Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 11:25 AM EST

PDB ID	:	6UIW
EMDB ID	:	EMD-20789
Title	:	Cryo-EM structure of human CALHM2 in a ruthenium red-bound inhibited state
Authors	:	Lu, W.; Du, J.; Choi, W.
Deposited on	:	2019-10-01
Resolution	:	2.70 Å(reported)

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

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

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

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

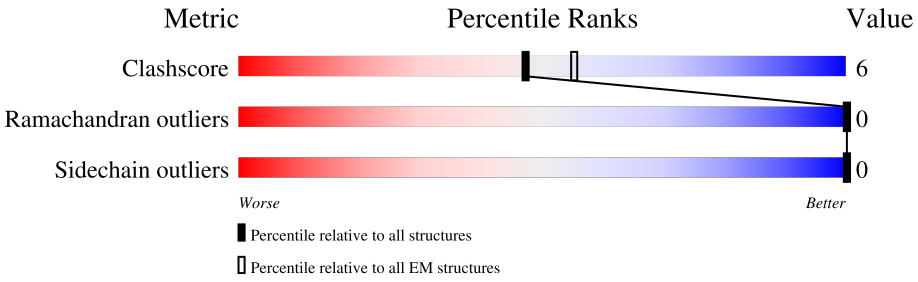
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	331	7% 77% 12% 11%
1	B	331	6% 76% 13% 11%
1	C	331	6% 77% 11% 11%
1	D	331	7% 78% 11% 11%
1	E	331	7% 77% 11% 11%
1	F	331	7% 77% 12% 11%
1	G	331	6% 77% 12% 11%
1	H	331	7% 77% 11% 11%

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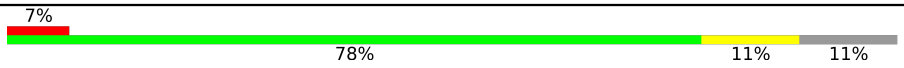
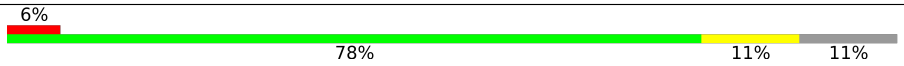
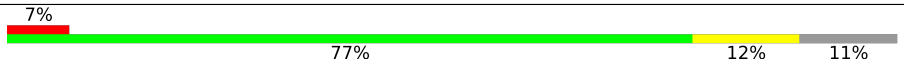
Mol	Chain	Length	Quality of chain
1	I	331	
1	J	331	
1	K	331	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23617 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 Calcium homeostasis modulator protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	B	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	C	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	D	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	E	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	F	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	G	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	H	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	I	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	J	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		
1	K	294	Total	C	N	O	S	0	0
			2128	1381	388	352	7		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	PHE	-	expression tag	UNP Q9HA72
A	325	GLU	-	expression tag	UNP Q9HA72
A	326	SER	-	expression tag	UNP Q9HA72
A	327	ARG	-	expression tag	UNP Q9HA72
A	328	LEU	-	expression tag	UNP Q9HA72
A	329	VAL	-	expression tag	UNP Q9HA72
A	330	PRO	-	expression tag	UNP Q9HA72
A	331	ARG	-	expression tag	UNP Q9HA72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	324	PHE	-	expression tag	UNP Q9HA72
B	325	GLU	-	expression tag	UNP Q9HA72
B	326	SER	-	expression tag	UNP Q9HA72
B	327	ARG	-	expression tag	UNP Q9HA72
B	328	LEU	-	expression tag	UNP Q9HA72
B	329	VAL	-	expression tag	UNP Q9HA72
B	330	PRO	-	expression tag	UNP Q9HA72
B	331	ARG	-	expression tag	UNP Q9HA72
C	324	PHE	-	expression tag	UNP Q9HA72
C	325	GLU	-	expression tag	UNP Q9HA72
C	326	SER	-	expression tag	UNP Q9HA72
C	327	ARG	-	expression tag	UNP Q9HA72
C	328	LEU	-	expression tag	UNP Q9HA72
C	329	VAL	-	expression tag	UNP Q9HA72
C	330	PRO	-	expression tag	UNP Q9HA72
C	331	ARG	-	expression tag	UNP Q9HA72
D	324	PHE	-	expression tag	UNP Q9HA72
D	325	GLU	-	expression tag	UNP Q9HA72
D	326	SER	-	expression tag	UNP Q9HA72
D	327	ARG	-	expression tag	UNP Q9HA72
D	328	LEU	-	expression tag	UNP Q9HA72
D	329	VAL	-	expression tag	UNP Q9HA72
D	330	PRO	-	expression tag	UNP Q9HA72
D	331	ARG	-	expression tag	UNP Q9HA72
E	324	PHE	-	expression tag	UNP Q9HA72
E	325	GLU	-	expression tag	UNP Q9HA72
E	326	SER	-	expression tag	UNP Q9HA72
E	327	ARG	-	expression tag	UNP Q9HA72
E	328	LEU	-	expression tag	UNP Q9HA72
E	329	VAL	-	expression tag	UNP Q9HA72
E	330	PRO	-	expression tag	UNP Q9HA72
E	331	ARG	-	expression tag	UNP Q9HA72
F	324	PHE	-	expression tag	UNP Q9HA72
F	325	GLU	-	expression tag	UNP Q9HA72
F	326	SER	-	expression tag	UNP Q9HA72
F	327	ARG	-	expression tag	UNP Q9HA72
F	328	LEU	-	expression tag	UNP Q9HA72
F	329	VAL	-	expression tag	UNP Q9HA72
F	330	PRO	-	expression tag	UNP Q9HA72
F	331	ARG	-	expression tag	UNP Q9HA72
G	324	PHE	-	expression tag	UNP Q9HA72
G	325	GLU	-	expression tag	UNP Q9HA72

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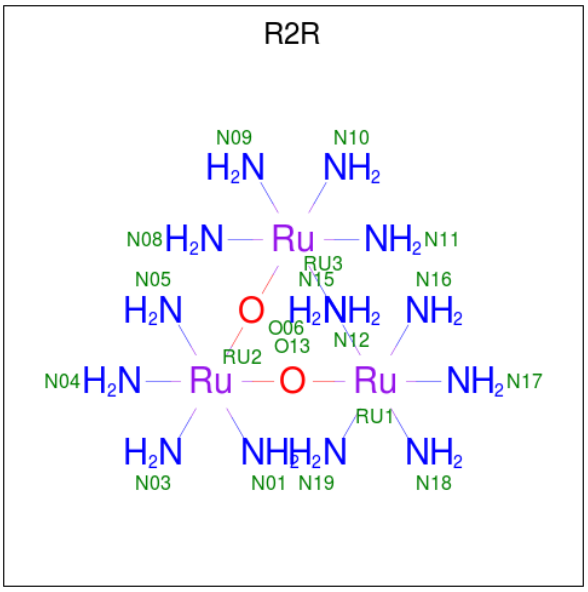
Chain	Residue	Modelled	Actual	Comment	Reference
G	326	SER	-	expression tag	UNP Q9HA72
G	327	ARG	-	expression tag	UNP Q9HA72
G	328	LEU	-	expression tag	UNP Q9HA72
G	329	VAL	-	expression tag	UNP Q9HA72
G	330	PRO	-	expression tag	UNP Q9HA72
G	331	ARG	-	expression tag	UNP Q9HA72
H	324	PHE	-	expression tag	UNP Q9HA72
H	325	GLU	-	expression tag	UNP Q9HA72
H	326	SER	-	expression tag	UNP Q9HA72
H	327	ARG	-	expression tag	UNP Q9HA72
H	328	LEU	-	expression tag	UNP Q9HA72
H	329	VAL	-	expression tag	UNP Q9HA72
H	330	PRO	-	expression tag	UNP Q9HA72
H	331	ARG	-	expression tag	UNP Q9HA72
I	324	PHE	-	expression tag	UNP Q9HA72
I	325	GLU	-	expression tag	UNP Q9HA72
I	326	SER	-	expression tag	UNP Q9HA72
I	327	ARG	-	expression tag	UNP Q9HA72
I	328	LEU	-	expression tag	UNP Q9HA72
I	329	VAL	-	expression tag	UNP Q9HA72
I	330	PRO	-	expression tag	UNP Q9HA72
I	331	ARG	-	expression tag	UNP Q9HA72
J	324	PHE	-	expression tag	UNP Q9HA72
J	325	GLU	-	expression tag	UNP Q9HA72
J	326	SER	-	expression tag	UNP Q9HA72
J	327	ARG	-	expression tag	UNP Q9HA72
J	328	LEU	-	expression tag	UNP Q9HA72
J	329	VAL	-	expression tag	UNP Q9HA72
J	330	PRO	-	expression tag	UNP Q9HA72
J	331	ARG	-	expression tag	UNP Q9HA72
K	324	PHE	-	expression tag	UNP Q9HA72
K	325	GLU	-	expression tag	UNP Q9HA72
K	326	SER	-	expression tag	UNP Q9HA72
K	327	ARG	-	expression tag	UNP Q9HA72
K	328	LEU	-	expression tag	UNP Q9HA72
K	329	VAL	-	expression tag	UNP Q9HA72
K	330	PRO	-	expression tag	UNP Q9HA72
K	331	ARG	-	expression tag	UNP Q9HA72

- Molecule 2 is ruthenium(6+) azanide pentaamino(oxido)ruthenium (1/4/2) (three-letter code: R2R) (formula: $H_{28}N_{14}O_2Ru_3$) (labeled as "Ligand of Interest" by depositor).



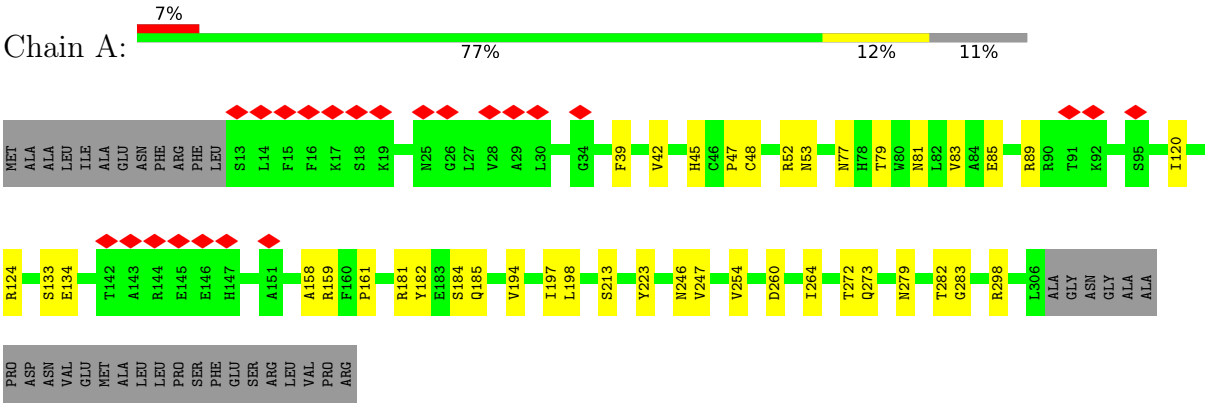
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	N	O	Ru	0
			19	14	2	3	
2	B	1	Total	N	O	Ru	0
			19	14	2	3	
2	C	1	Total	N	O	Ru	0
			19	14	2	3	
2	D	1	Total	N	O	Ru	0
			19	14	2	3	
2	E	1	Total	N	O	Ru	0
			19	14	2	3	
2	F	1	Total	N	O	Ru	0
			19	14	2	3	
2	G	1	Total	N	O	Ru	0
			19	14	2	3	
2	H	1	Total	N	O	Ru	0
			19	14	2	3	
2	I	1	Total	N	O	Ru	0
			19	14	2	3	
2	J	1	Total	N	O	Ru	0
			19	14	2	3	
2	K	1	Total	N	O	Ru	0
			19	14	2	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.

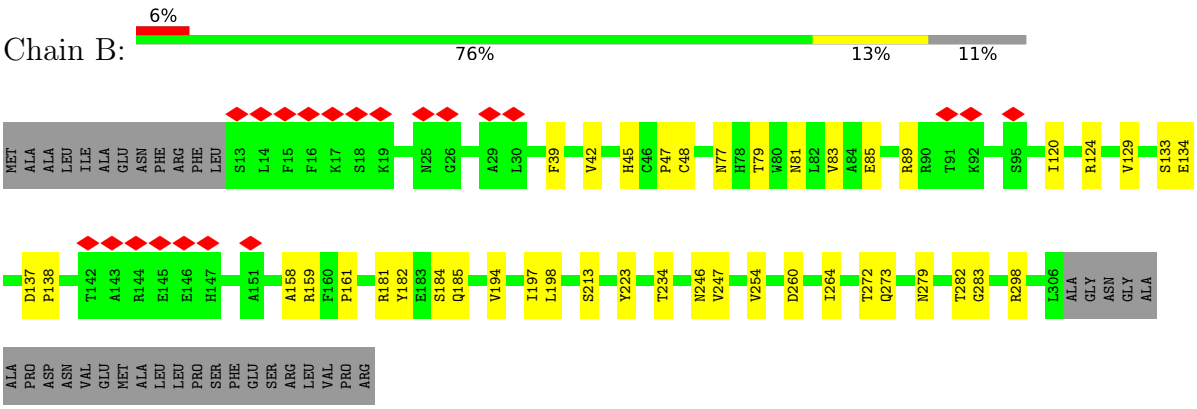
• Molecule 1: Calcium homeostasis modulator protein 2

Chain A:



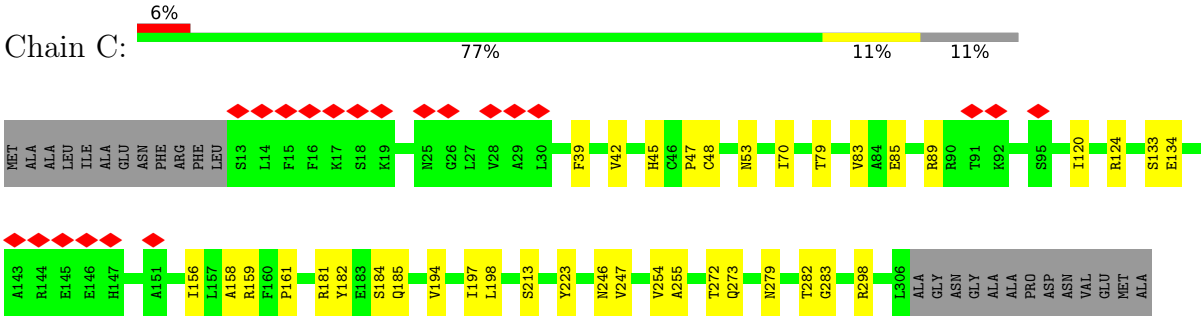
• Molecule 1: Calcium homeostasis modulator protein 2

Chain B:

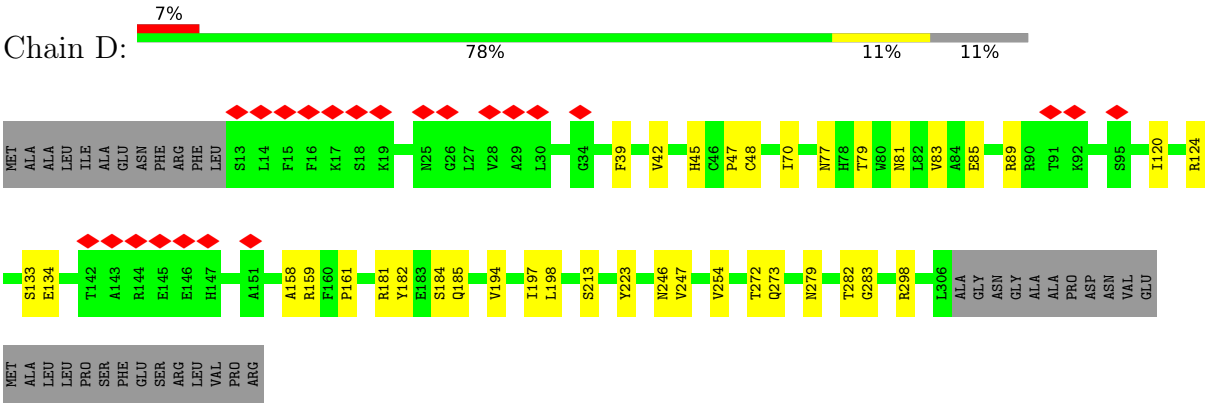


• Molecule 1: Calcium homeostasis modulator protein 2

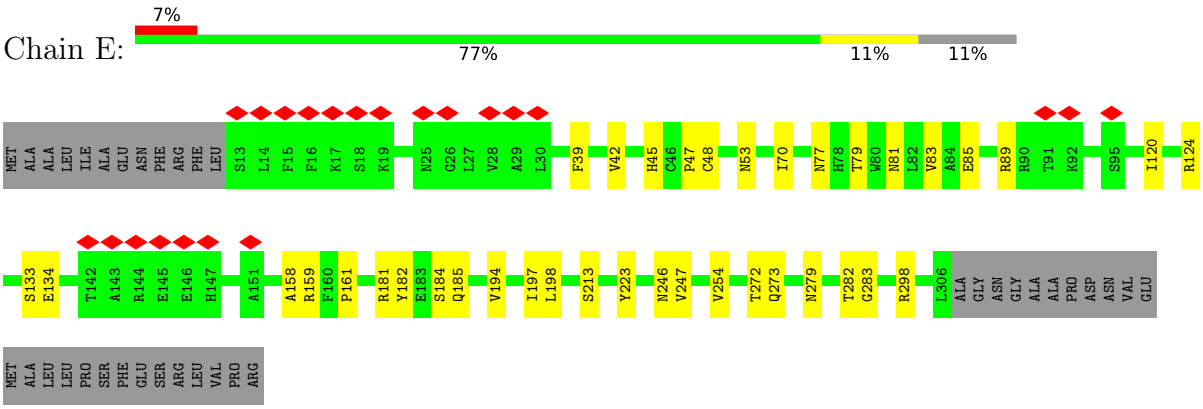
Chain C:



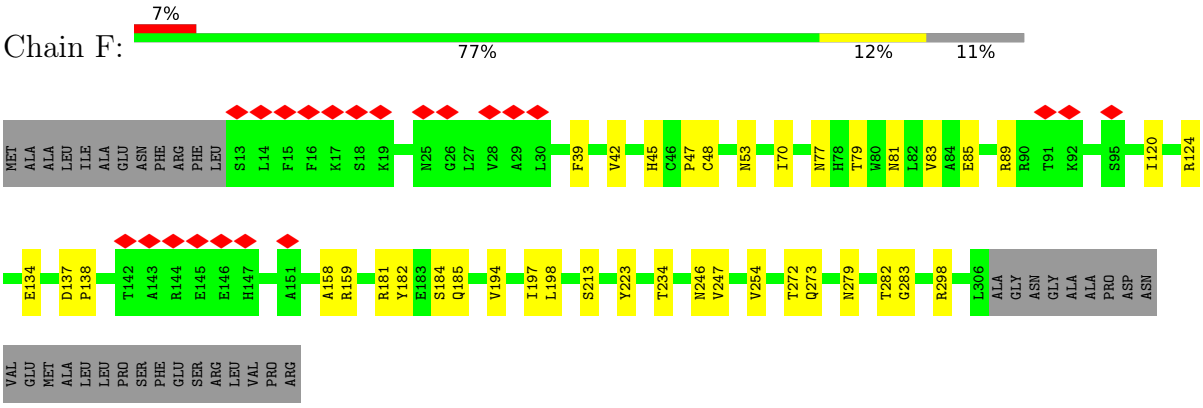
• Molecule 1: Calcium homeostasis modulator protein 2



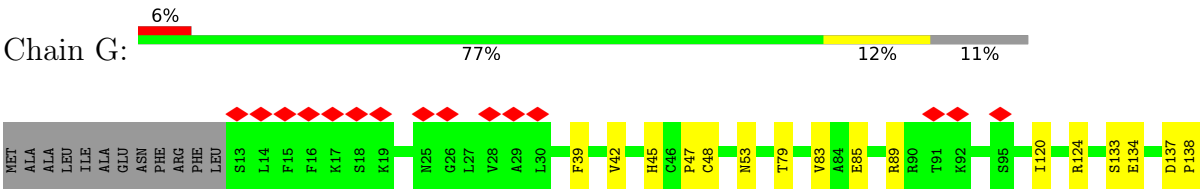
• Molecule 1: Calcium homeostasis modulator protein 2

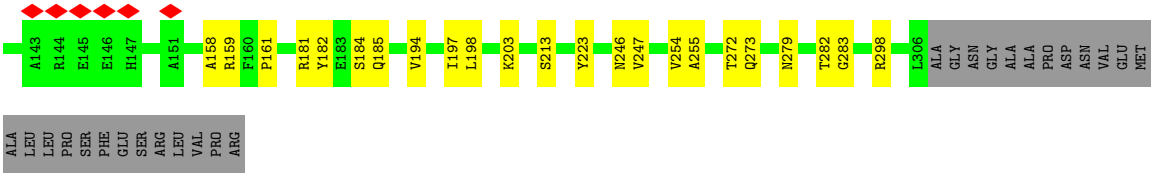


• Molecule 1: Calcium homeostasis modulator protein 2



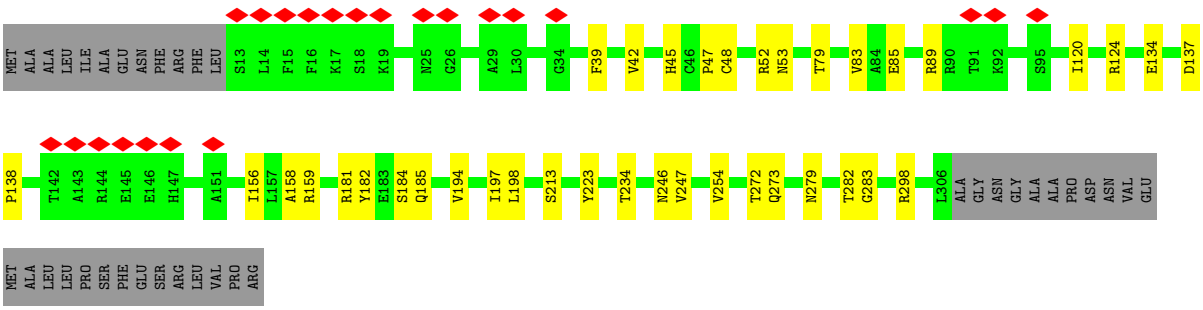
• Molecule 1: Calcium homeostasis modulator protein 2





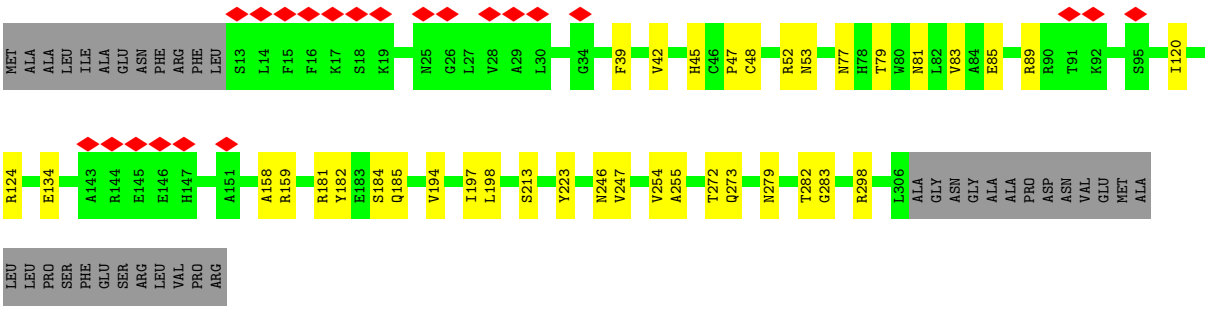
• Molecule 1: Calcium homeostasis modulator protein 2

Chain H:



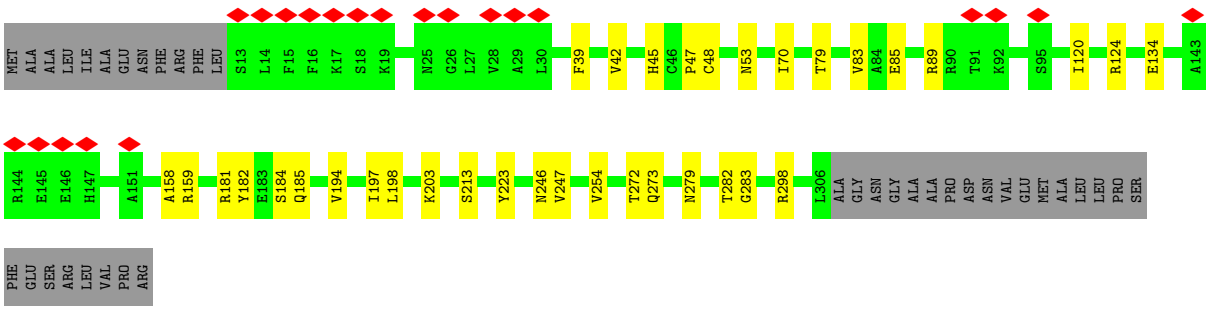
• Molecule 1: Calcium homeostasis modulator protein 2

Chain I:



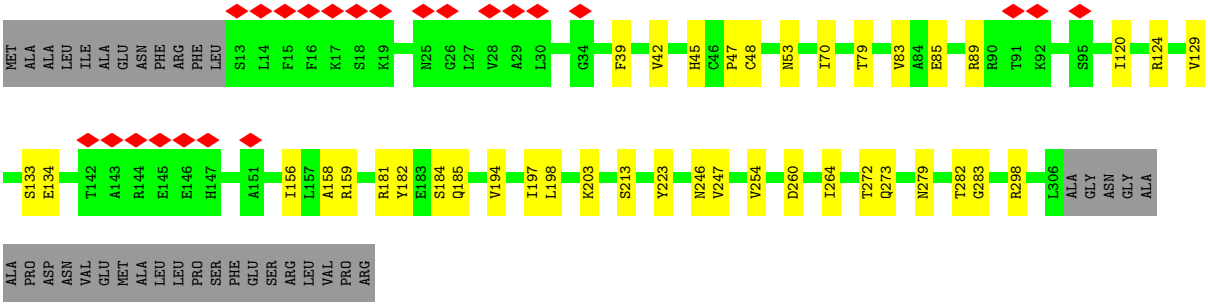
• Molecule 1: Calcium homeostasis modulator protein 2

Chain J:



• Molecule 1: Calcium homeostasis modulator protein 2

Chain K:


MET ALA ALA LEU ILE ALA GLU ASN PHE ARG PHE LEU
S13 L14 F15 F16 K17 S18 K19
N25 G26 L27 V28 A29 L30
G34
F39 V42 H45 C46 P47 C48 N53 I70 T79 V83 A84 E85 R89 R90 T91 K92 S95 I120 R124 V129
S133 E134
T142 A143 R144 E145 E146 H147
A151
I156 L157 A158 R159 R181 Y182 E183 S184 Q185 V194 I197 L198 K203 S213 Y223 N246 V247 V254 D260 I264 T272 Q273 N279 T282 G283 R298 L306
ALA GLY ASN GLY ALA
ALA PRO ASP ASN VAL GLU MET ALA LEU LEU PRO SER PHE GLU SER ARG LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	83728	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 ($e^-/Å^2$)	54.4	Depositor
Minimum defocus (nm)	1000.0	Depositor
Maximum defocus (nm)	2500.0	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	348.84, 348.84, 348.84	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.026, 1.026, 1.026	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R2R

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	0.49	0/2185	0.53	0/2999
1	B	0.49	0/2185	0.53	0/2999
1	C	0.49	0/2185	0.53	0/2999
1	D	0.49	0/2185	0.53	0/2999
1	E	0.49	0/2185	0.53	0/2999
1	F	0.49	0/2185	0.53	0/2999
1	G	0.49	0/2185	0.53	0/2999
1	H	0.49	0/2185	0.53	0/2999
1	I	0.49	0/2185	0.53	0/2999
1	J	0.49	0/2185	0.53	0/2999
1	K	0.49	0/2185	0.53	0/2999
All	All	0.49	0/24035	0.53	0/32989

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2128	0	1939	31	0
1	B	2128	0	1939	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2128	0	1939	30	0
1	D	2128	0	1939	28	0
1	E	2128	0	1939	29	0
1	F	2128	0	1939	31	0
1	G	2128	0	1939	31	0
1	H	2128	0	1939	32	0
1	I	2128	0	1939	31	0
1	J	2128	0	1939	29	0
1	K	2128	0	1939	32	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	0	0
2	E	19	0	0	0	0
2	F	19	0	0	0	0
2	G	19	0	0	0	0
2	H	19	0	0	0	0
2	I	19	0	0	0	0
2	J	19	0	0	0	0
2	K	19	0	0	0	0
All	All	23617	0	21329	289	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 6.

All (289) 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:120:ILE:O	1:C:124:ARG:HG2	1.44	1.18
1:I:120:ILE:O	1:I:124:ARG:HG2	1.44	1.18
1:J:120:ILE:O	1:J:124:ARG:HG2	1.44	1.18
1:K:120:ILE:O	1:K:124:ARG:HG2	1.44	1.18
1:H:120:ILE:O	1:H:124:ARG:HG2	1.44	1.18
1:G:120:ILE:O	1:G:124:ARG:HG2	1.44	1.18
1:A:120:ILE:O	1:A:124:ARG:HG2	1.44	1.17
1:F:120:ILE:O	1:F:124:ARG:HG2	1.44	1.17
1:B:120:ILE:O	1:B:124:ARG:HG2	1.44	1.16
1:E:120:ILE:O	1:E:124:ARG:HG2	1.44	1.16
1:D:120:ILE:O	1:D:124:ARG:HG2	1.44	1.15
1:J:124:ARG:HG3	1:J:124:ARG:HH11	1.36	0.91
1:G:124:ARG:HG3	1:G:124:ARG:HH11	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:ARG:HG3	1:F:124:ARG:HH11	1.36	0.91
1:K:124:ARG:HG3	1:K:124:ARG:HH11	1.36	0.91
1:C:124:ARG:HG3	1:C:124:ARG:HH11	1.36	0.90
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.36	0.89
1:H:124:ARG:HH11	1:H:124:ARG:HG3	1.36	0.89
1:E:124:ARG:HG3	1:E:124:ARG:HH11	1.36	0.89
1:I:124:ARG:HG3	1:I:124:ARG:HH11	1.36	0.89
1:D:124:ARG:HG3	1:D:124:ARG:HH11	1.36	0.89
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.36	0.88
1:A:124:ARG:HG3	1:A:124:ARG:NH1	2.09	0.68
1:C:124:ARG:HG3	1:C:124:ARG:NH1	2.09	0.68
1:K:124:ARG:HG3	1:K:124:ARG:NH1	2.09	0.68
1:D:124:ARG:HG3	1:D:124:ARG:NH1	2.09	0.67
1:G:124:ARG:HG3	1:G:124:ARG:NH1	2.09	0.64
1:A:45:HIS:HB3	1:K:181:ARG:HH21	1.64	0.63
1:J:124:ARG:HG3	1:J:124:ARG:NH1	2.09	0.63
1:F:181:ARG:HH21	1:G:45:HIS:HB3	1.63	0.63
1:H:124:ARG:HG3	1:H:124:ARG:NH1	2.09	0.63
1:B:181:ARG:HH21	1:C:45:HIS:HB3	1.64	0.63
1:H:181:ARG:HH21	1:I:45:HIS:HB3	1.62	0.62
1:I:181:ARG:HH21	1:J:45:HIS:HB3	1.65	0.61
1:J:181:ARG:HH21	1:K:45:HIS:HB3	1.65	0.61
1:D:181:ARG:HH21	1:E:45:HIS:HB3	1.64	0.61
1:C:181:ARG:HH21	1:D:45:HIS:HB3	1.66	0.61
1:E:124:ARG:HG3	1:E:124:ARG:NH1	2.09	0.61
1:E:181:ARG:HH21	1:F:45:HIS:HB3	1.64	0.61
1:F:124:ARG:HG3	1:F:124:ARG:NH1	2.09	0.60
1:A:181:ARG:HH21	1:B:45:HIS:HB3	1.66	0.60
1:H:223:TYR:OH	1:I:246:ASN:ND2	2.34	0.60
1:G:181:ARG:HH21	1:H:45:HIS:HB3	1.66	0.60
1:C:124:ARG:HH11	1:C:124:ARG:CG	2.14	0.59
1:I:124:ARG:HG3	1:I:124:ARG:NH1	2.09	0.59
1:I:223:TYR:OH	1:J:246:ASN:ND2	2.35	0.59
1:D:223:TYR:OH	1:E:246:ASN:ND2	2.35	0.58
1:E:223:TYR:OH	1:F:246:ASN:ND2	2.34	0.58
1:F:223:TYR:OH	1:G:246:ASN:ND2	2.35	0.58
1:C:223:TYR:OH	1:D:246:ASN:ND2	2.35	0.57
1:F:182:TYR:HB2	1:G:47:PRO:HB3	1.85	0.57
1:I:124:ARG:HH11	1:I:124:ARG:CG	2.14	0.57
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.09	0.57
1:B:223:TYR:OH	1:C:246:ASN:ND2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:TYR:HB2	1:I:47:PRO:HB3	1.86	0.57
1:J:182:TYR:HB2	1:K:47:PRO:HB3	1.85	0.57
1:D:182:TYR:HB2	1:E:47:PRO:HB3	1.86	0.56
1:A:182:TYR:HB2	1:B:47:PRO:HB3	1.85	0.56
1:H:124:ARG:HH11	1:H:124:ARG:CG	2.14	0.56
1:B:182:TYR:HB2	1:C:47:PRO:HB3	1.86	0.56
1:I:182:TYR:HB2	1:J:47:PRO:HB3	1.87	0.56
1:G:223:TYR:OH	1:H:246:ASN:ND2	2.35	0.56
1:A:246:ASN:ND2	1:K:223:TYR:OH	2.34	0.55
1:C:48:CYS:HB3	1:C:159:ARG:HA	1.89	0.55
1:G:182:TYR:HB2	1:H:47:PRO:HB3	1.88	0.55
1:K:48:CYS:HB3	1:K:159:ARG:HA	1.89	0.55
1:A:48:CYS:HB3	1:A:159:ARG:HA	1.89	0.55
1:G:124:ARG:HH11	1:G:124:ARG:CG	2.14	0.55
1:B:48:CYS:HB3	1:B:159:ARG:HA	1.89	0.55
1:E:48:CYS:HB3	1:E:159:ARG:HA	1.89	0.55
1:E:182:TYR:HB2	1:F:47:PRO:HB3	1.87	0.55
1:D:48:CYS:HB3	1:D:159:ARG:HA	1.89	0.55
1:I:48:CYS:HB3	1:I:159:ARG:HA	1.89	0.55
1:A:47:PRO:HB3	1:K:182:TYR:HB2	1.87	0.55
1:C:182:TYR:HB2	1:D:47:PRO:HB3	1.88	0.55
1:F:48:CYS:HB3	1:F:159:ARG:HA	1.89	0.55
1:G:48:CYS:HB3	1:G:159:ARG:HA	1.89	0.55
1:J:48:CYS:HB3	1:J:159:ARG:HA	1.89	0.55
1:J:223:TYR:OH	1:K:246:ASN:ND2	2.36	0.54
1:H:48:CYS:HB3	1:H:159:ARG:HA	1.89	0.54
1:A:223:TYR:OH	1:B:246:ASN:ND2	2.37	0.54
1:C:194:VAL:O	1:C:198:LEU:HB2	2.08	0.54
1:E:194:VAL:O	1:E:198:LEU:HB2	2.08	0.54
1:G:194:VAL:O	1:G:198:LEU:HB2	2.08	0.54
1:I:194:VAL:O	1:I:198:LEU:HB2	2.08	0.54
1:J:194:VAL:O	1:J:198:LEU:HB2	2.08	0.54
1:K:194:VAL:O	1:K:198:LEU:HB2	2.08	0.54
1:B:194:VAL:O	1:B:198:LEU:HB2	2.08	0.53
1:H:194:VAL:O	1:H:198:LEU:HB2	2.08	0.53
1:A:194:VAL:O	1:A:198:LEU:HB2	2.08	0.53
1:F:194:VAL:O	1:F:198:LEU:HB2	2.08	0.53
1:D:194:VAL:O	1:D:198:LEU:HB2	2.08	0.53
1:E:124:ARG:NH1	1:E:124:ARG:CG	2.73	0.52
1:K:124:ARG:NH1	1:K:124:ARG:CG	2.73	0.51
1:B:283:GLY:HA3	1:B:298:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:GLY:HA3	1:G:298:ARG:HH11	1.76	0.51
1:D:283:GLY:HA3	1:D:298:ARG:HH11	1.76	0.51
1:C:85:GLU:O	1:C:89:ARG:CB	2.59	0.51
1:H:85:GLU:O	1:H:89:ARG:CB	2.60	0.51
1:J:283:GLY:HA3	1:J:298:ARG:HH11	1.76	0.51
1:I:85:GLU:O	1:I:89:ARG:CB	2.59	0.50
1:A:283:GLY:HA3	1:A:298:ARG:HH11	1.76	0.50
1:F:124:ARG:NH1	1:F:124:ARG:CG	2.73	0.50
1:I:194:VAL:HA	1:I:197:ILE:HG12	1.93	0.50
1:E:85:GLU:O	1:E:89:ARG:CB	2.60	0.50
1:E:283:GLY:HA3	1:E:298:ARG:HH11	1.76	0.50
1:H:194:VAL:HA	1:H:197:ILE:HG12	1.94	0.50
1:I:283:GLY:HA3	1:I:298:ARG:HH11	1.76	0.50
1:K:283:GLY:HA3	1:K:298:ARG:HH11	1.76	0.50
1:A:85:GLU:O	1:A:89:ARG:CB	2.60	0.50
1:F:194:VAL:HA	1:F:197:ILE:HG12	1.94	0.50
1:C:283:GLY:HA3	1:C:298:ARG:HH11	1.76	0.50
1:F:283:GLY:HA3	1:F:298:ARG:HH11	1.76	0.50
1:G:194:VAL:HA	1:G:197:ILE:HG12	1.94	0.50
1:H:124:ARG:NH1	1:H:124:ARG:CG	2.73	0.50
1:E:194:VAL:HA	1:E:197:ILE:HG12	1.94	0.50
1:J:194:VAL:HA	1:J:197:ILE:HG12	1.94	0.50
1:G:85:GLU:O	1:G:89:ARG:CB	2.60	0.50
1:J:85:GLU:O	1:J:89:ARG:CB	2.60	0.50
1:K:85:GLU:O	1:K:89:ARG:CB	2.60	0.50
1:D:194:VAL:HA	1:D:197:ILE:HG12	1.94	0.49
1:F:85:GLU:O	1:F:89:ARG:CB	2.60	0.49
1:H:283:GLY:HA3	1:H:298:ARG:HH11	1.76	0.49
1:D:85:GLU:O	1:D:89:ARG:CB	2.60	0.49
1:I:124:ARG:NH1	1:I:124:ARG:CG	2.73	0.49
1:B:85:GLU:O	1:B:89:ARG:CB	2.59	0.49
1:K:194:VAL:HA	1:K:197:ILE:HG12	1.94	0.49
1:C:194:VAL:HA	1:C:197:ILE:HG12	1.94	0.49
1:A:194:VAL:HA	1:A:197:ILE:HG12	1.94	0.49
1:B:194:VAL:HA	1:B:197:ILE:HG12	1.94	0.48
1:E:279:ASN:HA	1:E:282:THR:HG22	1.97	0.47
1:C:279:ASN:HA	1:C:282:THR:HG22	1.97	0.47
1:G:279:ASN:HA	1:G:282:THR:HG22	1.97	0.47
1:I:279:ASN:HA	1:I:282:THR:HG22	1.97	0.47
1:H:279:ASN:HA	1:H:282:THR:HG22	1.97	0.47
1:F:279:ASN:HA	1:F:282:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:279:ASN:HA	1:J:282:THR:HG22	1.97	0.47
1:K:279:ASN:HA	1:K:282:THR:HG22	1.97	0.47
1:A:279:ASN:HA	1:A:282:THR:HG22	1.97	0.46
1:B:279:ASN:HA	1:B:282:THR:HG22	1.97	0.46
1:D:279:ASN:HA	1:D:282:THR:HG22	1.97	0.46
1:C:134:GLU:HB3	1:C:158:ALA:HB2	1.98	0.46
1:F:198:LEU:HD12	1:F:198:LEU:HA	1.84	0.46
1:B:124:ARG:NH1	1:B:124:ARG:CG	2.73	0.46
1:E:134:GLU:HB3	1:E:158:ALA:HB2	1.98	0.46
1:E:184:SER:OG	1:E:185:GLN:N	2.49	0.46
1:F:184:SER:OG	1:F:185:GLN:N	2.49	0.45
1:B:198:LEU:HD12	1:B:198:LEU:HA	1.84	0.45
1:D:184:SER:OG	1:D:185:GLN:N	2.49	0.45
1:H:213:SER:HB2	1:I:282:THR:HG21	1.98	0.45
1:A:134:GLU:HB3	1:A:158:ALA:HB2	1.98	0.45
1:G:184:SER:OG	1:G:185:GLN:N	2.49	0.45
1:I:134:GLU:HB3	1:I:158:ALA:HB2	1.98	0.45
1:C:184:SER:OG	1:C:185:GLN:N	2.49	0.45
1:D:134:GLU:HB3	1:D:158:ALA:HB2	1.98	0.45
1:H:184:SER:OG	1:H:185:GLN:N	2.49	0.45
1:B:134:GLU:HB3	1:B:158:ALA:HB2	1.98	0.45
1:C:124:ARG:NH1	1:C:124:ARG:CG	2.73	0.45
1:H:134:GLU:HB3	1:H:158:ALA:HB2	1.98	0.45
1:I:184:SER:OG	1:I:185:GLN:N	2.49	0.45
1:J:134:GLU:HB3	1:J:158:ALA:HB2	1.98	0.45
1:B:184:SER:OG	1:B:185:GLN:N	2.49	0.45
1:A:124:ARG:NH1	1:A:124:ARG:CG	2.73	0.45
1:J:184:SER:OG	1:J:185:GLN:N	2.49	0.45
1:F:213:SER:HB2	1:G:282:THR:HG21	1.99	0.45
1:G:134:GLU:HB3	1:G:158:ALA:HB2	1.98	0.45
1:F:134:GLU:HB3	1:F:158:ALA:HB2	1.98	0.45
1:D:124:ARG:NH1	1:D:124:ARG:CG	2.73	0.44
1:K:184:SER:OG	1:K:185:GLN:N	2.49	0.44
1:D:272:THR:OG1	1:D:273:GLN:N	2.51	0.44
1:K:134:GLU:HB3	1:K:158:ALA:HB2	1.98	0.44
1:B:272:THR:OG1	1:B:273:GLN:N	2.51	0.44
1:G:198:LEU:HD12	1:G:198:LEU:HA	1.84	0.44
1:A:272:THR:OG1	1:A:273:GLN:N	2.51	0.44
1:I:77:ASN:O	1:I:81:ASN:ND2	2.39	0.44
1:J:70:ILE:HD13	1:J:70:ILE:HA	1.86	0.44
1:E:213:SER:HB2	1:F:282:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:VAL:HG12	1:J:254:VAL:HG22	2.00	0.44
1:K:247:VAL:HG12	1:K:254:VAL:HG22	2.00	0.44
1:A:184:SER:OG	1:A:185:GLN:N	2.49	0.44
1:A:247:VAL:HG12	1:A:254:VAL:HG22	2.00	0.44
1:E:272:THR:OG1	1:E:273:GLN:N	2.51	0.44
1:B:247:VAL:HG12	1:B:254:VAL:HG22	2.00	0.44
1:C:247:VAL:HG12	1:C:254:VAL:HG22	2.00	0.44
1:G:272:THR:OG1	1:G:273:GLN:N	2.51	0.44
1:I:247:VAL:HG12	1:I:254:VAL:HG22	2.00	0.44
1:K:272:THR:OG1	1:K:273:GLN:N	2.51	0.43
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.84	0.43
1:J:213:SER:HB2	1:K:282:THR:HG21	2.00	0.43
1:C:272:THR:OG1	1:C:273:GLN:N	2.51	0.43
1:H:247:VAL:HG12	1:H:254:VAL:HG22	2.00	0.43
1:B:137:ASP:HA	1:B:138:PRO:HD3	1.93	0.43
1:B:213:SER:HB2	1:C:282:THR:HG21	1.99	0.43
1:D:213:SER:HB2	1:E:282:THR:HG21	2.00	0.43
1:D:247:VAL:HG12	1:D:254:VAL:HG22	2.00	0.43
1:K:156:ILE:HD12	1:K:156:ILE:HA	1.90	0.43
1:E:79:THR:O	1:E:83:VAL:HG23	2.19	0.43
1:I:272:THR:OG1	1:I:273:GLN:N	2.51	0.43
1:J:39:PHE:HA	1:J:42:VAL:HG22	2.01	0.43
1:K:39:PHE:HA	1:K:42:VAL:HG22	2.01	0.43
1:D:79:THR:O	1:D:83:VAL:HG23	2.19	0.43
1:E:247:VAL:HG12	1:E:254:VAL:HG22	2.00	0.43
1:F:79:THR:O	1:F:83:VAL:HG23	2.19	0.43
1:G:247:VAL:HG12	1:G:254:VAL:HG22	2.00	0.43
1:A:39:PHE:HA	1:A:42:VAL:HG22	2.01	0.43
1:F:247:VAL:HG12	1:F:254:VAL:HG22	2.00	0.43
1:H:39:PHE:HA	1:H:42:VAL:HG22	2.01	0.43
1:C:156:ILE:HD12	1:C:156:ILE:HA	1.90	0.43
1:F:77:ASN:O	1:F:81:ASN:ND2	2.39	0.43
1:I:39:PHE:HA	1:I:42:VAL:HG22	2.01	0.43
1:B:39:PHE:HA	1:B:42:VAL:HG22	2.01	0.42
1:C:79:THR:O	1:C:83:VAL:HG23	2.19	0.42
1:G:79:THR:O	1:G:83:VAL:HG23	2.19	0.42
1:B:129:VAL:O	1:B:133:SER:OG	2.32	0.42
1:C:39:PHE:HA	1:C:42:VAL:HG22	2.01	0.42
1:G:39:PHE:HA	1:G:42:VAL:HG22	2.01	0.42
1:H:198:LEU:HD12	1:H:198:LEU:HA	1.84	0.42
1:B:77:ASN:O	1:B:81:ASN:ND2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:HD13	1:E:70:ILE:HA	1.86	0.42
1:A:52:ARG:HE	1:A:52:ARG:HB2	1.74	0.42
1:G:213:SER:HB2	1:H:282:THR:HG21	2.02	0.42
1:H:272:THR:OG1	1:H:273:GLN:N	2.51	0.42
1:K:79:THR:O	1:K:83:VAL:HG23	2.19	0.42
1:J:79:THR:O	1:J:83:VAL:HG23	2.19	0.42
1:K:203:LYS:HE2	1:K:203:LYS:HB3	1.93	0.42
1:D:39:PHE:HA	1:D:42:VAL:HG22	2.01	0.42
1:A:282:THR:HG21	1:K:213:SER:HB2	2.01	0.42
1:D:70:ILE:HD13	1:D:70:ILE:HA	1.86	0.42
1:F:39:PHE:HA	1:F:42:VAL:HG22	2.01	0.42
1:H:79:THR:O	1:H:83:VAL:HG23	2.19	0.42
1:I:79:THR:O	1:I:83:VAL:HG23	2.19	0.42
1:G:203:LYS:HE2	1:G:203:LYS:HB3	1.93	0.42
1:H:234:THR:HB	1:I:255:ALA:H	1.85	0.42
1:K:129:VAL:O	1:K:133:SER:OG	2.32	0.42
1:H:156:ILE:HD12	1:H:156:ILE:HA	1.90	0.42
1:K:198:LEU:HD12	1:K:198:LEU:HA	1.84	0.42
1:B:79:THR:O	1:B:83:VAL:HG23	2.19	0.41
1:D:77:ASN:O	1:D:81:ASN:ND2	2.39	0.41
1:F:70:ILE:HD13	1:F:70:ILE:HA	1.86	0.41
1:A:79:THR:O	1:A:83:VAL:HG23	2.19	0.41
1:E:39:PHE:HA	1:E:42:VAL:HG22	2.01	0.41
1:I:213:SER:HB2	1:J:282:THR:HG21	2.02	0.41
1:D:181:ARG:HG2	1:D:185:GLN:HE21	1.86	0.41
1:I:181:ARG:HG2	1:I:185:GLN:HE21	1.86	0.41
1:J:47:PRO:HG2	1:J:53:ASN:HA	2.03	0.41
1:B:181:ARG:HG2	1:B:185:GLN:HE21	1.86	0.41
1:G:47:PRO:HG2	1:G:53:ASN:HA	2.03	0.41
1:A:77:ASN:O	1:A:81:ASN:ND2	2.39	0.41
1:F:272:THR:OG1	1:F:273:GLN:N	2.51	0.41
1:I:198:LEU:HD12	1:I:198:LEU:HA	1.84	0.41
1:G:181:ARG:HG2	1:G:185:GLN:HE21	1.86	0.41
1:H:47:PRO:HG2	1:H:53:ASN:HA	2.03	0.41
1:J:198:LEU:HD12	1:J:198:LEU:HA	1.84	0.41
1:K:181:ARG:HG2	1:K:185:GLN:HE21	1.86	0.41
1:F:181:ARG:HG2	1:F:185:GLN:HE21	1.86	0.41
1:J:203:LYS:HE2	1:J:203:LYS:HB3	1.93	0.41
1:I:47:PRO:HG2	1:I:53:ASN:HA	2.03	0.41
1:A:47:PRO:HG2	1:A:53:ASN:HA	2.03	0.41
1:C:133:SER:OG	1:C:161:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:SER:HB2	1:D:282:THR:HG21	2.02	0.41
1:E:47:PRO:HG2	1:E:53:ASN:HA	2.03	0.41
1:E:133:SER:OG	1:E:161:PRO:HD3	2.21	0.41
1:J:124:ARG:NH1	1:J:124:ARG:CG	2.73	0.41
1:A:133:SER:OG	1:A:161:PRO:HD3	2.21	0.41
1:A:181:ARG:HG2	1:A:185:GLN:HE21	1.86	0.41
1:A:213:SER:HB2	1:B:282:THR:HG21	2.02	0.41
1:E:77:ASN:O	1:E:81:ASN:ND2	2.39	0.41
1:F:137:ASP:HA	1:F:138:PRO:HD3	1.93	0.41
1:H:52:ARG:HE	1:H:52:ARG:HB2	1.74	0.41
1:B:234:THR:HB	1:C:255:ALA:H	1.86	0.40
1:H:137:ASP:HA	1:H:138:PRO:HD3	1.93	0.40
1:J:181:ARG:HG2	1:J:185:GLN:HE21	1.86	0.40
1:K:70:ILE:HD13	1:K:70:ILE:HA	1.86	0.40
1:C:47:PRO:HG2	1:C:53:ASN:HA	2.02	0.40
1:D:133:SER:OG	1:D:161:PRO:HD3	2.21	0.40
1:E:181:ARG:HG2	1:E:185:GLN:HE21	1.86	0.40
1:F:47:PRO:HG2	1:F:53:ASN:HA	2.02	0.40
1:J:272:THR:OG1	1:J:273:GLN:N	2.51	0.40
1:A:260:ASP:O	1:A:264:ILE:HG12	2.22	0.40
1:C:70:ILE:HD13	1:C:70:ILE:HA	1.86	0.40
1:F:234:THR:HB	1:G:255:ALA:H	1.87	0.40
1:G:133:SER:OG	1:G:161:PRO:HD3	2.21	0.40
1:G:137:ASP:HA	1:G:138:PRO:HD3	1.93	0.40
1:I:52:ARG:HE	1:I:52:ARG:HB2	1.74	0.40
1:K:47:PRO:HG2	1:K:53:ASN:HA	2.02	0.40
1:B:133:SER:OG	1:B:161:PRO:HD3	2.21	0.40
1:B:260:ASP:O	1:B:264:ILE:HG12	2.22	0.40
1:H:181:ARG:HG2	1:H:185:GLN:HE21	1.86	0.40
1:K:260:ASP:O	1:K:264:ILE:HG12	2.22	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	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	B	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	C	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	D	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	E	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	F	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	G	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	H	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	I	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	J	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
1	K	292/331 (88%)	283 (97%)	9 (3%)	0	100	100
All	All	3212/3641 (88%)	3113 (97%)	99 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/278 (65%)	181 (100%)	0	100	100
1	B	181/278 (65%)	181 (100%)	0	100	100
1	C	181/278 (65%)	181 (100%)	0	100	100
1	D	181/278 (65%)	181 (100%)	0	100	100
1	E	181/278 (65%)	181 (100%)	0	100	100
1	F	181/278 (65%)	181 (100%)	0	100	100
1	G	181/278 (65%)	181 (100%)	0	100	100
1	H	181/278 (65%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	181/278 (65%)	181 (100%)	0	100	100
1	J	181/278 (65%)	181 (100%)	0	100	100
1	K	181/278 (65%)	181 (100%)	0	100	100
All	All	1991/3058 (65%)	1991 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	226	ASN
1	A	232	GLN
1	A	246	ASN
1	A	279	ASN
1	B	81	ASN
1	B	185	GLN
1	B	226	ASN
1	B	232	GLN
1	B	246	ASN
1	B	279	ASN
1	C	81	ASN
1	C	185	GLN
1	C	226	ASN
1	C	232	GLN
1	C	246	ASN
1	C	279	ASN
1	D	185	GLN
1	D	226	ASN
1	D	232	GLN
1	D	246	ASN
1	D	279	ASN
1	E	81	ASN
1	E	185	GLN
1	E	226	ASN
1	E	232	GLN
1	E	246	ASN
1	E	279	ASN
1	F	81	ASN
1	F	185	GLN
1	F	226	ASN

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Mol	Chain	Res	Type
1	F	232	GLN
1	F	246	ASN
1	F	279	ASN
1	G	81	ASN
1	G	185	GLN
1	G	226	ASN
1	G	232	GLN
1	G	246	ASN
1	G	279	ASN
1	H	81	ASN
1	H	185	GLN
1	H	226	ASN
1	H	232	GLN
1	H	246	ASN
1	H	279	ASN
1	I	81	ASN
1	I	185	GLN
1	I	226	ASN
1	I	232	GLN
1	I	246	ASN
1	I	279	ASN
1	J	81	ASN
1	J	185	GLN
1	J	226	ASN
1	J	232	GLN
1	J	246	ASN
1	J	279	ASN
1	K	81	ASN
1	K	185	GLN
1	K	226	ASN
1	K	232	GLN
1	K	246	ASN
1	K	279	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	R2R	G	501	-	14,18,18	3.88	14 (100%)	-		
2	R2R	F	501	-	14,18,18	3.88	14 (100%)	-		
2	R2R	K	501	-	14,18,18	3.90	14 (100%)	-		
2	R2R	C	501	-	14,18,18	3.88	14 (100%)	-		
2	R2R	I	501	-	14,18,18	3.89	14 (100%)	-		
2	R2R	B	501	-	14,18,18	3.89	14 (100%)	-		
2	R2R	J	501	-	14,18,18	3.89	14 (100%)	-		
2	R2R	A	501	-	14,18,18	3.89	14 (100%)	-		
2	R2R	D	501	-	14,18,18	3.89	14 (100%)	-		
2	R2R	H	501	-	14,18,18	3.88	14 (100%)	-		
2	R2R	E	501	-	14,18,18	3.88	14 (100%)	-		

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	R2R	RU2-N01	-4.15	2.04	2.11
2	E	501	R2R	RU2-N01	-4.13	2.04	2.11
2	I	501	R2R	RU2-N05	-4.12	2.04	2.11
2	K	501	R2R	RU2-N05	-4.12	2.04	2.11
2	J	501	R2R	RU2-N05	-4.12	2.04	2.11
2	J	501	R2R	RU2-N01	-4.12	2.04	2.11
2	C	501	R2R	RU2-N01	-4.11	2.04	2.11
2	A	501	R2R	RU2-N01	-4.11	2.04	2.11
2	H	501	R2R	RU2-N01	-4.11	2.04	2.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	R2R	RU2-N01	-4.11	2.04	2.11
2	F	501	R2R	RU2-N01	-4.10	2.04	2.11
2	C	501	R2R	RU2-N05	-4.09	2.04	2.11
2	G	501	R2R	RU2-N05	-4.09	2.04	2.11
2	B	501	R2R	RU2-N01	-4.09	2.04	2.11
2	D	501	R2R	RU2-N01	-4.08	2.04	2.11
2	K	501	R2R	RU2-N01	-4.08	2.04	2.11
2	A	501	R2R	RU2-N05	-4.08	2.04	2.11
2	B	501	R2R	RU2-N03	-4.07	2.04	2.11
2	D	501	R2R	RU2-N05	-4.07	2.04	2.11
2	H	501	R2R	RU2-N05	-4.06	2.04	2.11
2	G	501	R2R	RU2-N04	-4.05	2.04	2.11
2	J	501	R2R	RU2-N03	-4.05	2.04	2.11
2	D	501	R2R	RU2-N03	-4.05	2.04	2.11
2	B	501	R2R	RU2-N05	-4.05	2.04	2.11
2	F	501	R2R	RU2-N05	-4.05	2.04	2.11
2	E	501	R2R	RU2-N04	-4.05	2.04	2.11
2	H	501	R2R	RU2-N04	-4.05	2.04	2.11
2	I	501	R2R	RU2-N03	-4.04	2.04	2.11
2	K	501	R2R	RU2-N04	-4.04	2.04	2.11
2	C	501	R2R	RU2-N03	-4.04	2.04	2.11
2	K	501	R2R	RU2-N03	-4.04	2.04	2.11
2	E	501	R2R	RU2-N05	-4.04	2.04	2.11
2	A	501	R2R	RU2-N03	-4.03	2.04	2.11
2	F	501	R2R	RU2-N03	-4.03	2.04	2.11
2	F	501	R2R	RU2-N04	-4.02	2.04	2.11
2	A	501	R2R	RU2-N04	-4.02	2.04	2.11
2	E	501	R2R	RU2-N03	-4.02	2.04	2.11
2	D	501	R2R	RU2-N04	-4.01	2.04	2.11
2	J	501	R2R	RU2-N04	-4.01	2.04	2.11
2	B	501	R2R	RU2-N04	-4.01	2.04	2.11
2	G	501	R2R	RU2-N03	-4.00	2.04	2.11
2	C	501	R2R	RU2-N04	-4.00	2.04	2.11
2	I	501	R2R	RU2-N04	-3.99	2.04	2.11
2	H	501	R2R	RU2-N03	-3.97	2.04	2.11
2	D	501	R2R	RU3-N10	-3.89	2.04	2.10
2	C	501	R2R	RU1-N17	-3.88	2.04	2.10
2	J	501	R2R	RU1-N18	-3.88	2.04	2.10
2	I	501	R2R	RU1-N17	-3.88	2.04	2.10
2	C	501	R2R	RU3-N10	-3.87	2.04	2.10
2	B	501	R2R	RU1-N18	-3.87	2.04	2.10
2	K	501	R2R	RU1-N18	-3.87	2.04	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	R2R	RU3-N10	-3.87	2.04	2.10
2	B	501	R2R	RU3-N09	-3.86	2.04	2.10
2	J	501	R2R	RU3-N09	-3.86	2.04	2.10
2	K	501	R2R	RU3-N09	-3.86	2.04	2.10
2	E	501	R2R	RU3-N09	-3.86	2.04	2.10
2	J	501	R2R	RU3-N11	-3.85	2.04	2.10
2	I	501	R2R	RU1-N18	-3.85	2.04	2.10
2	B	501	R2R	RU1-N17	-3.85	2.04	2.10
2	J	501	R2R	RU1-N17	-3.85	2.04	2.10
2	A	501	R2R	RU3-N09	-3.85	2.04	2.10
2	G	501	R2R	RU1-N19	-3.85	2.04	2.10
2	K	501	R2R	RU1-N17	-3.85	2.04	2.10
2	F	501	R2R	RU3-N09	-3.85	2.04	2.10
2	F	501	R2R	RU1-N17	-3.85	2.04	2.10
2	B	501	R2R	RU3-N12	-3.85	2.04	2.10
2	C	501	R2R	RU1-N19	-3.84	2.04	2.10
2	A	501	R2R	RU1-N18	-3.84	2.04	2.10
2	B	501	R2R	RU3-N10	-3.84	2.04	2.10
2	J	501	R2R	RU3-N10	-3.84	2.04	2.10
2	A	501	R2R	RU1-N17	-3.84	2.04	2.10
2	K	501	R2R	RU3-N10	-3.84	2.04	2.10
2	D	501	R2R	RU3-N09	-3.84	2.04	2.10
2	H	501	R2R	RU3-N09	-3.84	2.04	2.10
2	H	501	R2R	RU1-N17	-3.84	2.04	2.10
2	F	501	R2R	RU3-N10	-3.84	2.04	2.10
2	K	501	R2R	RU1-N19	-3.84	2.04	2.10
2	G	501	R2R	RU3-N11	-3.84	2.04	2.10
2	F	501	R2R	RU1-N18	-3.84	2.04	2.10
2	D	501	R2R	RU3-N11	-3.84	2.04	2.10
2	D	501	R2R	RU1-N19	-3.84	2.04	2.10
2	A	501	R2R	RU3-N10	-3.83	2.04	2.10
2	D	501	R2R	RU1-N16	-3.83	2.04	2.10
2	H	501	R2R	RU3-N10	-3.83	2.04	2.10
2	B	501	R2R	RU1-N19	-3.83	2.04	2.10
2	D	501	R2R	RU1-N17	-3.83	2.04	2.10
2	G	501	R2R	RU1-N18	-3.83	2.04	2.10
2	E	501	R2R	RU3-N10	-3.83	2.04	2.10
2	K	501	R2R	RU3-N12	-3.83	2.04	2.10
2	F	501	R2R	RU3-N11	-3.82	2.04	2.10
2	I	501	R2R	RU3-N11	-3.82	2.04	2.10
2	I	501	R2R	RU3-N12	-3.82	2.04	2.10
2	G	501	R2R	RU3-N09	-3.82	2.04	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	R2R	RU3-N09	-3.82	2.04	2.10
2	E	501	R2R	RU3-N11	-3.82	2.04	2.10
2	E	501	R2R	RU1-N19	-3.82	2.04	2.10
2	C	501	R2R	RU3-N09	-3.82	2.04	2.10
2	H	501	R2R	RU3-N11	-3.82	2.04	2.10
2	H	501	R2R	RU1-N19	-3.82	2.04	2.10
2	A	501	R2R	RU3-N11	-3.81	2.04	2.10
2	A	501	R2R	RU3-N12	-3.81	2.04	2.10
2	A	501	R2R	RU1-N19	-3.81	2.04	2.10
2	G	501	R2R	RU1-N16	-3.81	2.04	2.10
2	G	501	R2R	RU1-N17	-3.81	2.04	2.10
2	K	501	R2R	RU3-N11	-3.81	2.04	2.10
2	E	501	R2R	RU1-N18	-3.81	2.04	2.10
2	H	501	R2R	RU1-N18	-3.81	2.04	2.10
2	F	501	R2R	RU3-N12	-3.81	2.04	2.10
2	F	501	R2R	RU1-N19	-3.81	2.04	2.10
2	K	501	R2R	RU1-N15	-3.81	2.04	2.10
2	I	501	R2R	RU1-N19	-3.81	2.04	2.10
2	E	501	R2R	RU1-N17	-3.80	2.04	2.10
2	J	501	R2R	RU1-N19	-3.80	2.04	2.10
2	G	501	R2R	RU3-N10	-3.80	2.04	2.10
2	B	501	R2R	RU3-N11	-3.80	2.04	2.10
2	K	501	R2R	RU1-N16	-3.80	2.04	2.10
2	C	501	R2R	RU3-N12	-3.80	2.04	2.10
2	C	501	R2R	RU1-N18	-3.80	2.04	2.10
2	E	501	R2R	RU1-N16	-3.79	2.04	2.10
2	C	501	R2R	RU3-N11	-3.79	2.04	2.10
2	H	501	R2R	RU3-N12	-3.79	2.04	2.10
2	G	501	R2R	RU3-N12	-3.79	2.04	2.10
2	I	501	R2R	RU3-N08	-3.79	2.04	2.10
2	C	501	R2R	RU1-N15	-3.79	2.04	2.10
2	D	501	R2R	RU3-N12	-3.78	2.04	2.10
2	D	501	R2R	RU1-N18	-3.78	2.04	2.10
2	J	501	R2R	RU3-N12	-3.78	2.04	2.10
2	B	501	R2R	RU3-N08	-3.78	2.04	2.10
2	H	501	R2R	RU1-N16	-3.78	2.04	2.10
2	F	501	R2R	RU1-N16	-3.78	2.04	2.10
2	A	501	R2R	RU1-N16	-3.78	2.04	2.10
2	E	501	R2R	RU3-N12	-3.78	2.04	2.10
2	A	501	R2R	RU3-N08	-3.78	2.04	2.10
2	J	501	R2R	RU3-N08	-3.78	2.04	2.10
2	H	501	R2R	RU3-N08	-3.77	2.04	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	R2R	RU3-N08	-3.77	2.04	2.10
2	J	501	R2R	RU1-N16	-3.77	2.04	2.10
2	B	501	R2R	RU1-N16	-3.77	2.04	2.10
2	C	501	R2R	RU3-N08	-3.77	2.04	2.10
2	G	501	R2R	RU3-N08	-3.77	2.04	2.10
2	D	501	R2R	RU3-N08	-3.77	2.04	2.10
2	H	501	R2R	RU1-N15	-3.76	2.04	2.10
2	E	501	R2R	RU3-N08	-3.76	2.04	2.10
2	K	501	R2R	RU3-N08	-3.76	2.04	2.10
2	J	501	R2R	RU1-N15	-3.76	2.04	2.10
2	I	501	R2R	RU1-N15	-3.76	2.04	2.10
2	C	501	R2R	RU1-N16	-3.76	2.04	2.10
2	I	501	R2R	RU1-N16	-3.76	2.04	2.10
2	A	501	R2R	RU1-N15	-3.75	2.04	2.10
2	D	501	R2R	RU1-N15	-3.75	2.04	2.10
2	E	501	R2R	RU1-N15	-3.75	2.04	2.10
2	F	501	R2R	RU1-N15	-3.74	2.04	2.10
2	G	501	R2R	RU1-N15	-3.74	2.04	2.10
2	B	501	R2R	RU1-N15	-3.74	2.04	2.10

There are no bond angle outliers.

There are no chirality outliers.

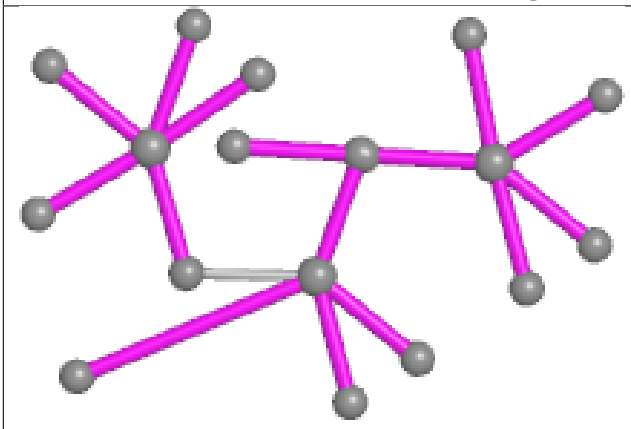
There are no torsion outliers.

There are no ring outliers.

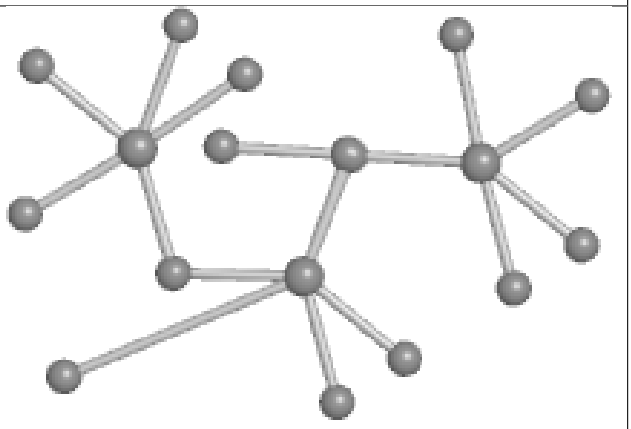
No monomer is involved in short contacts.

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.

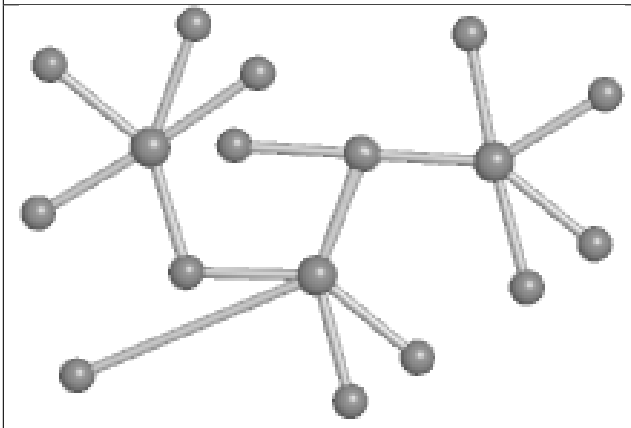
Ligand R2R G 501



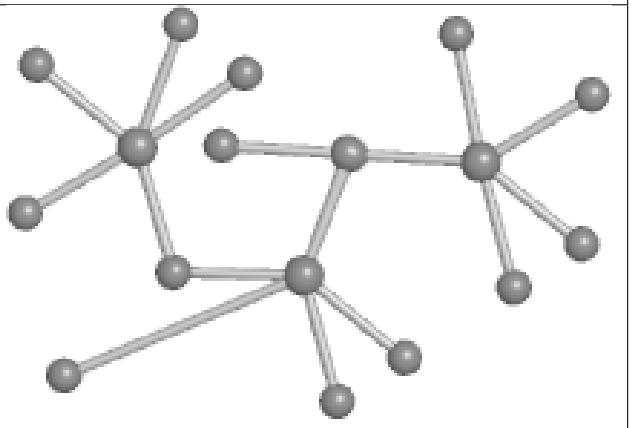
Bond lengths



Bond angles

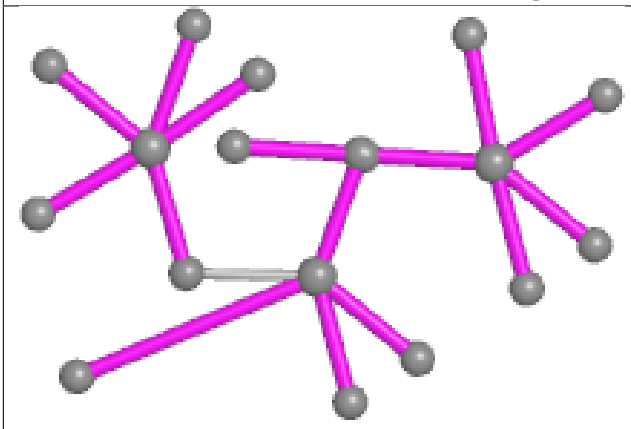


Torsions

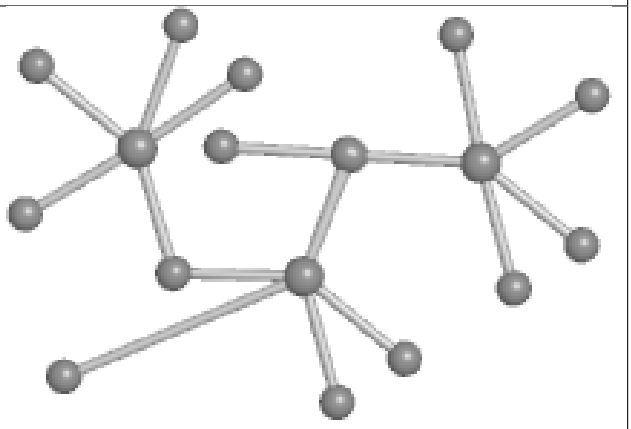


Rings

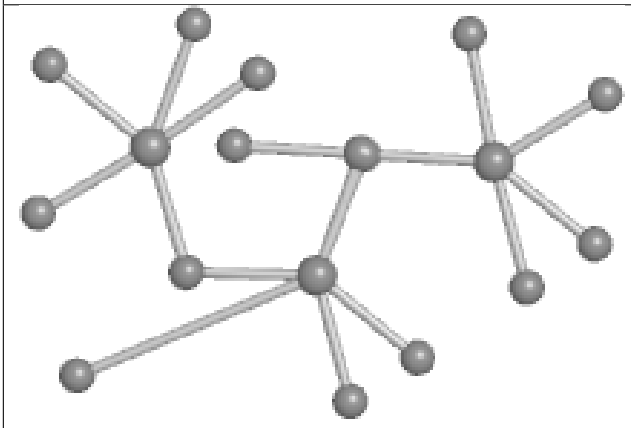
Ligand R2R F 501



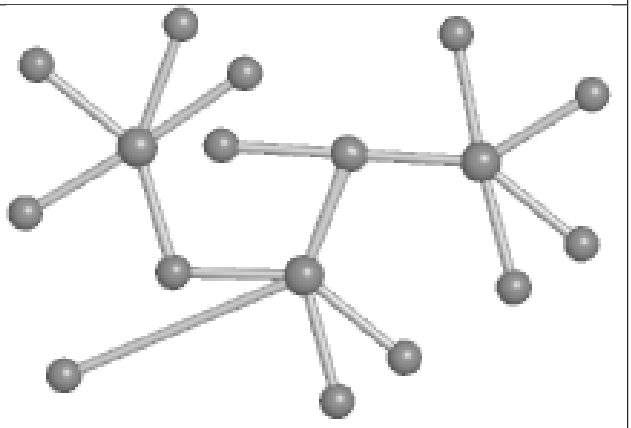
Bond lengths



Bond angles

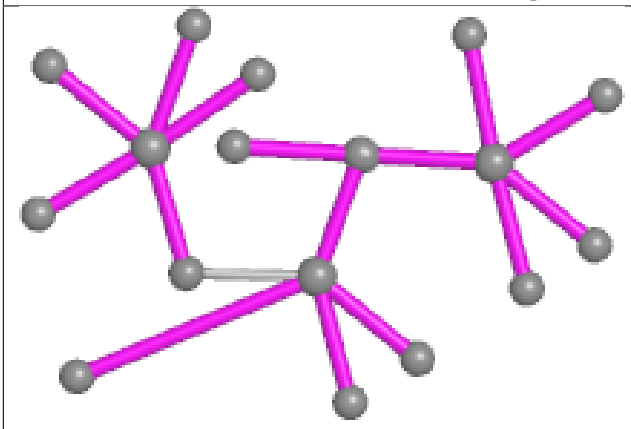


Torsions

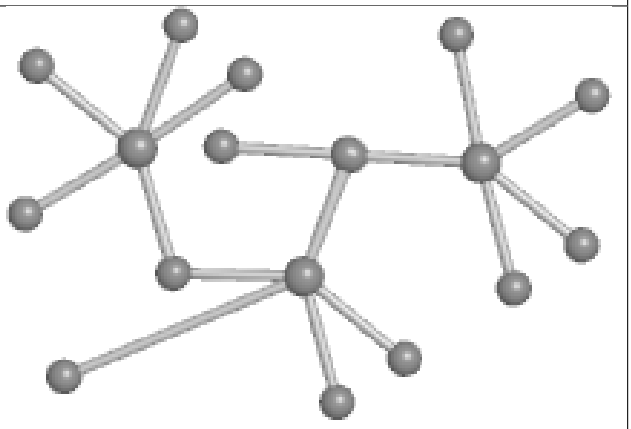


Rings

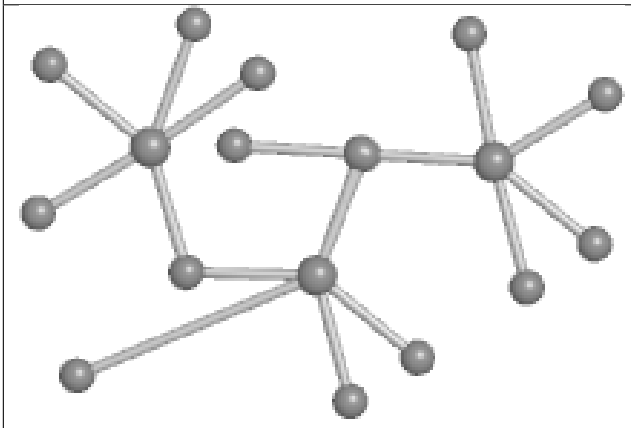
Ligand R2R K 501



Bond lengths



Bond angles



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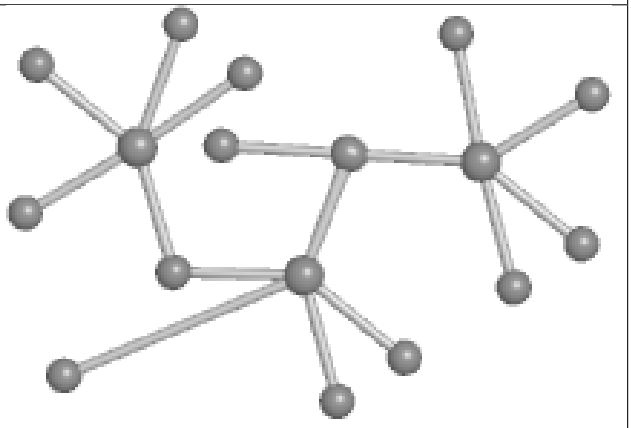
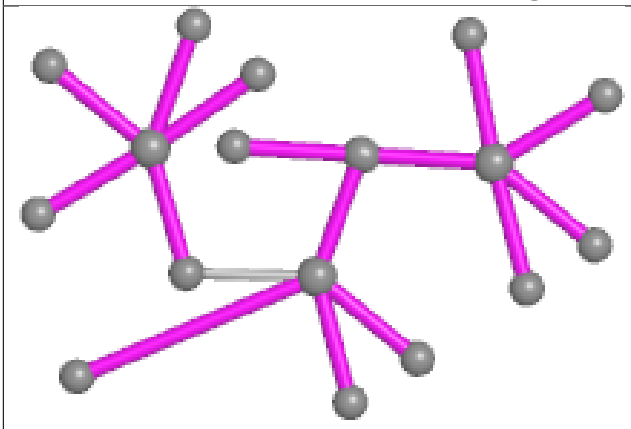
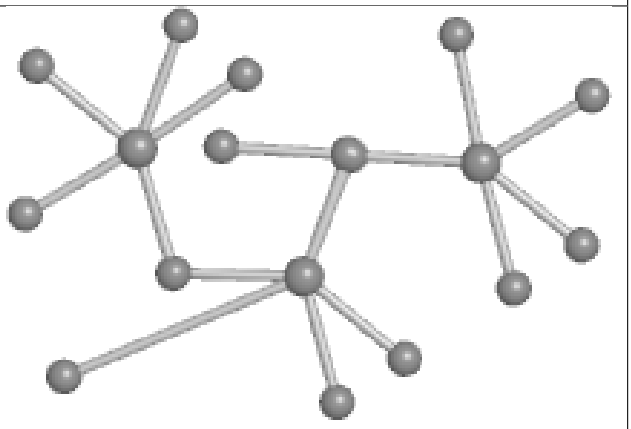


Rings

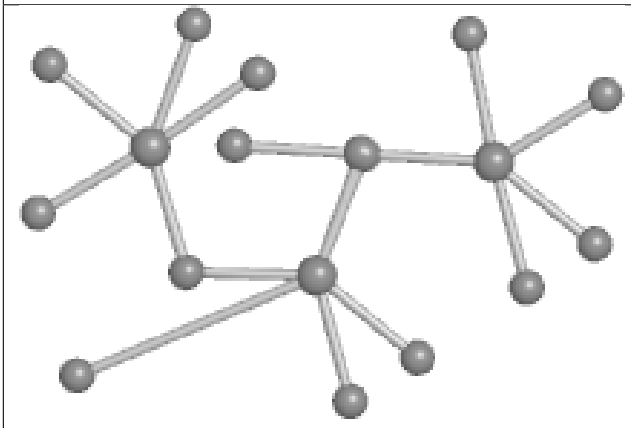
Ligand R2R C 501



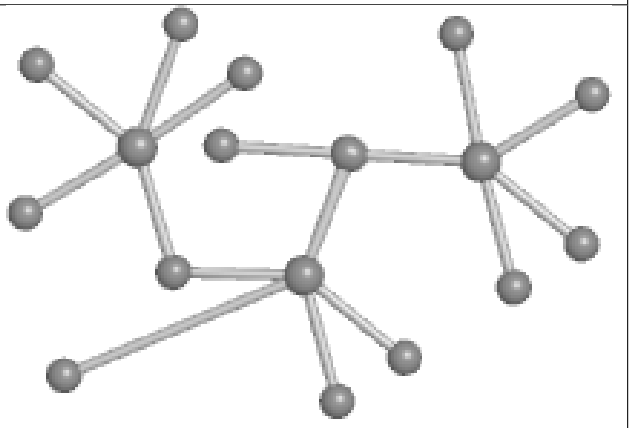
Bond lengths



Bond angles

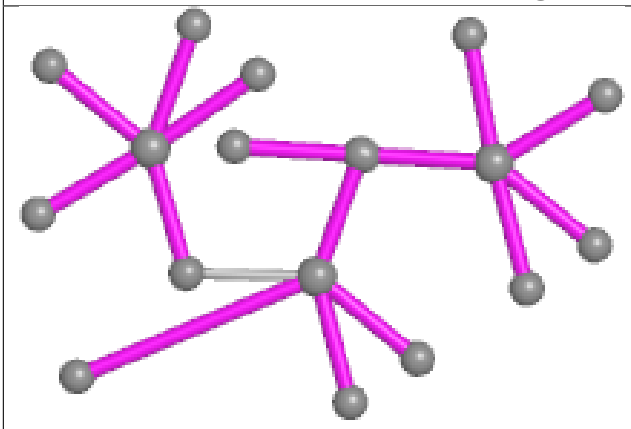


Torsions



Rings

Ligand R2R I 501



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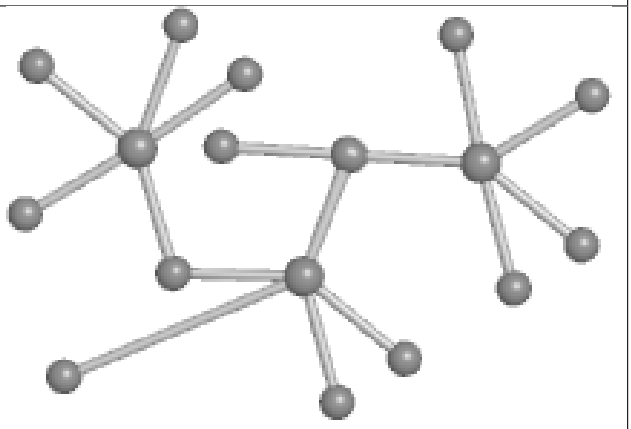
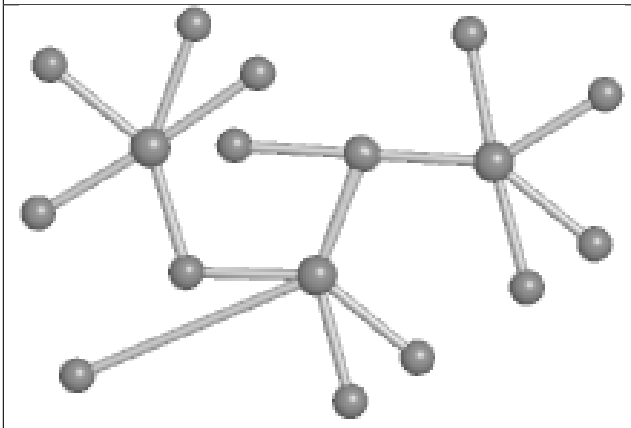


Bond angles



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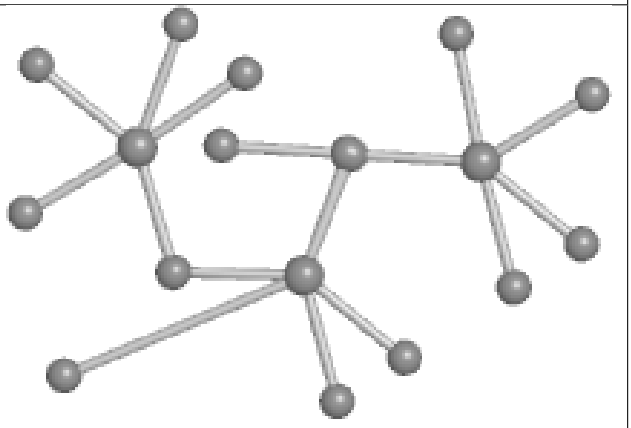
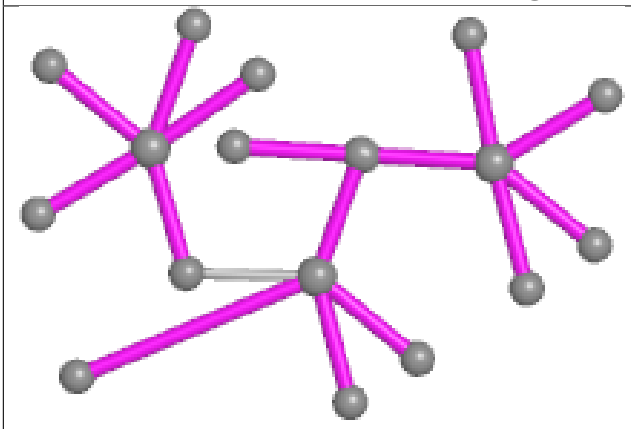


Rings

Ligand R2R B 501



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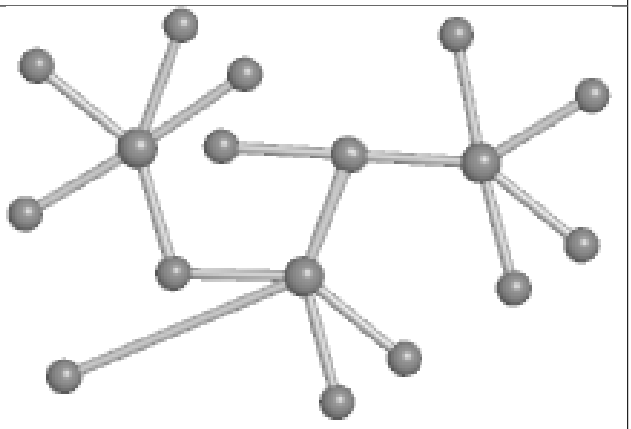
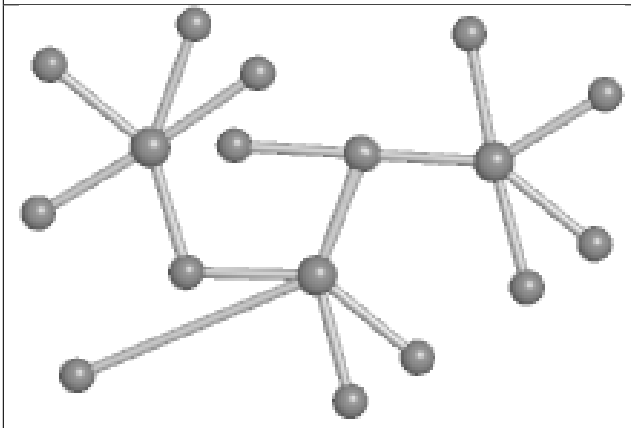


Bond angles



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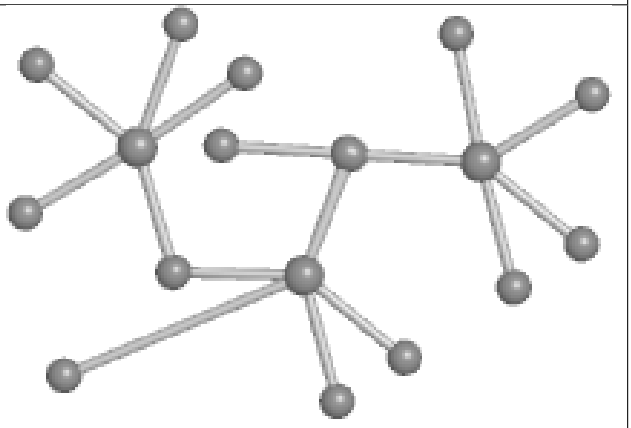
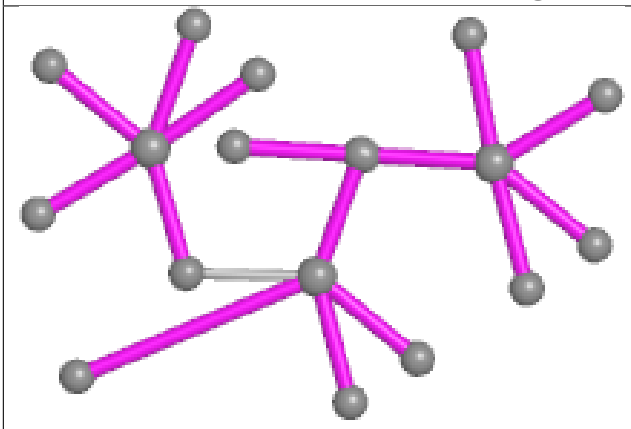


Rings

Ligand R2R J 501



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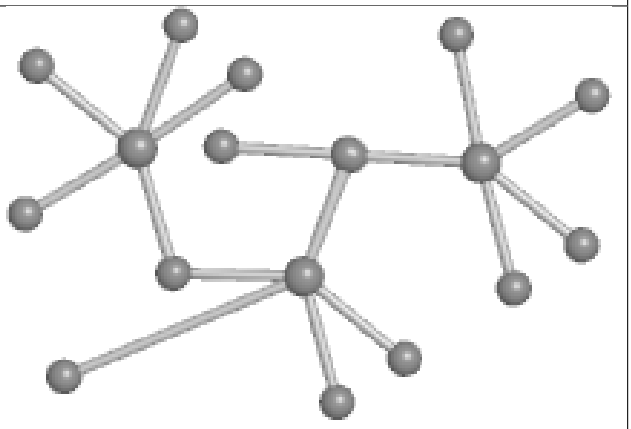
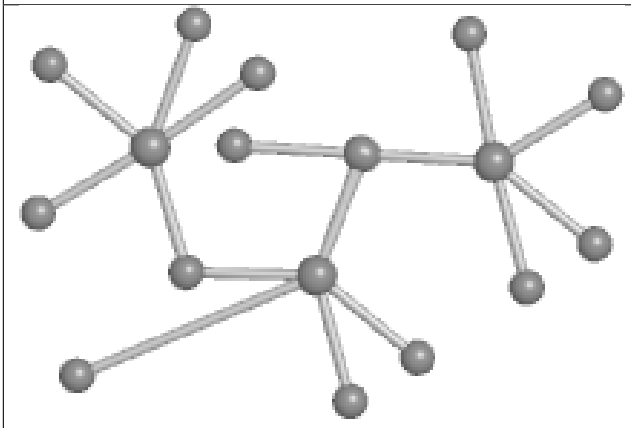


Bond angles



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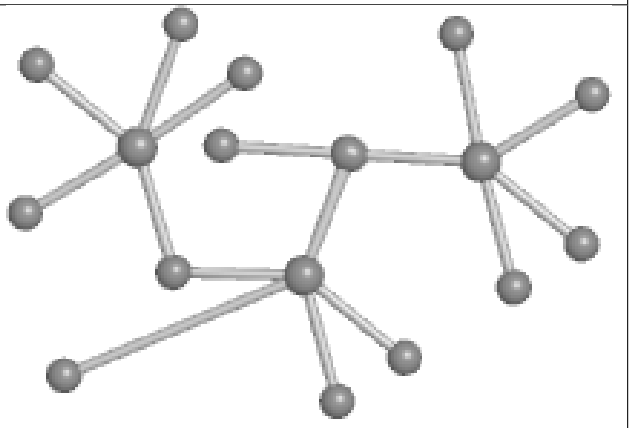
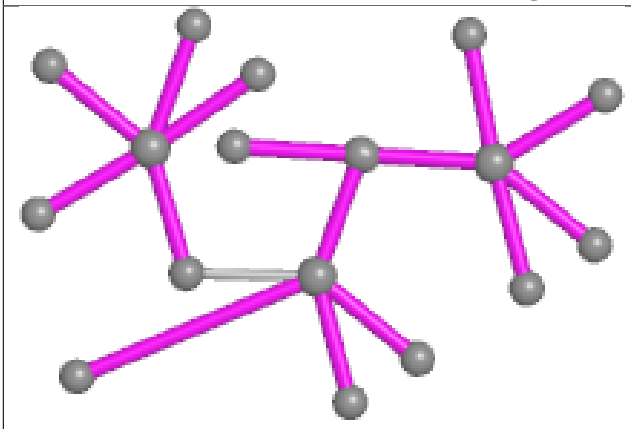
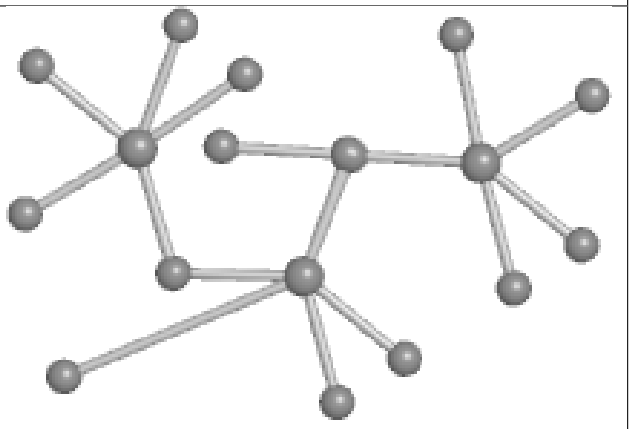


Rings

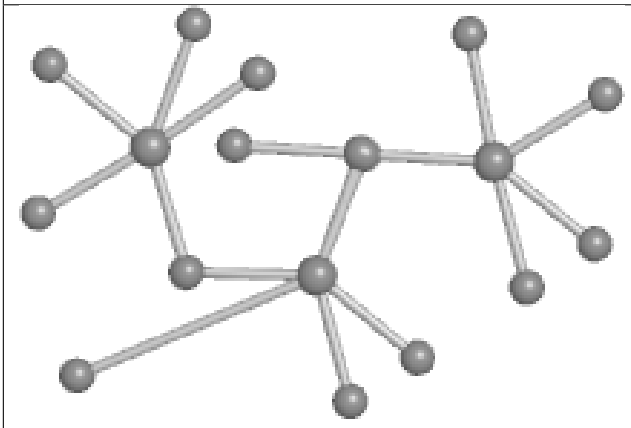
Ligand R2R A 501



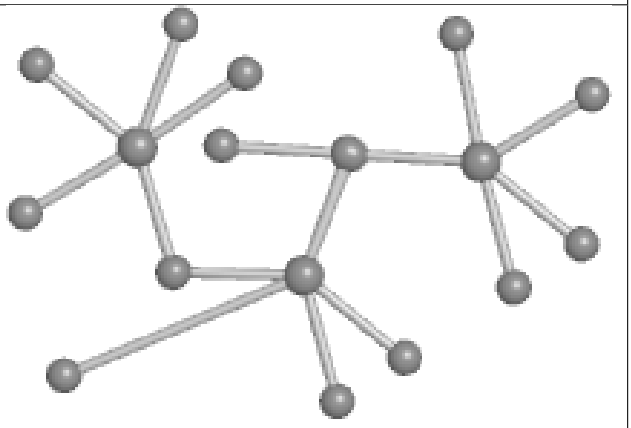
Bond lengths



Bond angles

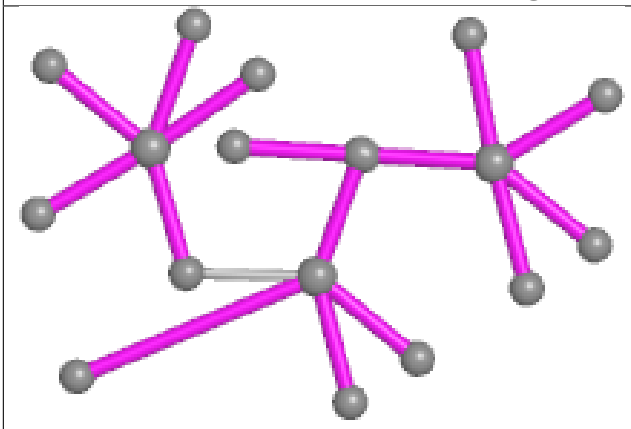


Torsions



Rings

Ligand R2R D 501



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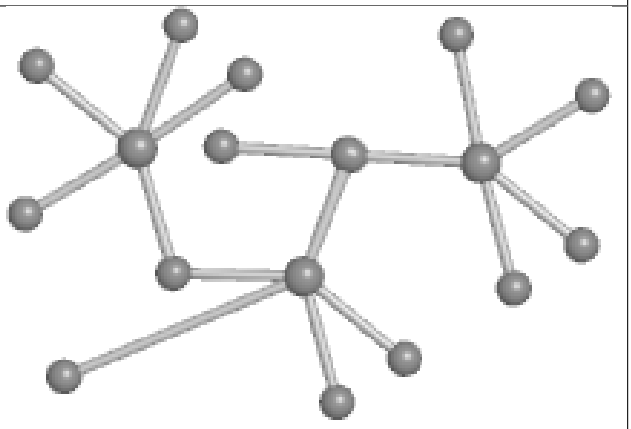
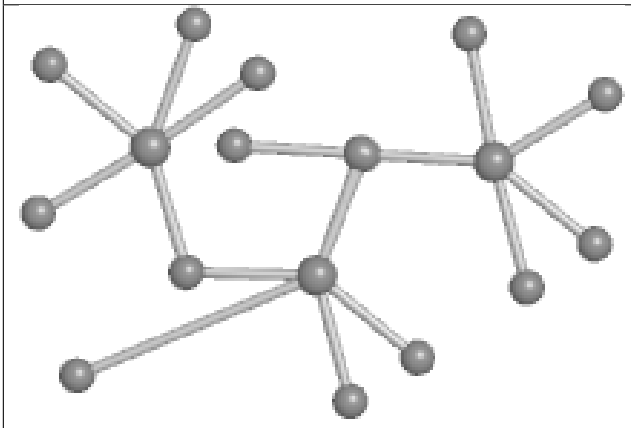
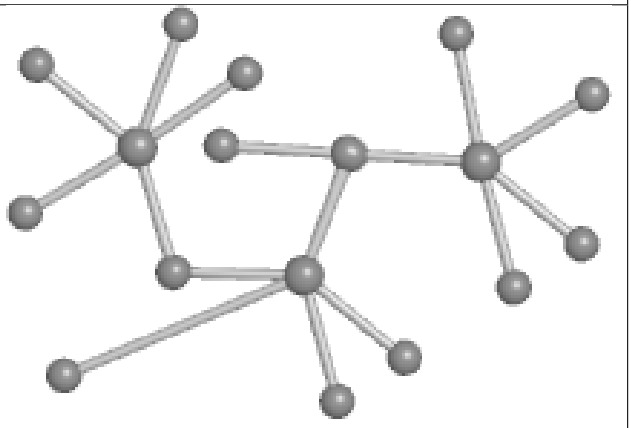


Bond angles

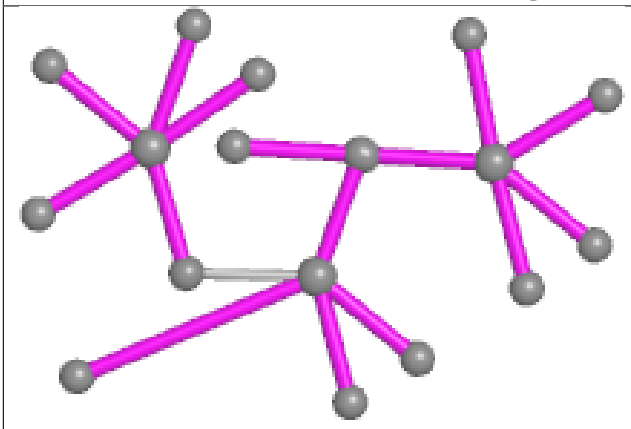


Torsions



Rings

Ligand R2R H 501



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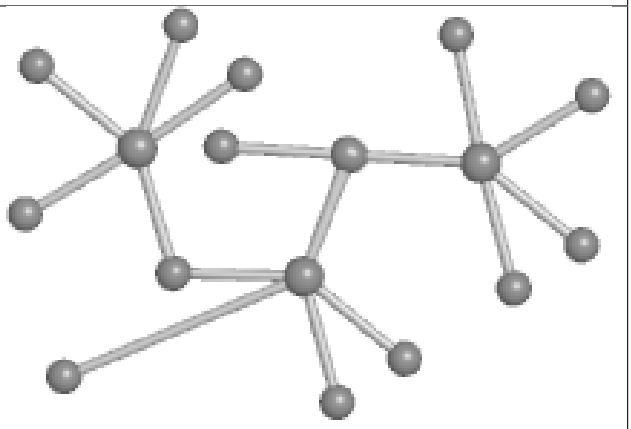
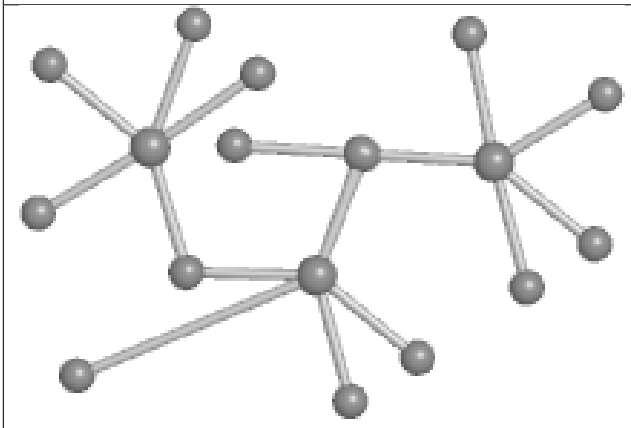


Bond angles



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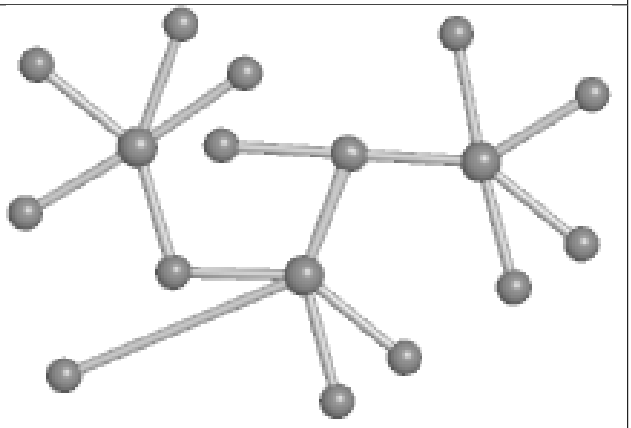
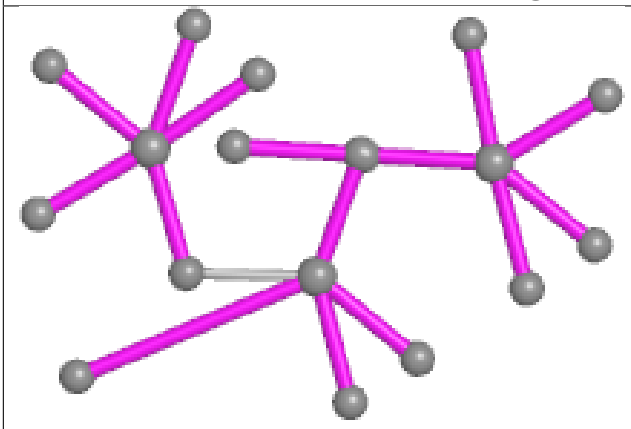


Rings

Ligand R2R E 501



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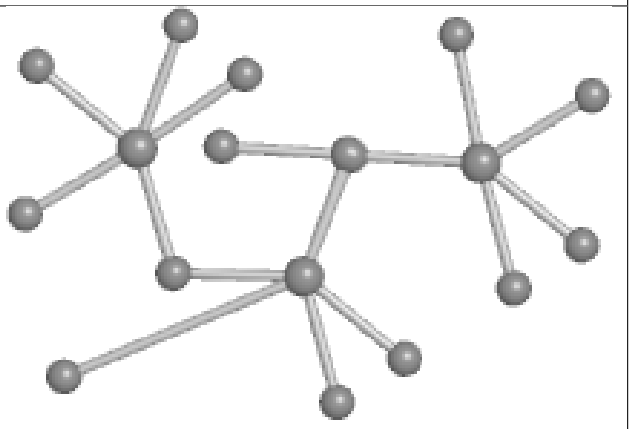
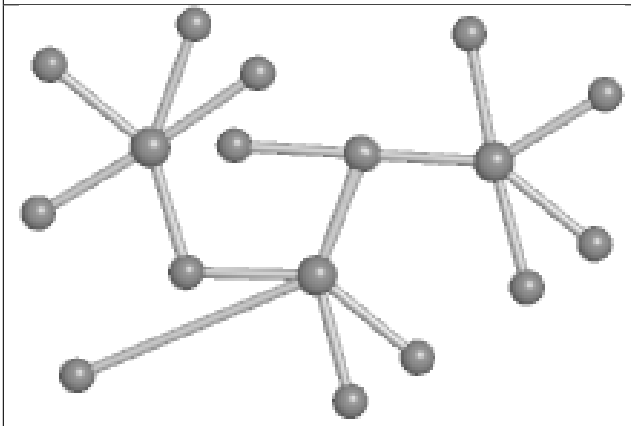
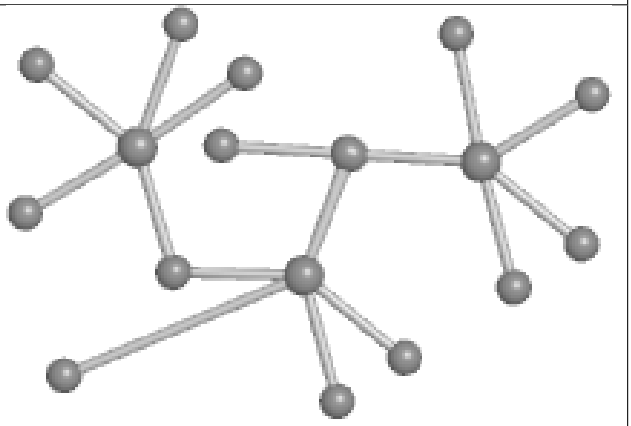


Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

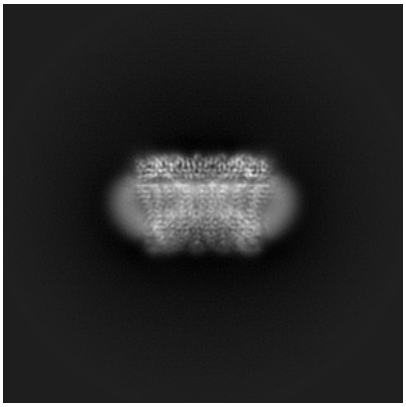
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20789. These allow visual inspection of the internal detail of the map and identification of artifacts.

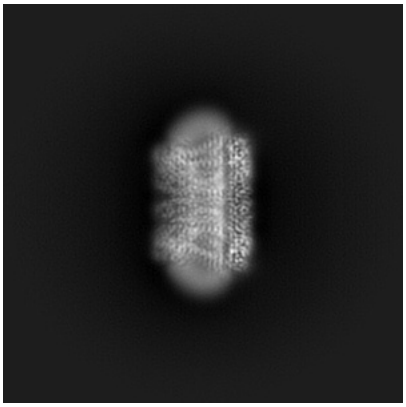
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

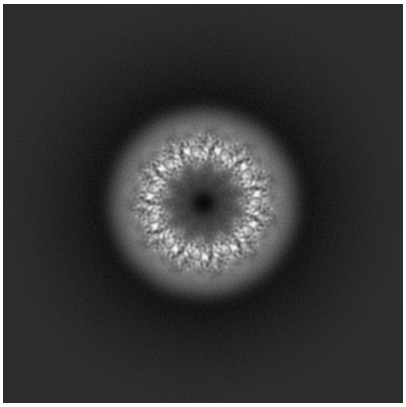
6.1.1 Primary map



X



Y

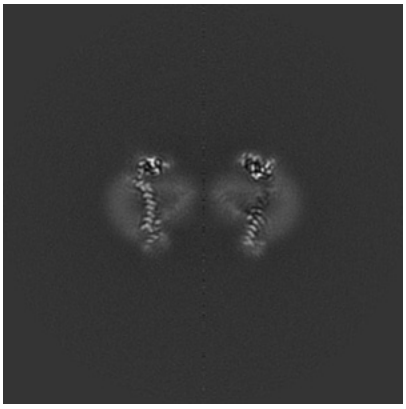


Z

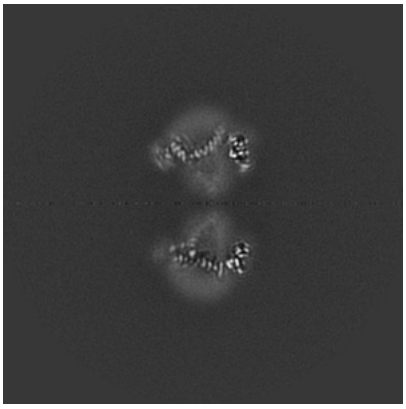
The images above show the map projected in three orthogonal directions.

6.2 Central slices

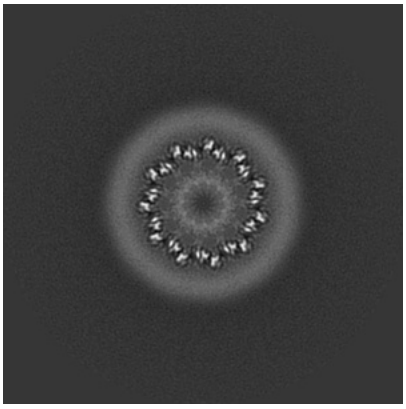
6.2.1 Primary map



X Index: 170



Y Index: 170

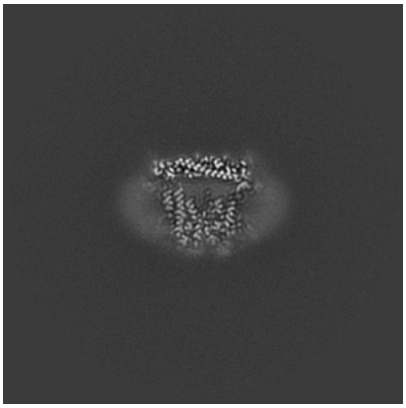


Z Index: 170

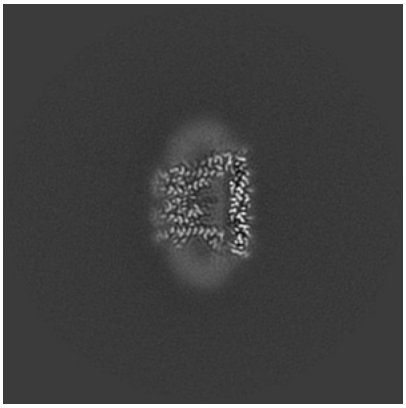
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

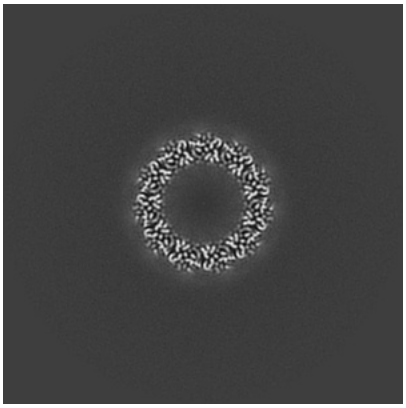
6.3.1 Primary map



X Index: 129



Y Index: 130

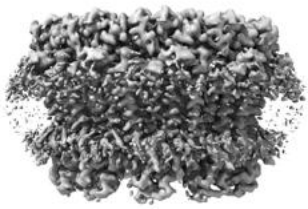


Z Index: 198

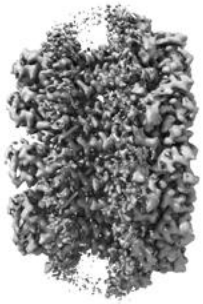
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

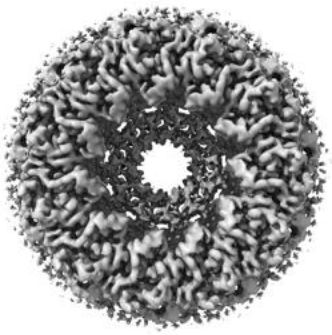
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

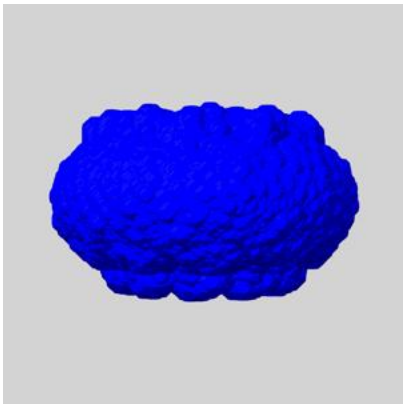
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

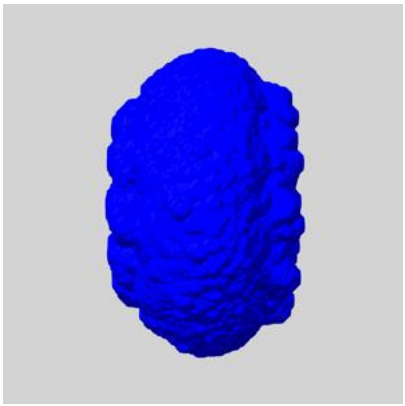
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

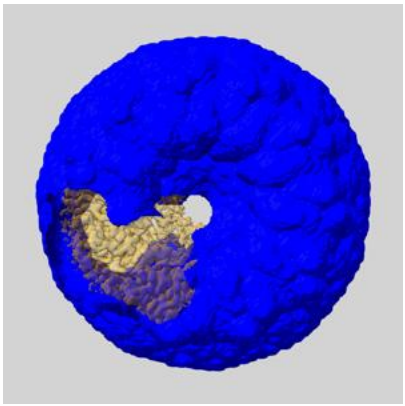
6.5.1 emd_20789_msk_1.map (i)



X



Y

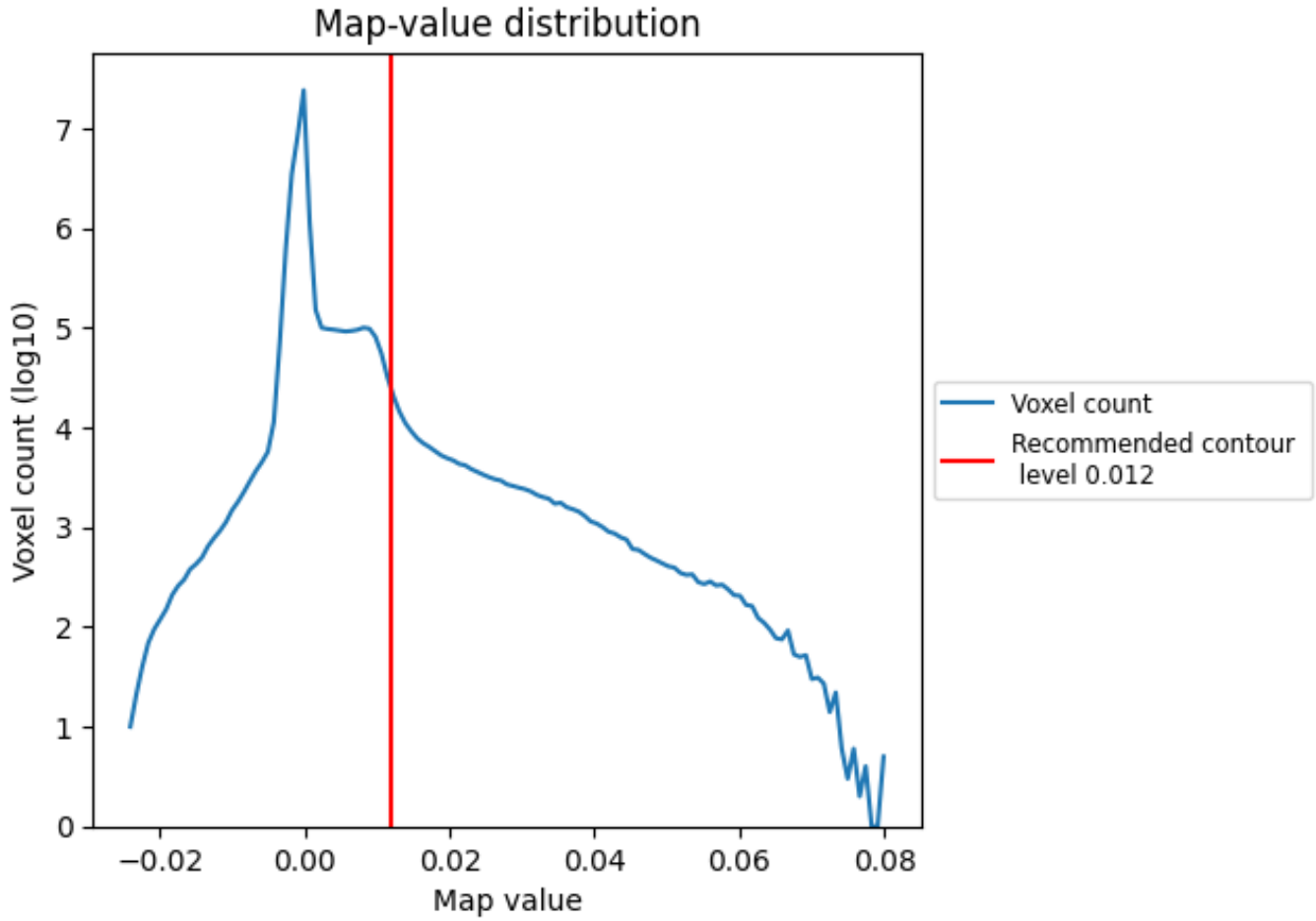


Z

7 Map analysis

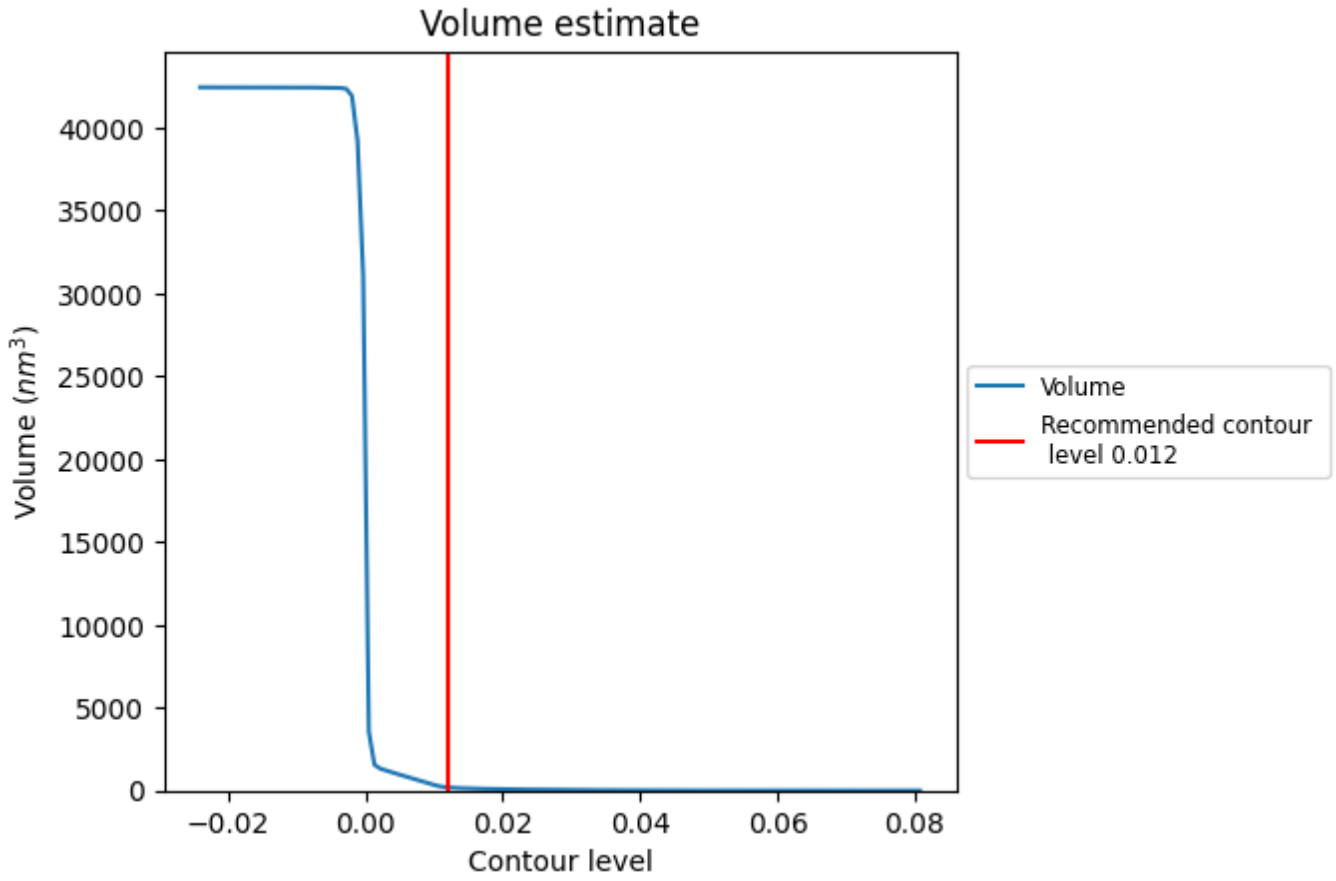
This section contains the results of statistical analysis of the map.

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.

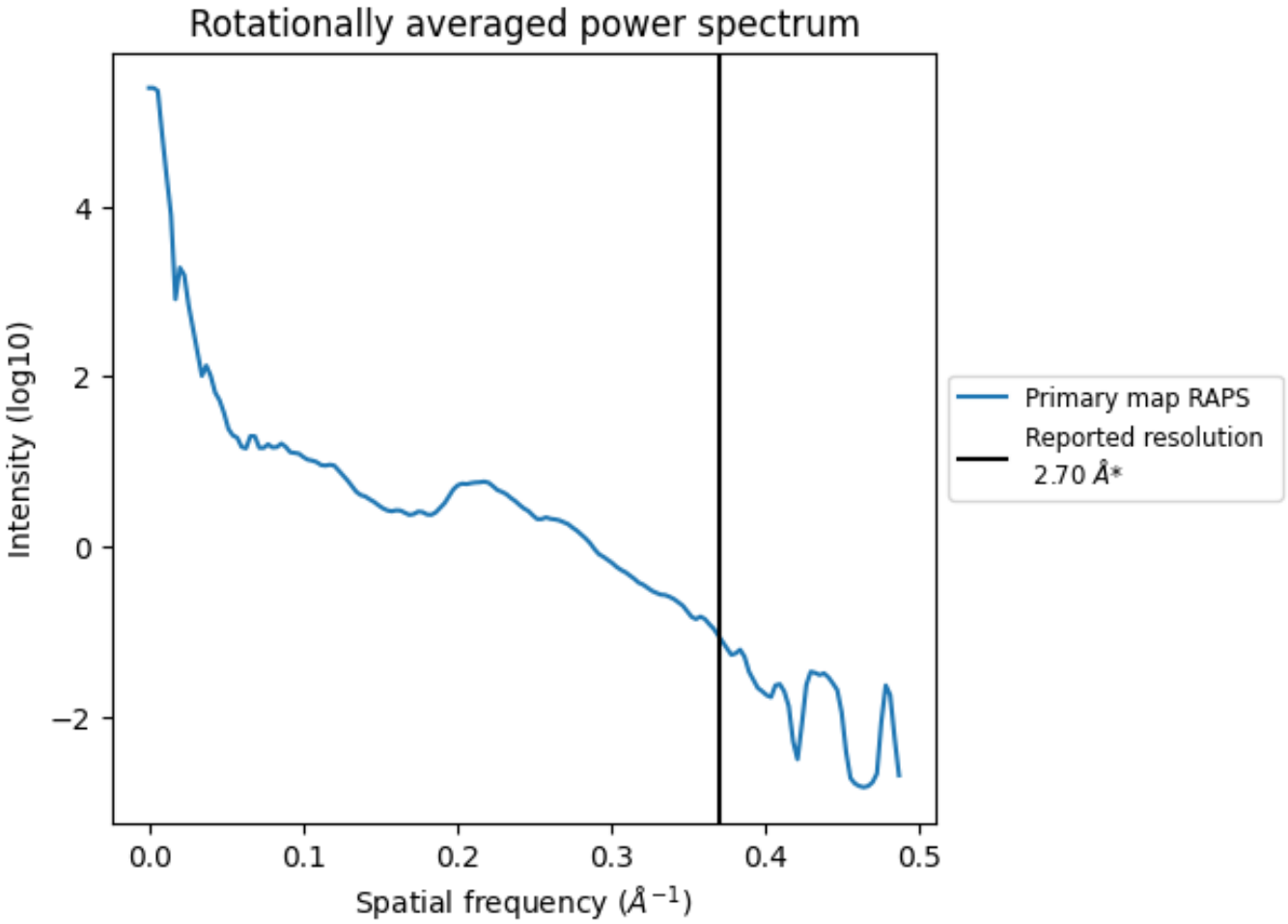
7.2 Volume estimate



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 0.370 Å^{-1}

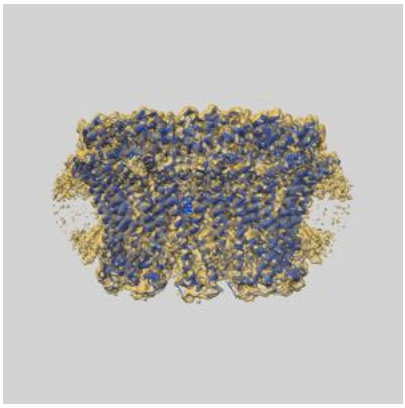
8 Fourier-Shell correlation (i)

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

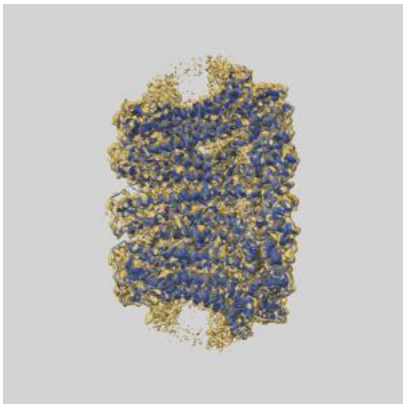
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20789 and PDB model 6UIW. Per-residue inclusion information can be found in section 3 on page 8.

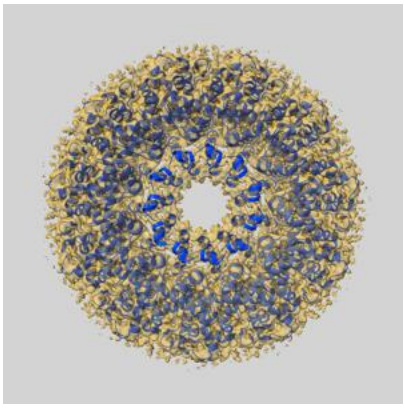
9.1 Map-model overlay



X



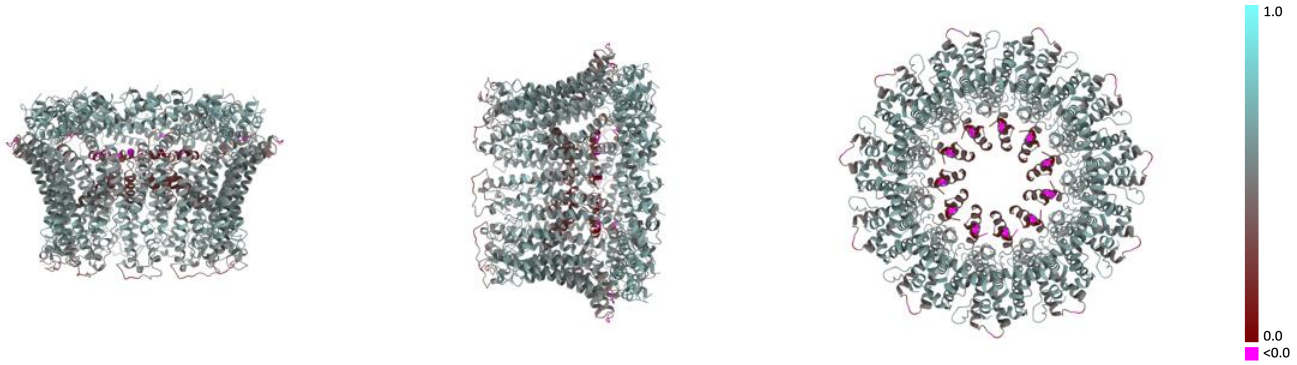
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

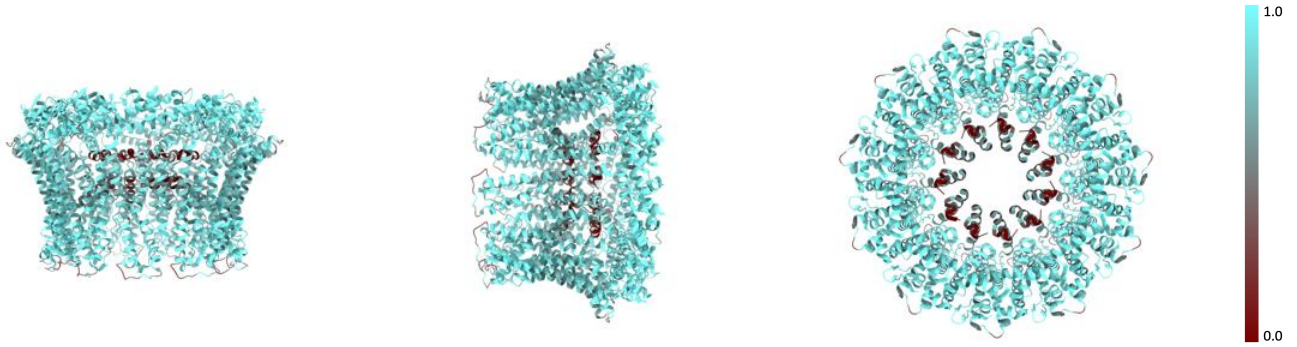
9.2 Q-score mapped to coordinate model (i)



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.

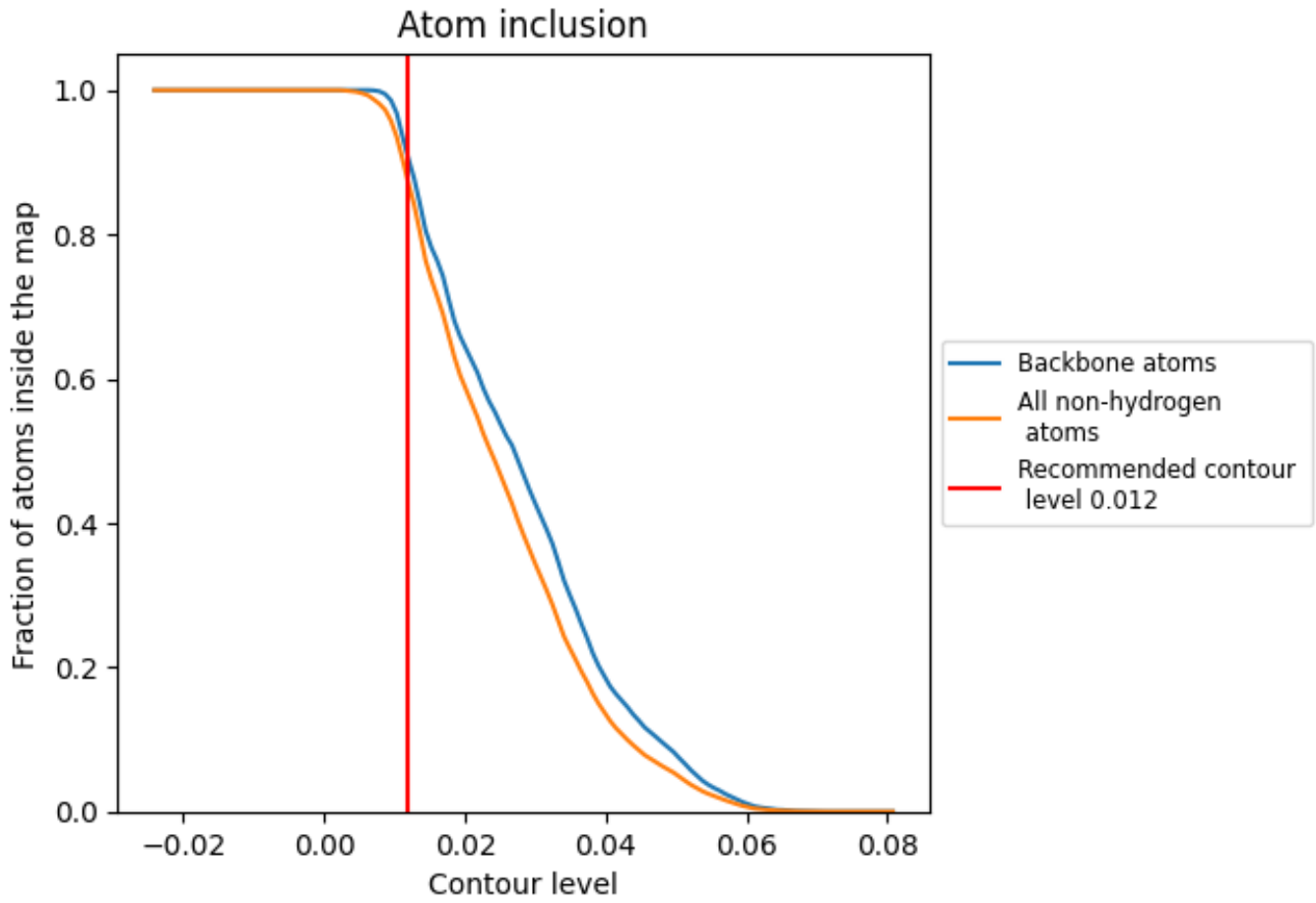
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8701	0.5230
A	0.8712	0.5230
B	0.8674	0.5220
C	0.8717	0.5240
D	0.8702	0.5230
E	0.8693	0.5240
F	0.8698	0.5240
G	0.8717	0.5240
H	0.8698	0.5240
I	0.8702	0.5210
J	0.8712	0.5220
K	0.8688	0.5220