Full wwPDB EM Validation Report ⓘ

May 26, 2024 – 10:34 AM EDT

PDB ID	:	7S4L
EMDB ID	:	EMD-24830
Title	:	CryoEM structure of Methylotuvimicrobium alcaliphilum 20Z pMMO in a POPC nanodisc at 2.46 Angstrom resolution
Authors	:	Koo, C.W.; Rosenzweig, A.C.
Deposited on	:	2021-09-09
Resolution	:	2.46 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:

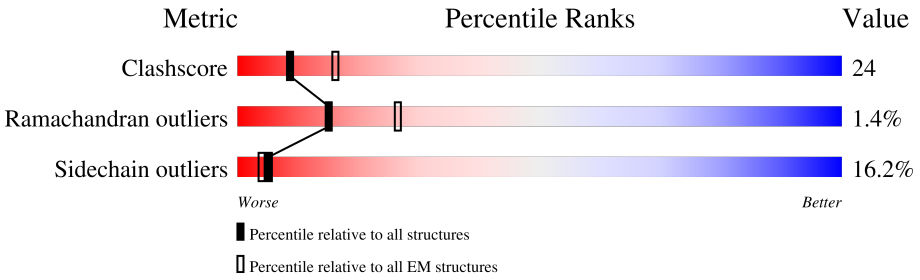
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.46 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	414	5% 64% 25% • 8%
1	D	414	6% 64% 25% • 8%
1	E	414	• 65% 24% • 8%
2	B	247	• 59% 30% 6% • •
2	F	247	• 57% 32% 7% • •
2	G	247	5% 59% 31% 6% • •
3	C	250	18% 40% 37% 15% 8%
3	H	250	18% 33% 46% 13% 8%

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Mol	Chain	Length	Quality of chain
3	I	250	19% 35% 43% 14% 8%

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
5	HXG	B	303	-	-	X	-
5	HXG	F	303	-	-	X	-
5	HXG	G	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22071 atoms, of which 918 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, B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			2970	1906	495	554	15		
1	D	382	Total	C	N	O	S	0	0
			2970	1906	495	554	15		
1	E	382	Total	C	N	O	S	0	0
			2970	1906	495	554	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	239	Total	C	N	O	S	0	0
			1953	1318	310	315	10		
2	F	239	Total	C	N	O	S	0	0
			1953	1318	310	315	10		
2	G	239	Total	C	N	O	S	0	0
			1953	1318	310	315	10		

- Molecule 3 is a protein called Particulate methane monooxygenase, C subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	231	Total	C	N	O	S	0	0
			1914	1290	297	320	7		
3	H	231	Total	C	N	O	S	0	0
			1914	1290	297	320	7		
3	I	231	Total	C	N	O	S	0	0
			1914	1290	297	320	7		

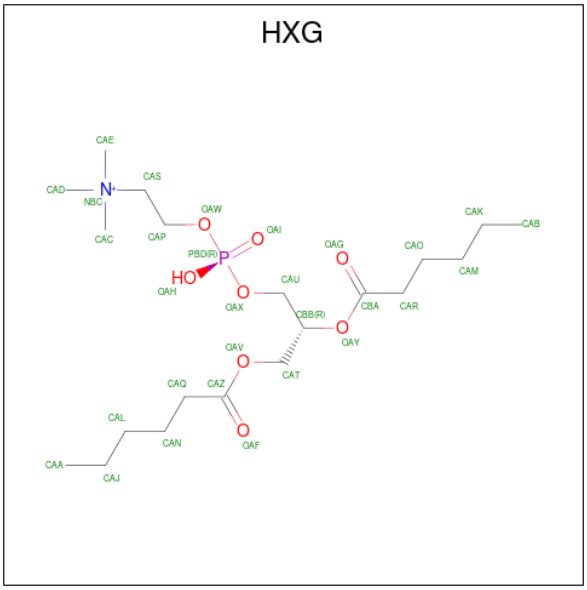
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	VAL	THR	conflict	UNP G4SZ62
H	75	VAL	THR	conflict	UNP G4SZ62
I	75	VAL	THR	conflict	UNP G4SZ62

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Cu 2 2	0
4	C	1	Total Cu 1 1	0
4	H	1	Total Cu 1 1	0
4	I	1	Total Cu 1 1	0
4	D	2	Total Cu 2 2	0
4	E	2	Total Cu 2 2	0

- Molecule 5 is 1,2-dihexanoyl-sn-glycero-3-phosphocholine (three-letter code: HXG) (formula: $C_{20}H_{41}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C H N O P 70 20 40 1 8 1	0
5	B	1	Total C H N O P 70 20 40 1 8 1	0
5	B	1	Total C H N O P 70 20 40 1 8 1	0
5	C	1	Total C H N O P 70 20 40 1 8 1	0

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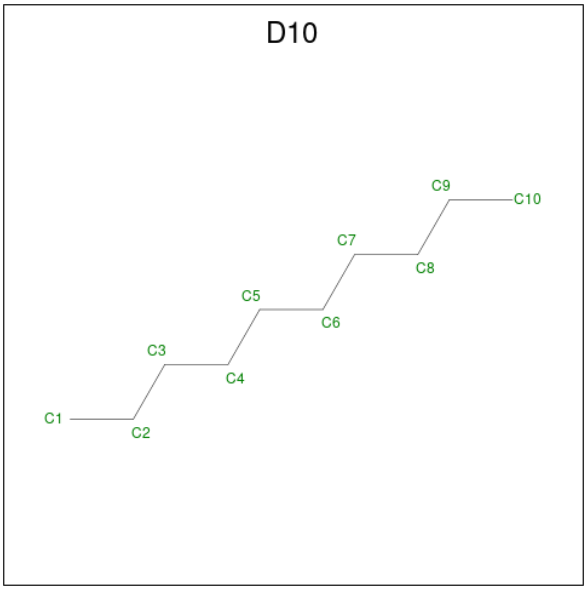
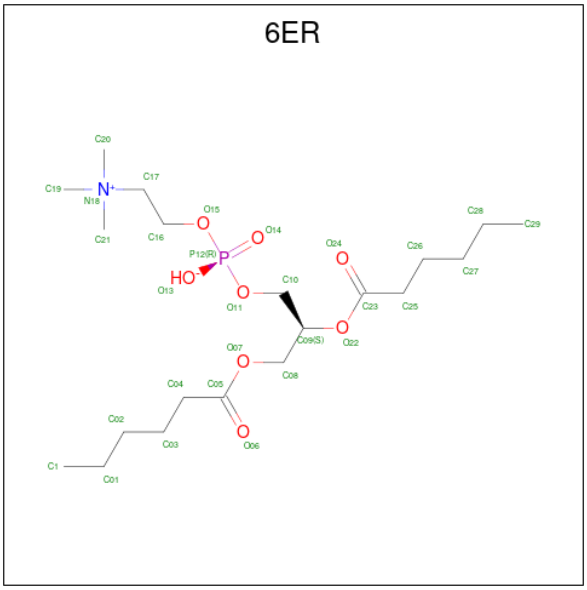
Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	H	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	H	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	I	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	I	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	F	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	F	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	F	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
5	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	

- Molecule 6 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total 32	C 10	H 22	0
6	B	1	Total 32	C 10	H 22	0
6	C	1	Total 32	C 10	H 22	0
6	H	1	Total 32	C 10	H 22	0
6	I	1	Total 32	C 10	H 22	0
6	F	1	Total 32	C 10	H 22	0
6	F	1	Total 32	C 10	H 22	0
6	G	1	Total 32	C 10	H 22	0
6	G	1	Total 32	C 10	H 22	0

- Molecule 7 is (S)-2,3-bis(hexanoyloxy)propyl(2-(trimethylammonio)ethyl)phosphate (three-letter code: 6ER) (formula: $C_{20}H_{41}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total 70	C 20	H 40	N 1	O 8	P 1	0
7	C	1	Total 70	C 20	H 40	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
7	I	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	

- Molecule 8 is water.

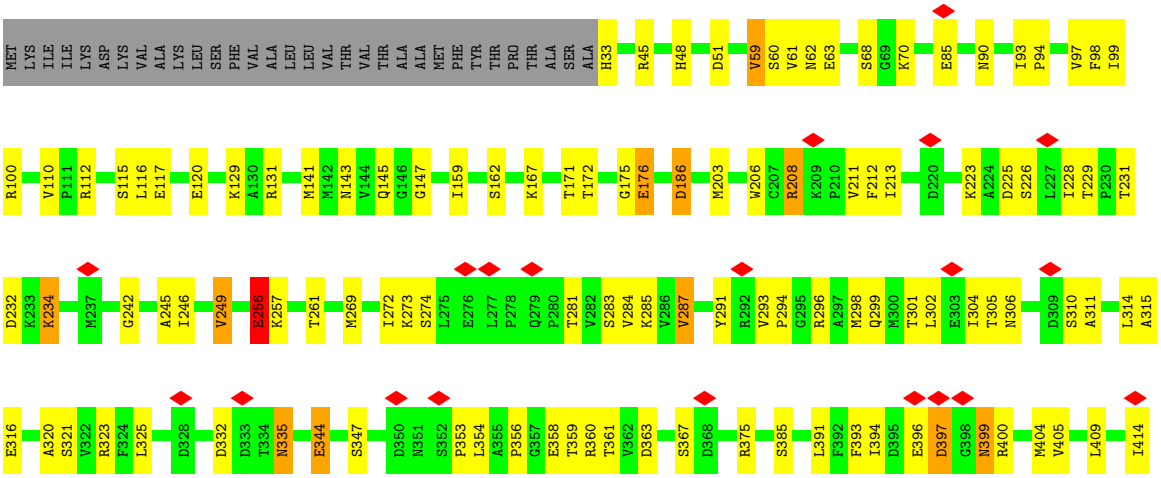
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	O	0
			1	1	
8	D	1	Total	O	0
			1	1	
8	E	1	Total	O	0
			1	1	

3 Residue-property plots (i)

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

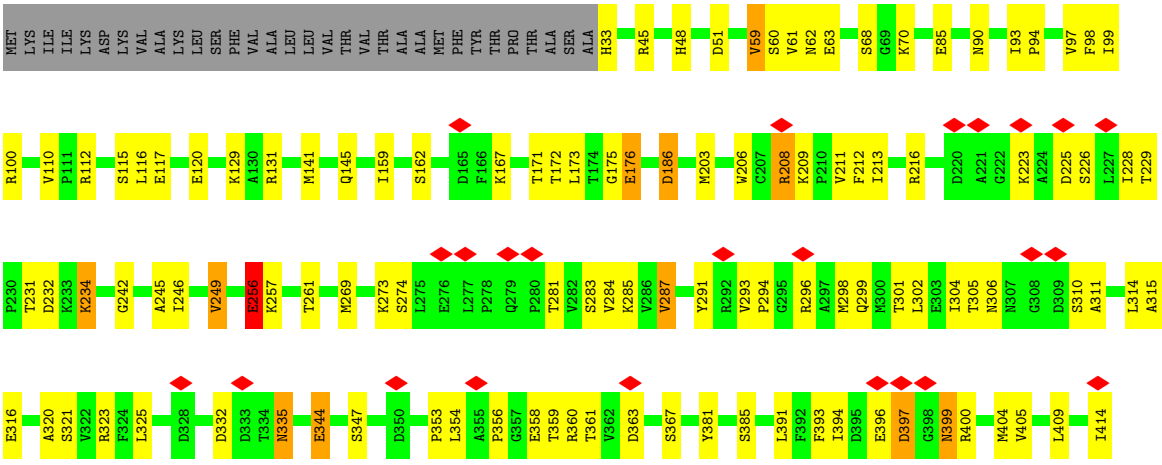
• Molecule 1: Particulate methane monooxygenase, B subunit

Chain A:



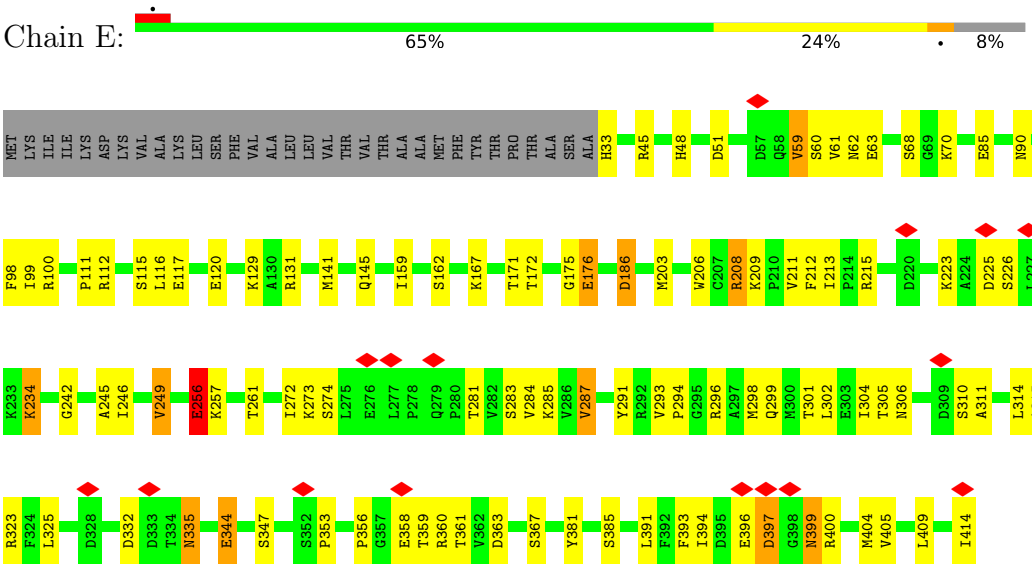
• Molecule 1: Particulate methane monooxygenase, B subunit

Chain D:



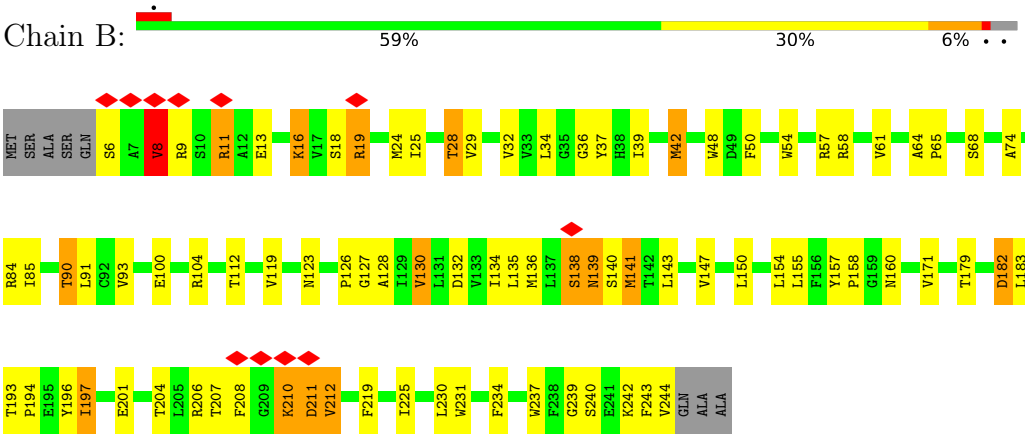
• Molecule 1: Particulate methane monooxygenase, B subunit

Chain E:



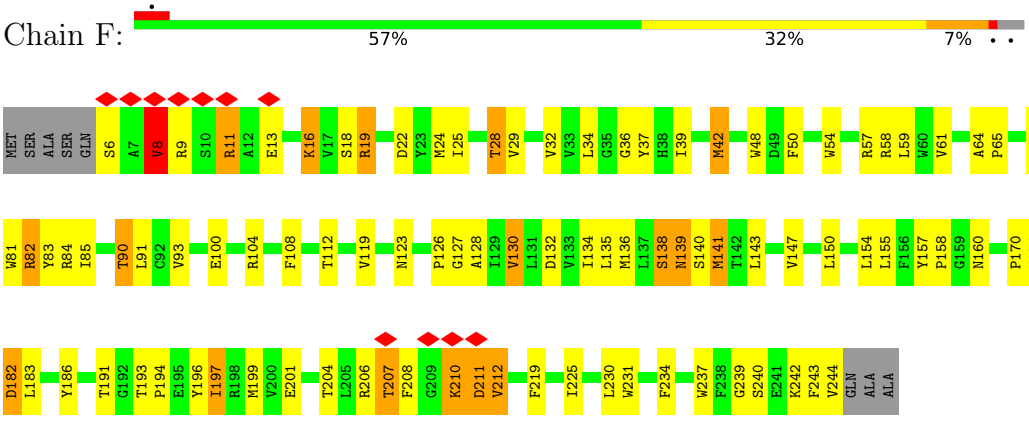
• Molecule 2: Particulate methane monooxygenase, A subunit

Chain B:



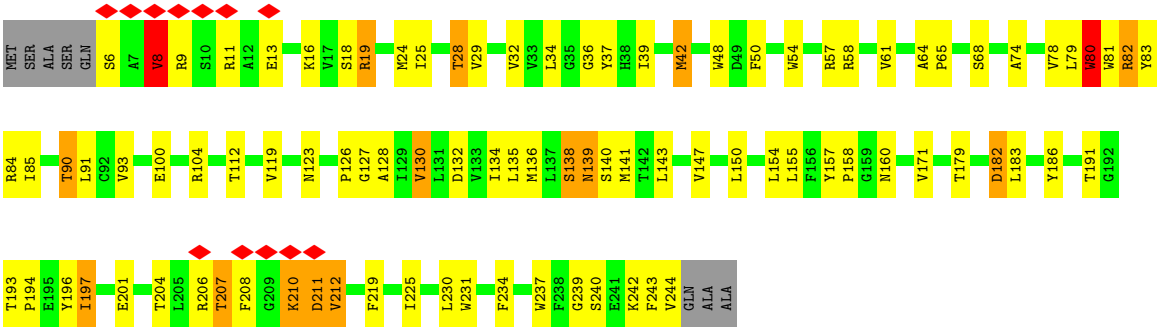
• Molecule 2: Particulate methane monooxygenase, A subunit

Chain F:



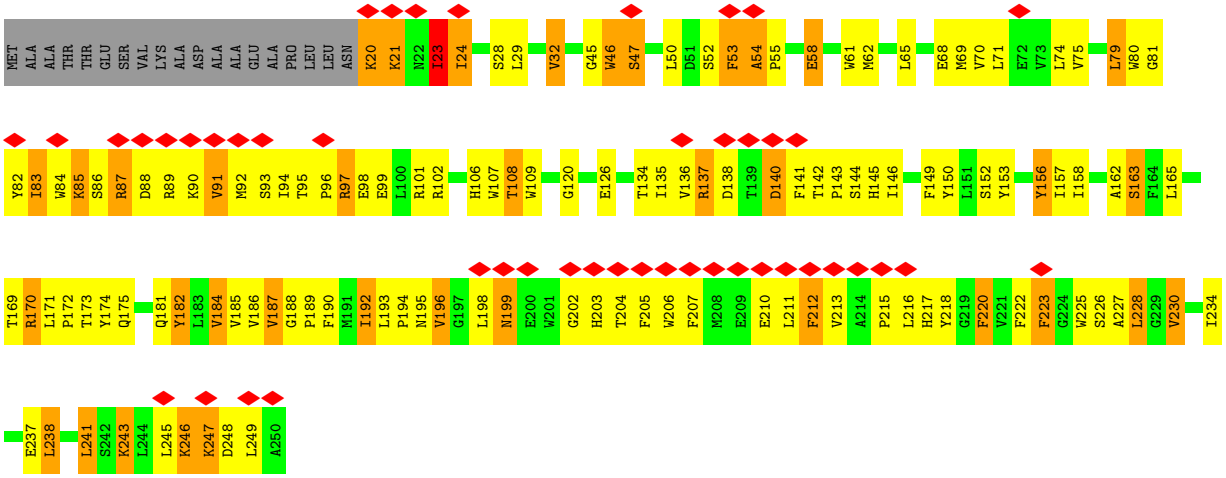
• Molecule 2: Particulate methane monooxygenase, A subunit

Chain G:



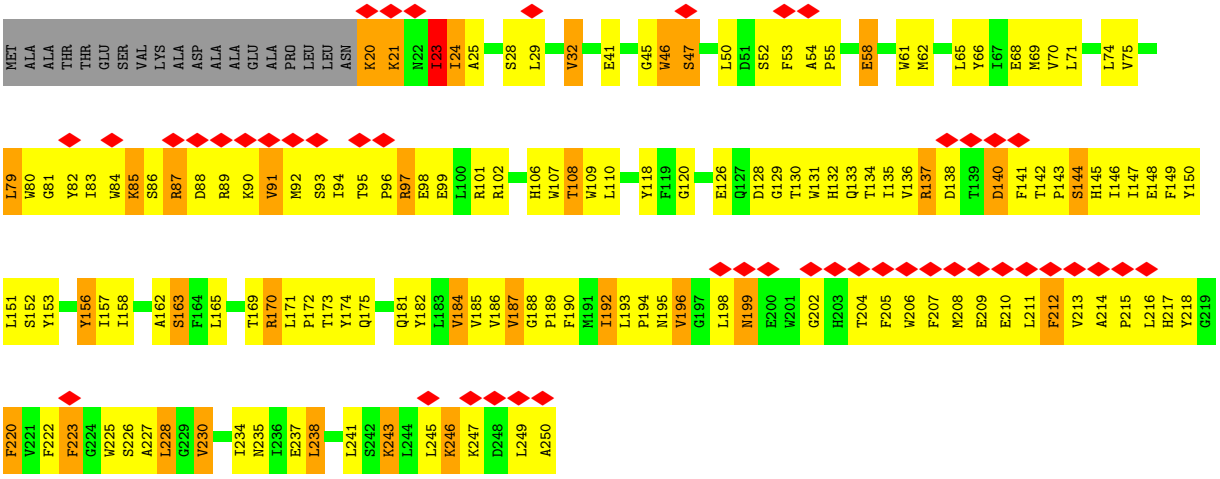
• Molecule 3: Particulate methane monooxygenase, C subunit

Chain C:



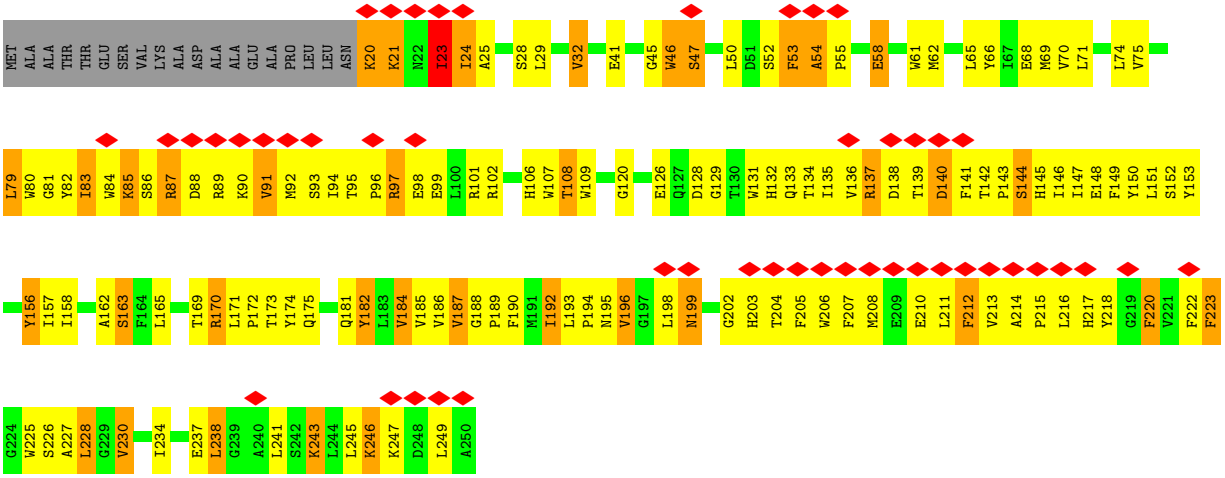
• Molecule 3: Particulate methane monooxygenase, C subunit

Chain H:



• Molecule 3: Particulate methane monooxygenase, C subunit

Chain I:


MET ALA ALA THR THR GLU SER VAL LYS ALA ASP ALA ALA GLU ALA PRO LEU LEU ASN K20 K21 N22 I23 I24 A25 S28 L29 V32 E41 G45 W46 S47 L50 D51 S52 F53 A54 P55 E58 W61 M62 L65 Y66 I67 E68 M69 V70 L71 L74 V75
L79 W80 G81 Y82 I83 W84 K85 S86 R87 D88 R89 K90 V91 M92 S93 I94 T95 P96 R97 E98 E99 L100 R101 R102 H106 W107 T108 W109 G120 E126 Q127 D128 G129 T130 W131 H132 Q133 T134 I135 V136 R137 D138 T139 D140 F141 T142 P143 S144 H145 I146 I147 E148 F149 Y150 L151 S152 Y153
Y156 I157 I158 A162 S163 F164 L165 T169 R170 L171 P172 T173 Y174 Q175 Q181 Y182 L183 V184 V185 V186 V187 G188 P189 F190 M191 I192 L193 P194 N195 V196 G197 L198 N199 G202 H203 T204 F205 W206 F207 M208 E209 E210 L211 F212 V213 A214 P215 L216 H217 Y218 G219 F220 V221 F222 F223
G224 W225 S226 A227 L228 G229 V230 I234 E237 L238 G239 A240 L241 S242 K243 L244 L245 K246 K247 D248 L249 A250

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443800	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 ($e^-/Å^2$)	64	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	0.137	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0272	Depositor
Map size (Å)	201.59999, 201.59999, 201.59999	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.525, 0.525, 0.525	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, HXG, 6ER, D10

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	0/3048	0.55	1/4155 (0.0%)
1	D	0.49	0/3048	0.55	1/4155 (0.0%)
1	E	0.49	0/3048	0.55	1/4155 (0.0%)
2	B	0.51	0/2029	0.52	0/2776
2	F	0.51	0/2029	0.52	0/2776
2	G	0.51	0/2029	0.52	0/2776
3	C	0.51	0/1985	0.57	0/2708
3	H	0.47	0/1985	0.53	0/2708
3	I	0.47	0/1985	0.53	0/2708
All	All	0.49	0/21186	0.54	3/28917 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	256	GLU	CA-CB-CG	5.66	125.86	113.40
1	E	256	GLU	CA-CB-CG	5.66	125.85	113.40
1	A	256	GLU	CA-CB-CG	5.66	125.84	113.40

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	2970	0	2921	69	0
1	D	2970	0	2921	72	0
1	E	2970	0	2921	67	0
2	B	1953	0	1917	124	0
2	F	1953	0	1917	131	0
2	G	1953	0	1917	123	0
3	C	1914	0	1869	165	0
3	H	1914	0	1869	171	0
3	I	1914	0	1869	172	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
5	B	90	120	120	42	0
5	C	60	80	80	0	0
5	F	90	120	120	45	0
5	G	90	120	120	43	0
5	H	60	80	80	1	0
5	I	60	80	80	1	0
6	B	20	44	44	1	0
6	C	10	22	22	4	0
6	F	20	44	44	1	0
6	G	20	44	44	1	0
6	H	10	22	22	4	0
6	I	10	22	22	4	0
7	B	30	40	0	8	0
7	C	30	40	0	7	0
7	I	30	40	0	8	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
All	All	21153	918	20919	998	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 24.

All (998) 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)
7:I:304:6ER:C19	6:I:305:D10:H11	1.31	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:237:TRP:CE2	5:G:303:HXG:H16	1.36	1.58
2:G:234:PHE:CE1	5:G:303:HXG:CAJ	1.87	1.57
2:F:237:TRP:CE2	5:F:303:HXG:H16	1.36	1.57
2:B:237:TRP:CE2	5:B:303:HXG:H16	1.36	1.56
7:C:304:6ER:C19	6:C:305:D10:H11	1.31	1.56
7:B:306:6ER:C19	6:H:301:D10:H11	1.31	1.53
2:B:234:PHE:CE1	5:B:303:HXG:CAJ	1.87	1.53
2:F:234:PHE:CE1	5:F:303:HXG:CAJ	1.87	1.52
2:B:234:PHE:CE1	5:B:303:HXG:H5	1.43	1.50
2:F:234:PHE:CE1	5:F:303:HXG:H5	1.43	1.46
2:G:234:PHE:CE1	5:G:303:HXG:H5	1.43	1.45
3:I:205:PHE:CZ	7:I:304:6ER:C21	2.00	1.44
2:B:237:TRP:NE1	5:B:303:HXG:H16	1.13	1.42
2:F:237:TRP:NE1	5:F:303:HXG:H16	1.13	1.41
2:G:237:TRP:NE1	5:G:303:HXG:H16	1.13	1.40
7:B:306:6ER:C21	3:H:205:PHE:CZ	2.05	1.39
2:G:237:TRP:NE1	5:G:303:HXG:CAR	1.88	1.36
3:C:205:PHE:CZ	7:C:304:6ER:C21	2.09	1.36
2:B:237:TRP:NE1	5:B:303:HXG:CAR	1.88	1.33
2:F:237:TRP:NE1	5:F:303:HXG:CAR	1.88	1.33
2:B:237:TRP:CE2	5:B:303:HXG:CAR	2.13	1.32
2:G:237:TRP:CE2	5:G:303:HXG:CAR	2.13	1.32
2:F:237:TRP:CE2	5:F:303:HXG:CAR	2.13	1.31
2:B:234:PHE:HE1	5:B:303:HXG:CAJ	1.29	1.29
3:I:21:LYS:HE3	3:I:108:THR:OG1	1.30	1.28
2:G:234:PHE:HE1	5:G:303:HXG:CAJ	1.29	1.28
3:H:21:LYS:HE3	3:H:108:THR:OG1	1.30	1.28
7:B:306:6ER:C19	6:H:301:D10:C1	2.13	1.26
2:F:234:PHE:HE1	5:F:303:HXG:CAJ	1.29	1.26
7:C:304:6ER:C19	6:C:305:D10:C1	2.13	1.26
7:I:304:6ER:C19	6:I:305:D10:C1	2.14	1.25
3:C:21:LYS:HE3	3:C:108:THR:OG1	1.30	1.24
2:F:234:PHE:CZ	5:F:303:HXG:H1	1.79	1.18
2:G:234:PHE:CZ	5:G:303:HXG:H1	1.79	1.17
2:B:234:PHE:CZ	5:B:303:HXG:H1	1.79	1.16
2:G:234:PHE:CD1	5:G:303:HXG:H5	1.86	1.11
2:B:234:PHE:CD1	5:B:303:HXG:H5	1.85	1.10
2:F:234:PHE:CD1	5:F:303:HXG:H5	1.86	1.10
2:B:237:TRP:CA	5:B:303:HXG:H33	1.83	1.08
2:G:237:TRP:CA	5:G:303:HXG:H33	1.83	1.08
2:F:237:TRP:CA	5:F:303:HXG:H33	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:SER:HB2	5:B:303:HXG:CAC	1.87	1.05
2:G:234:PHE:HE1	5:G:303:HXG:H4	0.90	1.05
2:F:240:SER:HB2	5:F:303:HXG:CAC	1.87	1.04
2:G:237:TRP:CD1	5:G:303:HXG:H16	1.92	1.04
2:B:237:TRP:CD1	5:B:303:HXG:H16	1.92	1.03
2:G:240:SER:HB2	5:G:303:HXG:CAC	1.87	1.03
2:F:237:TRP:CD1	5:F:303:HXG:H16	1.92	1.03
2:B:234:PHE:HE1	5:B:303:HXG:H4	0.90	1.02
3:I:142:THR:HG22	3:I:144:SER:H	1.21	1.02
2:F:234:PHE:HE1	5:F:303:HXG:H4	0.90	1.01
3:I:134:THR:HG21	2:G:112:THR:HG21	1.43	1.01
2:F:237:TRP:HA	5:F:303:HXG:H33	1.01	1.01
3:H:142:THR:HG22	3:H:144:SER:H	1.21	1.01
2:F:234:PHE:CE1	5:F:303:HXG:CAA	2.43	1.00
2:B:234:PHE:CE1	5:B:303:HXG:CAA	2.43	1.00
2:G:234:PHE:CE1	5:G:303:HXG:CAA	2.43	1.00
2:G:237:TRP:HA	5:G:303:HXG:H33	1.01	1.00
2:B:237:TRP:HA	5:B:303:HXG:H33	1.01	0.99
3:I:186:VAL:O	3:I:188:GLY:N	1.96	0.99
3:H:186:VAL:O	3:H:188:GLY:N	1.96	0.98
2:G:237:TRP:HA	5:G:303:HXG:CAD	1.94	0.98
3:C:186:VAL:O	3:C:188:GLY:N	1.96	0.98
2:F:237:TRP:HA	5:F:303:HXG:CAD	1.94	0.97
2:F:237:TRP:HE1	5:F:303:HXG:CBA	1.76	0.97
2:B:237:TRP:HA	5:B:303:HXG:CAD	1.94	0.97
2:B:237:TRP:HE1	5:B:303:HXG:CBA	1.76	0.97
2:G:237:TRP:HE1	5:G:303:HXG:CBA	1.76	0.96
3:H:91:VAL:HA	3:H:94:ILE:HG13	1.48	0.96
2:B:237:TRP:NE1	5:B:303:HXG:CBA	2.28	0.96
2:F:237:TRP:NE1	5:F:303:HXG:CBA	2.28	0.96
2:G:237:TRP:NE1	5:G:303:HXG:CBA	2.28	0.95
3:C:91:VAL:HA	3:C:94:ILE:HG13	1.48	0.94
3:I:91:VAL:HA	3:I:94:ILE:HG13	1.48	0.93
2:F:240:SER:HB2	5:F:303:HXG:H39	1.51	0.92
2:B:112:THR:HG21	3:C:134:THR:HG21	1.50	0.92
3:H:134:THR:HG21	2:F:112:THR:HG21	1.49	0.92
3:C:23:ILE:HD12	3:C:24:ILE:HD12	1.52	0.92
2:F:237:TRP:CZ2	5:F:303:HXG:H15	2.05	0.92
2:F:186:TYR:O	1:D:100:ARG:NH2	2.02	0.91
2:G:240:SER:HB2	5:G:303:HXG:H39	1.51	0.91
3:I:23:ILE:HD12	3:I:24:ILE:HD12	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:PHE:HZ	7:C:304:6ER:C21	1.81	0.91
2:G:237:TRP:CZ2	5:G:303:HXG:H15	2.05	0.91
2:F:234:PHE:HZ	5:F:303:HXG:H1	1.36	0.90
2:B:237:TRP:CZ2	5:B:303:HXG:H15	2.05	0.90
3:I:205:PHE:HZ	7:I:304:6ER:C21	1.72	0.90
2:F:234:PHE:CZ	5:F:303:HXG:CAA	2.55	0.90
3:H:23:ILE:HD12	3:H:24:ILE:CD1	2.02	0.90
3:H:23:ILE:HD12	3:H:24:ILE:HD12	1.51	0.90
3:C:23:ILE:HD12	3:C:24:ILE:CD1	2.02	0.90
2:G:234:PHE:CZ	5:G:303:HXG:CAA	2.55	0.89
2:B:237:TRP:CD1	5:B:303:HXG:H36	2.08	0.89
3:H:21:LYS:HE3	3:H:108:THR:HG1	1.35	0.89
2:B:240:SER:HB2	5:B:303:HXG:H39	1.51	0.89
2:F:237:TRP:CD1	5:F:303:HXG:H36	2.08	0.89
2:B:234:PHE:CZ	5:B:303:HXG:CAA	2.55	0.88
3:I:205:PHE:CE2	7:I:304:6ER:C21	2.56	0.88
2:G:237:TRP:CD1	5:G:303:HXG:H36	2.08	0.88
2:F:234:PHE:CE1	5:F:303:HXG:H4	1.80	0.88
3:I:23:ILE:HD12	3:I:24:ILE:CD1	2.02	0.88
3:C:21:LYS:HE3	3:C:108:THR:HG1	1.38	0.88
2:G:186:TYR:O	1:E:100:ARG:NH2	2.07	0.87
3:C:205:PHE:CE2	7:C:304:6ER:C21	2.58	0.87
2:B:25:ILE:O	2:B:29:VAL:HG12	1.75	0.87
2:B:234:PHE:HZ	5:B:303:HXG:H1	1.36	0.86
2:F:25:ILE:O	2:F:29:VAL:HG12	1.75	0.86
2:G:234:PHE:HZ	5:G:303:HXG:H1	1.36	0.86
2:F:240:SER:HB2	5:F:303:HXG:H40	1.57	0.86
2:G:25:ILE:O	2:G:29:VAL:HG12	1.75	0.85
1:E:310:SER:OG	1:E:396:GLU:OE1	1.95	0.85
1:A:310:SER:OG	1:A:396:GLU:OE1	1.95	0.85
2:F:237:TRP:CZ2	5:F:303:HXG:CAR	2.60	0.84
2:G:237:TRP:CZ2	5:G:303:HXG:CAR	2.60	0.84
1:A:62:ASN:HD21	1:A:167:LYS:H	1.25	0.84
2:B:237:TRP:CZ2	5:B:303:HXG:CAR	2.60	0.84
2:G:240:SER:HB2	5:G:303:HXG:H40	1.57	0.84
3:H:193:LEU:HB3	3:H:194:PRO:HD3	1.60	0.83
3:C:95:THR:HB	3:C:96:PRO:HD2	1.61	0.83
1:D:310:SER:OG	1:D:396:GLU:OE1	1.95	0.83
2:B:240:SER:HB2	5:B:303:HXG:H40	1.57	0.83
3:I:21:LYS:HE3	3:I:108:THR:HG1	1.40	0.83
3:I:193:LEU:HB3	3:I:194:PRO:HD3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASP:OD2	1:E:186:ASP:N	2.11	0.82
3:H:95:THR:HB	3:H:96:PRO:HD2	1.61	0.81
3:I:189:PRO:HA	3:I:223:PHE:CD1	2.15	0.81
2:F:234:PHE:CE1	5:F:303:HXG:H1	2.13	0.81
2:B:234:PHE:CE1	5:B:303:HXG:H1	2.13	0.81
3:I:95:THR:HB	3:I:96:PRO:HD2	1.61	0.81
3:H:189:PRO:HA	3:H:223:PHE:CD1	2.15	0.81
1:E:62:ASN:HD21	1:E:167:LYS:H	1.25	0.81
3:C:193:LEU:HB3	3:C:194:PRO:HD3	1.60	0.81
3:I:220:PHE:HD1	3:I:220:PHE:H	1.29	0.80
7:B:306:6ER:C21	3:H:205:PHE:HZ	1.86	0.80
3:C:220:PHE:HD1	3:C:220:PHE:H	1.29	0.80
1:D:62:ASN:HD21	1:D:167:LYS:H	1.25	0.80
1:A:100:ARG:NH2	2:B:186:TYR:O	2.14	0.79
3:C:189:PRO:HA	3:C:223:PHE:CD1	2.15	0.79
3:C:142:THR:HG22	3:C:144:SER:H	1.46	0.79
2:B:100:GLU:O	2:B:104:ARG:HG2	1.83	0.79
7:B:306:6ER:C21	3:H:205:PHE:CE2	2.66	0.79
2:F:100:GLU:O	2:F:104:ARG:HG2	1.83	0.79
2:F:237:TRP:CE2	5:F:303:HXG:H15	2.15	0.78
1:E:176:GLU:HA	1:E:176:GLU:OE2	1.84	0.78
2:B:234:PHE:CE1	5:B:303:HXG:H4	1.80	0.78
1:D:186:ASP:OD2	1:D:186:ASP:N	2.11	0.78
3:H:21:LYS:CE	3:H:108:THR:OG1	2.24	0.77
2:G:237:TRP:CD2	5:G:303:HXG:H16	2.17	0.77
3:C:21:LYS:CE	3:C:108:THR:OG1	2.24	0.77
3:H:220:PHE:HD1	3:H:220:PHE:H	1.29	0.77
2:B:123:ASN:H	2:B:160:ASN:HD21	1.32	0.77
3:I:211:LEU:HB2	3:I:212:PHE:CZ	2.20	0.77
3:H:97:ARG:HH11	2:F:8:VAL:HG12	1.48	0.77
2:F:123:ASN:H	2:F:160:ASN:HD21	1.32	0.77
2:G:100:GLU:O	2:G:104:ARG:HG2	1.83	0.77
7:C:304:6ER:C28	6:C:305:D10:H51	2.15	0.77
2:G:123:ASN:H	2:G:160:ASN:HD21	1.33	0.77
1:D:176:GLU:OE2	1:D:176:GLU:HA	1.84	0.77
2:G:234:PHE:CE1	5:G:303:HXG:H1	2.13	0.76
1:A:299:GLN:HE22	1:A:363:ASP:HB3	1.50	0.76
7:I:304:6ER:C28	6:I:305:D10:H51	2.15	0.76
3:C:211:LEU:HB2	3:C:212:PHE:CZ	2.20	0.76
1:D:299:GLN:HE22	1:D:363:ASP:HB3	1.50	0.76
3:I:21:LYS:CE	3:I:108:THR:OG1	2.24	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:VAL:HG12	3:C:187:VAL:H	1.51	0.76
1:A:176:GLU:OE2	1:A:176:GLU:HA	1.83	0.75
7:B:306:6ER:C28	6:H:301:D10:H51	2.15	0.75
3:H:186:VAL:O	3:H:189:PRO:HD2	1.86	0.75
3:C:186:VAL:O	3:C:189:PRO:HD2	1.86	0.75
2:F:237:TRP:CD2	5:F:303:HXG:H16	2.17	0.75
3:C:205:PHE:HB2	2:G:58:ARG:CZ	2.16	0.75
3:H:91:VAL:HG23	3:H:172:PRO:HD3	1.69	0.75
3:H:211:LEU:HB2	3:H:212:PHE:CZ	2.20	0.75
1:E:299:GLN:HE22	1:E:363:ASP:HB3	1.50	0.75
3:I:91:VAL:HG23	3:I:172:PRO:HD3	1.69	0.75
3:I:186:VAL:HG12	3:I:187:VAL:H	1.51	0.75
2:B:25:ILE:HG23	3:C:234:ILE:HD13	1.69	0.75
2:B:28:THR:HG21	3:C:107:TRP:HZ3	1.50	0.74
3:H:135:ILE:HA	2:F:191:THR:OG1	1.85	0.74
2:B:150:LEU:HD13	2:B:225:ILE:HD11	1.70	0.74
3:I:186:VAL:O	3:I:189:PRO:HD2	1.86	0.74
2:G:150:LEU:HD13	2:G:225:ILE:HD11	1.69	0.74
5:B:302:HXG:H26	6:G:304:D10:H91	1.69	0.73
3:C:91:VAL:HG23	3:C:172:PRO:HD3	1.69	0.73
2:G:234:PHE:CE1	5:G:303:HXG:H4	1.80	0.73
2:F:90:THR:OG1	2:F:132:ASP:OD2	2.07	0.73
1:A:93:ILE:H	2:B:191:THR:HG21	1.54	0.73
3:C:174:TYR:OH	3:C:237:GLU:OE1	2.04	0.73
1:A:287:VAL:HG23	1:A:301:THR:O	1.89	0.72
3:I:174:TYR:OH	3:I:237:GLU:OE1	2.04	0.72
3:I:230:VAL:HG21	2:G:32:VAL:HG11	1.69	0.72
2:G:90:THR:OG1	2:G:132:ASP:OD2	2.07	0.72
3:H:186:VAL:HG12	3:H:187:VAL:H	1.51	0.72
2:F:150:LEU:HD13	2:F:225:ILE:HD11	1.70	0.72
2:B:90:THR:OG1	2:B:132:ASP:OD2	2.07	0.72
2:B:237:TRP:NE1	5:B:303:HXG:OAY	2.23	0.72
1:E:287:VAL:HG23	1:E:301:THR:O	1.89	0.72
1:A:186:ASP:OD2	1:A:186:ASP:N	2.11	0.72
3:H:91:VAL:HB	3:H:99:GLU:HG3	1.72	0.72
3:H:46:TRP:O	3:H:50:LEU:HG	1.90	0.72
3:I:91:VAL:HB	3:I:99:GLU:HG3	1.72	0.72
3:C:58:GLU:HG2	3:C:62:MET:HB2	1.71	0.71
3:C:46:TRP:O	3:C:50:LEU:HG	1.90	0.71
3:H:97:ARG:NH1	2:F:8:VAL:HG12	2.06	0.71
2:F:237:TRP:NE1	5:F:303:HXG:OAY	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:VAL:HG23	1:D:301:THR:O	1.89	0.71
2:F:237:TRP:HE1	5:F:303:HXG:CAR	1.90	0.71
2:G:237:TRP:NE1	5:G:303:HXG:OAY	2.23	0.71
2:B:237:TRP:CD2	5:B:303:HXG:H16	2.17	0.71
7:B:306:6ER:C21	3:H:205:PHE:CE1	2.73	0.71
3:H:126:GLU:HG3	2:F:42:MET:HG3	1.73	0.71
3:C:91:VAL:HB	3:C:99:GLU:HG3	1.72	0.71
3:H:174:TYR:OH	3:H:237:GLU:OE1	2.04	0.71
6:F:304:D10:H91	5:G:302:HXG:H26	1.71	0.71
3:C:204:THR:HG23	2:G:207:THR:HA	1.73	0.71
3:I:46:TRP:O	3:I:50:LEU:HG	1.90	0.71
2:B:32:VAL:HG11	3:C:230:VAL:HG21	1.72	0.71
2:B:237:TRP:HB2	5:B:303:HXG:OAF	1.91	0.70
3:H:58:GLU:HG2	3:H:62:MET:HB2	1.71	0.70
3:I:230:VAL:HG21	2:G:32:VAL:CG1	2.21	0.70
2:G:237:TRP:HB2	5:G:303:HXG:OAF	1.91	0.70
2:B:28:THR:HG21	3:C:107:TRP:CZ3	2.25	0.70
3:I:58:GLU:HG2	3:I:62:MET:HB2	1.71	0.70
3:H:107:TRP:NE1	3:H:237:GLU:HG2	2.07	0.69
3:I:107:TRP:NE1	3:I:237:GLU:HG2	2.07	0.69
2:F:237:TRP:HB2	5:F:303:HXG:OAF	1.91	0.69
2:B:208:PHE:HD2	2:B:211:ASP:HB3	1.58	0.69
3:C:107:TRP:NE1	3:C:237:GLU:HG2	2.07	0.69
2:B:134:ILE:HD13	2:B:147:VAL:HG12	1.75	0.69
2:G:208:PHE:HD2	2:G:211:ASP:HB3	1.58	0.68
2:F:240:SER:CB	5:F:303:HXG:H40	2.24	0.68
1:A:245:ALA:O	1:A:249:VAL:HG23	1.94	0.68
7:C:304:6ER:C29	6:C:305:D10:H51	2.24	0.68
2:F:208:PHE:HD2	2:F:211:ASP:HB3	1.58	0.68
3:C:211:LEU:HB2	3:C:212:PHE:CE1	2.29	0.68
7:I:304:6ER:C29	6:I:305:D10:H51	2.24	0.68
1:D:245:ALA:O	1:D:249:VAL:HG23	1.94	0.68
7:B:306:6ER:C29	6:H:301:D10:H51	2.24	0.68
3:C:135:ILE:HG23	3:C:136:VAL:HG23	1.76	0.68
2:B:237:TRP:CD1	5:B:303:HXG:OAY	2.47	0.67
2:B:240:SER:CB	5:B:303:HXG:H40	2.24	0.67
3:H:135:ILE:HG23	3:H:136:VAL:HG23	1.76	0.67
2:G:237:TRP:CD1	5:G:303:HXG:OAY	2.47	0.67
1:E:245:ALA:O	1:E:249:VAL:HG23	1.94	0.67
2:F:134:ILE:HD13	2:F:147:VAL:HG12	1.75	0.67
2:B:32:VAL:CG1	3:C:230:VAL:HG21	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TRP:CD1	5:F:303:HXG:OAY	2.47	0.67
2:G:240:SER:CB	5:G:303:HXG:H40	2.24	0.67
3:H:89:ARG:HD2	3:H:170:ARG:HD2	1.77	0.67
3:I:107:TRP:CZ3	2:G:28:THR:HG21	2.30	0.67
2:B:58:ARG:CZ	3:H:205:PHE:HB2	2.25	0.67
3:I:211:LEU:HB2	3:I:212:PHE:CE1	2.29	0.67
2:G:134:ILE:HD13	2:G:147:VAL:HG12	1.75	0.67
3:H:79:LEU:HD21	3:H:162:ALA:HB2	1.77	0.66
3:H:142:THR:HG22	3:H:144:SER:N	2.03	0.66
3:I:135:ILE:HG23	3:I:136:VAL:HG23	1.76	0.66
3:H:211:LEU:HB2	3:H:212:PHE:CE1	2.29	0.66
3:C:89:ARG:HD2	3:C:170:ARG:HD2	1.77	0.66
3:I:89:ARG:HD2	3:I:170:ARG:HD2	1.77	0.66
2:F:237:TRP:CD1	5:F:303:HXG:CAE	2.80	0.65
3:I:142:THR:HG22	3:I:144:SER:N	2.03	0.65
3:I:107:TRP:HZ3	2:G:28:THR:HG21	1.60	0.65
3:I:79:LEU:HD21	3:I:162:ALA:HB2	1.77	0.65
3:C:89:ARG:HD2	3:C:170:ARG:HA	1.79	0.65
3:I:107:TRP:HE1	3:I:237:GLU:HG2	1.61	0.65
3:I:202:GLY:O	3:I:207:PHE:HA	1.98	0.65
3:C:79:LEU:HD21	3:C:162:ALA:HB2	1.77	0.64
1:A:48:HIS:HE1	1:A:404:MET:CE	2.10	0.64
3:H:202:GLY:O	3:H:207:PHE:HA	1.98	0.64
3:I:205:PHE:HB2	2:F:58:ARG:CZ	2.27	0.64
3:C:202:GLY:O	3:C:207:PHE:HA	1.98	0.64
3:H:107:TRP:HE1	3:H:237:GLU:HG2	1.61	0.64
3:I:131:TRP:NE1	3:I:136:VAL:HG21	2.13	0.64
2:F:240:SER:CB	5:F:303:HXG:CAC	2.73	0.64
1:A:48:HIS:HE1	1:A:404:MET:HE2	1.63	0.64
3:C:186:VAL:HG12	3:C:187:VAL:N	2.13	0.64
3:H:186:VAL:HG12	3:H:187:VAL:N	2.13	0.63
2:G:237:TRP:CD1	5:G:303:HXG:CAE	2.80	0.63
3:C:107:TRP:HE1	3:C:237:GLU:HG2	1.61	0.63
3:H:131:TRP:NE1	3:H:136:VAL:HG21	2.13	0.63
3:I:134:THR:OG1	3:I:135:ILE:N	2.31	0.63
1:D:48:HIS:HE1	1:D:404:MET:HE2	1.64	0.63
1:E:48:HIS:HE1	1:E:404:MET:CE	2.10	0.63
1:E:48:HIS:HE1	1:E:404:MET:HE2	1.64	0.63
2:B:219:PHE:CD1	3:H:198:LEU:HA	2.34	0.63
3:I:89:ARG:HD2	3:I:170:ARG:HA	1.79	0.63
1:D:48:HIS:HE1	1:D:404:MET:CE	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:THR:OG1	3:H:135:ILE:N	2.31	0.63
2:B:237:TRP:CD1	5:B:303:HXG:CAE	2.80	0.63
3:H:89:ARG:HD2	3:H:170:ARG:HA	1.79	0.63
1:D:48:HIS:CE1	1:D:404:MET:CE	2.82	0.63
1:E:48:HIS:CE1	1:E:404:MET:CE	2.82	0.63
3:I:186:VAL:HG12	3:I:187:VAL:N	2.13	0.62
2:G:237:TRP:HD1	5:G:303:HXG:CAE	2.12	0.62
1:A:48:HIS:CE1	1:A:404:MET:CE	2.82	0.62
3:I:135:ILE:HA	2:G:191:THR:OG1	1.99	0.62
2:B:237:TRP:HD1	5:B:303:HXG:CAE	2.12	0.62
3:I:134:THR:HG21	2:G:112:THR:CG2	2.24	0.62
3:C:192:ILE:HD13	3:C:223:PHE:CE2	2.35	0.62
3:C:140:ASP:O	3:C:141:PHE:HB2	2.00	0.62
3:C:181:GLN:HA	3:C:184:VAL:HG23	1.82	0.62
3:C:140:ASP:HB2	2:G:208:PHE:CG	2.34	0.62
2:F:237:TRP:HD1	5:F:303:HXG:CAE	2.12	0.62
2:B:32:VAL:HG11	3:C:230:VAL:CG2	2.30	0.61
3:I:192:ILE:HD13	3:I:223:PHE:CE2	2.35	0.61
1:E:294:PRO:O	1:E:414:ILE:HD11	2.00	0.61
3:H:181:GLN:HA	3:H:184:VAL:HG23	1.82	0.61
3:H:192:ILE:HD13	3:H:223:PHE:CE2	2.35	0.61
3:I:140:ASP:O	3:I:141:PHE:HB2	2.00	0.61
2:G:240:SER:CB	5:G:303:HXG:CAC	2.73	0.61
1:D:311:ALA:HB3	1:D:396:GLU:OE2	2.01	0.61
2:B:208:PHE:CG	3:H:140:ASP:HB2	2.36	0.61
2:B:237:TRP:CD1	5:B:303:HXG:OAV	2.54	0.61
3:I:181:GLN:HA	3:I:184:VAL:HG23	1.82	0.61
3:C:189:PRO:HA	3:C:223:PHE:HD1	1.65	0.61
1:D:294:PRO:O	1:D:414:ILE:HD11	2.00	0.61
2:G:244:VAL:C	5:G:302:HXG:H40	2.22	0.60
3:I:230:VAL:CG2	2:G:32:VAL:HG11	2.31	0.60
1:A:294:PRO:O	1:A:414:ILE:HD11	2.00	0.60
1:A:311:ALA:HB3	1:A:396:GLU:OE2	2.01	0.60
1:D:314:LEU:HD11	1:D:391:LEU:HD22	1.84	0.60
2:G:237:TRP:CD1	5:G:303:HXG:OAV	2.54	0.60
3:C:86:SER:HB2	3:C:169:THR:HB	1.82	0.60
3:H:107:TRP:HZ3	2:F:28:THR:HG21	1.66	0.60
3:H:192:ILE:HD12	3:H:220:PHE:HD2	1.67	0.60
2:F:244:VAL:C	5:F:302:HXG:H40	2.22	0.60
2:B:244:VAL:C	5:B:302:HXG:H40	2.22	0.60
3:C:202:GLY:C	3:C:216:LEU:HD22	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:THR:HA	2:B:197:ILE:HD11	1.84	0.60
3:C:80:TRP:HZ2	3:C:158:ILE:HA	1.66	0.60
3:C:134:THR:OG1	3:C:135:ILE:N	2.31	0.60
3:H:86:SER:HB2	3:H:169:THR:HB	1.82	0.60
3:H:140:ASP:O	3:H:141:PHE:HB2	2.00	0.60
3:H:202:GLY:C	3:H:216:LEU:HD22	2.22	0.60
3:I:86:SER:HB2	3:I:169:THR:HB	1.82	0.60
1:E:51:ASP:OD1	1:E:70:LYS:HE2	2.02	0.60
3:I:192:ILE:CD1	3:I:220:PHE:HD2	2.15	0.60
1:D:51:ASP:OD1	1:D:70:LYS:HE2	2.02	0.60
3:H:107:TRP:CZ3	2:F:28:THR:HG21	2.35	0.60
3:I:189:PRO:HB3	3:I:223:PHE:HE1	1.67	0.60
1:E:311:ALA:HB3	1:E:396:GLU:OE2	2.01	0.60
1:A:51:ASP:OD1	1:A:70:LYS:HE2	2.02	0.59
3:I:97:ARG:HH11	2:G:8:VAL:HG12	1.66	0.59
2:F:237:TRP:CD1	5:F:303:HXG:OAV	2.54	0.59
1:E:314:LEU:HD11	1:E:391:LEU:HD22	1.84	0.59
3:C:192:ILE:HD12	3:C:220:PHE:HD2	1.67	0.59
3:H:192:ILE:CD1	3:H:220:PHE:HD2	2.15	0.59
3:I:80:TRP:HZ2	3:I:158:ILE:HA	1.66	0.59
2:F:193:THR:HA	2:F:197:ILE:HD11	1.84	0.59
2:G:193:THR:HA	2:G:197:ILE:HD11	1.84	0.59
1:A:314:LEU:HD11	1:A:391:LEU:HD22	1.83	0.59
3:C:192:ILE:CD1	3:C:220:PHE:HD2	2.15	0.59
2:B:191:THR:OG1	3:C:135:ILE:HA	2.03	0.59
3:I:80:TRP:CZ2	3:I:158:ILE:HA	2.38	0.59
3:I:192:ILE:HD12	3:I:220:PHE:HD2	1.67	0.59
3:I:204:THR:HG23	2:F:207:THR:HA	1.84	0.59
2:B:25:ILE:CG2	3:C:234:ILE:HD13	2.32	0.58
3:H:80:TRP:HZ2	3:H:158:ILE:HA	1.67	0.58
2:B:240:SER:CB	5:B:303:HXG:CAC	2.73	0.58
3:I:145:HIS:HB2	3:I:149:PHE:CD2	2.38	0.58
3:I:202:GLY:C	3:I:216:LEU:HD22	2.22	0.58
3:C:143:PRO:HA	3:C:146:ILE:HD12	1.85	0.58
3:C:189:PRO:HB3	3:C:223:PHE:HE1	1.67	0.58
3:H:145:HIS:HB2	3:H:149:PHE:CD2	2.38	0.58
3:H:189:PRO:HB3	3:H:223:PHE:HE1	1.67	0.58
3:H:80:TRP:CZ2	3:H:158:ILE:HA	2.38	0.58
3:C:80:TRP:CZ2	3:C:158:ILE:HA	2.38	0.58
1:D:394:ILE:HA	1:D:399:ASN:O	2.04	0.58
3:H:142:THR:HG23	3:H:143:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:HB2	2:B:85:ILE:HG12	1.86	0.57
1:E:394:ILE:HA	1:E:399:ASN:O	2.04	0.57
3:C:102:ARG:HG3	3:C:170:ARG:HE	1.69	0.57
3:H:157:ILE:HD13	3:H:190:PHE:HD1	1.68	0.57
3:I:138:ASP:HB2	2:F:206:ARG:HH22	1.69	0.57
3:I:157:ILE:HD13	3:I:190:PHE:HD1	1.69	0.57
2:F:83:TYR:HB2	2:F:85:ILE:HG12	1.86	0.57
3:C:157:ILE:HD13	3:C:190:PHE:HD1	1.68	0.57
3:H:102:ARG:HG3	3:H:170:ARG:HE	1.70	0.57
3:I:142:THR:HG23	3:I:143:PRO:HD2	1.86	0.57
2:F:150:LEU:CD1	2:F:225:ILE:HD11	2.35	0.57
2:B:210:LYS:HB2	1:D:381:TYR:HB3	1.86	0.57
1:A:394:ILE:HA	1:A:399:ASN:O	2.04	0.57
2:B:57:ARG:NH2	2:B:201:GLU:OE2	2.36	0.57
1:A:212:PHE:HB3	3:C:238:LEU:HD21	1.87	0.56
3:I:134:THR:CG2	2:G:112:THR:HG21	2.27	0.56
2:G:237:TRP:HE1	5:G:303:HXG:CAR	1.90	0.56
2:G:150:LEU:CD1	2:G:225:ILE:HD11	2.35	0.56
2:B:42:MET:O	3:C:212:PHE:CE2	2.58	0.56
2:B:150:LEU:CD1	2:B:225:ILE:HD11	2.35	0.56
3:H:185:VAL:HG21	3:H:230:VAL:HG13	1.88	0.56
3:H:230:VAL:HG21	2:F:32:VAL:HG11	1.86	0.56
3:I:102:ARG:HG3	3:I:170:ARG:HE	1.69	0.56
3:C:138:ASP:HB2	2:G:206:ARG:HH22	1.70	0.56
3:I:243:LYS:HA	3:I:246:LYS:HG2	1.87	0.56
2:F:57:ARG:NH2	2:F:201:GLU:OE2	2.36	0.56
3:C:185:VAL:HG21	3:C:230:VAL:HG13	1.88	0.56
1:E:335:ASN:N	1:E:335:ASN:HD22	2.03	0.56
3:H:189:PRO:HA	3:H:223:PHE:HD1	1.65	0.56
1:A:375:ARG:NH1	2:G:208:PHE:HE1	2.04	0.56
2:G:83:TYR:HB2	2:G:85:ILE:HG12	1.86	0.56
3:C:243:LYS:HA	3:C:246:LYS:HG2	1.87	0.56
3:I:189:PRO:HA	3:I:223:PHE:HD1	1.65	0.56
3:I:131:TRP:HE1	3:I:136:VAL:HG21	1.71	0.56
3:C:193:LEU:HB3	3:C:194:PRO:CD	2.36	0.55
3:I:185:VAL:HG21	3:I:230:VAL:HG13	1.88	0.55
3:C:145:HIS:CE1	3:C:149:PHE:HE2	2.24	0.55
3:H:243:LYS:HA	3:H:246:LYS:HG2	1.87	0.55
3:C:204:THR:O	3:C:205:PHE:HB3	2.06	0.55
3:H:131:TRP:HE1	3:H:136:VAL:HG21	1.71	0.55
1:A:335:ASN:N	1:A:335:ASN:HD22	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:304:D10:H91	5:F:302:HXG:H26	1.88	0.55
3:I:134:THR:OG1	3:I:135:ILE:HG22	2.07	0.55
2:G:57:ARG:NH2	2:G:201:GLU:OE2	2.36	0.55
3:C:134:THR:OG1	3:C:135:ILE:HG22	2.07	0.55
3:I:204:THR:O	3:I:205:PHE:HB3	2.06	0.55
3:I:192:ILE:HA	3:I:195:ASN:HB3	1.88	0.55
1:E:316:GLU:OE2	1:E:323:ARG:HD2	2.07	0.55
3:C:192:ILE:HA	3:C:195:ASN:HB3	1.88	0.55
3:I:126:GLU:HG3	2:G:42:MET:HG3	1.89	0.55
3:H:192:ILE:HA	3:H:195:ASN:HB3	1.88	0.55
1:D:335:ASN:N	1:D:335:ASN:HD22	2.03	0.55
3:H:230:VAL:HG21	2:F:32:VAL:CG1	2.37	0.55
3:I:97:ARG:NH1	2:G:8:VAL:HG12	2.21	0.55
1:A:316:GLU:OE2	1:A:323:ARG:HD2	2.07	0.54
1:D:316:GLU:OE2	1:D:323:ARG:HD2	2.07	0.54
3:H:134:THR:OG1	3:H:135:ILE:HG22	2.07	0.54
3:I:193:LEU:HB3	3:I:194:PRO:CD	2.36	0.54
3:C:207:PHE:CG	2:G:206:ARG:HG3	2.41	0.54
3:H:193:LEU:HB3	3:H:194:PRO:CD	2.36	0.54
1:E:302:LEU:O	1:E:361:THR:HA	2.07	0.54
3:H:204:THR:O	3:H:205:PHE:HB3	2.06	0.54
1:A:302:LEU:O	1:A:361:THR:HA	2.07	0.54
2:F:138:SER:O	2:F:140:SER:N	2.41	0.54
1:D:397:ASP:OD1	1:D:397:ASP:N	2.40	0.54
3:C:142:THR:HG22	3:C:144:SER:N	2.20	0.54
3:H:192:ILE:HG21	3:H:223:PHE:CE2	2.43	0.54
2:G:58:ARG:HB2	2:G:212:VAL:HG12	1.90	0.54
1:E:48:HIS:CE1	1:E:404:MET:HE1	2.42	0.54
2:B:58:ARG:HB2	2:B:212:VAL:HG12	1.90	0.54
2:B:237:TRP:HE1	5:B:303:HXG:CAR	1.90	0.54
3:H:238:LEU:O	1:D:216:ARG:NE	2.41	0.54
1:D:48:HIS:CE1	1:D:404:MET:HE1	2.42	0.54
1:A:48:HIS:CE1	1:A:404:MET:HE1	2.42	0.54
3:C:192:ILE:HG21	3:C:223:PHE:CE2	2.43	0.53
3:H:153:TYR:HA	3:H:156:TYR:CE2	2.44	0.53
2:F:58:ARG:HB2	2:F:212:VAL:HG12	1.90	0.53
3:H:192:ILE:HD12	3:H:220:PHE:HB2	1.90	0.53
3:I:192:ILE:HG21	3:I:223:PHE:CE2	2.43	0.53
2:G:138:SER:O	2:G:140:SER:N	2.41	0.53
1:D:302:LEU:O	1:D:361:THR:HA	2.07	0.53
1:A:294:PRO:O	1:A:414:ILE:CD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:SER:O	2:B:140:SER:N	2.41	0.53
3:I:153:TYR:HA	3:I:156:TYR:CE2	2.44	0.53
2:B:42:MET:O	2:B:42:MET:HG2	2.09	0.53
2:F:42:MET:O	2:F:42:MET:HG2	2.09	0.53
2:B:50:PHE:CE2	3:C:212:PHE:HZ	2.27	0.53
3:C:192:ILE:HD12	3:C:220:PHE:HB2	1.90	0.53
3:C:196:VAL:HA	3:C:199:ASN:OD1	2.09	0.53
1:D:294:PRO:O	1:D:414:ILE:CD1	2.57	0.53
2:B:123:ASN:N	2:B:160:ASN:HD21	2.06	0.53
3:I:192:ILE:HD12	3:I:220:PHE:HB2	1.90	0.53
2:F:171:VAL:HG22	1:D:172:THR:HA	1.91	0.53
1:E:294:PRO:O	1:E:414:ILE:CD1	2.57	0.53
1:E:397:ASP:OD1	1:E:397:ASP:N	2.40	0.53
2:B:112:THR:CG2	3:C:134:THR:HG21	2.31	0.53
3:H:109:TRP:HB3	3:H:163:SER:HB2	1.90	0.53
3:C:192:ILE:O	3:C:195:ASN:HB3	2.09	0.53
1:D:316:GLU:HB2	1:D:325:LEU:CD2	2.39	0.53
1:E:316:GLU:HB2	1:E:325:LEU:CD2	2.39	0.53
3:C:165:LEU:O	3:C:169:THR:HG23	2.09	0.53
3:I:165:LEU:O	3:I:169:THR:HG23	2.09	0.53
3:I:212:PHE:HZ	2:G:50:PHE:CE2	2.27	0.53
1:A:316:GLU:HB2	1:A:325:LEU:CD2	2.39	0.52
3:C:184:VAL:O	3:C:189:PRO:HD3	2.10	0.52
1:E:59:VAL:HG12	1:E:63:GLU:HB3	1.91	0.52
1:A:97:VAL:O	1:A:131:ARG:HB3	2.09	0.52
3:H:41:GLU:HG3	3:H:147:ILE:HD12	1.92	0.52
3:I:171:LEU:O	3:I:175:GLN:NE2	2.35	0.52
1:A:90:ASN:HB3	1:A:141:MET:HG3	1.91	0.52
3:I:192:ILE:O	3:I:195:ASN:HB3	2.09	0.52
2:G:57:ARG:HH21	2:G:201:GLU:CD	2.12	0.52
1:D:90:ASN:HB3	1:D:141:MET:HG3	1.91	0.52
3:C:109:TRP:HB3	3:C:163:SER:HB2	1.91	0.52
3:I:196:VAL:HA	3:I:199:ASN:OD1	2.09	0.52
1:A:256:GLU:OE2	1:A:256:GLU:C	2.48	0.52
1:D:97:VAL:O	1:D:131:ARG:HB3	2.09	0.52
1:A:59:VAL:HG12	1:A:63:GLU:HB3	1.92	0.52
3:C:153:TYR:HA	3:C:156:TYR:CE2	2.43	0.52
3:H:165:LEU:O	3:H:169:THR:HG23	2.09	0.52
1:D:99:ILE:HG12	1:D:129:LYS:HB3	1.92	0.52
1:E:97:VAL:O	1:E:131:ARG:HB3	2.10	0.52
2:B:112:THR:HG21	3:C:134:THR:CG2	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:184:VAL:O	3:I:189:PRO:HD3	2.10	0.52
3:I:234:ILE:HD13	2:G:25:ILE:HG23	1.91	0.52
2:B:57:ARG:HH21	2:B:201:GLU:CD	2.12	0.52
3:I:142:THR:HB	3:I:145:HIS:NE2	2.25	0.52
3:I:109:TRP:HB3	3:I:163:SER:HB2	1.90	0.52
2:F:58:ARG:HB2	2:F:212:VAL:CG1	2.40	0.52
1:E:90:ASN:HB3	1:E:141:MET:HG3	1.91	0.52
3:H:95:THR:HB	3:H:96:PRO:CD	2.38	0.52
2:F:50:PHE:O	2:F:119:VAL:HA	2.10	0.52
2:F:57:ARG:HH21	2:F:201:GLU:CD	2.12	0.52
1:E:256:GLU:C	1:E:256:GLU:OE2	2.48	0.52
3:C:189:PRO:HA	3:C:223:PHE:CE1	2.45	0.51
3:H:184:VAL:O	3:H:189:PRO:HD3	2.10	0.51
2:F:157:TYR:HB3	2:F:158:PRO:HD3	1.92	0.51
2:B:58:ARG:HB2	2:B:212:VAL:CG1	2.40	0.51
3:H:189:PRO:HA	3:H:223:PHE:CE1	2.45	0.51
3:H:196:VAL:HA	3:H:199:ASN:OD1	2.09	0.51
2:G:42:MET:O	2:G:42:MET:HG2	2.09	0.51
2:G:157:TYR:HB3	2:G:158:PRO:HD3	1.92	0.51
2:B:157:TYR:HB3	2:B:158:PRO:HD3	1.92	0.51
3:C:82:TYR:HB3	3:C:85:LYS:HE3	1.93	0.51
3:I:41:GLU:HG3	3:I:147:ILE:HD12	1.92	0.51
3:I:135:ILE:O	3:I:137:ARG:NE	2.43	0.51
3:I:207:PHE:CG	2:F:206:ARG:HG3	2.46	0.51
2:G:58:ARG:HB2	2:G:212:VAL:CG1	2.40	0.51
1:D:256:GLU:OE2	1:D:256:GLU:C	2.48	0.51
3:H:192:ILE:O	3:H:195:ASN:HB3	2.09	0.51
2:F:123:ASN:N	2:F:160:ASN:HD21	2.06	0.51
1:E:172:THR:OG1	1:E:176:GLU:HB3	2.11	0.51
1:D:59:VAL:HG12	1:D:63:GLU:HB3	1.92	0.51
1:A:99:ILE:HG12	1:A:129:LYS:HB3	1.92	0.51
3:H:82:TYR:HB3	3:H:85:LYS:HE3	1.93	0.51
3:H:118:TYR:HD1	2:F:34:LEU:HD22	1.75	0.51
3:I:189:PRO:HA	3:I:223:PHE:CE1	2.45	0.51
1:A:397:ASP:OD1	1:A:397:ASP:N	2.40	0.51
3:H:142:THR:HB	3:H:145:HIS:NE2	2.25	0.51
2:B:50:PHE:O	2:B:119:VAL:HA	2.10	0.50
3:C:192:ILE:HG21	3:C:223:PHE:CZ	2.47	0.50
3:I:129:GLY:O	3:I:133:GLN:HG2	2.11	0.50
1:E:99:ILE:HG12	1:E:129:LYS:HB3	1.92	0.50
2:B:134:ILE:CD1	2:B:147:VAL:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:TRP:CG	5:B:303:HXG:H16	2.43	0.50
3:H:45:GLY:HA3	3:H:61:TRP:HZ2	1.77	0.50
3:C:107:TRP:HH2	3:C:234:ILE:HG12	1.77	0.50
3:H:46:TRP:CZ3	1:D:94:PRO:HB2	2.46	0.50
3:H:97:ARG:CZ	2:F:8:VAL:HA	2.42	0.50
3:I:189:PRO:HD3	3:I:226:SER:OG	2.11	0.50
2:F:134:ILE:HD13	2:F:147:VAL:CG1	2.42	0.50
2:B:36:GLY:O	2:B:39:ILE:HG22	2.12	0.50
3:C:65:LEU:HG	3:C:69:MET:HE2	1.93	0.50
3:H:192:ILE:HG21	3:H:223:PHE:CZ	2.47	0.50
1:A:172:THR:OG1	1:A:176:GLU:HB3	2.11	0.50
3:H:46:TRP:HZ3	1:D:94:PRO:HB2	1.77	0.50
3:I:140:ASP:HB2	2:F:208:PHE:CG	2.46	0.50
3:I:163:SER:HG	3:I:182:TYR:HH	1.58	0.50
2:F:237:TRP:CG	5:F:303:HXG:H16	2.43	0.50
2:G:36:GLY:O	2:G:39:ILE:HG22	2.12	0.50
2:G:50:PHE:O	2:G:119:VAL:HA	2.10	0.50
2:G:134:ILE:CD1	2:G:147:VAL:HG12	2.41	0.50
2:G:134:ILE:HD13	2:G:147:VAL:CG1	2.42	0.50
3:C:65:LEU:O	3:C:68:GLU:HG2	2.12	0.50
3:C:203:HIS:HB3	2:G:206:ARG:NH2	2.27	0.50
3:H:65:LEU:O	3:H:68:GLU:HG2	2.12	0.50
3:H:187:VAL:HA	3:H:190:PHE:HB3	1.94	0.50
2:G:37:TYR:OH	2:G:68:SER:O	2.26	0.50
3:C:189:PRO:HD3	3:C:226:SER:OG	2.11	0.50
3:H:65:LEU:HG	3:H:69:MET:HE2	1.93	0.50
3:I:192:ILE:HG21	3:I:223:PHE:CZ	2.47	0.50
3:I:202:GLY:O	3:I:216:LEU:HD22	2.12	0.50
2:B:134:ILE:HD13	2:B:147:VAL:CG1	2.42	0.49
3:H:189:PRO:HD3	3:H:226:SER:OG	2.11	0.49
1:D:172:THR:OG1	1:D:176:GLU:HB3	2.11	0.49
3:H:202:GLY:O	3:H:216:LEU:HD22	2.12	0.49
3:I:45:GLY:HA3	3:I:61:TRP:HZ2	1.77	0.49
3:I:82:TYR:HB3	3:I:85:LYS:HE3	1.93	0.49
3:H:129:GLY:O	3:H:133:GLN:HG2	2.11	0.49
2:F:36:GLY:O	2:F:39:ILE:HG22	2.12	0.49
3:C:135:ILE:O	3:C:137:ARG:NE	2.43	0.49
3:H:171:LEU:O	3:H:175:GLN:NE2	2.35	0.49
3:I:65:LEU:HG	3:I:69:MET:HE2	1.95	0.49
3:I:216:LEU:C	3:I:216:LEU:HD12	2.33	0.49
3:C:45:GLY:HA3	3:C:61:TRP:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:41:GLU:HG3	3:H:147:ILE:CD1	2.43	0.49
3:I:107:TRP:HH2	3:I:234:ILE:HG12	1.77	0.49
2:B:8:VAL:HG12	3:C:97:ARG:HH11	1.77	0.49
3:C:86:SER:CB	3:C:169:THR:HB	2.43	0.49
3:C:202:GLY:O	3:C:216:LEU:HD22	2.12	0.49
3:C:202:GLY:HA2	3:C:206:TRP:HB3	1.95	0.49
2:F:179:THR:OG1	2:F:182:ASP:OD1	2.31	0.49
2:B:206:ARG:HH22	3:H:138:ASP:HB2	1.77	0.49
3:C:140:ASP:HB2	2:G:208:PHE:HB2	1.95	0.49
2:B:130:VAL:HG21	2:B:155:LEU:CD1	2.43	0.49
2:B:237:TRP:CH2	5:B:303:HXG:H22	2.48	0.49
3:C:187:VAL:HA	3:C:190:PHE:HB3	1.94	0.49
3:H:107:TRP:HH2	3:H:234:ILE:HG12	1.77	0.49
3:I:41:GLU:HG3	3:I:147:ILE:CD1	2.43	0.49
3:I:65:LEU:O	3:I:68:GLU:HG2	2.12	0.49
3:I:187:VAL:HA	3:I:190:PHE:HB3	1.94	0.49
1:A:98:PHE:CZ	1:A:159:ILE:HD11	2.48	0.49
3:C:95:THR:HB	3:C:96:PRO:CD	2.38	0.49
3:H:216:LEU:HD12	3:H:216:LEU:C	2.33	0.49
2:B:78:VAL:HG11	2:B:239:GLY:HA3	1.95	0.48
1:D:98:PHE:CZ	1:D:159:ILE:HD11	2.48	0.48
1:E:98:PHE:CZ	1:E:159:ILE:HD11	2.48	0.48
3:C:47:SER:HA	3:C:50:LEU:HD12	1.95	0.48
3:C:94:ILE:HG21	3:C:98:GLU:HB3	1.96	0.48
2:F:194:PRO:O	2:F:197:ILE:HG12	2.13	0.48
2:B:42:MET:HG3	3:C:126:GLU:HG3	1.95	0.48
3:C:211:LEU:HB2	3:C:212:PHE:CE2	2.48	0.48
3:C:216:LEU:HD12	3:C:216:LEU:C	2.33	0.48
3:H:29:LEU:O	3:H:32:VAL:HG23	2.13	0.48
2:B:179:THR:OG1	2:B:182:ASP:OD1	2.31	0.48
3:H:97:ARG:HH11	2:F:8:VAL:CG1	2.23	0.48
3:H:135:ILE:O	3:H:137:ARG:NE	2.43	0.48
3:I:211:LEU:HB2	3:I:212:PHE:CE2	2.48	0.48
1:D:61:VAL:O	1:D:62:ASN:HB2	2.14	0.48
1:A:291:TYR:CD1	1:A:409:LEU:HG	2.49	0.48
2:B:34:LEU:C	2:B:34:LEU:HD23	2.34	0.48
3:H:211:LEU:HB2	3:H:212:PHE:CE2	2.48	0.48
3:H:212:PHE:CE2	2:F:42:MET:O	2.66	0.48
3:I:202:GLY:HA2	3:I:206:TRP:HB3	1.95	0.48
1:E:61:VAL:O	1:E:62:ASN:HB2	2.14	0.48
2:B:194:PRO:O	2:B:197:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:47:SER:HA	3:H:50:LEU:HD12	1.95	0.48
3:H:68:GLU:OE2	3:H:150:TYR:HB2	2.14	0.48
2:G:194:PRO:O	2:G:197:ILE:HG12	2.13	0.48
3:H:213:VAL:O	3:H:215:PRO:HD3	2.14	0.48
3:I:205:PHE:CE1	7:I:304:6ER:C21	2.84	0.48
2:G:34:LEU:C	2:G:34:LEU:HD23	2.34	0.48
2:G:123:ASN:N	2:G:160:ASN:HD21	2.06	0.48
3:C:213:VAL:O	3:C:215:PRO:HD3	2.14	0.48
3:H:94:ILE:HG21	3:H:98:GLU:HB3	1.96	0.48
3:I:47:SER:HA	3:I:50:LEU:HD12	1.95	0.48
2:F:37:TYR:OH	2:F:68:SER:O	2.26	0.48
2:F:130:VAL:HG21	2:F:155:LEU:CD1	2.43	0.48
1:D:115:SER:O	1:D:116:LEU:HD23	2.14	0.48
1:E:284:VAL:HG13	1:E:304:ILE:HG12	1.96	0.48
3:C:68:GLU:OE2	3:C:150:TYR:HB2	2.14	0.48
2:F:34:LEU:C	2:F:34:LEU:HD23	2.34	0.48
1:D:208:ARG:H	1:D:208:ARG:HG2	1.43	0.48
3:C:163:SER:HG	3:C:182:TYR:HH	1.60	0.48
3:H:192:ILE:HD12	3:H:220:PHE:CD2	2.48	0.48
3:I:20:LYS:HB3	3:I:101:ARG:HG3	1.95	0.48
3:I:128:ASP:OD1	3:I:132:HIS:NE2	2.47	0.48
2:F:78:VAL:HG11	2:F:239:GLY:HA3	1.95	0.48
2:G:81:TRP:HH2	2:G:135:LEU:HD11	1.79	0.48
1:A:61:VAL:O	1:A:62:ASN:HB2	2.14	0.47
1:A:172:THR:HA	2:B:171:VAL:HG22	1.96	0.47
3:C:20:LYS:HB3	3:C:101:ARG:HG3	1.95	0.47
3:C:29:LEU:O	3:C:32:VAL:HG23	2.13	0.47
3:C:192:ILE:HD12	3:C:220:PHE:CD2	2.48	0.47
3:H:20:LYS:HB3	3:H:101:ARG:HG3	1.95	0.47
1:D:284:VAL:HG13	1:D:304:ILE:HG12	1.96	0.47
1:D:291:TYR:CD1	1:D:409:LEU:HG	2.49	0.47
1:E:291:TYR:CD1	1:E:409:LEU:HG	2.49	0.47
1:E:360:ARG:HG2	1:E:361:THR:N	2.29	0.47
1:A:360:ARG:HG2	1:A:361:THR:N	2.29	0.47
2:G:130:VAL:HG21	2:G:155:LEU:CD1	2.43	0.47
2:G:179:THR:OG1	2:G:182:ASP:OD1	2.31	0.47
3:I:86:SER:CB	3:I:169:THR:HB	2.43	0.47
2:F:24:MET:O	2:F:28:THR:HG22	2.14	0.47
2:F:237:TRP:CH2	5:F:303:HXG:H22	2.48	0.47
2:G:24:MET:O	2:G:28:THR:HG22	2.14	0.47
2:G:237:TRP:CH2	5:G:303:HXG:H22	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG13	1:A:304:ILE:HG12	1.96	0.47
2:B:81:TRP:HH2	2:B:135:LEU:HD11	1.79	0.47
3:I:29:LEU:O	3:I:32:VAL:HG23	2.13	0.47
3:I:94:ILE:HG21	3:I:98:GLU:HB3	1.96	0.47
3:I:212:PHE:CE2	2:G:42:MET:O	2.68	0.47
1:E:115:SER:O	1:E:116:LEU:HD23	2.14	0.47
3:C:171:LEU:O	3:C:175:GLN:NE2	2.35	0.47
3:H:128:ASP:OD1	3:H:132:HIS:NE2	2.47	0.47
3:I:213:VAL:O	3:I:215:PRO:HD3	2.14	0.47
3:C:187:VAL:O	3:C:190:PHE:HB3	2.15	0.47
3:I:68:GLU:OE2	3:I:150:TYR:HB2	2.14	0.47
3:C:23:ILE:HD12	3:C:24:ILE:HD11	1.92	0.47
3:H:181:GLN:HA	3:H:184:VAL:CG2	2.44	0.47
3:H:187:VAL:O	3:H:190:PHE:HB3	2.15	0.47
3:I:187:VAL:O	3:I:190:PHE:HB3	2.15	0.47
2:F:81:TRP:HH2	2:F:135:LEU:HD11	1.79	0.47
2:F:170:PRO:HB2	1:D:173:LEU:HD12	1.96	0.47
2:G:48:TRP:HA	2:G:54:TRP:HB3	1.97	0.47
2:B:48:TRP:HA	2:B:54:TRP:HB3	1.97	0.47
3:H:202:GLY:HA2	3:H:206:TRP:HB3	1.95	0.47
2:F:80:TRP:CZ2	2:F:136:MET:HA	2.50	0.47
2:G:74:ALA:HB2	2:G:231:TRP:HE3	1.80	0.47
1:D:234:LYS:HB3	1:D:234:LYS:HE3	1.46	0.47
1:D:360:ARG:HG2	1:D:361:THR:N	2.30	0.47
2:B:24:MET:O	2:B:28:THR:HG22	2.14	0.47
2:B:80:TRP:CZ2	2:B:136:MET:HA	2.50	0.47
2:F:74:ALA:HB2	2:F:231:TRP:HE3	1.80	0.47
2:B:19:ARG:HD2	2:B:19:ARG:HA	1.42	0.47
3:H:86:SER:CB	3:H:169:THR:HB	2.43	0.47
2:G:80:TRP:CZ2	2:G:136:MET:HA	2.50	0.47
1:A:115:SER:O	1:A:116:LEU:HD23	2.14	0.46
3:C:212:PHE:CD1	3:C:212:PHE:N	2.84	0.46
3:I:181:GLN:HA	3:I:184:VAL:CG2	2.44	0.46
2:F:134:ILE:CD1	2:F:147:VAL:HG12	2.41	0.46
2:G:78:VAL:HG11	2:G:239:GLY:HA3	1.96	0.46
1:E:242:GLY:O	1:E:246:ILE:HG13	2.15	0.46
3:C:87:ARG:HA	3:C:87:ARG:HD3	1.64	0.46
3:H:23:ILE:HD12	3:H:24:ILE:HD11	1.92	0.46
3:H:235:ASN:O	1:D:216:ARG:NH2	2.48	0.46
2:B:219:PHE:HD1	3:H:198:LEU:HA	1.81	0.46
3:I:46:TRP:HZ3	1:E:94:PRO:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:225:TRP:O	3:I:228:LEU:HB2	2.16	0.46
3:C:142:THR:O	3:C:145:HIS:HB2	2.16	0.46
3:I:192:ILE:HD12	3:I:220:PHE:CD2	2.48	0.46
2:F:244:VAL:O	5:F:302:HXG:H40	2.16	0.46
2:G:237:TRP:CG	5:G:303:HXG:H16	2.44	0.46
2:G:242:LYS:HG2	2:G:243:PHE:N	2.31	0.46
1:D:242:GLY:O	1:D:246:ILE:HG13	2.15	0.46
1:A:93:ILE:O	2:B:191:THR:HG21	2.15	0.46
3:H:234:ILE:HD13	2:F:25:ILE:HG23	1.97	0.46
2:G:210:LYS:HE3	2:G:211:ASP:N	2.31	0.46
1:E:234:LYS:HB3	1:E:234:LYS:HE3	1.46	0.46
1:A:208:ARG:H	1:A:208:ARG:HG2	1.43	0.46
3:H:192:ILE:HB	3:H:223:PHE:CD2	2.51	0.46
3:I:102:ARG:HD2	3:I:170:ARG:NE	2.31	0.46
2:F:82:ARG:HD2	2:F:82:ARG:HA	1.61	0.46
3:C:53:PHE:HB3	3:C:54:ALA:H	1.40	0.46
3:C:181:GLN:HA	3:C:184:VAL:CG2	2.44	0.46
3:C:192:ILE:HB	3:C:223:PHE:CD2	2.51	0.46
3:H:29:LEU:H	3:H:29:LEU:HD23	1.81	0.46
3:H:102:ARG:HG3	3:H:170:ARG:NE	2.31	0.46
2:B:74:ALA:HB2	2:B:231:TRP:HE3	1.80	0.46
3:C:102:ARG:HD2	3:C:170:ARG:NE	2.31	0.46
3:H:225:TRP:O	3:H:228:LEU:HB2	2.16	0.46
3:I:29:LEU:HD23	3:I:29:LEU:H	1.81	0.46
3:I:203:HIS:HB3	2:F:206:ARG:NH2	2.31	0.46
2:F:48:TRP:HA	2:F:54:TRP:HB3	1.97	0.46
2:B:242:LYS:HG2	2:B:243:PHE:N	2.30	0.45
3:C:225:TRP:O	3:C:228:LEU:HB2	2.16	0.45
3:I:142:THR:HB	3:I:145:HIS:CE1	2.51	0.45
3:I:212:PHE:CD1	3:I:212:PHE:N	2.84	0.45
3:C:21:LYS:HD2	3:C:21:LYS:HA	1.36	0.45
1:A:393:PHE:O	1:A:400:ARG:HA	2.17	0.45
2:B:183:LEU:HD12	2:B:183:LEU:HA	1.80	0.45
3:H:71:LEU:O	3:H:75:VAL:HG23	2.16	0.45
3:H:135:ILE:HG23	3:H:136:VAL:N	2.31	0.45
3:H:212:PHE:CD1	3:H:212:PHE:N	2.84	0.45
3:I:141:PHE:CZ	3:I:146:ILE:HG13	2.52	0.45
2:F:210:LYS:HE3	2:F:211:ASP:N	2.31	0.45
2:G:183:LEU:HD12	2:G:183:LEU:HA	1.80	0.45
1:A:242:GLY:O	1:A:246:ILE:HG13	2.15	0.45
2:B:244:VAL:O	5:B:302:HXG:H40	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ARG:HH11	3:C:170:ARG:HD2	1.82	0.45
3:I:135:ILE:HG23	3:I:136:VAL:N	2.32	0.45
3:I:238:LEU:HD21	1:E:212:PHE:HB3	1.99	0.45
2:F:194:PRO:HD2	2:F:197:ILE:CD1	2.47	0.45
2:G:194:PRO:HD2	2:G:197:ILE:CD1	2.47	0.45
3:C:83:ILE:HD12	3:C:83:ILE:HA	1.71	0.45
3:C:135:ILE:HG23	3:C:136:VAL:N	2.32	0.45
3:H:89:ARG:HH11	3:H:170:ARG:HD2	1.81	0.45
3:H:202:GLY:HA3	3:H:216:LEU:HB2	1.99	0.45
3:I:45:GLY:HA3	3:I:61:TRP:CZ2	2.52	0.45
2:F:93:VAL:HG21	2:F:128:ALA:HB2	1.99	0.45
1:E:320:ALA:O	1:E:321:SER:HB2	2.17	0.45
3:C:98:GLU:O	3:C:102:ARG:HG2	2.17	0.45
3:H:98:GLU:O	3:H:102:ARG:HG2	2.17	0.45
3:I:95:THR:HB	3:I:96:PRO:CD	2.38	0.45
3:H:106:HIS:ND1	3:H:237:GLU:OE2	2.50	0.45
3:I:71:LEU:O	3:I:75:VAL:HG23	2.16	0.45
3:I:102:ARG:HG3	3:I:170:ARG:NE	2.31	0.45
3:I:106:HIS:ND1	3:I:237:GLU:OE2	2.50	0.45
2:G:93:VAL:HG21	2:G:128:ALA:HB2	1.99	0.45
2:G:244:VAL:O	5:G:302:HXG:H40	2.16	0.45
2:B:210:LYS:HE3	2:B:211:ASP:N	2.31	0.45
3:H:141:PHE:CZ	3:H:146:ILE:HG13	2.52	0.45
3:I:120:GLY:HA2	3:I:152:SER:HB3	1.99	0.45
3:I:192:ILE:HB	3:I:223:PHE:CD2	2.51	0.45
1:A:316:GLU:HB2	1:A:325:LEU:HD23	1.99	0.45
3:C:29:LEU:HD23	3:C:29:LEU:H	1.81	0.45
3:C:45:GLY:HA3	3:C:61:TRP:CZ2	2.52	0.45
3:H:217:HIS:HA	3:H:220:PHE:HE1	1.81	0.45
3:I:202:GLY:HA3	3:I:216:LEU:HB2	1.99	0.45
3:I:217:HIS:HA	3:I:220:PHE:HE1	1.81	0.45
2:G:171:VAL:HG22	1:E:172:THR:HA	1.99	0.45
1:A:272:ILE:HD13	1:A:272:ILE:HA	1.85	0.45
2:B:82:ARG:HD2	2:B:82:ARG:HA	1.61	0.45
3:C:140:ASP:HB2	2:G:208:PHE:CD1	2.51	0.45
3:I:98:GLU:O	3:I:102:ARG:HG2	2.17	0.45
2:F:64:ALA:HB3	2:F:65:PRO:HD3	1.99	0.45
2:F:210:LYS:HD2	2:F:210:LYS:HA	1.83	0.45
2:F:242:LYS:HG2	2:F:243:PHE:N	2.31	0.45
1:D:393:PHE:O	1:D:400:ARG:HA	2.17	0.45
3:C:106:HIS:ND1	3:C:237:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:HIS:O	2:G:206:ARG:HB3	2.17	0.44
3:I:83:ILE:HD12	3:I:83:ILE:HA	1.71	0.44
3:I:246:LYS:HE2	3:I:246:LYS:HB2	1.45	0.44
2:F:126:PRO:O	2:F:130:VAL:HG22	2.17	0.44
2:G:64:ALA:HB3	2:G:65:PRO:HD3	1.99	0.44
2:B:138:SER:O	2:B:139:ASN:C	2.55	0.44
3:C:71:LEU:O	3:C:75:VAL:HG23	2.16	0.44
3:H:102:ARG:HD2	3:H:170:ARG:NE	2.31	0.44
3:H:120:GLY:HA2	3:H:152:SER:HB3	1.99	0.44
3:H:142:THR:HB	3:H:145:HIS:CE1	2.51	0.44
2:F:19:ARG:HD2	2:F:19:ARG:HA	1.42	0.44
1:A:320:ALA:O	1:A:321:SER:HB2	2.17	0.44
3:H:45:GLY:HA3	3:H:61:TRP:CZ2	2.52	0.44
3:H:91:VAL:CG2	3:H:172:PRO:HD3	2.44	0.44
3:I:89:ARG:HH11	3:I:170:ARG:HD2	1.81	0.44
3:I:91:VAL:CG2	3:I:172:PRO:HD3	2.44	0.44
1:E:393:PHE:O	1:E:400:ARG:HA	2.17	0.44
3:H:210:GLU:OE1	3:H:213:VAL:HG12	2.18	0.44
2:F:196:TYR:CE1	1:D:145:GLN:HA	2.52	0.44
2:G:126:PRO:O	2:G:130:VAL:HG22	2.17	0.44
1:D:209:LYS:H	1:D:209:LYS:HG2	1.62	0.44
1:A:117:GLU:HB2	1:A:120:GLU:HG3	2.00	0.44
3:C:205:PHE:O	3:C:205:PHE:CG	2.70	0.44
3:C:210:GLU:OE1	3:C:213:VAL:HG12	2.18	0.44
3:C:241:LEU:HD12	3:C:241:LEU:HA	1.82	0.44
2:B:57:ARG:HD2	2:B:210:LYS:NZ	2.33	0.44
2:B:93:VAL:HG21	2:B:128:ALA:HB2	1.99	0.44
3:C:198:LEU:HA	2:G:219:PHE:CD1	2.53	0.44
3:C:202:GLY:HA3	3:C:216:LEU:HB2	1.99	0.44
3:H:126:GLU:HG3	2:F:42:MET:CG	2.46	0.44
1:A:234:LYS:HE3	1:A:234:LYS:HB3	1.46	0.44
2:B:64:ALA:HB3	2:B:65:PRO:HD3	1.99	0.44
3:H:205:PHE:CG	3:H:205:PHE:O	2.70	0.44
3:I:53:PHE:HB3	3:I:54:ALA:H	1.40	0.44
2:G:237:TRP:CD1	5:G:303:HXG:CAR	2.75	0.44
1:D:320:ALA:O	1:D:321:SER:HB2	2.17	0.44
1:E:117:GLU:HB2	1:E:120:GLU:HG3	2.00	0.44
1:A:85:GLU:OE1	1:A:85:GLU:N	2.51	0.44
1:A:110:VAL:HA	1:A:269:MET:HE1	1.98	0.44
3:C:217:HIS:HA	3:C:220:PHE:HE1	1.81	0.44
3:H:21:LYS:HD2	3:H:21:LYS:HA	1.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:PRO:O	2:B:130:VAL:HG22	2.17	0.44
3:I:210:GLU:OE1	3:I:213:VAL:HG12	2.18	0.44
2:F:57:ARG:HD2	2:F:210:LYS:NZ	2.33	0.44
2:G:138:SER:O	2:G:139:ASN:C	2.55	0.44
1:D:85:GLU:OE1	1:D:85:GLU:N	2.51	0.44
1:E:316:GLU:HB2	1:E:325:LEU:HD23	1.99	0.44
1:A:175:GLY:HA2	1:A:176:GLU:C	2.38	0.43
2:F:127:GLY:HA2	2:F:130:VAL:CG2	2.48	0.43
2:F:138:SER:O	2:F:139:ASN:C	2.55	0.43
2:F:237:TRP:CD1	5:F:303:HXG:CAR	2.75	0.43
1:D:117:GLU:HB2	1:D:120:GLU:HG3	2.00	0.43
3:C:120:GLY:HA2	3:C:152:SER:HB3	1.99	0.43
3:C:234:ILE:O	3:C:238:LEU:HB2	2.18	0.43
3:I:58:GLU:HG2	3:I:62:MET:CB	2.46	0.43
1:E:208:ARG:H	1:E:208:ARG:HG2	1.43	0.43
2:B:194:PRO:HD2	2:B:197:ILE:CD1	2.47	0.43
2:B:208:PHE:HB2	3:H:140:ASP:HB2	2.00	0.43
3:I:101:ARG:HG2	3:I:102:ARG:NH1	2.33	0.43
1:D:175:GLY:HA2	1:D:176:GLU:C	2.38	0.43
2:G:127:GLY:HA2	2:G:130:VAL:CG2	2.48	0.43
1:E:85:GLU:N	1:E:85:GLU:OE1	2.51	0.43
1:E:175:GLY:HA2	1:E:176:GLU:C	2.38	0.43
1:E:358:GLU:HG2	1:E:358:GLU:O	2.19	0.43
3:H:234:ILE:O	3:H:238:LEU:HB2	2.18	0.43
3:I:23:ILE:CD1	3:I:24:ILE:CD1	2.88	0.43
2:G:57:ARG:HD2	2:G:210:LYS:NZ	2.33	0.43
2:B:141:MET:O	2:B:141:MET:HG2	2.19	0.43
3:I:46:TRP:O	3:I:46:TRP:HE3	2.02	0.43
3:I:135:ILE:O	3:I:137:ARG:NH2	2.52	0.43
3:I:205:PHE:O	3:I:205:PHE:CG	2.70	0.43
1:D:358:GLU:O	1:D:358:GLU:HG2	2.19	0.43
2:B:127:GLY:HA2	2:B:130:VAL:CG2	2.48	0.43
3:C:101:ARG:HG2	3:C:102:ARG:NH1	2.33	0.43
3:I:140:ASP:HB2	2:F:208:PHE:HB2	1.99	0.43
3:I:145:HIS:HA	3:I:148:GLU:HB3	2.00	0.43
2:G:19:ARG:HA	2:G:19:ARG:HD2	1.42	0.43
2:G:196:TYR:CE1	1:E:145:GLN:HA	2.53	0.43
3:C:102:ARG:HG3	3:C:170:ARG:NE	2.31	0.43
3:I:46:TRP:CZ3	1:E:94:PRO:HB2	2.53	0.43
3:I:234:ILE:O	3:I:238:LEU:HB2	2.18	0.43
2:F:191:THR:HG21	1:D:93:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:GLU:OE1	1:D:344:GLU:N	2.50	0.43
3:C:238:LEU:HA	3:C:238:LEU:HD12	1.75	0.43
3:H:46:TRP:O	3:H:46:TRP:HE3	2.02	0.43
3:H:135:ILE:O	3:H:137:ARG:NH2	2.52	0.43
3:H:145:HIS:HA	3:H:148:GLU:HB3	2.00	0.43
3:H:230:VAL:O	3:H:234:ILE:HG13	2.19	0.43
1:A:99:ILE:O	1:A:99:ILE:HG13	2.19	0.43
1:A:344:GLU:OE1	1:A:344:GLU:N	2.50	0.43
2:G:150:LEU:O	2:G:154:LEU:HG	2.19	0.43
1:A:145:GLN:HA	2:B:196:TYR:CE1	2.53	0.42
1:A:315:ALA:HB2	1:A:394:ILE:HG13	2.01	0.42
3:H:101:ARG:HG2	3:H:102:ARG:NH1	2.33	0.42
3:H:230:VAL:CG2	2:F:32:VAL:HG11	2.48	0.42
2:F:180:LEU:HD23	2:F:180:LEU:HA	1.84	0.42
2:G:138:SER:OG	2:G:143:LEU:HD12	2.20	0.42
1:D:323:ARG:NH1	1:D:332:ASP:OD1	2.52	0.42
1:A:256:GLU:OE2	1:A:257:LYS:N	2.52	0.42
3:I:170:ARG:HD2	3:I:170:ARG:HA	1.93	0.42
2:F:150:LEU:O	2:F:154:LEU:HG	2.19	0.42
2:F:237:TRP:HD1	5:F:303:HXG:H37	1.85	0.42
1:D:99:ILE:O	1:D:99:ILE:HG13	2.19	0.42
2:B:37:TYR:OH	2:B:68:SER:O	2.26	0.42
2:B:150:LEU:O	2:B:154:LEU:HG	2.19	0.42
3:I:215:PRO:HA	3:I:218:TYR:CD2	2.55	0.42
2:F:183:LEU:HD12	2:F:183:LEU:HA	1.80	0.42
1:D:256:GLU:OE2	1:D:257:LYS:N	2.52	0.42
1:A:358:GLU:O	1:A:358:GLU:HG2	2.19	0.42
2:B:11:ARG:HA	3:C:248:ASP:HB3	2.01	0.42
3:C:172:PRO:O	3:C:175:GLN:HG2	2.20	0.42
1:E:256:GLU:OE2	1:E:257:LYS:N	2.52	0.42
1:A:399:ASN:OD1	1:A:399:ASN:N	2.53	0.42
2:B:208:PHE:CB	3:H:140:ASP:HB2	2.50	0.42
1:D:316:GLU:HB2	1:D:325:LEU:HD23	1.99	0.42
1:E:209:LYS:H	1:E:209:LYS:HG2	1.62	0.42
1:A:323:ARG:NH1	1:A:332:ASP:OD1	2.52	0.42
3:H:189:PRO:O	3:H:192:ILE:HG22	2.20	0.42
3:H:215:PRO:HA	3:H:218:TYR:CD2	2.55	0.42
2:B:191:THR:OG1	3:C:134:THR:O	2.21	0.42
3:C:81:GLY:HA3	3:C:84:TRP:CZ3	2.55	0.42
3:I:230:VAL:O	3:I:234:ILE:HG13	2.19	0.42
1:E:399:ASN:N	1:E:399:ASN:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TRP:CH2	1:A:232:ASP:HB3	2.55	0.42
2:B:138:SER:OG	2:B:143:LEU:HD12	2.20	0.42
3:C:204:THR:HG23	2:G:207:THR:CA	2.47	0.42
1:D:316:GLU:OE1	1:D:323:ARG:NH2	2.53	0.42
3:C:230:VAL:O	3:C:234:ILE:HG13	2.19	0.42
3:H:87:ARG:HA	3:H:87:ARG:NH1	2.35	0.42
3:I:81:GLY:HA3	3:I:84:TRP:CZ3	2.55	0.42
2:F:16:LYS:HA	2:F:16:LYS:HD3	1.93	0.42
1:E:206:TRP:CH2	1:E:232:ASP:HB3	2.55	0.42
1:A:316:GLU:OE1	1:A:323:ARG:NH2	2.53	0.42
3:C:46:TRP:O	3:C:46:TRP:HE3	2.02	0.42
3:H:70:VAL:HG23	3:H:71:LEU:N	2.35	0.42
3:H:147:ILE:O	3:H:151:LEU:HB3	2.19	0.42
2:G:83:TYR:HB3	1:E:215:ARG:HB2	2.02	0.42
2:G:191:THR:HG21	1:E:93:ILE:H	1.84	0.42
1:A:93:ILE:H	2:B:191:THR:CG2	2.26	0.41
3:I:147:ILE:O	3:I:151:LEU:HB3	2.19	0.41
2:F:138:SER:OG	2:F:143:LEU:HD12	2.20	0.41
3:C:21:LYS:HZ3	3:C:23:ILE:HG13	1.86	0.41
3:H:250:ALA:HB3	2:F:11:ARG:HH21	1.85	0.41
2:F:210:LYS:HB2	1:E:381:TYR:HB3	2.02	0.41
1:D:206:TRP:CH2	1:D:232:ASP:HB3	2.55	0.41
1:E:344:GLU:OE1	1:E:344:GLU:N	2.51	0.41
3:C:85:LYS:NZ	3:C:170:ARG:HB2	2.35	0.41
3:H:81:GLY:HA3	3:H:84:TRP:CZ3	2.55	0.41
3:I:189:PRO:O	3:I:192:ILE:HG22	2.20	0.41
3:C:189:PRO:O	3:C:192:ILE:HG22	2.20	0.41
3:I:21:LYS:HZ2	3:I:25:ALA:HB2	1.85	0.41
3:I:23:ILE:HD12	3:I:24:ILE:HD11	1.92	0.41
3:I:87:ARG:NH1	3:I:87:ARG:HA	2.35	0.41
1:E:323:ARG:NH1	1:E:332:ASP:OD1	2.52	0.41
1:A:94:PRO:HA	3:C:135:ILE:HB	2.02	0.41
1:A:147:GLY:O	3:C:207:PHE:CZ	2.74	0.41
3:H:85:LYS:NZ	3:H:170:ARG:HB2	2.35	0.41
3:H:134:THR:HG21	2:F:112:THR:CG2	2.36	0.41
3:H:165:LEU:HD23	3:H:165:LEU:HA	1.92	0.41
2:G:82:ARG:HD2	2:G:82:ARG:HA	1.62	0.41
1:D:110:VAL:HA	1:D:269:MET:HE1	2.03	0.41
1:D:399:ASN:OD1	1:D:399:ASN:N	2.53	0.41
3:C:215:PRO:HA	3:C:218:TYR:CD2	2.55	0.41
3:I:225:TRP:CD1	3:I:225:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:MET:O	2:F:141:MET:HG2	2.19	0.41
1:D:175:GLY:N	1:D:176:GLU:HB3	2.36	0.41
1:D:344:GLU:H	1:D:344:GLU:CD	2.23	0.41
1:D:354:LEU:HA	1:D:358:GLU:OE2	2.21	0.41
1:E:344:GLU:H	1:E:344:GLU:CD	2.23	0.41
1:A:354:LEU:HA	1:A:358:GLU:OE2	2.21	0.41
3:C:247:LYS:H	3:C:247:LYS:HG3	1.46	0.41
3:H:21:LYS:HZ1	3:H:25:ALA:HB2	1.86	0.41
3:H:209:GLU:OE2	3:H:209:GLU:N	2.54	0.41
3:I:66:TYR:HE1	5:I:303:HXG:OAF	2.04	0.41
2:F:22:ASP:HA	1:D:212:PHE:HD1	1.85	0.41
2:F:196:TYR:CD1	1:D:145:GLN:HB2	2.56	0.41
1:E:272:ILE:HD13	1:E:272:ILE:HA	1.85	0.41
3:I:70:VAL:HG23	3:I:71:LEU:N	2.35	0.41
1:E:315:ALA:HB2	1:E:394:ILE:HG13	2.01	0.41
1:E:316:GLU:OE1	1:E:323:ARG:NH2	2.53	0.41
1:A:344:GLU:H	1:A:344:GLU:CD	2.23	0.41
2:B:16:LYS:HA	2:B:16:LYS:HD3	1.93	0.41
3:C:70:VAL:HG23	3:C:71:LEU:N	2.35	0.41
3:C:87:ARG:HA	3:C:87:ARG:NH1	2.35	0.41
3:C:135:ILE:O	3:C:137:ARG:NH2	2.52	0.41
3:C:140:ASP:HB2	2:G:208:PHE:CB	2.50	0.41
3:C:145:HIS:CE1	3:C:149:PHE:CE2	3.07	0.41
3:C:220:PHE:CD1	3:C:220:PHE:N	2.79	0.41
3:H:58:GLU:HG2	3:H:62:MET:CB	2.46	0.41
3:H:110:LEU:HD23	3:H:110:LEU:HA	1.92	0.41
3:H:130:THR:OG1	2:F:108:PHE:CE2	2.70	0.41
3:H:172:PRO:O	3:H:175:GLN:HG2	2.20	0.41
3:H:220:PHE:CD1	3:H:220:PHE:N	2.79	0.41
3:I:87:ARG:HA	3:I:87:ARG:HD3	1.64	0.41
2:F:59:LEU:HD22	2:F:199:MET:HB3	2.03	0.41
1:D:315:ALA:HB2	1:D:394:ILE:HG13	2.01	0.41
2:B:127:GLY:O	2:B:130:VAL:HG23	2.21	0.41
3:C:246:LYS:HB2	3:C:246:LYS:HE2	1.45	0.41
3:H:66:TYR:HE1	5:H:304:HXG:OAF	2.03	0.41
3:I:186:VAL:CG1	3:I:187:VAL:N	2.84	0.41
1:E:99:ILE:O	1:E:99:ILE:HG13	2.19	0.41
1:A:143:ASN:HB3	2:B:196:TYR:CE2	2.56	0.40
1:D:409:LEU:HD12	1:D:409:LEU:HA	1.88	0.40
1:E:305:THR:HG22	1:E:359:THR:HG23	2.03	0.40
1:A:305:THR:HG22	1:A:359:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:PRO:O	3:I:175:GLN:HG2	2.20	0.40
3:I:198:LEU:HA	2:F:219:PHE:CD1	2.56	0.40
1:D:305:THR:HG22	1:D:359:THR:HG23	2.03	0.40
1:A:175:GLY:N	1:A:176:GLU:HB3	2.36	0.40
3:I:85:LYS:NZ	3:I:170:ARG:HB2	2.35	0.40
3:I:208:MET:CB	3:I:214:ALA:HB2	2.52	0.40
2:G:186:TYR:CE1	1:E:111:PRO:HA	2.56	0.40
3:C:102:ARG:HA	3:C:102:ARG:HD3	1.97	0.40
3:I:139:THR:O	3:I:140:ASP:HB3	2.21	0.40
1:E:291:TYR:HD1	1:E:409:LEU:HG	1.87	0.40
2:B:197:ILE:HG12	2:B:197:ILE:H	1.76	0.40
3:H:208:MET:HB3	3:H:214:ALA:HB2	2.03	0.40
1:D:291:TYR:HD1	1:D:409:LEU:HG	1.87	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	380/414 (92%)	350 (92%)	28 (7%)	2 (0%)	29	34
1	D	380/414 (92%)	350 (92%)	28 (7%)	2 (0%)	29	34
1	E	380/414 (92%)	350 (92%)	28 (7%)	2 (0%)	29	34
2	B	237/247 (96%)	211 (89%)	21 (9%)	5 (2%)	7	5
2	F	237/247 (96%)	211 (89%)	21 (9%)	5 (2%)	7	5
2	G	237/247 (96%)	211 (89%)	21 (9%)	5 (2%)	7	5
3	C	229/250 (92%)	187 (82%)	37 (16%)	5 (2%)	6	4
3	H	229/250 (92%)	187 (82%)	37 (16%)	5 (2%)	6	4
3	I	229/250 (92%)	187 (82%)	37 (16%)	5 (2%)	6	4
All	All	2538/2733 (93%)	2244 (88%)	258 (10%)	36 (1%)	15	9

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	187	VAL
3	H	187	VAL
3	I	187	VAL
2	B	8	VAL
2	B	139	ASN
3	C	54	ALA
3	C	55	PRO
3	H	54	ALA
3	H	55	PRO
3	I	54	ALA
3	I	55	PRO
2	F	8	VAL
2	F	139	ASN
2	G	8	VAL
2	G	139	ASN
2	B	9	ARG
2	B	211	ASP
3	C	23	ILE
3	H	23	ILE
3	I	23	ILE
2	F	9	ARG
2	F	211	ASP
2	G	9	ARG
2	G	211	ASP
2	B	80	TRP
2	F	80	TRP
2	G	80	TRP
1	A	353	PRO
3	C	227	ALA
3	H	227	ALA
3	I	227	ALA
1	D	353	PRO
1	E	353	PRO
1	A	356	PRO
1	D	356	PRO
1	E	356	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/343 (92%)	275 (87%)	42 (13%)	4	3
1	D	317/343 (92%)	275 (87%)	42 (13%)	4	3
1	E	317/343 (92%)	275 (87%)	42 (13%)	4	3
2	B	202/207 (98%)	176 (87%)	26 (13%)	4	3
2	F	202/207 (98%)	176 (87%)	26 (13%)	4	3
2	G	202/207 (98%)	176 (87%)	26 (13%)	4	3
3	C	197/211 (93%)	150 (76%)	47 (24%)	0	0
3	H	197/211 (93%)	149 (76%)	48 (24%)	0	0
3	I	197/211 (93%)	149 (76%)	48 (24%)	0	0
All	All	2148/2283 (94%)	1801 (84%)	347 (16%)	5	1

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	45	ARG
1	A	59	VAL
1	A	60	SER
1	A	68	SER
1	A	112	ARG
1	A	162	SER
1	A	171	THR
1	A	176	GLU
1	A	186	ASP
1	A	203	MET
1	A	208	ARG
1	A	211	VAL
1	A	213	ILE
1	A	223	LYS
1	A	225	ASP
1	A	226	SER
1	A	228	ILE
1	A	229	THR
1	A	231	THR
1	A	234	LYS
1	A	249	VAL
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	261	THR
1	A	273	LYS
1	A	274	SER
1	A	281	THR
1	A	283	SER
1	A	285	LYS
1	A	287	VAL
1	A	293	VAL
1	A	296	ARG
1	A	298	MET
1	A	306	ASN
1	A	335	ASN
1	A	344	GLU
1	A	347	SER
1	A	367	SER
1	A	385	SER
1	A	397	ASP
1	A	399	ASN
1	A	405	VAL
2	B	6	SER
2	B	8	VAL
2	B	11	ARG
2	B	13	GLU
2	B	16	LYS
2	B	18	SER
2	B	19	ARG
2	B	28	THR
2	B	42	MET
2	B	61	VAL
2	B	79	LEU
2	B	80	TRP
2	B	82	ARG
2	B	84	ARG
2	B	90	THR
2	B	91	LEU
2	B	130	VAL
2	B	138	SER
2	B	141	MET
2	B	182	ASP
2	B	197	ILE
2	B	204	THR
2	B	207	THR

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Mol	Chain	Res	Type
2	B	210	LYS
2	B	212	VAL
2	B	230	LEU
3	C	20	LYS
3	C	21	LYS
3	C	23	ILE
3	C	24	ILE
3	C	28	SER
3	C	32	VAL
3	C	46	TRP
3	C	47	SER
3	C	52	SER
3	C	53	PHE
3	C	58	GLU
3	C	74	LEU
3	C	79	LEU
3	C	83	ILE
3	C	85	LYS
3	C	87	ARG
3	C	88	ASP
3	C	90	LYS
3	C	91	VAL
3	C	92	MET
3	C	93	SER
3	C	97	ARG
3	C	108	THR
3	C	137	ARG
3	C	140	ASP
3	C	156	TYR
3	C	163	SER
3	C	170	ARG
3	C	173	THR
3	C	182	TYR
3	C	184	VAL
3	C	192	ILE
3	C	196	VAL
3	C	199	ASN
3	C	212	PHE
3	C	220	PHE
3	C	222	PHE
3	C	223	PHE
3	C	228	LEU

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Mol	Chain	Res	Type
3	C	230	VAL
3	C	238	LEU
3	C	241	LEU
3	C	243	LYS
3	C	245	LEU
3	C	246	LYS
3	C	247	LYS
3	C	249	LEU
3	H	20	LYS
3	H	21	LYS
3	H	23	ILE
3	H	24	ILE
3	H	28	SER
3	H	32	VAL
3	H	46	TRP
3	H	47	SER
3	H	52	SER
3	H	53	PHE
3	H	58	GLU
3	H	74	LEU
3	H	79	LEU
3	H	83	ILE
3	H	85	LYS
3	H	87	ARG
3	H	88	ASP
3	H	90	LYS
3	H	91	VAL
3	H	92	MET
3	H	93	SER
3	H	97	ARG
3	H	108	THR
3	H	137	ARG
3	H	140	ASP
3	H	144	SER
3	H	156	TYR
3	H	163	SER
3	H	170	ARG
3	H	173	THR
3	H	182	TYR
3	H	184	VAL
3	H	192	ILE
3	H	196	VAL

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Mol	Chain	Res	Type
3	H	199	ASN
3	H	212	PHE
3	H	220	PHE
3	H	222	PHE
3	H	223	PHE
3	H	228	LEU
3	H	230	VAL
3	H	238	LEU
3	H	241	LEU
3	H	243	LYS
3	H	245	LEU
3	H	246	LYS
3	H	247	LYS
3	H	249	LEU
3	I	20	LYS
3	I	21	LYS
3	I	23	ILE
3	I	24	ILE
3	I	28	SER
3	I	32	VAL
3	I	46	TRP
3	I	47	SER
3	I	52	SER
3	I	53	PHE
3	I	58	GLU
3	I	74	LEU
3	I	79	LEU
3	I	83	ILE
3	I	85	LYS
3	I	87	ARG
3	I	88	ASP
3	I	90	LYS
3	I	91	VAL
3	I	92	MET
3	I	93	SER
3	I	97	ARG
3	I	108	THR
3	I	137	ARG
3	I	140	ASP
3	I	144	SER
3	I	156	TYR
3	I	163	SER

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Mol	Chain	Res	Type
3	I	170	ARG
3	I	173	THR
3	I	182	TYR
3	I	184	VAL
3	I	192	ILE
3	I	196	VAL
3	I	199	ASN
3	I	212	PHE
3	I	220	PHE
3	I	222	PHE
3	I	223	PHE
3	I	228	LEU
3	I	230	VAL
3	I	238	LEU
3	I	241	LEU
3	I	243	LYS
3	I	245	LEU
3	I	246	LYS
3	I	247	LYS
3	I	249	LEU
2	F	6	SER
2	F	8	VAL
2	F	11	ARG
2	F	13	GLU
2	F	16	LYS
2	F	18	SER
2	F	19	ARG
2	F	28	THR
2	F	42	MET
2	F	61	VAL
2	F	79	LEU
2	F	80	TRP
2	F	82	ARG
2	F	84	ARG
2	F	90	THR
2	F	91	LEU
2	F	130	VAL
2	F	138	SER
2	F	141	MET
2	F	182	ASP
2	F	197	ILE
2	F	204	THR

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Mol	Chain	Res	Type
2	F	207	THR
2	F	210	LYS
2	F	212	VAL
2	F	230	LEU
2	G	6	SER
2	G	8	VAL
2	G	11	ARG
2	G	13	GLU
2	G	16	LYS
2	G	18	SER
2	G	19	ARG
2	G	28	THR
2	G	42	MET
2	G	61	VAL
2	G	79	LEU
2	G	80	TRP
2	G	82	ARG
2	G	84	ARG
2	G	90	THR
2	G	91	LEU
2	G	130	VAL
2	G	138	SER
2	G	141	MET
2	G	182	ASP
2	G	197	ILE
2	G	204	THR
2	G	207	THR
2	G	210	LYS
2	G	212	VAL
2	G	230	LEU
1	D	33	HIS
1	D	45	ARG
1	D	59	VAL
1	D	60	SER
1	D	68	SER
1	D	112	ARG
1	D	162	SER
1	D	171	THR
1	D	176	GLU
1	D	186	ASP
1	D	203	MET
1	D	208	ARG

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Mol	Chain	Res	Type
1	D	211	VAL
1	D	213	ILE
1	D	223	LYS
1	D	225	ASP
1	D	226	SER
1	D	228	ILE
1	D	229	THR
1	D	231	THR
1	D	234	LYS
1	D	249	VAL
1	D	256	GLU
1	D	261	THR
1	D	273	LYS
1	D	274	SER
1	D	281	THR
1	D	283	SER
1	D	285	LYS
1	D	287	VAL
1	D	293	VAL
1	D	296	ARG
1	D	298	MET
1	D	306	ASN
1	D	335	ASN
1	D	344	GLU
1	D	347	SER
1	D	367	SER
1	D	385	SER
1	D	397	ASP
1	D	399	ASN
1	D	405	VAL
1	E	33	HIS
1	E	45	ARG
1	E	59	VAL
1	E	60	SER
1	E	68	SER
1	E	112	ARG
1	E	162	SER
1	E	171	THR
1	E	176	GLU
1	E	186	ASP
1	E	203	MET
1	E	208	ARG

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Mol	Chain	Res	Type
1	E	211	VAL
1	E	213	ILE
1	E	223	LYS
1	E	225	ASP
1	E	226	SER
1	E	228	ILE
1	E	229	THR
1	E	231	THR
1	E	234	LYS
1	E	249	VAL
1	E	256	GLU
1	E	261	THR
1	E	273	LYS
1	E	274	SER
1	E	281	THR
1	E	283	SER
1	E	285	LYS
1	E	287	VAL
1	E	293	VAL
1	E	296	ARG
1	E	298	MET
1	E	306	ASN
1	E	335	ASN
1	E	344	GLU
1	E	347	SER
1	E	367	SER
1	E	385	SER
1	E	397	ASP
1	E	399	ASN
1	E	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	108	GLN
1	A	137	HIS
1	A	299	GLN
1	A	335	ASN
2	B	103	ASN
2	B	107	ASN
2	B	160	ASN

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Mol	Chain	Res	Type
2	B	232	HIS
3	C	176	GLN
3	C	181	GLN
3	H	176	GLN
3	H	181	GLN
3	I	176	GLN
3	I	181	GLN
2	F	103	ASN
2	F	107	ASN
2	F	160	ASN
2	F	232	HIS
2	G	103	ASN
2	G	107	ASN
2	G	160	ASN
2	G	232	HIS
1	D	62	ASN
1	D	108	GLN
1	D	137	HIS
1	D	299	GLN
1	D	335	ASN
1	E	62	ASN
1	E	108	GLN
1	E	137	HIS
1	E	299	GLN
1	E	335	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
7	6ER	B	306	-	29,29,29	0.39	0	35,37,37	0.52	0
6	D10	B	305	-	9,9,9	0.15	0	8,8,8	0.12	0
5	HXG	B	302	-	29,29,29	1.21	1 (3%)	35,37,37	1.15	2 (5%)
6	D10	H	301	-	9,9,9	0.10	0	8,8,8	0.06	0
6	D10	C	305	-	9,9,9	0.10	0	8,8,8	0.06	0
6	D10	G	304	-	9,9,9	0.10	0	8,8,8	0.10	0
5	HXG	H	304	-	29,29,29	0.33	0	35,37,37	0.45	0
5	HXG	F	301	-	29,29,29	1.19	3 (10%)	35,37,37	1.14	2 (5%)
6	D10	I	305	-	9,9,9	0.10	0	8,8,8	0.06	0
5	HXG	F	302	-	29,29,29	1.21	1 (3%)	35,37,37	1.15	2 (5%)
5	HXG	I	302	-	29,29,29	1.19	3 (10%)	35,37,37	1.07	2 (5%)
5	HXG	C	302	-	29,29,29	1.19	3 (10%)	35,37,37	1.07	2 (5%)
5	HXG	C	303	-	29,29,29	0.34	0	35,37,37	0.45	0
5	HXG	F	303	-	29,29,29	0.35	0	35,37,37	0.46	0
6	D10	G	305	-	9,9,9	0.15	0	8,8,8	0.12	0
7	6ER	C	304	-	29,29,29	0.39	0	35,37,37	0.52	0
5	HXG	I	303	-	29,29,29	0.33	0	35,37,37	0.45	0
6	D10	F	304	-	9,9,9	0.09	0	8,8,8	0.11	0
6	D10	B	304	-	9,9,9	0.10	0	8,8,8	0.10	0
5	HXG	B	301	-	29,29,29	1.19	3 (10%)	35,37,37	1.14	2 (5%)
5	HXG	B	303	-	29,29,29	0.35	0	35,37,37	0.46	0
5	HXG	G	301	-	29,29,29	1.19	3 (10%)	35,37,37	1.14	2 (5%)
7	6ER	I	304	-	29,29,29	0.39	0	35,37,37	0.52	0
6	D10	F	305	-	9,9,9	0.15	0	8,8,8	0.12	0
5	HXG	H	303	-	29,29,29	1.19	3 (10%)	35,37,37	1.07	2 (5%)
5	HXG	G	302	-	29,29,29	1.21	1 (3%)	35,37,37	1.15	2 (5%)
5	HXG	G	303	-	29,29,29	0.35	0	35,37,37	0.46	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
7	6ER	B	306	-	-	14/33/33/33	-
6	D10	B	305	-	-	1/7/7/7	-
5	HXG	B	302	-	-	16/33/33/33	-
6	D10	H	301	-	-	1/7/7/7	-
6	D10	C	305	-	-	1/7/7/7	-
6	D10	G	304	-	-	5/7/7/7	-
5	HXG	H	304	-	-	13/33/33/33	-
5	HXG	F	301	-	-	13/33/33/33	-
6	D10	I	305	-	-	1/7/7/7	-
5	HXG	F	302	-	-	16/33/33/33	-
5	HXG	I	302	-	-	12/33/33/33	-
5	HXG	C	302	-	-	12/33/33/33	-
5	HXG	C	303	-	-	13/33/33/33	-
5	HXG	F	303	-	-	12/33/33/33	-
6	D10	G	305	-	-	1/7/7/7	-
7	6ER	C	304	-	-	14/33/33/33	-
5	HXG	I	303	-	-	13/33/33/33	-
6	D10	F	304	-	-	5/7/7/7	-
6	D10	B	304	-	-	5/7/7/7	-
5	HXG	B	301	-	-	13/33/33/33	-
5	HXG	B	303	-	-	12/33/33/33	-
5	HXG	G	301	-	-	13/33/33/33	-
7	6ER	I	304	-	-	14/33/33/33	-
6	D10	F	305	-	-	1/7/7/7	-
5	HXG	H	303	-	-	12/33/33/33	-
5	HXG	G	302	-	-	16/33/33/33	-
5	HXG	G	303	-	-	12/33/33/33	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	301	HXG	PBD-OAW	3.99	1.75	1.59
5	B	301	HXG	PBD-OAW	3.99	1.75	1.59
5	F	301	HXG	PBD-OAW	3.98	1.75	1.59
5	B	302	HXG	PBD-OAW	3.71	1.74	1.59
5	G	302	HXG	PBD-OAW	3.70	1.74	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	302	HXG	PBD-OAW	3.69	1.74	1.59
5	C	302	HXG	PBD-OAW	3.54	1.73	1.59
5	H	303	HXG	PBD-OAW	3.53	1.73	1.59
5	I	302	HXG	PBD-OAW	3.53	1.73	1.59
5	I	302	HXG	OAY-CBB	-2.35	1.40	1.46
5	C	302	HXG	OAY-CBB	-2.33	1.40	1.46
5	H	303	HXG	OAY-CBB	-2.32	1.40	1.46
5	B	301	HXG	OAY-CBB	-2.27	1.40	1.46
5	F	301	HXG	OAY-CBB	-2.26	1.40	1.46
5	G	301	HXG	OAY-CBB	-2.26	1.40	1.46
5	B	301	HXG	OAX-CAU	-2.25	1.36	1.44
5	F	301	HXG	OAX-CAU	-2.24	1.36	1.44
5	G	301	HXG	OAX-CAU	-2.24	1.36	1.44
5	I	302	HXG	OAW-CAP	-2.08	1.36	1.44
5	H	303	HXG	OAW-CAP	-2.08	1.36	1.44
5	C	302	HXG	OAW-CAP	-2.08	1.36	1.44

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	302	HXG	OAH-PBD-OAI	3.32	128.64	112.24
5	B	302	HXG	OAH-PBD-OAI	3.31	128.62	112.24
5	G	302	HXG	OAH-PBD-OAI	3.31	128.61	112.24
5	G	301	HXG	OAH-PBD-OAI	3.22	128.15	112.24
5	B	301	HXG	OAH-PBD-OAI	3.21	128.12	112.24
5	F	301	HXG	OAH-PBD-OAI	3.21	128.11	112.24
5	I	302	HXG	OAH-PBD-OAI	3.16	127.86	112.24
5	H	303	HXG	OAH-PBD-OAI	3.16	127.86	112.24
5	C	302	HXG	OAH-PBD-OAI	3.15	127.83	112.24
5	F	302	HXG	OAY-CBA-CAR	3.01	117.98	111.50
5	B	302	HXG	OAY-CBA-CAR	2.99	117.94	111.50
5	G	302	HXG	OAY-CBA-CAR	2.96	117.89	111.50
5	I	302	HXG	OAY-CBA-CAR	2.31	116.48	111.50
5	H	303	HXG	OAY-CBA-CAR	2.31	116.48	111.50
5	C	302	HXG	OAY-CBA-CAR	2.29	116.44	111.50
5	F	301	HXG	OAY-CBA-CAR	2.13	116.09	111.50
5	B	301	HXG	OAY-CBA-CAR	2.13	116.08	111.50
5	G	301	HXG	OAY-CBA-CAR	2.12	116.07	111.50

There are no chirality outliers.

All (261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	HXG	CAU-OAX-PBD-OAI
5	B	301	HXG	OAW-CAP-CAS-NBC
5	B	302	HXG	CAU-OAX-PBD-OAW
5	B	302	HXG	CAP-OAW-PBD-OAH
5	B	302	HXG	OAW-CAP-CAS-NBC
5	C	302	HXG	CAU-OAX-PBD-OAH
5	C	302	HXG	CAP-OAW-PBD-OAX
5	C	302	HXG	CAP-OAW-PBD-OAI
5	C	302	HXG	CAP-OAW-PBD-OAH
5	C	303	HXG	OAV-CAT-CBB-OAY
5	C	303	HXG	CAU-OAX-PBD-OAI
5	H	303	HXG	CAU-OAX-PBD-OAH
5	H	303	HXG	CAP-OAW-PBD-OAX
5	H	303	HXG	CAP-OAW-PBD-OAI
5	H	303	HXG	CAP-OAW-PBD-OAH
5	H	304	HXG	OAV-CAT-CBB-OAY
5	H	304	HXG	CAU-OAX-PBD-OAI
5	I	302	HXG	CAU-OAX-PBD-OAH
5	I	302	HXG	CAP-OAW-PBD-OAX
5	I	302	HXG	CAP-OAW-PBD-OAI
5	I	302	HXG	CAP-OAW-PBD-OAH
5	I	303	HXG	OAV-CAT-CBB-OAY
5	I	303	HXG	CAU-OAX-PBD-OAI
5	F	301	HXG	CAU-OAX-PBD-OAI
5	F	301	HXG	OAW-CAP-CAS-NBC
5	F	302	HXG	CAU-OAX-PBD-OAW
5	F	302	HXG	CAP-OAW-PBD-OAH
5	F	302	HXG	OAW-CAP-CAS-NBC
5	G	301	HXG	CAU-OAX-PBD-OAI
5	G	301	HXG	OAW-CAP-CAS-NBC
5	G	302	HXG	CAU-OAX-PBD-OAW
5	G	302	HXG	CAP-OAW-PBD-OAH
5	G	302	HXG	OAW-CAP-CAS-NBC
7	B	306	6ER	O06-C05-O07-C08
7	C	304	6ER	O06-C05-O07-C08
7	I	304	6ER	O06-C05-O07-C08
5	C	303	HXG	OAG-CBA-OAY-CBB
5	H	304	HXG	OAG-CBA-OAY-CBB
5	I	303	HXG	OAG-CBA-OAY-CBB
5	C	303	HXG	CAQ-CAZ-OAV-CAT
5	H	304	HXG	CAQ-CAZ-OAV-CAT
5	I	303	HXG	CAQ-CAZ-OAV-CAT
7	B	306	6ER	C04-C05-O07-C08

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Mol	Chain	Res	Type	Atoms
7	C	304	6ER	C04-C05-O07-C08
7	I	304	6ER	C04-C05-O07-C08
5	B	303	HXG	OAF-CAZ-OAV-CAT
5	C	303	HXG	OAF-CAZ-OAV-CAT
5	H	304	HXG	OAF-CAZ-OAV-CAT
5	I	303	HXG	OAF-CAZ-OAV-CAT
5	F	303	HXG	OAF-CAZ-OAV-CAT
5	G	303	HXG	OAF-CAZ-OAV-CAT
5	B	303	HXG	CAQ-CAZ-OAV-CAT
5	F	303	HXG	CAQ-CAZ-OAV-CAT
5	G	303	HXG	CAQ-CAZ-OAV-CAT
5	C	303	HXG	CAR-CBA-OAY-CBB
5	H	304	HXG	CAR-CBA-OAY-CBB
5	I	303	HXG	CAR-CBA-OAY-CBB
5	B	302	HXG	CAQ-CAZ-OAV-CAT
5	F	302	HXG	CAQ-CAZ-OAV-CAT
5	G	302	HXG	CAQ-CAZ-OAV-CAT
5	B	303	HXG	CAR-CBA-OAY-CBB
5	F	303	HXG	CAR-CBA-OAY-CBB
5	G	303	HXG	CAR-CBA-OAY-CBB
5	B	302	HXG	OAF-CAZ-OAV-CAT
5	F	302	HXG	OAF-CAZ-OAV-CAT
5	G	302	HXG	OAF-CAZ-OAV-CAT
5	B	301	HXG	CAM-CAO-CAR-CBA
5	F	301	HXG	CAM-CAO-CAR-CBA
5	G	301	HXG	CAM-CAO-CAR-CBA
5	B	303	HXG	CAM-CAO-CAR-CBA
5	F	303	HXG	CAM-CAO-CAR-CBA
5	G	303	HXG	CAM-CAO-CAR-CBA
5	C	302	HXG	CAQ-CAZ-OAV-CAT
5	H	303	HXG	CAQ-CAZ-OAV-CAT
5	I	302	HXG	CAQ-CAZ-OAV-CAT
5	B	303	HXG	OAG-CBA-OAY-CBB
5	F	303	HXG	OAG-CBA-OAY-CBB
5	G	303	HXG	OAG-CBA-OAY-CBB
7	B	306	6ER	C25-C23-O22-C09
7	C	304	6ER	C25-C23-O22-C09
7	I	304	6ER	C25-C23-O22-C09
5	B	302	HXG	CAP-OAW-PBD-OAX
5	C	303	HXG	CAU-OAX-PBD-OAW
5	H	304	HXG	CAU-OAX-PBD-OAW
5	I	303	HXG	CAU-OAX-PBD-OAW

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Mol	Chain	Res	Type	Atoms
5	F	302	HXG	CAP-OAW-PBD-OAX
5	G	302	HXG	CAP-OAW-PBD-OAX
7	B	306	6ER	O24-C23-O22-C09
7	C	304	6ER	O24-C23-O22-C09
7	I	304	6ER	O24-C23-O22-C09
5	C	302	HXG	OAF-CAZ-OAV-CAT
5	H	303	HXG	OAF-CAZ-OAV-CAT
5	I	302	HXG	OAF-CAZ-OAV-CAT
5	C	302	HXG	CAJ-CAL-CAN-CAQ
5	H	303	HXG	CAJ-CAL-CAN-CAQ
5	I	302	HXG	CAJ-CAL-CAN-CAQ
5	B	301	HXG	OAG-CBA-OAY-CBB
5	F	301	HXG	OAG-CBA-OAY-CBB
5	G	301	HXG	OAG-CBA-OAY-CBB
5	B	301	HXG	CAR-CBA-OAY-CBB
5	F	301	HXG	CAR-CBA-OAY-CBB
5	G	301	HXG	CAR-CBA-OAY-CBB
7	B	306	6ER	C23-C25-C26-C27
7	C	304	6ER	C23-C25-C26-C27
7	I	304	6ER	C23-C25-C26-C27
7	B	306	6ER	C01-C02-C03-C04
7	C	304	6ER	C01-C02-C03-C04
7	I	304	6ER	C01-C02-C03-C04
5	G	302	HXG	CAL-CAN-CAQ-CAZ
5	B	302	HXG	CAL-CAN-CAQ-CAZ
5	F	302	HXG	CAL-CAN-CAQ-CAZ
6	B	305	D10	C4-C5-C6-C7
6	F	305	D10	C4-C5-C6-C7
6	G	305	D10	C4-C5-C6-C7
5	H	304	HXG	CAK-CAM-CAO-CAR
5	C	303	HXG	CAK-CAM-CAO-CAR
5	I	303	HXG	CAK-CAM-CAO-CAR
5	B	303	HXG	OAV-CAT-CBB-OAY
5	F	303	HXG	OAV-CAT-CBB-OAY
5	G	303	HXG	OAV-CAT-CBB-OAY
5	B	301	HXG	CAU-OAX-PBD-OAW
5	B	301	HXG	CAP-OAW-PBD-OAX
5	F	301	HXG	CAU-OAX-PBD-OAW
5	F	301	HXG	CAP-OAW-PBD-OAX
5	G	301	HXG	CAU-OAX-PBD-OAW
5	G	301	HXG	CAP-OAW-PBD-OAX
5	B	301	HXG	OAX-CAU-CBB-CAT

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Mol	Chain	Res	Type	Atoms
5	F	301	HXG	OAX-CAU-CBB-CAT
5	G	301	HXG	OAX-CAU-CBB-CAT
5	B	303	HXG	OAV-CAT-CBB-CAU
5	F	303	HXG	OAV-CAT-CBB-CAU
5	G	303	HXG	OAV-CAT-CBB-CAU
6	B	304	D10	C7-C8-C9-C10
6	F	304	D10	C7-C8-C9-C10
6	G	304	D10	C7-C8-C9-C10
5	C	302	HXG	OAX-CAU-CBB-CAT
5	H	303	HXG	OAX-CAU-CBB-CAT
5	I	302	HXG	OAX-CAU-CBB-CAT
7	B	306	6ER	C1-C01-C02-C03
7	C	304	6ER	C1-C01-C02-C03
7	I	304	6ER	C1-C01-C02-C03
5	B	302	HXG	CBB-CAU-OAX-PBD
5	F	302	HXG	CBB-CAU-OAX-PBD
5	G	302	HXG	CBB-CAU-OAX-PBD
5	B	302	HXG	OAV-CAT-CBB-CAU
5	F	302	HXG	OAV-CAT-CBB-CAU
5	G	302	HXG	OAV-CAT-CBB-CAU
5	C	302	HXG	OAX-CAU-CBB-OAY
5	H	303	HXG	OAX-CAU-CBB-OAY
5	I	302	HXG	OAX-CAU-CBB-OAY
5	B	301	HXG	CAT-CBB-OAY-CBA
5	F	301	HXG	CAT-CBB-OAY-CBA
5	G	301	HXG	CAT-CBB-OAY-CBA
5	C	303	HXG	OAV-CAT-CBB-CAU
5	H	304	HXG	OAV-CAT-CBB-CAU
5	I	303	HXG	OAV-CAT-CBB-CAU
5	C	303	HXG	CAA-CAJ-CAL-CAN
5	H	304	HXG	CAA-CAJ-CAL-CAN
5	I	303	HXG	CAA-CAJ-CAL-CAN
6	B	304	D10	C5-C6-C7-C8
6	F	304	D10	C5-C6-C7-C8
6	G	304	D10	C5-C6-C7-C8
5	B	302	HXG	CAU-OAX-PBD-OAH
5	C	303	HXG	CAU-OAX-PBD-OAH
5	H	304	HXG	CAU-OAX-PBD-OAH
5	I	303	HXG	CAU-OAX-PBD-OAH
5	F	302	HXG	CAU-OAX-PBD-OAH
5	G	302	HXG	CAU-OAX-PBD-OAH
5	B	302	HXG	CAS-CAP-OAW-PBD

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Mol	Chain	Res	Type	Atoms
5	C	302	HXG	CAS-CAP-OAW-PBD
5	H	303	HXG	CAS-CAP-OAW-PBD
5	I	302	HXG	CAS-CAP-OAW-PBD
5	F	302	HXG	CAS-CAP-OAW-PBD
5	G	302	HXG	CAS-CAP-OAW-PBD
7	B	306	6ER	C17-C16-O15-P12
7	C	304	6ER	C17-C16-O15-P12
7	I	304	6ER	C17-C16-O15-P12
5	H	304	HXG	CAB-CAK-CAM-CAO
5	C	303	HXG	CAB-CAK-CAM-CAO
5	I	303	HXG	CAB-CAK-CAM-CAO
5	B	302	HXG	OAV-CAT-CBB-OAY
5	F	302	HXG	OAV-CAT-CBB-OAY
5	G	302	HXG	OAV-CAT-CBB-OAY
7	B	306	6ER	O07-C08-C09-O22
7	C	304	6ER	O07-C08-C09-O22
7	I	304	6ER	O07-C08-C09-O22
5	I	302	HXG	CAO-CAR-CBA-OAY
7	B	306	6ER	C08-C09-O22-C23
7	C	304	6ER	C08-C09-O22-C23
7	I	304	6ER	C08-C09-O22-C23
6	F	304	D10	C6-C7-C8-C9
6	G	304	D10	C6-C7-C8-C9
5	C	302	HXG	CAO-CAR-CBA-OAY
5	H	303	HXG	CAO-CAR-CBA-OAY
6	B	304	D10	C6-C7-C8-C9
5	B	301	HXG	OAX-CAU-CBB-OAY
5	F	301	HXG	OAX-CAU-CBB-OAY
5	G	301	HXG	OAX-CAU-CBB-OAY
5	G	303	HXG	CAB-CAK-CAM-CAO
5	B	303	HXG	CAB-CAK-CAM-CAO
5	F	303	HXG	CAB-CAK-CAM-CAO
5	B	303	HXG	OAX-CAU-CBB-OAY
5	F	303	HXG	OAX-CAU-CBB-OAY
5	G	303	HXG	OAX-CAU-CBB-OAY
6	B	304	D10	C4-C5-C6-C7
6	F	304	D10	C4-C5-C6-C7
6	G	304	D10	C4-C5-C6-C7
7	B	306	6ER	O07-C08-C09-C10
7	C	304	6ER	O07-C08-C09-C10
7	I	304	6ER	O07-C08-C09-C10
6	C	305	D10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	H	301	D10	C5-C6-C7-C8
6	I	305	D10	C5-C6-C7-C8
5	F	301	HXG	OAV-CAT-CBB-OAY
5	B	303	HXG	CAO-CAR-CBA-OAY
5	F	303	HXG	CAO-CAR-CBA-OAY
5	G	303	HXG	CAO-CAR-CBA-OAY
5	G	302	HXG	CAA-CAJ-CAL-CAN
5	B	302	HXG	CAA-CAJ-CAL-CAN
5	F	302	HXG	CAA-CAJ-CAL-CAN
5	B	302	HXG	OAG-CBA-OAY-CBB
5	F	302	HXG	OAG-CBA-OAY-CBB
5	G	302	HXG	OAG-CBA-OAY-CBB
7	B	306	6ER	O22-C23-C25-C26
7	C	304	6ER	O22-C23-C25-C26
7	I	304	6ER	O22-C23-C25-C26
5	B	303	HXG	OAX-CAU-CBB-CAT
5	F	303	HXG	OAX-CAU-CBB-CAT
5	G	303	HXG	OAX-CAU-CBB-CAT
5	B	301	HXG	OAV-CAT-CBB-OAY
5	G	301	HXG	OAV-CAT-CBB-OAY
5	B	302	HXG	CAR-CBA-OAY-CBB
5	F	302	HXG	CAR-CBA-OAY-CBB
5	G	302	HXG	CAR-CBA-OAY-CBB
5	B	303	HXG	CAO-CAR-CBA-OAG
5	F	303	HXG	CAO-CAR-CBA-OAG
5	G	303	HXG	CAO-CAR-CBA-OAG
6	G	304	D10	C2-C3-C4-C5
6	B	304	D10	C2-C3-C4-C5
6	F	304	D10	C2-C3-C4-C5
7	C	304	6ER	O24-C23-C25-C26
7	I	304	6ER	O24-C23-C25-C26
7	B	306	6ER	O24-C23-C25-C26
5	B	301	HXG	CAU-OAX-PBD-OAH
5	B	301	HXG	CAP-OAW-PBD-OAI
5	C	303	HXG	CAP-OAW-PBD-OAI
5	H	304	HXG	CAP-OAW-PBD-OAI
5	I	303	HXG	CAP-OAW-PBD-OAI
5	F	301	HXG	CAU-OAX-PBD-OAH
5	F	301	HXG	CAP-OAW-PBD-OAI
5	G	301	HXG	CAU-OAX-PBD-OAH
5	G	301	HXG	CAP-OAW-PBD-OAI
7	B	306	6ER	C10-C09-O22-C23

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Mol	Chain	Res	Type	Atoms
7	C	304	6ER	C10-C09-O22-C23
7	I	304	6ER	C10-C09-O22-C23
5	B	302	HXG	CAO-CAR-CBA-OAY
5	F	302	HXG	CAO-CAR-CBA-OAY
5	G	302	HXG	CAO-CAR-CBA-OAY
5	H	303	HXG	CAK-CAM-CAO-CAR
5	C	302	HXG	CAK-CAM-CAO-CAR
5	I	302	HXG	CAK-CAM-CAO-CAR

There are no ring outliers.

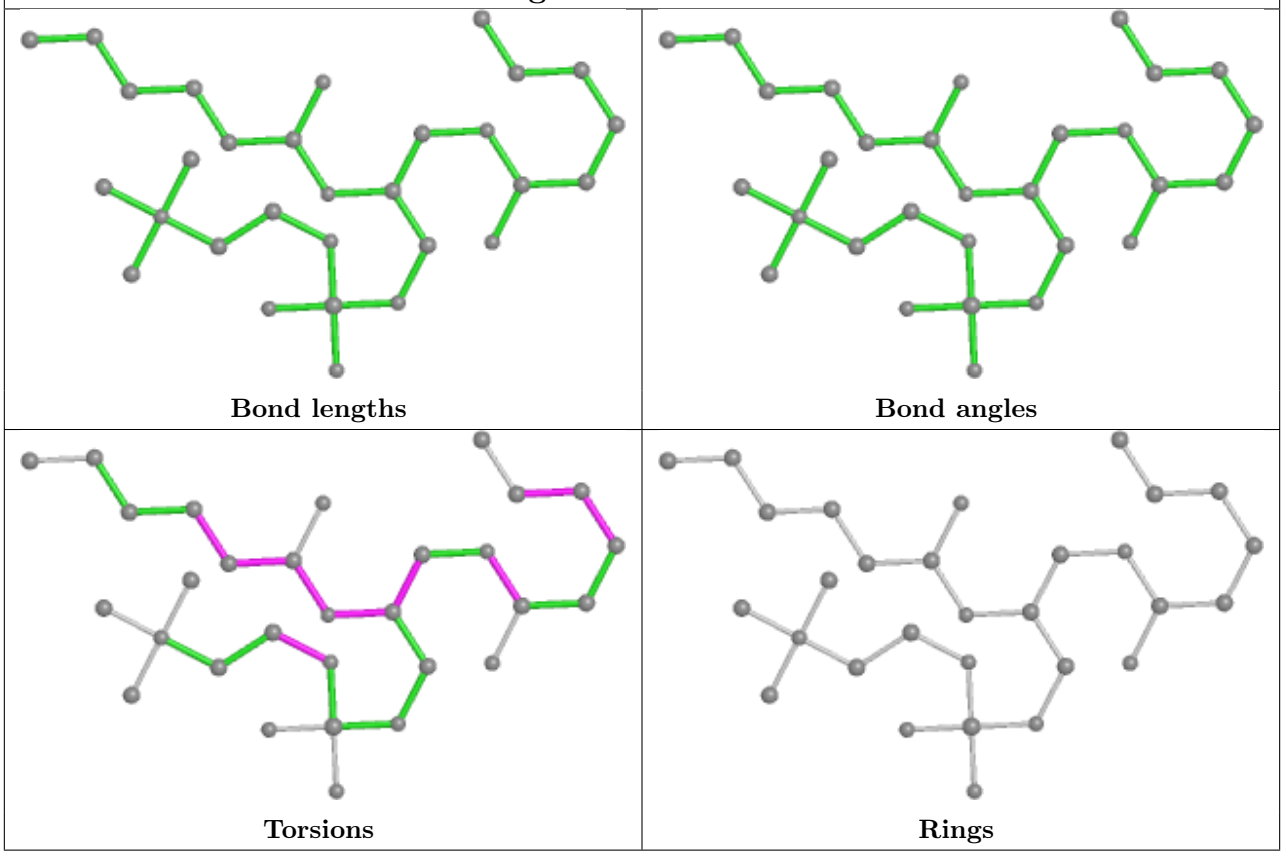
17 monomers are involved in 155 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	306	6ER	8	0
5	B	302	HXG	3	0
6	H	301	D10	4	0
6	C	305	D10	4	0
6	G	304	D10	1	0
5	H	304	HXG	1	0
6	I	305	D10	4	0
5	F	302	HXG	3	0
5	F	303	HXG	42	0
7	C	304	6ER	7	0
5	I	303	HXG	1	0
6	F	304	D10	1	0
6	B	304	D10	1	0
5	B	303	HXG	39	0
7	I	304	6ER	8	0
5	G	302	HXG	3	0
5	G	303	HXG	40	0

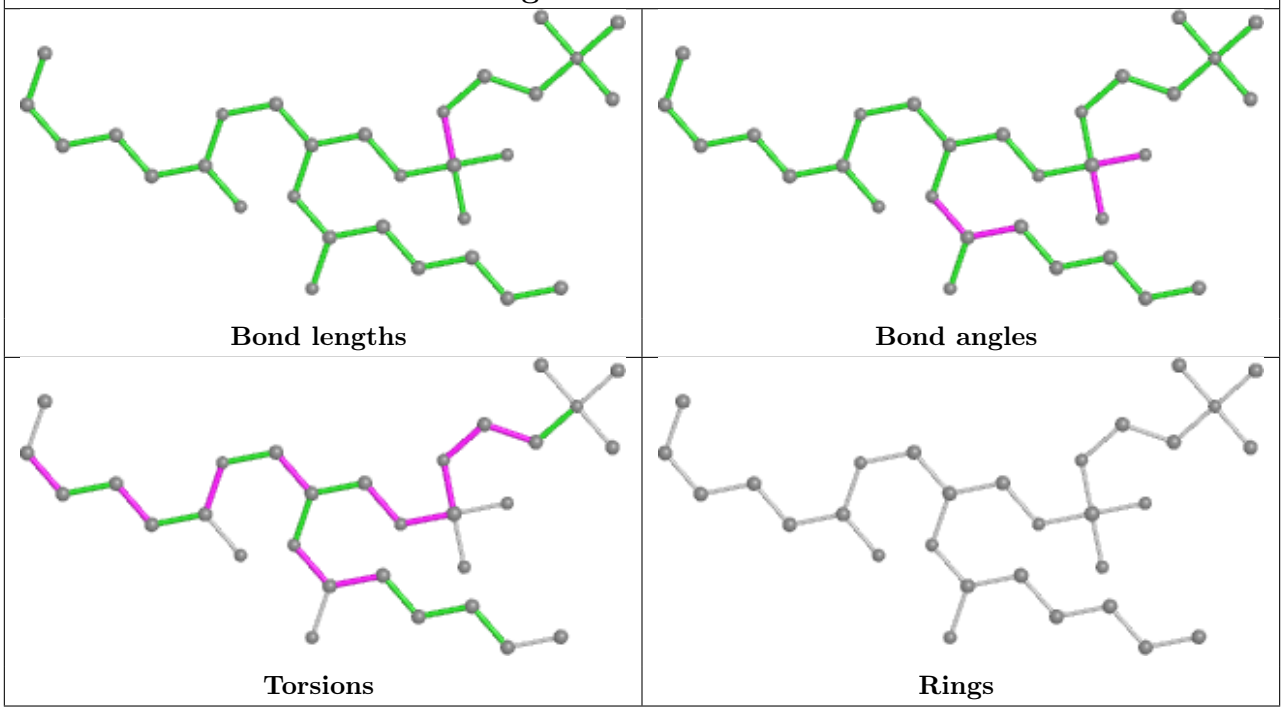
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

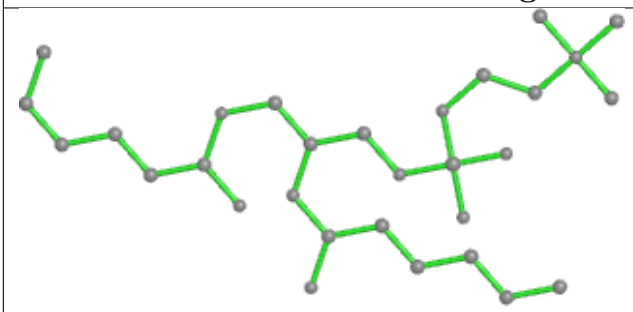
Ligand 6ER B 306



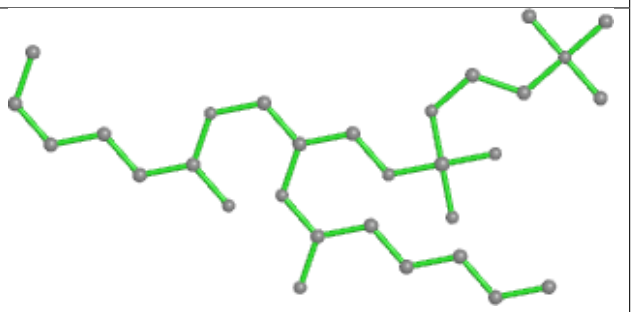
Ligand HXG B 302



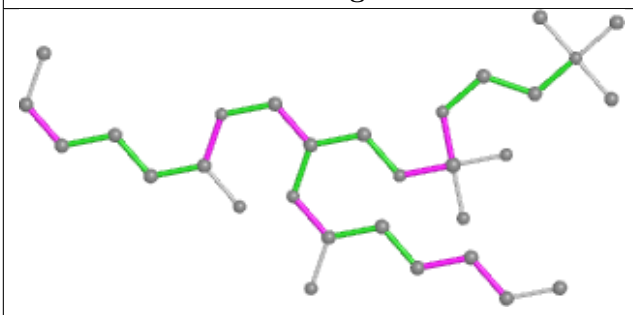
Ligand HXG H 304



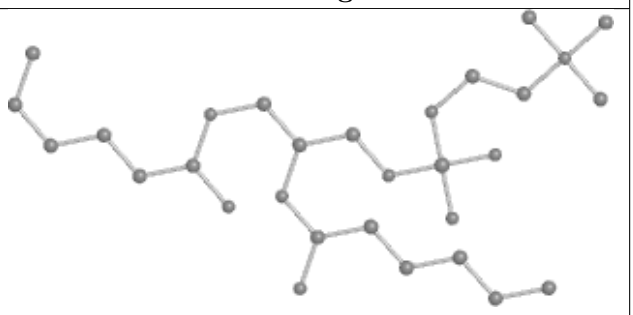
Bond lengths



Bond angles

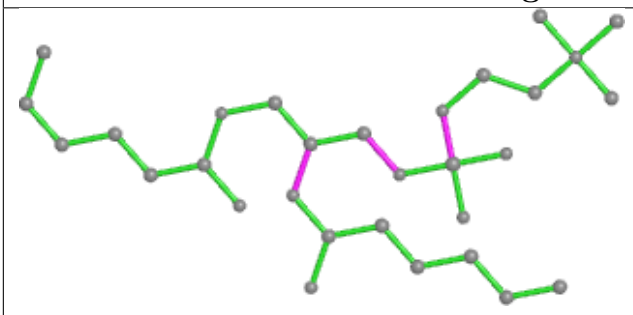


Torsions

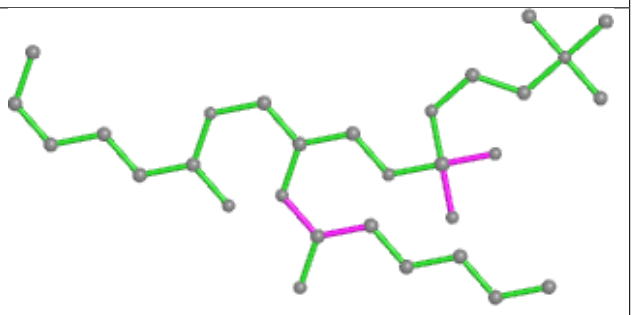


Rings

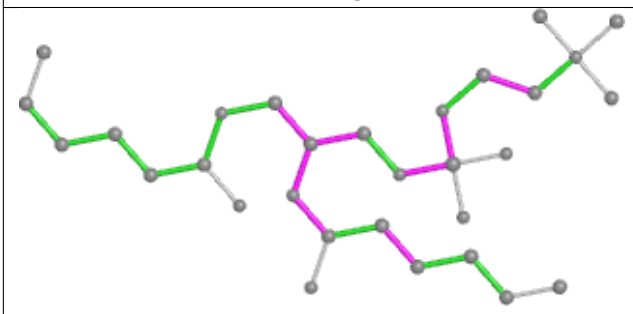
Ligand HXG F 301



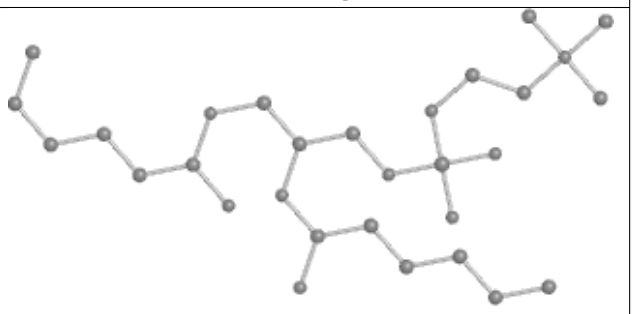
Bond lengths



Bond angles

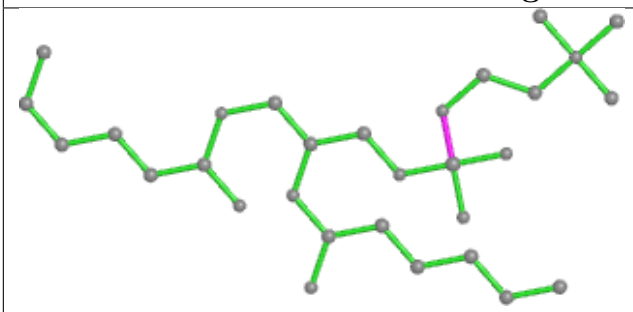


Torsions

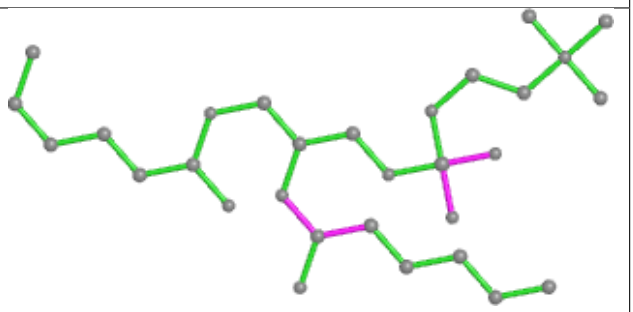


Rings

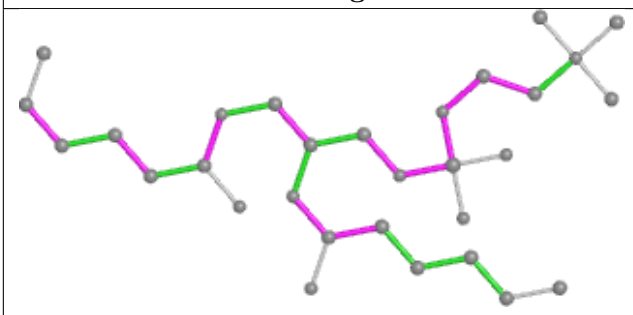
Ligand HXG F 302



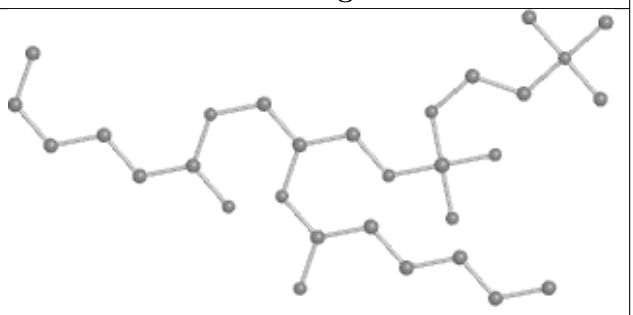
Bond lengths



Bond angles

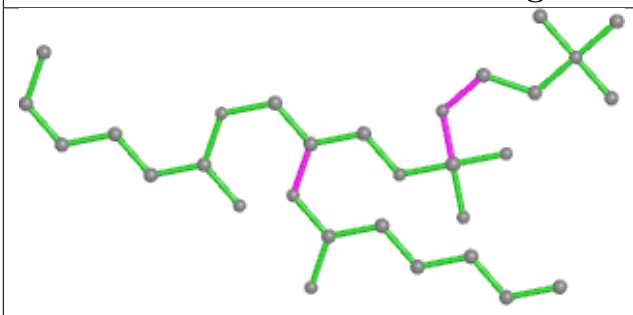


Torsions

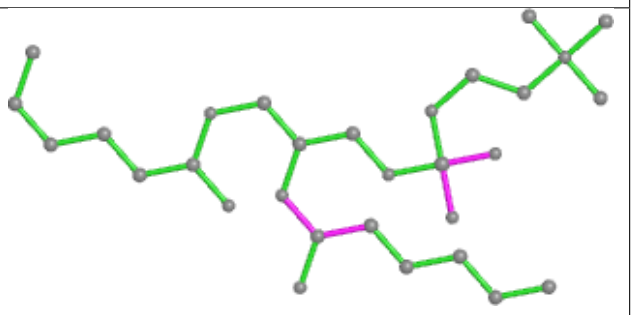


Rings

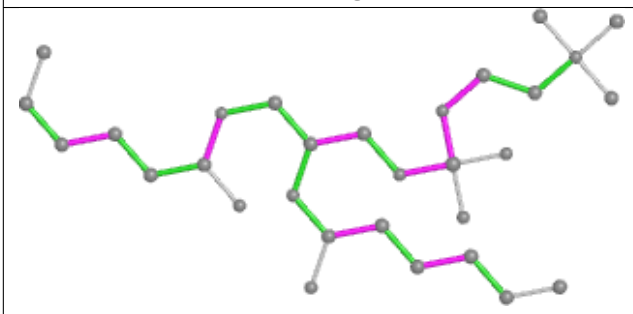
Ligand HXG I 302



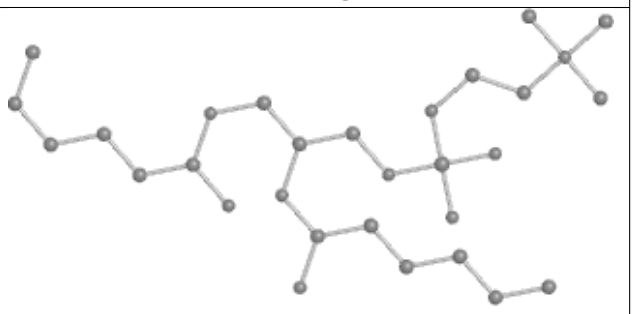
Bond lengths



Bond angles

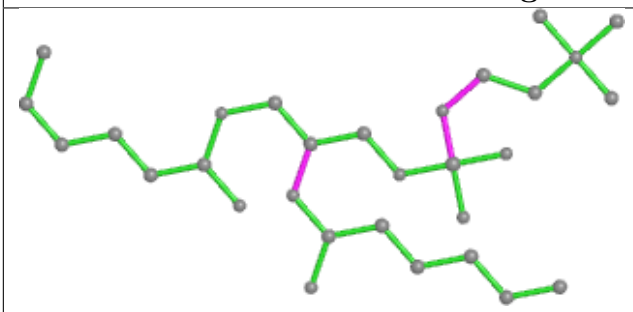


Torsions



Rings

Ligand HXG C 302



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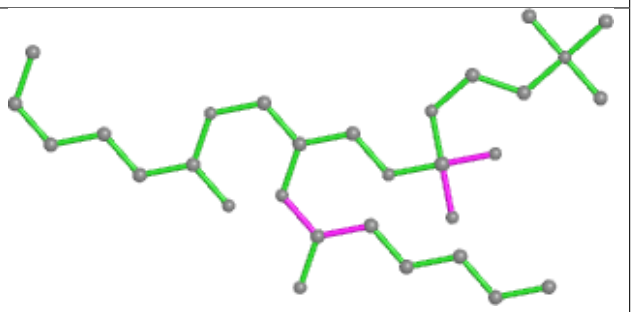

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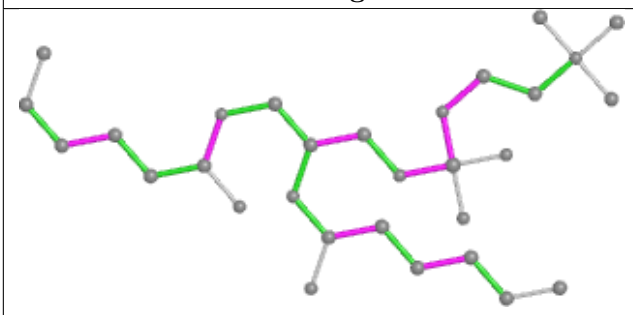
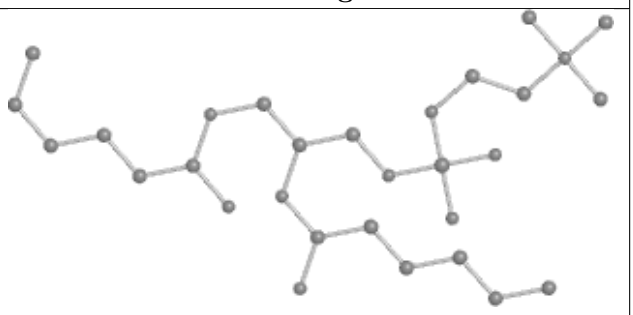
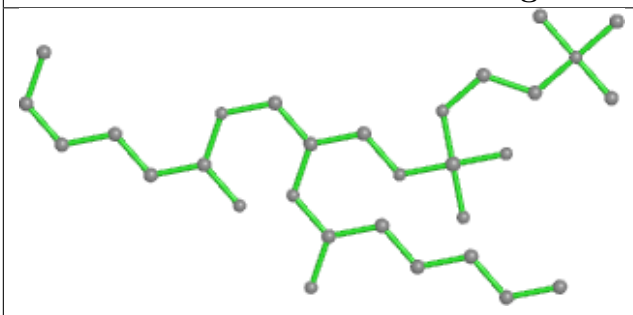


Torsions



Rings

Ligand HXG C 303



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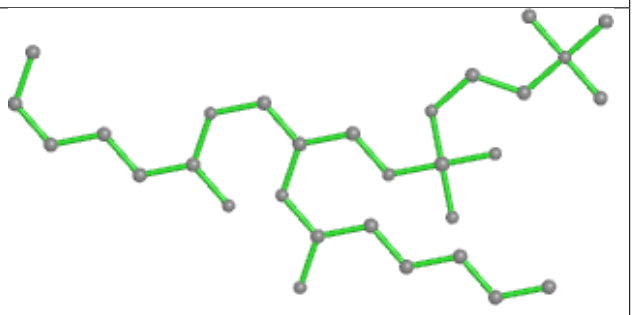
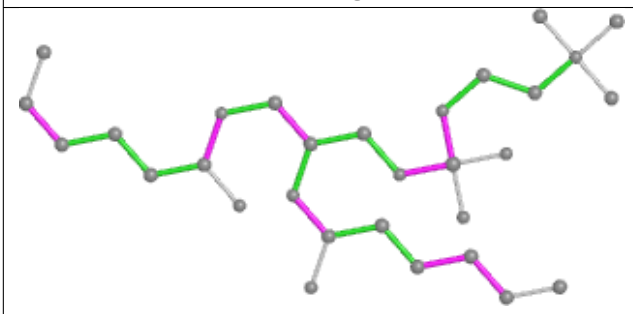


Bond angles



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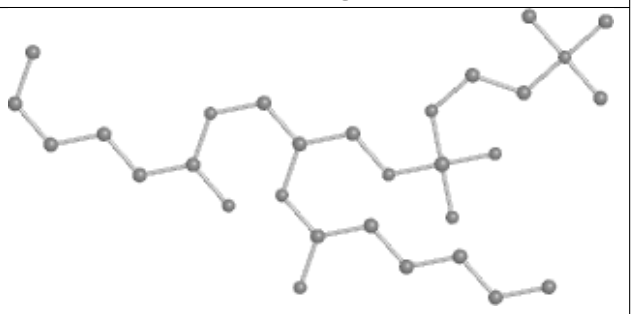
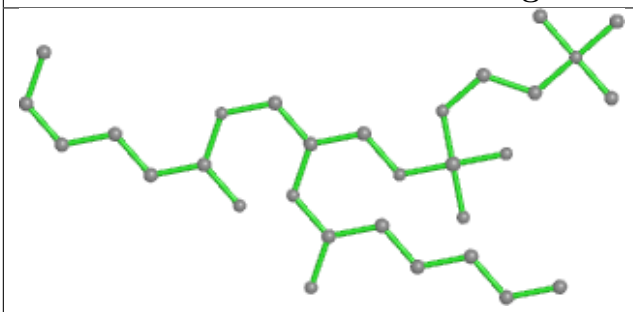
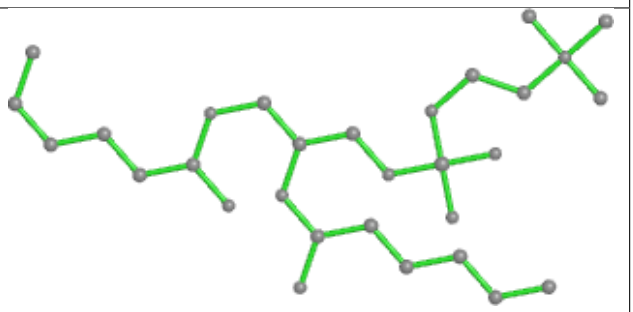


Rings

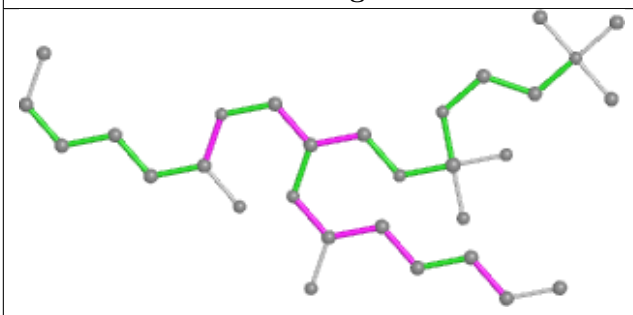
Ligand HXG F 303



Bond lengths



Bond angles



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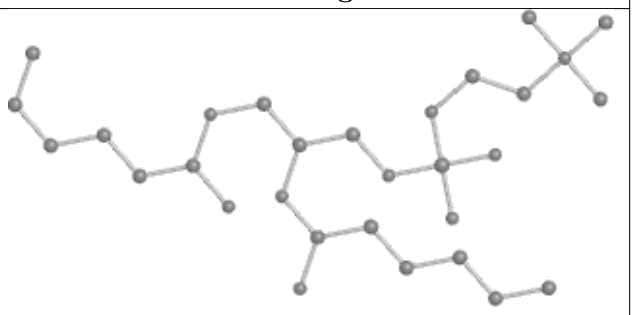
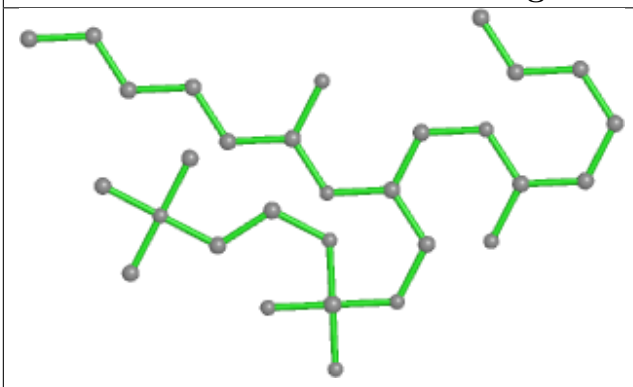
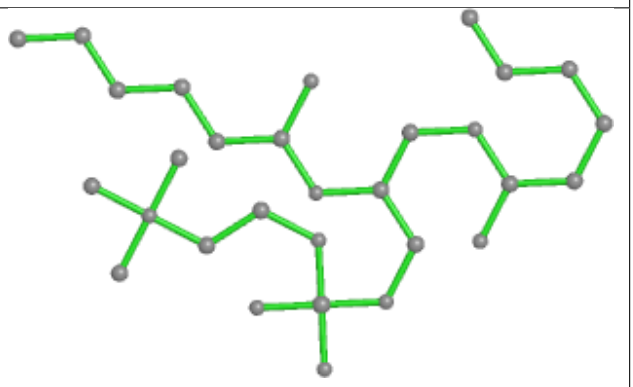


Rings

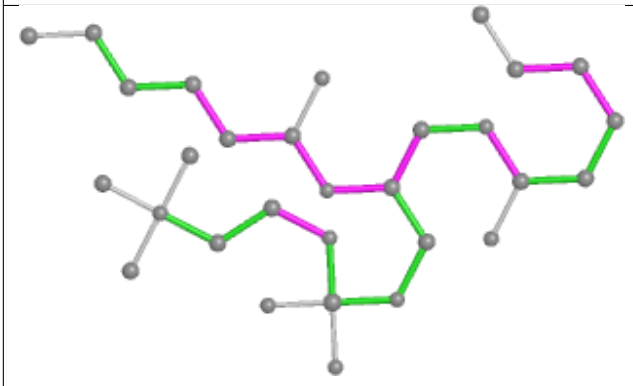
Ligand 6ER C 304



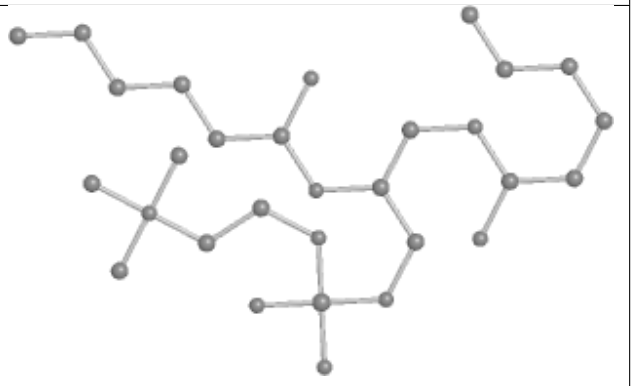
Bond lengths



Bond angles

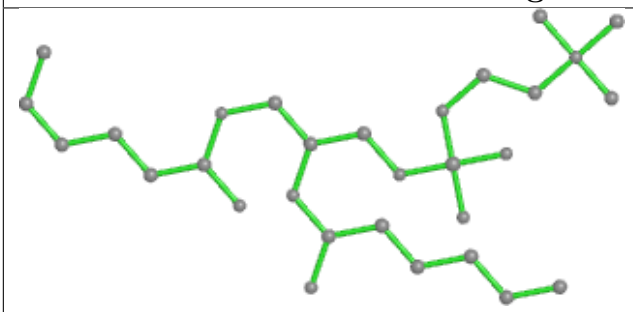


Torsions

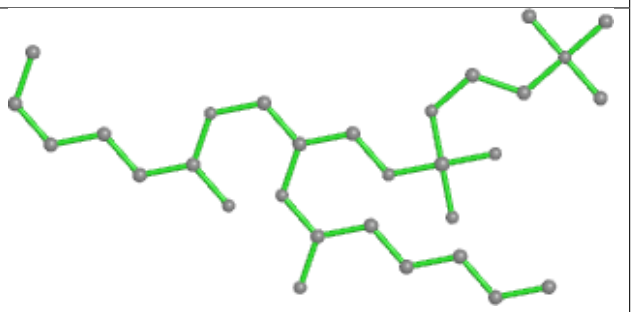


Rings

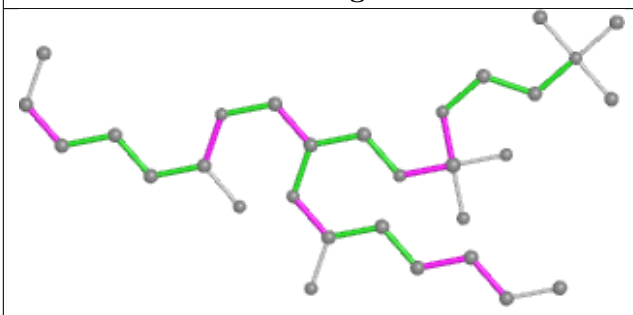
Ligand HXG I 303



Bond lengths



Bond angles



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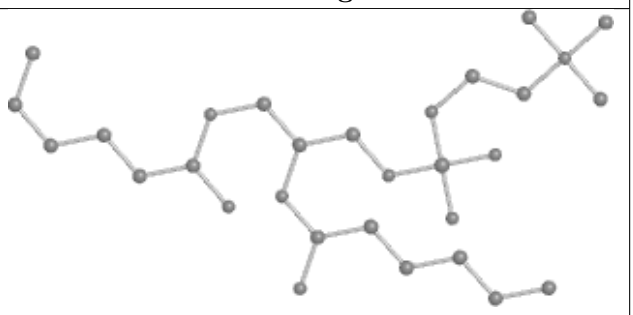
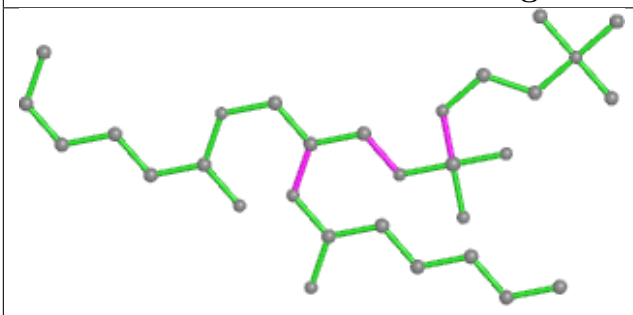


Rings

Ligand HXG B 301



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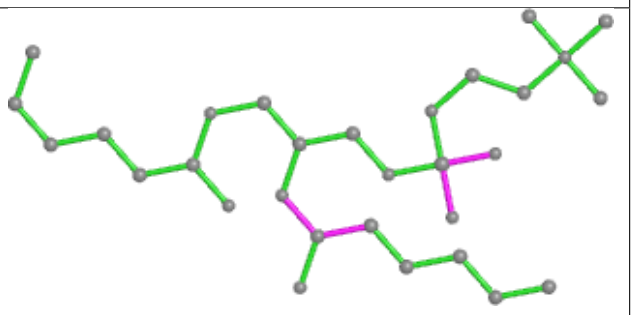
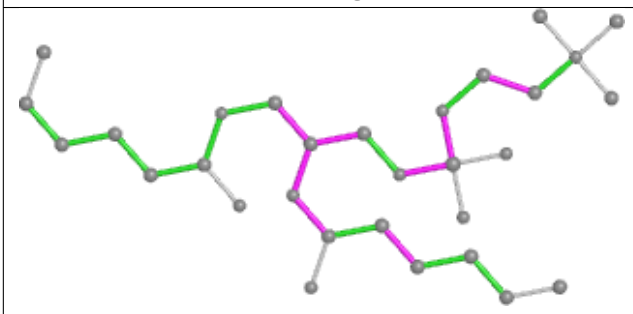


Bond angles



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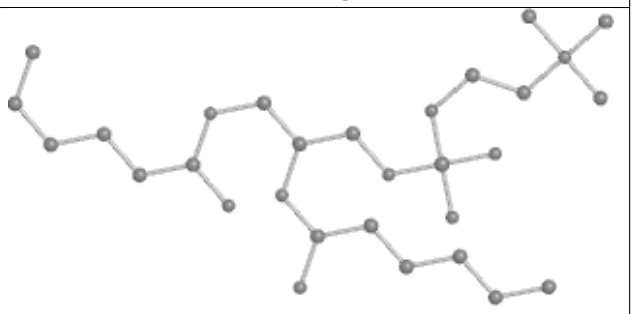
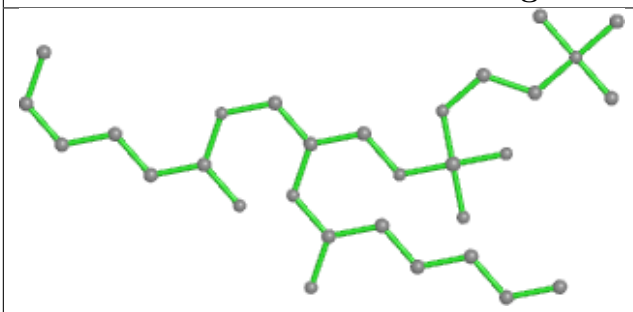


Rings

Ligand HXG B 303



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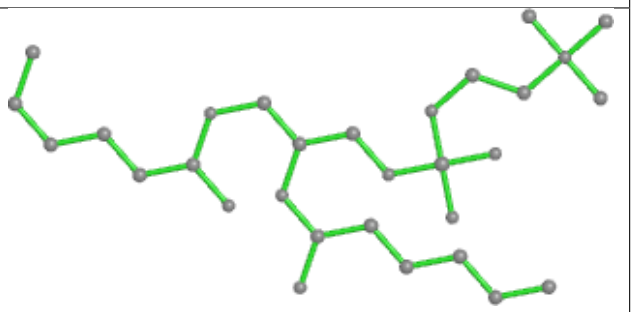
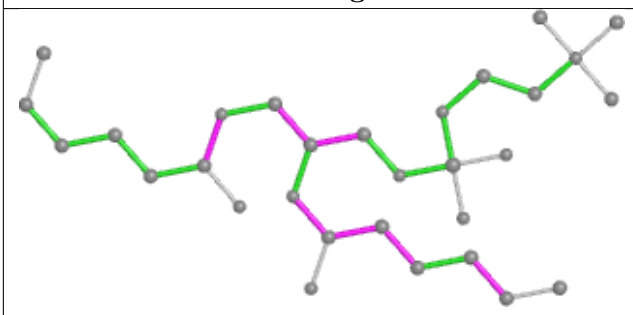
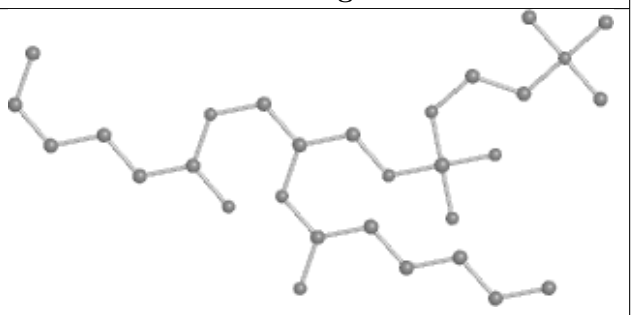


Bond angles

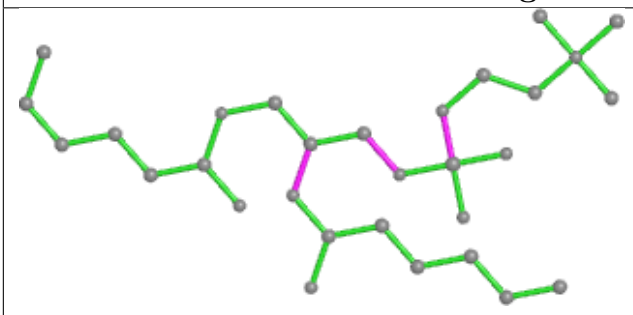


Torsions

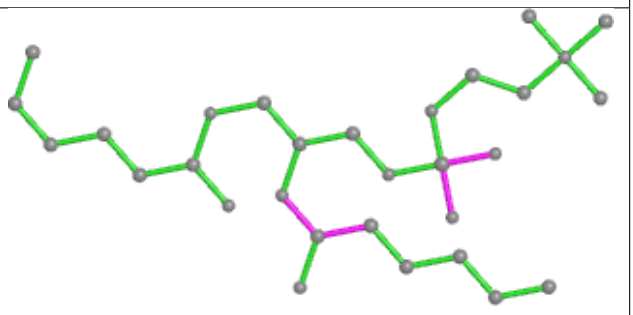


Rings

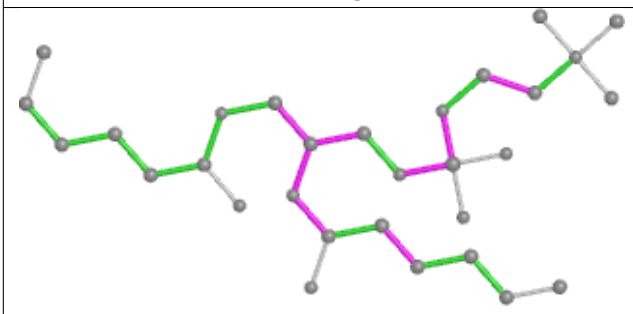
Ligand HXG G 301



Bond lengths



Bond angles



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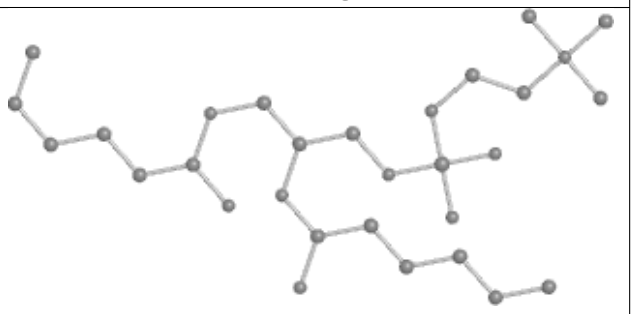
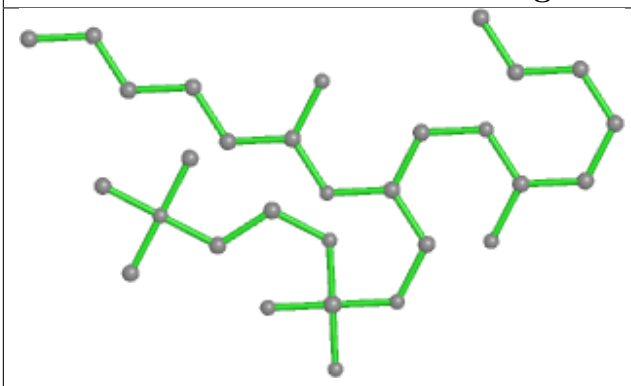
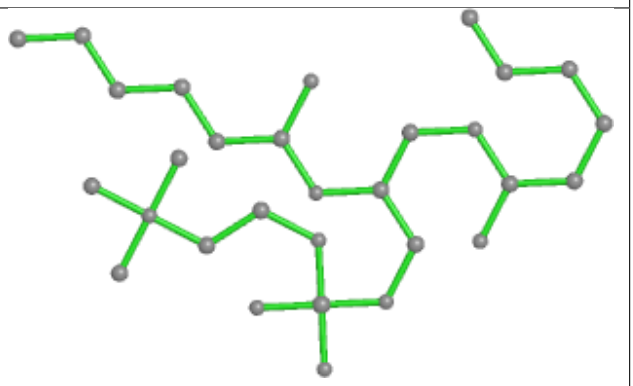


Rings

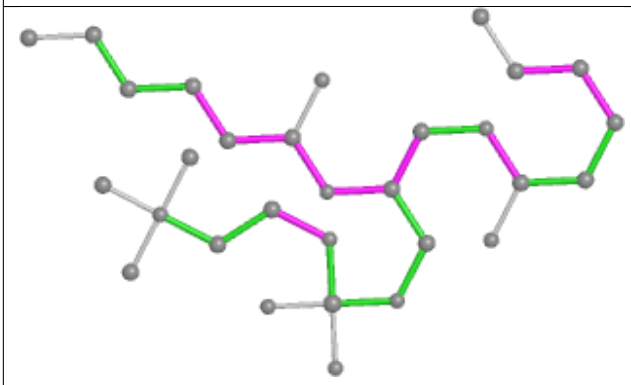
Ligand 6ER I 304



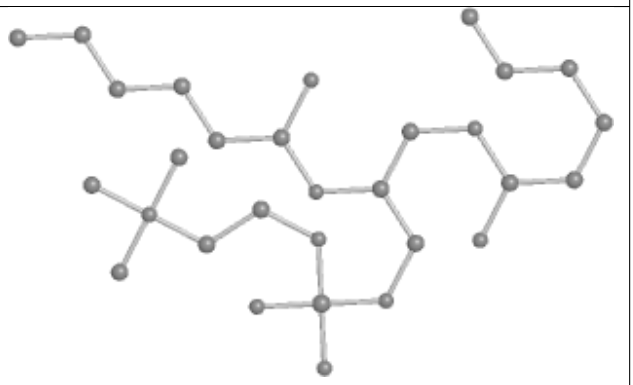
Bond lengths



Bond angles

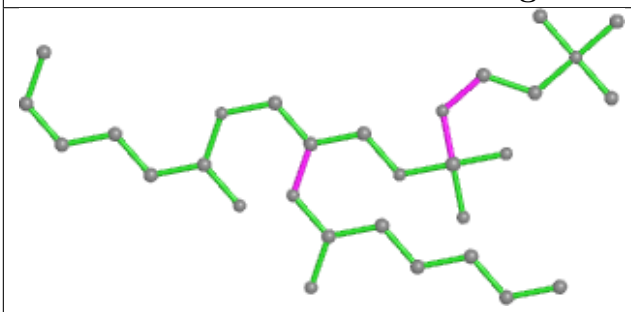


Torsions

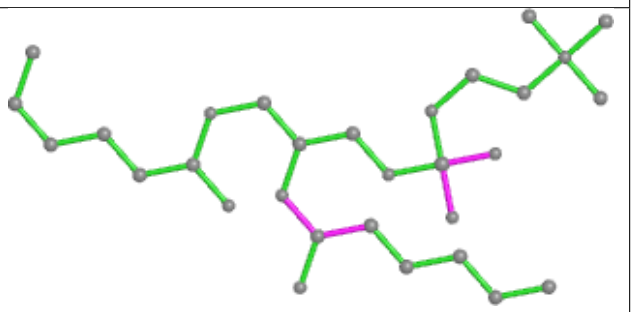


Rings

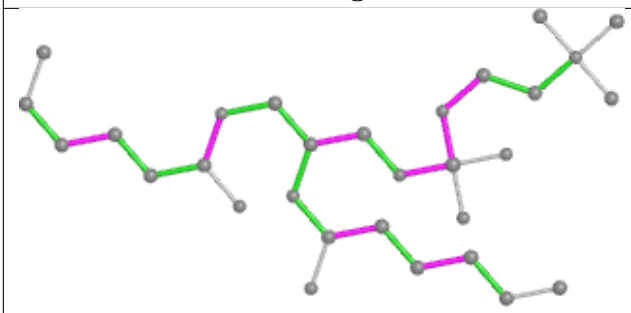
Ligand HXG H 303



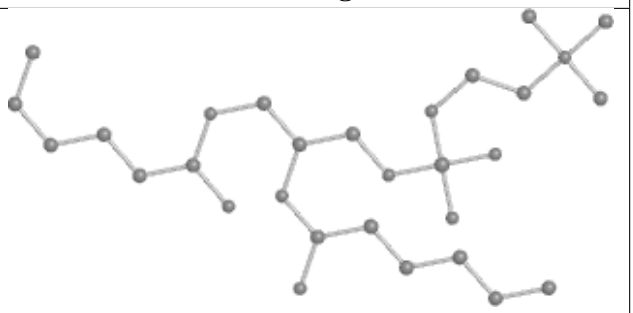
Bond lengths



Bond angles

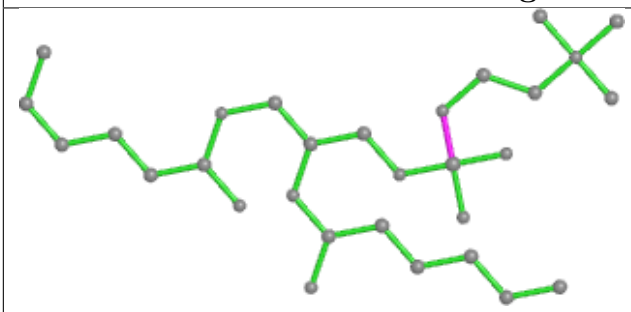


Torsions

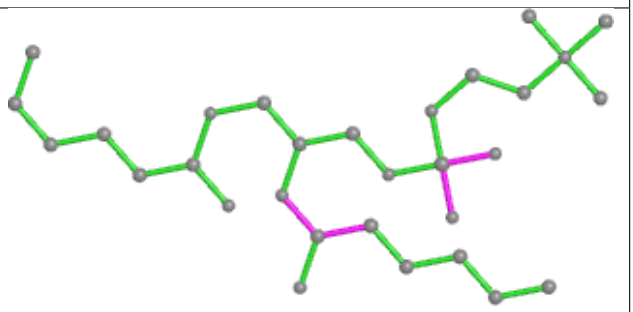


Rings

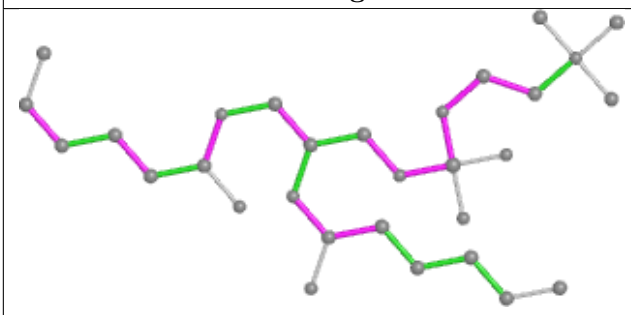
Ligand HXG G 302



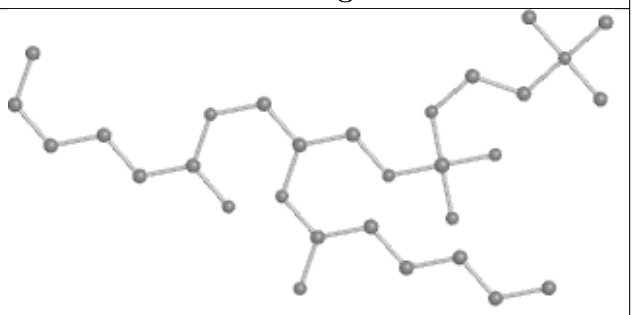
Bond lengths



Bond angles

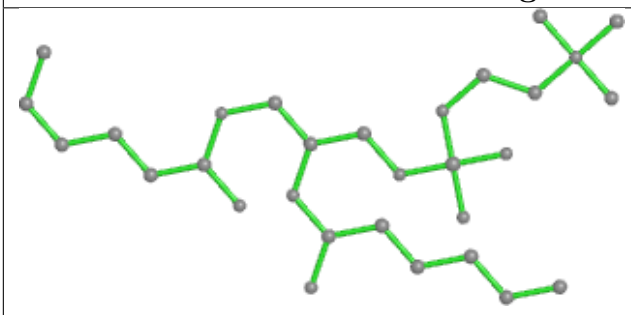


Torsions

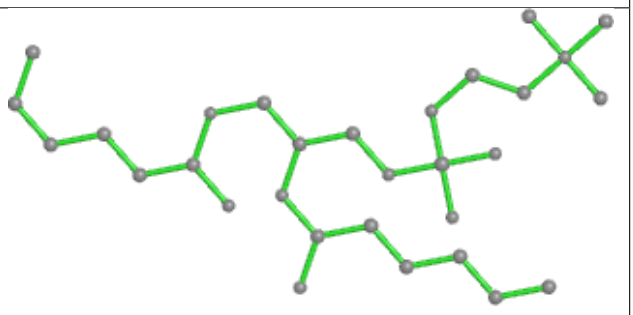


Rings

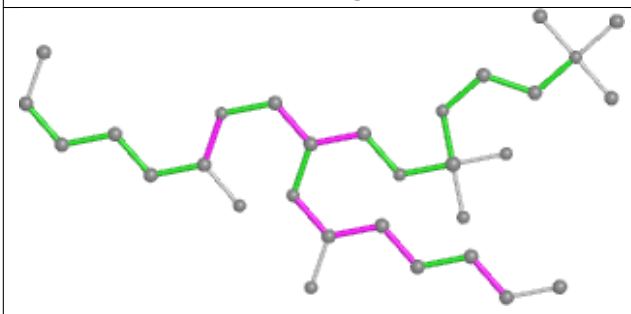
Ligand HXG G 303



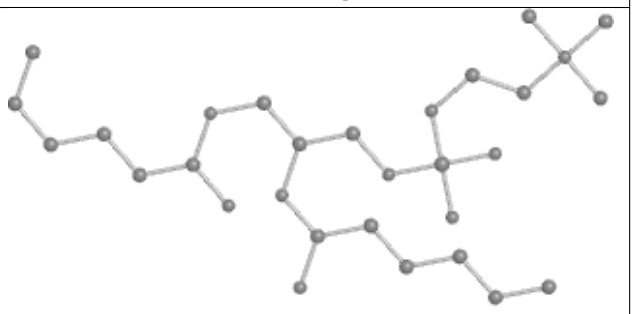
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

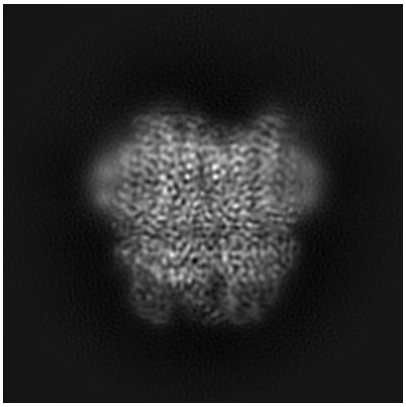
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24830. These allow visual inspection of the internal detail of the map and identification of artifacts.

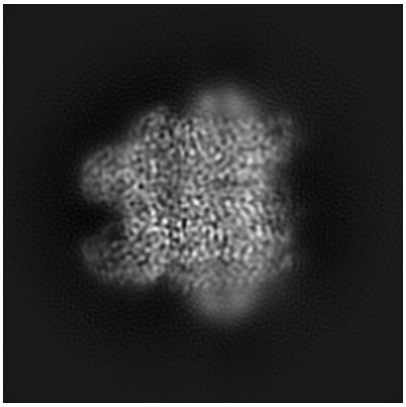
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

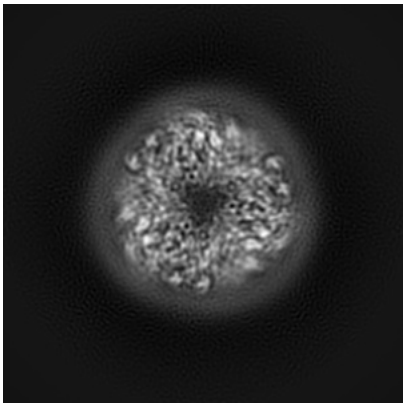
6.1.1 Primary map



X



Y

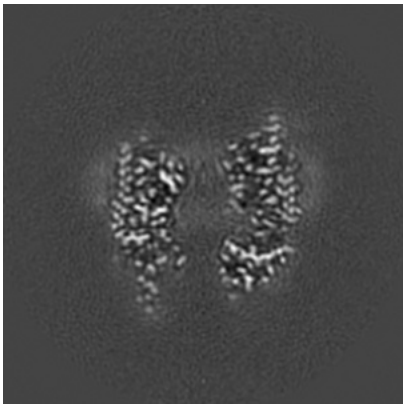


Z

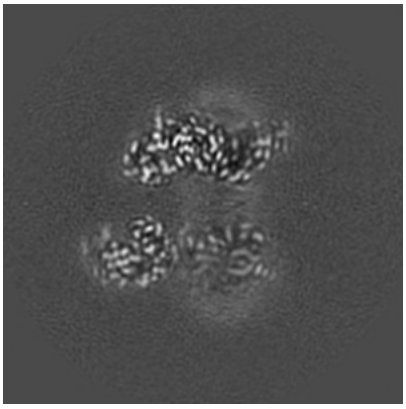
The images above show the map projected in three orthogonal directions.

6.2 Central slices

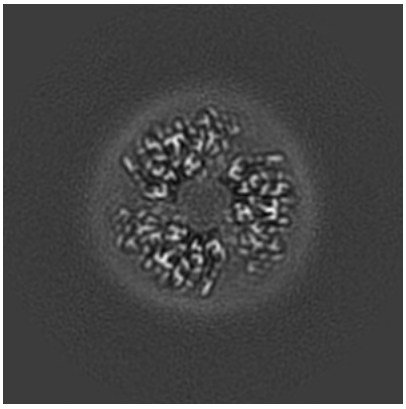
6.2.1 Primary map



X Index: 192



Y Index: 192

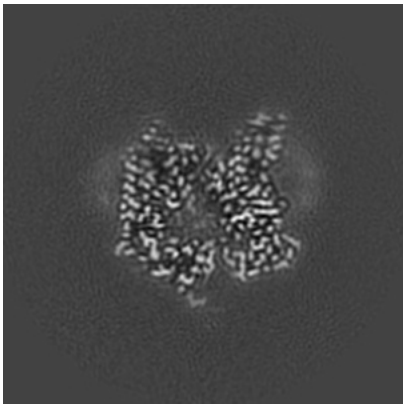


Z Index: 192

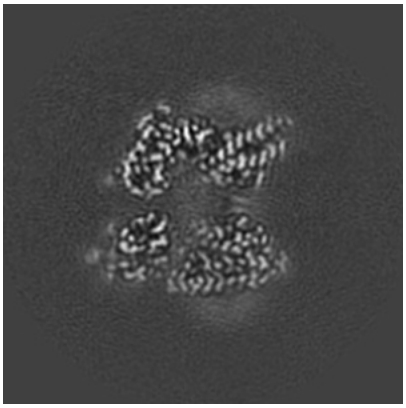
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

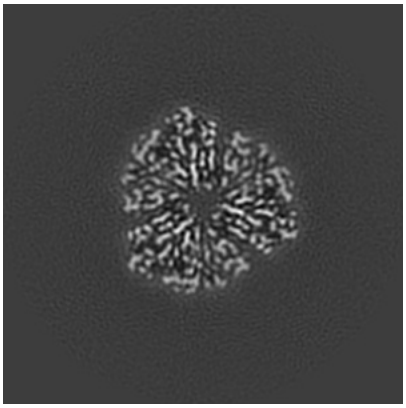
6.3.1 Primary map



X Index: 166



Y Index: 178

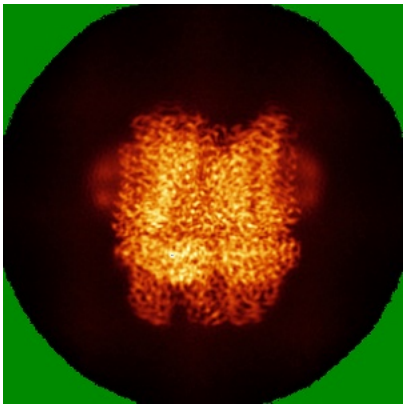


Z Index: 144

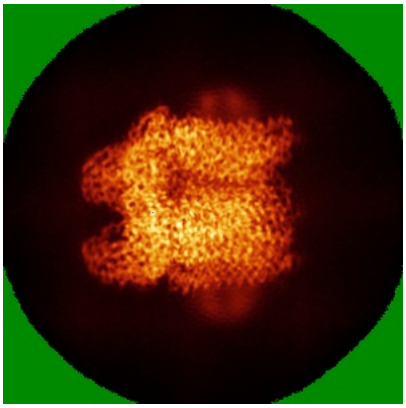
The images above show the largest variance slices of the map in three orthogonal directions.

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

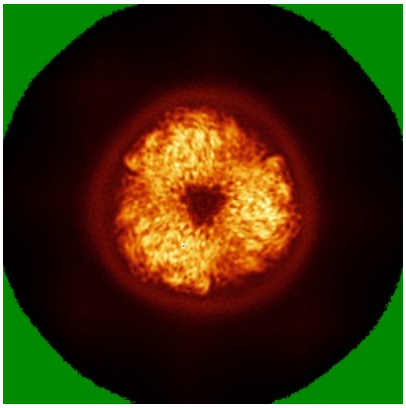
6.4.1 Primary map



X



Y

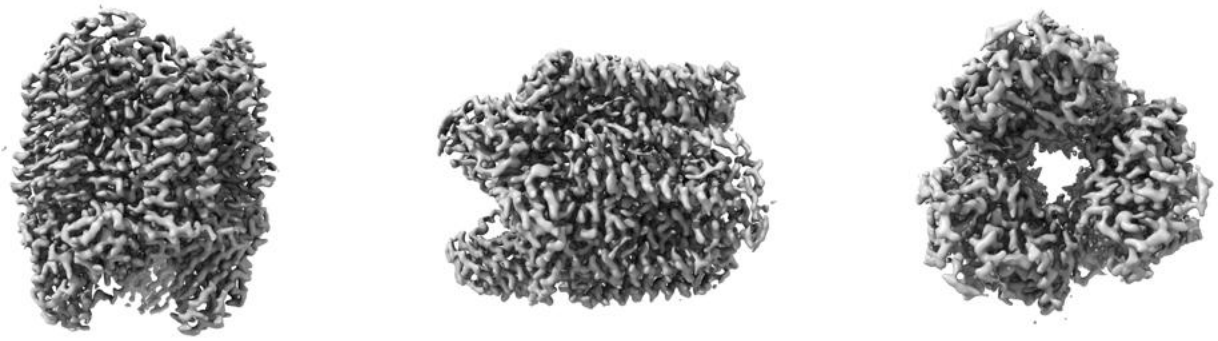


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0272. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

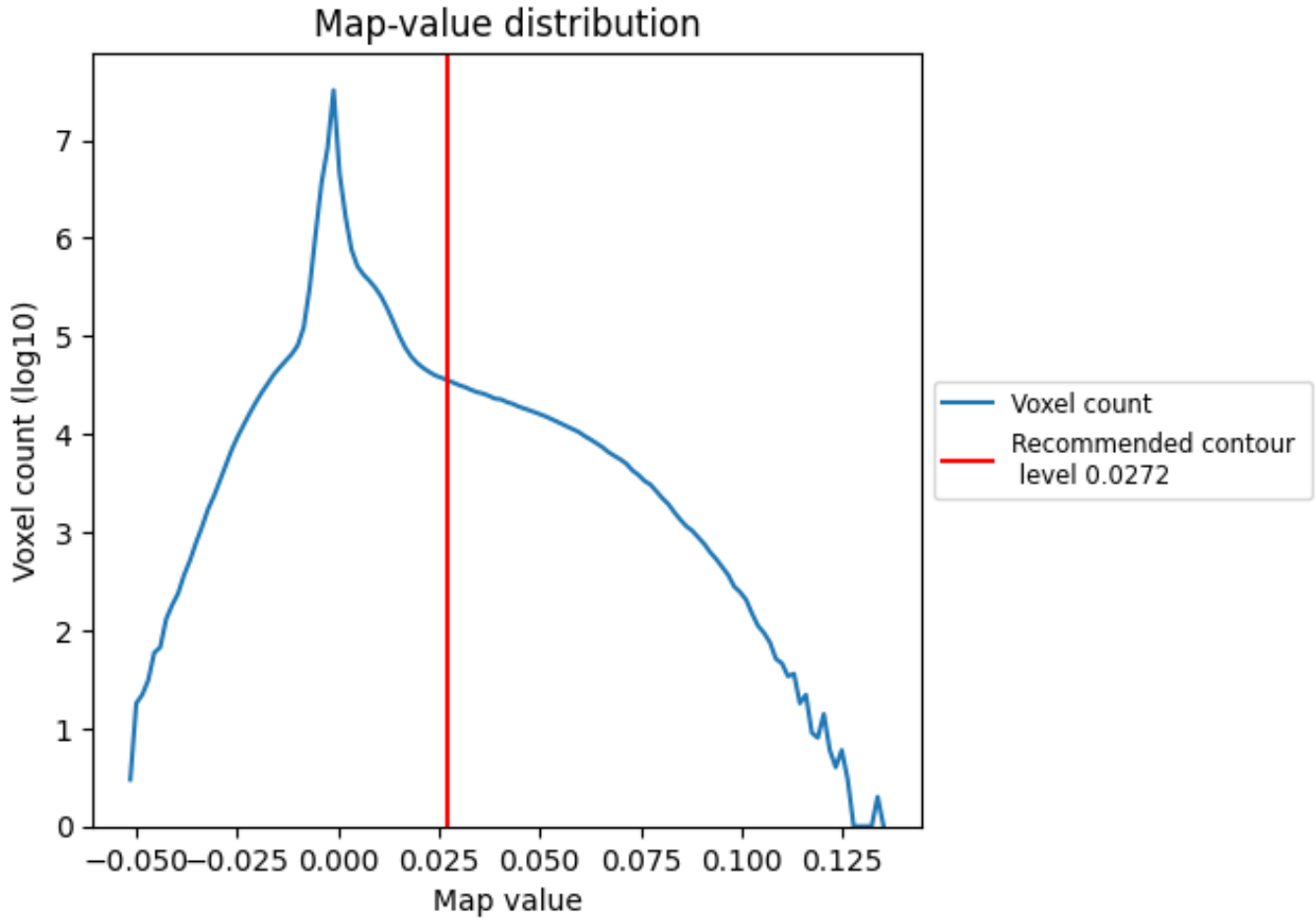
6.6 Mask visualisation (i)

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

7 Map analysis

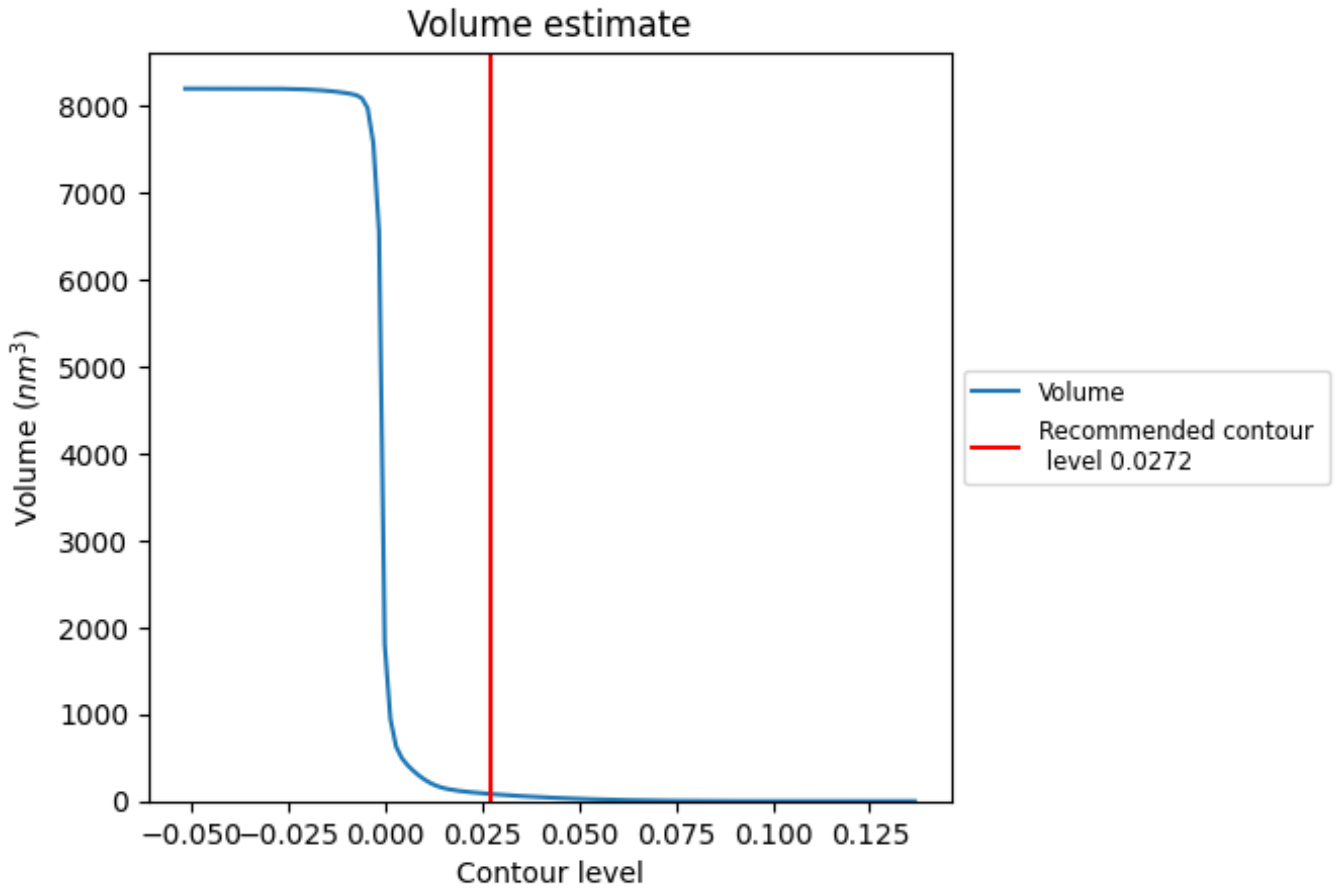
This section contains the results of statistical analysis of the map.

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.

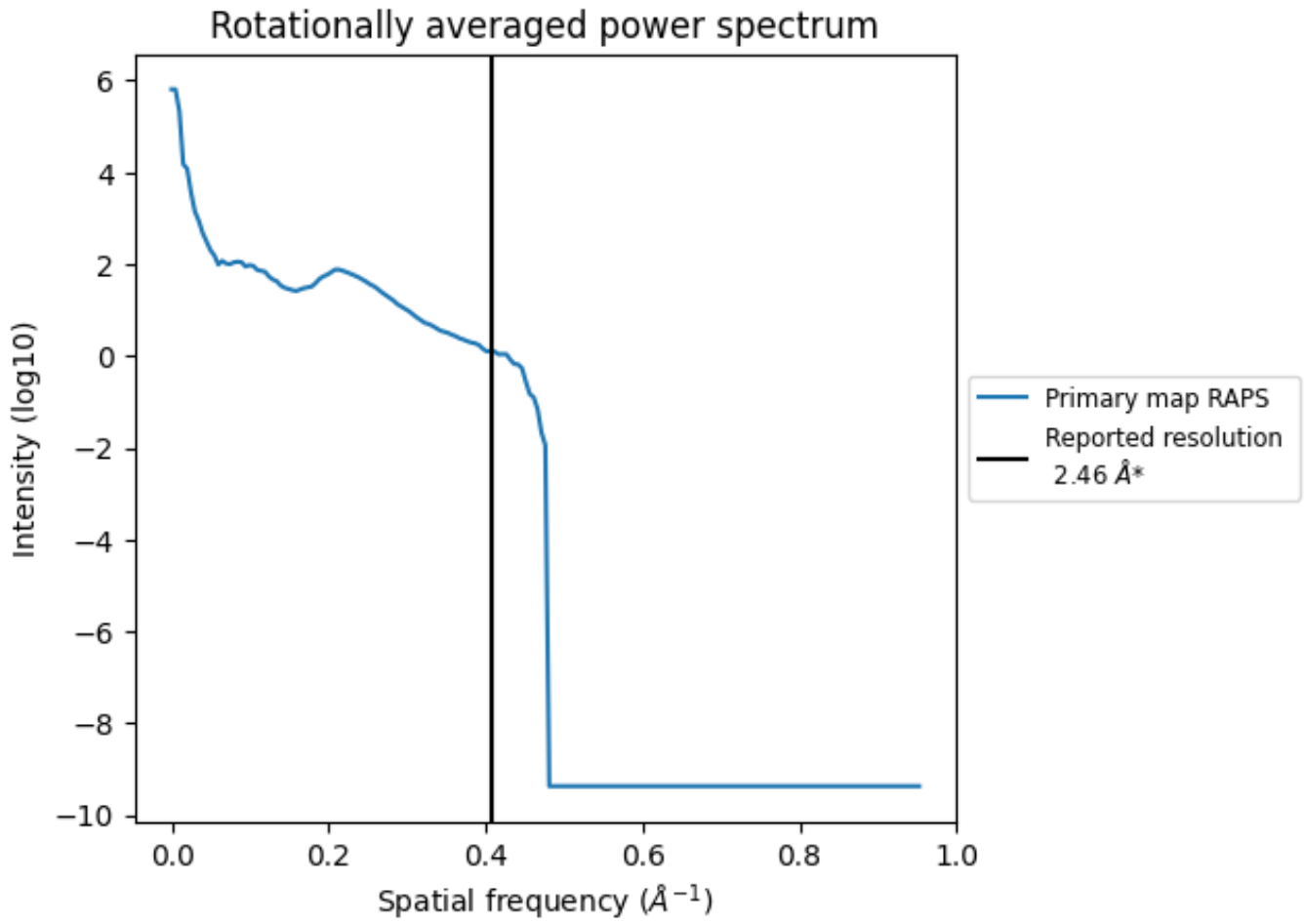
7.2 Volume estimate



The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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)

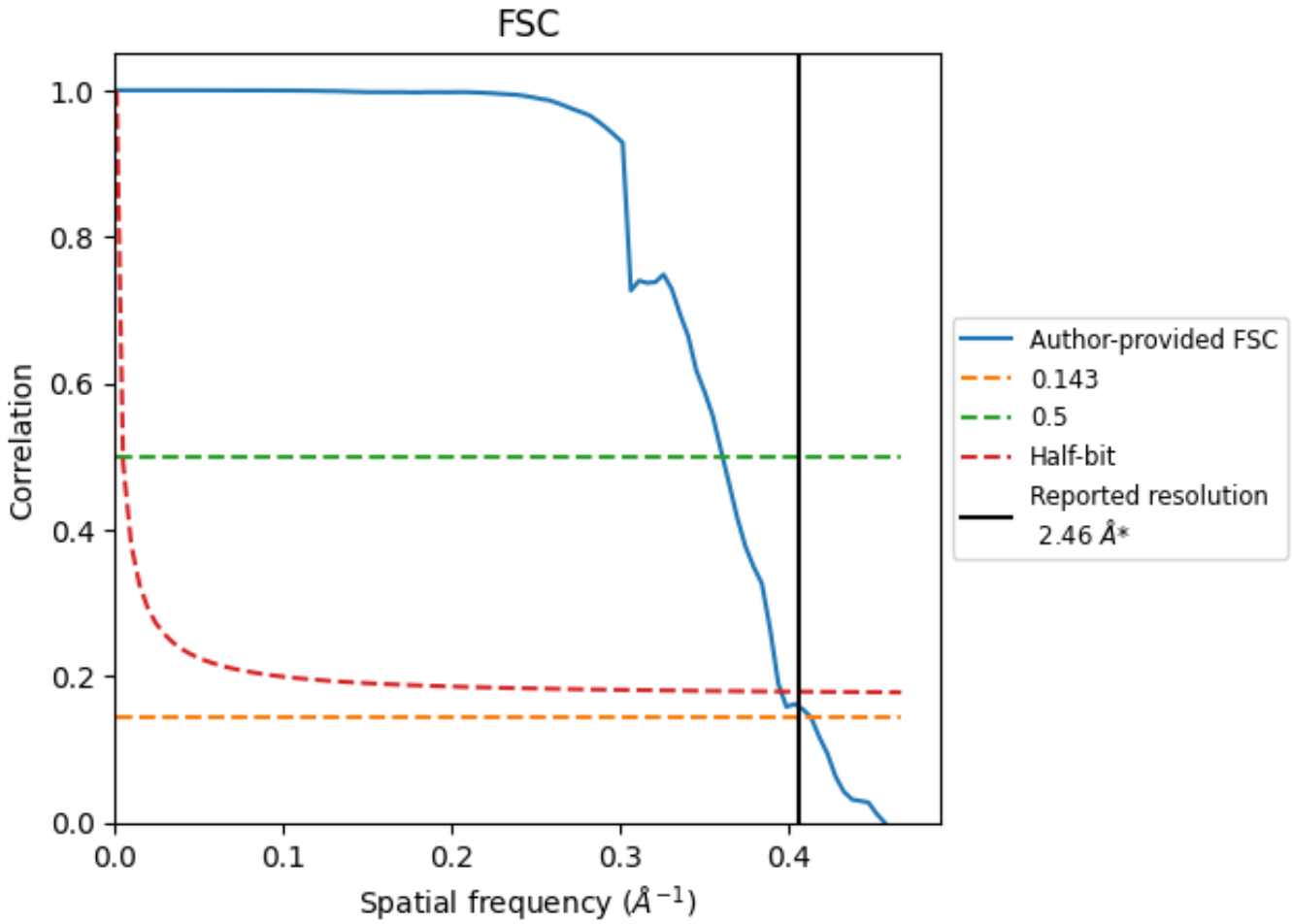


*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

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 0.407 Å^{-1}

8.2 Resolution estimates (i)

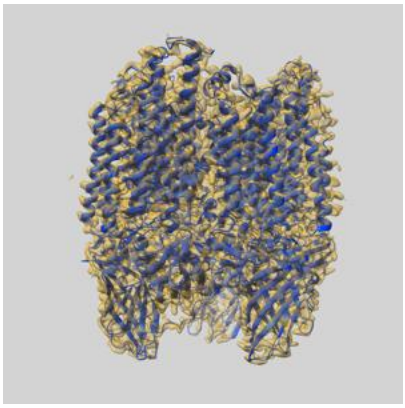
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	2.42	2.77	2.53
Unmasked-calculated*	-	-	-

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

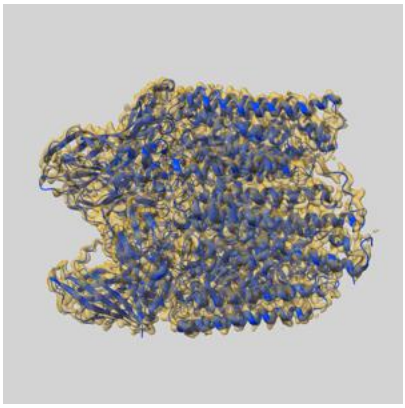
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24830 and PDB model 7S4L. Per-residue inclusion information can be found in section 3 on page 9.

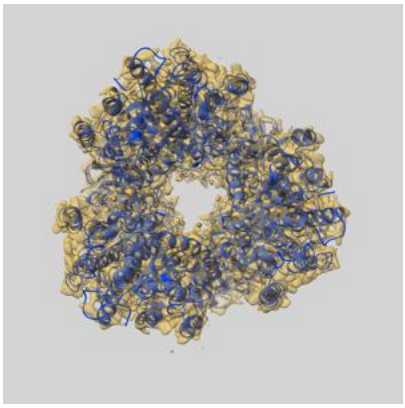
9.1 Map-model overlay



X



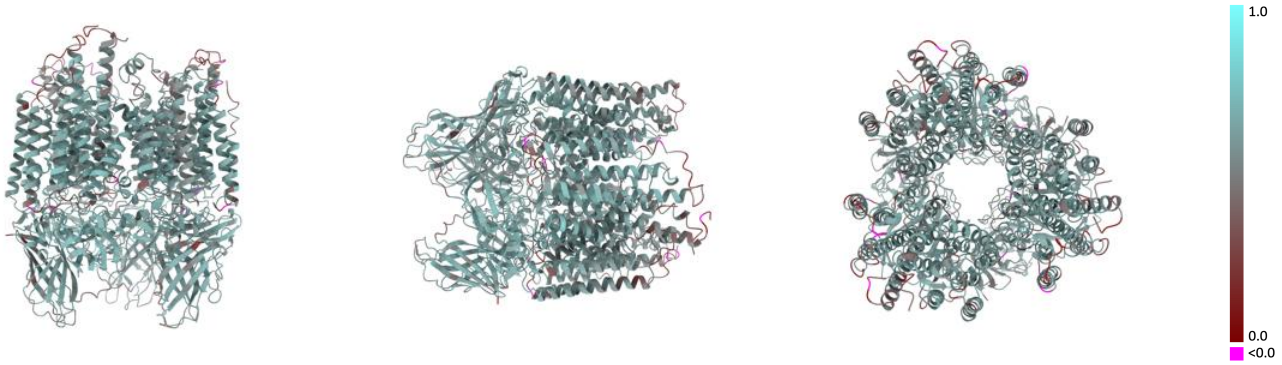
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0272 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.

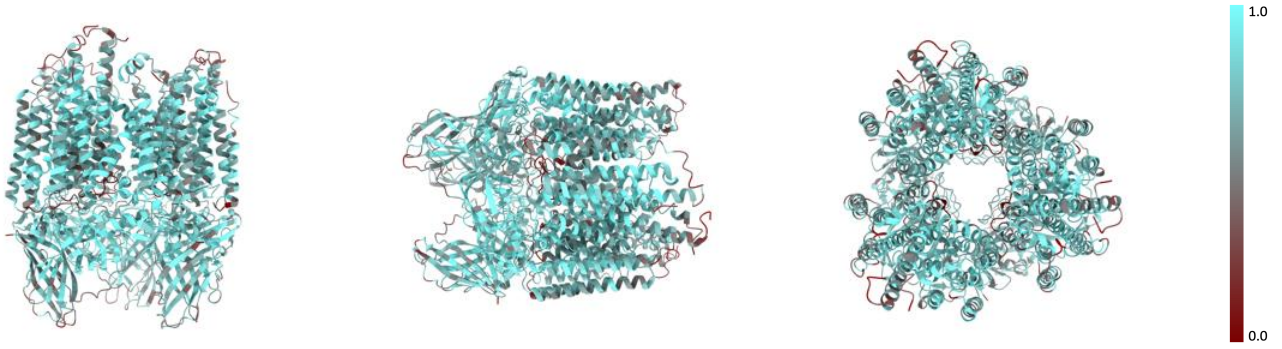
9.2 Q-score mapped to coordinate model



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.

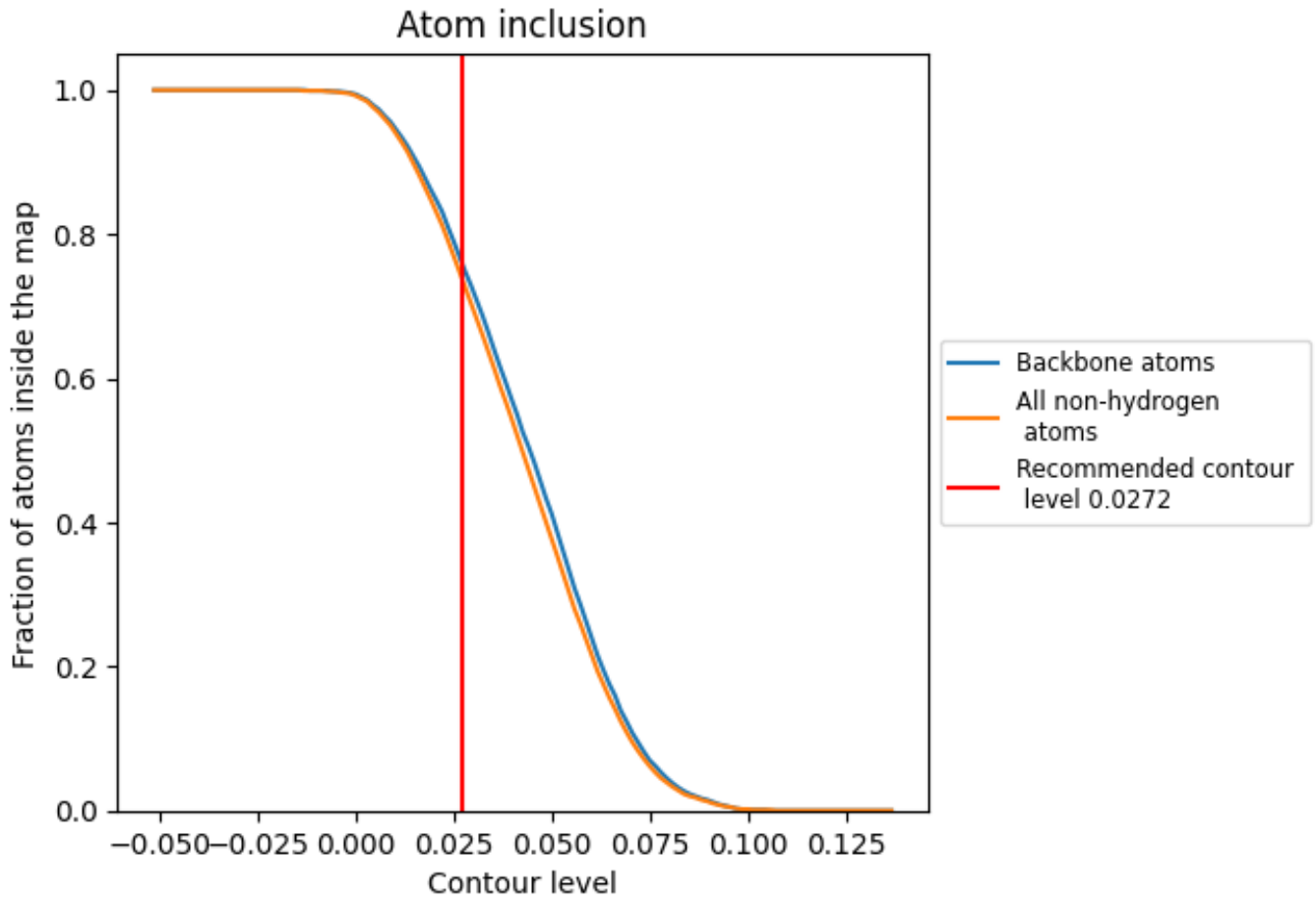
9.3 Atom inclusion mapped to coordinate model



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 (0.0272).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0272) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.5640
A	0.7580	0.5790
B	0.8050	0.5850
C	0.6370	0.5210
D	0.7610	0.5730
E	0.7990	0.5990
F	0.7900	0.5670
G	0.8110	0.5930
H	0.6550	0.5240
I	0.6200	0.5090