Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 01:52 PM JST

PDB ID	:	7D06
EMDB ID	:	EMD-30525
Title	:	Cryo EM structure of the nucleotide free Acinetobacter MlaFEDB complex
Authors	:	Zhang, Y.Y.; Fan, Q.X.; Chi, X.M.; Zhou, Q.; Li, Y.Y.
Deposited on	:	2020-09-09
Resolution	:	3.10 Å(reported)

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

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

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

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

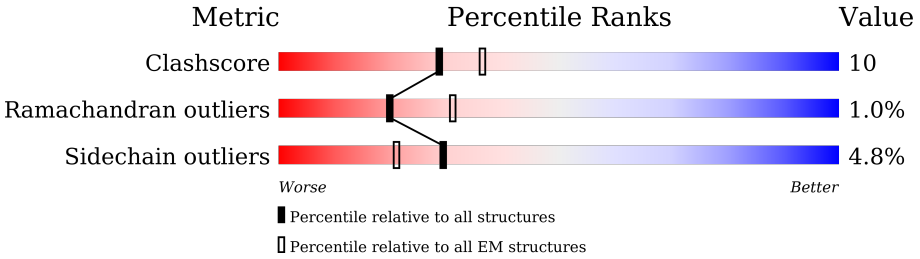
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	258	88% 11% •
1	D	258	87% 12% •
2	B	273	8% 79% 16% • •
2	E	273	6% 76% 17% • • •
3	C	103	33% 57% 29% 5% • 8%
3	F	103	37% 57% 28% 6% • 8%
4	G	226	22% 69% 14% • 15%
4	H	226	20% 75% 8% • 15%

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Mol	Chain	Length	Quality of chain
4	I	226	22% 69% 14% • 15%
4	J	226	21% 76% 8% 15%
4	K	226	20% 72% 11% • 15%
4	L	226	23% 69% 11% • • 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18328 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Intermembrane phospholipid transport system permease protein MlaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	256	1902	1244	309	333	16	0	0
1	D	256	1902	1244	309	333	16	0	0

- Molecule 2 is a protein called ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	263	2032	1284	350	390	8	0	0
2	E	263	2032	1284	350	390	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A0A086HZU3
E	1	MET	-	initiating methionine	UNP A0A086HZU3

- Molecule 3 is a protein called Anti-sigma factor antagonist.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	95	763	493	131	137	2	0	0
3	F	95	763	493	131	137	2	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	-	expression tag	UNP V5V9K5
C	96	LEU	-	expression tag	UNP V5V9K5

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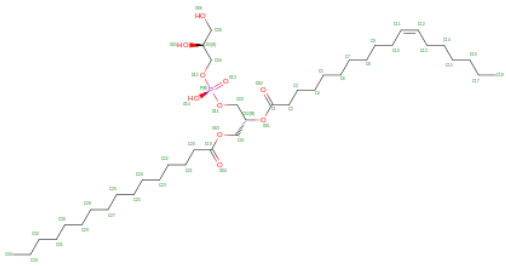
Chain	Residue	Modelled	Actual	Comment	Reference
C	97	GLU	-	expression tag	UNP V5V9K5
C	98	HIS	-	expression tag	UNP V5V9K5
C	99	HIS	-	expression tag	UNP V5V9K5
C	100	HIS	-	expression tag	UNP V5V9K5
C	101	HIS	-	expression tag	UNP V5V9K5
C	102	HIS	-	expression tag	UNP V5V9K5
C	103	HIS	-	expression tag	UNP V5V9K5
F	1	VAL	-	expression tag	UNP V5V9K5
F	96	LEU	-	expression tag	UNP V5V9K5
F	97	GLU	-	expression tag	UNP V5V9K5
F	98	HIS	-	expression tag	UNP V5V9K5
F	99	HIS	-	expression tag	UNP V5V9K5
F	100	HIS	-	expression tag	UNP V5V9K5
F	101	HIS	-	expression tag	UNP V5V9K5
F	102	HIS	-	expression tag	UNP V5V9K5
F	103	HIS	-	expression tag	UNP V5V9K5

- Molecule 4 is a protein called MCE family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	191	1391	880	233	272	6	0	0
4	H	191	1391	880	233	272	6	0	0
4	I	191	1391	880	233	272	6	0	0
4	J	191	1391	880	233	272	6	0	0
4	K	191	1391	880	233	272	6	0	0
4	L	191	1391	880	233	272	6	0	0

- Molecule 5 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

PGV



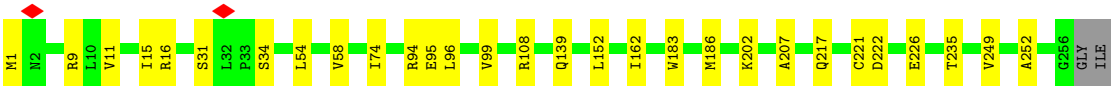
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
5	A	1	51	40	10	1	0
			Total	C	O	P	
5	A	1	51	40	10	1	0
			Total	C	O	P	
5	A	1	51	40	10	1	0
			Total	C	O	P	
5	A	1	51	40	10	1	0
			Total	C	O	P	
5	A	1	39	28	10	1	0
			Total	C	O	P	
5	A	1	51	40	10	1	0
			Total	C	O	P	
5	D	1	51	40	10	1	0
			Total	C	O	P	
5	D	1	51	40	10	1	0
			Total	C	O	P	
5	D	1	51	40	10	1	0
			Total	C	O	P	
5	D	1	51	40	10	1	0
			Total	C	O	P	
5	D	1	39	28	10	1	0
			Total	C	O	P	
5	I	1	51	40	10	1	0

3 Residue-property plots (i)

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

• Molecule 1: Intermembrane phospholipid transport system permease protein MlaE

Chain A:

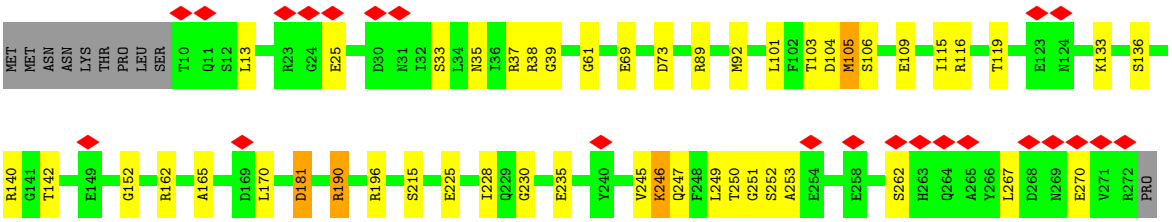


• Molecule 1: Intermembrane phospholipid transport system permease protein MlaE

Chain D:

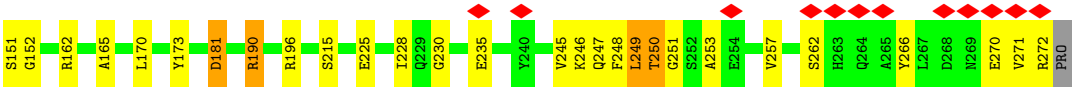
• Molecule 2: ABC transporter ATP-binding protein

Chain B:



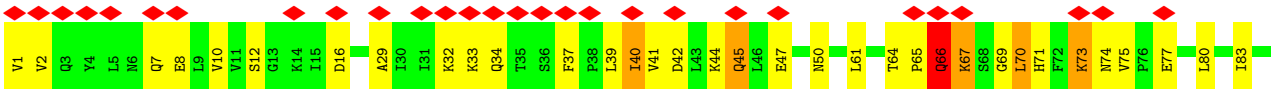
• Molecule 2: ABC transporter ATP-binding protein

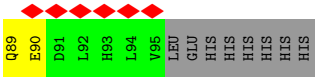
Chain E:



- Molecule 3: Anti-sigma factor antagonist

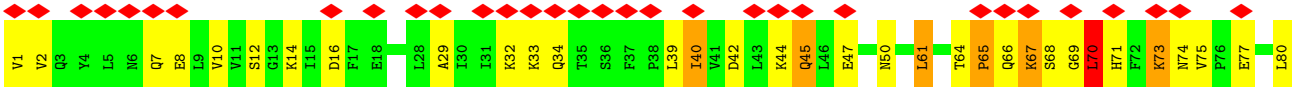
Chain C:

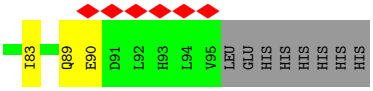




- Molecule 3: Anti-sigma factor antagonist

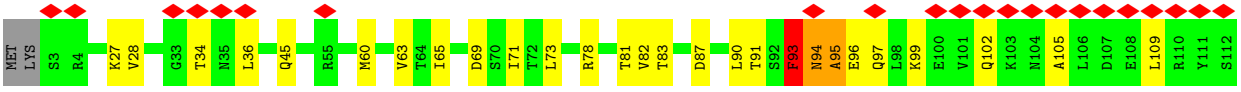
Chain F:

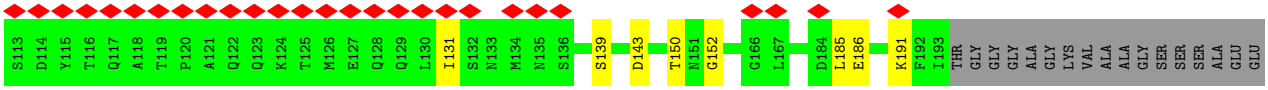




- Molecule 4: MCE family protein

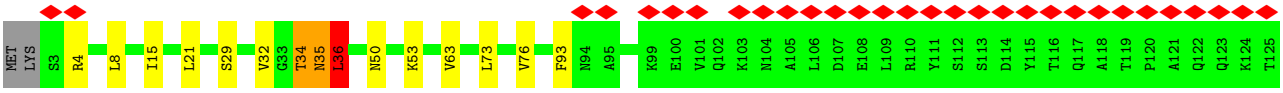
Chain G:

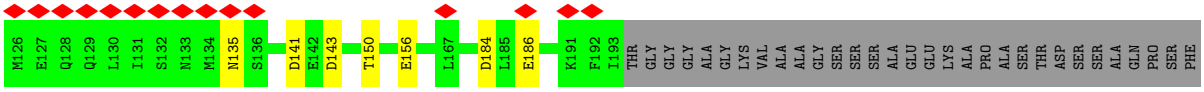




- Molecule 4: MCE family protein

Chain H:

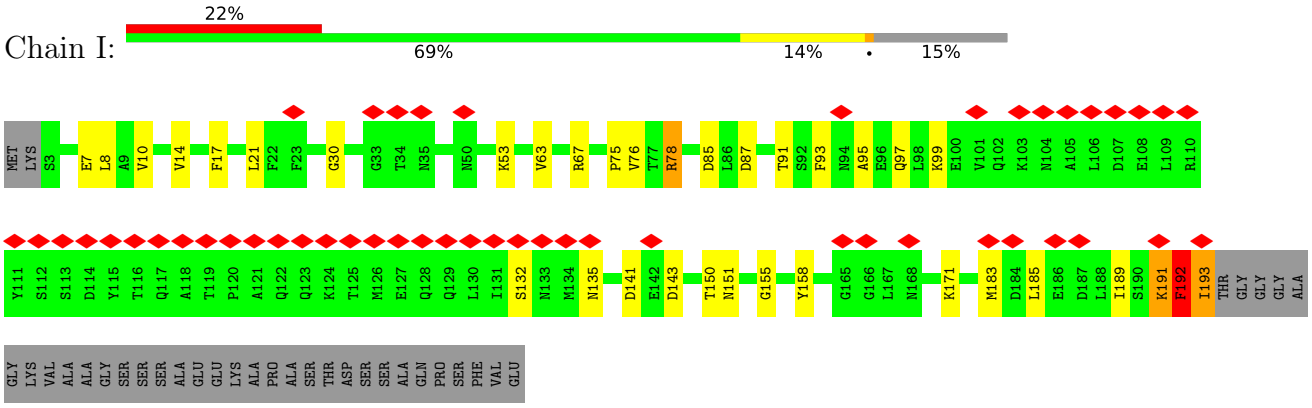




VAL
GLU

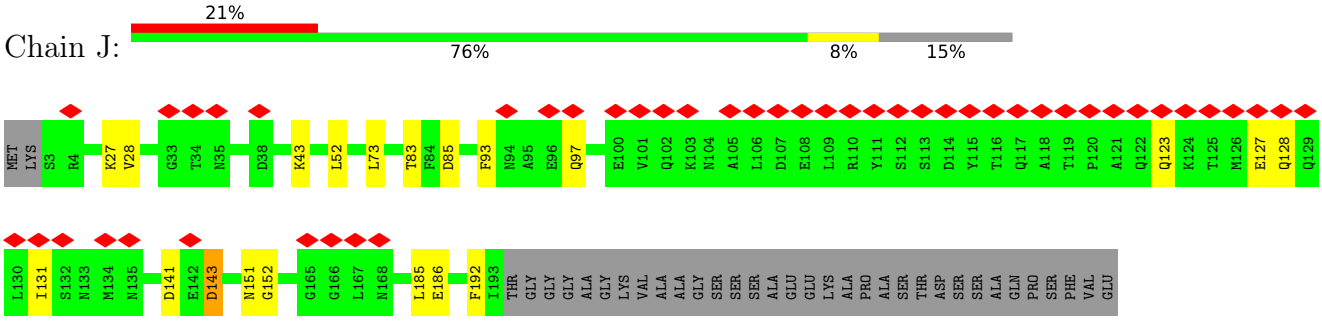
- Molecule 4: MCE family protein

Chain I:



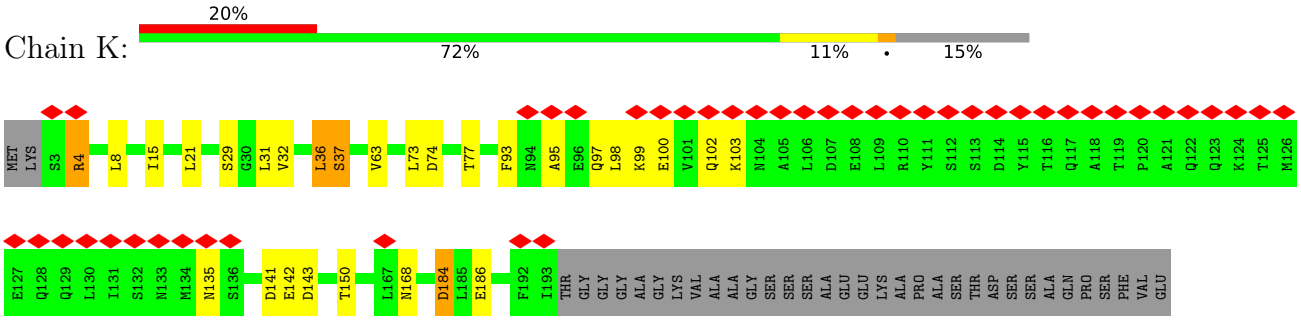
- Molecule 4: MCE family protein

Chain J:



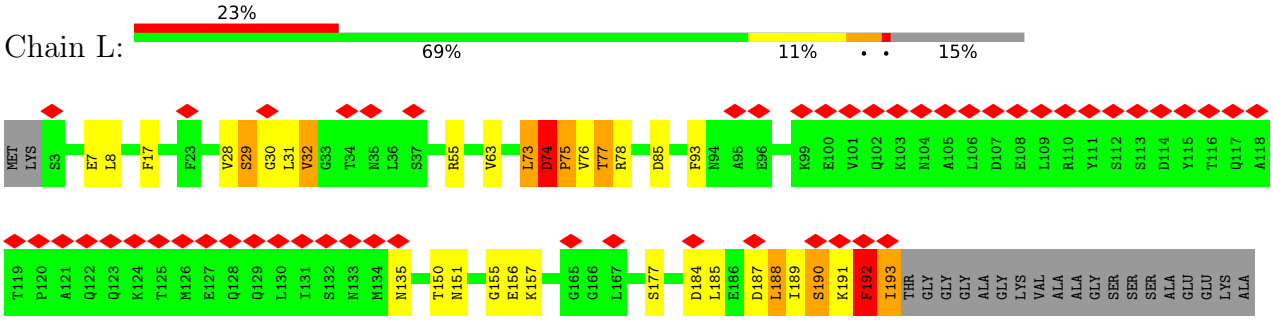
- Molecule 4: MCE family protein

Chain K:



- Molecule 4: MCE family protein

Chain L:



PRO
ALA
SER
THR
ASP
SER
SER
ALA
GLN
PRO
SER
PHE
VAL
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	217.40001, 217.40001, 217.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/1936	0.54	0/2627
1	D	0.46	0/1936	0.54	0/2627
2	B	0.40	0/2062	0.61	0/2790
2	E	0.40	0/2062	0.61	0/2790
3	C	0.38	0/776	0.70	0/1050
3	F	0.38	0/776	0.70	0/1050
4	G	0.40	0/1405	0.57	0/1902
4	H	0.35	0/1405	0.55	0/1902
4	I	0.40	0/1405	0.56	0/1902
4	J	0.58	1/1405 (0.1%)	0.63	0/1902
4	K	0.46	0/1405	0.58	0/1902
4	L	0.32	0/1405	0.55	0/1902
All	All	0.42	1/17978 (0.0%)	0.59	0/24346

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	52	LEU	C-N	-5.07	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1902	0	1994	34	0
1	D	1902	0	1994	42	0
2	B	2032	0	2063	28	0
2	E	2032	0	2063	28	0
3	C	763	0	795	30	0
3	F	763	0	795	25	0
4	G	1391	0	1370	48	0
4	H	1391	0	1370	44	0
4	I	1391	0	1370	53	0
4	J	1391	0	1369	24	0
4	K	1391	0	1370	54	0
4	L	1391	0	1370	56	0
5	A	294	0	431	28	0
5	D	243	0	355	30	0
5	I	51	0	76	3	0
All	All	18328	0	18785	387	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 10.

All (387) 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)
3:F:64:THR:CG2	3:F:65:PRO:HD2	1.32	1.59
3:C:64:THR:CG2	3:C:65:PRO:HD2	1.32	1.58
3:F:64:THR:CG2	3:F:65:PRO:CD	2.24	1.16
3:C:64:THR:HG23	3:C:65:PRO:CD	1.75	1.16
3:C:64:THR:CG2	3:C:65:PRO:CD	2.23	1.15
3:F:64:THR:HG23	3:F:65:PRO:CD	1.77	1.11
4:G:97:GLN:NE2	4:L:76:VAL:HB	1.70	1.06
1:A:16:ARG:NH1	4:H:4:ARG:HB3	1.71	1.06
3:C:37:PHE:HB2	3:C:65:PRO:HG3	1.39	1.05
4:G:90:LEU:O	4:L:75:PRO:HG3	1.57	1.04
4:G:191:LYS:HZ1	4:L:189:ILE:HG22	1.18	1.04
3:F:64:THR:HG22	3:F:65:PRO:HD2	1.35	1.04
4:G:191:LYS:NZ	4:L:189:ILE:HG22	1.72	1.03
4:I:185:LEU:HD21	4:J:152:GLY:O	1.56	1.03
1:D:186:MET:SD	4:J:28:VAL:HG13	1.99	1.02
3:C:64:THR:HG22	3:C:65:PRO:HD2	1.38	1.02
4:G:191:LYS:NZ	4:L:189:ILE:CG2	2.23	1.01
4:H:76:VAL:HG21	4:I:97:GLN:HG2	1.39	1.00
4:G:73:LEU:HD12	4:H:63:VAL:CG2	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLU:HG3	5:D:305:PGV:H251	1.44	0.96
4:H:76:VAL:CG2	4:I:97:GLN:HG2	1.96	0.95
4:J:186:GLU:OE2	4:K:150:THR:HG22	1.66	0.95
1:D:16:ARG:NH1	4:K:4:ARG:HB3	1.82	0.94
4:J:73:LEU:HG	4:K:63:VAL:HG11	1.48	0.93
4:G:191:LYS:HZ2	4:L:189:ILE:CG2	1.84	0.88
4:L:75:PRO:O	4:L:76:VAL:HG12	1.74	0.87
4:K:186:GLU:OE2	4:L:150:THR:HG22	1.74	0.87
4:I:78:ARG:CB	4:I:78:ARG:HH21	1.88	0.86
1:D:95:GLU:HG3	5:D:305:PGV:C25	2.05	0.86
4:L:77:THR:O	4:L:78:ARG:HG2	1.74	0.86
4:G:186:GLU:OE2	4:H:150:THR:HG22	1.76	0.86
4:H:73:LEU:HD13	4:I:63:VAL:HG11	1.57	0.86
4:H:73:LEU:HD13	4:I:63:VAL:CG1	2.06	0.85
4:K:36:LEU:CG	4:K:37:SER:H	1.89	0.85
4:K:36:LEU:HD23	4:K:37:SER:N	1.91	0.85
4:I:185:LEU:CD2	4:J:152:GLY:O	2.23	0.85
3:F:64:THR:HG23	3:F:65:PRO:HD2	0.86	0.84
4:G:63:VAL:CG1	4:L:73:LEU:HG	2.07	0.84
3:F:64:THR:HG22	3:F:65:PRO:CD	1.99	0.83
3:C:64:THR:HG23	3:C:65:PRO:HD2	0.82	0.82
4:G:73:LEU:HD12	4:H:63:VAL:HG21	1.60	0.81
4:G:97:GLN:NE2	4:L:76:VAL:CB	2.44	0.80
4:G:94:ASN:OD1	4:G:95:ALA:N	2.13	0.80
1:D:94:ARG:HD2	5:D:305:PGV:H211	1.64	0.79
3:C:37:PHE:CB	3:C:65:PRO:HG3	2.13	0.79
4:G:97:GLN:HE21	4:L:76:VAL:HB	1.46	0.79
3:C:64:THR:HG22	3:C:65:PRO:CD	2.01	0.79
4:L:187:ASP:HA	4:L:190:SER:OG	1.83	0.79
1:D:15:ILE:CD1	4:K:15:ILE:CD1	2.62	0.78
4:I:78:ARG:HH21	4:I:78:ARG:HB3	1.46	0.78
4:K:36:LEU:HG	4:K:37:SER:H	1.47	0.78
5:D:305:PGV:H32	5:D:305:PGV:P	2.24	0.77
1:D:76:VAL:HG22	4:H:156:GLU:HG3	1.65	0.77
1:A:183:TRP:HB2	4:L:55:ARG:HH22	1.47	0.77
3:F:65:PRO:O	3:F:66:GLN:HG2	1.85	0.77
4:I:76:VAL:CG2	4:J:97:GLN:HG2	2.15	0.76
4:J:73:LEU:HG	4:K:63:VAL:CG1	2.16	0.76
3:F:64:THR:HG21	3:F:69:GLY:O	1.86	0.75
4:G:63:VAL:HG11	4:L:73:LEU:HG	1.66	0.75
4:G:73:LEU:HD12	4:H:63:VAL:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:75:PRO:O	4:J:93:PHE:HE1	1.68	0.74
1:A:95:GLU:HG3	5:A:305:PGV:H251	1.69	0.74
3:F:68:SER:OG	3:F:69:GLY:N	2.20	0.74
2:E:105:MET:O	2:E:106:SER:OG	2.02	0.72
1:A:15:ILE:CD1	4:H:15:ILE:CD1	2.68	0.72
2:E:245:VAL:O	2:E:249:LEU:HB2	1.90	0.72
3:C:41:VAL:HG23	3:C:70:LEU:CD2	2.20	0.71
4:L:31:LEU:O	4:L:32:VAL:HG12	1.90	0.71
1:D:15:ILE:CD1	4:K:15:ILE:HD11	2.21	0.71
4:G:185:LEU:HB3	4:H:150:THR:HG21	1.71	0.71
4:G:191:LYS:HZ1	4:L:189:ILE:CG2	1.95	0.70
4:G:73:LEU:CD1	4:H:63:VAL:CG2	2.70	0.70
4:L:192:PHE:C	4:L:193:ILE:HG13	2.12	0.70
2:B:246:LYS:O	2:B:250:THR:HG22	1.92	0.69
3:C:64:THR:HG21	3:C:69:GLY:O	1.92	0.69
1:A:183:TRP:CB	4:L:55:ARG:HH22	2.04	0.69
5:A:305:PGV:H32	5:A:305:PGV:P	2.32	0.69
4:K:186:GLU:OE2	4:L:150:THR:CG2	2.40	0.69
4:K:36:LEU:CD2	4:K:37:SER:H	2.05	0.69
1:A:15:ILE:HG22	4:H:8:LEU:HD12	1.74	0.69
1:D:15:ILE:HG22	4:K:8:LEU:HD12	1.75	0.68
2:B:105:MET:O	2:B:106:SER:OG	2.08	0.68
4:J:185:LEU:HB3	4:K:150:THR:HG21	1.73	0.68
5:A:302:PGV:C34	4:H:21:LEU:HB3	2.25	0.67
4:L:187:ASP:O	4:L:191:LYS:HG2	1.95	0.67
5:D:302:PGV:C34	4:K:21:LEU:HB3	2.26	0.66
4:G:97:GLN:HE21	4:L:76:VAL:CB	2.05	0.66
1:A:16:ARG:HD3	4:H:4:ARG:HD3	1.77	0.66
2:B:245:VAL:O	2:B:249:LEU:HG	1.96	0.66
4:I:192:PHE:O	4:I:193:ILE:HB	1.96	0.65
5:A:306:PGV:H331	4:L:17:PHE:CE2	2.32	0.65
4:G:93:PHE:HB3	4:G:97:GLN:HG2	1.79	0.64
4:L:73:LEU:O	4:L:74:ASP:O	2.14	0.64
4:L:151:ASN:HB3	4:L:155:GLY:HA3	1.79	0.64
4:K:36:LEU:CG	4:K:37:SER:N	2.61	0.64
5:D:305:PGV:H32	5:D:305:PGV:O14	1.98	0.64
4:H:34:THR:OG1	4:H:35:ASN:N	2.30	0.63
5:D:305:PGV:H32	5:D:305:PGV:O13	1.99	0.63
1:D:15:ILE:HD13	4:K:15:ILE:HD11	1.82	0.62
1:D:252:ALA:O	4:K:29:SER:HB2	1.99	0.61
1:A:16:ARG:HH12	4:H:4:ARG:HB3	1.60	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:36:LEU:CD2	4:K:37:SER:N	2.60	0.61
1:D:95:GLU:CG	5:D:305:PGV:C25	2.77	0.61
2:E:247:GLN:O	2:E:251:GLY:N	2.28	0.61
4:G:73:LEU:CD1	4:H:63:VAL:HG21	2.31	0.60
4:I:189:ILE:HG23	4:J:192:PHE:CE1	2.36	0.60
2:B:104:ASP:O	2:B:105:MET:HG3	2.02	0.60
5:D:302:PGV:H343	4:K:21:LEU:HB3	1.84	0.59
4:I:78:ARG:HH21	4:I:78:ARG:CG	2.14	0.59
1:A:16:ARG:HH11	4:H:4:ARG:HB3	1.65	0.59
4:L:192:PHE:O	4:L:193:ILE:HG13	2.03	0.59
1:A:15:ILE:HG22	4:H:8:LEU:CD1	2.33	0.59
5:A:301:PGV:H22	5:A:302:PGV:H202	1.85	0.59
4:L:28:VAL:HG23	4:L:28:VAL:O	2.01	0.59
1:D:1:MET:SD	4:L:8:LEU:HD11	2.42	0.58
5:A:302:PGV:H343	4:H:21:LEU:CB	2.33	0.58
4:I:189:ILE:HG23	4:J:192:PHE:HE1	1.69	0.58
1:A:186:MET:SD	4:G:28:VAL:HG13	2.44	0.58
4:L:191:LYS:C	4:L:193:ILE:H	2.06	0.57
5:D:305:PGV:O12	5:D:305:PGV:O06	2.11	0.57
3:F:66:GLN:HG3	3:F:68:SER:H	1.69	0.57
5:D:301:PGV:H22	5:D:302:PGV:H202	1.84	0.57
1:D:9:ARG:HD3	4:L:7:GLU:OE2	2.03	0.57
4:I:85:ASP:N	4:I:85:ASP:OD1	2.36	0.57
1:A:1:MET:SD	4:I:8:LEU:HD21	2.45	0.57
1:A:15:ILE:HD13	4:H:15:ILE:HD11	1.86	0.57
3:C:37:PHE:CG	3:C:65:PRO:HD3	2.39	0.57
4:I:76:VAL:HG21	4:J:97:GLN:CG	2.35	0.57
4:G:94:ASN:CG	4:G:95:ALA:H	2.04	0.57
4:K:99:LYS:HA	4:K:102:GLN:HB2	1.86	0.57
1:A:183:TRP:HB2	4:L:55:ARG:NH2	2.18	0.57
4:I:151:ASN:HB3	4:I:155:GLY:HA3	1.87	0.57
4:J:143:ASP:OD1	4:J:143:ASP:N	2.36	0.56
4:H:76:VAL:HG21	4:I:97:GLN:CG	2.25	0.56
1:A:15:ILE:CD1	4:H:15:ILE:HD11	2.34	0.56
1:D:16:ARG:NH1	4:K:4:ARG:O	2.39	0.56
1:D:96:LEU:CD2	5:D:305:PGV:H331	2.35	0.56
5:D:305:PGV:C19	5:D:305:PGV:H031	2.35	0.56
5:D:302:PGV:H343	4:K:21:LEU:CB	2.35	0.56
4:I:76:VAL:HG22	4:J:97:GLN:HG2	1.87	0.56
4:K:73:LEU:HD13	4:L:63:VAL:CG1	2.36	0.56
4:H:141:ASP:OD1	4:H:141:ASP:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:CG1	2:B:249:LEU:HD11	2.36	0.56
5:A:305:PGV:H201	1:D:74:ILE:HD11	1.87	0.55
1:D:95:GLU:CG	5:D:305:PGV:H252	2.36	0.55
4:I:192:PHE:CD1	4:I:193:ILE:HG22	2.41	0.55
4:H:32:VAL:HG23	4:H:32:VAL:O	2.06	0.55
4:H:143:ASP:OD1	4:H:143:ASP:N	2.39	0.55
4:J:85:ASP:OD1	4:J:85:ASP:N	2.37	0.55
2:E:61:GLY:O	2:E:89:ARG:NH2	2.39	0.55
4:L:76:VAL:HG13	4:L:77:THR:N	2.21	0.55
4:L:77:THR:O	4:L:78:ARG:CG	2.51	0.55
3:C:41:VAL:CG2	3:C:70:LEU:CD2	2.85	0.55
4:G:69:ASP:HB3	4:G:83:THR:HG23	1.87	0.55
2:B:245:VAL:HG12	2:B:249:LEU:CD1	2.36	0.55
4:I:132:SER:O	4:I:171:LYS:NZ	2.39	0.55
1:A:221:CYS:SG	1:A:222:ASP:N	2.80	0.55
1:D:221:CYS:SG	1:D:222:ASP:N	2.80	0.55
2:B:61:GLY:O	2:B:89:ARG:NH2	2.39	0.55
4:I:17:PHE:CE2	5:I:301:PGV:H331	2.42	0.55
1:D:15:ILE:CD1	4:K:15:ILE:HD12	2.36	0.54
4:G:97:GLN:HE21	4:L:76:VAL:CG2	2.20	0.54
4:G:143:ASP:OD1	4:G:143:ASP:N	2.39	0.54
2:B:245:VAL:CG1	2:B:249:LEU:CD1	2.86	0.54
4:I:183:MET:HE2	4:I:191:LYS:HZ2	1.72	0.54
4:L:28:VAL:O	4:L:29:SER:HB3	2.07	0.54
1:A:139:GLN:NE2	5:A:304:PGV:O06	2.41	0.54
2:B:245:VAL:HG12	2:B:249:LEU:HD12	1.89	0.54
1:D:139:GLN:NE2	5:D:304:PGV:O06	2.41	0.54
4:J:128:GLN:HA	4:J:131:ILE:HG12	1.90	0.54
5:D:301:PGV:H12	5:D:302:PGV:H311	1.90	0.54
5:A:301:PGV:H12	5:A:302:PGV:H311	1.90	0.54
5:A:302:PGV:H343	4:H:21:LEU:HB3	1.89	0.53
3:C:73:LYS:HG3	3:C:74:ASN:H	1.73	0.53
2:E:104:ASP:OD1	2:E:104:ASP:N	2.40	0.53
4:K:36:LEU:CD2	4:K:36:LEU:H	2.20	0.53
3:F:73:LYS:HG3	3:F:74:ASN:H	1.73	0.53
1:A:34:SER:OG	5:A:304:PGV:O14	2.26	0.53
5:A:301:PGV:H201	1:D:58:VAL:HG11	1.90	0.53
4:K:31:LEU:O	4:K:32:VAL:HG12	2.10	0.52
1:A:15:ILE:CD1	4:H:15:ILE:HD12	2.40	0.52
4:H:186:GLU:OE2	4:I:150:THR:HG22	2.10	0.52
4:K:141:ASP:OD1	4:K:141:ASP:N	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:76:VAL:CG1	4:L:77:THR:N	2.73	0.52
4:I:183:MET:HE1	4:I:191:LYS:HZ1	1.75	0.52
1:D:15:ILE:HD12	4:K:15:ILE:HD12	1.91	0.52
4:K:95:ALA:HA	4:K:98:LEU:HB3	1.90	0.52
2:B:181:ASP:N	2:B:181:ASP:OD1	2.43	0.52
2:E:181:ASP:OD1	2:E:181:ASP:N	2.43	0.52
5:D:305:PGV:H031	5:D:305:PGV:O04	2.10	0.52
4:I:183:MET:CE	4:I:191:LYS:NZ	2.72	0.51
4:K:73:LEU:HD13	4:L:63:VAL:HG11	1.91	0.51
1:D:15:ILE:HD11	4:K:15:ILE:CD1	2.37	0.51
4:G:185:LEU:HB3	4:H:150:THR:CG2	2.36	0.51
3:F:70:LEU:O	3:F:71:HIS:HD2	1.94	0.51
1:D:9:ARG:HD3	4:L:7:GLU:CD	2.31	0.51
4:K:36:LEU:CD2	4:K:36:LEU:N	2.73	0.51
4:K:142:GLU:OE1	4:K:168:ASN:ND2	2.43	0.50
4:I:143:ASP:N	4:I:143:ASP:OD1	2.43	0.50
1:D:96:LEU:HD23	5:D:305:PGV:H331	1.94	0.50
4:K:135:ASN:OD1	4:K:135:ASN:N	2.45	0.50
4:G:152:GLY:O	4:L:185:LEU:HD22	2.11	0.50
2:B:101:LEU:HA	2:B:162:ARG:HH12	1.77	0.50
1:D:249:VAL:HG21	5:D:302:PGV:H301	1.94	0.50
4:G:27:LYS:HE2	4:L:30:GLY:HA3	1.94	0.50
1:D:15:ILE:HG22	4:K:8:LEU:CD1	2.41	0.50
1:A:252:ALA:O	4:H:29:SER:HB2	2.12	0.49
4:I:78:ARG:CG	4:I:78:ARG:NH2	2.73	0.49
1:D:34:SER:OG	5:D:304:PGV:O14	2.26	0.49
4:K:36:LEU:H	4:K:36:LEU:HD22	1.78	0.49
3:F:42:ASP:HB3	3:F:44:LYS:HG2	1.95	0.49
1:A:249:VAL:HG21	5:A:302:PGV:H301	1.94	0.49
2:E:39:GLY:O	2:E:196:ARG:NH2	2.46	0.49
4:I:93:PHE:HB3	4:I:97:GLN:HB2	1.95	0.49
3:C:42:ASP:HB3	3:C:44:LYS:HG2	1.95	0.48
1:D:16:ARG:HH12	4:K:4:ARG:HB3	1.69	0.48
2:E:115:ILE:O	2:E:119:THR:OG1	2.24	0.48
2:E:101:LEU:HA	2:E:162:ARG:HH12	1.77	0.48
4:I:76:VAL:CG2	4:J:97:GLN:CG	2.87	0.48
4:L:85:ASP:OD1	4:L:85:ASP:N	2.43	0.48
1:A:96:LEU:HD23	5:A:305:PGV:H321	1.95	0.48
2:E:247:GLN:OE1	2:E:257:VAL:HG22	2.13	0.48
2:B:39:GLY:O	2:B:196:ARG:NH2	2.46	0.48
3:C:41:VAL:CG2	3:C:70:LEU:HD21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:99:LYS:HA	4:G:102:GLN:HB2	1.95	0.48
1:D:16:ARG:NH1	4:K:4:ARG:CB	2.68	0.47
4:H:76:VAL:HG22	4:I:97:GLN:HB3	1.95	0.47
4:I:76:VAL:HG21	4:J:97:GLN:HG3	1.94	0.47
1:D:162:ILE:HD11	5:I:301:PGV:H12	1.96	0.47
4:J:43:LYS:HE3	4:J:83:THR:HG22	1.96	0.47
1:D:81:GLU:OE2	4:H:53:LYS:NZ	2.47	0.47
2:B:250:THR:HG23	2:B:252:SER:OG	2.15	0.47
4:I:95:ALA:O	4:I:99:LYS:NZ	2.46	0.47
4:J:141:ASP:OD1	4:J:141:ASP:N	2.47	0.47
1:A:162:ILE:HD11	5:A:306:PGV:H12	1.96	0.47
2:B:35:ASN:O	2:B:37:ARG:NH1	2.48	0.47
4:K:100:GLU:HA	4:K:103:LYS:HE2	1.95	0.47
1:A:9:ARG:HD3	4:I:7:GLU:OE2	2.14	0.47
3:C:66:GLN:HE21	3:C:67:LYS:H	1.62	0.47
4:I:192:PHE:CD1	4:I:192:PHE:C	2.86	0.47
4:J:185:LEU:HB3	4:K:150:THR:CG2	2.44	0.47
1:A:15:ILE:HD12	4:H:15:ILE:HD12	1.96	0.46
1:A:74:ILE:HD11	5:D:305:PGV:H201	1.97	0.46
1:D:13:GLU:OE2	4:K:4:ARG:NH1	2.47	0.46
2:E:35:ASN:O	2:E:37:ARG:NH1	2.48	0.46
4:J:151:ASN:OD1	4:J:151:ASN:N	2.47	0.46
4:K:31:LEU:O	4:K:32:VAL:CG1	2.63	0.46
2:E:109:GLU:OE2	2:E:116:ARG:NH1	2.38	0.46
3:F:29:ALA:HA	3:F:32:LYS:HG2	1.98	0.46
4:I:183:MET:CE	4:I:191:LYS:HZ2	2.28	0.46
4:G:63:VAL:HG11	4:L:73:LEU:CG	2.42	0.46
4:K:32:VAL:O	4:K:32:VAL:HG23	2.14	0.46
5:A:305:PGV:C20	1:D:74:ILE:HD11	2.45	0.46
4:H:34:THR:HB	4:H:36:LEU:HD22	1.98	0.46
2:B:247:GLN:O	2:B:251:GLY:N	2.37	0.46
1:D:180:GLY:HA3	4:I:67:ARG:NH1	2.31	0.46
5:D:302:PGV:H21	5:D:302:PGV:H52	1.71	0.46
3:C:29:ALA:HA	3:C:32:LYS:HG2	1.98	0.46
4:G:91:THR:O	4:G:139:SER:N	2.47	0.46
4:H:135:ASN:OD1	4:H:135:ASN:N	2.43	0.46
5:A:301:PGV:H72	5:A:301:PGV:H42	1.81	0.46
5:A:305:PGV:H031	5:A:305:PGV:C04	2.46	0.46
2:E:107:VAL:HG11	2:E:142:THR:O	2.15	0.46
3:F:16:ASP:OD1	3:F:16:ASP:N	2.49	0.46
3:C:64:THR:HG22	3:C:65:PRO:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:31:LEU:C	4:K:32:VAL:CG1	2.84	0.45
3:C:37:PHE:CD2	3:C:65:PRO:HD3	2.50	0.45
1:D:217:GLN:HG3	1:D:235:THR:HG22	1.99	0.45
4:H:76:VAL:CG2	4:I:97:GLN:CG	2.83	0.45
2:B:253:ALA:HB2	2:E:190:ARG:HH12	1.82	0.45
3:C:80:LEU:HA	3:C:83:ILE:HG12	1.98	0.45
5:D:304:PGV:H221	5:D:304:PGV:H252	1.79	0.45
4:L:156:GLU:HG2	4:L:157:LYS:H	1.82	0.45
3:C:41:VAL:HG23	3:C:70:LEU:HD22	1.97	0.45
3:F:66:GLN:O	3:F:68:SER:N	2.50	0.45
4:G:105:ALA:O	4:G:109:LEU:N	2.49	0.45
4:I:14:VAL:HG22	5:I:301:PGV:H282	1.99	0.45
4:K:36:LEU:HD23	4:K:36:LEU:C	2.37	0.45
4:K:74:ASP:OD2	4:K:77:THR:OG1	2.33	0.45
3:C:65:PRO:O	3:C:66:GLN:CB	2.65	0.45
4:G:73:LEU:CG	4:H:63:VAL:HG21	2.47	0.45
1:A:217:GLN:HG3	1:A:235:THR:HG22	1.99	0.45
1:A:94:ARG:O	1:A:202:LYS:NZ	2.47	0.45
5:D:304:PGV:H182	5:D:304:PGV:H151	1.83	0.45
3:F:80:LEU:HA	3:F:83:ILE:HG12	1.98	0.45
2:B:250:THR:CG2	2:B:252:SER:OG	2.65	0.45
2:B:115:ILE:O	2:B:119:THR:OG1	2.24	0.44
4:G:131:ILE:HD12	4:G:131:ILE:HA	1.90	0.44
1:A:54:LEU:HD13	5:A:306:PGV:H62	1.98	0.44
2:E:228:ILE:HG22	2:E:230:GLY:H	1.83	0.44
4:K:184:ASP:N	4:K:184:ASP:OD1	2.50	0.44
5:A:302:PGV:H343	4:H:21:LEU:HB2	1.99	0.44
5:A:305:PGV:H32	5:A:305:PGV:O14	2.17	0.44
2:E:133:LYS:HE3	2:E:165:ALA:HA	1.99	0.44
4:G:150:THR:CG2	4:L:185:LEU:HD21	2.47	0.44
3:C:16:ASP:OD1	3:C:16:ASP:N	2.49	0.44
2:E:38:ARG:NH2	2:E:73:ASP:OD1	2.51	0.44
4:G:191:LYS:CE	4:L:189:ILE:HG22	2.46	0.44
4:L:184:ASP:O	4:L:188:LEU:HD22	2.18	0.44
4:L:185:LEU:HA	4:L:188:LEU:HD23	1.99	0.44
5:A:304:PGV:H252	5:A:304:PGV:H221	1.79	0.43
2:B:228:ILE:HG22	2:B:230:GLY:H	1.83	0.43
5:A:301:PGV:H321	5:A:301:PGV:H291	1.78	0.43
2:B:13:LEU:HB2	2:B:38:ARG:HG2	2.00	0.43
3:C:40:ILE:HD11	3:C:73:LYS:HD3	2.00	0.43
3:C:44:LYS:HB2	3:C:45:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:PHE:O	2:E:103:THR:O	2.36	0.43
4:K:31:LEU:C	4:K:32:VAL:HG13	2.39	0.43
3:C:75:VAL:HG11	3:C:80:LEU:HB3	2.01	0.43
5:D:301:PGV:H291	5:D:301:PGV:H321	1.78	0.43
2:E:13:LEU:HB2	2:E:38:ARG:HG2	2.00	0.43
3:F:40:ILE:HD11	3:F:73:LYS:HD3	2.01	0.43
4:I:191:LYS:HE3	4:I:191:LYS:HB2	1.64	0.43
2:B:190:ARG:HH12	2:E:253:ALA:HB2	1.83	0.43
4:G:191:LYS:HZ2	4:L:189:ILE:HG21	1.79	0.43
4:K:36:LEU:N	4:K:36:LEU:HD22	2.33	0.43
3:F:44:LYS:HB2	3:F:45:GLN:HG2	2.00	0.43
4:G:60:MET:HB2	4:G:65:ILE:HD13	2.00	0.43
4:J:123:GLN:O	4:J:127:GLU:N	2.52	0.43
2:B:133:LYS:HE3	2:B:165:ALA:HA	2.00	0.43
4:I:87:ASP:O	4:I:91:THR:OG1	2.30	0.43
5:A:302:PGV:H52	5:A:302:PGV:H21	1.71	0.43
2:B:38:ARG:NH2	2:B:73:ASP:OD1	2.51	0.43
3:C:40:ILE:HB	3:C:71:HIS:HB2	2.01	0.43
3:F:34:GLN:HG2	3:F:39:LEU:HD22	2.01	0.43
4:H:50:ASN:ND2	4:I:158:TYR:OH	2.51	0.43
4:L:135:ASN:OD1	4:L:135:ASN:N	2.46	0.43
4:L:184:ASP:OD1	4:L:187:ASP:HB2	2.18	0.43
4:I:135:ASN:OD1	4:I:135:ASN:N	2.52	0.43
4:K:143:ASP:OD1	4:K:143:ASP:N	2.51	0.43
2:B:109:GLU:OE2	2:B:116:ARG:NH1	2.38	0.43
1:D:94:ARG:O	1:D:202:LYS:NZ	2.47	0.42
4:I:183:MET:HE2	4:I:191:LYS:NZ	2.32	0.42
2:E:246:LYS:O	2:E:250:THR:OG1	2.34	0.42
4:L:177:SER:O	4:L:177:SER:OG	2.31	0.42
4:L:73:LEU:O	4:L:73:LEU:HD22	2.18	0.42
5:A:305:PGV:H251	5:A:305:PGV:H282	1.77	0.42
2:B:246:LYS:HA	2:B:246:LYS:HD3	1.66	0.42
3:C:67:LYS:HD3	3:C:67:LYS:HA	1.85	0.42
5:D:305:PGV:O14	5:D:305:PGV:H41	2.20	0.42
2:B:140:ARG:HH11	2:E:266:TYR:HB2	1.84	0.42
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.91	0.42
1:A:11:VAL:HG21	4:I:10:VAL:HG12	2.00	0.42
2:E:151:SER:O	2:E:151:SER:OG	2.35	0.42
3:F:40:ILE:HB	3:F:71:HIS:HB2	2.01	0.42
4:G:63:VAL:HG13	4:L:73:LEU:HG	1.96	0.42
4:L:73:LEU:O	4:L:74:ASP:CG	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:14:LYS:HE2	3:F:14:LYS:HB3	1.89	0.42
3:F:50:ASN:N	3:F:50:ASN:OD1	2.53	0.42
3:F:75:VAL:HG11	3:F:80:LEU:HB3	2.01	0.42
4:G:93:PHE:O	4:G:94:ASN:HB3	2.20	0.42
1:A:99:VAL:CG1	5:A:305:PGV:H342	2.50	0.42
3:C:34:GLN:HG2	3:C:39:LEU:HD22	2.01	0.42
3:F:61:LEU:HD13	3:F:61:LEU:HA	1.93	0.42
4:G:34:THR:O	4:G:34:THR:OG1	2.37	0.42
4:I:30:GLY:HA3	4:J:27:LYS:HE3	2.02	0.42
1:D:188:ASN:HD21	4:I:53:LYS:HE3	1.84	0.42
2:E:245:VAL:O	2:E:245:VAL:HG12	2.19	0.42
5:A:304:PGV:H151	5:A:304:PGV:H182	1.83	0.41
2:B:92:MET:HG2	2:B:170:LEU:HD23	2.02	0.41
4:G:71:ILE:HG23	4:G:82:VAL:HG22	2.01	0.41
4:K:93:PHE:HB2	4:K:97:GLN:HB2	2.01	0.41
4:G:95:ALA:O	4:G:97:GLN:N	2.53	0.41
1:A:11:VAL:CG2	4:I:10:VAL:HG12	2.51	0.41
5:A:302:PGV:C34	4:H:21:LEU:CB	2.95	0.41
5:D:305:PGV:H251	5:D:305:PGV:H282	1.72	0.41
1:A:58:VAL:HG11	5:D:301:PGV:H201	2.02	0.41
4:I:192:PHE:CE1	4:I:193:ILE:HG22	2.56	0.41
5:D:305:PGV:H201	5:D:305:PGV:H232	1.70	0.41
2:E:92:MET:HG2	2:E:170:LEU:HD23	2.03	0.41
2:E:95:LEU:HD23	2:E:173:TYR:HD2	1.86	0.41
4:I:183:MET:HE1	4:I:191:LYS:NZ	2.35	0.41
4:I:21:LEU:HD23	4:I:21:LEU:HA	1.95	0.41
1:D:152:LEU:HB3	1:D:207:ALA:HB2	2.03	0.41
4:G:150:THR:HG23	4:L:185:LEU:HD21	2.02	0.41
4:H:184:ASP:OD1	4:H:184:ASP:N	2.43	0.41
1:A:152:LEU:HB3	1:A:207:ALA:HB2	2.03	0.40
3:C:50:ASN:OD1	3:C:50:ASN:N	2.53	0.40
2:E:248:PHE:CD1	2:E:248:PHE:C	2.94	0.40
4:G:36:LEU:HD12	4:G:87:ASP:HB2	2.03	0.40
4:I:141:ASP:OD1	4:I:141:ASP:N	2.52	0.40
1:D:202:LYS:HG2	1:D:250:LEU:HD13	2.04	0.40
2:E:271:VAL:HG23	2:E:272:ARG:H	1.86	0.40
1:D:252:ALA:O	4:K:29:SER:CB	2.67	0.40
4:G:45:GLN:OE1	4:G:81:THR:OG1	2.39	0.40
4:G:78:ARG:HE	4:G:78:ARG:HB2	1.77	0.40
4:K:150:THR:O	4:K:150:THR:OG1	2.33	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	254/258 (98%)	248 (98%)	6 (2%)	0	100	100
1	D	254/258 (98%)	248 (98%)	6 (2%)	0	100	100
2	B	261/273 (96%)	225 (86%)	33 (13%)	3 (1%)	14	46
2	E	261/273 (96%)	225 (86%)	32 (12%)	4 (2%)	10	39
3	C	93/103 (90%)	72 (77%)	20 (22%)	1 (1%)	14	46
3	F	93/103 (90%)	69 (74%)	21 (23%)	3 (3%)	4	22
4	G	189/226 (84%)	160 (85%)	25 (13%)	4 (2%)	7	30
4	H	189/226 (84%)	169 (89%)	18 (10%)	2 (1%)	14	46
4	I	189/226 (84%)	167 (88%)	21 (11%)	1 (0%)	29	64
4	J	189/226 (84%)	165 (87%)	24 (13%)	0	100	100
4	K	189/226 (84%)	175 (93%)	13 (7%)	1 (0%)	29	64
4	L	189/226 (84%)	159 (84%)	25 (13%)	5 (3%)	5	26
All	All	2350/2624 (90%)	2082 (89%)	244 (10%)	24 (1%)	20	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	103	THR
2	B	105	MET
2	E	103	THR
4	G	93	PHE
4	G	94	ASN
4	L	74	ASP
2	B	152	GLY
2	E	104	ASP
2	E	105	MET
2	E	152	GLY
3	F	67	LYS
4	G	95	ALA

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Mol	Chain	Res	Type
4	L	32	VAL
3	F	70	LEU
4	G	96	GLU
4	H	36	LEU
3	C	66	GLN
4	H	34	THR
4	L	29	SER
3	F	65	PRO
4	I	192	PHE
4	L	192	PHE
4	K	37	SER
4	L	75	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	204/205 (100%)	201 (98%)	3 (2%)	65	85
1	D	204/205 (100%)	201 (98%)	3 (2%)	65	85
2	B	219/229 (96%)	206 (94%)	13 (6%)	19	50
2	E	219/229 (96%)	203 (93%)	16 (7%)	14	43
3	C	85/93 (91%)	67 (79%)	18 (21%)	1	5
3	F	85/93 (91%)	68 (80%)	17 (20%)	1	5
4	G	143/186 (77%)	142 (99%)	1 (1%)	84	93
4	H	143/186 (77%)	140 (98%)	3 (2%)	53	79
4	I	143/186 (77%)	139 (97%)	4 (3%)	43	73
4	J	143/186 (77%)	142 (99%)	1 (1%)	84	93
4	K	143/186 (77%)	140 (98%)	3 (2%)	53	79
4	L	143/186 (77%)	135 (94%)	8 (6%)	21	52
All	All	1874/2170 (86%)	1784 (95%)	90 (5%)	29	58

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	108	ARG
1	A	226	GLU
2	B	25	GLU
2	B	33	SER
2	B	69	GLU
2	B	136	SER
2	B	142	THR
2	B	181	ASP
2	B	190	ARG
2	B	215	SER
2	B	225	GLU
2	B	235	GLU
2	B	246	LYS
2	B	262	SER
2	B	270	GLU
3	C	1	VAL
3	C	2	VAL
3	C	7	GLN
3	C	8	GLU
3	C	10	VAL
3	C	12	SER
3	C	33	LYS
3	C	40	ILE
3	C	45	GLN
3	C	47	GLU
3	C	61	LEU
3	C	66	GLN
3	C	67	LYS
3	C	70	LEU
3	C	73	LYS
3	C	77	GLU
3	C	89	GLN
3	C	90	GLU
1	D	31	SER
1	D	108	ARG
1	D	226	GLU
2	E	25	GLU
2	E	33	SER
2	E	69	GLU
2	E	103	THR
2	E	105	MET
2	E	136	SER

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Mol	Chain	Res	Type
2	E	142	THR
2	E	181	ASP
2	E	190	ARG
2	E	215	SER
2	E	225	GLU
2	E	235	GLU
2	E	249	LEU
2	E	250	THR
2	E	262	SER
2	E	270	GLU
3	F	1	VAL
3	F	2	VAL
3	F	7	GLN
3	F	8	GLU
3	F	10	VAL
3	F	12	SER
3	F	33	LYS
3	F	40	ILE
3	F	45	GLN
3	F	47	GLU
3	F	61	LEU
3	F	67	LYS
3	F	70	LEU
3	F	73	LYS
3	F	77	GLU
3	F	89	GLN
3	F	90	GLU
4	G	93	PHE
4	H	35	ASN
4	H	36	LEU
4	H	93	PHE
4	I	78	ARG
4	I	191	LYS
4	I	192	PHE
4	I	193	ILE
4	J	143	ASP
4	K	4	ARG
4	K	36	LEU
4	K	184	ASP
4	L	73	LEU
4	L	74	ASP
4	L	77	THR

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Mol	Chain	Res	Type
4	L	93	PHE
4	L	188	LEU
4	L	190	SER
4	L	192	PHE
4	L	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	139	GLN
1	A	191	GLN
2	B	35	ASN
3	C	66	GLN
3	C	93	HIS
1	D	46	HIS
1	D	139	GLN
1	D	191	GLN
2	E	35	ASN
3	F	71	HIS
4	G	45	GLN
4	G	97	GLN
4	H	45	GLN
4	H	50	ASN
4	I	45	GLN
4	K	45	GLN
4	L	50	ASN
4	L	128	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PGV	D	302	-	50,50,50	1.36	5 (10%)	53,56,56	1.65	4 (7%)
5	PGV	A	302	-	50,50,50	1.36	5 (10%)	53,56,56	1.65	4 (7%)
5	PGV	A	301	-	50,50,50	1.37	5 (10%)	53,56,56	1.67	3 (5%)
5	PGV	A	306	-	50,50,50	1.37	5 (10%)	53,56,56	1.66	4 (7%)
5	PGV	I	301	-	50,50,50	1.37	5 (10%)	53,56,56	1.66	4 (7%)
5	PGV	D	304	-	50,50,50	1.39	5 (10%)	53,56,56	1.61	3 (5%)
5	PGV	A	303	-	50,50,50	1.40	5 (10%)	53,56,56	1.55	3 (5%)
5	PGV	A	304	-	50,50,50	1.39	5 (10%)	53,56,56	1.61	3 (5%)
5	PGV	D	303	-	50,50,50	1.39	5 (10%)	53,56,56	1.55	3 (5%)
5	PGV	D	301	-	50,50,50	1.37	5 (10%)	53,56,56	1.67	3 (5%)
5	PGV	A	305	-	38,38,50	1.18	3 (7%)	41,44,56	1.79	3 (7%)
5	PGV	D	305	-	38,38,50	1.18	3 (7%)	41,44,56	1.79	3 (7%)

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
5	PGV	D	302	-	-	30/55/55/55	-
5	PGV	A	302	-	-	30/55/55/55	-
5	PGV	A	301	-	-	39/55/55/55	-
5	PGV	A	306	-	-	28/55/55/55	-
5	PGV	I	301	-	-	28/55/55/55	-
5	PGV	D	304	-	-	29/55/55/55	-
5	PGV	A	303	-	-	35/55/55/55	-
5	PGV	A	304	-	-	29/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGV	D	303	-	-	35/55/55/55	-
5	PGV	D	301	-	-	39/55/55/55	-
5	PGV	A	305	-	-	22/43/43/55	-
5	PGV	D	305	-	-	31/43/43/55	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	PGV	C9-C10	-4.51	1.34	1.52
5	D	304	PGV	C9-C10	-4.49	1.34	1.52
5	A	306	PGV	C9-C10	-4.45	1.34	1.52
5	I	301	PGV	C9-C10	-4.42	1.34	1.52
5	D	301	PGV	C9-C10	-4.41	1.34	1.52
5	A	301	PGV	C9-C10	-4.39	1.34	1.52
5	A	302	PGV	C9-C10	-4.38	1.34	1.52
5	A	303	PGV	C9-C10	-4.37	1.34	1.52
5	D	302	PGV	C9-C10	-4.36	1.34	1.52
5	D	303	PGV	C9-C10	-4.36	1.34	1.52
5	A	304	PGV	C12-C11	4.13	1.55	1.31
5	A	303	PGV	C12-C11	4.13	1.55	1.31
5	D	304	PGV	C12-C11	4.12	1.55	1.31
5	D	303	PGV	C12-C11	4.12	1.55	1.31
5	D	302	PGV	C12-C11	4.12	1.55	1.31
5	A	306	PGV	C12-C11	4.12	1.55	1.31
5	I	301	PGV	C12-C11	4.11	1.55	1.31
5	A	302	PGV	C12-C11	4.10	1.55	1.31
5	A	301	PGV	C12-C11	4.08	1.55	1.31
5	D	301	PGV	C12-C11	4.08	1.55	1.31
5	A	303	PGV	O03-C19	3.13	1.42	1.33
5	D	303	PGV	O03-C19	3.12	1.42	1.33
5	D	301	PGV	O01-C1	2.94	1.42	1.34
5	A	302	PGV	O01-C02	-2.94	1.39	1.46
5	A	301	PGV	O01-C1	2.92	1.42	1.34
5	D	302	PGV	O01-C02	-2.89	1.39	1.46
5	I	301	PGV	O03-C19	2.88	1.41	1.33
5	A	306	PGV	O03-C19	2.88	1.41	1.33
5	A	305	PGV	O03-C19	2.86	1.41	1.33
5	A	302	PGV	O03-C19	2.81	1.41	1.33
5	D	305	PGV	O03-C19	2.81	1.41	1.33
5	D	304	PGV	O03-C19	2.80	1.41	1.33
5	D	302	PGV	O03-C19	2.79	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	PGV	O03-C19	2.79	1.41	1.33
5	D	301	PGV	O03-C19	2.74	1.41	1.33
5	A	301	PGV	O03-C19	2.74	1.41	1.33
5	A	304	PGV	O01-C02	-2.73	1.39	1.46
5	D	304	PGV	O01-C02	-2.70	1.39	1.46
5	D	305	PGV	O01-C1	2.69	1.41	1.34
5	A	303	PGV	O01-C02	-2.63	1.40	1.46
5	I	301	PGV	O01-C1	2.63	1.41	1.34
5	A	304	PGV	O01-C1	2.62	1.41	1.34
5	A	303	PGV	O01-C1	2.61	1.41	1.34
5	D	303	PGV	O01-C1	2.61	1.41	1.34
5	A	305	PGV	O01-C1	2.61	1.41	1.34
5	D	304	PGV	O01-C1	2.60	1.41	1.34
5	A	306	PGV	O01-C1	2.60	1.41	1.34
5	D	303	PGV	O01-C02	-2.59	1.40	1.46
5	A	305	PGV	O01-C02	-2.52	1.40	1.46
5	I	301	PGV	O01-C02	-2.50	1.40	1.46
5	A	306	PGV	O01-C02	-2.49	1.40	1.46
5	D	305	PGV	O01-C02	-2.38	1.40	1.46
5	A	302	PGV	O01-C1	2.31	1.40	1.34
5	D	302	PGV	O01-C1	2.30	1.40	1.34
5	D	301	PGV	O01-C02	-2.10	1.41	1.46
5	A	301	PGV	O01-C02	-2.09	1.41	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	305	PGV	C21-C20-C19	-9.19	80.19	113.62
5	A	301	PGV	C21-C20-C19	-8.94	81.12	113.62
5	D	301	PGV	C21-C20-C19	-8.93	81.14	113.62
5	A	305	PGV	C21-C20-C19	-8.84	81.47	113.62
5	A	306	PGV	C21-C20-C19	-8.66	82.13	113.62
5	I	301	PGV	C21-C20-C19	-8.65	82.15	113.62
5	D	304	PGV	C21-C20-C19	-8.36	83.22	113.62
5	A	304	PGV	C21-C20-C19	-8.34	83.28	113.62
5	A	302	PGV	C21-C20-C19	-8.21	83.77	113.62
5	D	302	PGV	C21-C20-C19	-8.20	83.82	113.62
5	D	303	PGV	C21-C20-C19	-7.78	85.33	113.62
5	A	303	PGV	C21-C20-C19	-7.78	85.33	113.62
5	D	304	PGV	O01-C1-C2	4.26	120.69	111.50
5	A	304	PGV	O01-C1-C2	4.25	120.66	111.50
5	D	301	PGV	O01-C1-C2	4.21	120.57	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	PGV	O01-C1-C2	4.19	120.54	111.50
5	D	302	PGV	O01-C1-C2	4.18	120.50	111.50
5	A	302	PGV	O01-C1-C2	4.17	120.49	111.50
5	A	305	PGV	O01-C1-C2	4.10	120.34	111.50
5	I	301	PGV	O01-C1-C2	3.98	120.08	111.50
5	A	306	PGV	O01-C1-C2	3.96	120.04	111.50
5	A	303	PGV	O01-C1-C2	3.96	120.03	111.50
5	D	303	PGV	O01-C1-C2	3.94	120.00	111.50
5	D	305	PGV	O01-C1-C2	3.62	119.29	111.50
5	D	305	PGV	O03-C19-C20	2.71	120.41	111.91
5	A	305	PGV	O03-C19-C20	2.59	120.02	111.91
5	D	302	PGV	O03-C19-C20	2.56	119.93	111.91
5	A	302	PGV	O03-C19-C20	2.55	119.90	111.91
5	D	303	PGV	O03-C19-C20	2.48	119.69	111.91
5	A	303	PGV	O03-C19-C20	2.47	119.65	111.91
5	A	306	PGV	O03-C19-C20	2.46	119.64	111.91
5	I	301	PGV	O03-C19-C20	2.46	119.61	111.91
5	D	301	PGV	O03-C19-C20	2.41	119.46	111.91
5	A	301	PGV	O03-C19-C20	2.40	119.43	111.91
5	A	304	PGV	O03-C19-C20	2.38	119.36	111.91
5	D	304	PGV	O03-C19-C20	2.35	119.27	111.91
5	D	302	PGV	C13-C12-C11	-2.08	108.73	124.73
5	A	302	PGV	C13-C12-C11	-2.08	108.80	124.73
5	I	301	PGV	C10-C11-C12	-2.07	108.84	124.73
5	A	306	PGV	C10-C11-C12	-2.06	108.88	124.73

There are no chirality outliers.

All (375) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	PGV	C04-O12-P-O11
5	A	301	PGV	C04-C05-C06-O06
5	A	302	PGV	C04-O12-P-O14
5	A	302	PGV	C04-C05-C06-O06
5	A	302	PGV	C2-C1-O01-C02
5	A	302	PGV	C11-C10-C9-C8
5	A	303	PGV	C04-O12-P-O13
5	A	303	PGV	C04-O12-P-O14
5	A	303	PGV	C11-C10-C9-C8
5	A	303	PGV	C10-C11-C12-C13
5	A	304	PGV	O12-C04-C05-O05
5	A	306	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	D	301	PGV	C04-O12-P-O11
5	D	301	PGV	C04-C05-C06-O06
5	D	302	PGV	C04-O12-P-O14
5	D	302	PGV	C04-C05-C06-O06
5	D	302	PGV	C2-C1-O01-C02
5	D	302	PGV	C11-C10-C9-C8
5	D	303	PGV	C04-O12-P-O13
5	D	303	PGV	C04-O12-P-O14
5	D	303	PGV	C11-C10-C9-C8
5	D	303	PGV	C10-C11-C12-C13
5	D	304	PGV	O12-C04-C05-O05
5	D	305	PGV	C03-O11-P-O13
5	D	305	PGV	C03-O11-P-O14
5	D	305	PGV	C04-O12-P-O13
5	I	301	PGV	C11-C10-C9-C8
5	A	304	PGV	O04-C19-O03-C01
5	D	304	PGV	O04-C19-O03-C01
5	A	305	PGV	O04-C19-O03-C01
5	A	301	PGV	O02-C1-O01-C02
5	A	302	PGV	O02-C1-O01-C02
5	D	301	PGV	O02-C1-O01-C02
5	D	302	PGV	O02-C1-O01-C02
5	A	304	PGV	C20-C19-O03-C01
5	A	305	PGV	C20-C19-O03-C01
5	D	304	PGV	C20-C19-O03-C01
5	D	305	PGV	C20-C19-O03-C01
5	A	301	PGV	C2-C1-O01-C02
5	D	301	PGV	C2-C1-O01-C02
5	A	301	PGV	C10-C11-C12-C13
5	A	304	PGV	C10-C11-C12-C13
5	D	301	PGV	C10-C11-C12-C13
5	D	304	PGV	C10-C11-C12-C13
5	D	305	PGV	O04-C19-O03-C01
5	A	302	PGV	O12-C04-C05-O05
5	A	305	PGV	O12-C04-C05-O05
5	D	302	PGV	O12-C04-C05-O05
5	A	304	PGV	O12-C04-C05-C06
5	D	304	PGV	O12-C04-C05-C06
5	A	302	PGV	C20-C19-O03-C01
5	A	303	PGV	C20-C19-O03-C01
5	A	306	PGV	C20-C19-O03-C01
5	D	302	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
5	D	303	PGV	C20-C19-O03-C01
5	I	301	PGV	C20-C19-O03-C01
5	A	304	PGV	C20-C21-C22-C23
5	D	304	PGV	C20-C21-C22-C23
5	I	301	PGV	O04-C19-O03-C01
5	I	301	PGV	C2-C1-O01-C02
5	A	303	PGV	O04-C19-O03-C01
5	A	306	PGV	O04-C19-O03-C01
5	D	303	PGV	O04-C19-O03-C01
5	A	304	PGV	C19-C20-C21-C22
5	D	304	PGV	C19-C20-C21-C22
5	D	305	PGV	C19-C20-C21-C22
5	A	306	PGV	C10-C11-C12-C13
5	I	301	PGV	C10-C11-C12-C13
5	A	301	PGV	C1-C2-C3-C4
5	A	303	PGV	C19-C20-C21-C22
5	D	301	PGV	C1-C2-C3-C4
5	D	303	PGV	C19-C20-C21-C22
5	D	305	PGV	C1-C2-C3-C4
5	A	306	PGV	C2-C1-O01-C02
5	A	302	PGV	O04-C19-O03-C01
5	D	302	PGV	O04-C19-O03-C01
5	A	301	PGV	C03-O11-P-O12
5	A	302	PGV	C04-O12-P-O11
5	A	303	PGV	C03-O11-P-O12
5	A	303	PGV	C04-O12-P-O11
5	D	301	PGV	C03-O11-P-O12
5	D	302	PGV	C04-O12-P-O11
5	D	303	PGV	C03-O11-P-O12
5	D	303	PGV	C04-O12-P-O11
5	D	305	PGV	C03-O11-P-O12
5	A	305	PGV	O12-C04-C05-C06
5	A	306	PGV	O02-C1-O01-C02
5	I	301	PGV	O02-C1-O01-C02
5	A	301	PGV	C12-C13-C14-C15
5	D	301	PGV	C12-C13-C14-C15
5	D	305	PGV	C2-C1-O01-C02
5	A	301	PGV	C13-C14-C15-C16
5	A	304	PGV	C5-C6-C7-C8
5	A	305	PGV	C28-C29-C30-C31
5	D	301	PGV	C13-C14-C15-C16
5	D	304	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	D	305	PGV	O02-C1-O01-C02
5	A	303	PGV	C27-C28-C29-C30
5	D	303	PGV	C27-C28-C29-C30
5	A	301	PGV	O12-C04-C05-O05
5	D	301	PGV	O12-C04-C05-O05
5	A	301	PGV	C27-C28-C29-C30
5	D	301	PGV	C27-C28-C29-C30
5	D	305	PGV	C29-C30-C31-C32
5	A	301	PGV	C23-C24-C25-C26
5	A	306	PGV	C30-C31-C32-C33
5	D	301	PGV	C23-C24-C25-C26
5	I	301	PGV	C28-C29-C30-C31
5	I	301	PGV	C30-C31-C32-C33
5	A	306	PGV	C28-C29-C30-C31
5	A	301	PGV	C28-C29-C30-C31
5	A	303	PGV	C04-C05-C06-O06
5	A	306	PGV	C04-C05-C06-O06
5	D	303	PGV	C04-C05-C06-O06
5	D	305	PGV	C04-C05-C06-O06
5	I	301	PGV	C04-C05-C06-O06
5	A	302	PGV	C5-C6-C7-C8
5	A	304	PGV	C28-C29-C30-C31
5	A	306	PGV	C5-C6-C7-C8
5	A	306	PGV	C22-C23-C24-C25
5	D	301	PGV	C28-C29-C30-C31
5	D	302	PGV	C5-C6-C7-C8
5	D	304	PGV	C28-C29-C30-C31
5	I	301	PGV	C5-C6-C7-C8
5	I	301	PGV	C22-C23-C24-C25
5	A	303	PGV	C2-C3-C4-C5
5	A	305	PGV	C23-C24-C25-C26
5	A	305	PGV	C24-C25-C26-C27
5	D	303	PGV	C2-C3-C4-C5
5	D	304	PGV	C25-C26-C27-C28
5	A	301	PGV	C26-C27-C28-C29
5	A	304	PGV	C25-C26-C27-C28
5	D	301	PGV	C26-C27-C28-C29
5	A	304	PGV	C14-C15-C16-C17
5	A	305	PGV	C29-C30-C31-C32
5	D	304	PGV	C14-C15-C16-C17
5	A	303	PGV	C7-C8-C9-C10
5	D	303	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	A	301	PGV	C6-C7-C8-C9
5	D	301	PGV	C6-C7-C8-C9
5	D	305	PGV	C24-C25-C26-C27
5	D	305	PGV	C2-C3-C4-C5
5	A	305	PGV	C2-C1-O01-C02
5	A	301	PGV	O05-C05-C06-O06
5	A	302	PGV	O05-C05-C06-O06
5	D	301	PGV	O05-C05-C06-O06
5	D	302	PGV	O05-C05-C06-O06
5	D	305	PGV	C23-C24-C25-C26
5	A	306	PGV	O12-C04-C05-O05
5	I	301	PGV	O12-C04-C05-O05
5	A	301	PGV	C2-C3-C4-C5
5	D	301	PGV	C2-C3-C4-C5
5	A	306	PGV	C21-C22-C23-C24
5	I	301	PGV	C21-C22-C23-C24
5	A	306	PGV	C26-C27-C28-C29
5	I	301	PGV	C26-C27-C28-C29
5	A	305	PGV	O02-C1-O01-C02
5	A	304	PGV	C13-C14-C15-C16
5	A	306	PGV	C29-C30-C31-C32
5	D	304	PGV	C13-C14-C15-C16
5	I	301	PGV	C29-C30-C31-C32
5	A	302	PGV	C25-C26-C27-C28
5	A	304	PGV	C30-C31-C32-C33
5	D	302	PGV	C25-C26-C27-C28
5	D	304	PGV	C30-C31-C32-C33
5	A	306	PGV	C19-C20-C21-C22
5	I	301	PGV	C19-C20-C21-C22
5	A	304	PGV	C29-C30-C31-C32
5	D	304	PGV	C29-C30-C31-C32
5	D	303	PGV	C21-C22-C23-C24
5	A	303	PGV	C2-C1-O01-C02
5	D	303	PGV	C2-C1-O01-C02
5	A	303	PGV	C21-C22-C23-C24
5	A	303	PGV	C12-C13-C14-C15
5	D	303	PGV	C12-C13-C14-C15
5	A	304	PGV	C1-C2-C3-C4
5	D	304	PGV	C1-C2-C3-C4
5	A	306	PGV	C24-C25-C26-C27
5	I	301	PGV	C24-C25-C26-C27
5	A	306	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
5	I	301	PGV	O12-C04-C05-C06
5	A	302	PGV	O03-C01-C02-C03
5	A	304	PGV	O03-C01-C02-C03
5	D	302	PGV	O03-C01-C02-C03
5	D	304	PGV	O03-C01-C02-C03
5	A	306	PGV	C14-C15-C16-C17
5	I	301	PGV	C14-C15-C16-C17
5	A	304	PGV	C9-C10-C11-C12
5	D	304	PGV	C9-C10-C11-C12
5	A	303	PGV	C31-C32-C33-C34
5	D	303	PGV	C31-C32-C33-C34
5	A	301	PGV	C25-C26-C27-C28
5	A	305	PGV	C3-C4-C5-C6
5	D	301	PGV	C25-C26-C27-C28
5	A	303	PGV	C14-C15-C16-C17
5	D	303	PGV	C14-C15-C16-C17
5	A	301	PGV	C21-C22-C23-C24
5	D	301	PGV	C21-C22-C23-C24
5	D	302	PGV	C28-C29-C30-C31
5	A	303	PGV	O02-C1-O01-C02
5	D	303	PGV	O02-C1-O01-C02
5	A	302	PGV	C28-C29-C30-C31
5	A	305	PGV	C31-C32-C33-C34
5	A	304	PGV	C04-C05-C06-O06
5	D	304	PGV	C04-C05-C06-O06
5	A	303	PGV	C5-C6-C7-C8
5	D	303	PGV	C5-C6-C7-C8
5	A	303	PGV	C3-C4-C5-C6
5	D	303	PGV	C3-C4-C5-C6
5	A	301	PGV	C01-C02-C03-O11
5	A	303	PGV	C01-C02-C03-O11
5	D	301	PGV	C01-C02-C03-O11
5	D	303	PGV	C01-C02-C03-O11
5	A	301	PGV	C19-C20-C21-C22
5	D	301	PGV	C19-C20-C21-C22
5	A	305	PGV	C27-C28-C29-C30
5	A	303	PGV	C22-C23-C24-C25
5	D	303	PGV	C22-C23-C24-C25
5	A	303	PGV	C28-C29-C30-C31
5	D	303	PGV	C28-C29-C30-C31
5	D	305	PGV	C04-O12-P-O11
5	A	306	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
5	I	301	PGV	O01-C02-C03-O11
5	D	305	PGV	C27-C28-C29-C30
5	A	304	PGV	O03-C01-C02-O01
5	D	304	PGV	O03-C01-C02-O01
5	A	302	PGV	O12-C04-C05-C06
5	D	302	PGV	O12-C04-C05-C06
5	A	304	PGV	C24-C25-C26-C27
5	D	304	PGV	C24-C25-C26-C27
5	D	305	PGV	C31-C32-C33-C34
5	D	302	PGV	C13-C14-C15-C16
5	A	302	PGV	C13-C14-C15-C16
5	A	306	PGV	C01-C02-C03-O11
5	I	301	PGV	C01-C02-C03-O11
5	A	302	PGV	C24-C25-C26-C27
5	D	302	PGV	C24-C25-C26-C27
5	D	301	PGV	C29-C30-C31-C32
5	D	305	PGV	C02-C01-O03-C19
5	A	301	PGV	C29-C30-C31-C32
5	A	302	PGV	O03-C01-C02-O01
5	A	303	PGV	O03-C01-C02-O01
5	D	302	PGV	O03-C01-C02-O01
5	D	303	PGV	O03-C01-C02-O01
5	A	305	PGV	C26-C27-C28-C29
5	A	303	PGV	C23-C24-C25-C26
5	A	303	PGV	C24-C25-C26-C27
5	D	303	PGV	C24-C25-C26-C27
5	D	303	PGV	C23-C24-C25-C26
5	D	301	PGV	C22-C23-C24-C25
5	A	301	PGV	C22-C23-C24-C25
5	A	302	PGV	C31-C32-C33-C34
5	D	302	PGV	C31-C32-C33-C34
5	A	301	PGV	C03-O11-P-O14
5	A	302	PGV	C03-O11-P-O13
5	A	303	PGV	C03-O11-P-O14
5	A	304	PGV	C03-O11-P-O13
5	D	301	PGV	C03-O11-P-O14
5	D	302	PGV	C03-O11-P-O13
5	D	303	PGV	C03-O11-P-O14
5	D	304	PGV	C03-O11-P-O13
5	A	305	PGV	C30-C31-C32-C33
5	A	301	PGV	C7-C8-C9-C10
5	D	301	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	I	301	PGV	C25-C26-C27-C28
5	A	306	PGV	C25-C26-C27-C28
5	A	305	PGV	C1-C2-C3-C4
5	A	303	PGV	O01-C02-C03-O11
5	D	303	PGV	O01-C02-C03-O11
5	D	305	PGV	O03-C01-C02-O01
5	D	303	PGV	C29-C30-C31-C32
5	A	303	PGV	C29-C30-C31-C32
5	I	301	PGV	C3-C4-C5-C6
5	A	306	PGV	C3-C4-C5-C6
5	D	305	PGV	C26-C27-C28-C29
5	A	305	PGV	C25-C26-C27-C28
5	A	301	PGV	C01-C02-O01-C1
5	D	301	PGV	C01-C02-O01-C1
5	D	305	PGV	C03-C02-O01-C1
5	A	306	PGV	C15-C16-C17-C18
5	I	301	PGV	C15-C16-C17-C18
5	A	302	PGV	C05-C04-O12-P
5	D	302	PGV	C05-C04-O12-P
5	A	301	PGV	O01-C02-C03-O11
5	D	301	PGV	O01-C02-C03-O11
5	A	302	PGV	C14-C15-C16-C17
5	D	302	PGV	C14-C15-C16-C17
5	A	302	PGV	C11-C12-C13-C14
5	D	302	PGV	C11-C12-C13-C14
5	A	304	PGV	C04-O12-P-O11
5	D	304	PGV	C04-O12-P-O11
5	A	303	PGV	O03-C01-C02-C03
5	D	303	PGV	O03-C01-C02-C03
5	A	301	PGV	C20-C19-O03-C01
5	D	301	PGV	C20-C19-O03-C01
5	D	304	PGV	C4-C5-C6-C7
5	A	304	PGV	C4-C5-C6-C7
5	A	304	PGV	O02-C1-O01-C02
5	D	304	PGV	O02-C1-O01-C02
5	A	302	PGV	C23-C24-C25-C26
5	D	302	PGV	C23-C24-C25-C26
5	D	305	PGV	C25-C26-C27-C28
5	D	305	PGV	C3-C4-C5-C6
5	D	305	PGV	C20-C21-C22-C23
5	A	301	PGV	O12-C04-C05-C06
5	D	301	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
5	A	302	PGV	C29-C30-C31-C32
5	D	302	PGV	C29-C30-C31-C32
5	A	303	PGV	C25-C26-C27-C28
5	D	303	PGV	C25-C26-C27-C28
5	A	302	PGV	C1-C2-C3-C4
5	D	302	PGV	C1-C2-C3-C4
5	D	305	PGV	C01-C02-C03-O11
5	A	301	PGV	O04-C19-O03-C01
5	D	301	PGV	O04-C19-O03-C01
5	D	305	PGV	O03-C01-C02-C03
5	A	301	PGV	C3-C4-C5-C6
5	D	301	PGV	C3-C4-C5-C6
5	A	306	PGV	O05-C05-C06-O06
5	I	301	PGV	O05-C05-C06-O06
5	A	305	PGV	C22-C23-C24-C25
5	A	304	PGV	C2-C1-O01-C02
5	D	304	PGV	C2-C1-O01-C02
5	A	301	PGV	O03-C19-C20-C21
5	D	301	PGV	O03-C19-C20-C21
5	D	304	PGV	C22-C23-C24-C25
5	A	304	PGV	C22-C23-C24-C25
5	A	301	PGV	C11-C12-C13-C14
5	D	301	PGV	C11-C12-C13-C14
5	A	306	PGV	O03-C19-C20-C21
5	D	305	PGV	C22-C23-C24-C25
5	I	301	PGV	O03-C19-C20-C21
5	A	302	PGV	O01-C1-C2-C3
5	A	305	PGV	C20-C21-C22-C23
5	D	302	PGV	O01-C1-C2-C3
5	A	304	PGV	O03-C19-C20-C21
5	D	304	PGV	O03-C19-C20-C21
5	D	301	PGV	C14-C15-C16-C17
5	A	305	PGV	O03-C19-C20-C21
5	D	305	PGV	O03-C19-C20-C21
5	A	301	PGV	C14-C15-C16-C17
5	I	301	PGV	C13-C14-C15-C16
5	A	301	PGV	C20-C21-C22-C23
5	A	306	PGV	C13-C14-C15-C16
5	D	301	PGV	C20-C21-C22-C23
5	A	301	PGV	C24-C25-C26-C27
5	D	301	PGV	C24-C25-C26-C27
5	A	305	PGV	O04-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
5	D	301	PGV	O04-C19-C20-C21
5	A	306	PGV	O04-C19-C20-C21
5	I	301	PGV	O04-C19-C20-C21
5	A	304	PGV	C6-C7-C8-C9
5	D	304	PGV	C6-C7-C8-C9
5	A	301	PGV	O04-C19-C20-C21
5	A	301	PGV	C05-C04-O12-P
5	D	301	PGV	C05-C04-O12-P
5	A	301	PGV	C04-O12-P-O14
5	A	303	PGV	C03-O11-P-O13
5	D	301	PGV	C04-O12-P-O14
5	D	303	PGV	C03-O11-P-O13
5	A	304	PGV	O04-C19-C20-C21
5	D	304	PGV	O04-C19-C20-C21
5	A	302	PGV	O03-C19-C20-C21
5	A	303	PGV	O03-C19-C20-C21
5	D	302	PGV	O03-C19-C20-C21
5	D	303	PGV	O03-C19-C20-C21
5	A	303	PGV	O04-C19-C20-C21
5	D	303	PGV	O04-C19-C20-C21
5	D	305	PGV	C28-C29-C30-C31
5	A	302	PGV	O04-C19-C20-C21
5	D	302	PGV	O04-C19-C20-C21
5	A	305	PGV	O01-C1-C2-C3
5	A	302	PGV	O02-C1-C2-C3
5	D	302	PGV	O02-C1-C2-C3
5	D	305	PGV	O04-C19-C20-C21

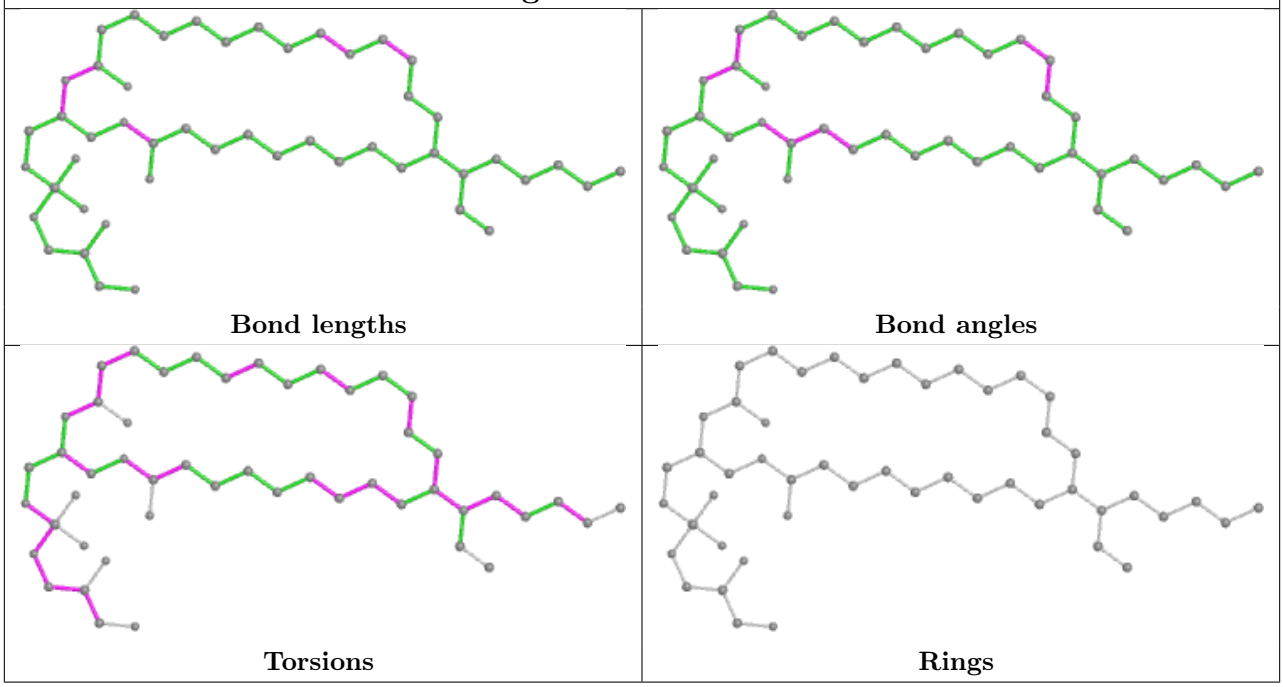
There are no ring outliers.

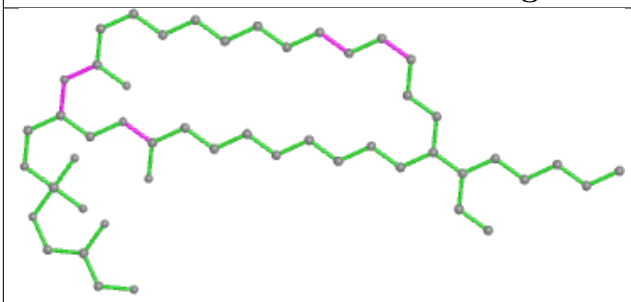
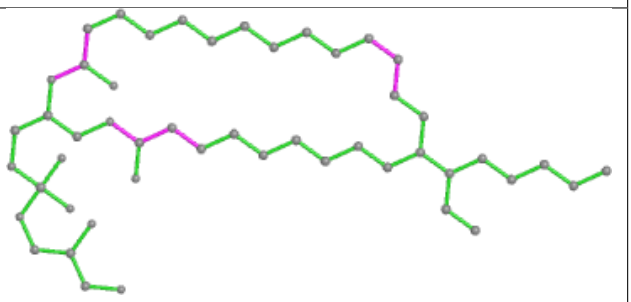
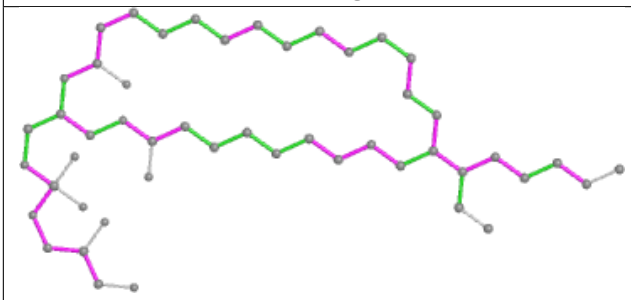
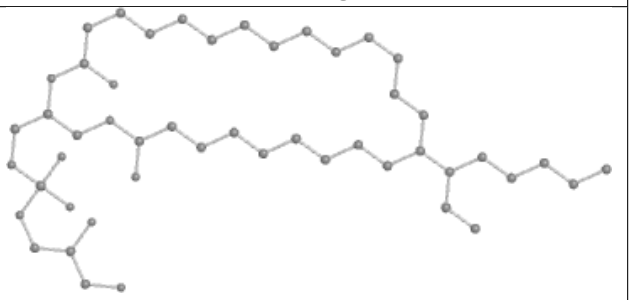
10 monomers are involved in 61 short contacts:

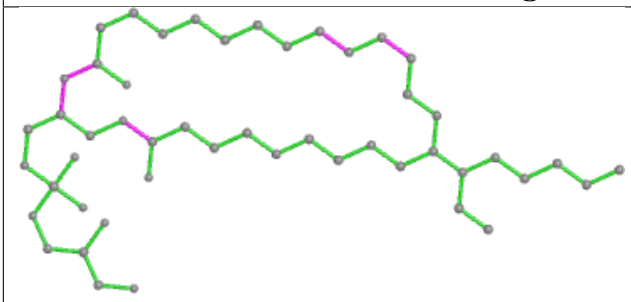
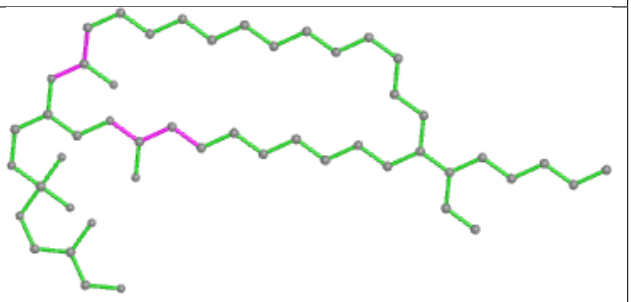
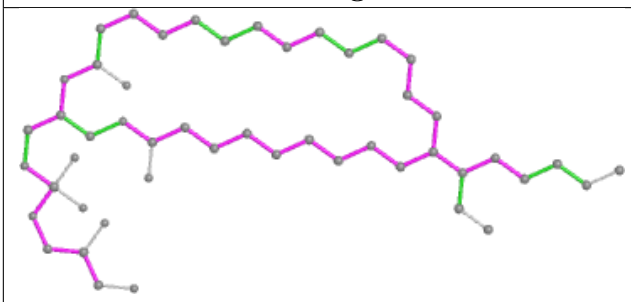
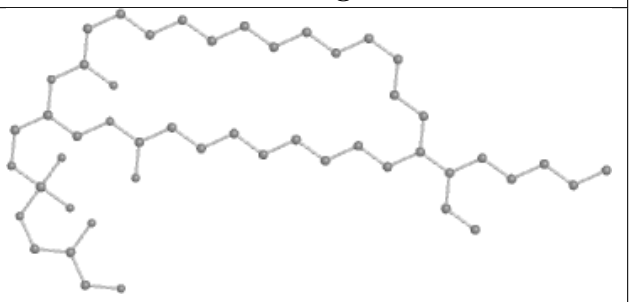
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	302	PGV	7	0
5	A	302	PGV	9	0
5	A	301	PGV	5	0
5	A	306	PGV	3	0
5	I	301	PGV	3	0
5	D	304	PGV	4	0
5	A	304	PGV	4	0
5	D	301	PGV	4	0
5	A	305	PGV	9	0
5	D	305	PGV	17	0

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 PGV D 302



Ligand PGV A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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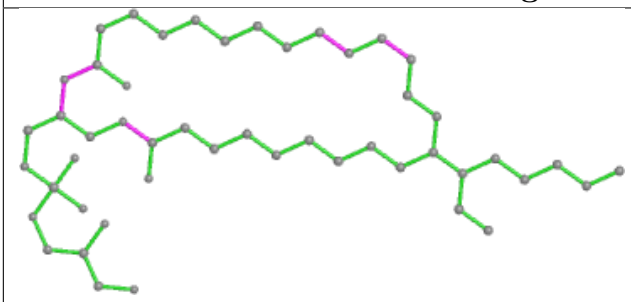
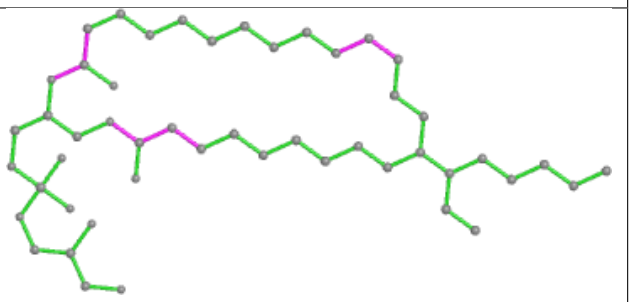
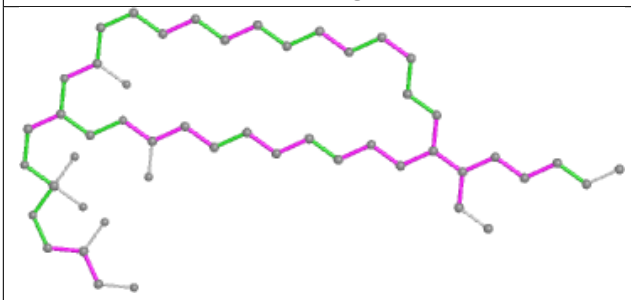
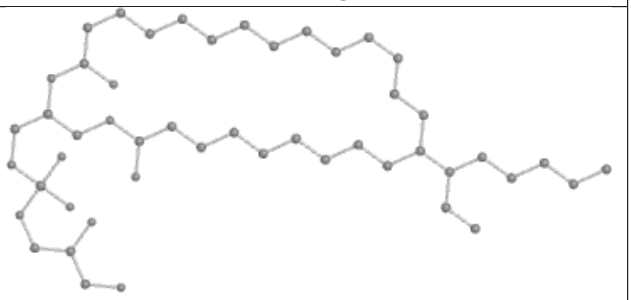
 Bond lengths	 Bond angles
 Torsions	 Rings

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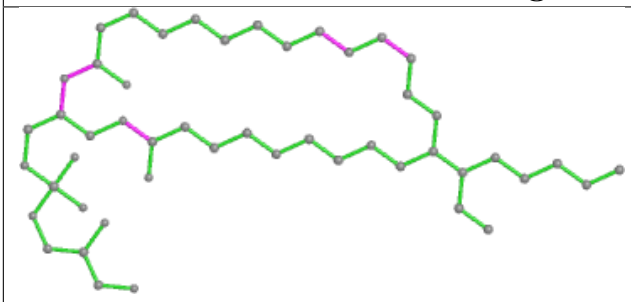
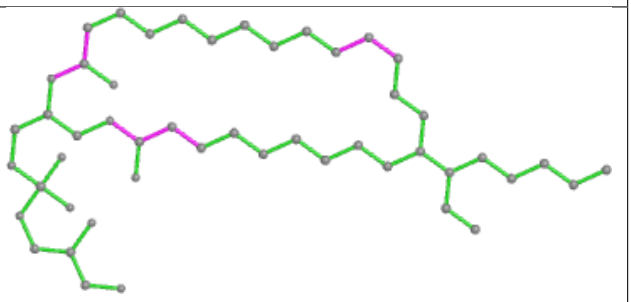
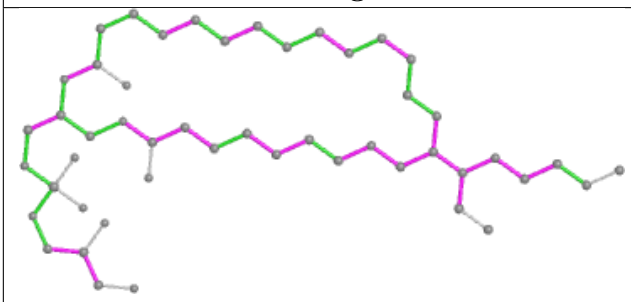
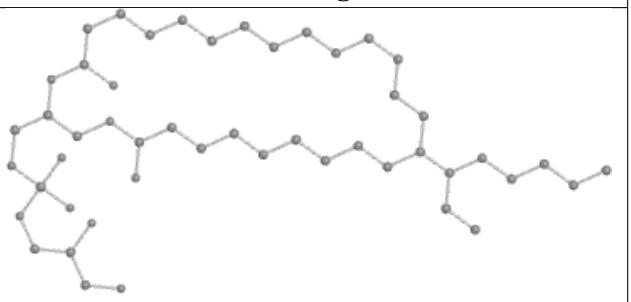
 Bond lengths	 Bond angles
 Torsions	 Rings

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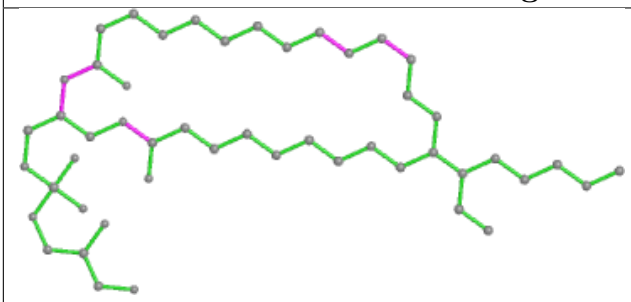
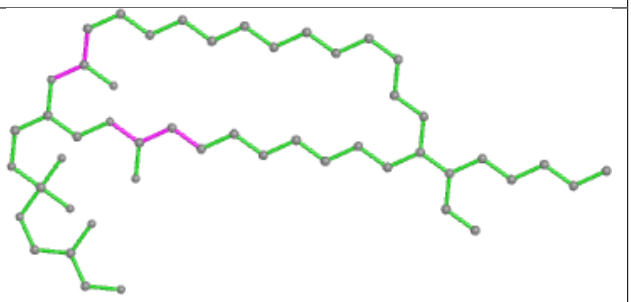
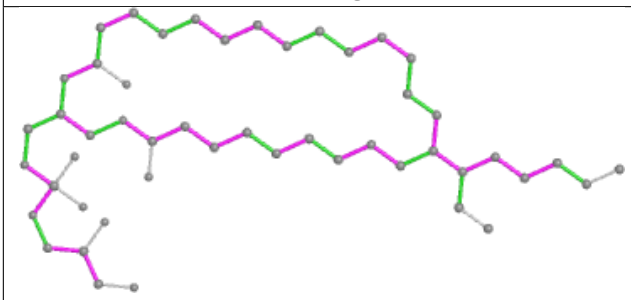
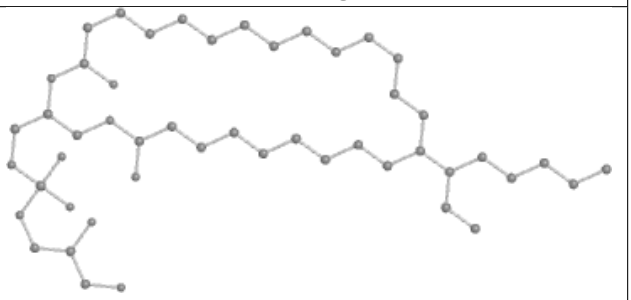
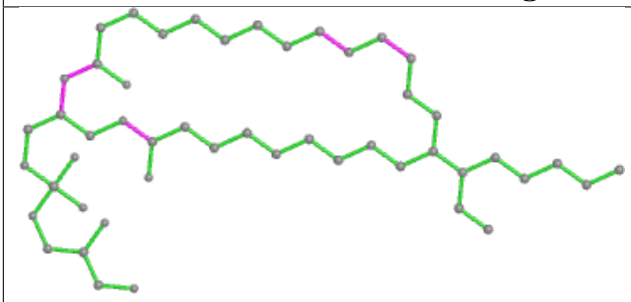
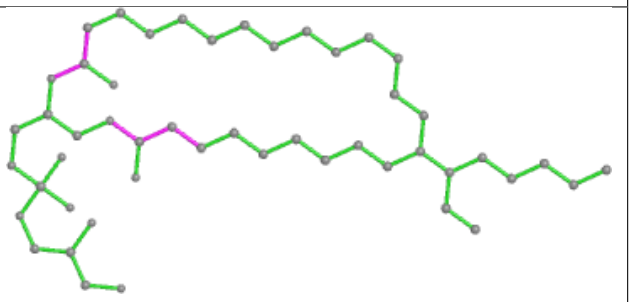
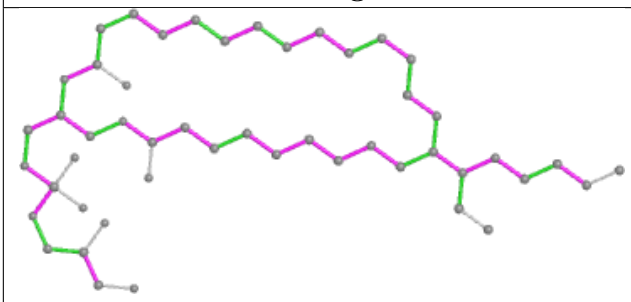
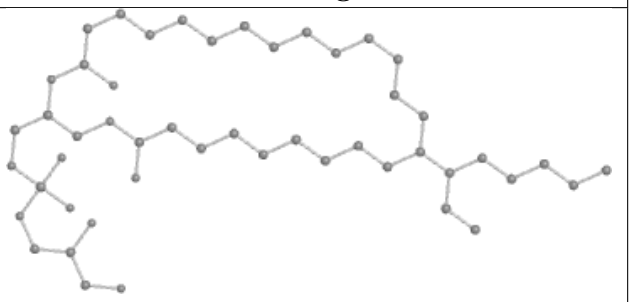
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV A 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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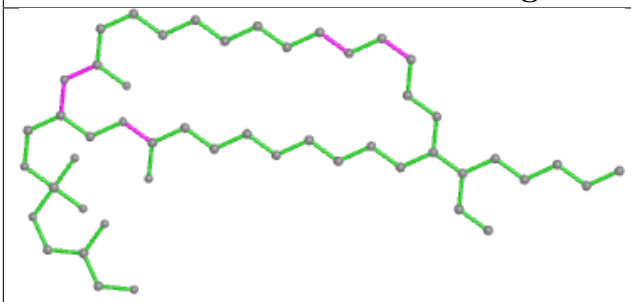
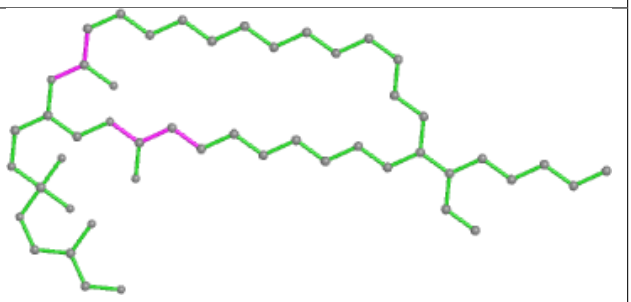
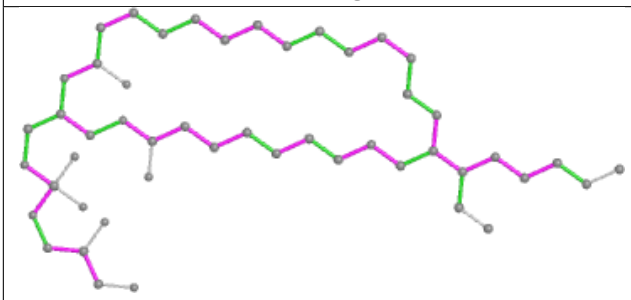
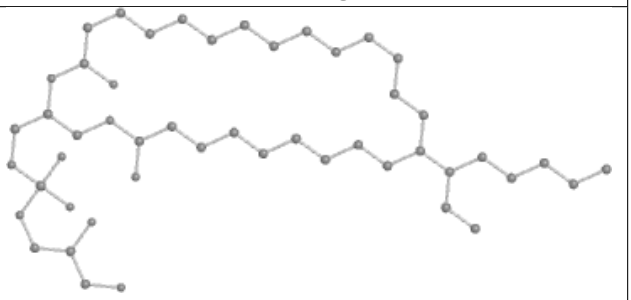
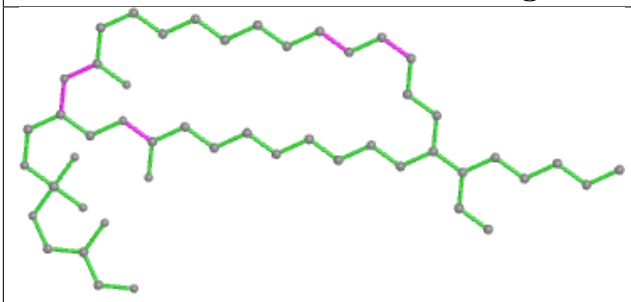
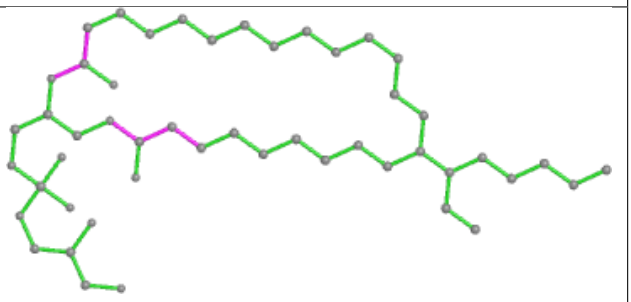
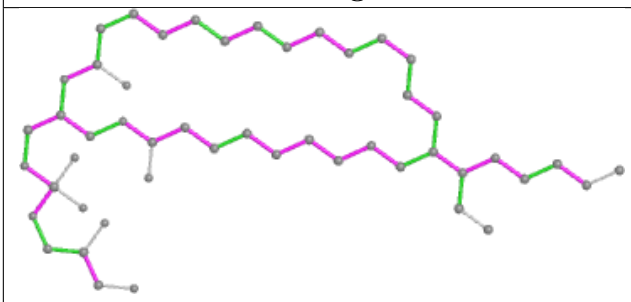
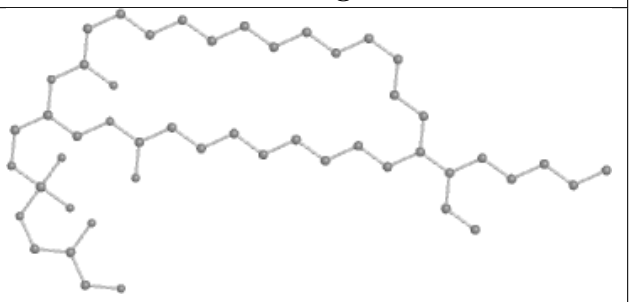
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV D 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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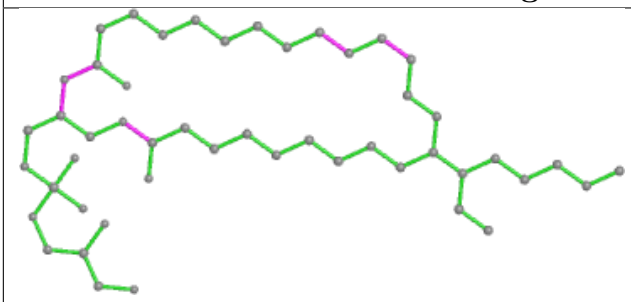
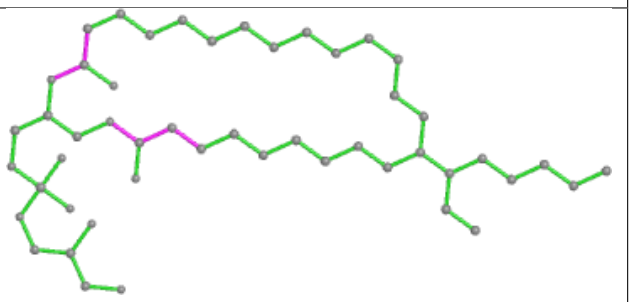
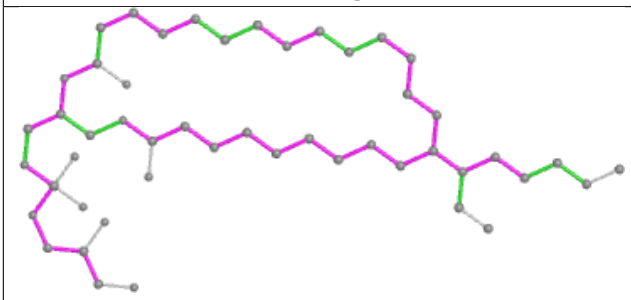
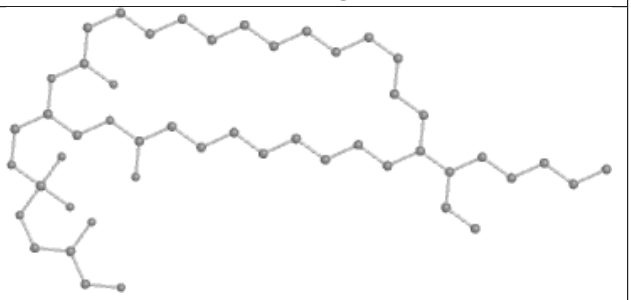
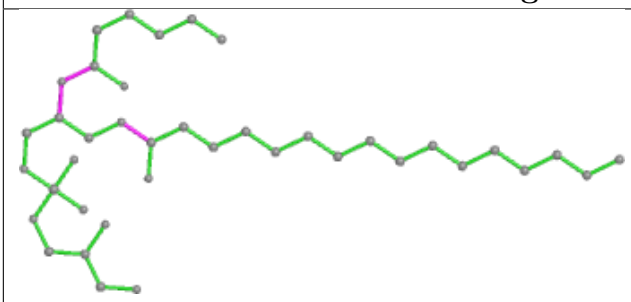
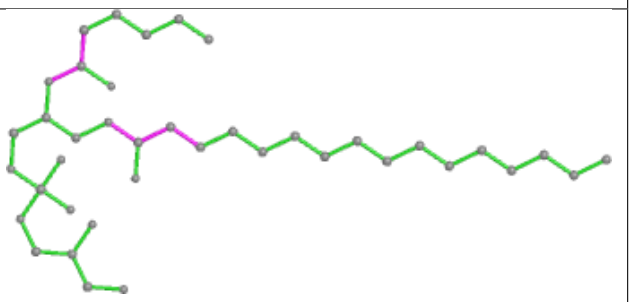
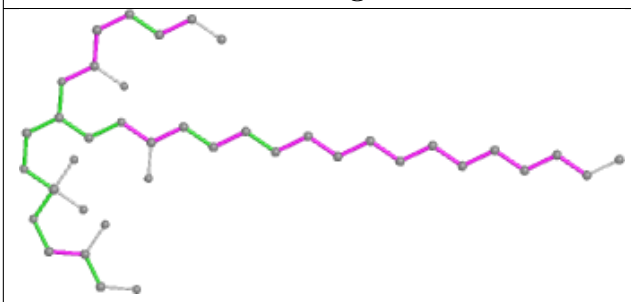
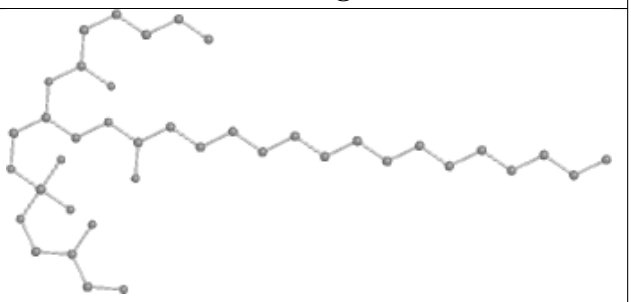
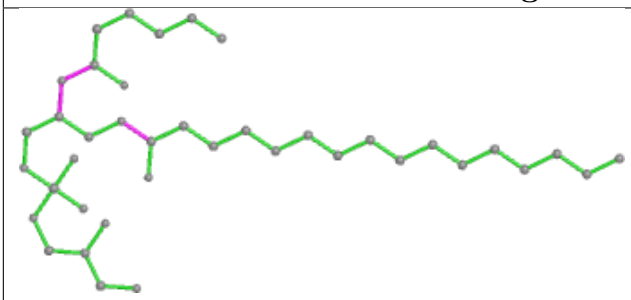
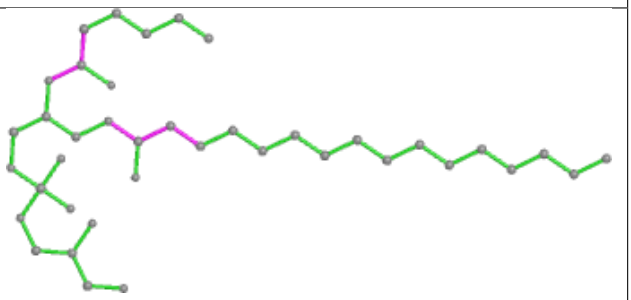
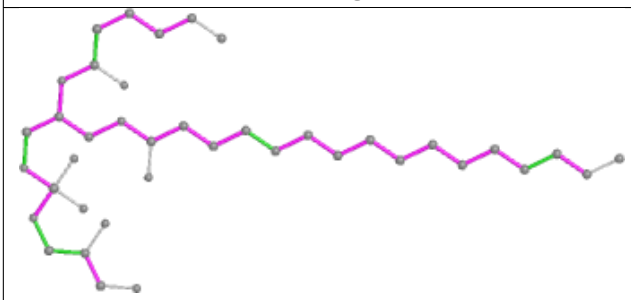
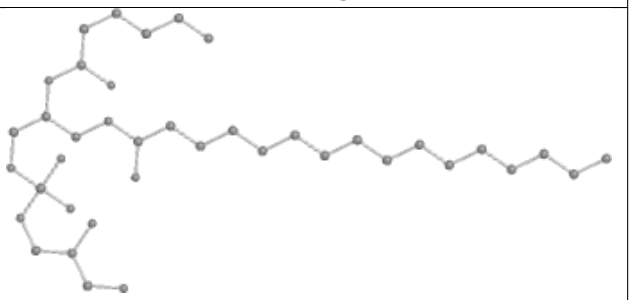
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV A 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV D 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

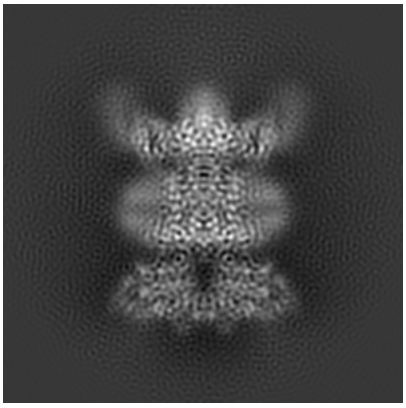
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30525. These allow visual inspection of the internal detail of the map and identification of artifacts.

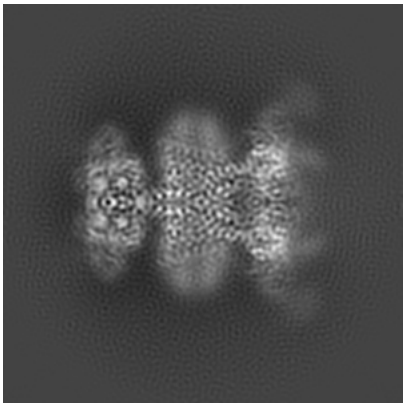
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

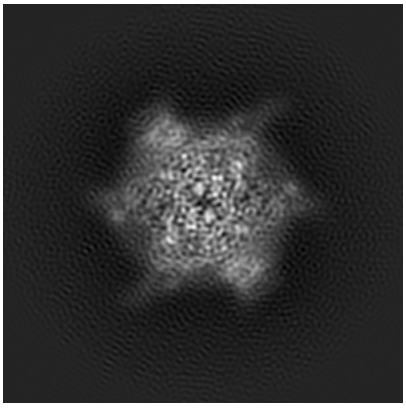
6.1.1 Primary map



X



Y

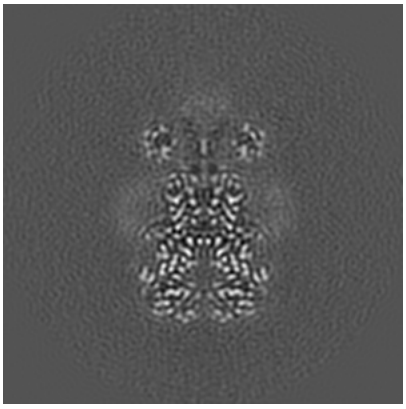


Z

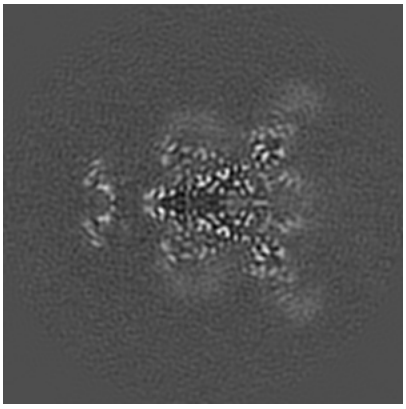
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

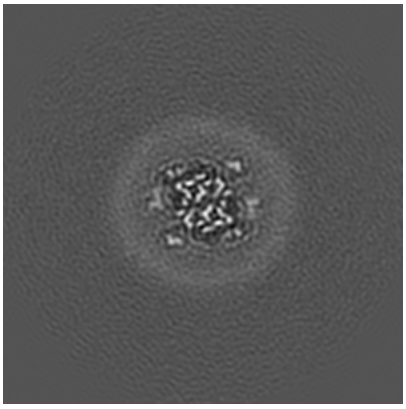
6.2.1 Primary map



X Index: 100



Y Index: 100

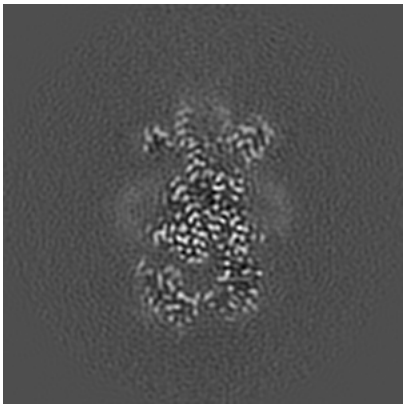


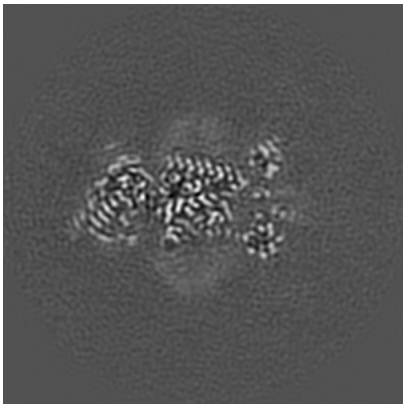
Z Index: 100

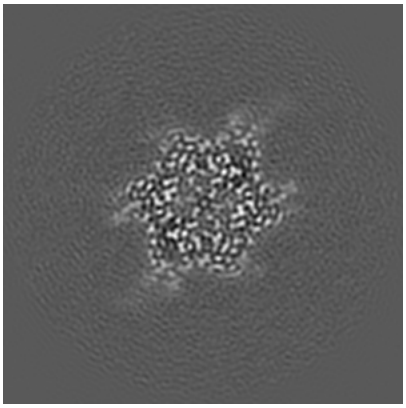
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 95

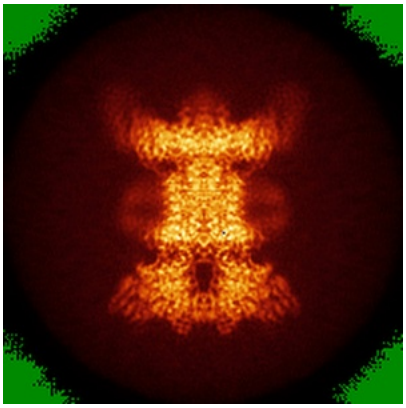

Y Index: 87

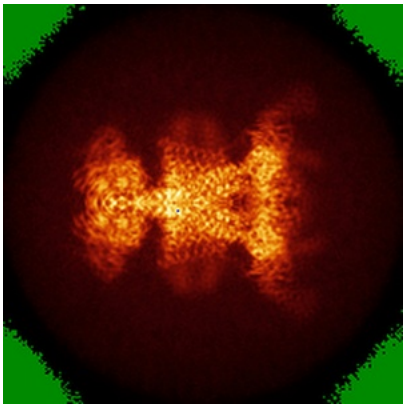

Z Index: 130

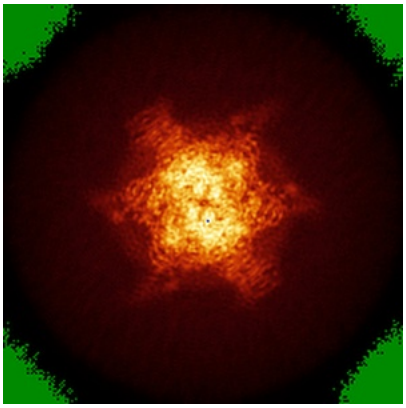
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

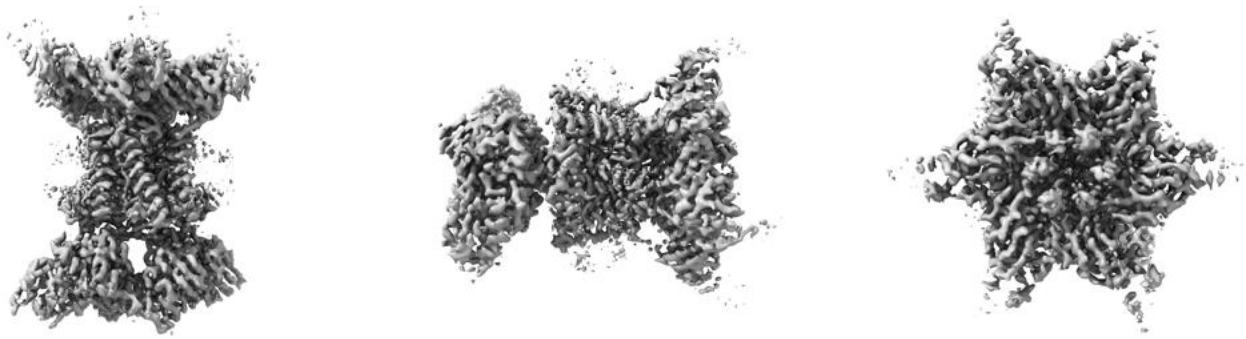

Y


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

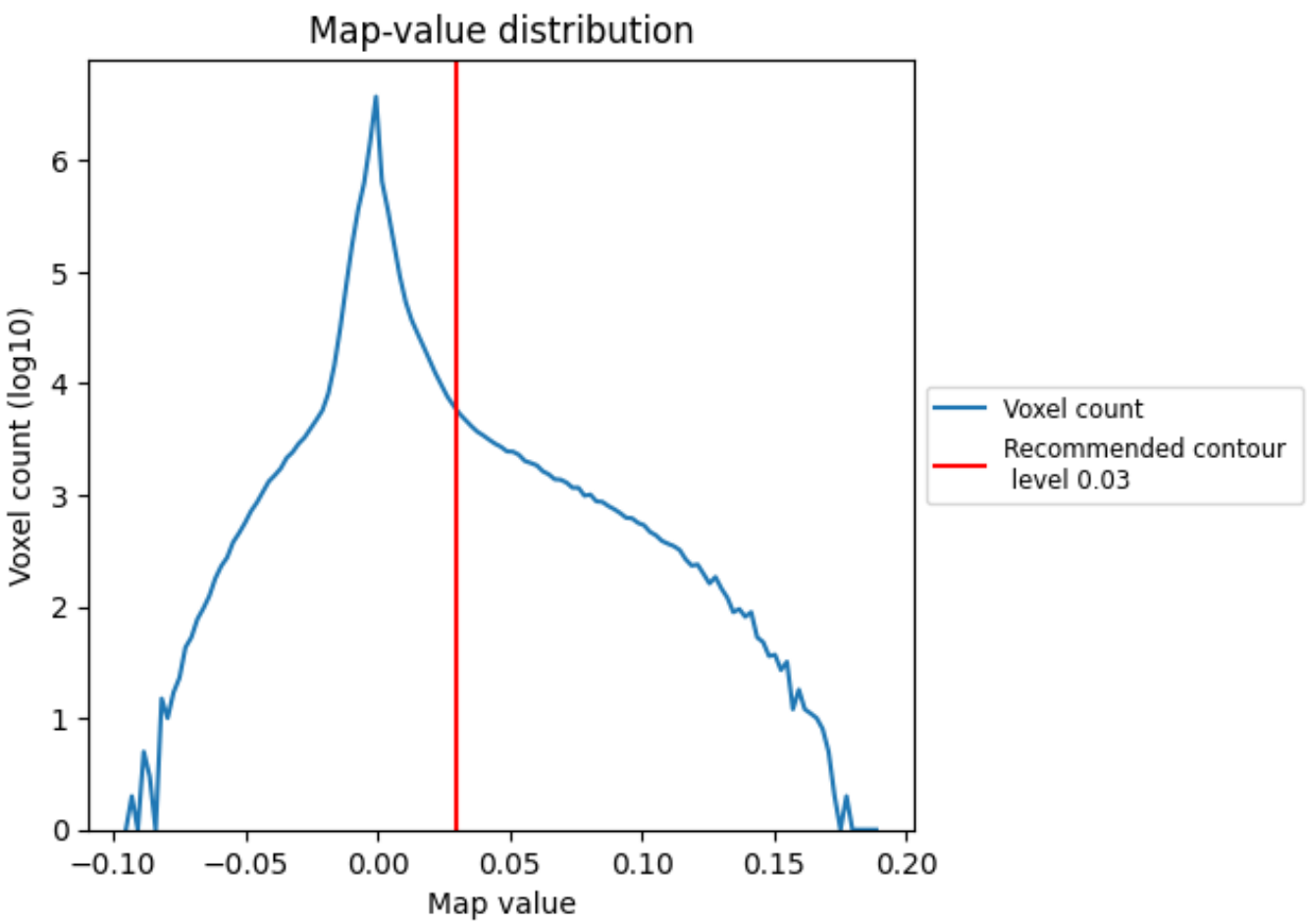
6.6 Mask visualisation (i)

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

7 Map analysis (i)

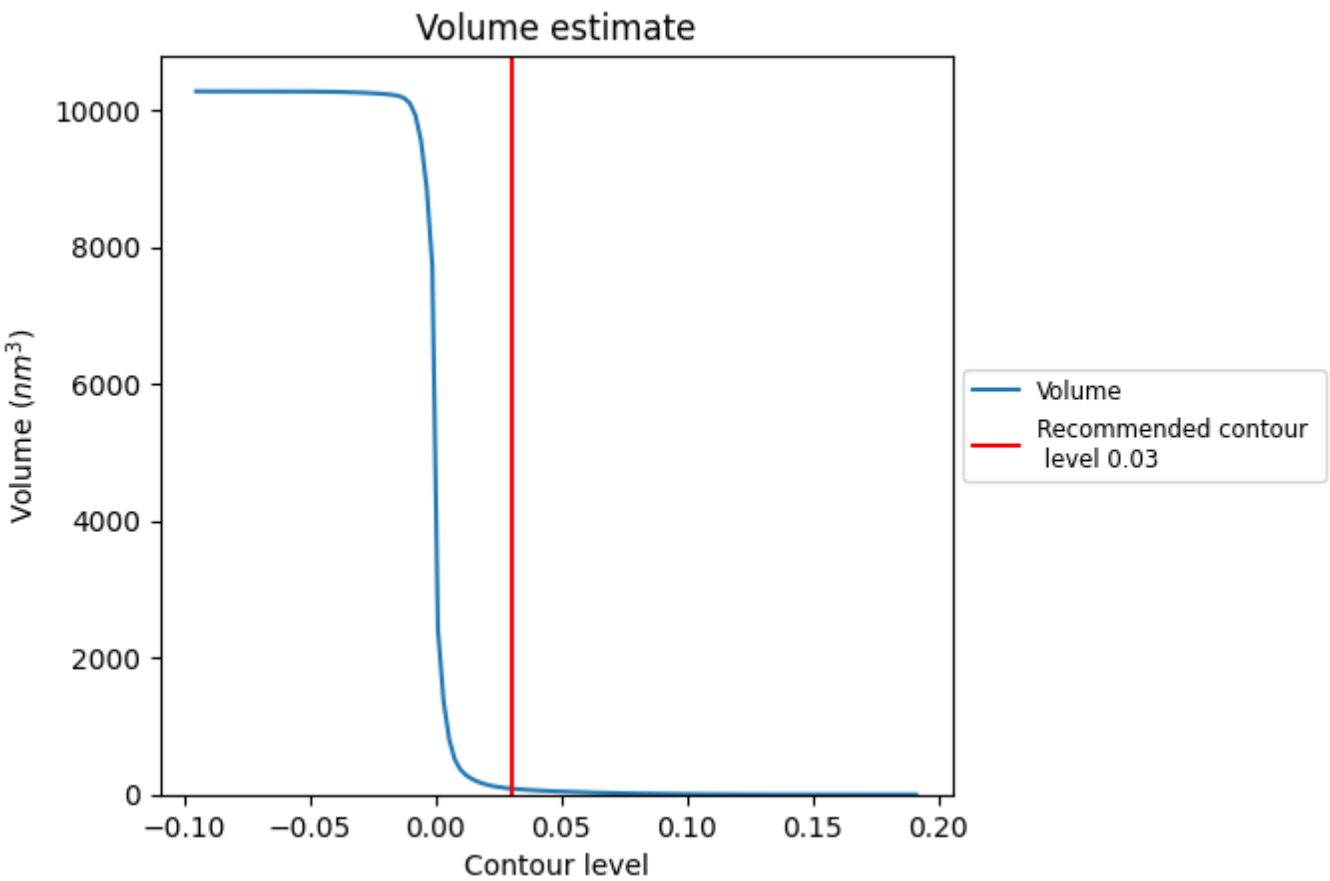
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

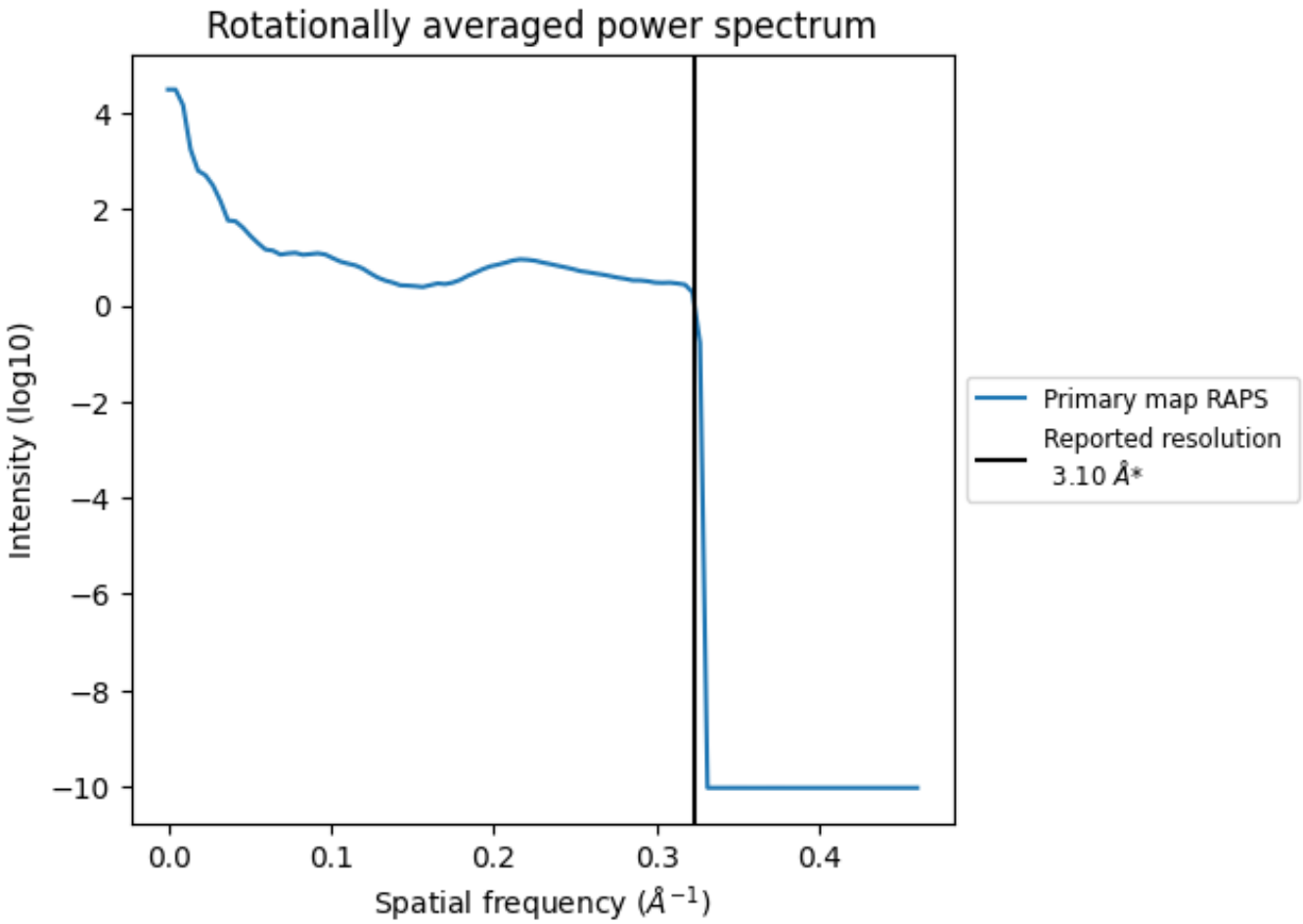
7.2 Volume estimate (i)



The volume at the recommended contour level is 88 nm^3; this corresponds to an approximate mass of 79 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 0.323 Å^{-1}

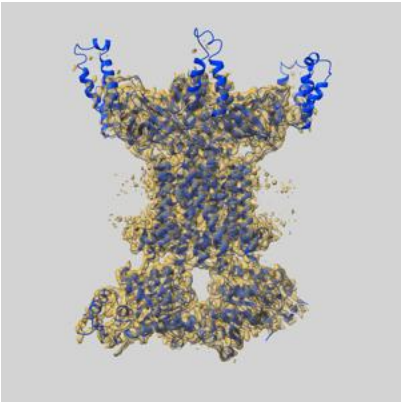
8 Fourier-Shell correlation (i)

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

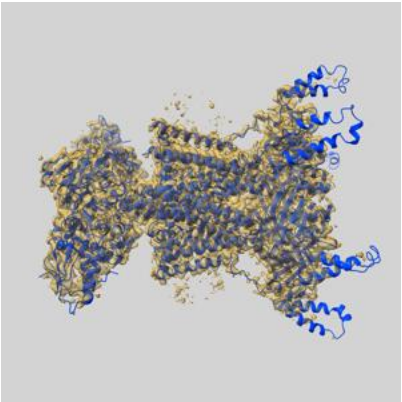
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30525 and PDB model 7D06. Per-residue inclusion information can be found in section 3 on page 7.

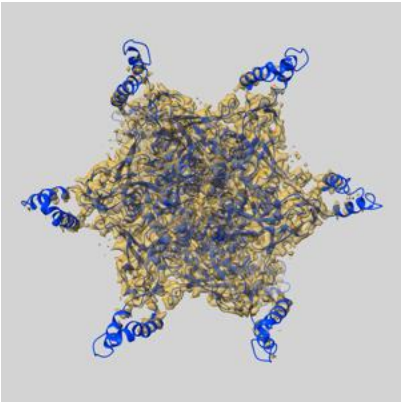
9.1 Map-model overlay (i)



X



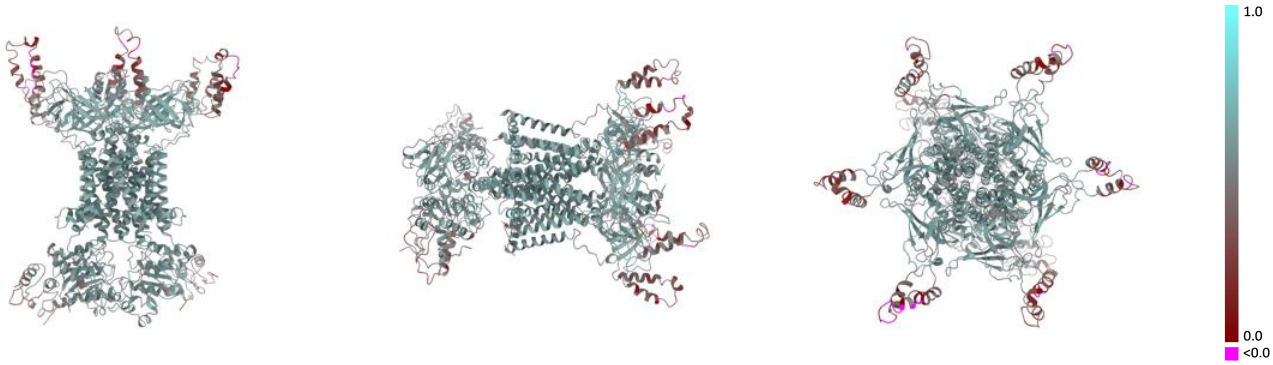
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

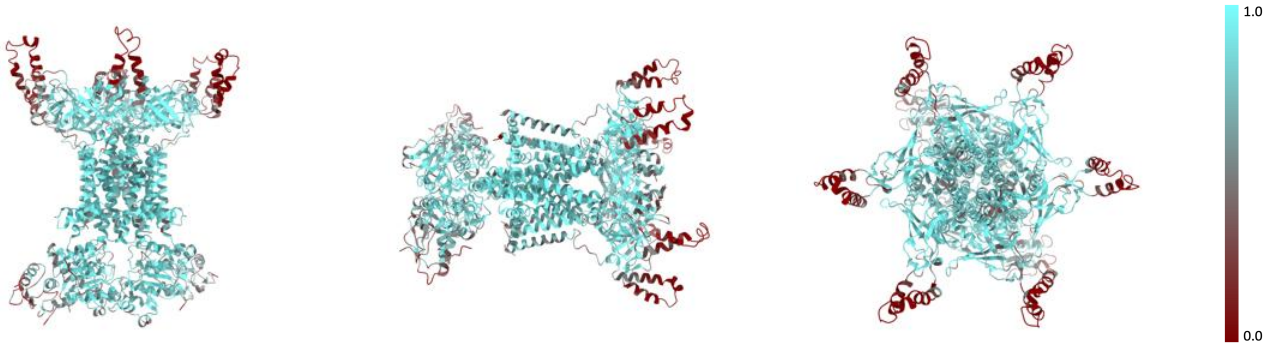
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

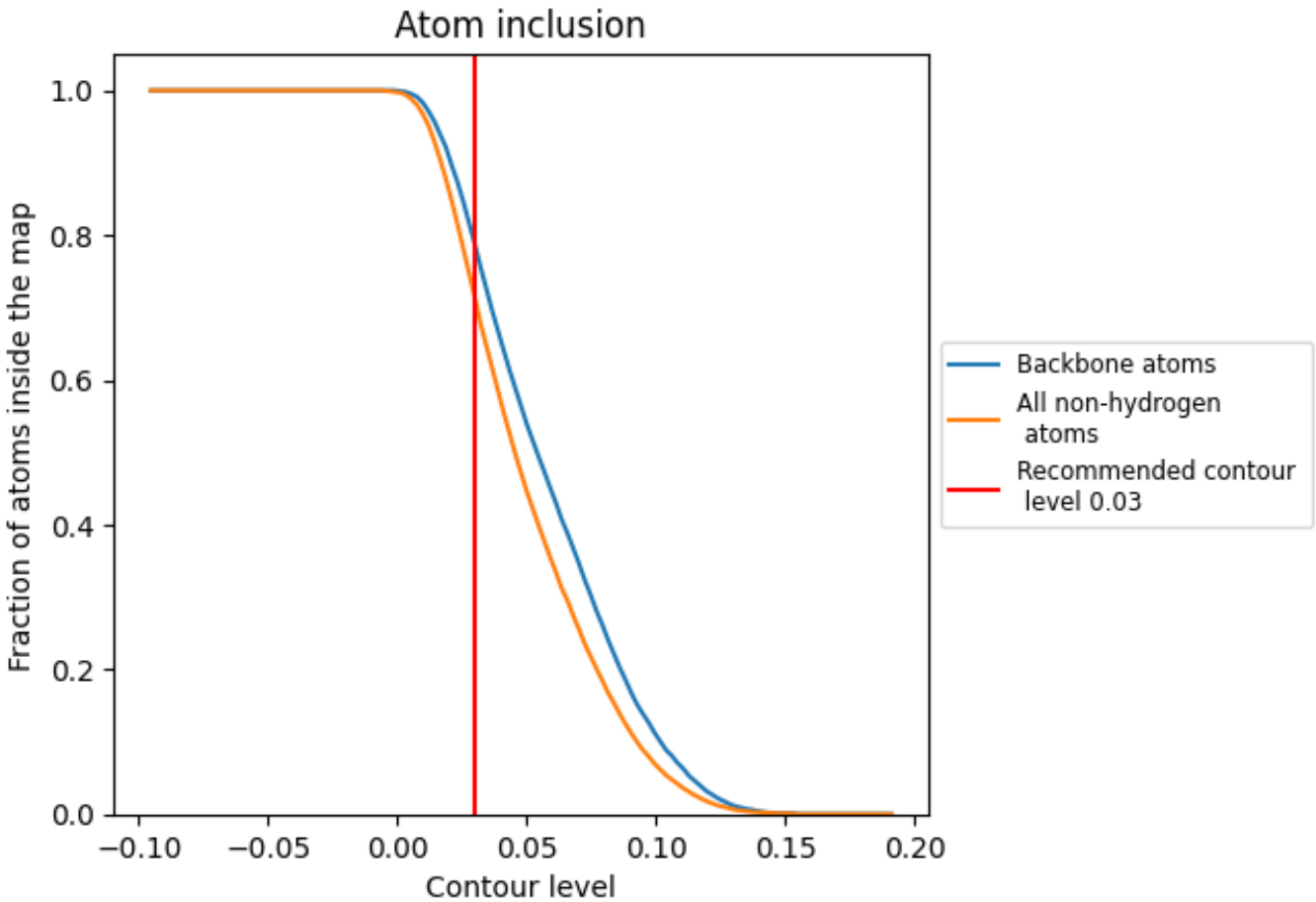
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.5330
A	0.8580	0.5940
B	0.7640	0.5380
C	0.5030	0.4560
D	0.8620	0.5930
E	0.7650	0.5430
F	0.4890	0.4340
G	0.6540	0.5150
H	0.6720	0.5030
I	0.6280	0.5110
J	0.6620	0.5250
K	0.6720	0.5180
L	0.6320	0.5090