model overlay



X



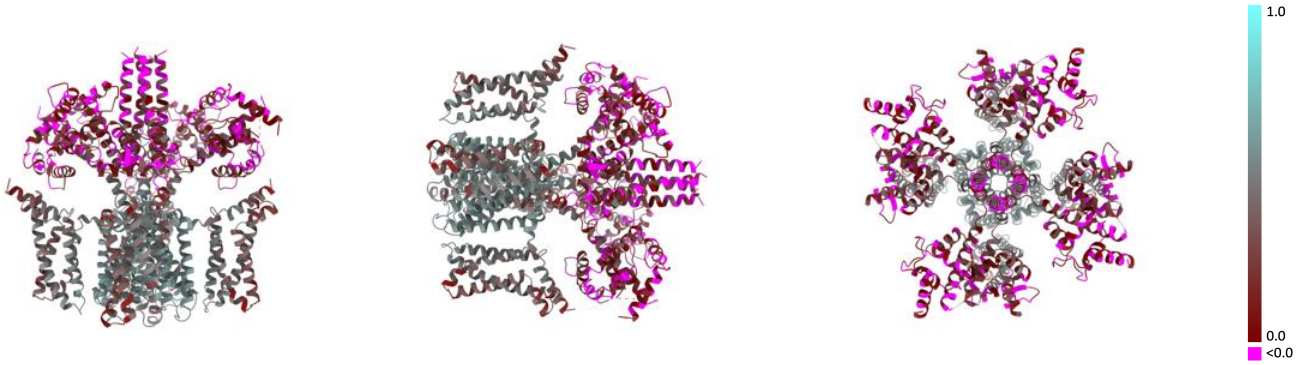
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

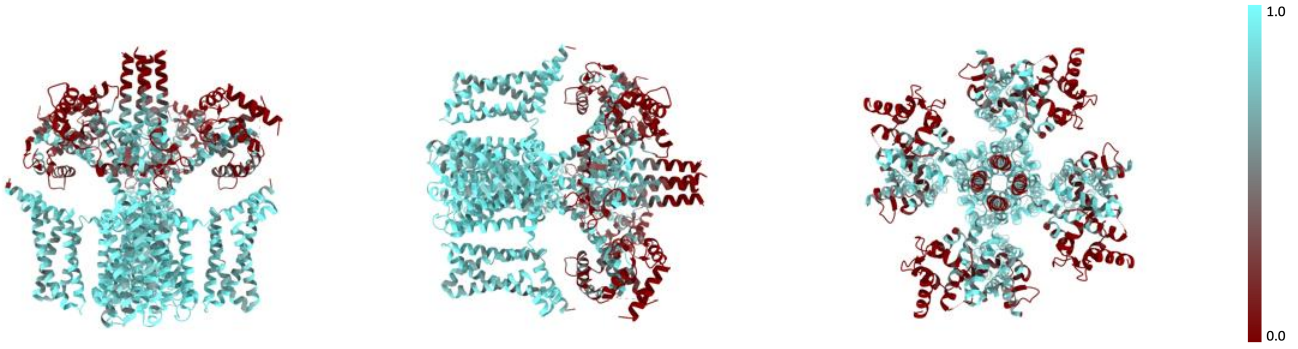
9.2 Q-score mapped to coordinate model (i)



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.

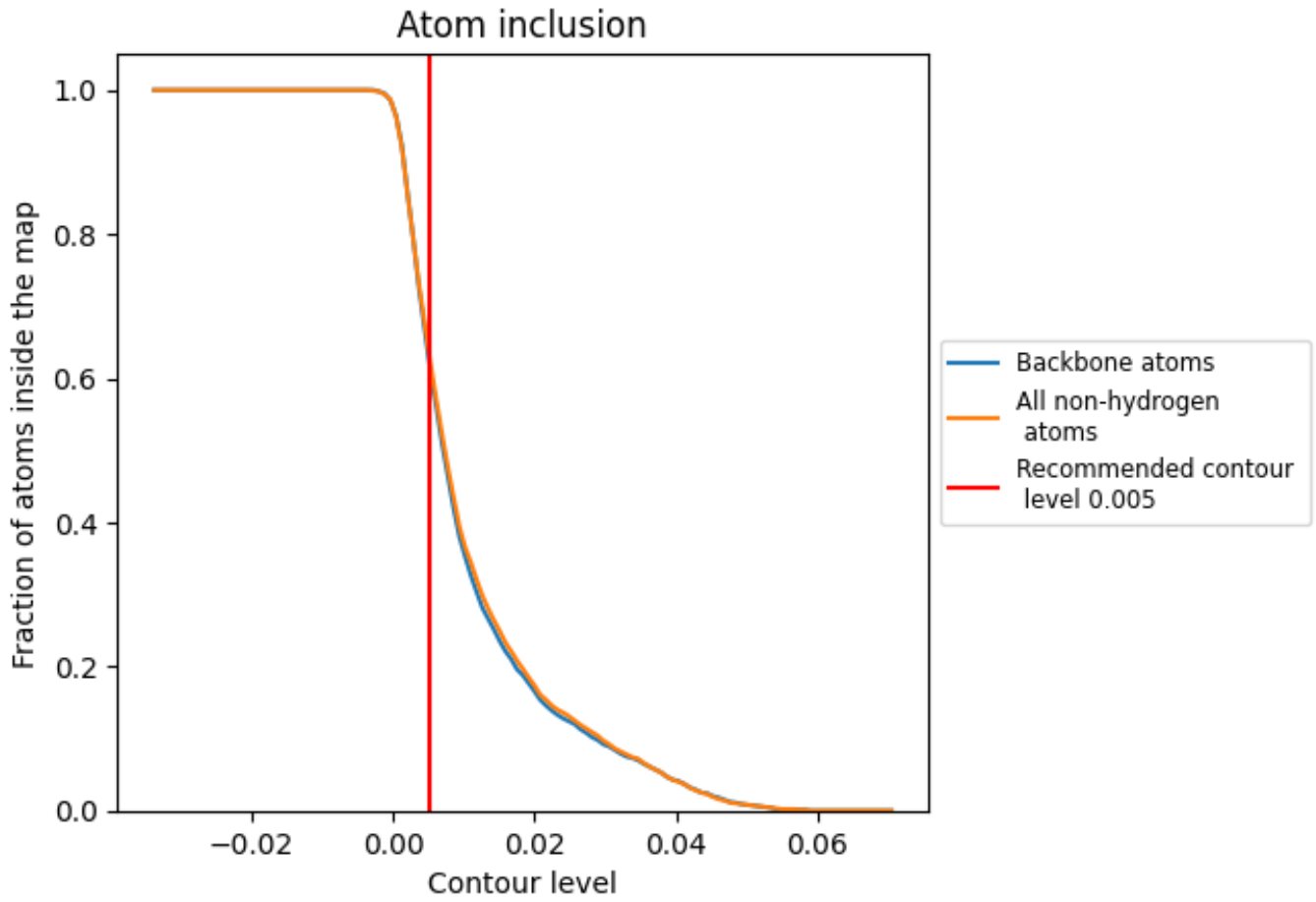
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6390	0.3060
A	0.8170	0.3880
B	0.8160	0.3860
C	0.2290	0.0970
D	0.8160	0.3860
E	0.2280	0.0990
F	0.2290	0.0970
G	0.8150	0.3840
H	0.2290	0.0970