Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:06 AM EST

PDB ID	:	7S4M
EMDB ID	:	EMD-24831
Title	:	CryoEM structure of Methylocystis sp. str. Rockwell pMMO in a POPC nanodisc at 2.42 Angstrom resolution
Authors	:	Koo, C.W.; Rosenzweig, A.C.
Deposited on	:	2021-09-09
Resolution	:	2.42 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:

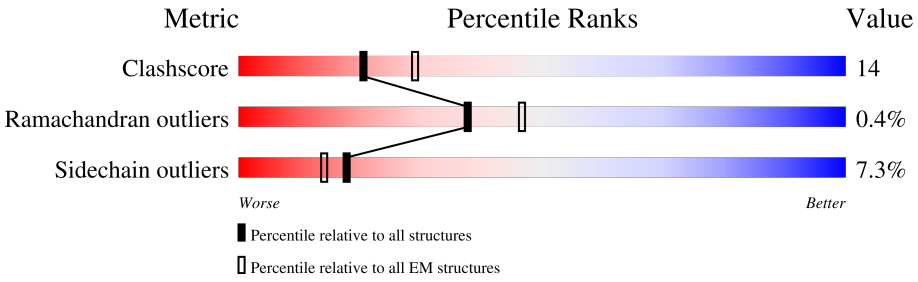
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.42 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	388	14% 79% 19% ·
1	E	388	16% 77% 19% ·
1	I	388	15% 80% 17% ·
2	B	244	8% 62% 35% ·
2	F	244	8% 68% 29% ·
2	J	244	7% 64% 33% ·
3	C	241	24% 67% 30% ·
3	G	241	27% 62% 35% ·

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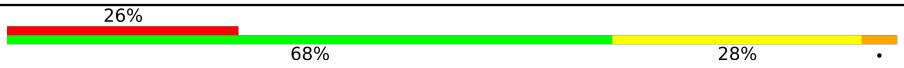
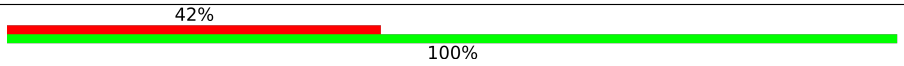
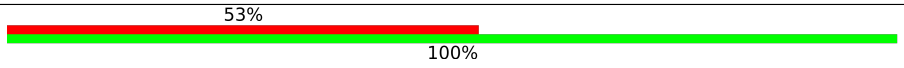
Mol	Chain	Length	Quality of chain
3	K	241	
4	D	19	
4	H	19	
4	N	19	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	D10	B	303	-	-	X	-
7	D10	F	303	-	-	X	-
7	D10	G	305	-	-	X	-
7	D10	J	303	-	-	X	-
7	D10	K	305	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22419 atoms, of which 690 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 Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		
1	E	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		
1	I	388	Total	C	N	O	S	0	0
			3026	1946	521	555	4		

- Molecule 2 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		
2	B	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		
2	J	244	Total	C	N	O	S	0	0
			1974	1336	311	316	11		

- Molecule 3 is a protein called Ammonia monooxygenase/methane monooxygenase, subunit C family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		
3	C	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		
3	K	241	Total	C	N	O	S	0	0
			1982	1337	311	325	9		

- Molecule 4 is a protein called Unidentified Helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	19	Total	C	N	O	0	0
			95	57	19	19		

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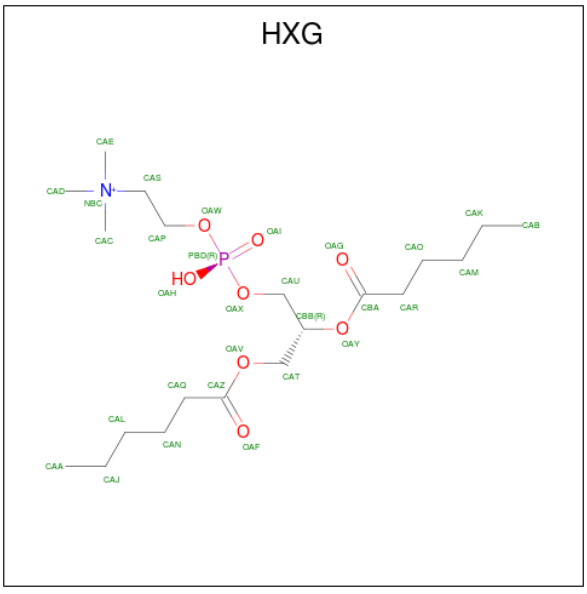
Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	19	Total	C	N	O	0	0
			95	57	19	19		
4	H	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

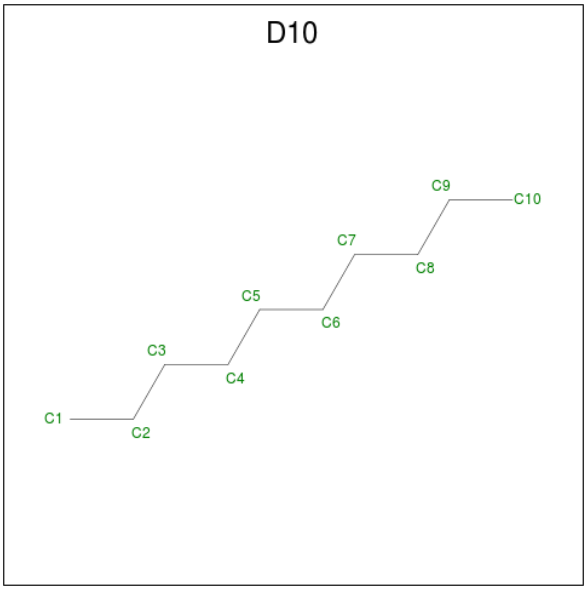
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Cu	0
			1	1	
5	G	1	Total	Cu	0
			1	1	
5	C	1	Total	Cu	0
			1	1	
5	K	1	Total	Cu	0
			1	1	
5	E	1	Total	Cu	0
			1	1	
5	I	1	Total	Cu	0
			1	1	

- Molecule 6 is 1,2-dihexanoyl-sn-glycero-3-phosphocholine (three-letter code: HXG) (formula: $C_{20}H_{41}NO_8P$) (labeled as "Ligand of Interest" by depositor).



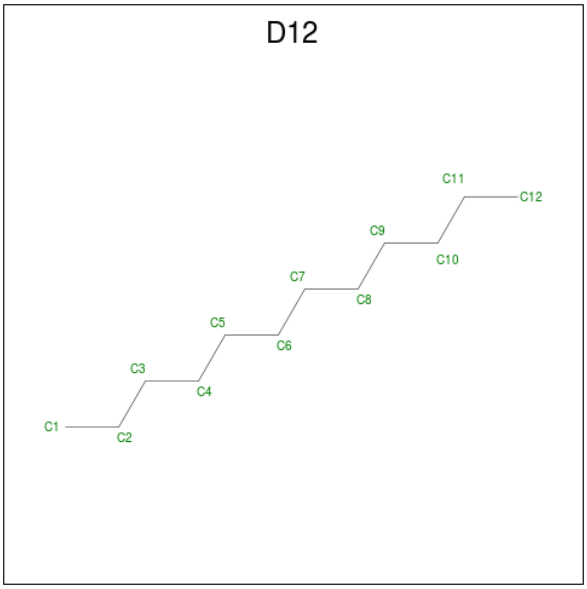
Mol	Chain	Residues	Atoms						AltConf
6	F	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	F	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	B	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	B	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	J	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	J	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	G	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	G	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	C	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	C	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	K	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	
6	K	1	Total	C	H	N	O	P	0
			140	40	80	2	16	2	

- Molecule 7 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	H	0
			32	10	22	
7	B	1	Total	C	H	0
			32	10	22	
7	J	1	Total	C	H	0
			32	10	22	
7	G	1	Total	C	H	0
			32	10	22	
7	C	1	Total	C	H	0
			32	10	22	
7	K	1	Total	C	H	0
			32	10	22	

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	G	1	Total	C	H	0
			38	12	26	
8	C	1	Total	C	H	0
			38	12	26	
8	K	1	Total	C	H	0
			38	12	26	

- Molecule 9 is water.

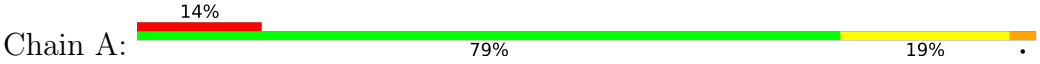
Mol	Chain	Residues	Atoms	AltConf
9	A	6	Total O 6 6	0
9	F	3	Total O 3 3	0
9	B	4	Total O 4 4	0
9	J	6	Total O 6 6	0
9	G	1	Total O 1 1	0
9	C	1	Total O 1 1	0
9	K	2	Total O 2 2	0
9	N	3	Total O 3 3	0
9	E	5	Total O 5 5	0
9	I	5	Total O 5 5	0

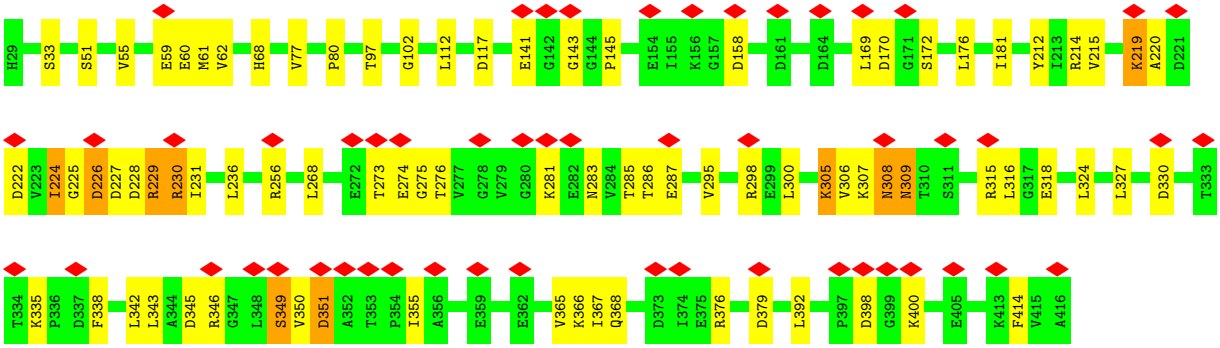
3 Residue-property plots (i)

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

• Molecule 1: Particulate methane monooxygenase alpha subunit

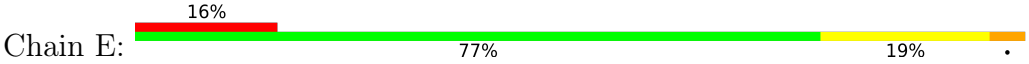
Chain A:

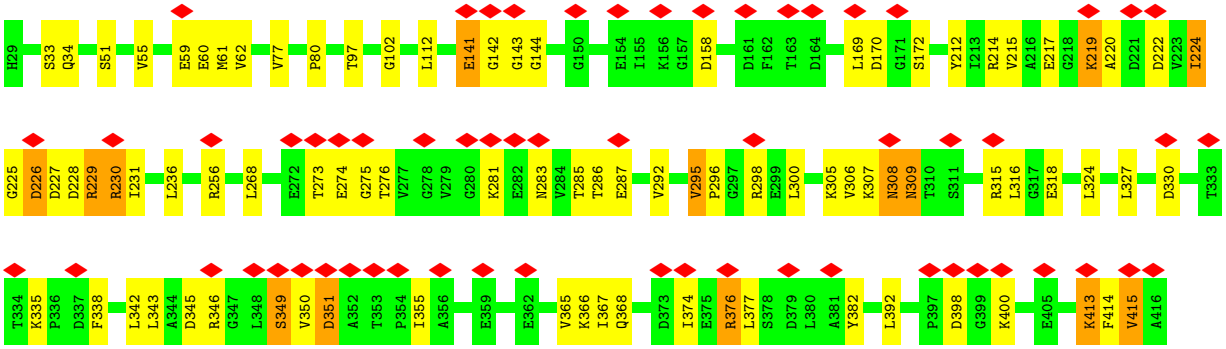




• Molecule 1: Particulate methane monooxygenase alpha subunit

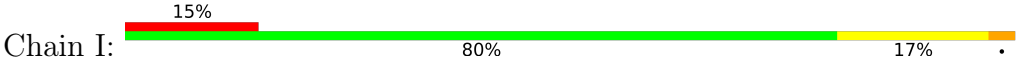
Chain E:

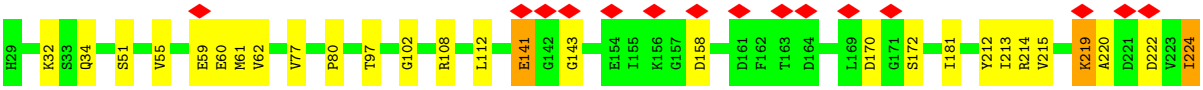


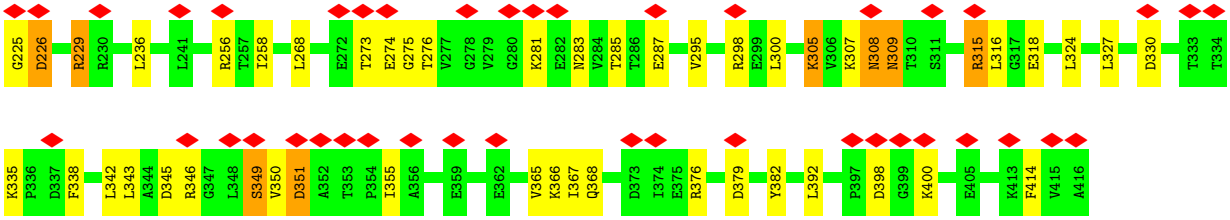


• Molecule 1: Particulate methane monooxygenase alpha subunit

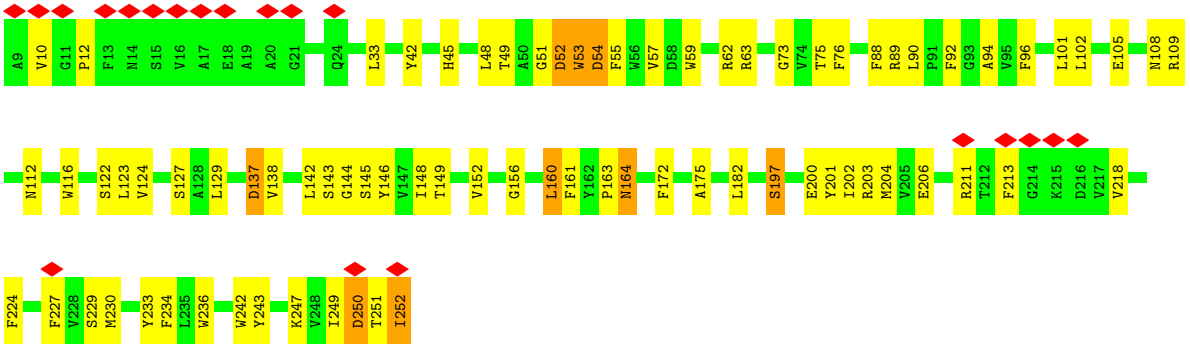
Chain I:



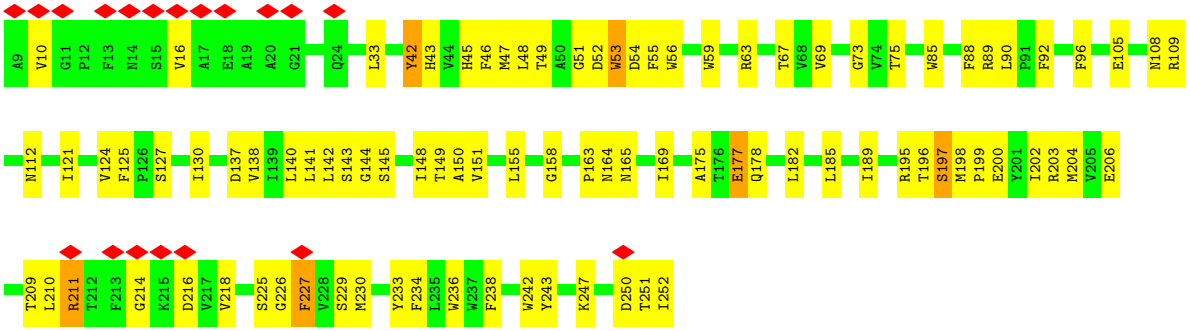




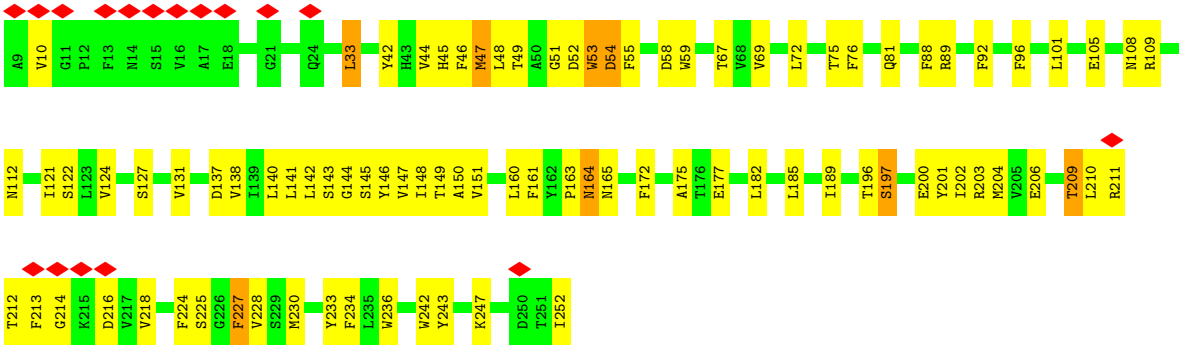
• Molecule 2: Particulate methane monooxygenase beta subunit



• Molecule 2: Particulate methane monooxygenase beta subunit

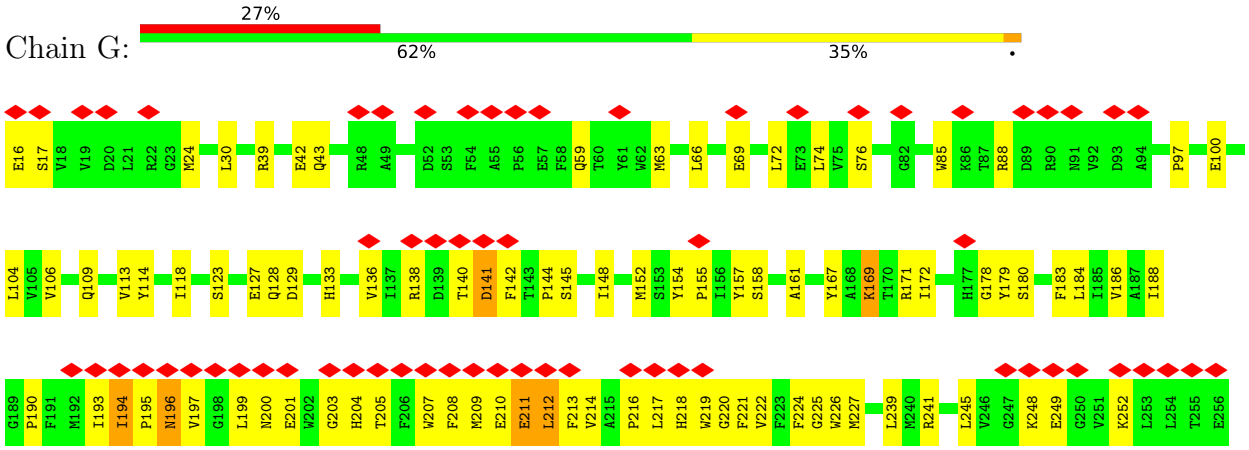


• Molecule 2: Particulate methane monooxygenase beta subunit



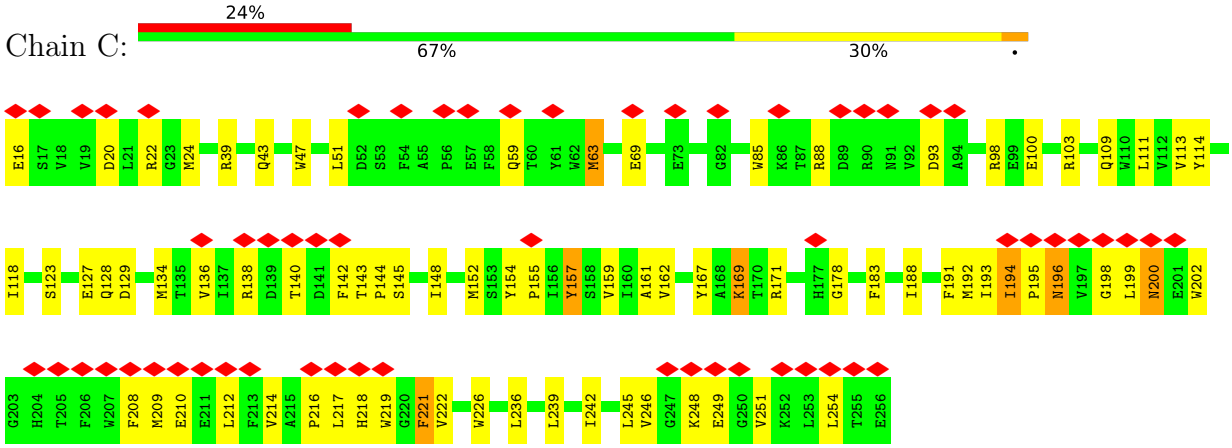
• Molecule 3: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

Chain G:



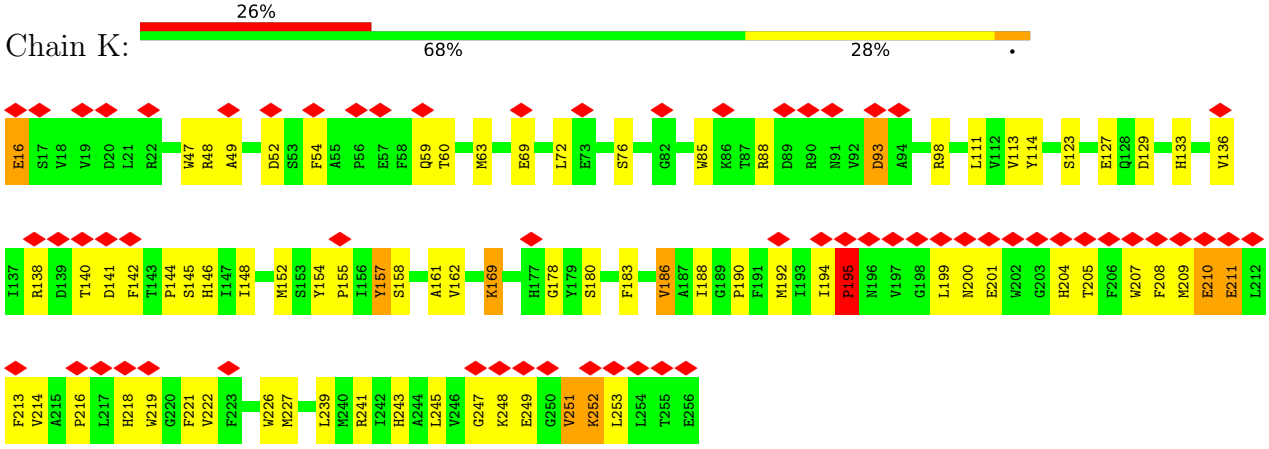
• Molecule 3: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

Chain C:



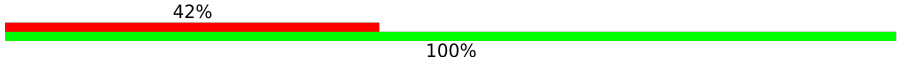
• Molecule 3: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

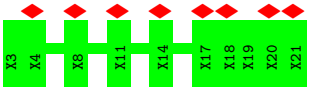
Chain K:



• Molecule 4: Unidentified Helix

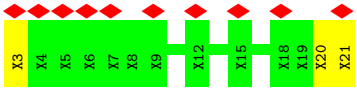
Chain D:





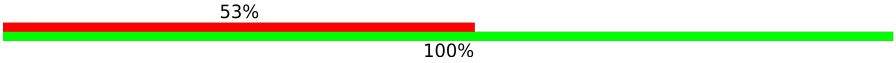
• Molecule 4: Unidentified Helix

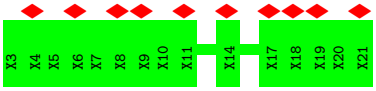
Chain N:



• Molecule 4: Unidentified Helix

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490196	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 ($e^-/Å^2$)	1.02	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.419	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0758	Depositor
Map size (Å)	199.68, 199.68, 199.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.52, 0.52, 0.52	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, D10, D12, HXG

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	0.40	0/3103	0.56	0/4227
1	E	0.41	0/3103	0.57	0/4227
1	I	0.41	0/3103	0.56	0/4227
2	B	0.32	0/2052	0.50	0/2814
2	F	0.32	0/2052	0.50	1/2814 (0.0%)
2	J	0.32	0/2052	0.50	0/2814
3	C	0.30	0/2052	0.51	0/2801
3	G	0.31	0/2052	0.53	0/2801
3	K	0.34	0/2052	0.57	2/2801 (0.1%)
All	All	0.36	0/21621	0.54	3/29526 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	2
1	I	0	2
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	208	PHE	CB-CA-C	6.86	124.12	110.40
2	F	33	LEU	CA-CB-CG	5.71	128.43	115.30
3	K	195	PRO	CB-CA-C	-5.12	99.19	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ASP	Peptide
1	A	308	ASN	Peptide
1	E	226	ASP	Peptide
1	E	308	ASN	Peptide
1	I	226	ASP	Peptide
1	I	308	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3026	0	3015	44	0
1	E	3026	0	3015	56	0
1	I	3026	0	3015	51	0
2	B	1974	0	1932	101	0
2	F	1974	0	1932	94	0
2	J	1974	0	1932	111	0
3	C	1982	0	1960	70	0
3	G	1982	0	1960	103	0
3	K	1982	0	1960	66	0
4	D	95	0	21	0	0
4	H	95	0	21	0	0
4	N	95	0	22	6	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
6	B	60	80	80	4	0
6	C	60	80	80	3	0
6	F	60	80	80	2	0
6	G	60	80	80	10	0
6	J	60	80	80	3	0
6	K	60	80	80	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	22	22	11	0
7	C	10	22	22	1	0
7	F	10	22	22	11	0
7	G	10	22	22	9	0
7	J	10	22	22	10	0
7	K	10	22	22	10	0
8	C	12	26	26	0	0
8	G	12	26	26	2	0
8	K	12	26	26	2	0
9	A	6	0	0	0	0
9	B	4	0	0	3	0
9	C	1	0	0	6	0
9	E	5	0	0	0	0
9	F	3	0	0	0	0
9	G	1	0	0	0	0
9	I	5	0	0	2	0
9	J	6	0	0	6	0
9	K	2	0	0	0	0
9	N	3	0	0	5	0
All	All	21729	690	21475	584	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 14.

All (584) 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)
2:J:214:GLY:HA2	9:J:404:HOH:O	1.38	1.19
2:J:252:ILE:CD1	6:K:302:HXG:H11	1.80	1.12
2:J:252:ILE:HD11	6:K:302:HXG:H11	1.12	1.10
2:F:243:TYR:CZ	7:F:303:D10:H101	1.91	1.05
9:J:402:HOH:O	3:G:209:MET:SD	2.14	1.05
2:B:243:TYR:CZ	7:B:303:D10:H101	1.92	1.05
2:J:252:ILE:HD11	6:K:302:HXG:CAQ	1.92	0.99
2:J:216:ASP:HB2	7:G:305:D10:H32	1.45	0.96
2:B:216:ASP:HB2	7:K:305:D10:H32	1.46	0.95
2:J:148:ILE:HD11	6:G:302:HXG:H9	1.45	0.95
3:K:142:PHE:HE2	7:K:305:D10:H82	1.30	0.95
9:J:404:HOH:O	1:E:382:TYR:HE2	1.48	0.94
3:G:209:MET:HG3	1:E:142:GLY:C	1.88	0.93
9:B:404:HOH:O	1:I:382:TYR:HE2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:142:PHE:CE2	7:K:305:D10:H82	2.07	0.90
2:J:243:TYR:CZ	7:J:303:D10:H101	2.06	0.90
3:C:100:GLU:HG2	3:C:245:LEU:HD11	1.55	0.88
4:N:21:UNK:C	9:N:103:HOH:O	2.22	0.87
2:B:243:TYR:CZ	7:B:303:D10:C10	2.58	0.87
9:J:404:HOH:O	1:E:382:TYR:CE2	2.26	0.87
2:F:243:TYR:CZ	7:F:303:D10:C10	2.58	0.86
2:B:199:PRO:HD2	2:B:202:ILE:HD12	1.57	0.86
3:G:209:MET:HG3	1:E:142:GLY:O	1.76	0.85
9:B:404:HOH:O	1:I:382:TYR:CE2	2.27	0.84
2:B:148:ILE:HD11	6:K:302:HXG:H6	1.62	0.80
3:C:195:PRO:CA	9:C:401:HOH:O	2.29	0.80
3:C:195:PRO:O	9:C:401:HOH:O	2.01	0.78
2:F:249:ILE:HD11	2:F:252:ILE:HG22	1.65	0.77
3:K:141:ASP:OD2	7:K:305:D10:H13	1.83	0.77
2:B:51:GLY:HA2	2:B:52:ASP:HB3	1.66	0.77
2:J:51:GLY:HA2	2:J:52:ASP:HB3	1.67	0.77
2:F:51:GLY:HA2	2:F:52:ASP:HB3	1.68	0.76
3:K:142:PHE:HE2	7:K:305:D10:C8	1.97	0.76
2:J:108:ASN:ND2	3:K:127:GLU:HB3	1.99	0.76
3:C:195:PRO:C	9:C:401:HOH:O	2.25	0.76
2:F:108:ASN:ND2	3:G:127:GLU:HB3	2.00	0.76
2:B:67:THR:HA	2:B:225:SER:HB3	1.67	0.75
2:B:216:ASP:HB2	7:K:305:D10:C3	2.17	0.75
3:G:59:GLN:HA	3:G:63:MET:HB2	1.67	0.74
3:K:192:MET:HA	3:K:195:PRO:HG2	1.68	0.74
2:F:108:ASN:HD22	3:G:127:GLU:HB3	1.53	0.74
3:K:59:GLN:HA	3:K:63:MET:HB2	1.69	0.73
3:C:59:GLN:HA	3:C:63:MET:HB2	1.69	0.73
2:F:252:ILE:HG21	3:G:184:LEU:HD11	1.70	0.72
2:J:242:TRP:HB3	7:J:303:D10:H62	1.72	0.72
3:G:141:ASP:OD2	7:G:305:D10:H13	1.89	0.72
2:J:247:LYS:NZ	7:J:303:D10:H13	2.05	0.71
2:J:227:PHE:CE1	3:G:195:PRO:HB3	2.25	0.70
3:C:142:PHE:HE2	7:C:305:D10:H51	1.56	0.70
3:C:198:GLY:O	3:C:202:TRP:N	2.23	0.70
2:J:45:HIS:HA	3:K:222:VAL:HG13	1.74	0.70
2:F:249:ILE:CD1	2:F:252:ILE:HG22	2.21	0.69
2:J:216:ASP:HB2	7:G:305:D10:C3	2.22	0.69
2:B:242:TRP:HB3	7:B:303:D10:H62	1.75	0.69
2:B:49:THR:HG23	3:C:222:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:HIS:HA	3:G:222:VAL:HG13	1.75	0.68
2:F:227:PHE:HA	2:F:230:MET:HG3	1.74	0.68
2:B:108:ASN:ND2	2:B:112:ASN:OD1	2.27	0.68
2:J:243:TYR:CZ	7:J:303:D10:C10	2.76	0.68
3:G:196:ASN:HA	3:G:199:LEU:HB3	1.74	0.67
2:J:224:PHE:HD1	3:G:199:LEU:HA	1.59	0.67
3:C:208:PHE:HB2	3:C:217:LEU:HD11	1.74	0.67
3:K:252:LYS:HE3	3:K:253:LEU:HG	1.77	0.67
2:F:242:TRP:HB3	7:F:303:D10:H62	1.76	0.67
2:J:48:LEU:HD13	3:K:221:PHE:HB3	1.77	0.67
3:C:195:PRO:CB	9:C:401:HOH:O	2.43	0.66
2:F:202:ILE:HD11	3:G:212:LEU:HB2	1.75	0.66
1:A:376:ARG:NH2	1:A:379:ASP:OD2	2.29	0.66
2:F:108:ASN:OD1	2:F:112:ASN:ND2	2.24	0.66
2:B:48:LEU:HD13	3:C:221:PHE:HB3	1.75	0.66
2:J:146:TYR:HA	2:J:149:THR:HG22	1.78	0.66
3:C:85:TRP:CH2	6:C:302:HXG:H27	2.31	0.66
2:F:227:PHE:CD2	9:C:401:HOH:O	2.47	0.66
2:F:211:ARG:NH1	3:C:209:MET:O	2.28	0.65
2:B:243:TYR:OH	7:B:303:D10:H101	1.96	0.65
3:G:133:HIS:HB3	3:G:211:GLU:HG2	1.77	0.64
3:G:100:GLU:HG2	3:G:245:LEU:HD11	1.79	0.64
1:I:376:ARG:NH2	1:I:379:ASP:OD2	2.29	0.64
1:A:176:LEU:HD21	2:B:185:LEU:HD22	1.80	0.64
3:C:24:MET:HB2	3:C:109:GLN:HB3	1.80	0.64
2:F:243:TYR:CE2	7:F:303:D10:H101	2.33	0.64
3:G:248:LYS:HE2	3:G:248:LYS:HA	1.79	0.64
3:G:209:MET:CG	1:E:142:GLY:O	2.46	0.64
3:G:142:PHE:CE2	7:G:305:D10:H82	2.33	0.63
2:J:216:ASP:CB	7:G:305:D10:H32	2.23	0.63
3:K:248:LYS:HE2	3:K:248:LYS:HA	1.79	0.63
1:I:273:THR:O	1:I:276:THR:OG1	2.17	0.63
2:F:252:ILE:HD12	2:J:147:VAL:HB	1.80	0.63
1:E:273:THR:O	1:E:276:THR:OG1	2.17	0.63
4:N:21:UNK:O	9:N:101:HOH:O	2.16	0.63
2:J:10:VAL:HG13	3:K:249:GLU:HG2	1.79	0.62
3:G:196:ASN:O	3:G:200:ASN:N	2.24	0.62
3:G:142:PHE:HE2	7:G:305:D10:H82	1.64	0.62
3:G:138:ARG:NH2	3:G:201:GLU:OE2	2.32	0.62
1:I:214:ARG:HG3	1:I:219:LYS:HD2	1.82	0.62
1:A:273:THR:O	1:A:276:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:LYS:NZ	7:B:303:D10:H13	2.15	0.62
2:B:243:TYR:CE2	7:B:303:D10:H101	2.35	0.61
1:A:77:VAL:HG13	1:A:143:GLY:HA3	1.82	0.61
2:B:148:ILE:HD12	8:K:303:D12:H42	1.80	0.61
2:F:200:GLU:OE2	2:F:203:ARG:NH2	2.32	0.61
1:A:214:ARG:HG3	1:A:219:LYS:HD2	1.82	0.61
2:F:48:LEU:HD13	3:G:221:PHE:HB3	1.82	0.61
2:J:161:PHE:O	2:J:164:ASN:ND2	2.34	0.61
1:E:77:VAL:HG13	1:E:143:GLY:HA3	1.82	0.61
3:G:252:LYS:HE3	1:E:217:GLU:OE1	2.01	0.61
2:B:243:TYR:OH	7:B:303:D10:C10	2.47	0.61
1:I:77:VAL:HG13	1:I:143:GLY:HA3	1.82	0.61
2:F:197:SER:OG	3:G:133:HIS:O	2.19	0.61
9:J:402:HOH:O	3:G:209:MET:CE	2.45	0.61
3:G:196:ASN:HB2	3:G:221:PHE:CE2	2.36	0.61
4:N:20:UNK:CA	9:N:102:HOH:O	2.48	0.60
2:F:243:TYR:OH	7:F:303:D10:H101	2.00	0.60
3:K:200:ASN:OD1	3:K:204:HIS:ND1	2.34	0.60
1:E:214:ARG:HG3	1:E:219:LYS:HD2	1.82	0.60
2:F:175:ALA:HB1	2:F:182:LEU:HD11	1.84	0.60
1:A:236:LEU:HB2	2:B:138:VAL:HG11	1.84	0.60
1:E:398:ASP:OD1	1:E:398:ASP:N	2.31	0.60
2:B:46:PHE:HZ	2:B:69:VAL:HG13	1.65	0.60
2:B:209:THR:OG1	9:B:401:HOH:O	2.16	0.59
3:C:140:THR:HG23	3:C:142:PHE:H	1.66	0.59
2:B:148:ILE:CD1	6:K:302:HXG:H6	2.32	0.59
2:J:175:ALA:HB1	2:J:182:LEU:HD11	1.84	0.59
3:K:129:ASP:OD1	3:K:145:SER:OG	2.20	0.59
2:F:243:TYR:OH	7:F:303:D10:C10	2.51	0.58
1:E:324:LEU:HD13	1:E:377:LEU:HD11	1.84	0.58
2:F:250:ASP:OD1	2:F:250:ASP:N	2.36	0.58
3:G:200:ASN:O	3:G:204:HIS:N	2.27	0.58
2:F:252:ILE:C	2:J:145:SER:HB2	2.24	0.58
2:J:144:GLY:HA3	6:G:302:HXG:H38	1.84	0.58
4:N:20:UNK:CB	9:N:102:HOH:O	2.51	0.58
1:E:227:ASP:HA	1:E:230:ARG:HG3	1.86	0.58
3:K:136:VAL:HG23	3:K:138:ARG:H	1.68	0.58
3:K:200:ASN:O	3:K:204:HIS:N	2.29	0.58
2:B:227:PHE:CE1	3:K:195:PRO:HG3	2.38	0.58
2:J:143:SER:OG	2:J:144:GLY:N	2.37	0.58
3:G:136:VAL:HG23	3:G:138:ARG:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:VAL:HG13	3:C:249:GLU:HG2	1.85	0.57
1:E:228:ASP:HA	1:E:231:ILE:HD12	1.86	0.57
1:A:227:ASP:HA	1:A:230:ARG:HG3	1.86	0.57
1:A:414:PHE:HB3	1:E:256:ARG:HD3	1.86	0.57
2:J:148:ILE:HD11	6:G:302:HXG:CAN	2.27	0.57
2:B:175:ALA:HB1	2:B:182:LEU:HD11	1.85	0.57
3:K:85:TRP:O	3:K:88:ARG:NH1	2.34	0.57
2:J:138:VAL:HG11	1:I:236:LEU:HB2	1.86	0.57
2:B:48:LEU:HB3	3:C:218:HIS:HB3	1.86	0.57
1:A:228:ASP:HA	1:A:231:ILE:HD12	1.86	0.57
3:G:216:PRO:HA	3:G:219:TRP:CG	2.40	0.56
1:A:80:PRO:HB2	1:A:112:LEU:HB2	1.87	0.56
2:F:89:ARG:O	1:E:224:ILE:HG13	2.04	0.56
1:A:256:ARG:HD3	1:I:414:PHE:HB3	1.87	0.56
2:F:51:GLY:HA3	2:F:53:TRP:H	1.69	0.56
3:G:141:ASP:N	3:G:141:ASP:OD1	2.39	0.56
1:I:225:GLY:HA2	1:I:229:ARG:HH22	1.71	0.56
2:J:213:PHE:HB3	1:E:33:SER:HB2	1.87	0.56
3:K:216:PRO:HA	3:K:219:TRP:CG	2.41	0.56
1:I:80:PRO:HB2	1:I:112:LEU:HB2	1.87	0.56
3:G:193:ILE:C	3:G:195:PRO:HD3	2.27	0.56
2:B:144:GLY:HA3	6:K:302:HXG:H38	1.88	0.56
3:K:133:HIS:HB3	3:K:211:GLU:HG2	1.87	0.55
1:A:225:GLY:HA2	1:A:229:ARG:HH22	1.71	0.55
2:B:195:ARG:HB3	3:C:134:MET:HE2	1.87	0.55
3:K:192:MET:CA	3:K:195:PRO:HG2	2.34	0.55
2:J:209:THR:HG22	2:J:211:ARG:H	1.70	0.55
2:J:211:ARG:HH22	3:G:209:MET:HE1	1.72	0.55
3:G:74:LEU:HA	8:G:303:D12:H121	1.87	0.55
2:B:59:TRP:HZ2	2:B:202:ILE:HG22	1.71	0.55
3:G:114:TYR:CE1	3:G:161:ALA:HB2	2.42	0.54
1:E:80:PRO:HB2	1:E:112:LEU:HB2	1.87	0.54
2:J:51:GLY:HA3	2:J:53:TRP:H	1.73	0.54
1:E:225:GLY:HA2	1:E:229:ARG:HH22	1.71	0.54
3:G:113:VAL:HG21	6:G:304:HXG:H8	1.88	0.54
2:J:88:PHE:CE2	1:I:212:TYR:HB2	2.42	0.54
2:J:252:ILE:HD12	6:K:302:HXG:H7	1.89	0.54
3:G:195:PRO:HD2	3:G:196:ASN:H	1.72	0.54
3:K:169:LYS:NZ	3:K:178:GLY:O	2.40	0.54
3:K:188:ILE:HD11	6:K:302:HXG:H1	1.89	0.54
2:F:54:ASP:OD1	2:F:127:SER:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:51:GLY:CA	2:J:52:ASP:HB3	2.37	0.54
1:I:398:ASP:OD1	1:I:398:ASP:N	2.31	0.54
2:B:51:GLY:CA	2:B:52:ASP:HB3	2.36	0.54
2:J:148:ILE:CD1	6:G:302:HXG:H9	2.31	0.54
1:A:33:SER:HB2	2:F:213:PHE:HB3	1.89	0.53
2:J:81:GLN:OE1	2:J:233:TYR:OH	2.18	0.53
1:A:51:SER:HB2	1:A:62:VAL:H	1.73	0.53
1:E:376:ARG:CZ	1:E:376:ARG:HB3	2.32	0.53
1:A:145:PRO:HD3	2:F:211:ARG:NH1	2.23	0.53
2:F:224:PHE:HA	2:F:227:PHE:CZ	2.43	0.53
2:B:108:ASN:OD1	3:C:127:GLU:HB3	2.08	0.53
2:J:42:TYR:CD1	2:J:76:PHE:HB2	2.42	0.53
1:A:324:LEU:HG	1:A:342:LEU:HD22	1.91	0.53
2:F:88:PHE:CE2	1:E:212:TYR:HB2	2.44	0.53
3:G:129:ASP:OD1	3:G:145:SER:OG	2.21	0.53
3:C:85:TRP:O	3:C:88:ARG:NH1	2.34	0.53
2:J:247:LYS:HZ2	7:J:303:D10:H13	1.74	0.53
1:E:414:PHE:HB3	1:I:256:ARG:HD3	1.89	0.53
2:F:247:LYS:NZ	7:F:303:D10:H13	2.24	0.53
2:F:146:TYR:HA	2:F:149:THR:HG22	1.90	0.52
3:K:113:VAL:HG21	6:K:304:HXG:H8	1.91	0.52
2:F:138:VAL:HG11	1:E:236:LEU:HB2	1.90	0.52
2:J:216:ASP:CB	7:G:305:D10:C3	2.85	0.52
3:G:85:TRP:O	3:G:88:ARG:NH1	2.37	0.52
3:C:193:ILE:HA	3:C:196:ASN:HB3	1.91	0.52
2:F:211:ARG:NH1	3:C:210:GLU:OE1	2.41	0.52
3:G:154:TYR:HA	3:G:157:TYR:CE2	2.45	0.52
2:F:252:ILE:HD11	6:G:302:HXG:H7	1.91	0.52
2:J:243:TYR:OH	7:J:303:D10:H101	2.08	0.52
3:G:24:MET:HB2	3:G:109:GLN:HB3	1.92	0.52
1:E:51:SER:HB2	1:E:62:VAL:H	1.73	0.52
3:K:72:LEU:O	3:K:76:SER:OG	2.26	0.52
1:E:292:VAL:HG13	1:E:413:LYS:HB2	1.92	0.52
2:B:140:LEU:HD13	2:B:149:THR:HG21	1.90	0.52
2:B:211:ARG:HG3	3:K:204:HIS:O	2.10	0.52
2:J:49:THR:HB	2:J:72:LEU:HD13	1.91	0.52
1:I:51:SER:HB2	1:I:62:VAL:H	1.73	0.52
2:F:143:SER:OG	2:F:144:GLY:N	2.42	0.52
2:B:252:ILE:HD11	6:C:302:HXG:H11	1.91	0.52
1:E:324:LEU:HG	1:E:342:LEU:HD22	1.91	0.52
1:A:224:ILE:HG13	2:B:89:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:216:PRO:HB3	3:K:219:TRP:CE3	2.45	0.52
2:F:102:LEU:HD11	2:F:129:LEU:H	1.75	0.51
3:C:114:TYR:O	3:C:118:ILE:HG22	2.10	0.51
3:C:248:LYS:HA	3:C:248:LYS:HE2	1.92	0.51
2:F:10:VAL:HG23	3:G:249:GLU:HG2	1.91	0.51
2:J:210:LEU:O	1:E:34:GLN:HG2	2.11	0.51
3:G:106:VAL:HG11	6:G:304:HXG:OAH	2.11	0.51
3:G:69:GLU:OE2	3:G:152:MET:HB2	2.11	0.51
3:G:188:ILE:HD11	6:G:302:HXG:H1	1.93	0.51
3:K:142:PHE:CE2	7:K:305:D10:C8	2.81	0.51
2:B:150:ALA:O	2:B:230:MET:HG2	2.11	0.51
1:I:338:PHE:HB3	1:I:343:LEU:HD13	1.92	0.51
2:J:49:THR:HG23	3:K:222:VAL:HG21	1.92	0.51
1:I:324:LEU:HG	1:I:342:LEU:HD22	1.91	0.51
2:B:51:GLY:HA3	2:B:53:TRP:H	1.76	0.50
2:F:51:GLY:HA3	2:F:53:TRP:N	2.27	0.50
2:F:51:GLY:CA	2:F:52:ASP:HB3	2.39	0.50
2:B:45:HIS:HA	3:C:222:VAL:HG22	1.93	0.50
2:F:75:THR:HB	2:F:236:TRP:CD2	2.47	0.50
2:F:252:ILE:HD12	2:J:147:VAL:CB	2.41	0.50
2:B:105:GLU:O	2:B:109:ARG:HG2	2.12	0.50
2:B:54:ASP:OD1	2:B:127:SER:OG	2.24	0.50
2:J:105:GLU:O	2:J:109:ARG:HG2	2.11	0.50
2:F:105:GLU:O	2:F:109:ARG:HG2	2.11	0.50
3:G:222:VAL:HG12	3:G:226:TRP:NE1	2.27	0.50
3:C:129:ASP:OD1	3:C:145:SER:OG	2.23	0.50
3:K:154:TYR:HA	3:K:157:TYR:CE2	2.46	0.50
3:K:218:HIS:O	3:K:221:PHE:HB2	2.11	0.50
2:J:142:LEU:HA	1:I:229:ARG:HG2	1.94	0.49
2:J:200:GLU:HG3	1:I:108:ARG:HA	1.94	0.49
2:J:127:SER:HB2	2:J:165:ASN:HD21	1.78	0.49
3:K:138:ARG:NH2	3:K:201:GLU:OE2	2.46	0.49
2:B:243:TYR:CE1	7:B:303:D10:H103	2.47	0.49
2:J:33:LEU:HD13	3:K:111:LEU:HB3	1.92	0.49
2:J:55:PHE:O	2:J:124:VAL:HA	2.13	0.49
3:C:47:TRP:HD1	3:C:51:LEU:HD11	1.77	0.49
3:K:141:ASP:OD1	3:K:141:ASP:N	2.43	0.49
2:F:48:LEU:HD22	3:G:218:HIS:HB3	1.95	0.49
2:F:243:TYR:CZ	7:F:303:D10:H103	2.45	0.49
2:J:88:PHE:CD2	1:I:212:TYR:HB2	2.47	0.49
3:C:16:GLU:O	3:C:98:ARG:NH2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:54:ASP:OD1	2:J:127:SER:N	2.45	0.49
3:K:114:TYR:CE1	3:K:161:ALA:HB2	2.47	0.49
2:F:243:TYR:CE1	7:F:303:D10:H103	2.47	0.49
2:B:155:LEU:HD13	2:B:227:PHE:CD2	2.48	0.49
2:B:216:ASP:CB	7:K:305:D10:H32	2.32	0.49
2:F:229:SER:O	2:F:233:TYR:N	2.33	0.49
2:B:148:ILE:HD11	6:K:302:HXG:CAL	2.39	0.48
2:J:224:PHE:HE1	3:G:199:LEU:HG	1.78	0.48
3:G:142:PHE:HE2	7:G:305:D10:C8	2.26	0.48
3:K:219:TRP:HA	3:K:222:VAL:HG23	1.95	0.48
2:J:202:ILE:HD12	3:K:210:GLU:HB3	1.94	0.48
1:I:315:ARG:CG	9:I:603:HOH:O	2.61	0.48
1:A:181:ILE:HD13	2:B:121:ILE:HB	1.95	0.48
2:B:143:SER:OG	2:B:144:GLY:N	2.46	0.48
2:B:200:GLU:OE2	2:B:203:ARG:NH2	2.45	0.48
1:I:214:ARG:HA	1:I:219:LYS:HE2	1.95	0.48
2:B:112:ASN:ND2	3:C:128:GLN:OE1	2.47	0.48
3:K:16:GLU:N	3:K:98:ARG:HE	2.12	0.48
1:A:300:LEU:HB3	1:A:367:ILE:HB	1.96	0.48
1:A:338:PHE:HB3	1:A:343:LEU:HD13	1.95	0.48
1:I:300:LEU:HB3	1:I:367:ILE:HB	1.96	0.48
1:A:274:GLU:OE1	1:A:400:LYS:NZ	2.41	0.48
1:A:366:LYS:NZ	1:A:368:GLN:OE1	2.43	0.48
2:F:42:TYR:CD1	2:F:76:PHE:HB2	2.48	0.48
1:E:55:VAL:HG22	1:E:59:GLU:HB3	1.96	0.48
1:E:374:ILE:C	1:E:376:ARG:H	2.17	0.48
3:G:190:PRO:HA	3:G:193:ILE:HG12	1.96	0.48
2:B:16:VAL:HG22	3:C:254:LEU:HD11	1.96	0.48
2:J:49:THR:O	3:K:214:VAL:HG13	2.14	0.48
1:A:55:VAL:HG22	1:A:59:GLU:HB3	1.96	0.48
2:J:150:ALA:O	2:J:230:MET:HG2	2.14	0.48
1:I:55:VAL:HG22	1:I:59:GLU:HB3	1.96	0.48
3:G:208:PHE:CE2	3:G:216:PRO:HD2	2.49	0.47
1:E:214:ARG:HA	1:E:219:LYS:HE2	1.95	0.47
1:E:374:ILE:C	1:E:376:ARG:N	2.68	0.47
2:J:42:TYR:CD2	2:J:101:LEU:HB2	2.49	0.47
3:C:69:GLU:OE1	3:C:152:MET:HE2	2.13	0.47
2:F:142:LEU:HD23	1:E:229:ARG:HG2	1.97	0.47
3:C:154:TYR:HA	3:C:157:TYR:CE2	2.48	0.47
1:E:338:PHE:HB3	1:E:343:LEU:HD13	1.95	0.47
2:F:252:ILE:HG23	3:G:179:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASP:CB	7:K:305:D10:C3	2.89	0.47
2:B:243:TYR:CZ	7:B:303:D10:H103	2.44	0.47
2:F:52:ASP:HB2	3:G:213:PHE:HB2	1.97	0.47
2:J:142:LEU:HD23	1:I:229:ARG:HG2	1.96	0.47
3:G:196:ASN:HD22	3:G:199:LEU:HD22	1.79	0.47
1:I:170:ASP:OD1	1:I:172:SER:OG	2.27	0.47
2:J:224:PHE:CD1	3:G:199:LEU:HA	2.45	0.47
3:C:200:ASN:C	3:C:200:ASN:HD22	2.15	0.47
1:A:214:ARG:HA	1:A:219:LYS:HE2	1.95	0.47
2:F:156:GLY:O	2:F:160:LEU:HB2	2.14	0.47
2:F:161:PHE:O	2:F:164:ASN:ND2	2.48	0.47
2:J:48:LEU:HD13	3:K:221:PHE:CB	2.44	0.47
3:C:113:VAL:HG21	6:C:304:HXG:H4	1.97	0.47
1:E:300:LEU:HB3	1:E:367:ILE:HB	1.96	0.47
1:I:214:ARG:HE	1:I:214:ARG:HB2	1.60	0.47
1:I:366:LYS:NZ	1:I:368:GLN:OE1	2.43	0.47
3:G:196:ASN:HD21	3:G:220:GLY:HA3	1.78	0.47
1:E:60:GLU:OE2	1:E:97:THR:OG1	2.33	0.47
2:B:43:HIS:NE2	3:C:127:GLU:OE2	2.43	0.47
2:J:75:THR:HB	2:J:236:TRP:CD2	2.49	0.47
3:K:162:VAL:HG21	8:K:303:D12:H102	1.97	0.47
2:B:145:SER:HB2	2:J:252:ILE:HG13	1.96	0.47
1:E:274:GLU:OE1	1:E:400:LYS:NZ	2.41	0.47
1:A:229:ARG:HG2	2:B:142:LEU:HD23	1.97	0.46
3:C:39:ARG:NH1	3:C:43:GLN:HB2	2.30	0.46
1:E:33:SER:HA	1:E:376:ARG:HH12	1.81	0.46
2:F:227:PHE:HZ	3:C:198:GLY:HA3	1.80	0.46
2:J:185:LEU:HD12	2:J:185:LEU:HA	1.75	0.46
3:G:39:ARG:HH12	3:G:43:GLN:HB2	1.80	0.46
1:E:170:ASP:OD1	1:E:172:SER:OG	2.27	0.46
1:I:60:GLU:OE2	1:I:97:THR:OG1	2.33	0.46
1:A:102:GLY:HA3	1:A:268:LEU:HB3	1.98	0.46
1:A:316:LEU:HD11	1:A:392:LEU:HD22	1.97	0.46
2:F:42:TYR:CD2	2:F:101:LEU:HB2	2.50	0.46
2:F:252:ILE:HD11	6:G:302:HXG:H4	1.97	0.46
2:B:75:THR:HB	2:B:236:TRP:CD2	2.51	0.46
2:B:216:ASP:HB3	7:K:305:D10:H41	1.98	0.46
1:E:316:LEU:HD11	1:E:392:LEU:HD22	1.98	0.46
1:I:102:GLY:HA3	1:I:268:LEU:HB3	1.98	0.46
2:J:227:PHE:HD1	2:J:227:PHE:O	1.98	0.46
2:J:227:PHE:CE2	3:G:195:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:196:ASN:N	3:G:196:ASN:OD1	2.49	0.46
3:C:169:LYS:NZ	3:C:178:GLY:O	2.49	0.46
3:C:194:ILE:HG23	3:C:195:PRO:HD2	1.97	0.46
1:A:212:TYR:HB2	2:B:88:PHE:CE2	2.50	0.46
2:F:142:LEU:HA	1:E:229:ARG:HG2	1.98	0.46
2:F:218:VAL:HG21	6:F:301:HXG:H35	1.98	0.46
2:J:243:TYR:CE1	7:J:303:D10:C10	2.99	0.46
3:C:216:PRO:HA	3:C:219:TRP:CD2	2.51	0.46
1:I:274:GLU:OE1	1:I:400:LYS:NZ	2.41	0.46
1:I:316:LEU:HD11	1:I:392:LEU:HD22	1.98	0.46
2:F:145:SER:HB2	2:B:252:ILE:HG13	1.97	0.46
2:J:51:GLY:HA3	2:J:53:TRP:N	2.31	0.46
3:G:144:PRO:O	3:G:148:ILE:HG12	2.16	0.46
2:J:218:VAL:HG21	6:J:301:HXG:H35	1.97	0.46
9:J:401:HOH:O	3:G:195:PRO:HB2	2.15	0.46
3:G:39:ARG:NH1	3:G:43:GLN:HB2	2.31	0.46
3:G:154:TYR:HB2	3:G:155:PRO:HD3	1.98	0.46
3:C:134:MET:HA	3:C:134:MET:HE3	1.98	0.46
2:B:127:SER:HB2	2:B:165:ASN:HD21	1.79	0.45
2:B:158:GLY:HA3	2:B:226:GLY:CA	2.46	0.45
3:K:188:ILE:HD11	6:K:302:HXG:CAA	2.45	0.45
2:F:236:TRP:HH2	3:G:226:TRP:CD1	2.34	0.45
3:K:186:VAL:O	3:K:190:PRO:HG2	2.16	0.45
2:F:247:LYS:HZ2	7:F:303:D10:H13	1.79	0.45
2:J:243:TYR:CE1	7:J:303:D10:H103	2.51	0.45
3:G:114:TYR:CZ	3:G:118:ILE:HD11	2.50	0.45
2:F:88:PHE:CD2	1:E:212:TYR:HB2	2.50	0.45
2:B:51:GLY:HA3	2:B:53:TRP:N	2.31	0.45
3:G:72:LEU:O	3:G:76:SER:OG	2.29	0.45
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.81	0.45
2:F:243:TYR:CE1	7:F:303:D10:C10	2.99	0.45
1:E:366:LYS:NZ	1:E:368:GLN:OE1	2.43	0.45
2:F:62:ARG:NH2	2:F:206:GLU:OE2	2.40	0.45
2:J:89:ARG:O	1:I:224:ILE:HG13	2.16	0.45
3:G:16:GLU:HG2	3:G:17:SER:H	1.82	0.45
1:A:229:ARG:HG2	2:B:142:LEU:HA	1.99	0.45
2:J:54:ASP:OD1	2:J:127:SER:OG	2.31	0.45
2:F:227:PHE:HD2	9:C:401:HOH:O	1.95	0.45
2:B:247:LYS:HZ1	7:B:303:D10:H13	1.80	0.45
2:F:49:THR:O	3:G:214:VAL:HG13	2.17	0.45
2:J:211:ARG:CZ	3:G:209:MET:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:241:ARG:HA	3:K:241:ARG:HD2	1.68	0.45
2:J:67:THR:HA	2:J:225:SER:HB3	1.98	0.45
2:J:140:LEU:HD13	2:J:149:THR:HG21	1.98	0.45
2:J:141:LEU:HD11	1:I:224:ILE:HD12	1.98	0.45
3:C:236:LEU:HD23	3:C:236:LEU:HA	1.83	0.45
1:A:170:ASP:OD1	1:A:172:SER:OG	2.27	0.44
2:F:75:THR:HB	2:F:236:TRP:CE2	2.52	0.44
2:B:63:ARG:HB3	2:B:206:GLU:HB2	1.99	0.44
2:B:75:THR:HB	2:B:236:TRP:CE2	2.52	0.44
2:J:236:TRP:HH2	3:K:226:TRP:CD1	2.35	0.44
3:G:154:TYR:CE2	3:G:193:ILE:HG22	2.53	0.44
3:G:193:ILE:HD13	3:G:193:ILE:HA	1.75	0.44
3:G:194:ILE:N	3:G:195:PRO:HD3	2.32	0.44
3:K:222:VAL:HG12	3:K:226:TRP:NE1	2.32	0.44
2:F:92:PHE:O	2:F:96:PHE:HB2	2.17	0.44
2:F:94:ALA:HB3	2:F:137:ASP:OD2	2.17	0.44
2:F:202:ILE:HG12	2:F:202:ILE:O	2.18	0.44
3:K:243:HIS:CD2	1:I:213:ILE:HG12	2.52	0.44
1:E:102:GLY:HA3	1:E:268:LEU:HB3	1.98	0.44
2:F:197:SER:HB2	3:G:211:GLU:HB2	1.99	0.44
3:K:141:ASP:O	3:K:146:HIS:ND1	2.48	0.44
2:F:55:PHE:O	2:F:124:VAL:HA	2.17	0.44
2:F:247:LYS:HE3	2:F:247:LYS:HB2	1.67	0.44
2:B:202:ILE:HD11	3:C:210:GLU:HG3	1.99	0.44
2:B:243:TYR:CE1	7:B:303:D10:C10	3.00	0.44
3:C:200:ASN:HB2	3:C:221:PHE:CE2	2.52	0.44
2:B:151:VAL:O	2:B:230:MET:HE2	2.18	0.44
2:J:212:THR:O	2:J:212:THR:OG1	2.34	0.44
2:B:55:PHE:O	2:B:124:VAL:HA	2.16	0.44
3:G:194:ILE:O	3:G:197:VAL:HG23	2.18	0.44
3:C:114:TYR:CE1	3:C:161:ALA:HB2	2.52	0.44
2:F:249:ILE:HD11	2:F:252:ILE:CG2	2.42	0.44
2:B:247:LYS:HE3	2:B:247:LYS:HB2	1.68	0.44
2:J:197:SER:OG	3:K:133:HIS:O	2.35	0.44
3:K:249:GLU:O	3:K:253:LEU:HB2	2.17	0.44
1:A:283:ASN:O	1:A:309:ASN:HB3	2.17	0.44
2:J:141:LEU:CD1	1:I:224:ILE:HD12	2.48	0.44
3:G:197:VAL:O	3:G:201:GLU:HB2	2.17	0.44
3:C:210:GLU:OE1	3:C:210:GLU:HA	2.17	0.44
1:E:283:ASN:O	1:E:309:ASN:HB3	2.17	0.44
2:B:218:VAL:HG21	6:B:301:HXG:H35	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:VAL:O	3:C:162:VAL:HG12	2.18	0.44
1:E:295:VAL:HA	1:E:296:PRO:HA	1.86	0.44
3:G:219:TRP:HA	3:G:222:VAL:HG23	2.00	0.43
3:C:188:ILE:O	3:C:192:MET:N	2.50	0.43
1:E:214:ARG:HD3	1:E:222:ASP:OD2	2.18	0.43
1:E:296:PRO:HD2	1:E:415:VAL:HG22	2.00	0.43
2:F:252:ILE:HD11	6:G:302:HXG:CAJ	2.48	0.43
2:B:163:PRO:HD3	6:B:301:HXG:H17	2.01	0.43
3:G:138:ARG:HH22	3:G:141:ASP:HA	1.83	0.43
3:K:60:THR:HG23	4:N:3:UNK:HA	2.01	0.43
3:K:154:TYR:HB2	3:K:155:PRO:HD3	2.01	0.43
2:J:185:LEU:O	2:J:189:ILE:HG13	2.18	0.43
1:E:215:VAL:HG22	1:E:220:ALA:CB	2.48	0.43
1:I:283:ASN:O	1:I:309:ASN:HB3	2.17	0.43
2:J:148:ILE:HD13	8:G:303:D12:H21	2.00	0.43
2:J:202:ILE:O	2:J:202:ILE:HG12	2.18	0.43
2:J:247:LYS:HZ1	7:J:303:D10:H13	1.80	0.43
3:G:241:ARG:HD2	3:G:241:ARG:HA	1.68	0.43
1:E:273:THR:HA	1:E:274:GLU:HA	1.71	0.43
1:I:214:ARG:HD3	1:I:222:ASP:OD2	2.19	0.43
1:A:305:LYS:HE2	1:A:305:LYS:HB2	1.77	0.43
1:E:169:LEU:HD23	1:E:169:LEU:HA	1.80	0.43
2:B:56:TRP:CH2	3:C:134:MET:HG3	2.54	0.43
2:B:85:TRP:O	2:B:89:ARG:HD3	2.19	0.43
2:J:196:THR:OG1	2:J:197:SER:N	2.52	0.43
1:I:32:LYS:O	1:I:376:ARG:NH1	2.49	0.43
2:F:48:LEU:HD13	3:G:221:PHE:CB	2.48	0.43
2:B:53:TRP:CZ3	3:C:214:VAL:HG21	2.54	0.43
2:B:250:ASP:OD1	2:B:251:THR:N	2.52	0.43
3:C:136:VAL:HG23	3:C:138:ARG:H	1.83	0.43
3:K:144:PRO:O	3:K:148:ILE:HG12	2.18	0.43
1:I:215:VAL:HG22	1:I:220:ALA:CB	2.48	0.43
1:I:273:THR:HA	1:I:274:GLU:HA	1.71	0.43
1:A:68:HIS:ND1	1:A:117:ASP:OD1	2.44	0.43
2:J:108:ASN:OD1	2:J:112:ASN:HB2	2.19	0.43
2:J:131:VAL:HG12	2:J:160:LEU:HD13	1.99	0.43
2:J:163:PRO:HG3	6:J:301:HXG:H15	2.00	0.43
3:G:169:LYS:NZ	3:G:178:GLY:O	2.52	0.43
3:G:216:PRO:HA	3:G:219:TRP:CD2	2.53	0.43
3:G:239:LEU:HB3	1:E:212:TYR:CE2	2.54	0.43
1:A:60:GLU:OE2	1:A:97:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:ARG:HB3	2:F:206:GLU:HB2	2.01	0.43
2:J:151:VAL:HA	2:J:230:MET:HG2	2.00	0.43
3:G:208:PHE:HB2	3:G:217:LEU:HD11	2.01	0.43
1:A:212:TYR:CE2	3:C:239:LEU:HB3	2.54	0.42
1:A:215:VAL:HG22	1:A:220:ALA:CB	2.48	0.42
2:F:252:ILE:HD12	2:J:147:VAL:CG2	2.49	0.42
2:B:145:SER:HB2	2:J:252:ILE:O	2.19	0.42
3:K:201:GLU:O	3:K:205:THR:HG23	2.19	0.42
2:J:47:MET:HE2	2:J:47:MET:HB2	1.88	0.42
3:G:167:TYR:CE1	3:G:171:ARG:HG3	2.54	0.42
1:I:315:ARG:CD	9:I:603:HOH:O	2.67	0.42
2:F:227:PHE:CZ	3:C:198:GLY:HA3	2.54	0.42
2:B:33:LEU:HD13	3:C:111:LEU:HB3	1.99	0.42
3:K:239:LEU:HB3	1:I:212:TYR:CE2	2.54	0.42
2:B:177:GLU:O	2:B:178:GLN:NE2	2.52	0.42
2:J:228:VAL:HG22	3:G:199:LEU:HD12	2.02	0.42
2:F:163:PRO:HG3	6:F:301:HXG:H15	2.02	0.42
2:J:247:LYS:HB2	2:J:247:LYS:HE3	1.75	0.42
3:G:193:ILE:HD11	3:G:225:GLY:N	2.35	0.42
3:C:191:PHE:O	3:C:195:PRO:HD2	2.19	0.42
3:K:138:ARG:NH2	3:K:141:ASP:HA	2.34	0.42
1:E:275:GLY:HA2	1:E:276:THR:HB	2.01	0.42
1:I:225:GLY:HA2	1:I:229:ARG:NH2	2.35	0.42
2:J:163:PRO:HD3	6:J:301:HXG:H17	2.02	0.42
3:G:203:GLY:C	3:G:217:LEU:HD13	2.40	0.42
1:A:214:ARG:HD3	1:A:222:ASP:OD2	2.19	0.42
2:B:185:LEU:O	2:B:189:ILE:HG13	2.20	0.42
1:I:275:GLY:HA2	1:I:276:THR:HB	2.01	0.42
2:B:16:VAL:HG22	3:C:254:LEU:HD21	2.02	0.42
3:G:138:ARG:NH2	3:G:141:ASP:HA	2.35	0.42
3:C:39:ARG:HH12	3:C:43:GLN:HB2	1.83	0.42
3:K:247:GLY:O	3:K:251:VAL:HG12	2.19	0.42
4:N:20:UNK:HA	9:N:102:HOH:O	2.19	0.42
1:A:275:GLY:HA2	1:A:276:THR:HB	2.01	0.42
2:J:182:LEU:HD21	1:I:258:ILE:HD13	2.01	0.42
2:J:243:TYR:OH	7:J:303:D10:C10	2.66	0.42
2:F:201:TYR:CE1	1:E:141:GLU:HA	2.55	0.42
2:B:210:LEU:O	1:I:34:GLN:HG2	2.20	0.42
3:G:218:HIS:O	3:G:221:PHE:HB2	2.19	0.42
3:C:148:ILE:O	3:C:152:MET:HB3	2.20	0.42
1:I:305:LYS:HB2	1:I:305:LYS:HE2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:LEU:HB3	3:G:218:HIS:HB3	2.01	0.41
2:F:59:TRP:CZ2	2:F:203:ARG:HA	2.56	0.41
2:B:90:LEU:HB3	2:B:92:PHE:CE2	2.55	0.41
2:B:214:GLY:HA3	1:I:376:ARG:NH2	2.35	0.41
2:J:200:GLU:OE2	2:J:203:ARG:NH2	2.46	0.41
3:K:140:THR:HG23	3:K:142:PHE:H	1.85	0.41
2:F:12:PRO:HB3	3:G:97:PRO:HB2	2.02	0.41
2:J:211:ARG:O	3:G:205:THR:HG22	2.21	0.41
3:G:140:THR:HG23	3:G:142:PHE:H	1.84	0.41
3:C:144:PRO:O	3:C:148:ILE:HG12	2.20	0.41
3:K:190:PRO:HD3	3:K:227:MET:HB2	2.02	0.41
2:B:46:PHE:CZ	2:B:69:VAL:HG13	2.51	0.41
2:B:198:MET:HB2	3:C:134:MET:HE1	2.01	0.41
2:J:52:ASP:HB2	3:K:213:PHE:HB2	2.01	0.41
2:B:42:TYR:OH	2:B:73:GLY:O	2.21	0.41
2:J:121:ILE:HB	1:I:181:ILE:HD13	2.01	0.41
2:B:67:THR:HA	2:B:225:SER:CB	2.45	0.41
1:E:225:GLY:HA2	1:E:229:ARG:NH2	2.35	0.41
2:F:49:THR:HG23	3:G:222:VAL:HG21	2.01	0.41
2:J:109:ARG:HA	2:J:109:ARG:HD3	1.90	0.41
3:G:210:GLU:OE2	1:E:144:GLY:HA2	2.20	0.41
3:C:196:ASN:O	3:C:199:LEU:HD12	2.21	0.41
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.80	0.41
2:F:116:TRP:HB2	3:G:39:ARG:NH2	2.35	0.41
2:B:54:ASP:OD1	2:B:127:SER:N	2.52	0.41
3:K:93:ASP:OD1	3:K:93:ASP:N	2.54	0.41
2:F:122:SER:HB2	2:F:172:PHE:CE1	2.56	0.41
2:B:229:SER:O	2:B:233:TYR:N	2.40	0.41
2:B:236:TRP:HH2	3:C:226:TRP:CD1	2.39	0.41
2:B:238:PHE:HE1	6:B:302:HXG:H39	1.86	0.41
2:J:58:ASP:OD1	2:J:58:ASP:N	2.51	0.41
2:B:163:PRO:HG3	6:B:301:HXG:H15	2.03	0.41
2:B:185:LEU:HD23	2:B:185:LEU:HA	1.81	0.41
2:J:122:SER:HB2	2:J:172:PHE:CE1	2.56	0.41
2:J:201:TYR:CE1	1:I:141:GLU:HA	2.56	0.41
2:J:216:ASP:HB3	7:G:305:D10:H41	2.03	0.41
3:G:30:LEU:HD23	3:G:30:LEU:HA	1.91	0.41
3:G:245:LEU:HD23	3:G:245:LEU:HA	1.81	0.41
3:C:167:TYR:CE1	3:C:171:ARG:HG3	2.56	0.41
2:F:42:TYR:OH	2:F:73:GLY:O	2.19	0.41
2:B:230:MET:H	2:B:230:MET:HG3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:92:PHE:O	2:J:96:PHE:HB2	2.20	0.41
3:G:224:PHE:HA	3:G:227:MET:HG2	2.01	0.41
3:C:20:ASP:OD1	3:C:22:ARG:HB2	2.21	0.41
3:C:217:LEU:H	3:C:217:LEU:HG	1.64	0.41
1:I:349:SER:O	1:I:365:VAL:HA	2.21	0.41
1:A:224:ILE:HD12	2:B:141:LEU:HD11	2.04	0.40
2:B:92:PHE:O	2:B:96:PHE:HB2	2.22	0.40
2:B:227:PHE:HE1	3:K:195:PRO:HG3	1.86	0.40
2:J:59:TRP:CZ2	2:J:203:ARG:HA	2.56	0.40
3:C:47:TRP:CD1	3:C:51:LEU:HD11	2.55	0.40
3:C:103:ARG:HD3	3:C:171:ARG:HB3	2.03	0.40
3:K:69:GLU:OE2	3:K:152:MET:HB2	2.21	0.40
1:A:286:THR:HG22	1:A:306:VAL:HG22	2.03	0.40
1:A:398:ASP:OD1	1:A:398:ASP:N	2.31	0.40
2:F:57:VAL:HG12	2:F:123:LEU:HD12	2.03	0.40
2:B:125:PHE:HZ	2:B:169:ILE:HG22	1.86	0.40
2:B:196:THR:OG1	2:B:197:SER:N	2.55	0.40
2:J:46:PHE:HZ	2:J:69:VAL:HG13	1.87	0.40
3:G:104:LEU:HD23	3:G:172:ILE:HD13	2.03	0.40
3:C:154:TYR:HB2	3:C:155:PRO:HD3	2.03	0.40
2:B:130:ILE:HD13	2:B:130:ILE:HA	1.97	0.40
2:J:46:PHE:CZ	2:J:69:VAL:HG13	2.57	0.40
3:G:222:VAL:HG12	3:G:226:TRP:HE1	1.86	0.40
1:E:286:THR:HG22	1:E:306:VAL:HG22	2.03	0.40
1:E:349:SER:O	1:E:365:VAL:HA	2.21	0.40
2:F:90:LEU:HB3	2:F:92:PHE:CE2	2.57	0.40
2:F:202:ILE:HD12	3:G:210:GLU:HB2	2.03	0.40
3:G:42:GLU:OE2	3:G:128:GLN:NE2	2.46	0.40
3:G:66:LEU:HA	3:G:69:GLU:OE1	2.21	0.40
3:K:48:ARG:O	3:K:49:ALA:HB3	2.22	0.40
1:A:225:GLY:HA2	1:A:229:ARG:NH2	2.35	0.40
1:A:349:SER:O	1:A:365:VAL:HA	2.21	0.40
2:F:148:ILE:O	2:F:152:VAL:HG12	2.22	0.40
2:J:44:VAL:HG13	2:J:48:LEU:HD12	2.02	0.40
3:C:242:ILE:O	3:C:246:VAL:HG22	2.21	0.40
3:K:52:ASP:OD1	3:K:54:PHE:N	2.46	0.40
3:K:245:LEU:HD23	3:K:245:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	359 (93%)	24 (6%)	3 (1%)	19	27
1	E	386/388 (100%)	357 (92%)	26 (7%)	3 (1%)	19	27
1	I	386/388 (100%)	357 (92%)	26 (7%)	3 (1%)	19	27
2	B	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
2	F	242/244 (99%)	233 (96%)	9 (4%)	0	100	100
2	J	242/244 (99%)	233 (96%)	9 (4%)	0	100	100
3	C	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
3	G	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
3	K	239/241 (99%)	223 (93%)	14 (6%)	2 (1%)	19	27
All	All	2601/2619 (99%)	2446 (94%)	144 (6%)	11 (0%)	38	47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	A	351	ASP
1	E	309	ASN
1	E	351	ASP
1	I	309	ASN
1	I	351	ASP
3	K	207	TRP
1	A	349	SER
3	K	195	PRO
1	E	349	SER
1	I	349	SER

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	319/319 (100%)	293 (92%)	26 (8%)	11	16
1	E	319/319 (100%)	290 (91%)	29 (9%)	9	13
1	I	319/319 (100%)	294 (92%)	25 (8%)	12	19
2	B	202/202 (100%)	191 (95%)	11 (5%)	22	34
2	F	202/202 (100%)	190 (94%)	12 (6%)	19	30
2	J	202/202 (100%)	189 (94%)	13 (6%)	17	27
3	C	205/205 (100%)	192 (94%)	13 (6%)	18	27
3	G	205/205 (100%)	193 (94%)	12 (6%)	19	30
3	K	205/205 (100%)	187 (91%)	18 (9%)	10	14
All	All	2178/2178 (100%)	2019 (93%)	159 (7%)	18	21

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	141	GLU
1	A	158	ASP
1	A	219	LYS
1	A	224	ILE
1	A	226	ASP
1	A	229	ARG
1	A	230	ARG
1	A	281	LYS
1	A	285	THR
1	A	287	GLU
1	A	295	VAL
1	A	298	ARG
1	A	305	LYS
1	A	307	LYS
1	A	308	ASN
1	A	315	ARG
1	A	318	GLU

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Mol	Chain	Res	Type
1	A	327	LEU
1	A	330	ASP
1	A	335	LYS
1	A	345	ASP
1	A	346	ARG
1	A	350	VAL
1	A	351	ASP
1	A	355	ILE
2	F	52	ASP
2	F	53	TRP
2	F	54	ASP
2	F	137	ASP
2	F	160	LEU
2	F	164	ASN
2	F	197	SER
2	F	204	MET
2	F	234	PHE
2	F	250	ASP
2	F	251	THR
2	F	252	ILE
2	B	42	TYR
2	B	47	MET
2	B	53	TRP
2	B	137	ASP
2	B	164	ASN
2	B	177	GLU
2	B	197	SER
2	B	204	MET
2	B	211	ARG
2	B	227	PHE
2	B	234	PHE
2	J	33	LEU
2	J	47	MET
2	J	53	TRP
2	J	54	ASP
2	J	137	ASP
2	J	164	ASN
2	J	177	GLU
2	J	197	SER
2	J	204	MET
2	J	206	GLU
2	J	209	THR

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Mol	Chain	Res	Type
2	J	227	PHE
2	J	234	PHE
3	G	123	SER
3	G	141	ASP
3	G	158	SER
3	G	169	LYS
3	G	180	SER
3	G	183	PHE
3	G	186	VAL
3	G	194	ILE
3	G	196	ASN
3	G	207	TRP
3	G	211	GLU
3	G	212	LEU
3	C	63	MET
3	C	93	ASP
3	C	123	SER
3	C	143	THR
3	C	157	TYR
3	C	169	LYS
3	C	183	PHE
3	C	194	ILE
3	C	196	ASN
3	C	200	ASN
3	C	212	LEU
3	C	221	PHE
3	C	251	VAL
3	K	16	GLU
3	K	47	TRP
3	K	93	ASP
3	K	123	SER
3	K	157	TYR
3	K	158	SER
3	K	169	LYS
3	K	180	SER
3	K	183	PHE
3	K	186	VAL
3	K	194	ILE
3	K	195	PRO
3	K	199	LEU
3	K	209	MET
3	K	210	GLU

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Mol	Chain	Res	Type
3	K	211	GLU
3	K	251	VAL
3	K	252	LYS
1	E	61	MET
1	E	141	GLU
1	E	158	ASP
1	E	219	LYS
1	E	224	ILE
1	E	226	ASP
1	E	229	ARG
1	E	230	ARG
1	E	281	LYS
1	E	285	THR
1	E	287	GLU
1	E	295	VAL
1	E	298	ARG
1	E	305	LYS
1	E	307	LYS
1	E	308	ASN
1	E	315	ARG
1	E	318	GLU
1	E	327	LEU
1	E	330	ASP
1	E	335	LYS
1	E	345	ASP
1	E	346	ARG
1	E	350	VAL
1	E	351	ASP
1	E	355	ILE
1	E	376	ARG
1	E	413	LYS
1	E	415	VAL
1	I	61	MET
1	I	141	GLU
1	I	158	ASP
1	I	219	LYS
1	I	224	ILE
1	I	226	ASP
1	I	229	ARG
1	I	281	LYS
1	I	285	THR
1	I	287	GLU

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Mol	Chain	Res	Type
1	I	295	VAL
1	I	298	ARG
1	I	305	LYS
1	I	307	LYS
1	I	308	ASN
1	I	315	ARG
1	I	318	GLU
1	I	327	LEU
1	I	330	ASP
1	I	335	LYS
1	I	345	ASP
1	I	346	ARG
1	I	350	VAL
1	I	351	ASP
1	I	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
2	B	108	ASN
2	B	112	ASN
2	B	178	GLN
3	C	196	ASN
3	C	200	ASN
3	K	128	GLN
3	K	218	HIS
3	K	243	HIS
1	E	387	GLN
1	I	387	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 for Mogul analysis.

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	$\#\|Z\|>2$
8	D12	G	303	-	11,11,11	0.78	0	10,10,10	0.14	0
6	HXG	B	301	-	29,29,29	0.80	0	35,37,37	0.91	2 (5%)
6	HXG	J	301	-	29,29,29	0.79	0	35,37,37	0.89	2 (5%)
8	D12	C	303	-	11,11,11	0.82	0	10,10,10	0.07	0
7	D10	B	303	-	9,9,9	0.10	0	8,8,8	0.06	0
7	D10	J	303	-	9,9,9	0.10	0	8,8,8	0.06	0
7	D10	F	303	-	9,9,9	0.09	0	8,8,8	0.06	0
8	D12	K	303	-	11,11,11	0.83	0	10,10,10	0.16	0
6	HXG	K	304	-	29,29,29	0.82	0	35,37,37	0.77	2 (5%)
6	HXG	F	302	-	29,29,29	0.82	0	35,37,37	0.56	0
6	HXG	C	302	-	29,29,29	0.34	0	35,37,37	0.49	0
6	HXG	K	302	-	29,29,29	0.34	0	35,37,37	0.48	0
7	D10	G	305	-	9,9,9	0.12	0	8,8,8	0.22	0
6	HXG	F	301	-	29,29,29	0.79	0	35,37,37	0.90	2 (5%)
7	D10	K	305	-	9,9,9	0.12	0	8,8,8	0.22	0
6	HXG	G	302	-	29,29,29	0.34	0	35,37,37	0.49	0
6	HXG	J	302	-	29,29,29	0.76	0	35,37,37	0.74	1 (2%)
6	HXG	B	302	-	29,29,29	0.78	0	35,37,37	0.76	2 (5%)
6	HXG	C	304	-	29,29,29	0.84	0	35,37,37	0.80	2 (5%)
6	HXG	G	304	-	29,29,29	0.85	0	35,37,37	0.67	0
7	D10	C	305	-	9,9,9	0.12	0	8,8,8	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D12	G	303	-	-	0/9/9/9	-
6	HXG	B	301	-	-	9/33/33/33	-
6	HXG	J	301	-	-	9/33/33/33	-
8	D12	C	303	-	-	1/9/9/9	-
7	D10	B	303	-	-	2/7/7/7	-
7	D10	J	303	-	-	2/7/7/7	-
7	D10	F	303	-	-	2/7/7/7	-
8	D12	K	303	-	-	1/9/9/9	-
6	HXG	K	304	-	-	12/33/33/33	-
6	HXG	F	302	-	-	7/33/33/33	-
6	HXG	C	302	-	-	11/33/33/33	-
6	HXG	K	302	-	-	11/33/33/33	-
7	D10	G	305	-	-	2/7/7/7	-
6	HXG	F	301	-	-	9/33/33/33	-
7	D10	K	305	-	-	2/7/7/7	-
6	HXG	G	302	-	-	11/33/33/33	-
6	HXG	J	302	-	-	6/33/33/33	-
6	HXG	B	302	-	-	10/33/33/33	-
6	HXG	C	304	-	-	12/33/33/33	-
6	HXG	G	304	-	-	7/33/33/33	-
7	D10	C	305	-	-	2/7/7/7	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	301	HXG	OAY-CBA-CAR	3.66	119.39	111.50
6	F	301	HXG	OAY-CBA-CAR	3.65	119.36	111.50
6	J	301	HXG	OAY-CBA-CAR	3.57	119.19	111.50
6	K	304	HXG	OAY-CBA-CAR	2.86	117.66	111.50
6	J	302	HXG	OAY-CBA-CAR	2.83	117.60	111.50
6	B	302	HXG	OAY-CBA-CAR	2.71	117.35	111.50
6	C	304	HXG	OAY-CBA-CAR	2.52	116.94	111.50
6	B	301	HXG	OAY-CBA-OAG	-2.34	118.05	123.70
6	K	304	HXG	OAY-CBA-OAG	-2.32	118.10	123.70
6	F	301	HXG	OAY-CBA-OAG	-2.30	118.14	123.70
6	J	301	HXG	OAY-CBA-OAG	-2.25	118.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	302	HXG	OAY-CBA-OAG	-2.22	118.34	123.70
6	C	304	HXG	OAY-CBA-OAG	-2.13	118.55	123.70

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	301	HXG	CAR-CBA-OAY-CBB
6	F	301	HXG	CAU-OAX-PBD-OAH
6	B	301	HXG	CAR-CBA-OAY-CBB
6	B	301	HXG	CAU-OAX-PBD-OAH
6	B	302	HXG	OAG-CBA-OAY-CBB
6	B	302	HXG	CAR-CBA-OAY-CBB
6	J	301	HXG	CAR-CBA-OAY-CBB
6	J	301	HXG	CAU-OAX-PBD-OAH
6	J	302	HXG	CAR-CBA-OAY-CBB
6	J	302	HXG	CAU-OAX-PBD-OAI
6	G	302	HXG	OAG-CBA-OAY-CBB
6	G	302	HXG	CAR-CBA-OAY-CBB
6	G	302	HXG	CAU-OAX-PBD-OAI
6	G	302	HXG	OAW-CAP-CAS-NBC
6	G	304	HXG	CAR-CBA-OAY-CBB
6	C	302	HXG	OAG-CBA-OAY-CBB
6	C	302	HXG	CAR-CBA-OAY-CBB
6	C	302	HXG	CAU-OAX-PBD-OAI
6	C	302	HXG	OAW-CAP-CAS-NBC
6	C	304	HXG	OAG-CBA-OAY-CBB
6	C	304	HXG	CAU-OAX-PBD-OAH
6	K	302	HXG	OAG-CBA-OAY-CBB
6	K	302	HXG	CAR-CBA-OAY-CBB
6	K	302	HXG	CAU-OAX-PBD-OAI
6	K	302	HXG	OAW-CAP-CAS-NBC
6	K	304	HXG	CAR-CBA-OAY-CBB
6	K	304	HXG	CAU-OAX-PBD-OAW
6	F	302	HXG	OAF-CAZ-OAV-CAT
6	K	304	HXG	OAF-CAZ-OAV-CAT
6	F	301	HXG	OAG-CBA-OAY-CBB
6	B	301	HXG	OAG-CBA-OAY-CBB
6	J	301	HXG	OAG-CBA-OAY-CBB
6	G	304	HXG	OAG-CBA-OAY-CBB
6	K	304	HXG	OAG-CBA-OAY-CBB
6	F	301	HXG	CAQ-CAZ-OAV-CAT

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Mol	Chain	Res	Type	Atoms
6	B	301	HXG	CAQ-CAZ-OAV-CAT
6	B	302	HXG	CAQ-CAZ-OAV-CAT
6	J	301	HXG	CAQ-CAZ-OAV-CAT
6	K	304	HXG	CAQ-CAZ-OAV-CAT
6	C	304	HXG	CAR-CBA-OAY-CBB
6	F	302	HXG	CAQ-CAZ-OAV-CAT
6	G	304	HXG	CAQ-CAZ-OAV-CAT
6	J	302	HXG	OAG-CBA-OAY-CBB
6	J	301	HXG	OAF-CAZ-OAV-CAT
6	G	302	HXG	CAQ-CAZ-OAV-CAT
6	C	302	HXG	CAQ-CAZ-OAV-CAT
6	K	302	HXG	CAQ-CAZ-OAV-CAT
6	F	301	HXG	OAF-CAZ-OAV-CAT
6	B	301	HXG	OAF-CAZ-OAV-CAT
6	B	302	HXG	OAF-CAZ-OAV-CAT
6	F	302	HXG	CAR-CBA-OAY-CBB
6	G	304	HXG	OAF-CAZ-OAV-CAT
6	G	302	HXG	OAF-CAZ-OAV-CAT
6	C	302	HXG	OAF-CAZ-OAV-CAT
6	K	302	HXG	OAF-CAZ-OAV-CAT
6	J	302	HXG	CAQ-CAZ-OAV-CAT
6	F	302	HXG	OAG-CBA-OAY-CBB
6	J	302	HXG	OAF-CAZ-OAV-CAT
6	G	302	HXG	CAL-CAN-CAQ-CAZ
6	C	302	HXG	CAL-CAN-CAQ-CAZ
6	K	302	HXG	CAL-CAN-CAQ-CAZ
6	F	301	HXG	CAU-OAX-PBD-OAW
6	B	301	HXG	CAU-OAX-PBD-OAW
6	B	302	HXG	CAU-OAX-PBD-OAW
6	J	301	HXG	CAU-OAX-PBD-OAW
6	K	304	HXG	CAK-CAM-CAO-CAR
6	G	304	HXG	CAL-CAN-CAQ-CAZ
6	C	304	HXG	CAP-OAW-PBD-OAX
6	K	304	HXG	CBB-CAU-OAX-PBD
6	C	304	HXG	CAQ-CAZ-OAV-CAT
6	B	301	HXG	CBB-CAU-OAX-PBD
6	C	304	HXG	OAF-CAZ-OAV-CAT
6	C	304	HXG	CAU-OAX-PBD-OAW
7	K	305	D10	C5-C6-C7-C8
7	G	305	D10	C5-C6-C7-C8
7	C	305	D10	C5-C6-C7-C8
6	F	301	HXG	CBB-CAU-OAX-PBD

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Mol	Chain	Res	Type	Atoms
6	J	301	HXG	CBB-CAU-OAX-PBD
6	F	301	HXG	CAU-CBB-OAY-CBA
6	B	301	HXG	CAU-CBB-OAY-CBA
6	J	301	HXG	CAU-CBB-OAY-CBA
6	C	304	HXG	CAT-CBB-OAY-CBA
7	K	305	D10	C2-C3-C4-C5
7	G	305	D10	C2-C3-C4-C5
7	C	305	D10	C2-C3-C4-C5
7	B	303	D10	C5-C6-C7-C8
7	F	303	D10	C5-C6-C7-C8
7	J	303	D10	C5-C6-C7-C8
6	J	302	HXG	CAU-OAX-PBD-OAW
6	G	304	HXG	CBB-CAU-OAX-PBD
6	B	302	HXG	CAU-OAX-PBD-OAH
6	C	304	HXG	CAU-OAX-PBD-OAI
6	C	304	HXG	CAP-OAW-PBD-OAI
6	C	304	HXG	CAP-OAW-PBD-OAH
6	K	304	HXG	CAU-OAX-PBD-OAH
6	C	304	HXG	CAL-CAN-CAQ-CAZ
6	F	301	HXG	OAW-CAP-CAS-NBC
6	B	301	HXG	OAW-CAP-CAS-NBC
6	J	301	HXG	OAW-CAP-CAS-NBC
6	F	302	HXG	CAU-OAX-PBD-OAW
6	G	302	HXG	CAU-OAX-PBD-OAW
6	G	304	HXG	CAU-OAX-PBD-OAW
6	C	302	HXG	CAU-OAX-PBD-OAW
6	K	302	HXG	CAU-OAX-PBD-OAW
6	F	302	HXG	CAL-CAN-CAQ-CAZ
6	K	304	HXG	OAX-CAU-CBB-OAY
8	C	303	D12	C7-C8-C9-C10
6	G	302	HXG	CAO-CAR-CBA-OAY
6	C	302	HXG	CAO-CAR-CBA-OAY
6	K	302	HXG	CAO-CAR-CBA-OAY
7	J	303	D10	C3-C4-C5-C6
7	B	303	D10	C3-C4-C5-C6
7	F	303	D10	C3-C4-C5-C6
6	F	302	HXG	OAX-CAU-CBB-OAY
6	B	302	HXG	OAX-CAU-CBB-OAY
6	B	302	HXG	CBB-CAU-OAX-PBD
8	K	303	D12	C6-C7-C8-C9
6	B	302	HXG	CAO-CAR-CBA-OAY
6	K	304	HXG	CAN-CAQ-CAZ-OAV

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Mol	Chain	Res	Type	Atoms
6	K	304	HXG	CAN-CAQ-CAZ-OAF
6	K	304	HXG	CAT-CBB-OAY-CBA
6	G	302	HXG	CAN-CAQ-CAZ-OAV
6	C	302	HXG	CAN-CAQ-CAZ-OAV
6	K	302	HXG	CAN-CAQ-CAZ-OAV
6	B	302	HXG	CAO-CAR-CBA-OAG
6	G	302	HXG	CAN-CAQ-CAZ-OAF
6	C	302	HXG	CAN-CAQ-CAZ-OAF
6	K	302	HXG	CAN-CAQ-CAZ-OAF

There are no ring outliers.

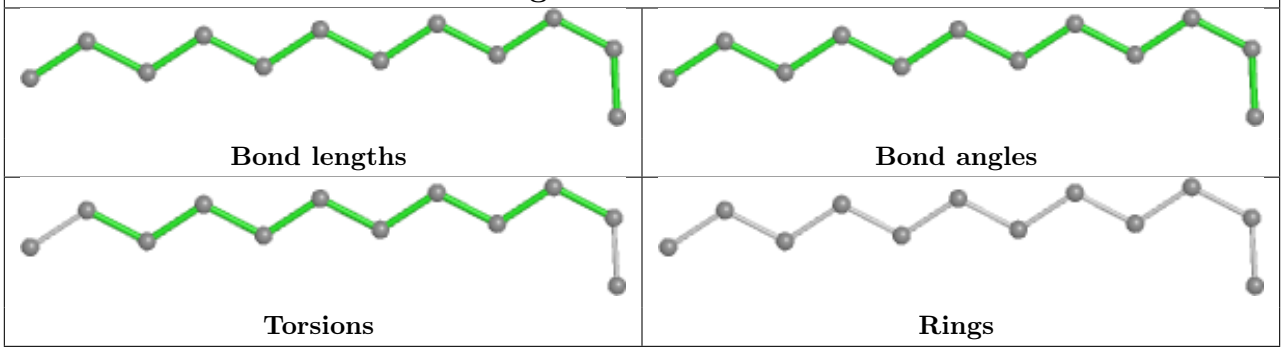
18 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	303	D12	2	0
6	B	301	HXG	3	0
6	J	301	HXG	3	0
7	B	303	D10	11	0
7	J	303	D10	10	0
7	F	303	D10	11	0
8	K	303	D12	2	0
6	K	304	HXG	1	0
6	C	302	HXG	2	0
6	K	302	HXG	10	0
7	G	305	D10	9	0
6	F	301	HXG	2	0
7	K	305	D10	10	0
6	G	302	HXG	8	0
6	B	302	HXG	1	0
6	C	304	HXG	1	0
6	G	304	HXG	2	0
7	C	305	D10	1	0

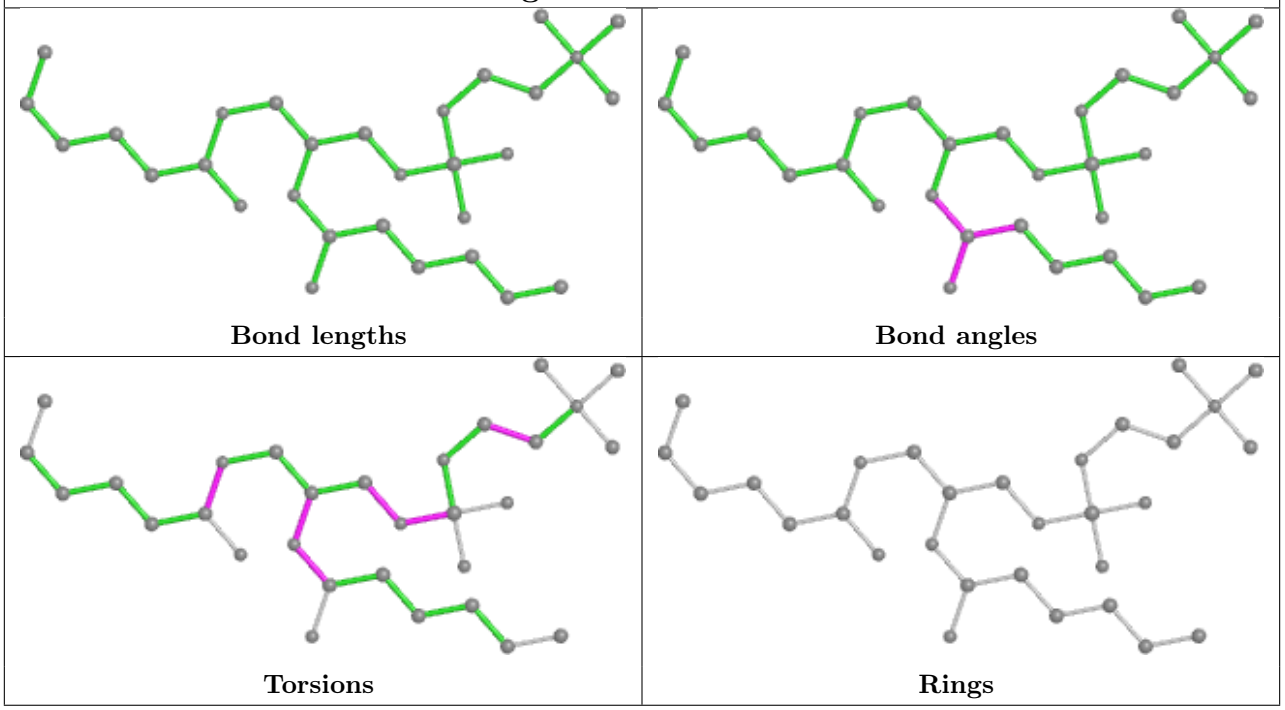
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand D12 G 303



Ligand HXG B 301



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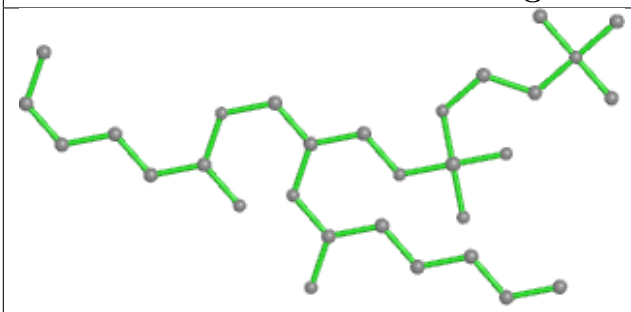
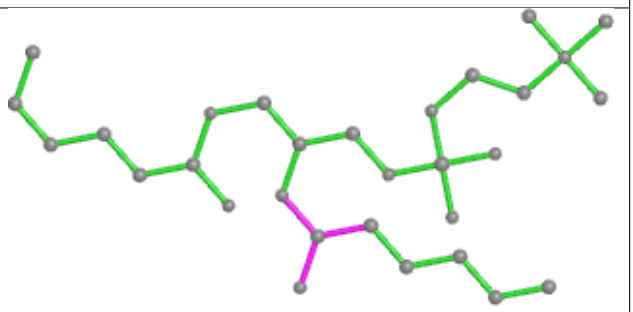
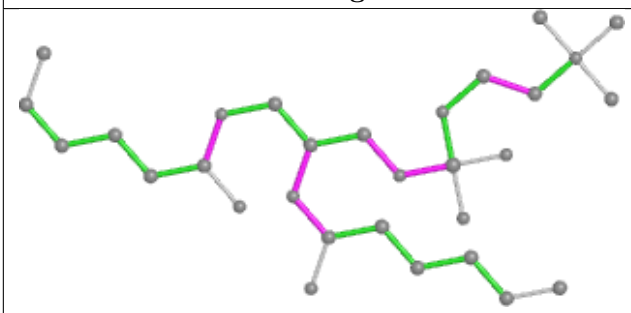


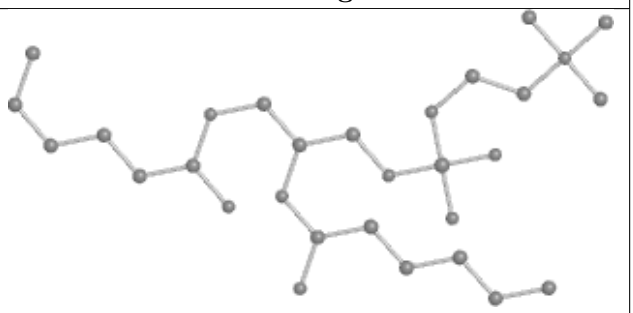
Bond lengths



Bond angles

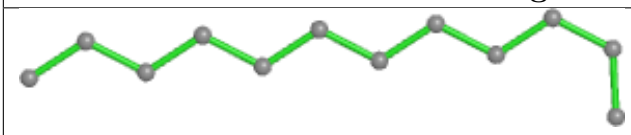


Torsions

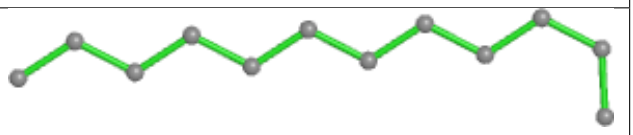


Rings

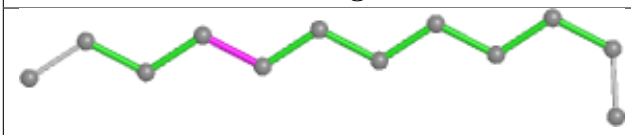
Ligand D12 C 303



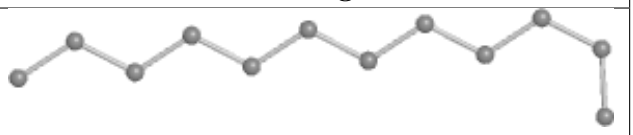
Bond lengths



Bond angles

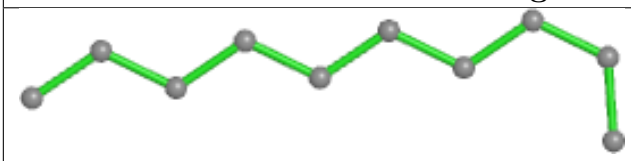


Torsions

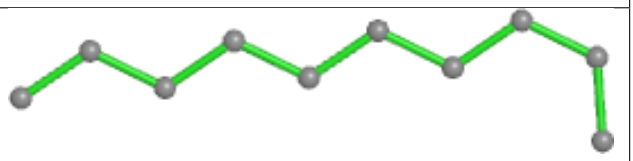


Rings

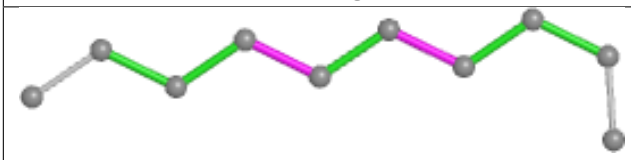
Ligand D10 B 303



Bond lengths



Bond angles



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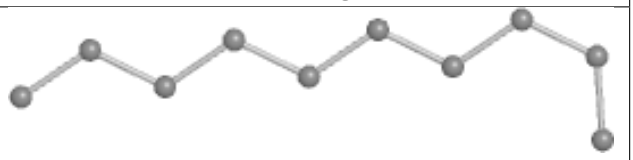
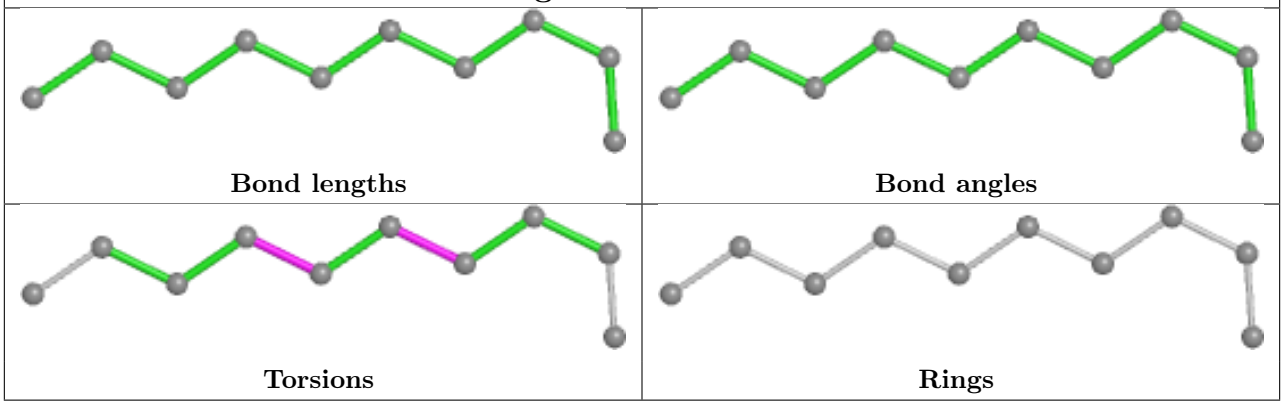


Rings

Ligand D10 J 303



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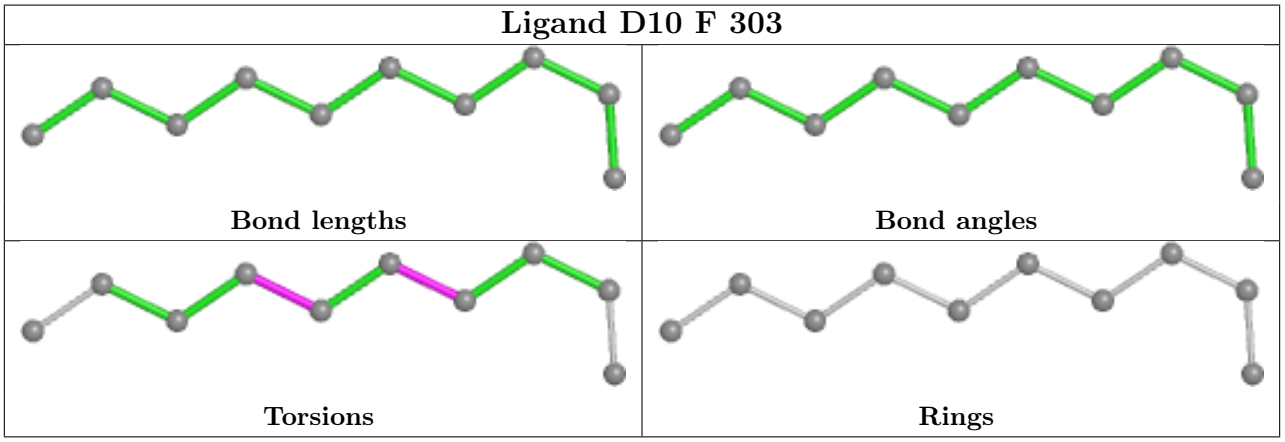

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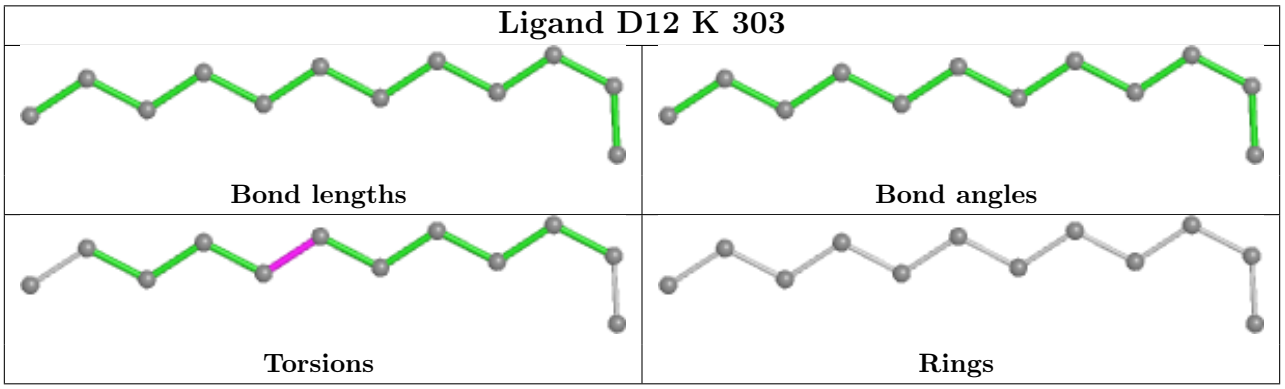
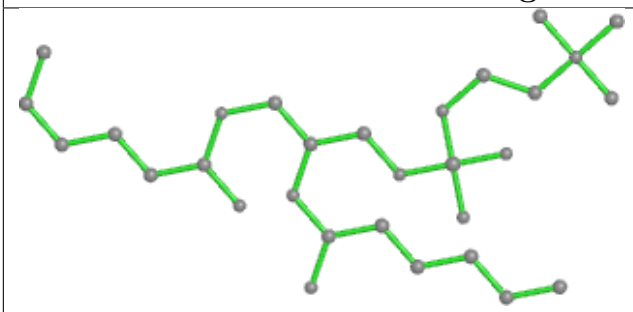
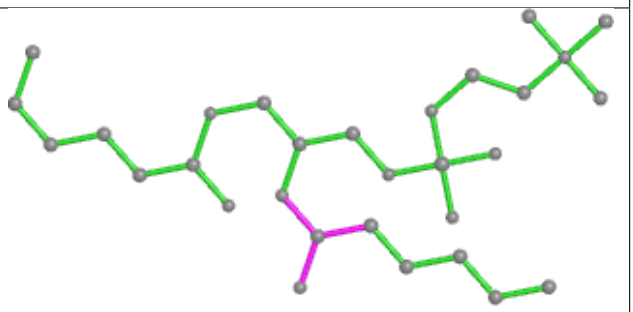


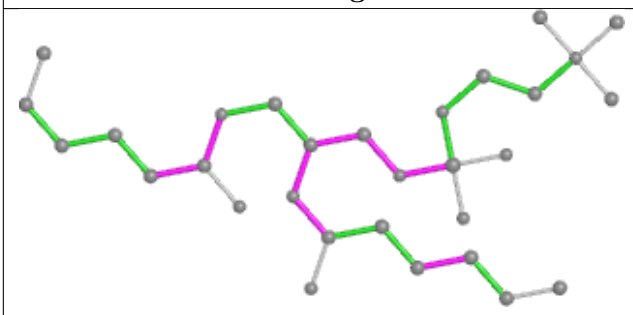
Ligand HXG K 304



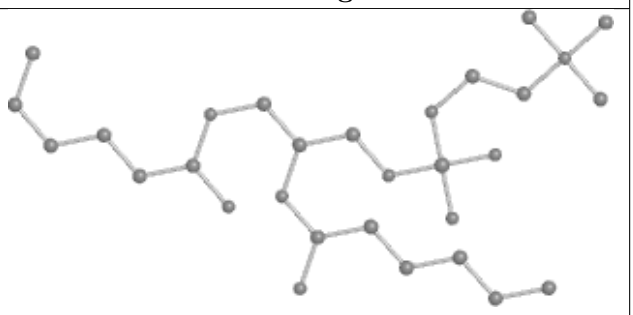
Bond lengths



Bond angles

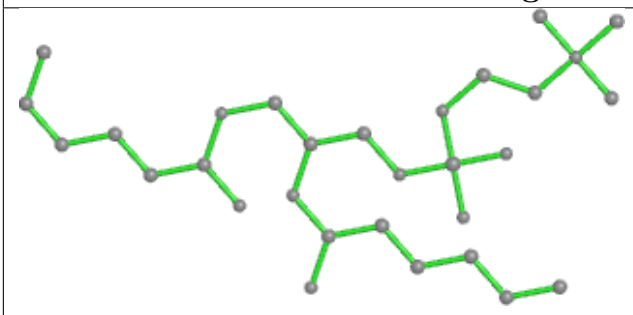


Torsions



Rings

Ligand HXG F 302



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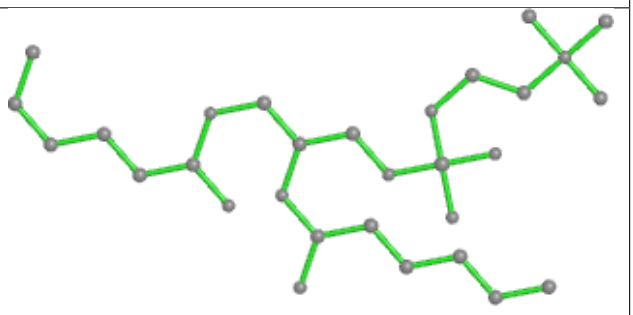
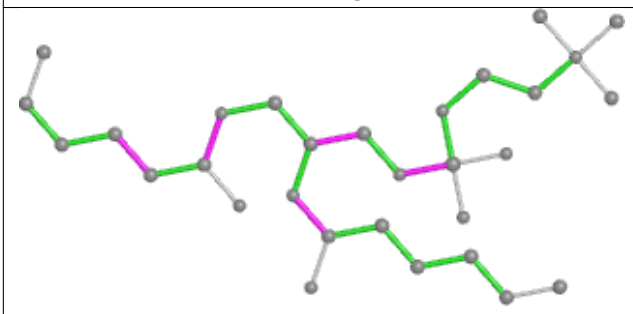


Bond angles



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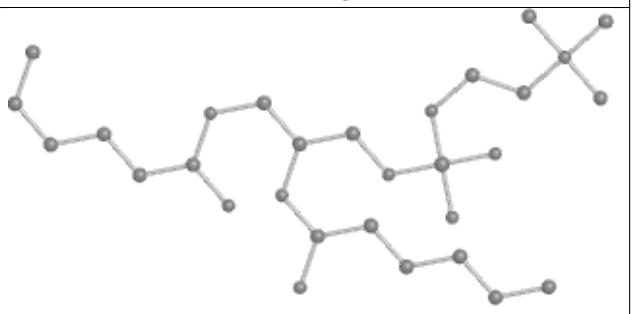
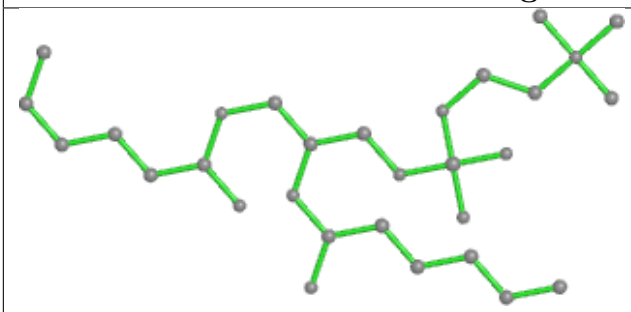
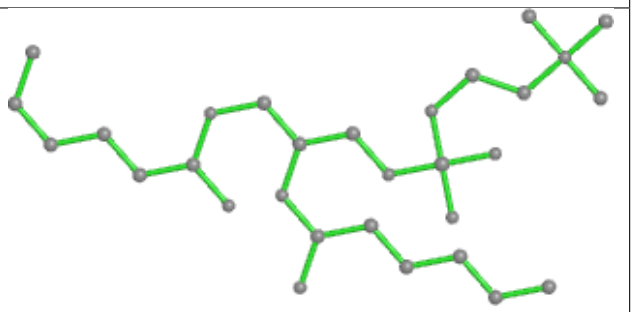


Rings

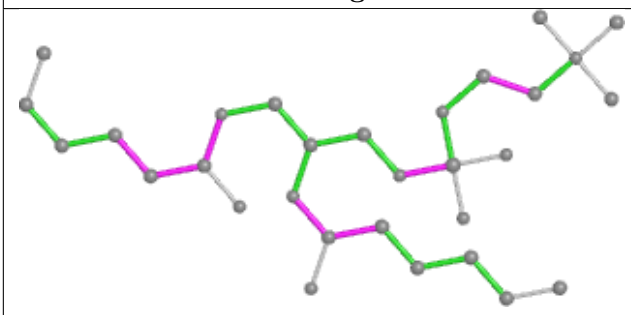
Ligand HXG C 302



Bond lengths



Bond angles



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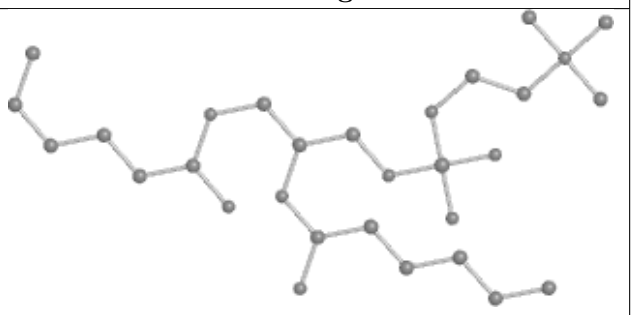
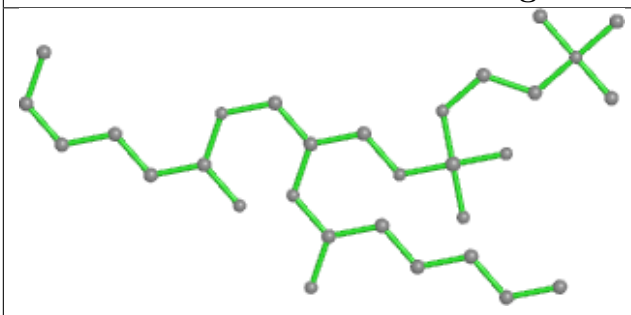
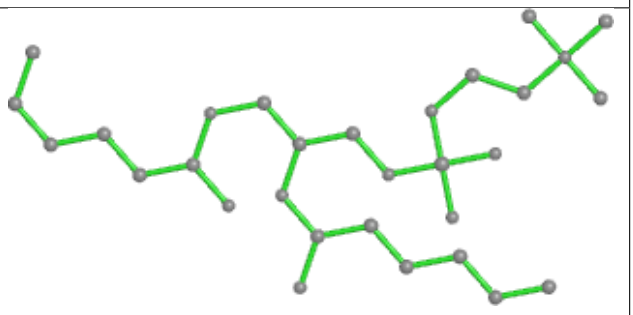


Rings

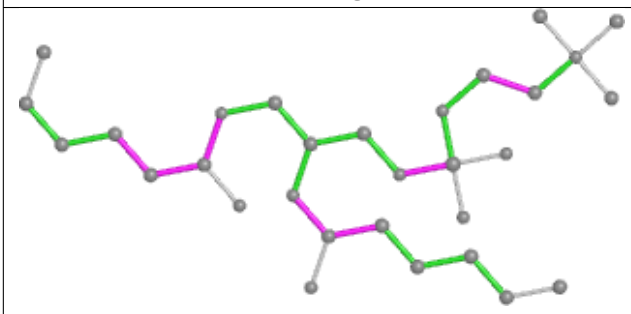
Ligand HXG K 302



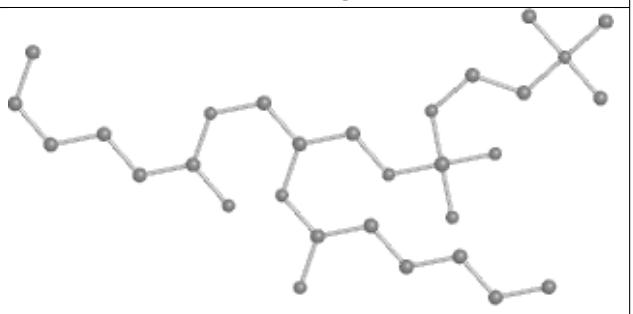
Bond lengths



Bond angles

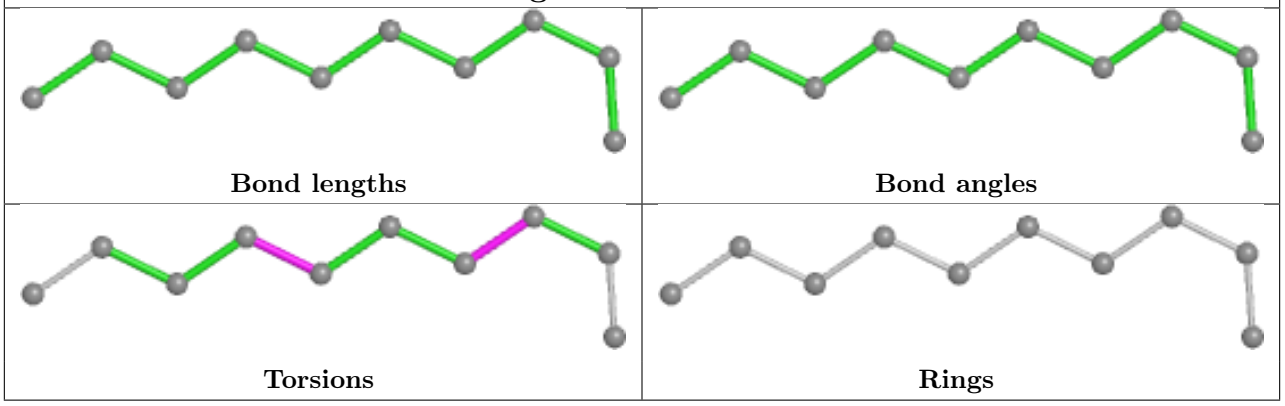


Torsions

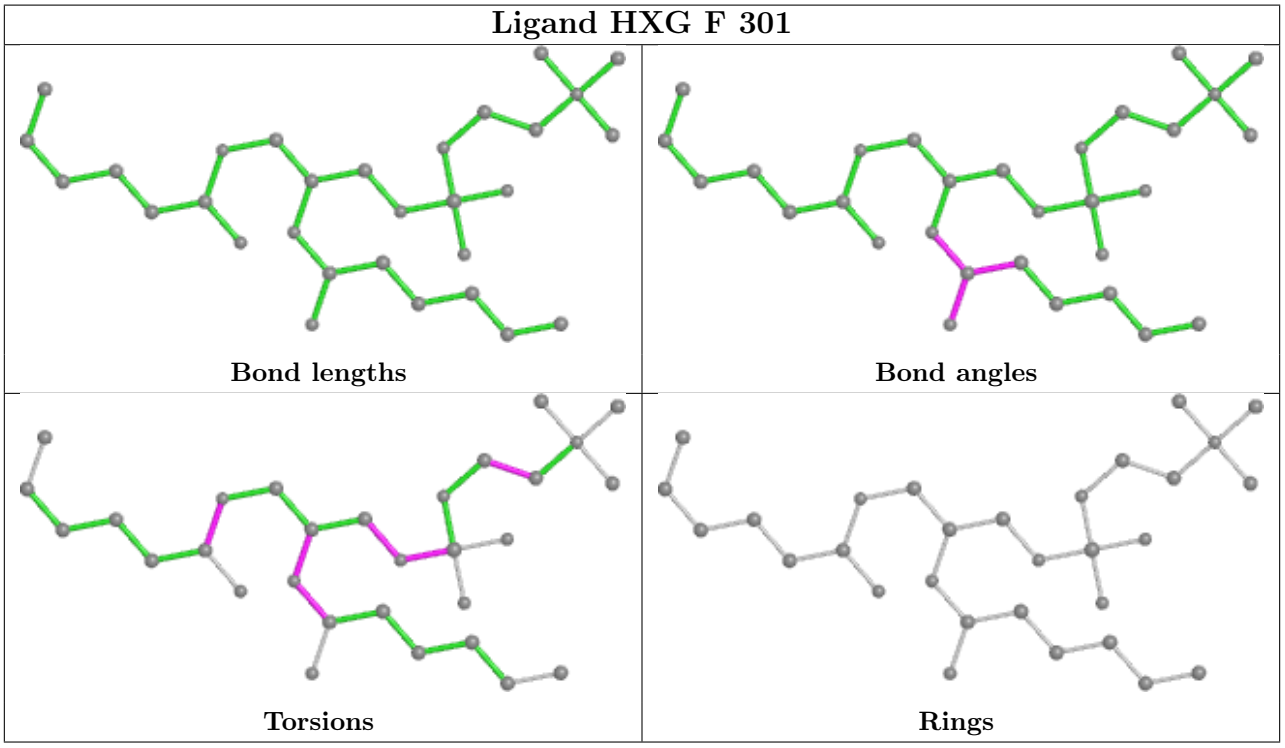


Rings

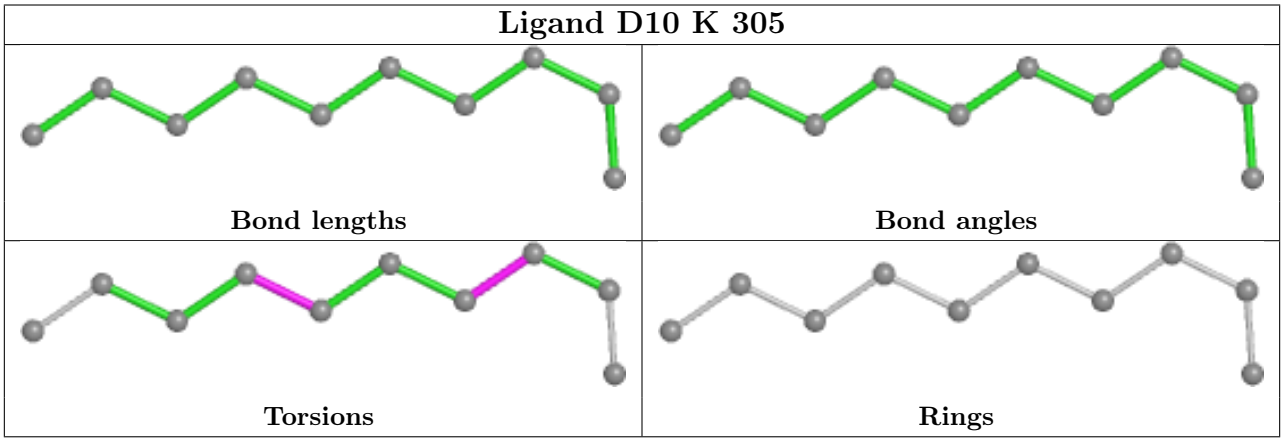
Ligand D10 G 305



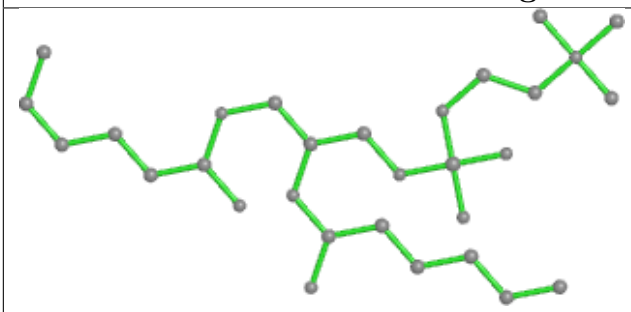
Ligand HXG F 301



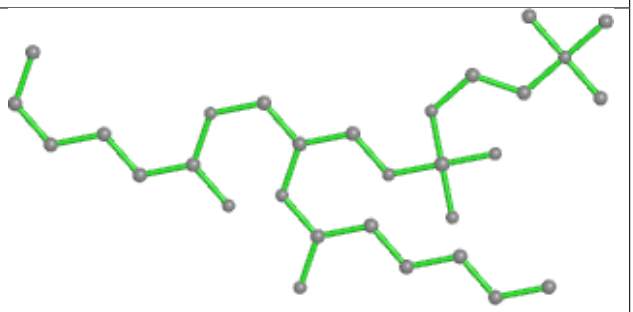
Ligand D10 K 305



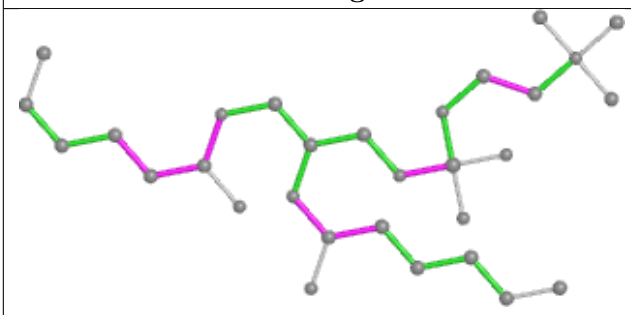
Ligand HXG G 302



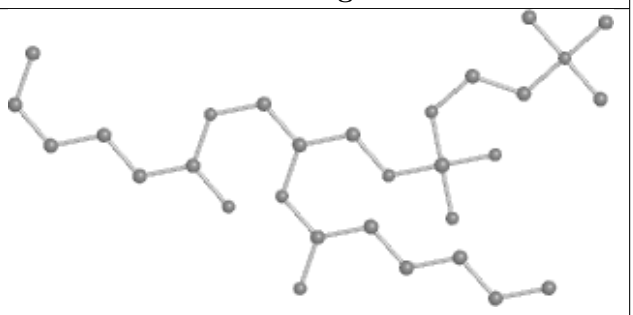
Bond lengths



Bond angles

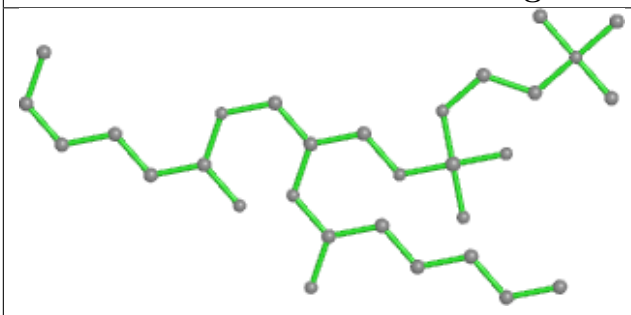


Torsions

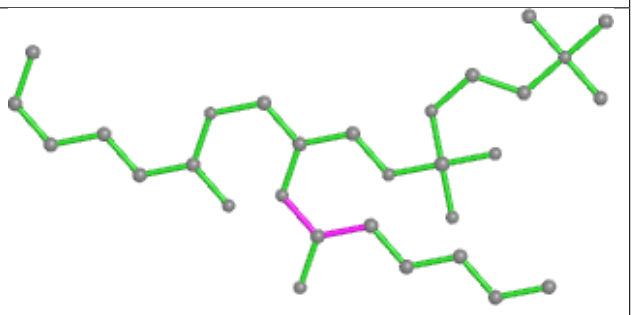


Rings

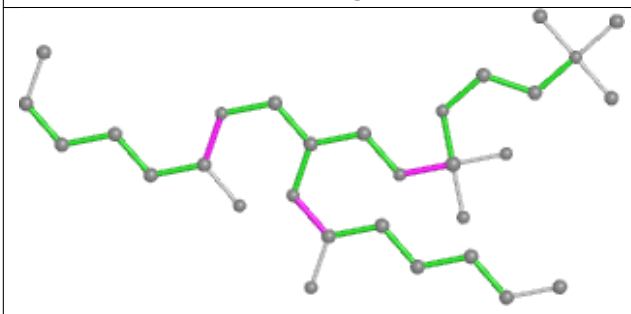
Ligand HXG J 302



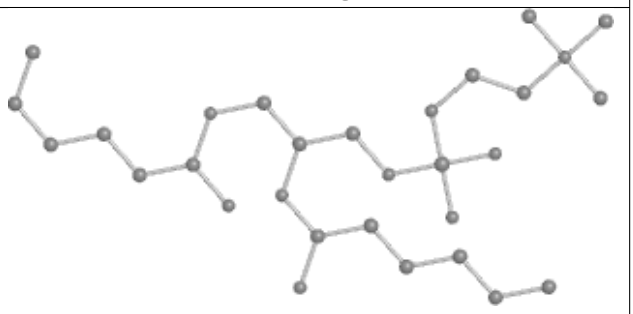
Bond lengths



Bond angles

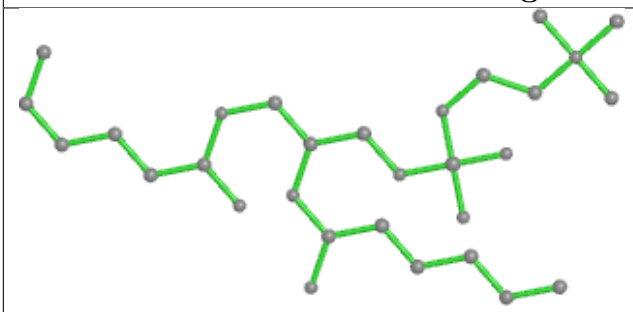


Torsions

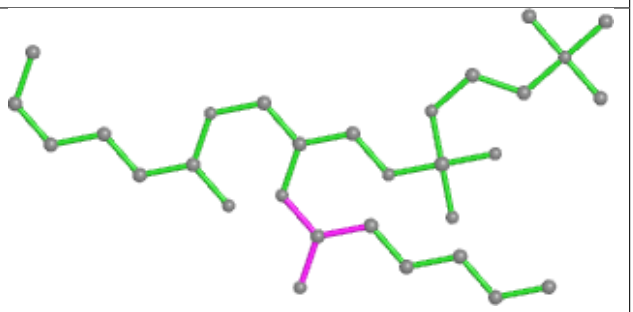


Rings

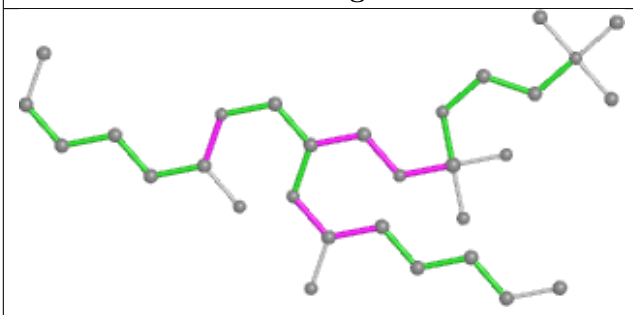
Ligand HXG B 302



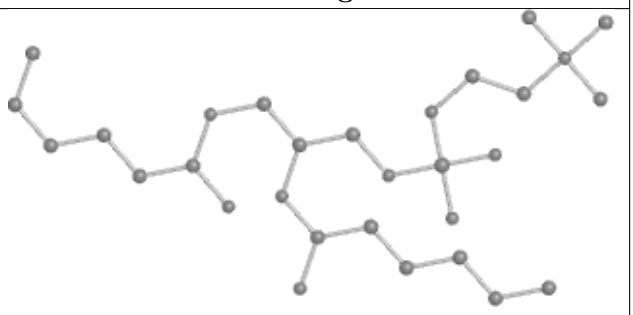
Bond lengths



Bond angles

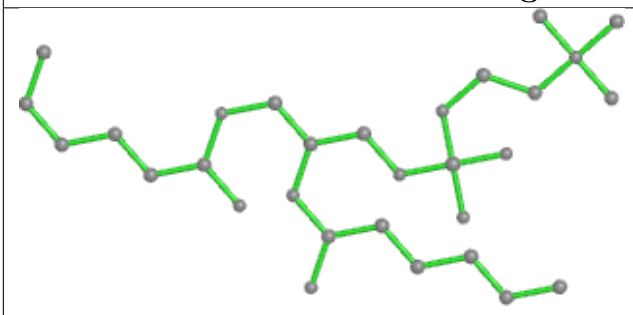


Torsions

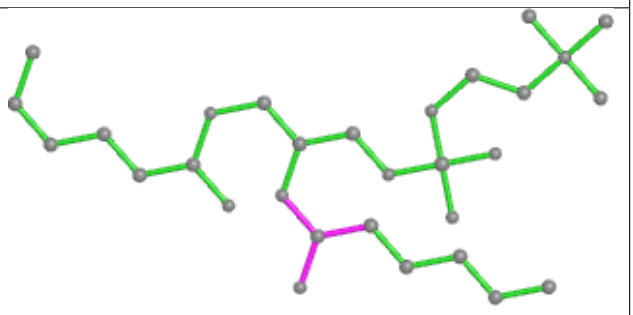


Rings

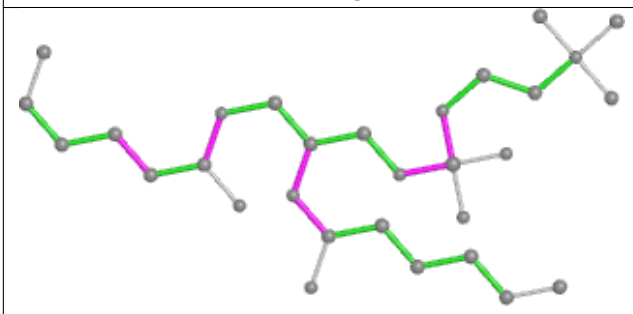
Ligand HXG C 304



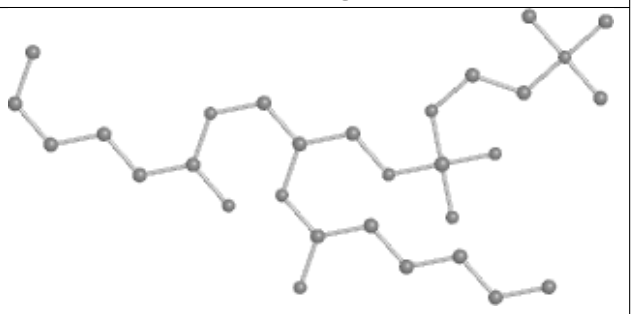
Bond lengths



Bond angles

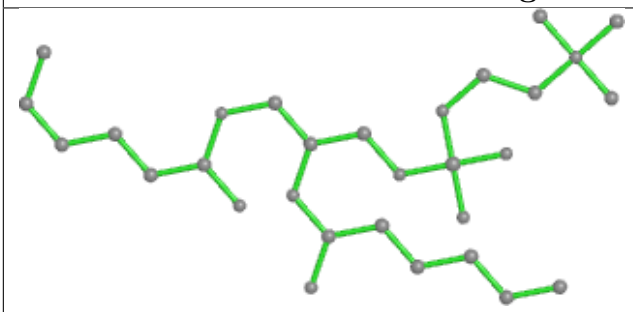


Torsions

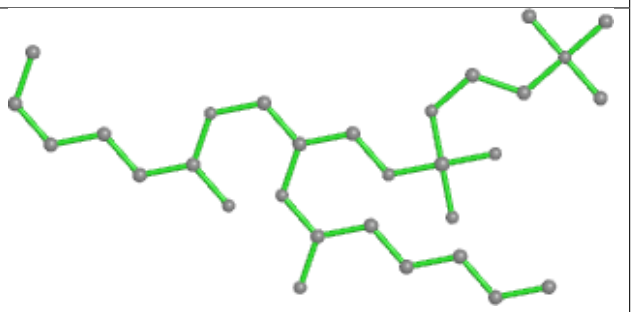


Rings

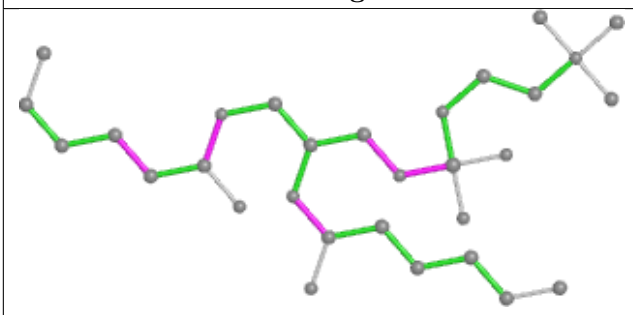
Ligand HXG G 304



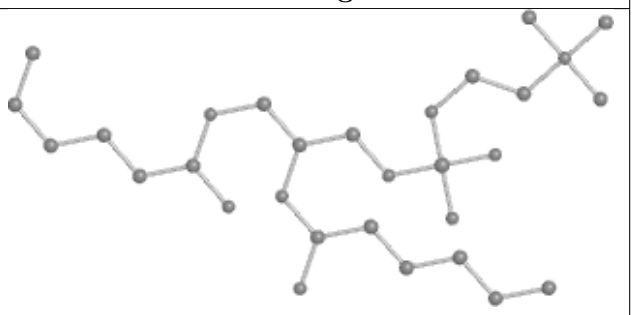
Bond lengths



Bond angles

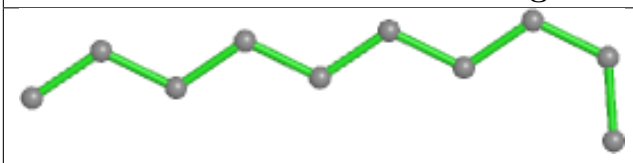


Torsions

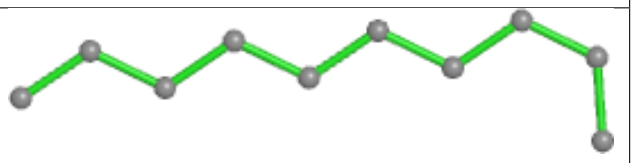


Rings

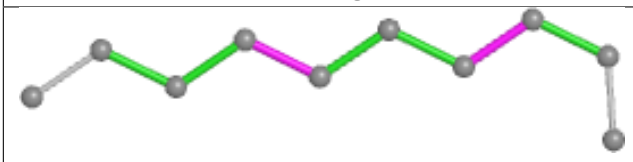
Ligand D10 C 305



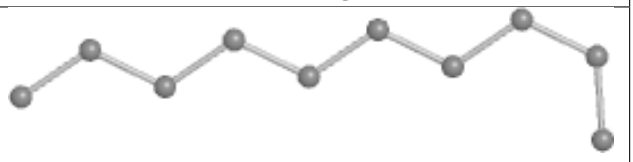
Bond lengths



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.

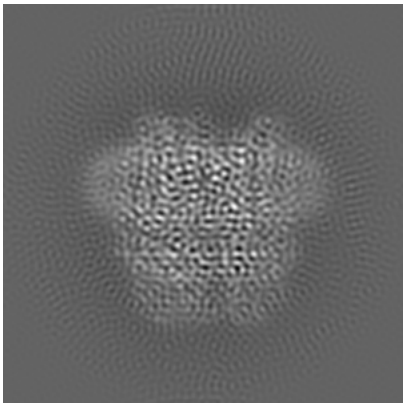
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24831. These allow visual inspection of the internal detail of the map and identification of artifacts.

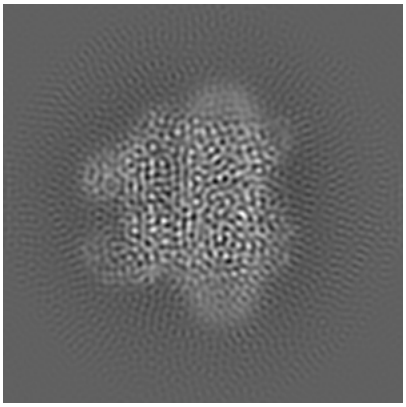
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

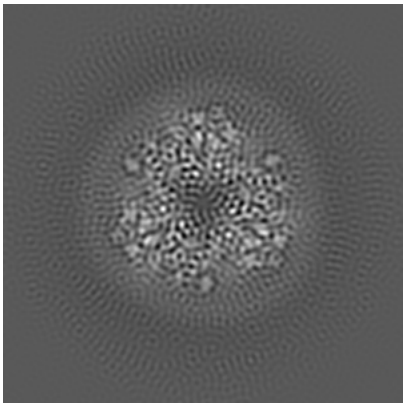
6.1.1 Primary map



X



Y

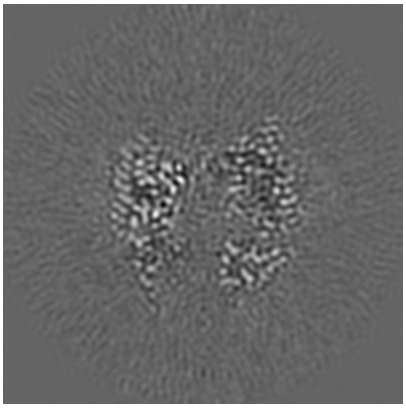


Z

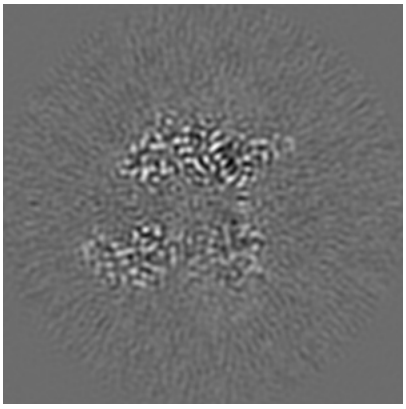
The images above show the map projected in three orthogonal directions.

6.2 Central slices

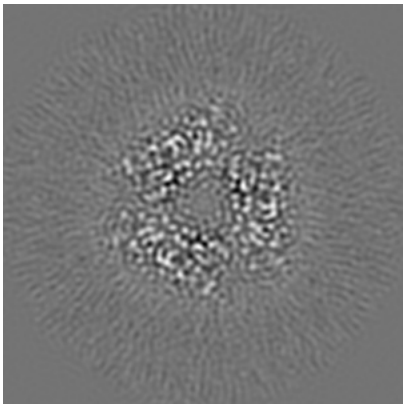
6.2.1 Primary map



X Index: 192



Y Index: 192

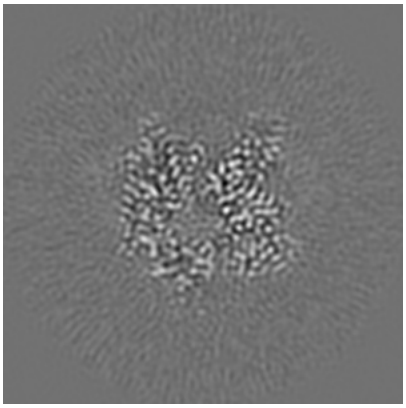


Z Index: 192

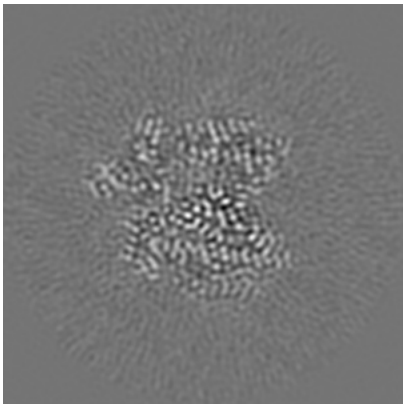
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

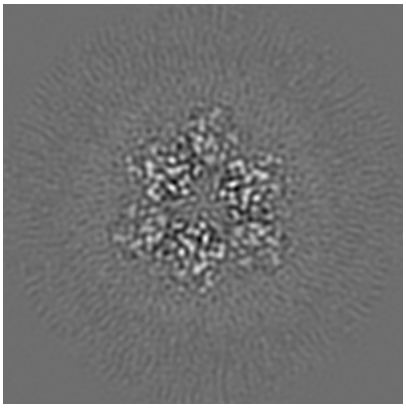
6.3.1 Primary map



X Index: 165



Y Index: 158



Z Index: 213

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 0.0758. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

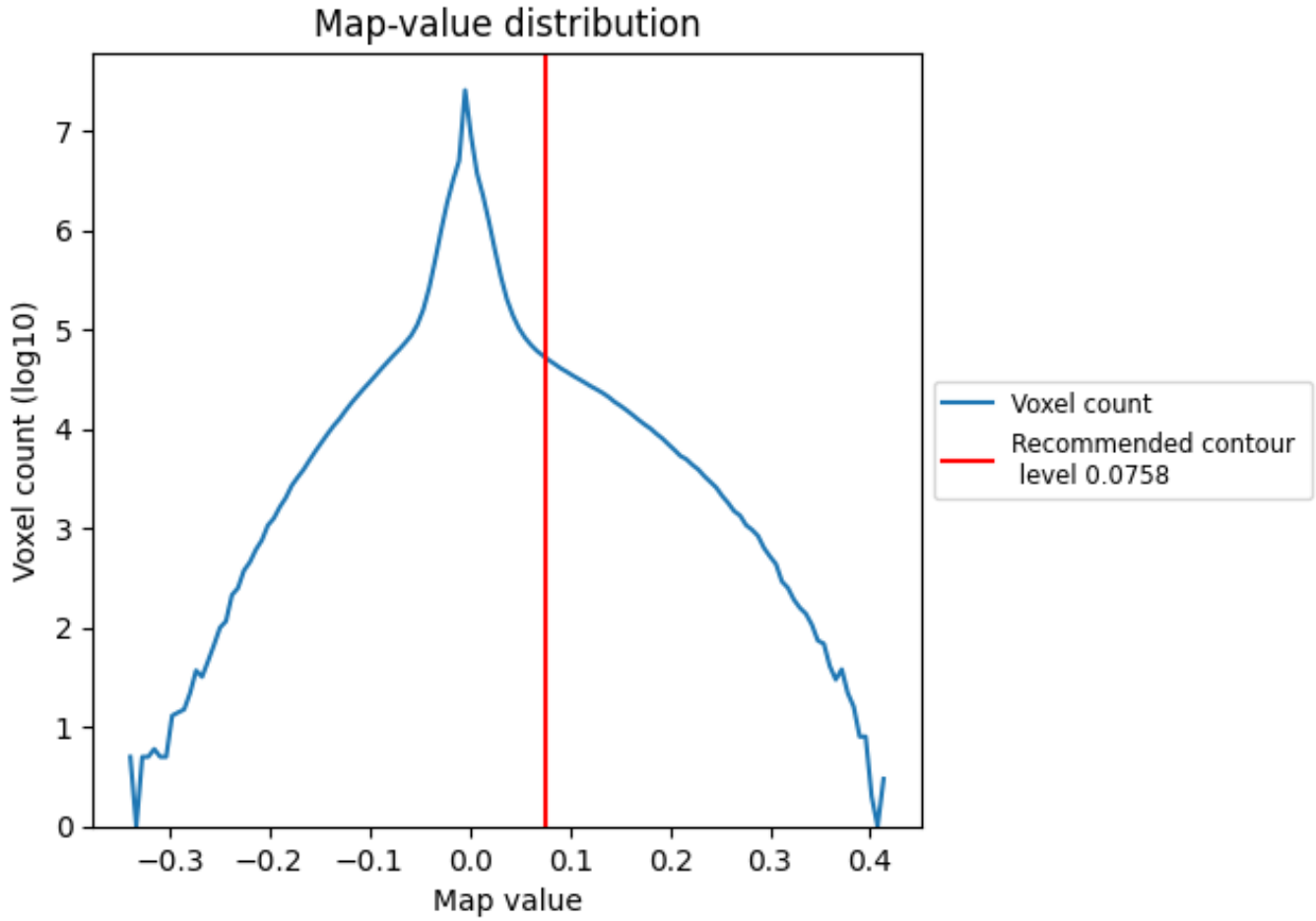
6.5 Mask visualisation (i)

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

7 Map analysis

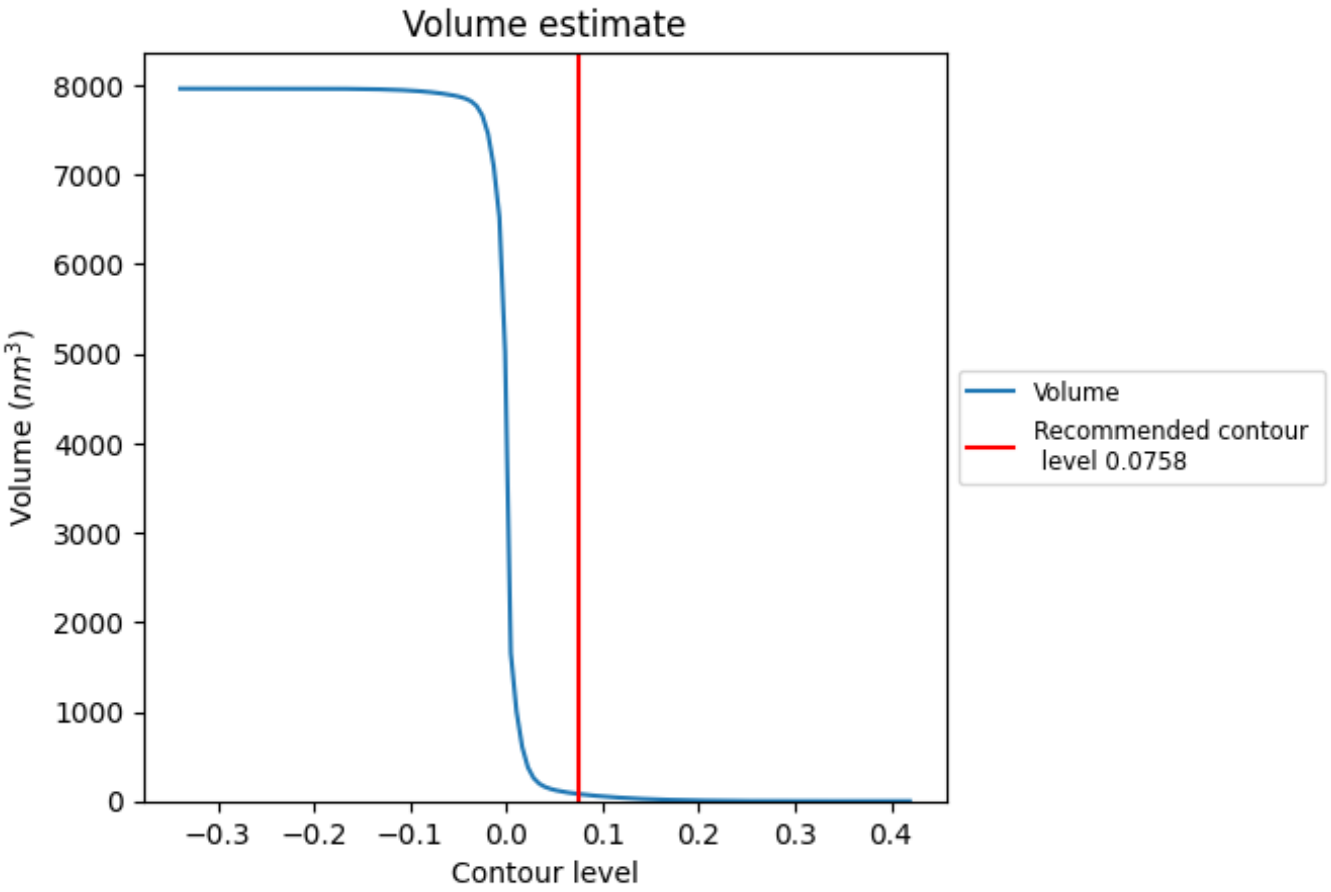
This section contains the results of statistical analysis of the map.

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.

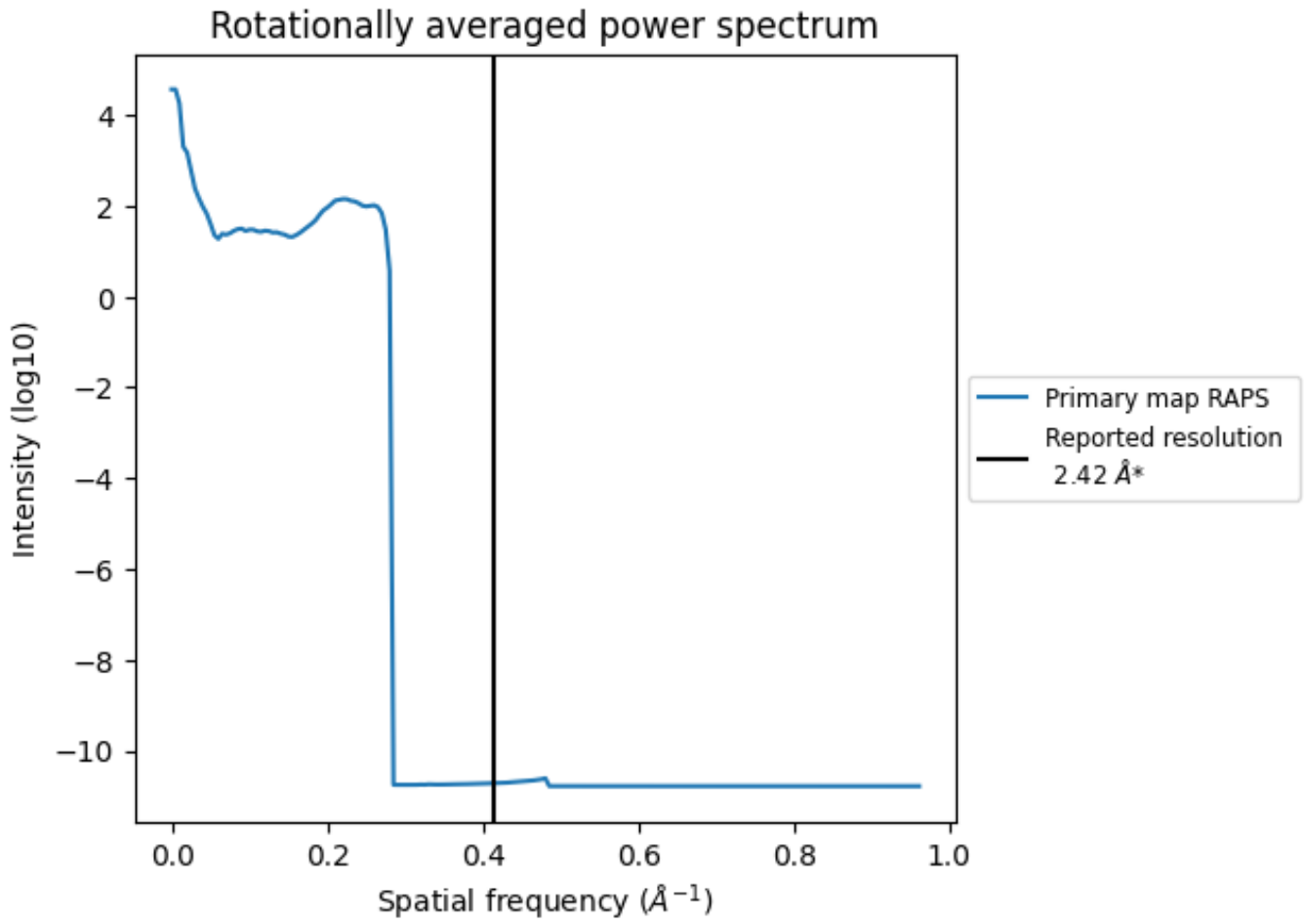
7.2 Volume estimate



The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 71 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)

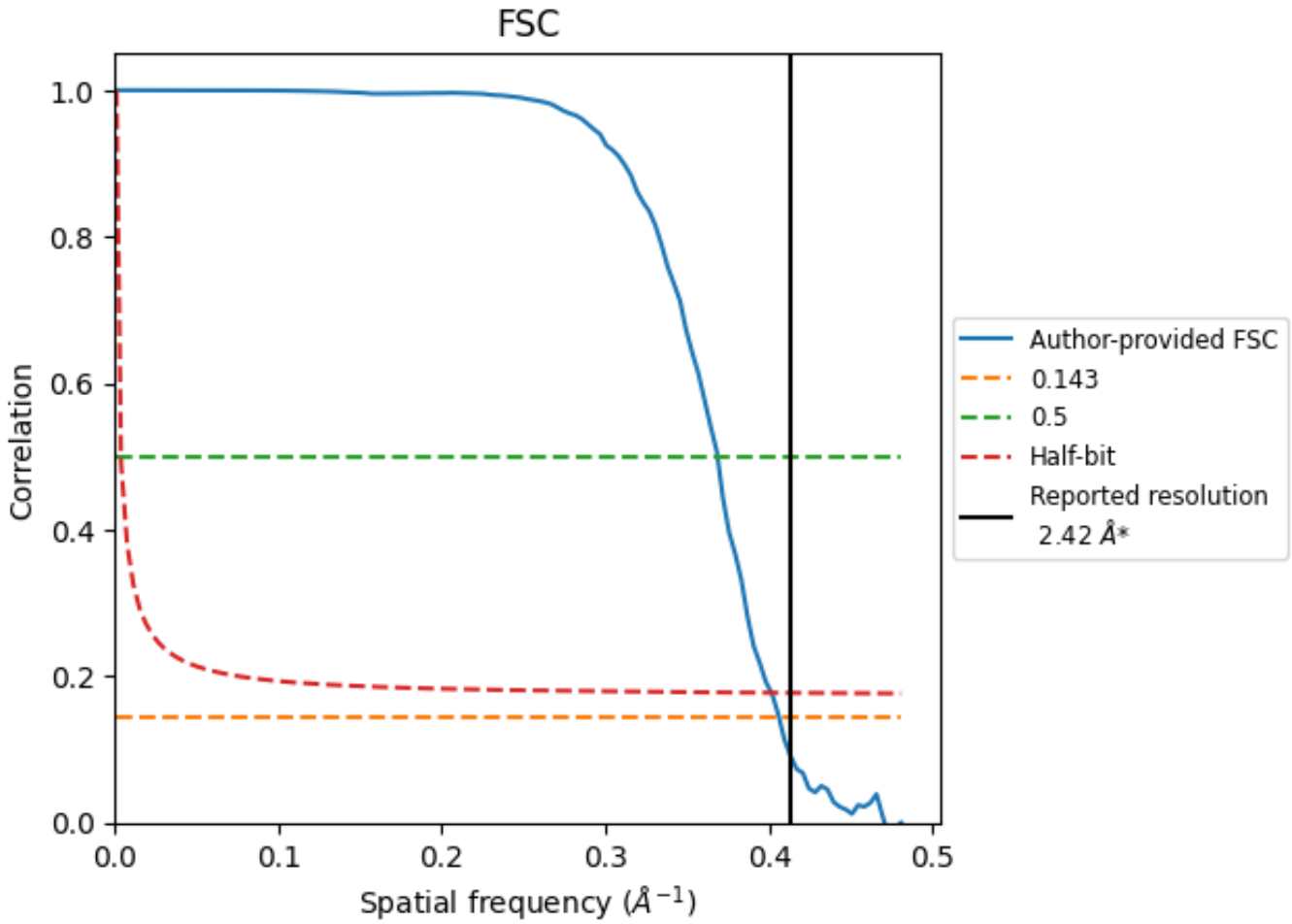


*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

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 0.413 Å^{-1}

8.2 Resolution estimates (i)

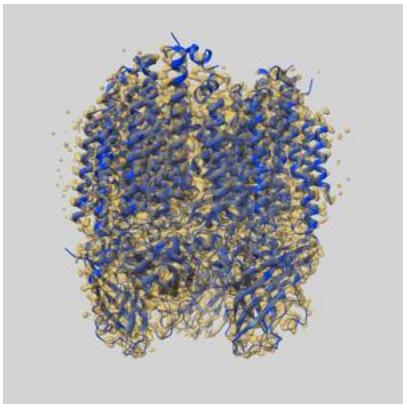
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.46	2.71	2.49
Unmasked-calculated*	-	-	-

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

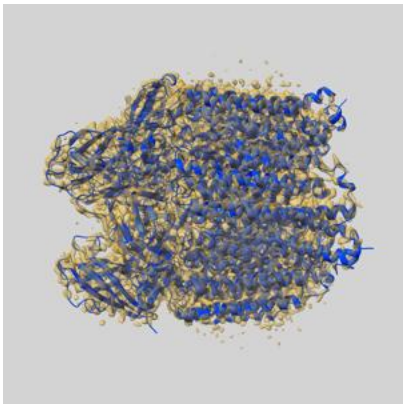
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24831 and PDB model 7S4M. Per-residue inclusion information can be found in section 3 on page 9.

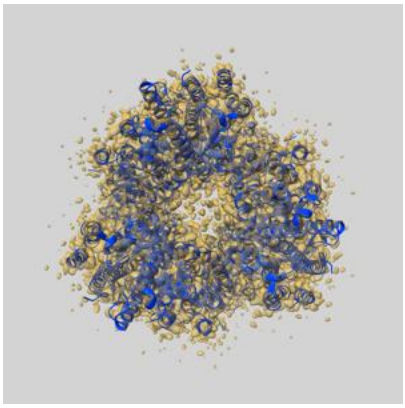
9.1 Map-model overlay



X



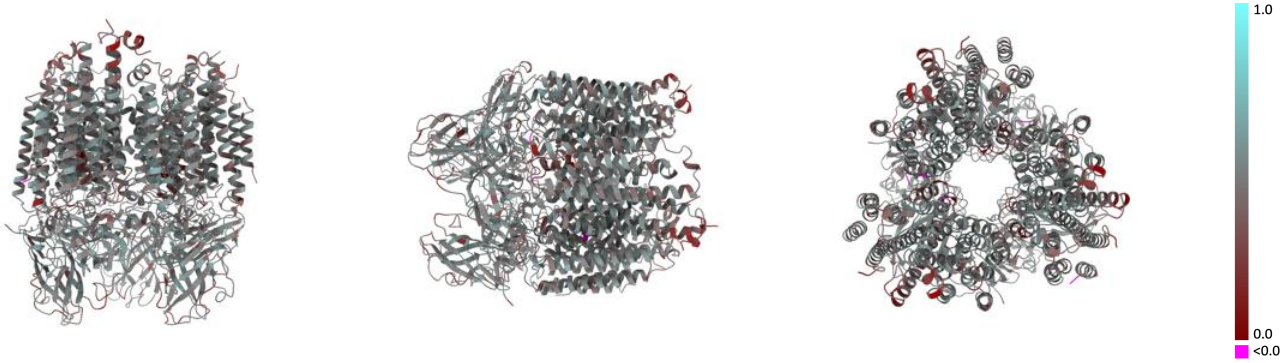
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0758 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

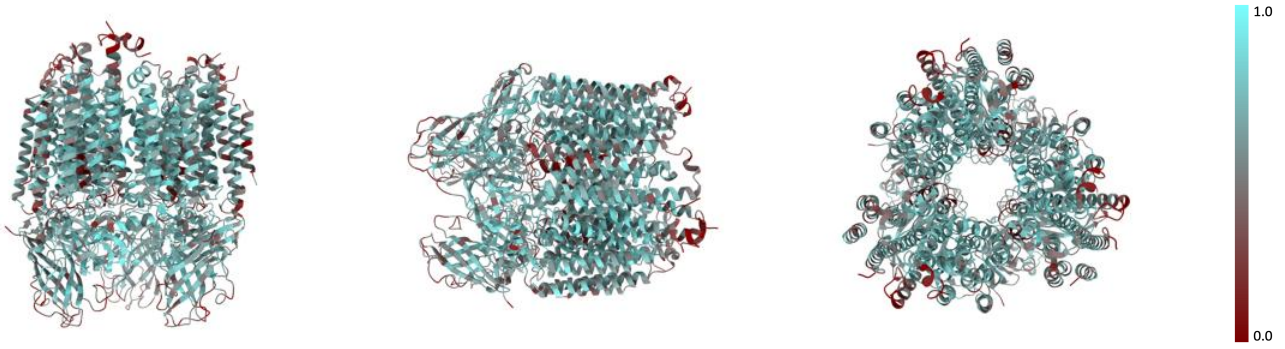
9.2 Q-score mapped to coordinate model



X Y Z

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

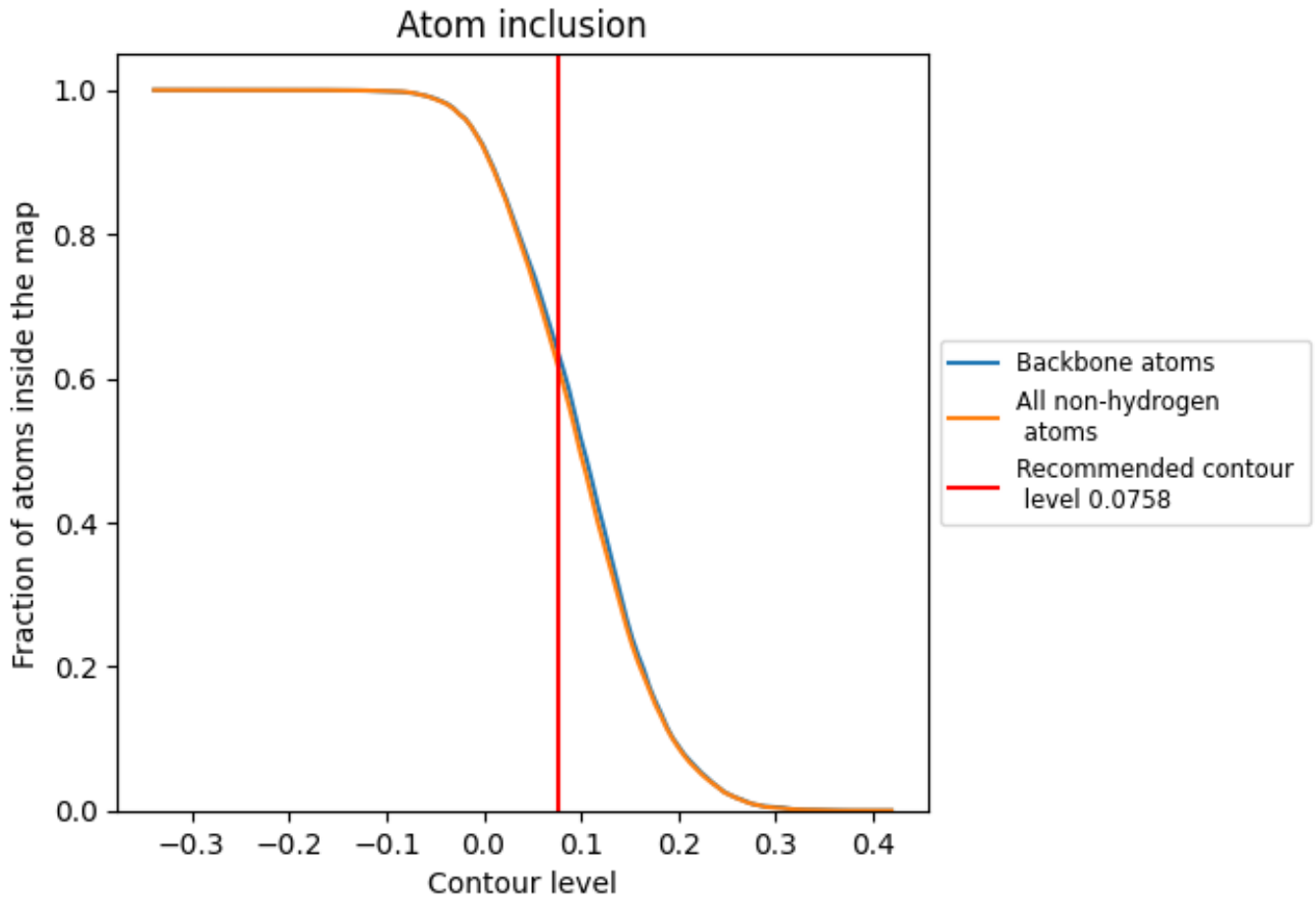
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0758).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 62% 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 (0.0758) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6199	0.4610
A	0.6195	0.4750
B	0.7125	0.4790
C	0.5568	0.4310
D	0.5263	0.4600
E	0.6148	0.4700
F	0.7065	0.4740
G	0.5444	0.4260
H	0.4737	0.4510
I	0.6175	0.4730
J	0.7135	0.4780
K	0.5488	0.4280
N	0.4632	0.4100