Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 11:52 PM JST

PDB ID	:	6K7Y
EMDB ID	:	EMD-9945
Title	:	Intact human mitochondrial calcium uniporter complex with MICU1/MICU2 subunits
Authors	:	Zhuo, W.; Zhou, H.; Yang, M.
Deposited on	:	2019-06-10
Resolution	:	3.60 Å(reported)
Based on initial models	:	4NSC, 6K7X, 6AGH

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:

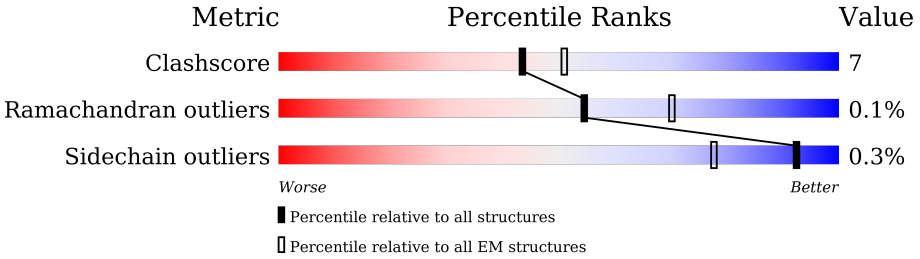
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.60 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	276	82% 17%
1	B	276	5% 84% 14%
1	C	276	88% 12%
1	D	276	87% 12%
1	N	276	84% 15%
1	O	276	5% 86% 13%
1	P	276	87% 13%
1	Q	276	87% 12%

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Mol	Chain	Length	Quality of chain
2	E	54	85% 15%
2	F	54	98%
2	G	54	6% 91% 9%
2	H	54	6% 85% 15%
2	R	54	87% 13%
2	S	54	91% 9%
2	T	54	6% 91% 9%
2	U	54	6% 85% 15%
3	I	476	50% 13% 36%
3	V	476	52% 12% 36%
4	J	336	76% 19% 5%
4	W	336	75% 20% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 32956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Calcium uniporter protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	273	2253	1443	392	410	8	0	0
1	B	273	2253	1443	392	410	8	0	0
1	C	276	2274	1456	396	414	8	0	0
1	D	273	2253	1443	392	410	8	0	0
1	N	273	2253	1443	392	410	8	0	0
1	O	273	2253	1443	392	410	8	0	0
1	P	276	2274	1456	396	414	8	0	0
1	Q	273	2253	1443	392	410	8	0	0

- Molecule 2 is a protein called Essential MCU regulator, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	54	423	286	66	70	1	0	0
2	F	54	423	286	66	70	1	0	0
2	G	54	423	286	66	70	1	0	0
2	H	54	423	286	66	70	1	0	0
2	R	54	423	286	66	70	1	0	0
2	S	54	423	286	66	70	1	0	0
2	T	54	423	286	66	70	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	U	54	423	286	66	70	1	0	0

- Molecule 3 is a protein called Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	306	2406	1533	407	453	13	0	0
3	V	306	2406	1533	407	453	13	0	0

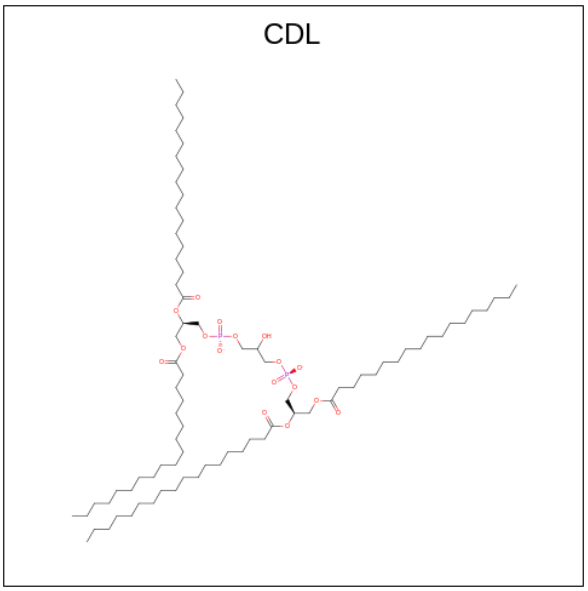
- Molecule 4 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	319	2602	1667	444	474	17	0	0
4	W	319	2602	1667	444	474	17	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

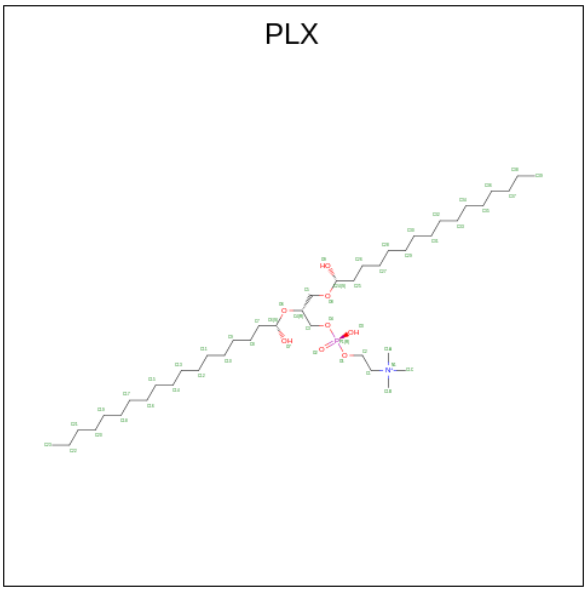
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0
5	N	1	1	1	0

- Molecule 6 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
6	A	1	100	81	17	2	0
6	B	1	100	81	17	2	0
6	C	1	100	81	17	2	0
6	H	1	100	81	17	2	0
6	N	1	100	81	17	2	0
6	O	1	100	81	17	2	0
6	P	1	100	81	17	2	0
6	Q	1	100	81	17	2	0

- Molecule 7 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	A	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	B	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	B	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	C	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	C	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	C	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	D	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	N	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	N	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	O	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	O	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	P	1	52	42	1	8	1	0
			Total	C	N	O	P	
7	P	1	34	26	1	6	1	0

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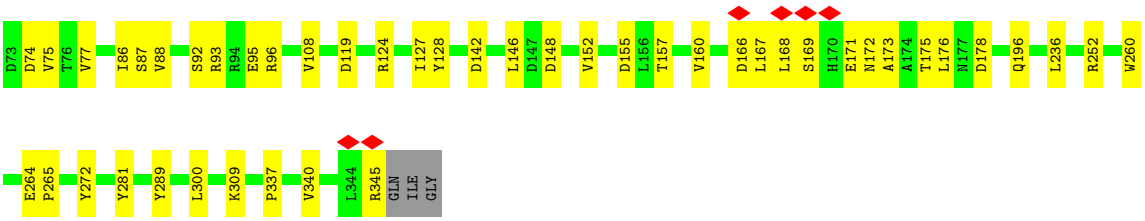
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	P	1	34	26	1	6	1	0
			Total	C	N	O	P	
7	Q	1	52	42	1	8	1	0

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.

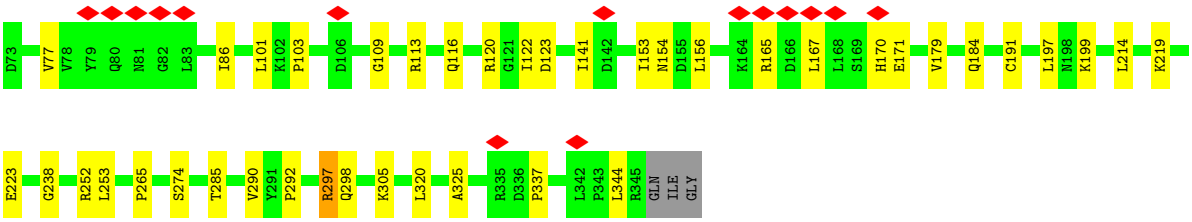
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain A:



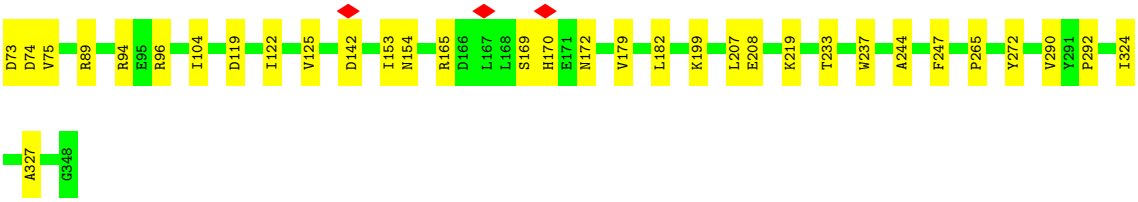
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain B:



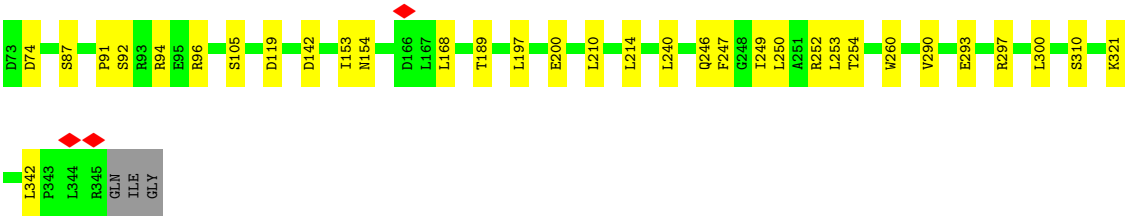
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain C:



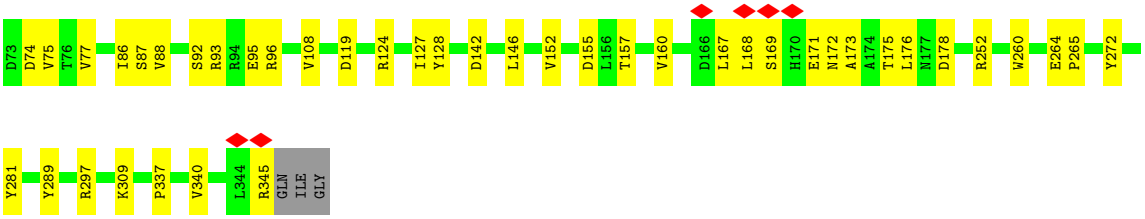
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain D:



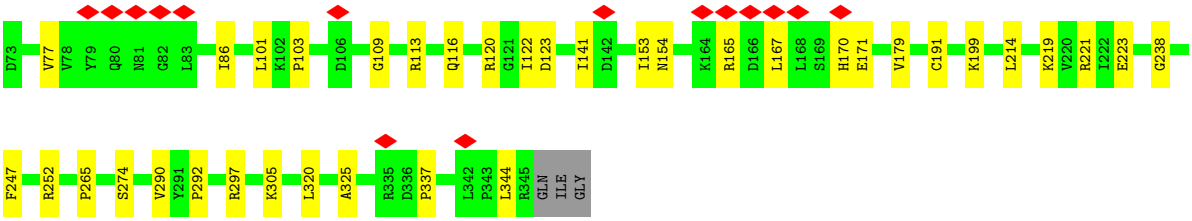
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain N:



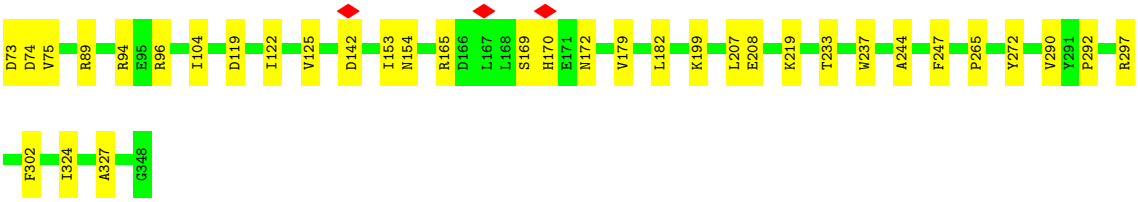
• Molecule 1: Calcium uniporter protein, mitochondrial

Chain O:



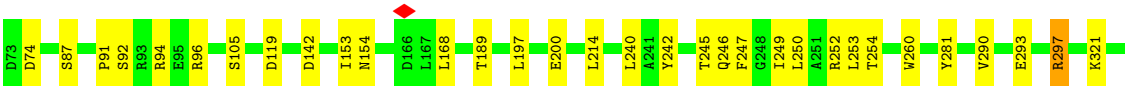
• Molecule 1: Calcium uniporter protein, mitochondrial

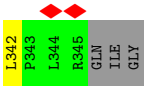
Chain P:



• Molecule 1: Calcium uniporter protein, mitochondrial

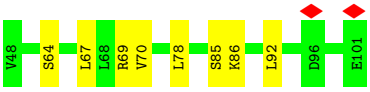
Chain Q:





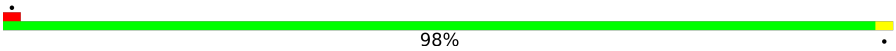
• Molecule 2: Essential MCU regulator, mitochondrial

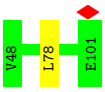
Chain E:



• Molecule 2: Essential MCU regulator, mitochondrial

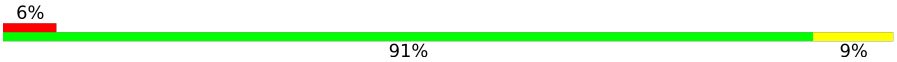
Chain F:





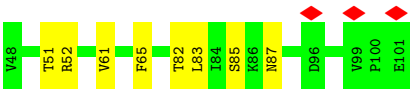
• Molecule 2: Essential MCU regulator, mitochondrial

Chain G:



• Molecule 2: Essential MCU regulator, mitochondrial

Chain H:

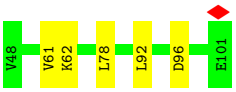


• Molecule 2: Essential MCU regulator, mitochondrial

Chain R:

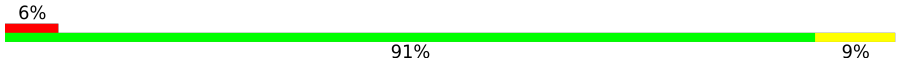
• Molecule 2: Essential MCU regulator, mitochondrial

Chain S:



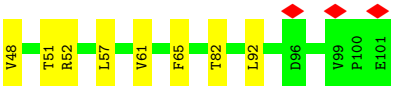
• Molecule 2: Essential MCU regulator, mitochondrial

Chain T:



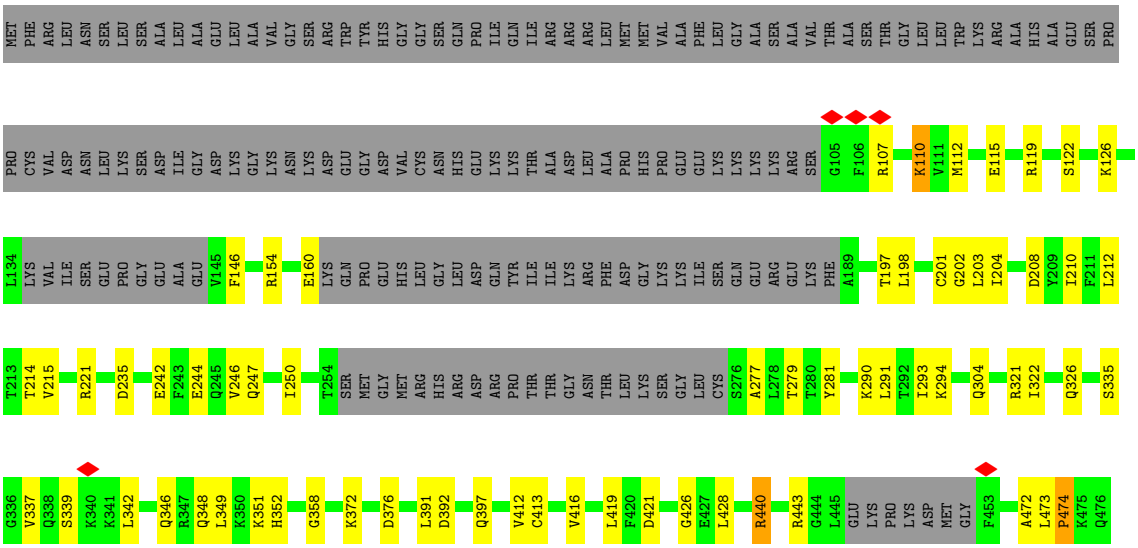
• Molecule 2: Essential MCU regulator, mitochondrial

Chain U:



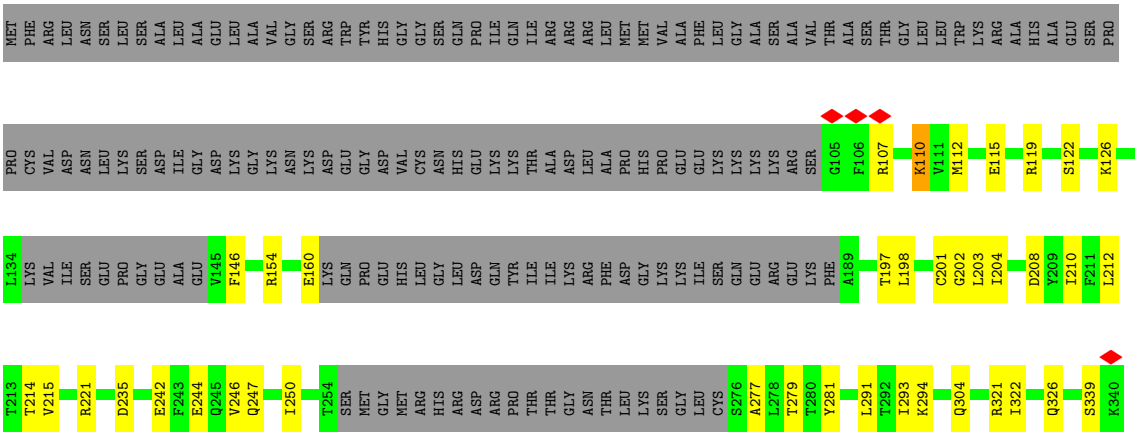
• Molecule 3: Calcium uptake protein 1, mitochondrial

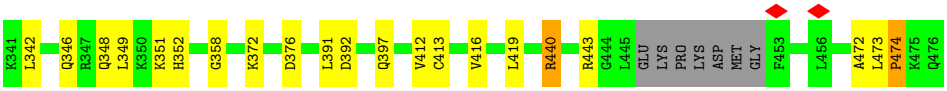
Chain I:



• Molecule 3: Calcium uptake protein 1, mitochondrial

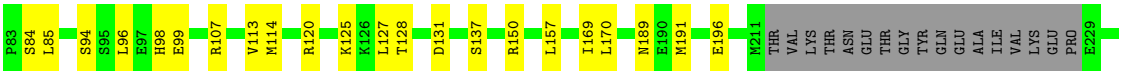
Chain V:

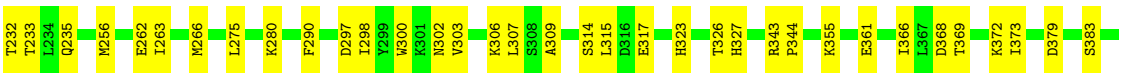


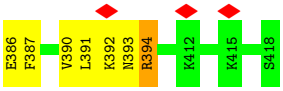


• Molecule 4: Calcium uptake protein 2, mitochondrial

Chain J:

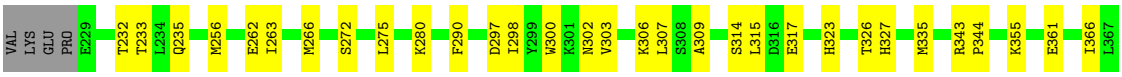


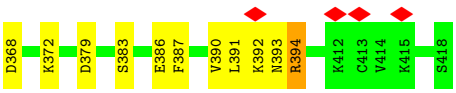




• Molecule 4: Calcium uptake protein 2, mitochondrial

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91728	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 K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	78.091	Depositor
Minimum map value	-39.142	Depositor
Average map value	0.103	Depositor
Map value standard deviation	1.837	Depositor
Recommended contour level	12.0	Depositor
Map size (Å)	392.75998, 392.75998, 392.75998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: CA, PLX, CDL

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	0.33	0/2299	0.42	0/3113
1	B	0.32	0/2299	0.44	0/3113
1	C	0.32	0/2320	0.44	0/3141
1	D	0.33	0/2299	0.42	0/3113
1	N	0.33	0/2299	0.42	0/3113
1	O	0.31	0/2299	0.45	0/3113
1	P	0.32	0/2320	0.44	0/3141
1	Q	0.33	0/2299	0.42	0/3113
2	E	0.30	0/433	0.43	0/588
2	F	0.30	0/433	0.40	0/588
2	G	0.30	0/433	0.44	0/588
2	H	0.30	0/433	0.41	0/588
2	R	0.30	0/433	0.42	0/588
2	S	0.30	0/433	0.40	0/588
2	T	0.30	0/433	0.44	0/588
2	U	0.30	0/433	0.41	0/588
3	I	0.28	0/2446	0.42	0/3285
3	V	0.28	0/2446	0.42	0/3285
4	J	0.30	0/2656	0.44	0/3554
4	W	0.30	0/2656	0.44	0/3554
All	All	0.31	0/32102	0.43	0/43342

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	2253	0	2283	36	0
1	B	2253	0	2283	38	0
1	C	2274	0	2305	25	0
1	D	2253	0	2283	28	0
1	N	2253	0	2283	33	0
1	O	2253	0	2283	30	0
1	P	2274	0	2305	28	0
1	Q	2253	0	2283	28	0
2	E	423	0	454	8	0
2	F	423	0	454	1	0
2	G	423	0	454	6	0
2	H	423	0	454	7	0
2	R	423	0	454	7	0
2	S	423	0	454	5	0
2	T	423	0	454	4	0
2	U	423	0	454	6	0
3	I	2406	0	2310	42	0
3	V	2406	0	2310	38	0
4	J	2602	0	2531	47	0
4	W	2602	0	2531	52	0
5	A	1	0	0	0	0
5	N	1	0	0	0	0
6	A	100	0	156	6	0
6	B	100	0	155	6	0
6	C	100	0	155	6	0
6	H	100	0	156	6	0
6	N	100	0	156	6	0
6	O	100	0	155	6	0
6	P	100	0	155	9	0
6	Q	100	0	156	10	0
7	A	86	0	141	3	0
7	B	86	0	141	5	0
7	C	120	0	194	5	0
7	D	52	0	88	4	0
7	N	86	0	141	1	0
7	O	86	0	141	4	0
7	P	120	0	194	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Q	52	0	88	3	0
All	All	32956	0	33994	465	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 7.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HH11	2:G:60:PRO:HB2	1.38	0.88
1:Q:252:ARG:HH11	2:R:86:LYS:HG3	1.45	0.82
1:D:252:ARG:HH11	2:E:86:LYS:HG3	1.45	0.79
1:B:274:SER:HB2	7:B:402:PLX:H24	1.68	0.76
1:O:274:SER:HB2	7:O:402:PLX:H24	1.68	0.76
1:N:297:ARG:NH2	6:N:402:CDL:OA3	2.20	0.74
6:B:401:CDL:H532	6:B:401:CDL:H582	1.69	0.74
4:J:343:ARG:NH2	4:J:344:PRO:O	2.22	0.73
6:O:401:CDL:H582	6:O:401:CDL:H532	1.69	0.73
6:H:201:CDL:HB31	6:H:201:CDL:H512	1.69	0.73
6:Q:401:CDL:HB31	6:Q:401:CDL:H512	1.69	0.73
1:B:103:PRO:HD2	1:C:208:GLU:OE1	1.89	0.73
1:A:172:ASN:OD1	1:A:173:ALA:N	2.22	0.73
1:N:172:ASN:OD1	1:N:173:ALA:N	2.22	0.72
1:Q:297:ARG:NH2	6:Q:401:CDL:OA4	2.22	0.72
4:W:343:ARG:NH2	4:W:344:PRO:O	2.22	0.72
1:B:297:ARG:NH1	2:G:60:PRO:HB2	2.04	0.71
1:O:103:PRO:HD2	1:P:208:GLU:OE1	1.89	0.71
1:B:290:VAL:HG12	1:B:292:PRO:HD2	1.72	0.71
4:J:170:LEU:HD11	4:J:263:ILE:HG13	1.74	0.70
4:W:94:SER:O	4:W:120:ARG:NH2	2.24	0.70
3:I:397:GLN:NE2	3:I:413:CYS:SG	2.65	0.70
4:J:94:SER:O	4:J:120:ARG:NH2	2.24	0.69
1:O:290:VAL:HG12	1:O:292:PRO:HD2	1.72	0.69
4:W:150:ARG:NH1	4:W:262:GLU:OE2	2.25	0.69
4:W:170:LEU:HD11	4:W:263:ILE:HG13	1.74	0.69
3:I:201:CYS:SG	3:I:202:GLY:N	2.66	0.69
3:V:397:GLN:NE2	3:V:413:CYS:SG	2.65	0.68
1:N:340:VAL:HA	1:N:345:ARG:HH11	1.58	0.68
4:J:150:ARG:NH1	4:J:262:GLU:OE2	2.25	0.68
1:P:297:ARG:NH1	6:P:401:CDL:OA4	2.24	0.68
1:A:340:VAL:HA	1:A:345:ARG:HH11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:201:CYS:SG	3:V:202:GLY:N	2.66	0.68
1:P:73:ASP:HB2	1:P:89:ARG:HH11	1.60	0.67
4:W:302:ASN:OD1	4:W:306:LYS:NZ	2.24	0.67
6:O:401:CDL:H132	6:O:401:CDL:H731	1.77	0.67
4:J:290:PHE:HE1	4:J:391:LEU:HD13	1.61	0.66
4:J:107:ARG:HH11	4:W:275:LEU:HD22	1.61	0.66
1:A:77:VAL:HG22	1:A:86:ILE:HG12	1.78	0.66
6:B:401:CDL:H132	6:B:401:CDL:H731	1.77	0.66
6:C:401:CDL:H542	7:C:402:PLX:H152	1.77	0.66
1:N:176:LEU:HD21	1:P:182:LEU:HD23	1.78	0.66
4:W:290:PHE:HE1	4:W:391:LEU:HD13	1.61	0.66
3:V:122:SER:HB2	3:V:126:LYS:HD3	1.77	0.66
1:N:77:VAL:HG22	1:N:86:ILE:HG12	1.78	0.66
1:C:73:ASP:HB2	1:C:89:ARG:HH11	1.60	0.65
4:W:298:ILE:O	4:W:302:ASN:ND2	2.29	0.65
4:J:298:ILE:O	4:J:302:ASN:ND2	2.29	0.65
4:J:275:LEU:HD22	4:W:107:ARG:HH11	1.61	0.65
1:A:176:LEU:HD21	1:C:182:LEU:HD23	1.78	0.64
3:I:122:SER:HB2	3:I:126:LYS:HD3	1.77	0.64
6:P:401:CDL:H542	7:P:402:PLX:H152	1.80	0.64
4:J:302:ASN:OD1	4:J:306:LYS:NZ	2.24	0.63
1:N:337:PRO:O	1:O:199:LYS:NZ	2.31	0.63
3:V:293:ILE:HG23	3:V:294:LYS:HD3	1.81	0.62
1:A:337:PRO:O	1:B:199:LYS:NZ	2.31	0.62
6:C:401:CDL:H192	7:C:403:PLX:H211	1.81	0.62
1:B:77:VAL:HG22	1:B:86:ILE:HG12	1.82	0.62
3:I:293:ILE:HG23	3:I:294:LYS:HD3	1.81	0.61
1:O:77:VAL:HG22	1:O:86:ILE:HG12	1.82	0.61
1:O:179:VAL:HG11	1:Q:168:LEU:HD11	1.83	0.61
6:P:401:CDL:CB7	6:P:401:CDL:HB32	2.31	0.61
6:C:401:CDL:CB7	6:C:401:CDL:HB32	2.31	0.60
4:J:125:LYS:HD3	4:W:309:ALA:HB3	1.83	0.60
4:W:290:PHE:O	4:W:393:ASN:ND2	2.35	0.60
1:B:179:VAL:HG11	1:D:168:LEU:HD11	1.83	0.60
1:Q:91:PRO:O	1:Q:94:ARG:NH1	2.35	0.60
4:W:392:LYS:O	4:W:394:ARG:NH2	2.35	0.60
4:J:309:ALA:HB3	4:W:125:LYS:HD3	1.83	0.60
4:J:392:LYS:O	4:J:394:ARG:NH2	2.35	0.60
1:B:305:LYS:NZ	6:B:401:CDL:OB4	2.30	0.59
3:I:126:LYS:H	3:I:126:LYS:HD2	1.68	0.59
3:I:346:GLN:HA	3:I:349:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:290:PHE:O	4:J:393:ASN:ND2	2.35	0.58
6:A:402:CDL:OB2	6:A:402:CDL:HB61	2.03	0.58
3:V:126:LYS:H	3:V:126:LYS:HD2	1.68	0.58
1:D:91:PRO:O	1:D:94:ARG:NH1	2.35	0.58
3:V:346:GLN:HA	3:V:349:LEU:HD12	1.85	0.58
1:D:153:ILE:HG22	1:D:154:ASN:H	1.68	0.58
4:J:96:LEU:HB3	4:J:127:LEU:HD11	1.86	0.58
6:N:402:CDL:HA22	2:S:62:LYS:HD3	1.86	0.58
1:D:297:ARG:NH1	2:H:61:VAL:O	2.37	0.58
1:B:86:ILE:HD12	1:B:101:LEU:HD21	1.85	0.57
3:I:349:LEU:HD11	3:I:419:LEU:HD12	1.85	0.57
1:Q:153:ILE:HG22	1:Q:154:ASN:H	1.68	0.57
4:J:386:GLU:O	4:J:390:VAL:HB	2.04	0.57
6:N:402:CDL:OB2	6:N:402:CDL:HB61	2.03	0.57
1:O:297:ARG:HD2	2:T:60:PRO:HG2	1.86	0.57
4:W:386:GLU:O	4:W:390:VAL:HB	2.05	0.57
1:O:86:ILE:HD12	1:O:101:LEU:HD21	1.86	0.57
3:V:349:LEU:HD11	3:V:419:LEU:HD12	1.85	0.57
4:W:96:LEU:HB3	4:W:127:LEU:HD11	1.86	0.57
1:B:297:ARG:HH11	2:G:60:PRO:CB	2.13	0.57
6:A:402:CDL:H532	7:A:403:PLX:H141	1.87	0.56
6:O:401:CDL:HA32	6:O:401:CDL:OA7	2.05	0.56
1:D:74:ASP:O	1:D:96:ARG:NH2	2.39	0.56
1:Q:74:ASP:O	1:Q:96:ARG:NH2	2.39	0.55
6:B:401:CDL:OA7	6:B:401:CDL:HA32	2.05	0.55
6:A:402:CDL:C53	7:A:403:PLX:H141	2.37	0.55
1:B:123:ASP:H	1:B:154:ASN:ND2	2.05	0.55
1:D:200:GLU:HG3	1:D:342:LEU:HD11	1.88	0.55
1:O:123:ASP:H	1:O:154:ASN:ND2	2.05	0.55
1:B:337:PRO:HG2	1:B:344:LEU:HD12	1.89	0.54
3:V:112:MET:O	3:V:115:GLU:HG3	2.07	0.54
1:P:207:LEU:HD13	1:P:327:ALA:HB3	1.89	0.54
1:Q:200:GLU:HG3	1:Q:342:LEU:HD11	1.88	0.54
1:P:153:ILE:HG22	1:P:154:ASN:H	1.73	0.54
1:P:122:ILE:HG22	1:P:125:VAL:HG22	1.90	0.54
1:C:74:ASP:O	1:C:96:ARG:NH2	2.40	0.53
3:I:112:MET:O	3:I:115:GLU:HG3	2.07	0.53
1:C:122:ILE:HG22	1:C:125:VAL:HG22	1.90	0.53
3:I:277:ALA:HB3	3:I:279:THR:HG23	1.90	0.53
3:V:210:ILE:O	3:V:214:THR:HG23	2.09	0.53
1:D:297:ARG:NH2	6:H:201:CDL:OA4	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:210:ILE:O	3:I:214:THR:HG23	2.09	0.53
1:C:153:ILE:HG22	1:C:154:ASN:H	1.72	0.53
3:I:212:LEU:HA	3:I:215:VAL:HG12	1.90	0.53
1:O:337:PRO:HG2	1:O:344:LEU:HD12	1.89	0.53
1:C:207:LEU:HD13	1:C:327:ALA:HB3	1.90	0.53
1:A:92:SER:OG	1:A:119:ASP:OD1	2.19	0.53
6:C:401:CDL:H861	2:E:67:LEU:HD23	1.90	0.53
1:N:176:LEU:HD22	1:P:179:VAL:HG13	1.90	0.53
1:A:176:LEU:HD22	1:C:179:VAL:HG13	1.90	0.52
3:V:154:ARG:NH2	3:V:160:GLU:O	2.42	0.52
1:A:171:GLU:OE1	1:A:171:GLU:N	2.42	0.52
1:O:116:GLN:HA	1:O:122:ILE:HD11	1.92	0.52
3:I:154:ARG:NH2	3:I:160:GLU:O	2.42	0.52
6:P:401:CDL:HB32	6:P:401:CDL:C71	2.40	0.52
3:V:212:LEU:HA	3:V:215:VAL:HG12	1.90	0.52
3:V:277:ALA:HB3	3:V:279:THR:HG23	1.90	0.52
4:W:317:GLU:HB3	4:W:366:ILE:HD11	1.91	0.52
1:Q:249:ILE:HG13	2:R:85:SER:HB2	1.92	0.52
1:Q:297:ARG:NH1	2:U:61:VAL:O	2.42	0.52
4:W:314:SER:OG	4:W:315:LEU:N	2.43	0.52
3:V:146:PHE:HB3	3:V:203:LEU:HB3	1.92	0.52
4:W:114:MET:SD	4:W:266:MET:HB3	2.50	0.52
4:J:114:MET:SD	4:J:266:MET:HB3	2.50	0.51
6:C:401:CDL:HB32	6:C:401:CDL:C71	2.40	0.51
4:J:150:ARG:HH11	4:J:266:MET:HE2	1.75	0.51
3:I:146:PHE:HB3	3:I:203:LEU:HB3	1.92	0.51
1:N:171:GLU:N	1:N:171:GLU:OE1	2.42	0.51
2:H:65:PHE:H	6:H:201:CDL:H842	1.75	0.51
1:B:153:ILE:HG22	1:B:154:ASN:H	1.76	0.51
4:W:157:LEU:N	4:W:233:THR:OG1	2.39	0.51
4:J:157:LEU:N	4:J:233:THR:OG1	2.39	0.50
1:N:152:VAL:HG22	1:N:157:THR:HG22	1.93	0.50
1:P:74:ASP:O	1:P:96:ARG:NH2	2.40	0.50
1:D:249:ILE:HG13	2:E:85:SER:HB2	1.92	0.50
4:J:317:GLU:HB3	4:J:366:ILE:HD11	1.91	0.50
6:A:402:CDL:H792	6:A:402:CDL:H751	1.94	0.50
1:B:116:GLN:HA	1:B:122:ILE:HD11	1.92	0.50
2:E:64:SER:O	2:E:69:ARG:NH1	2.45	0.50
1:O:153:ILE:HG22	1:O:154:ASN:H	1.76	0.50
6:P:401:CDL:HB61	6:P:401:CDL:OB7	2.10	0.50
1:N:155:ASP:OD1	1:N:155:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:297:ARG:NH1	2:S:61:VAL:O	2.45	0.50
6:C:401:CDL:OB7	6:C:401:CDL:HB61	2.10	0.50
4:J:314:SER:OG	4:J:315:LEU:N	2.43	0.50
1:A:152:VAL:HG22	1:A:157:THR:HG22	1.93	0.49
1:O:219:LYS:O	1:O:223:GLU:HG2	2.12	0.49
1:N:142:ASP:OD1	1:N:142:ASP:N	2.45	0.49
1:O:214:LEU:HD12	1:O:320:LEU:HB3	1.94	0.49
4:W:306:LYS:HB3	4:W:372:LYS:HD2	1.94	0.49
1:C:94:ARG:HE	1:Q:94:ARG:NH2	2.10	0.49
6:N:402:CDL:H751	6:N:402:CDL:H792	1.94	0.49
4:W:157:LEU:O	4:W:232:THR:OG1	2.30	0.49
4:W:326:THR:HG23	4:W:327:HIS:CD2	2.47	0.49
4:J:306:LYS:HB3	4:J:372:LYS:HD2	1.94	0.49
4:J:326:THR:HG23	4:J:327:HIS:CD2	2.47	0.49
4:J:387:PHE:O	4:J:391:LEU:HB3	2.13	0.49
2:R:64:SER:O	2:R:69:ARG:NH1	2.45	0.49
4:J:157:LEU:O	4:J:232:THR:OG1	2.30	0.49
1:O:247:PHE:HE2	6:Q:401:CDL:H451	1.77	0.49
6:Q:401:CDL:H842	2:U:65:PHE:H	1.77	0.49
1:C:169:SER:HB3	1:C:172:ASN:ND2	2.27	0.49
1:P:169:SER:HB3	1:P:172:ASN:ND2	2.27	0.49
1:D:142:ASP:OD1	1:D:142:ASP:N	2.46	0.49
1:P:290:VAL:HG12	1:P:292:PRO:HD2	1.95	0.49
4:W:128:THR:H	4:W:131:ASP:HB2	1.78	0.49
1:A:155:ASP:OD1	1:A:155:ASP:N	2.43	0.49
1:B:219:LYS:O	1:B:223:GLU:HG2	2.12	0.49
4:J:275:LEU:HD22	4:W:107:ARG:NH1	2.28	0.49
1:O:103:PRO:HA	1:O:141:ILE:HB	1.95	0.49
1:B:252:ARG:HD3	2:H:82:THR:HG23	1.95	0.48
4:J:128:THR:H	4:J:131:ASP:HB2	1.78	0.48
4:J:300:TRP:HA	4:J:303:VAL:HG12	1.95	0.48
7:O:402:PLX:H301	7:O:402:PLX:H271	1.60	0.48
1:D:94:ARG:NH2	1:P:94:ARG:HE	2.10	0.48
3:I:321:ARG:HB3	3:I:358:GLY:HA3	1.95	0.48
3:I:348:GLN:NE2	3:I:352:HIS:HB2	2.28	0.48
1:O:305:LYS:NZ	6:O:401:CDL:OB4	2.30	0.48
1:C:169:SER:OG	1:C:170:HIS:N	2.47	0.48
1:O:252:ARG:HD3	2:U:82:THR:HG23	1.95	0.48
1:P:169:SER:OG	1:P:170:HIS:N	2.47	0.48
1:C:290:VAL:HG12	1:C:292:PRO:HD2	1.95	0.48
4:W:300:TRP:HA	4:W:303:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:107:ARG:NH1	4:W:275:LEU:HD22	2.28	0.48
3:V:107:ARG:O	3:V:110:LYS:HG3	2.14	0.48
3:V:348:GLN:NE2	3:V:352:HIS:HB2	2.28	0.48
1:B:103:PRO:HA	1:B:141:ILE:HB	1.95	0.48
1:C:74:ASP:OD1	1:C:75:VAL:N	2.46	0.48
7:C:402:PLX:H101	7:C:402:PLX:H72	1.50	0.48
6:H:201:CDL:HB61	6:H:201:CDL:H712	1.45	0.48
3:I:112:MET:HB2	3:I:112:MET:HE3	1.70	0.48
1:Q:281:TYR:CD2	6:Q:401:CDL:HA61	2.49	0.48
1:B:214:LEU:HD12	1:B:320:LEU:HB3	1.95	0.48
1:P:272:TYR:HD2	1:Q:247:PHE:HD1	1.62	0.47
1:Q:142:ASP:OD1	1:Q:142:ASP:N	2.46	0.47
4:W:387:PHE:O	4:W:391:LEU:HB3	2.13	0.47
1:A:172:ASN:HA	1:A:175:THR:HB	1.96	0.47
1:N:75:VAL:HB	1:N:160:VAL:HG22	1.96	0.47
1:D:250:LEU:O	1:D:254:THR:HG23	2.15	0.47
3:I:235:ASP:OD1	3:I:235:ASP:N	2.47	0.47
1:N:172:ASN:HA	1:N:175:THR:HB	1.96	0.47
1:P:244:ALA:HB1	2:S:78:LEU:HD12	1.96	0.47
1:B:170:HIS:O	1:B:170:HIS:ND1	2.47	0.47
1:O:170:HIS:O	1:O:170:HIS:ND1	2.47	0.47
1:Q:250:LEU:O	1:Q:254:THR:HG23	2.15	0.47
3:V:321:ARG:HB3	3:V:358:GLY:HA3	1.95	0.47
1:C:244:ALA:HB1	2:F:78:LEU:HD12	1.96	0.47
1:N:92:SER:OG	1:N:119:ASP:OD1	2.19	0.47
4:W:355:LYS:HD3	4:W:361:GLU:HB3	1.97	0.47
7:B:402:PLX:H322	7:B:402:PLX:H351	1.67	0.47
1:C:119:ASP:HB3	1:C:122:ILE:HD11	1.97	0.47
1:C:272:TYR:HD2	1:D:247:PHE:HD1	1.62	0.47
4:J:113:VAL:HG11	4:J:263:ILE:HD12	1.97	0.47
4:J:355:LYS:HD3	4:J:361:GLU:HB3	1.97	0.47
1:Q:281:TYR:HD2	6:Q:401:CDL:HA61	1.77	0.47
1:A:142:ASP:OD1	1:A:142:ASP:N	2.45	0.47
1:B:305:LYS:HG2	1:B:305:LYS:O	2.15	0.47
3:I:107:ARG:O	3:I:110:LYS:HG3	2.14	0.47
3:I:412:VAL:O	3:I:416:VAL:HG23	2.15	0.47
6:Q:401:CDL:H712	6:Q:401:CDL:HB61	1.45	0.47
1:D:214:LEU:HD21	1:D:321:LYS:HE3	1.97	0.47
3:V:412:VAL:O	3:V:416:VAL:HG23	2.15	0.47
4:W:137:SER:O	4:W:137:SER:OG	2.29	0.47
1:A:75:VAL:HB	1:A:160:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:120:ARG:HD3	1:O:120:ARG:HA	1.74	0.46
6:O:401:CDL:OB7	6:O:401:CDL:HB31	2.14	0.46
1:Q:92:SER:OG	1:Q:119:ASP:OD2	2.31	0.46
1:P:119:ASP:HB3	1:P:122:ILE:HD11	1.97	0.46
3:I:321:ARG:HD3	3:I:358:GLY:HA3	1.97	0.46
6:Q:401:CDL:H712	6:Q:401:CDL:H741	1.60	0.46
3:V:440:ARG:O	3:V:443:ARG:HG2	2.16	0.46
4:W:113:VAL:HG11	4:W:263:ILE:HD12	1.97	0.46
1:C:104:ILE:HG21	1:D:197:LEU:HB3	1.98	0.46
1:B:238:GLY:HA2	7:B:402:PLX:H202	1.98	0.46
4:J:189:ASN:ND2	4:J:191:MET:O	2.49	0.46
1:O:238:GLY:HA2	7:O:402:PLX:H202	1.98	0.46
7:P:402:PLX:H1B3	7:P:402:PLX:H21	1.70	0.46
3:V:235:ASP:N	3:V:235:ASP:OD1	2.47	0.46
2:G:90:ALA:O	2:G:94:GLU:HG2	2.16	0.46
4:J:137:SER:O	4:J:137:SER:OG	2.29	0.46
1:P:302:PHE:HE1	6:P:401:CDL:HB31	1.81	0.46
4:W:189:ASN:ND2	4:W:191:MET:O	2.49	0.46
1:P:207:LEU:HD11	1:P:324:ILE:HG23	1.98	0.46
1:Q:246:GLN:HA	1:Q:249:ILE:HG22	1.98	0.46
3:V:291:LEU:H	3:V:291:LEU:HD23	1.80	0.46
1:N:108:VAL:HG13	1:N:127:ILE:HD12	1.98	0.46
1:Q:214:LEU:HD21	1:Q:321:LYS:HE3	1.97	0.46
1:A:87:SER:OG	1:A:96:ARG:NH2	2.49	0.45
1:B:285:THR:HG22	1:B:297:ARG:HH21	1.81	0.45
3:I:291:LEU:HD23	3:I:291:LEU:H	1.80	0.45
1:O:305:LYS:O	1:O:305:LYS:HG2	2.15	0.45
6:P:401:CDL:H171	6:P:401:CDL:H142	1.74	0.45
2:T:90:ALA:O	2:T:94:GLU:HG2	2.16	0.45
3:V:321:ARG:HD3	3:V:358:GLY:HA3	1.97	0.45
4:W:379:ASP:N	4:W:379:ASP:OD1	2.50	0.45
6:H:201:CDL:H822	6:H:201:CDL:H852	1.43	0.45
3:I:440:ARG:O	3:I:443:ARG:HG2	2.16	0.45
4:J:84:SER:OG	4:J:85:LEU:N	2.50	0.45
4:J:196:GLU:N	4:J:196:GLU:OE1	2.49	0.45
1:N:87:SER:OG	1:N:96:ARG:NH2	2.49	0.45
1:N:146:LEU:HD21	1:Q:189:THR:HG22	1.99	0.45
1:N:168:LEU:HG	1:N:169:SER:H	1.82	0.45
1:N:281:TYR:CD2	1:N:289:TYR:HB2	2.51	0.45
1:A:146:LEU:HD21	1:D:189:THR:HG22	1.99	0.45
3:I:339:SER:HG	3:I:342:LEU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:ASP:OD1	1:N:74:ASP:N	2.49	0.45
1:A:168:LEU:HG	1:A:169:SER:H	1.82	0.45
6:B:401:CDL:OB7	6:B:401:CDL:HB31	2.14	0.45
1:N:252:ARG:HD3	2:T:82:THR:HG23	1.98	0.45
3:V:244:GLU:O	3:V:247:GLN:HG3	2.17	0.45
4:W:84:SER:OG	4:W:85:LEU:N	2.50	0.45
4:W:196:GLU:OE1	4:W:196:GLU:N	2.49	0.45
1:B:171:GLU:OE2	1:D:105:SER:OG	2.26	0.45
1:C:265:PRO:HG3	1:D:260:TRP:CD2	2.52	0.45
4:J:379:ASP:N	4:J:379:ASP:OD1	2.50	0.45
1:A:281:TYR:CD2	1:A:289:TYR:HB2	2.51	0.45
7:D:401:PLX:H21	7:D:401:PLX:H1C3	1.73	0.45
3:I:290:LYS:H	3:I:290:LYS:HG2	1.60	0.45
1:P:104:ILE:HG21	1:Q:197:LEU:HB3	1.98	0.45
1:N:272:TYR:HD2	1:P:247:PHE:HD1	1.65	0.45
1:P:219:LYS:HE2	1:P:219:LYS:HB3	1.79	0.45
7:P:404:PLX:H21	7:P:404:PLX:H1B3	1.77	0.45
1:D:246:GLN:HA	1:D:249:ILE:HG22	1.98	0.45
3:V:443:ARG:HA	3:V:443:ARG:HD2	1.82	0.45
1:N:167:LEU:HG	1:N:171:GLU:HG2	1.99	0.44
1:A:108:VAL:HG13	1:A:127:ILE:HD12	1.98	0.44
1:C:199:LYS:HD2	1:C:199:LYS:HA	1.79	0.44
3:I:115:GLU:CD	3:I:119:ARG:HH12	2.21	0.44
1:P:265:PRO:HG3	1:Q:260:TRP:CD2	2.52	0.44
7:P:403:PLX:H1C3	7:P:403:PLX:H21	1.75	0.44
1:A:264:GLU:N	1:A:265:PRO:HD2	2.33	0.44
1:C:207:LEU:HD11	1:C:324:ILE:HG23	1.98	0.44
4:J:169:ILE:HD13	4:J:256:MET:HG2	2.00	0.44
6:A:402:CDL:H641	6:A:402:CDL:H612	1.89	0.44
6:H:201:CDL:H712	6:H:201:CDL:H741	1.60	0.44
1:O:123:ASP:H	1:O:154:ASN:HD22	1.65	0.44
3:V:348:GLN:HE22	3:V:352:HIS:HB2	1.82	0.44
6:A:402:CDL:H261	6:A:402:CDL:H232	1.81	0.44
1:C:122:ILE:HG23	1:C:153:ILE:HG23	1.99	0.44
1:D:87:SER:OG	1:D:96:ARG:NE	2.50	0.44
3:I:348:GLN:HE22	3:I:352:HIS:HB2	1.82	0.44
1:N:264:GLU:N	1:N:265:PRO:HD2	2.33	0.44
1:P:122:ILE:HG23	1:P:153:ILE:HG23	1.99	0.44
3:V:322:ILE:HG23	3:V:326:GLN:HB2	2.00	0.44
1:A:74:ASP:OD1	1:A:74:ASP:N	2.49	0.44
3:I:247:GLN:O	3:I:250:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:GLY:O	1:O:113:ARG:HG2	2.18	0.44
1:A:272:TYR:HD2	1:C:247:PHE:HD1	1.65	0.44
1:N:340:VAL:HG11	1:O:191:CYS:SG	2.57	0.44
3:V:247:GLN:O	3:V:250:ILE:HG22	2.17	0.44
3:V:339:SER:HG	3:V:342:LEU:H	1.64	0.44
4:W:105:THR:OG1	4:W:108:ASP:OD1	2.33	0.44
4:W:326:THR:HG23	4:W:327:HIS:HD2	1.82	0.44
1:A:74:ASP:O	1:A:96:ARG:NH1	2.37	0.44
1:A:124:ARG:NH2	1:A:128:TYR:OH	2.50	0.44
1:A:167:LEU:HG	1:A:171:GLU:HG2	1.99	0.44
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.83	0.44
1:B:109:GLY:O	1:B:113:ARG:HG2	2.18	0.44
3:I:244:GLU:O	3:I:247:GLN:HG3	2.17	0.44
1:A:340:VAL:HG11	1:B:191:CYS:SG	2.58	0.43
1:B:120:ARG:HA	1:B:120:ARG:HD3	1.74	0.43
3:I:221:ARG:NH2	3:I:376:ASP:OD2	2.50	0.43
4:J:386:GLU:HG2	4:J:387:PHE:N	2.33	0.43
7:Q:402:PLX:H1C3	7:Q:402:PLX:H21	1.73	0.43
1:P:74:ASP:OD1	1:P:75:VAL:N	2.46	0.43
1:A:75:VAL:HG22	1:A:88:VAL:HG12	2.00	0.43
1:B:285:THR:CG2	1:B:297:ARG:HH21	2.31	0.43
1:N:75:VAL:HG22	1:N:88:VAL:HG12	2.00	0.43
3:V:221:ARG:NH2	3:V:376:ASP:OD2	2.50	0.43
4:W:386:GLU:HG2	4:W:387:PHE:N	2.33	0.43
1:B:123:ASP:H	1:B:154:ASN:HD22	1.65	0.43
3:I:421:ASP:OD2	3:I:426:GLY:N	2.40	0.43
4:J:98:HIS:CE1	4:J:99:GLU:HG3	2.54	0.43
1:A:309:LYS:HE3	1:A:309:LYS:HB2	1.86	0.43
1:C:142:ASP:N	1:C:142:ASP:OD1	2.52	0.43
7:C:404:PLX:H21	7:C:404:PLX:H1B3	1.77	0.43
3:V:304:GLN:HE22	3:V:372:LYS:HD3	1.83	0.43
1:D:92:SER:OG	1:D:119:ASP:OD2	2.31	0.43
3:I:428:LEU:HD12	3:I:428:LEU:HA	1.88	0.43
6:O:401:CDL:H742	6:O:401:CDL:H712	1.72	0.43
3:V:115:GLU:CD	3:V:119:ARG:HH12	2.21	0.43
1:Q:290:VAL:HG23	1:Q:293:GLU:HB2	2.00	0.43
1:A:252:ARG:HD3	2:G:82:THR:HG23	2.01	0.43
4:J:326:THR:HG23	4:J:327:HIS:HD2	1.82	0.43
1:A:93:ARG:O	1:A:95:GLU:N	2.52	0.43
7:C:403:PLX:H21	7:C:403:PLX:H1C3	1.75	0.43
4:J:128:THR:HG23	4:J:131:ASP:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:171:GLU:OE2	1:Q:105:SER:OG	2.27	0.43
2:E:92:LEU:HD23	2:E:92:LEU:HA	1.88	0.43
3:I:322:ILE:HG23	3:I:326:GLN:HB2	2.00	0.43
4:J:323:HIS:O	4:J:326:THR:HG22	2.19	0.43
4:W:169:ILE:HD13	4:W:256:MET:HG2	2.00	0.43
7:A:404:PLX:H1C3	7:A:404:PLX:H21	1.78	0.42
3:I:391:LEU:HG	3:I:392:ASP:H	1.84	0.42
6:N:402:CDL:H261	6:N:402:CDL:H232	1.81	0.42
1:P:142:ASP:OD1	1:P:142:ASP:N	2.52	0.42
4:W:128:THR:HG23	4:W:131:ASP:H	1.84	0.42
3:I:304:GLN:HE22	3:I:372:LYS:HD3	1.83	0.42
1:Q:87:SER:OG	1:Q:96:ARG:NE	2.50	0.42
2:R:92:LEU:HD23	2:R:92:LEU:HA	1.88	0.42
3:V:391:LEU:HG	3:V:392:ASP:H	1.84	0.42
1:N:93:ARG:O	1:N:95:GLU:N	2.52	0.42
1:N:175:THR:O	1:N:178:ASP:HB3	2.20	0.42
6:N:402:CDL:H641	6:N:402:CDL:H612	1.89	0.42
7:P:402:PLX:H101	7:P:402:PLX:H72	1.50	0.42
4:W:98:HIS:CE1	4:W:99:GLU:HG3	2.54	0.42
2:H:83:LEU:O	2:H:87:ASN:ND2	2.44	0.42
3:I:242:GLU:O	3:I:246:VAL:HG22	2.20	0.42
1:D:290:VAL:HG23	1:D:293:GLU:HB2	2.00	0.42
1:O:325:ALA:HB2	2:T:53:SER:HB3	2.00	0.42
7:D:401:PLX:H121	7:D:401:PLX:H152	1.67	0.42
1:Q:253:LEU:HG	2:R:85:SER:OG	2.20	0.42
4:W:297:ASP:N	4:W:297:ASP:OD1	2.53	0.42
4:W:323:HIS:O	4:W:326:THR:HG22	2.19	0.42
1:A:175:THR:O	1:A:178:ASP:HB3	2.20	0.42
7:D:401:PLX:H311	7:D:401:PLX:H342	1.94	0.42
4:J:368:ASP:O	4:J:372:LYS:HG2	2.20	0.42
4:W:280:LYS:HB3	4:W:307:LEU:HD21	2.02	0.42
1:A:166:ASP:OD1	1:A:166:ASP:N	2.48	0.42
1:C:233:THR:HG22	1:C:237:TRP:CD1	2.55	0.42
7:O:402:PLX:H351	7:O:402:PLX:H322	1.67	0.42
4:W:150:ARG:HH11	4:W:266:MET:HE2	1.85	0.42
4:W:335:MET:HE3	4:W:335:MET:HB2	1.89	0.42
1:N:124:ARG:NH2	1:N:128:TYR:OH	2.50	0.41
3:I:335:SER:O	3:I:337:VAL:N	2.52	0.41
6:Q:401:CDL:HB31	6:Q:401:CDL:C51	2.46	0.41
1:P:233:THR:HG22	1:P:237:TRP:CD1	2.55	0.41
6:Q:401:CDL:OA7	7:Q:402:PLX:H321	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:368:ASP:O	4:W:372:LYS:HG2	2.20	0.41
1:B:197:LEU:HD12	1:B:197:LEU:HA	1.88	0.41
7:D:401:PLX:H24	7:D:401:PLX:H72	2.02	0.41
3:I:440:ARG:O	3:I:440:ARG:NH2	2.50	0.41
1:P:302:PHE:CE1	6:P:401:CDL:HB31	2.56	0.41
2:S:96:ASP:HB3	3:V:339:SER:O	2.21	0.41
6:P:401:CDL:H802	6:P:401:CDL:H832	1.82	0.41
3:V:197:THR:HG21	3:V:281:TYR:HD1	1.85	0.41
3:V:242:GLU:O	3:V:246:VAL:HG22	2.20	0.41
1:B:165:ARG:NH1	1:B:167:LEU:H	2.19	0.41
1:C:219:LYS:HE2	1:C:219:LYS:HB3	1.79	0.41
1:D:210:LEU:HD23	1:D:210:LEU:HA	1.93	0.41
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.91	0.41
1:B:253:LEU:HG	2:H:85:SER:OG	2.21	0.41
1:B:298:GLN:NE2	6:B:401:CDL:OB3	2.47	0.41
2:S:92:LEU:HD23	2:S:92:LEU:HA	1.91	0.41
2:U:51:THR:HG22	2:U:52:ARG:N	2.36	0.41
1:B:325:ALA:HB2	2:G:53:SER:HB3	2.02	0.41
4:W:290:PHE:CE1	4:W:391:LEU:HD13	2.49	0.41
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.90	0.41
7:B:402:PLX:H21	7:B:402:PLX:H1A2	1.85	0.41
1:D:253:LEU:HG	2:E:85:SER:OG	2.20	0.41
2:H:51:THR:HG22	2:H:52:ARG:N	2.36	0.41
3:I:197:THR:HG21	3:I:281:TYR:HD1	1.85	0.41
3:I:198:LEU:HD22	3:I:198:LEU:H	1.86	0.41
1:N:74:ASP:O	1:N:96:ARG:NH1	2.37	0.41
1:N:309:LYS:HB2	1:N:309:LYS:HE3	1.86	0.41
7:N:403:PLX:H1B3	7:N:403:PLX:H22	1.74	0.41
1:Q:242:TYR:HA	1:Q:245:THR:HG22	2.03	0.41
7:Q:402:PLX:H24	7:Q:402:PLX:H72	2.02	0.41
3:V:204:ILE:HG22	3:V:208:ASP:HB2	2.02	0.41
4:W:185:ASP:HA	4:W:196:GLU:HG2	2.03	0.41
4:W:232:THR:HG23	4:W:235:GLN:H	1.86	0.41
1:A:148:ASP:N	1:A:148:ASP:OD1	2.54	0.41
3:I:204:ILE:HG22	3:I:208:ASP:HB2	2.02	0.41
3:I:348:GLN:HE21	3:I:351:LYS:NZ	2.19	0.41
1:Q:247:PHE:HD2	2:R:78:LEU:HD11	1.86	0.41
3:V:348:GLN:HE21	3:V:351:LYS:NZ	2.19	0.41
1:D:310:SER:O	1:D:310:SER:OG	2.36	0.40
1:N:260:TRP:CG	1:O:265:PRO:HG3	2.56	0.40
1:O:165:ARG:NH1	1:O:167:LEU:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:344:PRO:HA	4:W:383:SER:HA	2.03	0.40
1:B:252:ARG:HB2	2:H:82:THR:HG23	2.04	0.40
2:U:48:VAL:HG13	2:U:57:LEU:HD11	2.03	0.40
4:W:272:SER:O	4:W:272:SER:OG	2.39	0.40
1:A:196:GLN:NE2	1:B:184:GLN:HG3	2.36	0.40
1:D:247:PHE:HD2	2:E:78:LEU:HD11	1.86	0.40
3:I:472:ALA:O	3:I:474:PRO:N	2.54	0.40
4:J:280:LYS:HB3	4:J:307:LEU:HD21	2.02	0.40
4:J:297:ASP:OD1	4:J:297:ASP:N	2.53	0.40
4:J:344:PRO:HA	4:J:383:SER:HA	2.03	0.40
1:P:199:LYS:HD2	1:P:199:LYS:HA	1.79	0.40
3:V:472:ALA:O	3:V:474:PRO:N	2.54	0.40
1:A:260:TRP:CG	1:B:265:PRO:HG3	2.56	0.40
7:B:402:PLX:H271	7:B:402:PLX:H301	1.60	0.40
1:D:240:LEU:HD21	2:E:70:VAL:HG23	2.04	0.40
4:J:232:THR:HG23	4:J:235:GLN:H	1.86	0.40
4:J:369:THR:O	4:J:373:ILE:HG13	2.22	0.40
2:U:92:LEU:HD23	2:U:92:LEU:HA	1.85	0.40
3:V:198:LEU:H	3:V:198:LEU:HD22	1.86	0.40
1:D:300:LEU:HD23	1:D:300:LEU:HA	1.89	0.40
1:O:221:ARG:HE	1:O:221:ARG:HB3	1.65	0.40
1:Q:240:LEU:HD21	2:R:70:VAL:HG23	2.04	0.40
4:W:104:MET:HG3	4:W:108:ASP:HB2	2.04	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	271/276 (98%)	257 (95%)	14 (5%)	0	100	100
1	B	271/276 (98%)	262 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	D	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
1	N	271/276 (98%)	257 (95%)	14 (5%)	0	100	100
1	O	271/276 (98%)	262 (97%)	9 (3%)	0	100	100
1	P	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	Q	271/276 (98%)	261 (96%)	10 (4%)	0	100	100
2	E	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
2	F	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
2	G	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
2	H	52/54 (96%)	52 (100%)	0	0	100	100
2	R	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
2	S	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
2	T	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
2	U	52/54 (96%)	52 (100%)	0	0	100	100
3	I	296/476 (62%)	268 (90%)	26 (9%)	2 (1%)	22	61
3	V	296/476 (62%)	268 (90%)	26 (9%)	2 (1%)	22	61
4	J	315/336 (94%)	300 (95%)	15 (5%)	0	100	100
4	W	315/336 (94%)	299 (95%)	16 (5%)	0	100	100
All	All	3812/4264 (89%)	3629 (95%)	179 (5%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	473	LEU
3	I	474	PRO
3	V	473	LEU
3	V	474	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	245/247 (99%)	245 (100%)	0	100	100
1	B	245/247 (99%)	244 (100%)	1 (0%)	91	97
1	C	247/247 (100%)	246 (100%)	1 (0%)	91	97
1	D	245/247 (99%)	245 (100%)	0	100	100
1	N	245/247 (99%)	245 (100%)	0	100	100
1	O	245/247 (99%)	245 (100%)	0	100	100
1	P	247/247 (100%)	246 (100%)	1 (0%)	91	97
1	Q	245/247 (99%)	244 (100%)	1 (0%)	91	97
2	E	48/48 (100%)	48 (100%)	0	100	100
2	F	48/48 (100%)	48 (100%)	0	100	100
2	G	48/48 (100%)	48 (100%)	0	100	100
2	H	48/48 (100%)	48 (100%)	0	100	100
2	R	48/48 (100%)	48 (100%)	0	100	100
2	S	48/48 (100%)	48 (100%)	0	100	100
2	T	48/48 (100%)	48 (100%)	0	100	100
2	U	48/48 (100%)	48 (100%)	0	100	100
3	I	250/413 (60%)	248 (99%)	2 (1%)	81	91
3	V	250/413 (60%)	248 (99%)	2 (1%)	81	91
4	J	277/308 (90%)	276 (100%)	1 (0%)	91	97
4	W	277/308 (90%)	276 (100%)	1 (0%)	91	97
All	All	3402/3802 (90%)	3392 (100%)	10 (0%)	92	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	ARG
1	C	165	ARG
3	I	110	LYS
3	I	440	ARG
4	J	394	ARG
1	P	165	ARG
1	Q	297	ARG
3	V	110	LYS
3	V	440	ARG
4	W	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	185	GLN
1	A	195	HIS
1	A	196	GLN
1	A	298	GLN
1	A	318	ASN
1	A	319	GLN
1	A	339	GLN
1	A	341	HIS
1	B	195	HIS
1	B	213	GLN
1	B	318	ASN
1	C	80	GLN
1	C	185	GLN
1	C	196	GLN
1	C	213	GLN
1	D	80	GLN
1	D	114	GLN
1	D	196	GLN
1	D	213	GLN
1	D	246	GLN
2	E	87	ASN
2	H	95	HIS
3	I	116	ASN
3	I	159	ASN
3	I	245	GLN
3	I	300	GLN
3	I	348	GLN
3	I	385	HIS
3	I	397	GLN
3	I	398	GLN
3	I	411	HIS
4	J	98	HIS
4	J	117	GLN
4	J	178	HIS
4	J	235	GLN
4	J	260	GLN
1	N	80	GLN
1	N	185	GLN
1	N	195	HIS
1	N	196	GLN

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Mol	Chain	Res	Type
1	N	298	GLN
1	N	318	ASN
1	N	319	GLN
1	N	339	GLN
1	N	341	HIS
1	O	195	HIS
1	O	213	GLN
1	O	318	ASN
1	P	80	GLN
1	P	185	GLN
1	P	196	GLN
1	P	213	GLN
1	Q	80	GLN
1	Q	114	GLN
1	Q	196	GLN
1	Q	213	GLN
1	Q	246	GLN
2	R	87	ASN
2	U	95	HIS
3	V	116	ASN
3	V	159	ASN
3	V	245	GLN
3	V	300	GLN
3	V	348	GLN
3	V	385	HIS
3	V	397	GLN
3	V	398	GLN
3	V	411	HIS
4	W	98	HIS
4	W	117	GLN
4	W	235	GLN
4	W	260	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)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	PLX	Q	402	-	51,51,51	1.03	5 (9%)	55,59,59	0.95	2 (3%)
7	PLX	C	404	-	33,33,51	1.27	4 (12%)	37,40,59	0.90	1 (2%)
7	PLX	A	404	-	33,33,51	1.26	3 (9%)	37,40,59	0.87	1 (2%)
7	PLX	O	402	-	51,51,51	1.05	4 (7%)	55,59,59	0.85	1 (1%)
7	PLX	D	401	-	51,51,51	1.03	4 (7%)	55,59,59	0.94	2 (3%)
7	PLX	B	402	-	51,51,51	1.05	4 (7%)	55,59,59	0.85	1 (1%)
6	CDL	C	401	-	99,99,99	0.28	0	105,111,111	0.77	4 (3%)
6	CDL	A	402	-	99,99,99	0.27	0	105,111,111	0.53	1 (0%)
7	PLX	N	403	-	51,51,51	1.04	4 (7%)	55,59,59	0.95	2 (3%)
7	PLX	N	404	-	33,33,51	1.26	3 (9%)	37,40,59	0.87	1 (2%)
7	PLX	O	403	-	33,33,51	1.26	4 (12%)	37,40,59	0.91	1 (2%)
6	CDL	N	402	-	99,99,99	0.27	0	105,111,111	0.52	1 (0%)
7	PLX	C	402	-	51,51,51	1.03	4 (7%)	55,59,59	0.91	2 (3%)
7	PLX	P	404	-	33,33,51	1.27	4 (12%)	37,40,59	0.90	1 (2%)
6	CDL	P	401	-	99,99,99	0.28	0	105,111,111	0.77	4 (3%)
6	CDL	O	401	-	99,99,99	0.26	0	105,111,111	0.71	4 (3%)
7	PLX	P	402	-	51,51,51	1.03	4 (7%)	55,59,59	0.91	2 (3%)
6	CDL	B	401	-	99,99,99	0.26	0	105,111,111	0.71	4 (3%)
6	CDL	H	201	-	99,99,99	0.29	0	105,111,111	0.57	1 (0%)
7	PLX	C	403	-	33,33,51	1.27	3 (9%)	37,40,59	0.91	1 (2%)
7	PLX	A	403	-	51,51,51	1.04	4 (7%)	55,59,59	0.95	2 (3%)
7	PLX	B	403	-	33,33,51	1.25	4 (12%)	37,40,59	0.91	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PLX	P	403	-	33,33,51	1.27	3 (9%)	37,40,59	0.91	1 (2%)
6	CDL	Q	401	-	99,99,99	0.28	0	105,111,111	0.57	1 (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	PLX	Q	402	-	-	29/55/55/55	-
7	PLX	C	404	-	-	18/35/35/55	-
7	PLX	A	404	-	-	16/35/35/55	-
7	PLX	O	402	-	-	28/55/55/55	-
7	PLX	D	401	-	-	29/55/55/55	-
7	PLX	B	402	-	-	28/55/55/55	-
6	CDL	C	401	-	-	62/110/110/110	-
6	CDL	A	402	-	-	61/110/110/110	-
7	PLX	N	403	-	-	20/55/55/55	-
7	PLX	N	404	-	-	16/35/35/55	-
7	PLX	O	403	-	-	18/35/35/55	-
6	CDL	N	402	-	-	61/110/110/110	-
7	PLX	C	402	-	-	26/55/55/55	-
7	PLX	P	404	-	-	18/35/35/55	-
6	CDL	P	401	-	-	62/110/110/110	-
6	CDL	O	401	-	-	62/110/110/110	-
7	PLX	P	402	-	-	26/55/55/55	-
6	CDL	B	401	-	-	62/110/110/110	-
6	CDL	H	201	-	-	61/110/110/110	-
7	PLX	C	403	-	-	16/35/35/55	-
7	PLX	A	403	-	-	20/55/55/55	-
7	PLX	B	403	-	-	18/35/35/55	-
7	PLX	P	403	-	-	16/35/35/55	-
6	CDL	Q	401	-	-	61/110/110/110	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	403	PLX	O6-C4	-3.76	1.40	1.44
7	P	403	PLX	O6-C4	-3.76	1.40	1.44
7	C	404	PLX	O6-C4	-3.49	1.40	1.44
7	P	404	PLX	O6-C4	-3.49	1.40	1.44
7	O	403	PLX	O6-C4	-3.48	1.40	1.44
7	B	403	PLX	O6-C4	-3.42	1.40	1.44
7	A	404	PLX	O6-C4	-3.36	1.41	1.44
7	N	404	PLX	O6-C4	-3.36	1.41	1.44
7	A	403	PLX	O6-C4	-3.06	1.40	1.44
7	N	403	PLX	O6-C4	-3.06	1.40	1.44
7	B	402	PLX	O6-C4	-2.87	1.40	1.44
7	O	402	PLX	O6-C4	-2.87	1.40	1.44
7	C	402	PLX	O6-C4	-2.84	1.40	1.44
7	P	402	PLX	O6-C4	-2.84	1.40	1.44
7	D	401	PLX	O6-C4	-2.82	1.40	1.44
7	Q	402	PLX	O6-C4	-2.82	1.40	1.44
7	C	404	PLX	C7-C6	2.60	1.56	1.50
7	P	404	PLX	C7-C6	2.60	1.56	1.50
7	A	404	PLX	C7-C6	2.54	1.56	1.50
7	N	404	PLX	C7-C6	2.54	1.56	1.50
7	B	403	PLX	C7-C6	2.50	1.56	1.50
7	B	402	PLX	C7-C6	2.47	1.56	1.50
7	O	402	PLX	C7-C6	2.47	1.56	1.50
7	O	403	PLX	C7-C6	2.44	1.55	1.50
7	P	403	PLX	C7-C6	2.38	1.55	1.50
7	C	403	PLX	C7-C6	2.37	1.55	1.50
7	C	402	PLX	C7-C6	2.33	1.55	1.50
7	P	402	PLX	C7-C6	2.33	1.55	1.50
7	Q	402	PLX	C7-C6	2.31	1.55	1.50
7	A	403	PLX	C7-C6	2.30	1.55	1.50
7	N	403	PLX	C7-C6	2.30	1.55	1.50
7	D	401	PLX	C7-C6	2.29	1.55	1.50
7	B	402	PLX	C1B-N1	-2.21	1.43	1.50
7	O	402	PLX	C1B-N1	-2.21	1.43	1.50
7	D	401	PLX	C1B-N1	-2.17	1.43	1.50
7	Q	402	PLX	C1B-N1	-2.17	1.43	1.50
7	A	403	PLX	C1B-N1	-2.12	1.43	1.50
7	N	403	PLX	C1B-N1	-2.12	1.43	1.50
7	C	404	PLX	P1-O1	2.12	1.67	1.59
7	P	404	PLX	P1-O1	2.12	1.67	1.59
7	C	402	PLX	C1B-N1	-2.10	1.43	1.50
7	P	402	PLX	C1B-N1	-2.10	1.43	1.50
7	N	403	PLX	P1-O3	-2.09	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	402	PLX	P1-O3	-2.09	1.45	1.55
7	B	402	PLX	P1-O3	-2.08	1.45	1.55
7	C	403	PLX	P1-O1	2.08	1.67	1.59
7	A	403	PLX	P1-O3	-2.07	1.45	1.55
7	C	402	PLX	P1-O3	-2.07	1.45	1.55
7	P	403	PLX	P1-O1	2.06	1.67	1.59
7	O	403	PLX	P1-O1	2.06	1.67	1.59
7	P	402	PLX	P1-O3	-2.06	1.45	1.55
7	B	403	PLX	P1-O1	2.05	1.67	1.59
7	N	404	PLX	P1-O1	2.05	1.67	1.59
7	B	403	PLX	C1B-N1	-2.04	1.44	1.50
7	O	403	PLX	C1B-N1	-2.04	1.44	1.50
7	D	401	PLX	P1-O3	-2.04	1.45	1.55
7	Q	402	PLX	P1-O3	-2.04	1.45	1.55
7	A	404	PLX	P1-O1	2.03	1.67	1.59
7	Q	402	PLX	C1C-N1	-2.01	1.44	1.50
7	C	404	PLX	C1B-N1	-2.00	1.44	1.50
7	P	404	PLX	C1B-N1	-2.00	1.44	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	401	CDL	OB6-CB5-C51	3.13	118.25	111.50
6	H	201	CDL	OB6-CB5-C51	3.11	118.20	111.50
6	C	401	CDL	O1-C1-CA2	2.90	119.73	109.56
6	P	401	CDL	O1-C1-CA2	2.89	119.71	109.56
6	P	401	CDL	O1-C1-CB2	2.89	119.71	109.56
6	C	401	CDL	O1-C1-CB2	2.88	119.67	109.56
6	B	401	CDL	CB2-C1-CA2	2.73	120.83	112.79
6	O	401	CDL	CB2-C1-CA2	2.73	120.83	112.79
6	B	401	CDL	O1-C1-CB2	2.67	118.91	109.56
6	O	401	CDL	O1-C1-CB2	2.66	118.90	109.56
6	C	401	CDL	CB2-C1-CA2	2.63	120.51	112.79
6	P	401	CDL	CB2-C1-CA2	2.62	120.49	112.79
6	B	401	CDL	O1-C1-CA2	2.46	118.18	109.56
6	O	401	CDL	O1-C1-CA2	2.46	118.17	109.56
6	O	401	CDL	OB5-PB2-OB3	2.36	118.30	109.07
7	C	404	PLX	O3-P1-O2	-2.36	100.56	112.24
6	B	401	CDL	OB5-PB2-OB3	2.36	118.29	109.07
7	P	404	PLX	O3-P1-O2	-2.35	100.61	112.24
6	C	401	CDL	OB6-CB5-C51	2.33	116.53	111.50
6	P	401	CDL	OB6-CB5-C51	2.32	116.51	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	403	PLX	C8-C7-C6	-2.30	108.07	113.38
7	N	403	PLX	C8-C7-C6	-2.30	108.07	113.38
7	A	404	PLX	O3-P1-O2	-2.29	100.91	112.24
7	N	404	PLX	O3-P1-O2	-2.29	100.92	112.24
7	P	403	PLX	O3-P1-O2	-2.25	101.12	112.24
7	C	403	PLX	O3-P1-O2	-2.24	101.15	112.24
7	A	403	PLX	O3-P1-O2	-2.22	101.28	112.24
7	N	403	PLX	O3-P1-O2	-2.21	101.33	112.24
7	P	402	PLX	O3-P1-O2	-2.21	101.33	112.24
7	C	402	PLX	O3-P1-O2	-2.20	101.34	112.24
7	D	401	PLX	O3-P1-O2	-2.20	101.34	112.24
7	Q	402	PLX	O3-P1-O2	-2.20	101.34	112.24
7	B	403	PLX	O3-P1-O2	-2.19	101.41	112.24
7	O	403	PLX	O3-P1-O2	-2.19	101.41	112.24
7	B	402	PLX	O3-P1-O2	-2.17	101.51	112.24
7	O	402	PLX	O3-P1-O2	-2.16	101.55	112.24
7	C	402	PLX	C2-C1-N1	-2.08	108.82	115.78
7	P	402	PLX	C2-C1-N1	-2.08	108.82	115.78
7	Q	402	PLX	C26-C25-C24	-2.08	108.58	113.38
6	A	402	CDL	OB6-CB5-C51	2.07	115.97	111.50
7	D	401	PLX	C26-C25-C24	-2.06	108.62	113.38
6	N	402	CDL	OB6-CB5-C51	2.03	115.88	111.50

There are no chirality outliers.

All (834) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	402	CDL	CA2-OA2-PA1-OA3
6	A	402	CDL	CA2-OA2-PA1-OA4
6	A	402	CDL	CA2-OA2-PA1-OA5
6	A	402	CDL	CA3-OA5-PA1-OA3
6	A	402	CDL	CA3-OA5-PA1-OA4
6	A	402	CDL	CA3-CA4-OA6-CA5
6	A	402	CDL	OA6-CA4-CA6-OA8
6	A	402	CDL	C11-CA5-OA6-CA4
6	A	402	CDL	CB2-OB2-PB2-OB4
6	B	401	CDL	O1-C1-CA2-OA2
6	B	401	CDL	CA2-OA2-PA1-OA3
6	B	401	CDL	CA2-OA2-PA1-OA4
6	B	401	CDL	CA2-OA2-PA1-OA5
6	B	401	CDL	C51-CB5-OB6-CB4
6	C	401	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
6	C	401	CDL	CA3-OA5-PA1-OA4
6	C	401	CDL	CB2-OB2-PB2-OB3
6	C	401	CDL	CB2-OB2-PB2-OB4
6	C	401	CDL	CB2-OB2-PB2-OB5
6	C	401	CDL	CB3-OB5-PB2-OB4
6	H	201	CDL	CA3-OA5-PA1-OA3
6	H	201	CDL	CA3-OA5-PA1-OA4
6	H	201	CDL	CB3-OB5-PB2-OB3
6	H	201	CDL	OB7-CB5-OB6-CB4
6	H	201	CDL	C51-CB5-OB6-CB4
6	H	201	CDL	OB9-CB7-OB8-CB6
6	H	201	CDL	C71-CB7-OB8-CB6
6	N	402	CDL	CA2-OA2-PA1-OA3
6	N	402	CDL	CA2-OA2-PA1-OA4
6	N	402	CDL	CA2-OA2-PA1-OA5
6	N	402	CDL	CA3-OA5-PA1-OA3
6	N	402	CDL	CA3-OA5-PA1-OA4
6	N	402	CDL	CA3-CA4-OA6-CA5
6	N	402	CDL	OA6-CA4-CA6-OA8
6	N	402	CDL	C11-CA5-OA6-CA4
6	N	402	CDL	CB2-OB2-PB2-OB4
6	O	401	CDL	O1-C1-CA2-OA2
6	O	401	CDL	CA2-OA2-PA1-OA3
6	O	401	CDL	CA2-OA2-PA1-OA4
6	O	401	CDL	CA2-OA2-PA1-OA5
6	O	401	CDL	C51-CB5-OB6-CB4
6	P	401	CDL	CA2-OA2-PA1-OA3
6	P	401	CDL	CA3-OA5-PA1-OA4
6	P	401	CDL	CB2-OB2-PB2-OB3
6	P	401	CDL	CB2-OB2-PB2-OB4
6	P	401	CDL	CB2-OB2-PB2-OB5
6	P	401	CDL	CB3-OB5-PB2-OB4
6	Q	401	CDL	CA3-OA5-PA1-OA3
6	Q	401	CDL	CA3-OA5-PA1-OA4
6	Q	401	CDL	CB3-OB5-PB2-OB3
6	Q	401	CDL	OB7-CB5-OB6-CB4
6	Q	401	CDL	C51-CB5-OB6-CB4
6	Q	401	CDL	OB9-CB7-OB8-CB6
6	Q	401	CDL	C71-CB7-OB8-CB6
7	A	403	PLX	C3-O4-P1-O2
7	A	403	PLX	C3-O4-P1-O3
7	A	403	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
7	A	403	PLX	O9-C24-C25-C26
7	A	404	PLX	O7-C6-O6-C4
7	A	404	PLX	N1-C1-C2-O1
7	B	402	PLX	O7-C6-C7-C8
7	B	402	PLX	O7-C6-O6-C4
7	B	402	PLX	C2-O1-P1-O4
7	B	402	PLX	C2-O1-P1-O2
7	B	402	PLX	C2-O1-P1-O3
7	B	402	PLX	O9-C24-C25-C26
7	B	403	PLX	O7-C6-O6-C4
7	B	403	PLX	C3-O4-P1-O2
7	B	403	PLX	C2-O1-P1-O4
7	C	402	PLX	O7-C6-C7-C8
7	C	402	PLX	C3-O4-P1-O2
7	C	402	PLX	N1-C1-C2-O1
7	C	402	PLX	O9-C24-O8-C5
7	C	403	PLX	O7-C6-C7-C8
7	C	403	PLX	O7-C6-O6-C4
7	C	404	PLX	C3-C4-O6-C6
7	C	404	PLX	O4-C3-C4-O6
7	C	404	PLX	O4-C3-C4-C5
7	C	404	PLX	C3-O4-P1-O3
7	C	404	PLX	C2-O1-P1-O3
7	D	401	PLX	O7-C6-C7-C8
7	D	401	PLX	O7-C6-O6-C4
7	D	401	PLX	C2-O1-P1-O3
7	D	401	PLX	N1-C1-C2-O1
7	D	401	PLX	O9-C24-O8-C5
7	N	403	PLX	C3-O4-P1-O2
7	N	403	PLX	C3-O4-P1-O3
7	N	403	PLX	C2-O1-P1-O2
7	N	403	PLX	O9-C24-C25-C26
7	N	404	PLX	O7-C6-O6-C4
7	N	404	PLX	N1-C1-C2-O1
7	O	402	PLX	O7-C6-C7-C8
7	O	402	PLX	O7-C6-O6-C4
7	O	402	PLX	C2-O1-P1-O4
7	O	402	PLX	C2-O1-P1-O2
7	O	402	PLX	C2-O1-P1-O3
7	O	402	PLX	O9-C24-C25-C26
7	O	403	PLX	O7-C6-O6-C4
7	O	403	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
7	O	403	PLX	C2-O1-P1-O4
7	P	402	PLX	O7-C6-C7-C8
7	P	402	PLX	C3-O4-P1-O2
7	P	402	PLX	N1-C1-C2-O1
7	P	402	PLX	O9-C24-O8-C5
7	P	403	PLX	O7-C6-C7-C8
7	P	403	PLX	O7-C6-O6-C4
7	P	404	PLX	C3-C4-O6-C6
7	P	404	PLX	O4-C3-C4-O6
7	P	404	PLX	O4-C3-C4-C5
7	P	404	PLX	C3-O4-P1-O3
7	P	404	PLX	C2-O1-P1-O3
7	Q	402	PLX	O7-C6-C7-C8
7	Q	402	PLX	O7-C6-O6-C4
7	Q	402	PLX	C2-O1-P1-O3
7	Q	402	PLX	N1-C1-C2-O1
7	Q	402	PLX	O9-C24-O8-C5
6	B	401	CDL	OB9-CB7-OB8-CB6
6	O	401	CDL	OB9-CB7-OB8-CB6
6	B	401	CDL	C71-CB7-OB8-CB6
6	O	401	CDL	C71-CB7-OB8-CB6
6	A	402	CDL	OA7-CA5-OA6-CA4
6	N	402	CDL	OA7-CA5-OA6-CA4
6	B	401	CDL	OB7-CB5-OB6-CB4
6	O	401	CDL	OB7-CB5-OB6-CB4
6	B	401	CDL	O1-C1-CB2-OB2
6	C	401	CDL	O1-C1-CB2-OB2
6	O	401	CDL	O1-C1-CB2-OB2
6	P	401	CDL	O1-C1-CB2-OB2
6	A	402	CDL	C51-CB5-OB6-CB4
6	N	402	CDL	C51-CB5-OB6-CB4
6	H	201	CDL	C34-C35-C36-C37
6	Q	401	CDL	C34-C35-C36-C37
6	A	402	CDL	C76-C77-C78-C79
6	C	401	CDL	C80-C81-C82-C83
6	N	402	CDL	C76-C77-C78-C79
6	P	401	CDL	C80-C81-C82-C83
6	C	401	CDL	C14-C15-C16-C17
6	P	401	CDL	C14-C15-C16-C17
6	H	201	CDL	C82-C83-C84-C85
6	Q	401	CDL	C82-C83-C84-C85
7	C	402	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	P	402	PLX	C7-C8-C9-C10
6	H	201	CDL	CA2-C1-CB2-OB2
6	Q	401	CDL	CA2-C1-CB2-OB2
6	C	401	CDL	C71-CB7-OB8-CB6
6	P	401	CDL	C71-CB7-OB8-CB6
6	B	401	CDL	C71-C72-C73-C74
6	O	401	CDL	C71-C72-C73-C74
6	H	201	CDL	C54-C55-C56-C57
6	Q	401	CDL	C54-C55-C56-C57
6	H	201	CDL	O1-C1-CB2-OB2
6	Q	401	CDL	O1-C1-CB2-OB2
6	C	401	CDL	OB9-CB7-OB8-CB6
6	P	401	CDL	OB9-CB7-OB8-CB6
6	A	402	CDL	C13-C14-C15-C16
6	H	201	CDL	C31-C32-C33-C34
6	Q	401	CDL	C31-C32-C33-C34
6	H	201	CDL	CA7-C31-C32-C33
6	Q	401	CDL	CA7-C31-C32-C33
6	N	402	CDL	C13-C14-C15-C16
7	B	402	PLX	C29-C30-C31-C32
7	O	402	PLX	C29-C30-C31-C32
6	A	402	CDL	OB7-CB5-OB6-CB4
6	N	402	CDL	OB7-CB5-OB6-CB4
6	P	401	CDL	C74-C75-C76-C77
6	C	401	CDL	C74-C75-C76-C77
6	H	201	CDL	C71-C72-C73-C74
6	Q	401	CDL	C71-C72-C73-C74
6	C	401	CDL	O1-C1-CA2-OA2
6	P	401	CDL	O1-C1-CA2-OA2
6	A	402	CDL	CB7-C71-C72-C73
6	N	402	CDL	CB7-C71-C72-C73
6	B	401	CDL	C55-C56-C57-C58
6	O	401	CDL	C55-C56-C57-C58
6	A	402	CDL	CA3-OA5-PA1-OA2
6	A	402	CDL	CB2-OB2-PB2-OB5
6	B	401	CDL	CA3-OA5-PA1-OA2
6	C	401	CDL	CA2-OA2-PA1-OA5
6	C	401	CDL	CA3-OA5-PA1-OA2
6	C	401	CDL	CB3-OB5-PB2-OB2
6	H	201	CDL	CA3-OA5-PA1-OA2
6	N	402	CDL	CA3-OA5-PA1-OA2
6	N	402	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
6	O	401	CDL	CA3-OA5-PA1-OA2
6	P	401	CDL	CA2-OA2-PA1-OA5
6	P	401	CDL	CA3-OA5-PA1-OA2
6	P	401	CDL	CB3-OB5-PB2-OB2
6	Q	401	CDL	CA3-OA5-PA1-OA2
7	A	403	PLX	C3-O4-P1-O1
7	A	403	PLX	C2-O1-P1-O4
7	A	404	PLX	C2-O1-P1-O4
7	B	403	PLX	C3-O4-P1-O1
7	C	402	PLX	C2-O1-P1-O4
7	C	404	PLX	C3-O4-P1-O1
7	C	404	PLX	C2-O1-P1-O4
7	D	401	PLX	C2-O1-P1-O4
7	N	403	PLX	C3-O4-P1-O1
7	N	403	PLX	C2-O1-P1-O4
7	N	404	PLX	C2-O1-P1-O4
7	O	403	PLX	C3-O4-P1-O1
7	P	402	PLX	C2-O1-P1-O4
7	P	404	PLX	C3-O4-P1-O1
7	P	404	PLX	C2-O1-P1-O4
7	Q	402	PLX	C2-O1-P1-O4
6	B	401	CDL	CB7-C71-C72-C73
6	O	401	CDL	CB7-C71-C72-C73
7	A	403	PLX	O8-C24-C25-C26
7	B	402	PLX	O8-C24-C25-C26
7	N	403	PLX	O8-C24-C25-C26
7	O	402	PLX	O8-C24-C25-C26
6	B	401	CDL	C57-C58-C59-C60
6	H	201	CDL	C61-C62-C63-C64
6	O	401	CDL	C57-C58-C59-C60
6	Q	401	CDL	C61-C62-C63-C64
7	O	402	PLX	C13-C14-C15-C16
6	A	402	CDL	C72-C73-C74-C75
6	B	401	CDL	C54-C55-C56-C57
6	C	401	CDL	C72-C73-C74-C75
6	N	402	CDL	C72-C73-C74-C75
6	O	401	CDL	C54-C55-C56-C57
6	P	401	CDL	C72-C73-C74-C75
7	B	402	PLX	C14-C15-C16-C17
7	B	402	PLX	C13-C14-C15-C16
7	B	403	PLX	C7-C8-C9-C10
7	O	402	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	O	403	PLX	C7-C8-C9-C10
6	C	401	CDL	C83-C84-C85-C86
6	H	201	CDL	C36-C37-C38-C39
6	H	201	CDL	C38-C39-C40-C41
6	P	401	CDL	C83-C84-C85-C86
6	Q	401	CDL	C36-C37-C38-C39
6	Q	401	CDL	C38-C39-C40-C41
7	D	401	PLX	C28-C29-C30-C31
7	Q	402	PLX	C28-C29-C30-C31
6	A	402	CDL	CB6-CB4-OB6-CB5
6	N	402	CDL	CB6-CB4-OB6-CB5
6	A	402	CDL	C42-C43-C44-C45
6	C	401	CDL	C42-C43-C44-C45
6	H	201	CDL	C13-C14-C15-C16
6	N	402	CDL	C42-C43-C44-C45
6	P	401	CDL	C42-C43-C44-C45
6	Q	401	CDL	C13-C14-C15-C16
6	A	402	CDL	C71-C72-C73-C74
6	C	401	CDL	C76-C77-C78-C79
6	H	201	CDL	C15-C16-C17-C18
6	N	402	CDL	C71-C72-C73-C74
6	P	401	CDL	C76-C77-C78-C79
6	Q	401	CDL	C15-C16-C17-C18
7	C	404	PLX	C12-C13-C14-C15
7	P	404	PLX	C12-C13-C14-C15
6	A	402	CDL	C39-C40-C41-C42
6	N	402	CDL	C39-C40-C41-C42
7	B	402	PLX	C26-C27-C28-C29
7	O	402	PLX	C26-C27-C28-C29
6	A	402	CDL	C40-C41-C42-C43
6	N	402	CDL	C40-C41-C42-C43
7	C	402	PLX	C30-C31-C32-C33
7	P	402	PLX	C30-C31-C32-C33
6	B	401	CDL	C13-C14-C15-C16
6	B	401	CDL	C18-C19-C20-C21
6	C	401	CDL	C12-C13-C14-C15
6	O	401	CDL	C13-C14-C15-C16
6	O	401	CDL	C18-C19-C20-C21
6	P	401	CDL	C12-C13-C14-C15
6	A	402	CDL	C14-C15-C16-C17
6	B	401	CDL	C19-C20-C21-C22
6	B	401	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
6	C	401	CDL	C61-C62-C63-C64
6	H	201	CDL	C80-C81-C82-C83
6	N	402	CDL	C14-C15-C16-C17
6	N	402	CDL	C81-C82-C83-C84
6	O	401	CDL	C19-C20-C21-C22
6	O	401	CDL	C36-C37-C38-C39
6	P	401	CDL	C61-C62-C63-C64
6	Q	401	CDL	C80-C81-C82-C83
7	A	404	PLX	C10-C11-C12-C13
7	C	402	PLX	C32-C33-C34-C35
7	P	402	PLX	C32-C33-C34-C35
6	A	402	CDL	C81-C82-C83-C84
6	B	401	CDL	C82-C83-C84-C85
6	H	201	CDL	C12-C13-C14-C15
6	O	401	CDL	C82-C83-C84-C85
6	Q	401	CDL	C12-C13-C14-C15
7	N	404	PLX	C10-C11-C12-C13
6	A	402	CDL	C60-C61-C62-C63
6	C	401	CDL	C78-C79-C80-C81
6	P	401	CDL	C78-C79-C80-C81
6	C	401	CDL	C36-C37-C38-C39
6	C	401	CDL	C71-C72-C73-C74
6	H	201	CDL	C18-C19-C20-C21
6	N	402	CDL	C60-C61-C62-C63
6	P	401	CDL	C36-C37-C38-C39
6	P	401	CDL	C71-C72-C73-C74
6	Q	401	CDL	C18-C19-C20-C21
7	B	402	PLX	C11-C10-C9-C8
7	D	401	PLX	C26-C27-C28-C29
7	O	402	PLX	C11-C10-C9-C8
7	Q	402	PLX	C26-C27-C28-C29
6	A	402	CDL	C15-C16-C17-C18
6	N	402	CDL	C15-C16-C17-C18
6	A	402	CDL	C54-C55-C56-C57
6	B	401	CDL	C43-C44-C45-C46
6	H	201	CDL	C39-C40-C41-C42
6	N	402	CDL	C54-C55-C56-C57
6	O	401	CDL	C43-C44-C45-C46
6	Q	401	CDL	C39-C40-C41-C42
6	B	401	CDL	C17-C18-C19-C20
6	O	401	CDL	C17-C18-C19-C20
6	C	401	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
6	P	401	CDL	C77-C78-C79-C80
6	H	201	CDL	C21-C22-C23-C24
6	P	401	CDL	C39-C40-C41-C42
6	Q	401	CDL	C21-C22-C23-C24
6	Q	401	CDL	C81-C82-C83-C84
7	C	403	PLX	C11-C12-C13-C14
7	P	403	PLX	C11-C12-C13-C14
7	C	402	PLX	C3-C4-C5-O8
6	C	401	CDL	C39-C40-C41-C42
6	H	201	CDL	C81-C82-C83-C84
7	B	403	PLX	C9-C10-C11-C12
7	O	403	PLX	C9-C10-C11-C12
6	H	201	CDL	C77-C78-C79-C80
6	Q	401	CDL	C77-C78-C79-C80
7	B	402	PLX	C31-C32-C33-C34
7	O	402	PLX	C31-C32-C33-C34
7	A	404	PLX	O7-C6-C7-C8
7	B	403	PLX	O7-C6-C7-C8
7	N	404	PLX	O7-C6-C7-C8
7	O	403	PLX	O7-C6-C7-C8
6	A	402	CDL	C16-C17-C18-C19
6	B	401	CDL	C60-C61-C62-C63
6	C	401	CDL	C81-C82-C83-C84
6	N	402	CDL	C16-C17-C18-C19
6	O	401	CDL	C60-C61-C62-C63
6	P	401	CDL	C81-C82-C83-C84
6	B	401	CDL	C21-C22-C23-C24
6	A	402	CDL	O1-C1-CB2-OB2
6	N	402	CDL	O1-C1-CB2-OB2
6	A	402	CDL	C73-C74-C75-C76
6	N	402	CDL	C73-C74-C75-C76
6	O	401	CDL	C21-C22-C23-C24
6	C	401	CDL	C17-C18-C19-C20
6	P	401	CDL	C17-C18-C19-C20
6	C	401	CDL	CA2-C1-CB2-OB2
6	P	401	CDL	CA2-C1-CB2-OB2
6	H	201	CDL	C72-C73-C74-C75
6	Q	401	CDL	C72-C73-C74-C75
7	B	402	PLX	C35-C36-C37-C38
7	O	402	PLX	C35-C36-C37-C38
7	C	402	PLX	C29-C30-C31-C32
7	C	403	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	P	402	PLX	C29-C30-C31-C32
7	P	403	PLX	C9-C10-C11-C12
6	A	402	CDL	C32-C33-C34-C35
6	N	402	CDL	C32-C33-C34-C35
7	C	402	PLX	C11-C10-C9-C8
7	P	402	PLX	C11-C10-C9-C8
7	P	403	PLX	C13-C14-C15-C16
6	H	201	CDL	CB5-C51-C52-C53
6	Q	401	CDL	CB5-C51-C52-C53
6	B	401	CDL	C84-C85-C86-C87
6	O	401	CDL	C84-C85-C86-C87
7	C	403	PLX	C13-C14-C15-C16
6	C	401	CDL	C11-C12-C13-C14
6	O	401	CDL	C11-C12-C13-C14
6	P	401	CDL	C11-C12-C13-C14
7	D	401	PLX	C14-C15-C16-C17
7	Q	402	PLX	C14-C15-C16-C17
6	B	401	CDL	C11-C12-C13-C14
6	H	201	CDL	C83-C84-C85-C86
6	O	401	CDL	C31-C32-C33-C34
7	P	402	PLX	C10-C11-C12-C13
6	A	402	CDL	C61-C62-C63-C64
6	B	401	CDL	C31-C32-C33-C34
6	N	402	CDL	C61-C62-C63-C64
6	Q	401	CDL	C83-C84-C85-C86
7	C	402	PLX	C10-C11-C12-C13
7	B	402	PLX	C17-C18-C19-C20
7	D	401	PLX	C15-C16-C17-C18
7	O	402	PLX	C17-C18-C19-C20
7	Q	402	PLX	C15-C16-C17-C18
6	H	201	CDL	C22-C23-C24-C25
6	H	201	CDL	C24-C25-C26-C27
6	Q	401	CDL	C22-C23-C24-C25
6	Q	401	CDL	C24-C25-C26-C27
7	B	402	PLX	C18-C19-C20-C21
7	O	402	PLX	C18-C19-C20-C21
6	C	401	CDL	CA5-C11-C12-C13
7	C	403	PLX	C11-C10-C9-C8
7	P	403	PLX	C11-C10-C9-C8
6	H	201	CDL	C73-C74-C75-C76
6	O	401	CDL	C74-C75-C76-C77
6	Q	401	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
6	B	401	CDL	C74-C75-C76-C77
6	C	401	CDL	C31-C32-C33-C34
6	C	401	CDL	C53-C54-C55-C56
6	P	401	CDL	C53-C54-C55-C56
6	P	401	CDL	CA5-C11-C12-C13
6	C	401	CDL	OB5-CB3-CB4-OB6
6	P	401	CDL	OB5-CB3-CB4-OB6
6	A	402	CDL	C20-C21-C22-C23
6	C	401	CDL	C20-C21-C22-C23
6	N	402	CDL	C20-C21-C22-C23
6	P	401	CDL	C20-C21-C22-C23
6	P	401	CDL	C31-C32-C33-C34
6	B	401	CDL	OA7-CA5-OA6-CA4
6	O	401	CDL	OA7-CA5-OA6-CA4
7	A	404	PLX	C16-C17-C18-C19
6	H	201	CDL	C55-C56-C57-C58
6	Q	401	CDL	C55-C56-C57-C58
7	N	404	PLX	C16-C17-C18-C19
6	C	401	CDL	C15-C16-C17-C18
6	P	401	CDL	C15-C16-C17-C18
6	C	401	CDL	C32-C33-C34-C35
6	P	401	CDL	C32-C33-C34-C35
6	B	401	CDL	C11-CA5-OA6-CA4
6	O	401	CDL	C11-CA5-OA6-CA4
7	C	404	PLX	C19-C20-C21-C22
7	D	401	PLX	C11-C10-C9-C8
7	P	404	PLX	C19-C20-C21-C22
6	B	401	CDL	C22-C23-C24-C25
6	O	401	CDL	C22-C23-C24-C25
7	Q	402	PLX	C11-C10-C9-C8
6	H	201	CDL	C11-C12-C13-C14
6	Q	401	CDL	C11-C12-C13-C14
6	C	401	CDL	C63-C64-C65-C66
6	P	401	CDL	C63-C64-C65-C66
6	C	401	CDL	CB5-C51-C52-C53
6	P	401	CDL	CB5-C51-C52-C53
6	N	402	CDL	C31-CA7-OA8-CA6
6	A	402	CDL	CA2-C1-CB2-OB2
6	B	401	CDL	CB2-C1-CA2-OA2
6	N	402	CDL	CA2-C1-CB2-OB2
6	O	401	CDL	CB2-C1-CA2-OA2
6	O	401	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
7	A	404	PLX	C15-C16-C17-C18
7	N	404	PLX	C15-C16-C17-C18
6	B	401	CDL	C37-C38-C39-C40
7	C	404	PLX	C14-C15-C16-C17
7	O	402	PLX	C30-C31-C32-C33
7	P	404	PLX	C14-C15-C16-C17
7	B	402	PLX	C30-C31-C32-C33
6	C	401	CDL	CA3-CA4-CA6-OA8
6	H	201	CDL	CB3-CB4-CB6-OB8
6	P	401	CDL	CA3-CA4-CA6-OA8
6	Q	401	CDL	CB3-CB4-CB6-OB8
7	P	402	PLX	C3-C4-C5-O8
6	A	402	CDL	C31-CA7-OA8-CA6
6	A	402	CDL	C64-C65-C66-C67
6	N	402	CDL	C64-C65-C66-C67
6	A	402	CDL	C12-C13-C14-C15
6	N	402	CDL	C12-C13-C14-C15
7	C	403	PLX	C12-C13-C14-C15
6	C	401	CDL	C44-C45-C46-C47
7	P	403	PLX	C12-C13-C14-C15
6	P	401	CDL	C44-C45-C46-C47
7	B	403	PLX	C11-C12-C13-C14
7	O	403	PLX	C11-C12-C13-C14
6	N	402	CDL	C11-C12-C13-C14
6	A	402	CDL	C11-C12-C13-C14
6	N	402	CDL	C34-C35-C36-C37
7	C	404	PLX	C9-C10-C11-C12
7	P	404	PLX	C9-C10-C11-C12
6	A	402	CDL	C34-C35-C36-C37
7	C	404	PLX	C20-C21-C22-C23
7	P	404	PLX	C20-C21-C22-C23
6	B	401	CDL	C52-C53-C54-C55
6	O	401	CDL	C52-C53-C54-C55
6	C	401	CDL	C33-C34-C35-C36
6	P	401	CDL	C33-C34-C35-C36
7	A	403	PLX	C30-C31-C32-C33
7	N	403	PLX	C30-C31-C32-C33
6	C	401	CDL	CB7-C71-C72-C73
6	A	402	CDL	OA9-CA7-OA8-CA6
6	N	402	CDL	OA9-CA7-OA8-CA6
6	P	401	CDL	CB7-C71-C72-C73
6	O	401	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
7	D	401	PLX	C11-C12-C13-C14
7	Q	402	PLX	C11-C12-C13-C14
6	A	402	CDL	C36-C37-C38-C39
6	B	401	CDL	C51-C52-C53-C54
6	H	201	CDL	C74-C75-C76-C77
6	N	402	CDL	C36-C37-C38-C39
7	B	402	PLX	C27-C28-C29-C30
6	Q	401	CDL	C74-C75-C76-C77
7	O	402	PLX	C27-C28-C29-C30
7	A	404	PLX	C9-C10-C11-C12
7	N	404	PLX	C9-C10-C11-C12
6	A	402	CDL	C44-C45-C46-C47
6	C	401	CDL	C82-C83-C84-C85
6	N	402	CDL	C44-C45-C46-C47
6	P	401	CDL	C82-C83-C84-C85
7	N	404	PLX	C7-C8-C9-C10
6	C	401	CDL	C60-C61-C62-C63
6	P	401	CDL	C60-C61-C62-C63
7	A	404	PLX	C7-C8-C9-C10
6	C	401	CDL	OB5-CB3-CB4-CB6
6	H	201	CDL	OA5-CA3-CA4-CA6
6	P	401	CDL	OB5-CB3-CB4-CB6
6	Q	401	CDL	OA5-CA3-CA4-CA6
7	B	402	PLX	C16-C17-C18-C19
7	O	402	PLX	C16-C17-C18-C19
6	H	201	CDL	C79-C80-C81-C82
6	Q	401	CDL	C79-C80-C81-C82
7	A	403	PLX	C34-C35-C36-C37
7	N	403	PLX	C34-C35-C36-C37
6	B	401	CDL	C64-C65-C66-C67
6	O	401	CDL	C64-C65-C66-C67
6	B	401	CDL	C61-C62-C63-C64
6	C	401	CDL	C23-C24-C25-C26
6	O	401	CDL	C61-C62-C63-C64
6	P	401	CDL	C23-C24-C25-C26
6	P	401	CDL	C56-C57-C58-C59
6	Q	401	CDL	C76-C77-C78-C79
6	C	401	CDL	C56-C57-C58-C59
6	H	201	CDL	C76-C77-C78-C79
7	B	403	PLX	O4-C3-C4-C5
7	O	403	PLX	O4-C3-C4-C5
7	B	403	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	C	402	PLX	C17-C18-C19-C20
7	D	401	PLX	C7-C8-C9-C10
7	O	403	PLX	C12-C13-C14-C15
7	P	402	PLX	C17-C18-C19-C20
7	Q	402	PLX	C7-C8-C9-C10
6	C	401	CDL	C58-C59-C60-C61
6	P	401	CDL	C58-C59-C60-C61
6	H	201	CDL	CB3-OB5-PB2-OB2
6	Q	401	CDL	CB3-OB5-PB2-OB2
7	C	402	PLX	C3-C4-O6-C6
7	P	402	PLX	C3-C4-O6-C6
7	A	403	PLX	O7-C6-C7-C8
7	C	404	PLX	O7-C6-C7-C8
7	N	403	PLX	O7-C6-C7-C8
7	P	404	PLX	O7-C6-C7-C8
6	O	401	CDL	C77-C78-C79-C80
7	C	403	PLX	C7-C8-C9-C10
6	H	201	CDL	OA5-CA3-CA4-OA6
6	Q	401	CDL	OA5-CA3-CA4-OA6
6	B	401	CDL	C77-C78-C79-C80
7	P	403	PLX	C7-C8-C9-C10
6	N	402	CDL	CA7-C31-C32-C33
6	C	401	CDL	C73-C74-C75-C76
6	P	401	CDL	C73-C74-C75-C76
7	B	403	PLX	O4-C3-C4-O6
7	O	403	PLX	O4-C3-C4-O6
6	B	401	CDL	C53-C54-C55-C56
6	O	401	CDL	C53-C54-C55-C56
7	A	404	PLX	C11-C12-C13-C14
7	N	404	PLX	C11-C12-C13-C14
6	A	402	CDL	C63-C64-C65-C66
6	Q	401	CDL	C63-C64-C65-C66
6	A	402	CDL	CA7-C31-C32-C33
6	H	201	CDL	C63-C64-C65-C66
6	N	402	CDL	C63-C64-C65-C66
7	O	402	PLX	C25-C26-C27-C28
7	B	402	PLX	C25-C26-C27-C28
7	D	401	PLX	C18-C19-C20-C21
7	Q	402	PLX	C18-C19-C20-C21
6	A	402	CDL	C38-C39-C40-C41
6	A	402	CDL	CB4-CB3-OB5-PB2
6	H	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
6	N	402	CDL	CB4-CB3-OB5-PB2
6	Q	401	CDL	C1-CB2-OB2-PB2
6	N	402	CDL	C38-C39-C40-C41
6	H	201	CDL	C44-C45-C46-C47
6	Q	401	CDL	C44-C45-C46-C47
7	O	403	PLX	C14-C15-C16-C17
7	B	403	PLX	C14-C15-C16-C17
7	C	402	PLX	C27-C28-C29-C30
7	C	403	PLX	O6-C6-C7-C8
7	P	402	PLX	O6-C6-C7-C8
7	P	403	PLX	O6-C6-C7-C8
7	P	402	PLX	C27-C28-C29-C30
7	A	403	PLX	C10-C11-C12-C13
7	N	403	PLX	C10-C11-C12-C13
6	B	401	CDL	C73-C74-C75-C76
6	H	201	CDL	C20-C21-C22-C23
6	O	401	CDL	C73-C74-C75-C76
6	Q	401	CDL	C20-C21-C22-C23
7	P	403	PLX	C20-C21-C22-C23
7	C	403	PLX	C20-C21-C22-C23
6	A	402	CDL	CA3-CA4-CA6-OA8
6	N	402	CDL	CA3-CA4-CA6-OA8
7	D	401	PLX	C3-C4-C5-O8
7	Q	402	PLX	C3-C4-C5-O8
6	A	402	CDL	OB5-CB3-CB4-OB6
6	N	402	CDL	OB5-CB3-CB4-OB6
7	D	401	PLX	O4-C3-C4-O6
7	Q	402	PLX	O4-C3-C4-O6
6	B	401	CDL	C79-C80-C81-C82
7	A	403	PLX	C31-C32-C33-C34
7	N	403	PLX	C31-C32-C33-C34
6	C	401	CDL	C38-C39-C40-C41
6	O	401	CDL	C79-C80-C81-C82
6	P	401	CDL	C38-C39-C40-C41
7	A	403	PLX	C24-C25-C26-C27
7	N	403	PLX	C24-C25-C26-C27
6	C	401	CDL	OA6-CA4-CA6-OA8
6	P	401	CDL	OA6-CA4-CA6-OA8
7	C	403	PLX	C14-C15-C16-C17
7	P	403	PLX	C14-C15-C16-C17
7	B	402	PLX	C6-C7-C8-C9
7	O	402	PLX	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	B	401	CDL	C16-C17-C18-C19
6	O	401	CDL	C16-C17-C18-C19
7	P	402	PLX	C12-C13-C14-C15
6	B	401	CDL	CB2-OB2-PB2-OB5
6	O	401	CDL	CB2-OB2-PB2-OB5
7	C	402	PLX	C3-O4-P1-O1
7	P	402	PLX	C3-O4-P1-O1
7	C	402	PLX	C12-C13-C14-C15
6	C	401	CDL	C1-CB2-OB2-PB2
6	P	401	CDL	C1-CB2-OB2-PB2
6	B	401	CDL	CA3-OA5-PA1-OA3
6	B	401	CDL	CA3-OA5-PA1-OA4
6	C	401	CDL	CA2-OA2-PA1-OA4
6	O	401	CDL	CA3-OA5-PA1-OA3
6	O	401	CDL	CA3-OA5-PA1-OA4
6	P	401	CDL	CA2-OA2-PA1-OA4
7	A	404	PLX	C2-O1-P1-O3
7	B	403	PLX	C3-O4-P1-O3
7	C	402	PLX	C2-O1-P1-O2
7	C	402	PLX	C2-O1-P1-O3
7	C	404	PLX	C3-O4-P1-O2
7	C	404	PLX	C2-O1-P1-O2
7	D	401	PLX	C2-O1-P1-O2
7	N	404	PLX	C2-O1-P1-O3
7	O	403	PLX	C3-O4-P1-O3
7	P	402	PLX	C2-O1-P1-O2
7	P	402	PLX	C2-O1-P1-O3
7	P	404	PLX	C3-O4-P1-O2
7	P	404	PLX	C2-O1-P1-O2
7	Q	402	PLX	C2-O1-P1-O2
6	C	401	CDL	C13-C14-C15-C16
6	P	401	CDL	C13-C14-C15-C16
6	A	402	CDL	OA5-CA3-CA4-CA6
6	A	402	CDL	OB5-CB3-CB4-CB6
6	B	401	CDL	OB5-CB3-CB4-CB6
6	N	402	CDL	OA5-CA3-CA4-CA6
6	N	402	CDL	OB5-CB3-CB4-CB6
6	O	401	CDL	OB5-CB3-CB4-CB6
6	B	401	CDL	C34-C35-C36-C37
6	N	402	CDL	C53-C54-C55-C56
7	D	401	PLX	C13-C14-C15-C16
6	A	402	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
6	O	401	CDL	C34-C35-C36-C37
7	Q	402	PLX	C13-C14-C15-C16
6	C	401	CDL	C64-C65-C66-C67
6	P	401	CDL	C64-C65-C66-C67
6	B	401	CDL	OB5-CB3-CB4-OB6
6	H	201	CDL	OB5-CB3-CB4-OB6
6	O	401	CDL	OB5-CB3-CB4-OB6
6	Q	401	CDL	OB5-CB3-CB4-OB6
7	B	402	PLX	C20-C21-C22-C23
7	O	402	PLX	C20-C21-C22-C23
7	A	404	PLX	C11-C10-C9-C8
7	N	404	PLX	C11-C10-C9-C8
7	A	403	PLX	N1-C1-C2-O1
7	B	403	PLX	N1-C1-C2-O1
7	C	403	PLX	N1-C1-C2-O1
7	C	404	PLX	N1-C1-C2-O1
7	N	403	PLX	N1-C1-C2-O1
7	O	403	PLX	N1-C1-C2-O1
7	P	403	PLX	N1-C1-C2-O1
7	P	404	PLX	N1-C1-C2-O1
6	A	402	CDL	OB6-CB4-CB6-OB8
6	N	402	CDL	OB6-CB4-CB6-OB8
7	C	402	PLX	O6-C4-C5-O8
7	P	402	PLX	O6-C4-C5-O8
7	B	403	PLX	C4-C3-O4-P1
7	O	403	PLX	C4-C3-O4-P1
7	C	402	PLX	C9-C10-C11-C12
7	P	402	PLX	C9-C10-C11-C12
7	D	401	PLX	C16-C17-C18-C19
7	Q	402	PLX	C16-C17-C18-C19
6	B	401	CDL	C23-C24-C25-C26
6	O	401	CDL	C23-C24-C25-C26
7	B	402	PLX	C11-C12-C13-C14
7	O	402	PLX	C11-C12-C13-C14
7	C	402	PLX	O6-C6-C7-C8
7	D	401	PLX	O6-C6-C7-C8
7	Q	402	PLX	O6-C6-C7-C8
6	H	201	CDL	C42-C43-C44-C45
6	Q	401	CDL	C42-C43-C44-C45
7	B	402	PLX	C7-C8-C9-C10
7	O	402	PLX	C7-C8-C9-C10
7	N	403	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
7	A	403	PLX	C28-C29-C30-C31
7	D	401	PLX	C36-C37-C38-C39
7	Q	402	PLX	C36-C37-C38-C39
7	B	402	PLX	C15-C16-C17-C18
7	O	402	PLX	C15-C16-C17-C18
6	B	401	CDL	C32-C33-C34-C35
6	O	401	CDL	C32-C33-C34-C35
7	B	403	PLX	C18-C19-C20-C21
7	O	403	PLX	C18-C19-C20-C21
6	B	401	CDL	C59-C60-C61-C62
6	O	401	CDL	C59-C60-C61-C62
7	N	403	PLX	C11-C10-C9-C8
7	A	403	PLX	C11-C10-C9-C8
6	H	201	CDL	C57-C58-C59-C60
6	Q	401	CDL	C57-C58-C59-C60
6	A	402	CDL	C1-CA2-OA2-PA1
6	N	402	CDL	C1-CA2-OA2-PA1
7	D	401	PLX	C4-C3-O4-P1
7	Q	402	PLX	C4-C3-O4-P1
6	B	401	CDL	C35-C36-C37-C38
6	O	401	CDL	C35-C36-C37-C38
7	B	402	PLX	C28-C29-C30-C31
7	O	402	PLX	C28-C29-C30-C31
6	C	401	CDL	OA5-CA3-CA4-OA6
6	P	401	CDL	OA5-CA3-CA4-OA6
7	O	402	PLX	C32-C33-C34-C35
7	B	402	PLX	C32-C33-C34-C35
7	C	402	PLX	C24-C25-C26-C27
7	C	404	PLX	C6-C7-C8-C9
7	P	404	PLX	C6-C7-C8-C9
7	C	404	PLX	O6-C6-C7-C8
7	P	404	PLX	O6-C6-C7-C8
6	A	402	CDL	C1-CB2-OB2-PB2
6	N	402	CDL	C1-CB2-OB2-PB2
6	N	402	CDL	C83-C84-C85-C86
6	A	402	CDL	C83-C84-C85-C86
6	B	401	CDL	C33-C34-C35-C36
7	A	403	PLX	C16-C17-C18-C19
6	A	402	CDL	C59-C60-C61-C62
6	N	402	CDL	C59-C60-C61-C62
6	O	401	CDL	C33-C34-C35-C36
7	N	403	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	P	402	PLX	C24-C25-C26-C27
6	A	402	CDL	C22-C23-C24-C25
6	Q	401	CDL	C56-C57-C58-C59
6	A	402	CDL	C52-C53-C54-C55
6	N	402	CDL	C22-C23-C24-C25
6	N	402	CDL	C52-C53-C54-C55
7	D	401	PLX	C29-C30-C31-C32
7	Q	402	PLX	C29-C30-C31-C32
6	H	201	CDL	C56-C57-C58-C59
6	B	401	CDL	CA3-CA4-OA6-CA5
6	B	401	CDL	CB3-CB4-OB6-CB5
6	O	401	CDL	CA3-CA4-OA6-CA5
6	O	401	CDL	CB3-CB4-OB6-CB5
6	Q	401	CDL	C41-C42-C43-C44
6	H	201	CDL	C41-C42-C43-C44
7	A	404	PLX	C6-C7-C8-C9
7	N	404	PLX	C6-C7-C8-C9
6	C	401	CDL	OA5-CA3-CA4-CA6
6	P	401	CDL	OA5-CA3-CA4-CA6
6	A	402	CDL	C79-C80-C81-C82
7	D	401	PLX	O6-C4-C5-O8
7	Q	402	PLX	O6-C4-C5-O8
7	C	403	PLX	C16-C17-C18-C19
6	N	402	CDL	C79-C80-C81-C82
7	P	403	PLX	C16-C17-C18-C19
6	P	401	CDL	C21-C22-C23-C24
6	C	401	CDL	C21-C22-C23-C24
7	A	404	PLX	C13-C14-C15-C16
7	N	404	PLX	C13-C14-C15-C16
7	Q	402	PLX	C6-C7-C8-C9
7	D	401	PLX	C4-C5-O8-C24
7	Q	402	PLX	C4-C5-O8-C24
6	Q	401	CDL	C40-C41-C42-C43
6	H	201	CDL	C40-C41-C42-C43
7	D	401	PLX	C6-C7-C8-C9
6	H	201	CDL	C16-C17-C18-C19
6	Q	401	CDL	C16-C17-C18-C19
7	B	402	PLX	O6-C6-C7-C8
7	O	402	PLX	O6-C6-C7-C8
6	Q	401	CDL	C32-C31-CA7-OA8
6	H	201	CDL	C32-C31-CA7-OA8
7	B	403	PLX	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	O	403	PLX	C6-C7-C8-C9
7	C	402	PLX	C15-C16-C17-C18
7	P	402	PLX	C15-C16-C17-C18
6	H	201	CDL	C72-C71-CB7-OB8
6	Q	401	CDL	C72-C71-CB7-OB8
6	B	401	CDL	CB6-CB4-OB6-CB5
6	H	201	CDL	CA3-CA4-OA6-CA5
6	O	401	CDL	CB6-CB4-OB6-CB5
6	Q	401	CDL	CA3-CA4-OA6-CA5
7	A	403	PLX	C20-C21-C22-C23
7	N	403	PLX	C20-C21-C22-C23
7	A	404	PLX	C7-C6-O6-C4
7	N	404	PLX	C7-C6-O6-C4
6	B	401	CDL	C62-C63-C64-C65
6	O	401	CDL	C62-C63-C64-C65
6	A	402	CDL	C21-C22-C23-C24
6	N	402	CDL	C21-C22-C23-C24
7	C	402	PLX	C6-C7-C8-C9
7	P	402	PLX	C6-C7-C8-C9
7	A	403	PLX	C36-C37-C38-C39
7	N	403	PLX	C36-C37-C38-C39
7	D	401	PLX	O4-C3-C4-C5
7	Q	402	PLX	O4-C3-C4-C5
6	C	401	CDL	C72-C71-CB7-OB8
6	P	401	CDL	C72-C71-CB7-OB8
6	B	401	CDL	C12-C11-CA5-OA6
6	O	401	CDL	C12-C11-CA5-OA6
7	C	402	PLX	O9-C24-C25-C26
7	D	401	PLX	O9-C24-C25-C26
7	P	402	PLX	O9-C24-C25-C26
7	Q	402	PLX	O9-C24-C25-C26
7	C	403	PLX	C6-C7-C8-C9
7	P	403	PLX	C6-C7-C8-C9
6	Q	401	CDL	C32-C31-CA7-OA9
7	P	403	PLX	C15-C16-C17-C18
7	C	403	PLX	C15-C16-C17-C18
6	H	201	CDL	C32-C31-CA7-OA9
6	H	201	CDL	C72-C71-CB7-OB9
6	Q	401	CDL	C72-C71-CB7-OB9
6	C	401	CDL	C72-C71-CB7-OB9
6	P	401	CDL	C72-C71-CB7-OB9
7	A	404	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
7	C	403	PLX	C3-O4-P1-O2
7	N	404	PLX	C3-O4-P1-O2
7	P	403	PLX	C3-O4-P1-O2
7	Q	402	PLX	C20-C21-C22-C23
7	D	401	PLX	C20-C21-C22-C23
6	B	401	CDL	C80-C81-C82-C83
6	O	401	CDL	C80-C81-C82-C83
6	B	401	CDL	CA6-CA4-OA6-CA5
6	H	201	CDL	CA6-CA4-OA6-CA5
6	O	401	CDL	CA6-CA4-OA6-CA5
6	Q	401	CDL	CA6-CA4-OA6-CA5
6	B	401	CDL	C12-C11-CA5-OA7
6	O	401	CDL	C12-C11-CA5-OA7
6	B	401	CDL	C72-C73-C74-C75
6	O	401	CDL	C72-C73-C74-C75
7	A	403	PLX	C6-C7-C8-C9
7	N	403	PLX	C6-C7-C8-C9
6	Q	401	CDL	C84-C85-C86-C87
6	H	201	CDL	C84-C85-C86-C87
7	B	403	PLX	C13-C14-C15-C16
7	O	403	PLX	C13-C14-C15-C16

There are no ring outliers.

21 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Q	402	PLX	3	0
7	C	404	PLX	1	0
7	A	404	PLX	1	0
7	O	402	PLX	4	0
7	D	401	PLX	4	0
7	B	402	PLX	5	0
6	C	401	CDL	6	0
6	A	402	CDL	6	0
7	N	403	PLX	1	0
6	N	402	CDL	6	0
7	C	402	PLX	2	0
7	P	404	PLX	1	0
6	P	401	CDL	9	0
6	O	401	CDL	6	0
7	P	402	PLX	3	0
6	B	401	CDL	6	0

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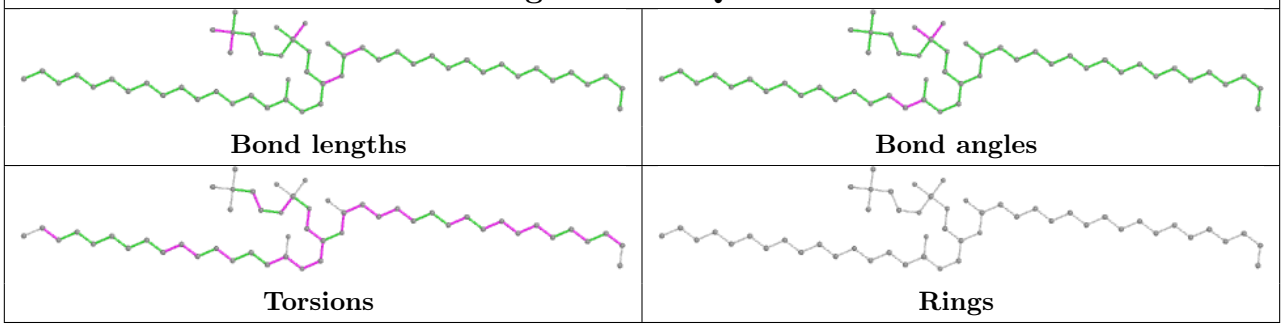
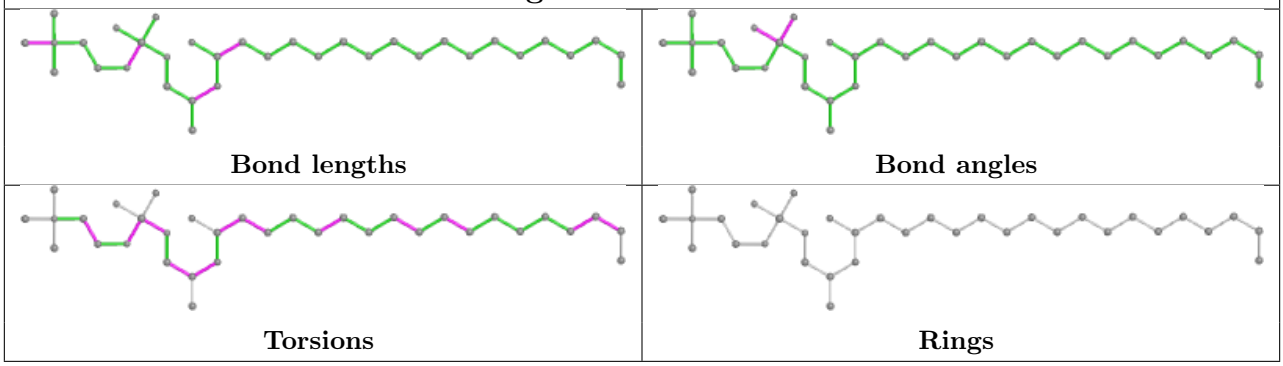
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	201	CDL	6	0
7	C	403	PLX	2	0
7	A	403	PLX	2	0
7	P	403	PLX	1	0
6	Q	401	CDL	10	0

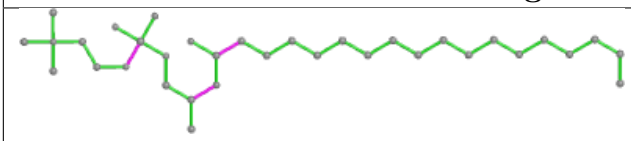
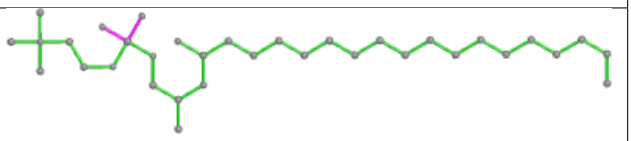
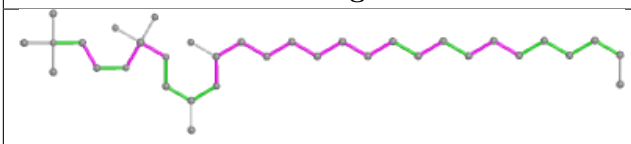
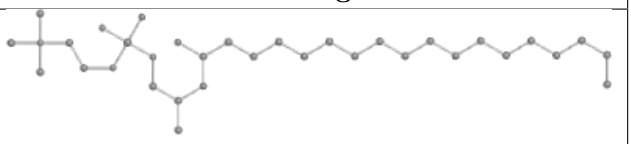
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

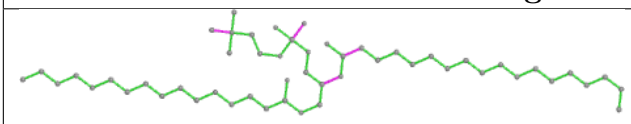
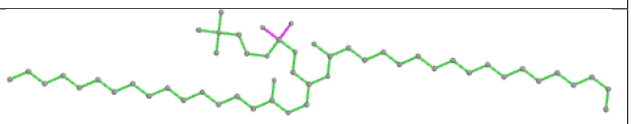
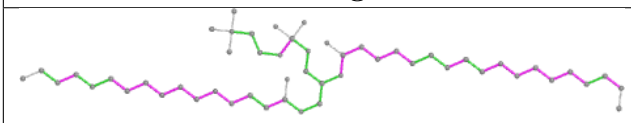
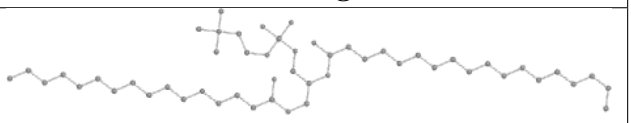
Ligand PLX Q 402

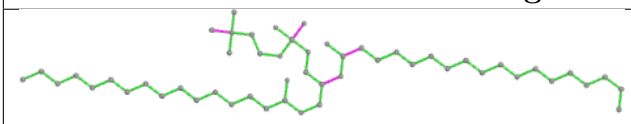
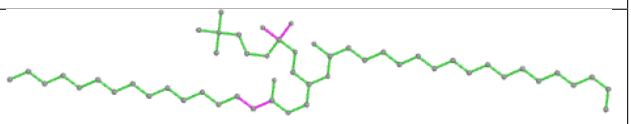
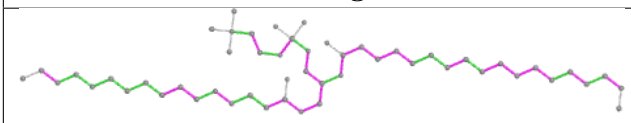
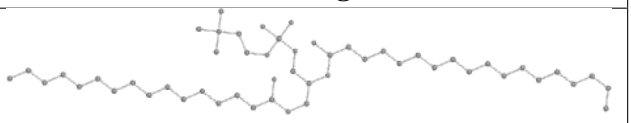


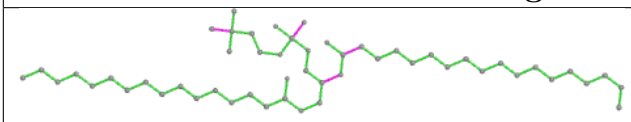
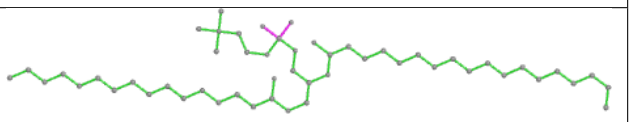
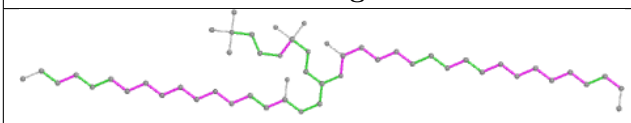
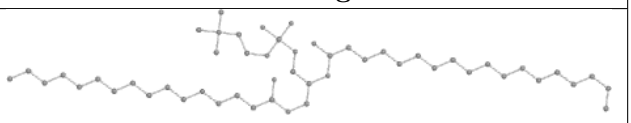
Ligand PLX C 404



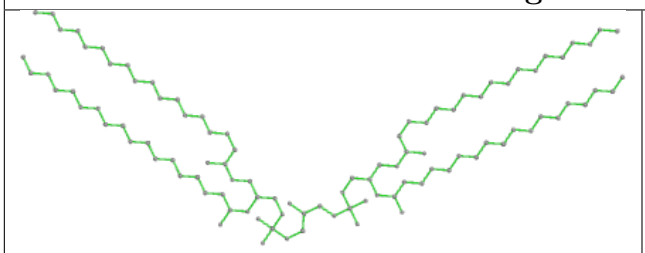
Ligand PLX A 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX O 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

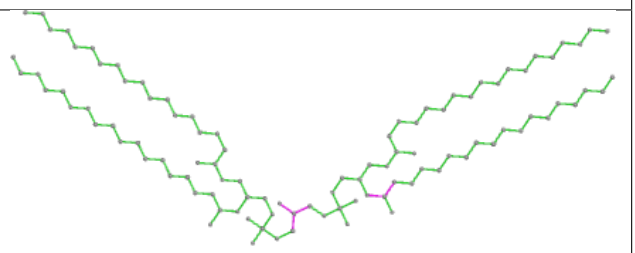
Ligand PLX D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX B 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL C 401



Bond lengths



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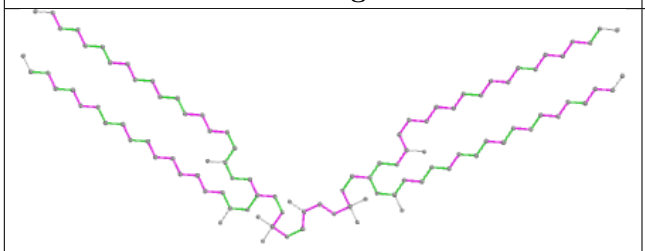

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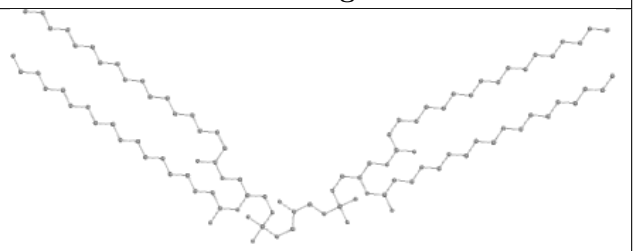
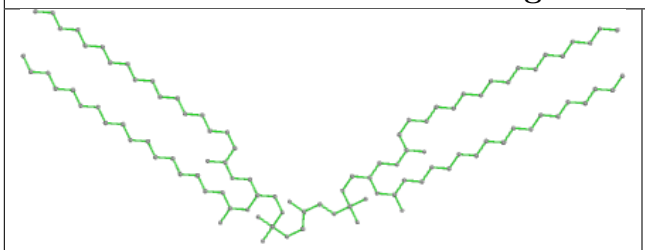


Rings

Ligand CDL A 402



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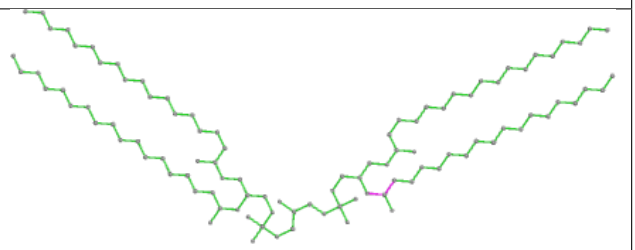

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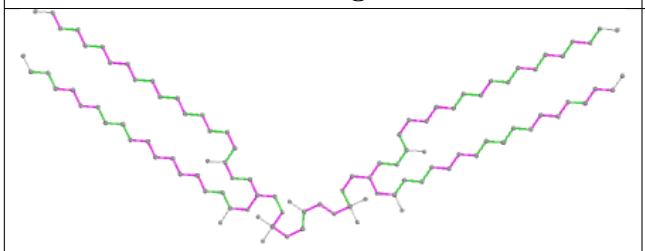

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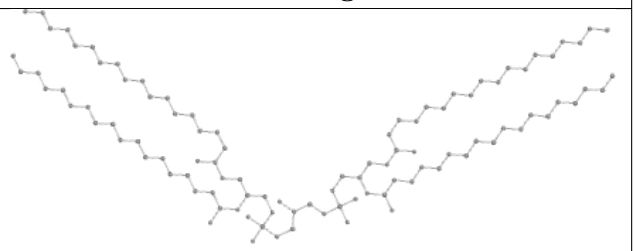
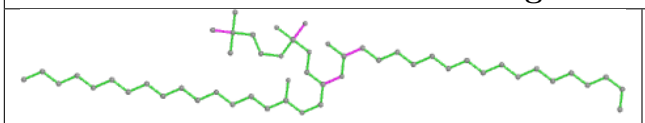


Rings

Ligand PLX N 403



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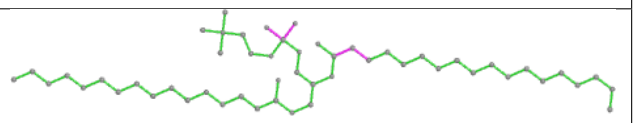
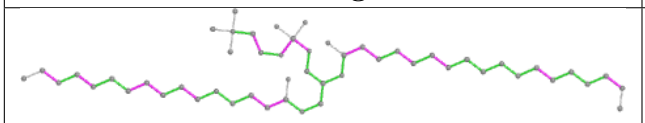


Bond angles



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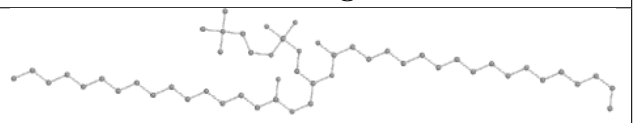
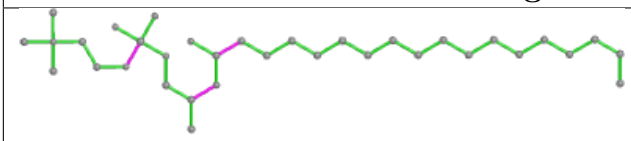


Rings

Ligand PLX N 404



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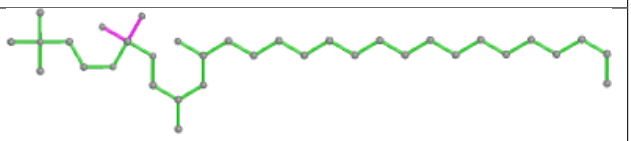
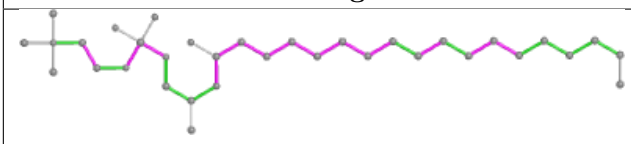


Bond angles



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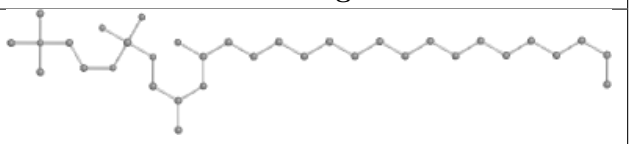
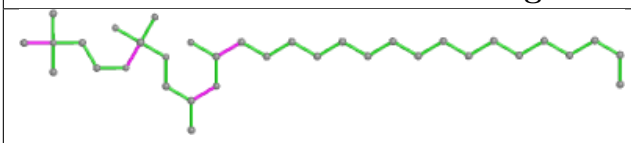
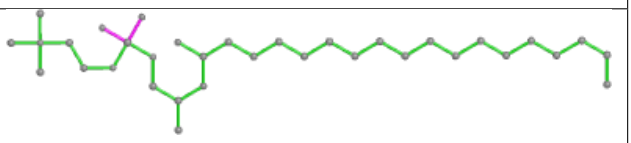


Rings

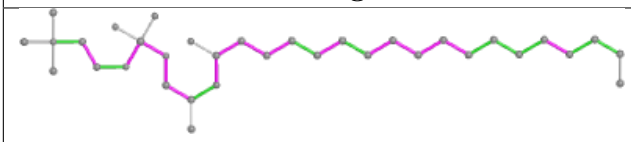
Ligand PLX O 403



Bond lengths



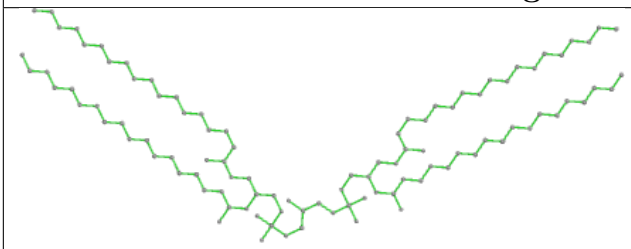
Bond angles



Torsions

Rings

Ligand CDL N 402



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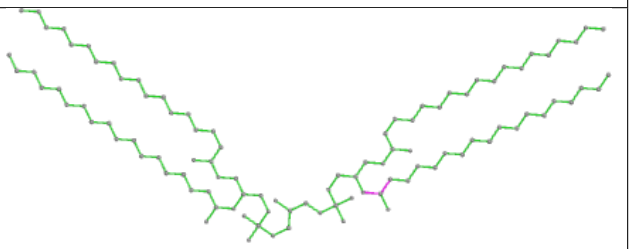
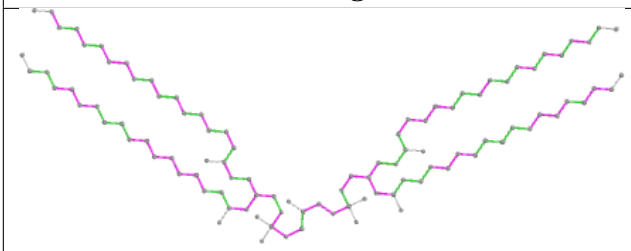
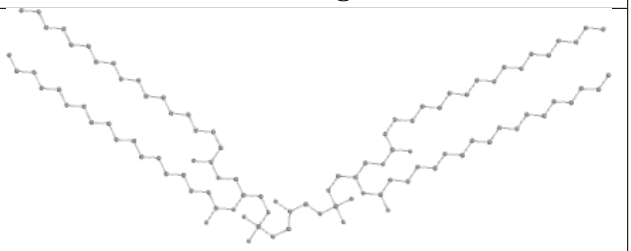


Bond angles

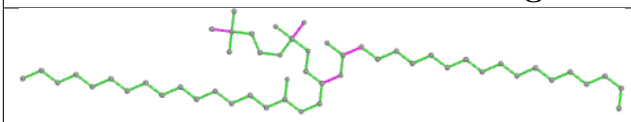


Torsions



Rings

Ligand PLX C 402



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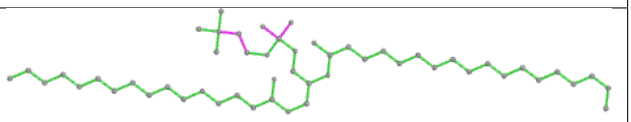
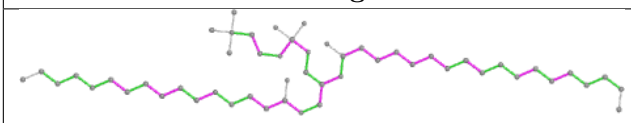
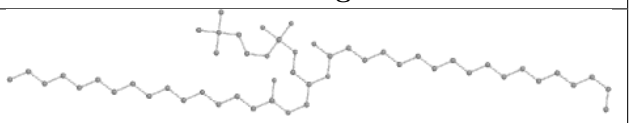


Bond angles

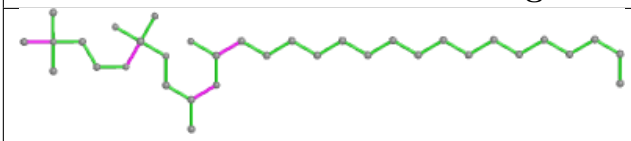


Torsions



Rings

Ligand PLX P 404



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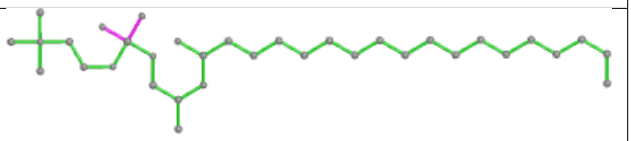
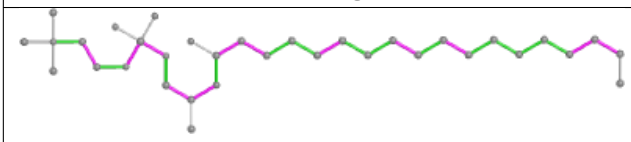


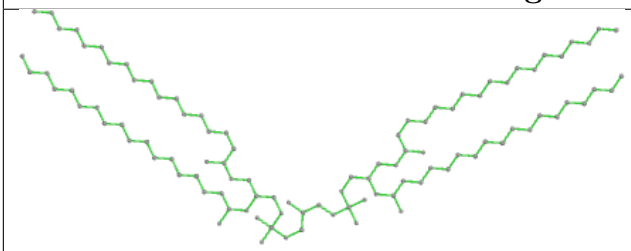
Bond angles



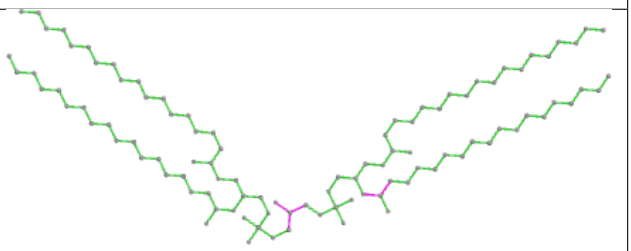
Torsions

Rings

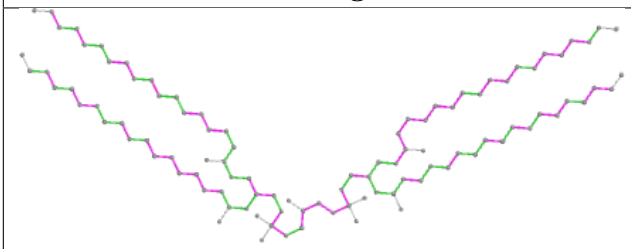
Ligand CDL P 401



Bond lengths



Bond angles



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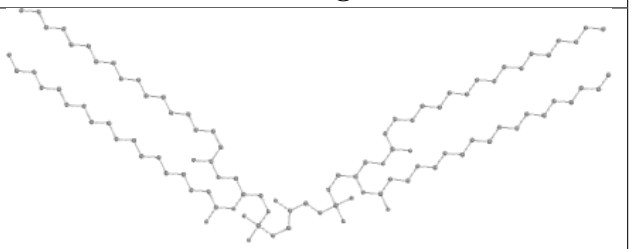
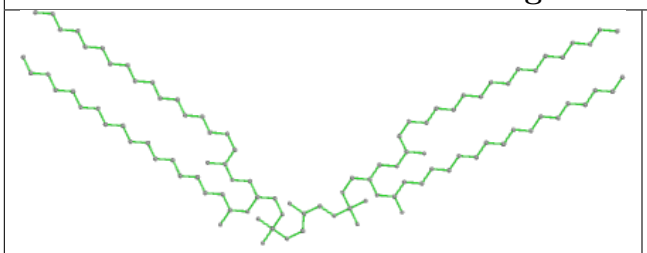


Rings

Ligand CDL O 401



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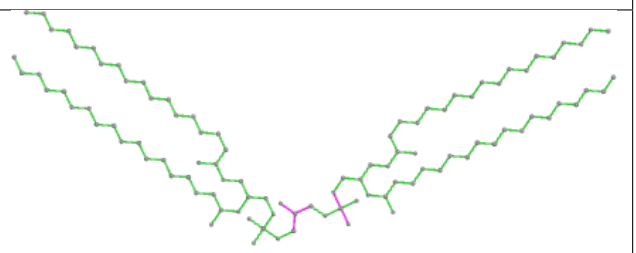
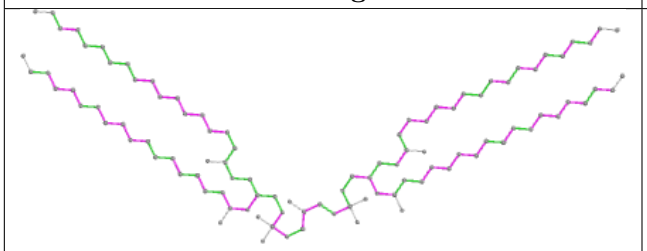


Bond angles



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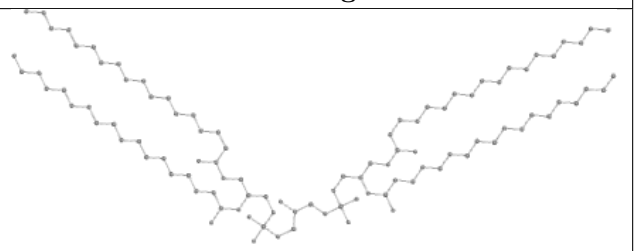
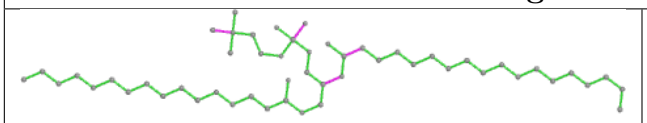


Rings

Ligand PLX P 402



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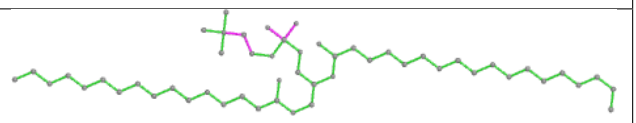
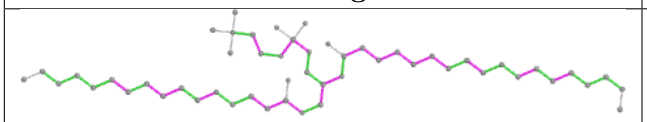


Bond angles



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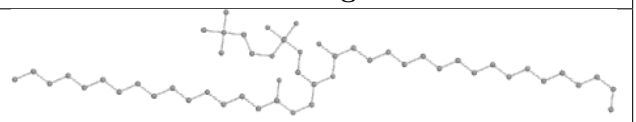
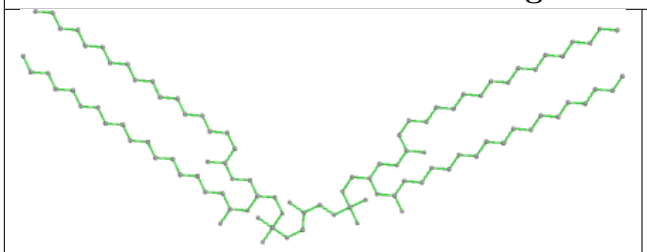
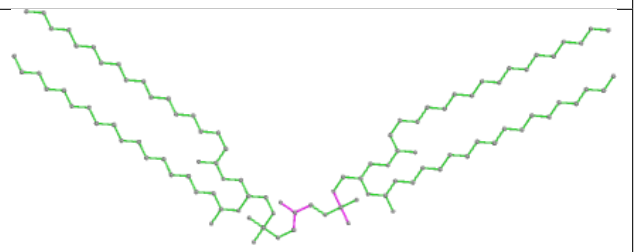


Rings

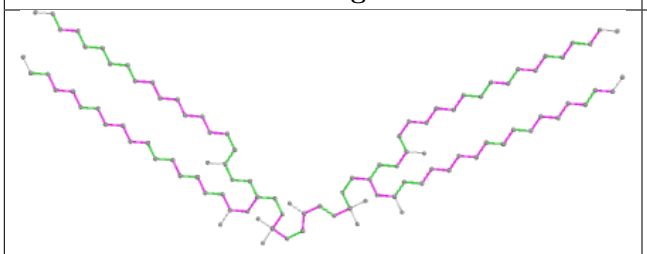
Ligand CDL B 401



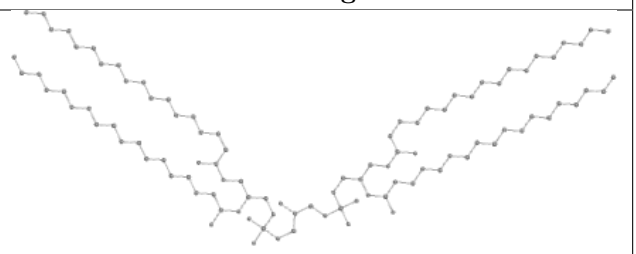
Bond lengths



Bond angles

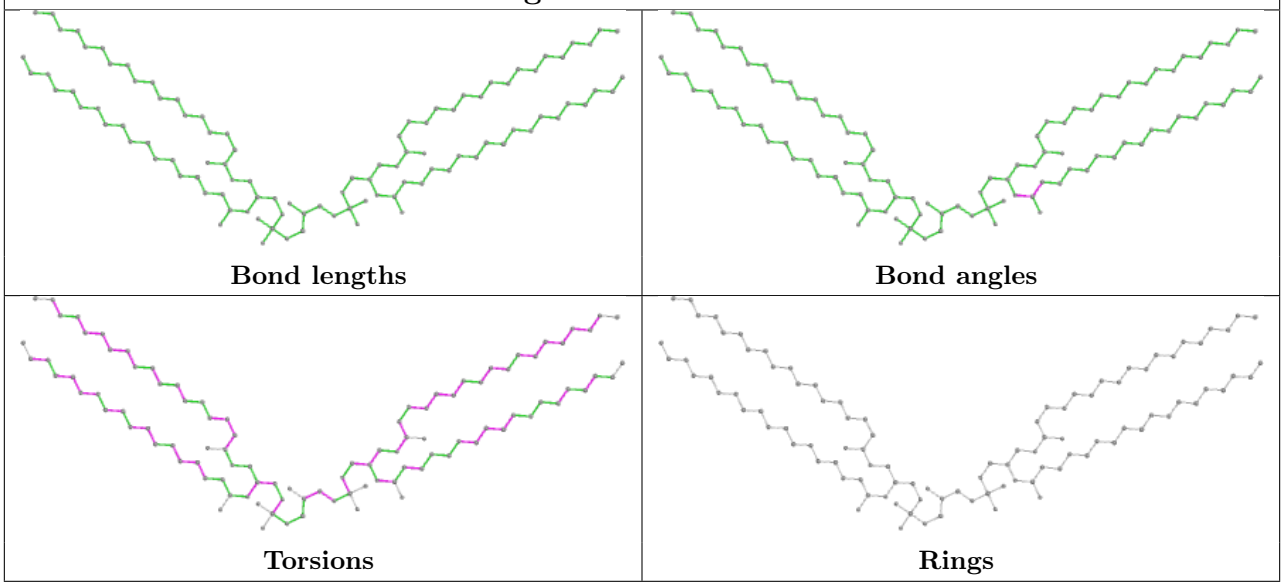


Torsions

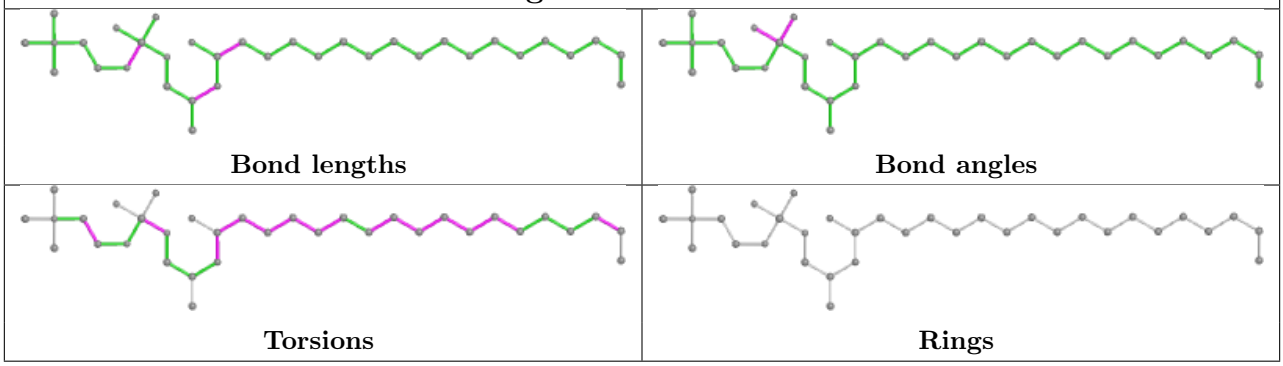


Rings

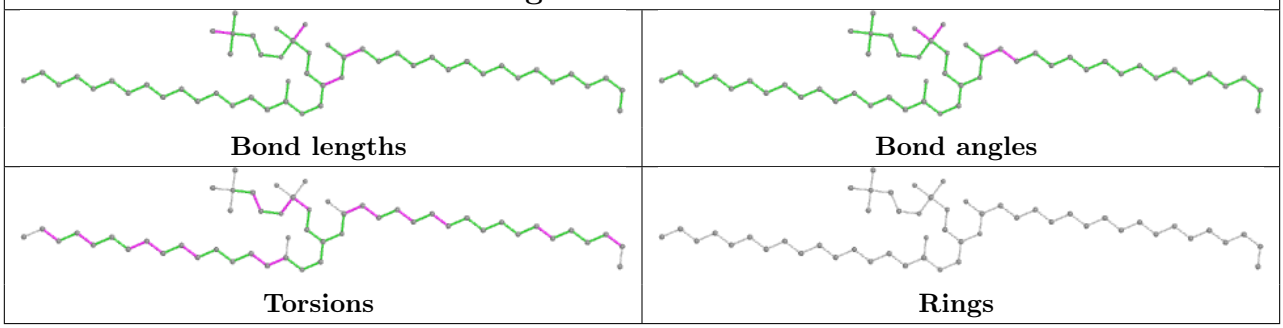
Ligand CDL H 201

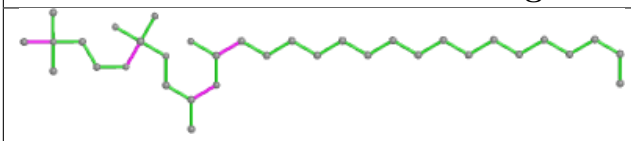
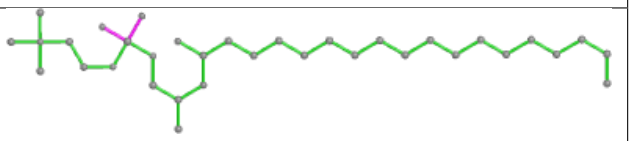
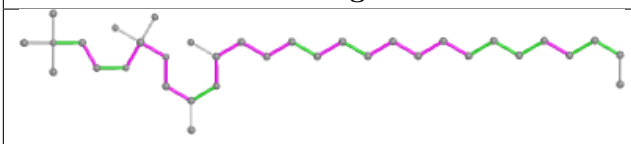
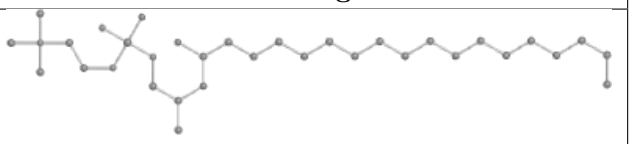


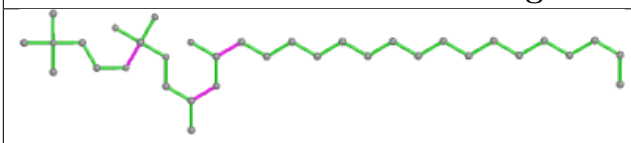
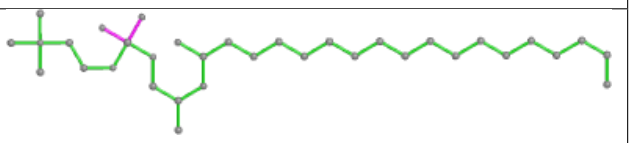
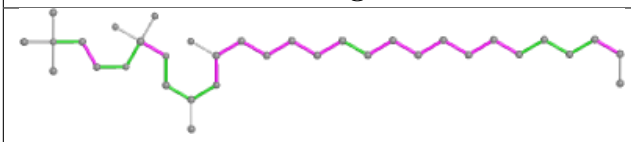
Ligand PLX C 403

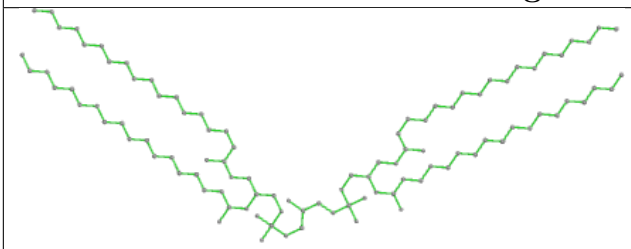
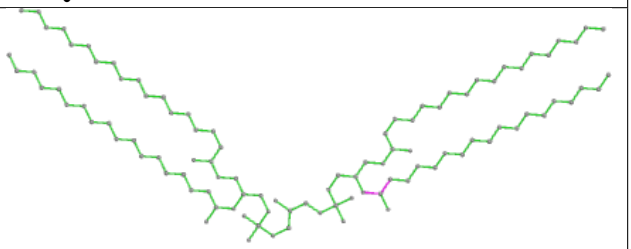
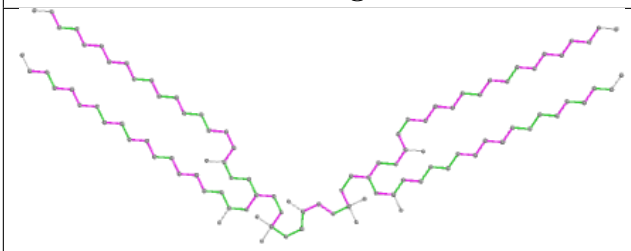
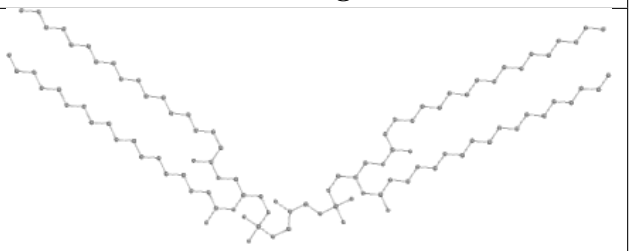


Ligand PLX A 403



Ligand PLX B 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX P 403	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CDL Q 401	
 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.

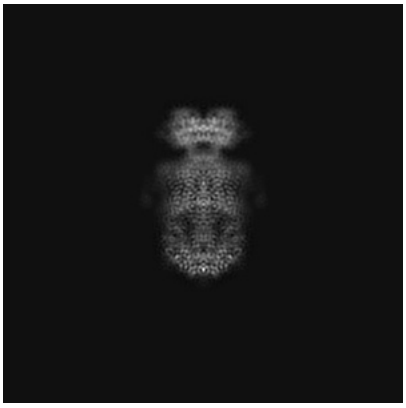
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9945. These allow visual inspection of the internal detail of the map and identification of artifacts.

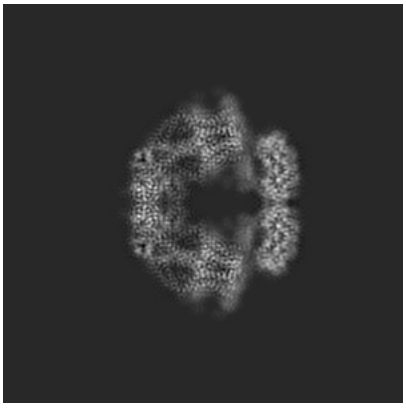
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

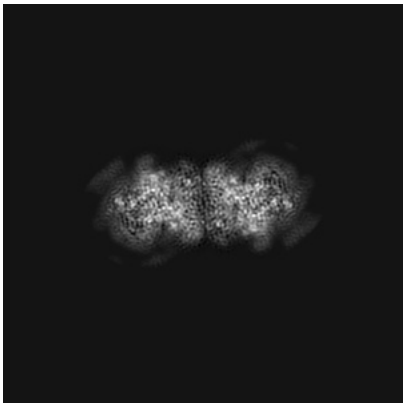
6.1.1 Primary map



X



Y



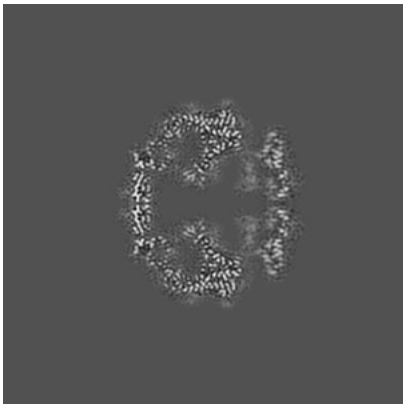
Z

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

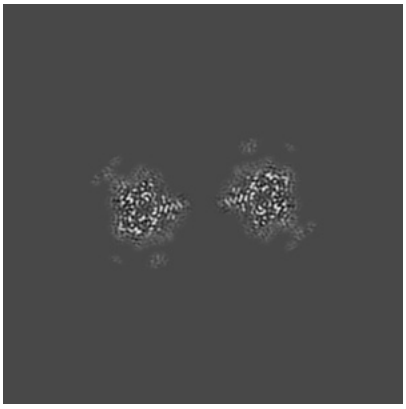
6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



Y Index: 180

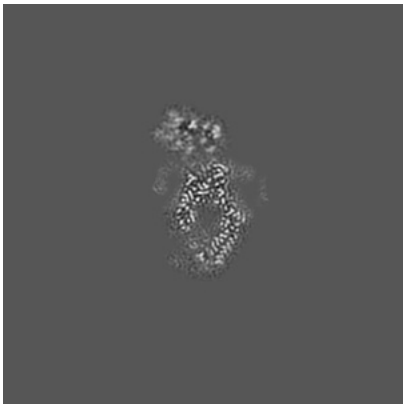


Z Index: 180

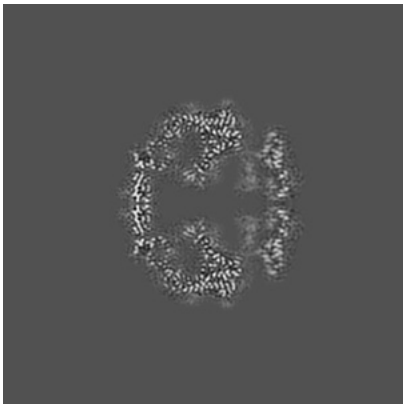
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

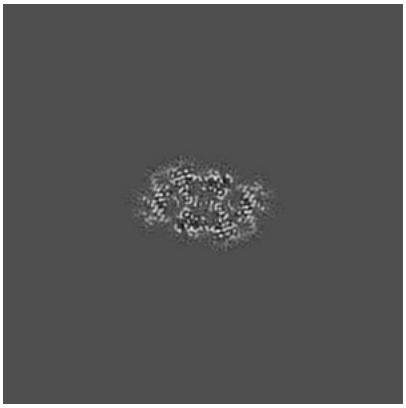
6.3.1 Primary map



X Index: 229



Y Index: 180

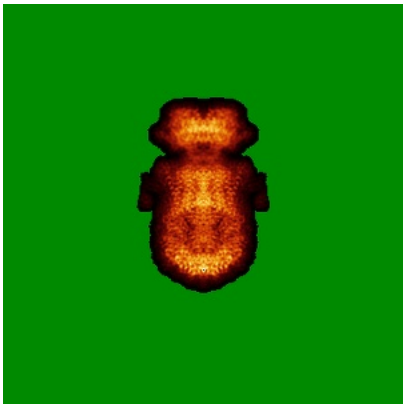


Z Index: 131

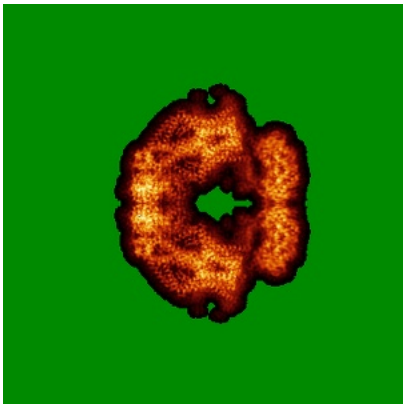
The images above show the largest variance slices of the map in three orthogonal directions.

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

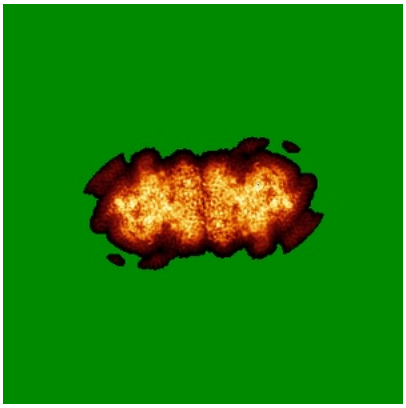
6.4.1 Primary map



X



Y

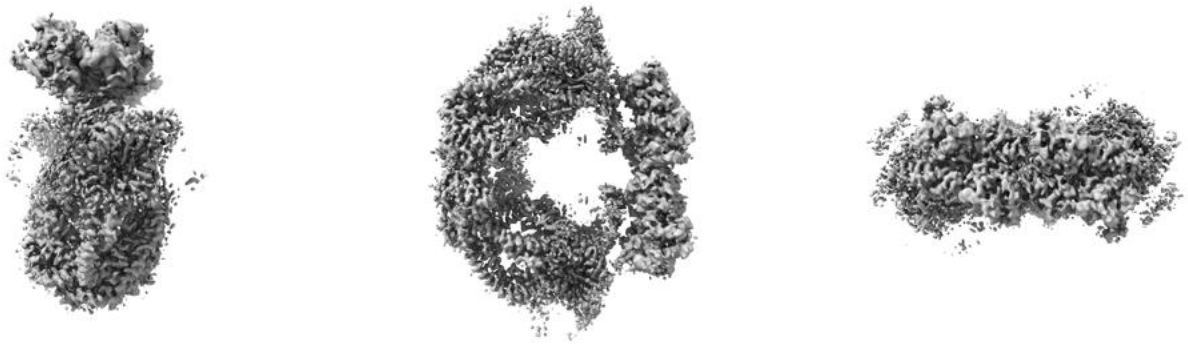


Z

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

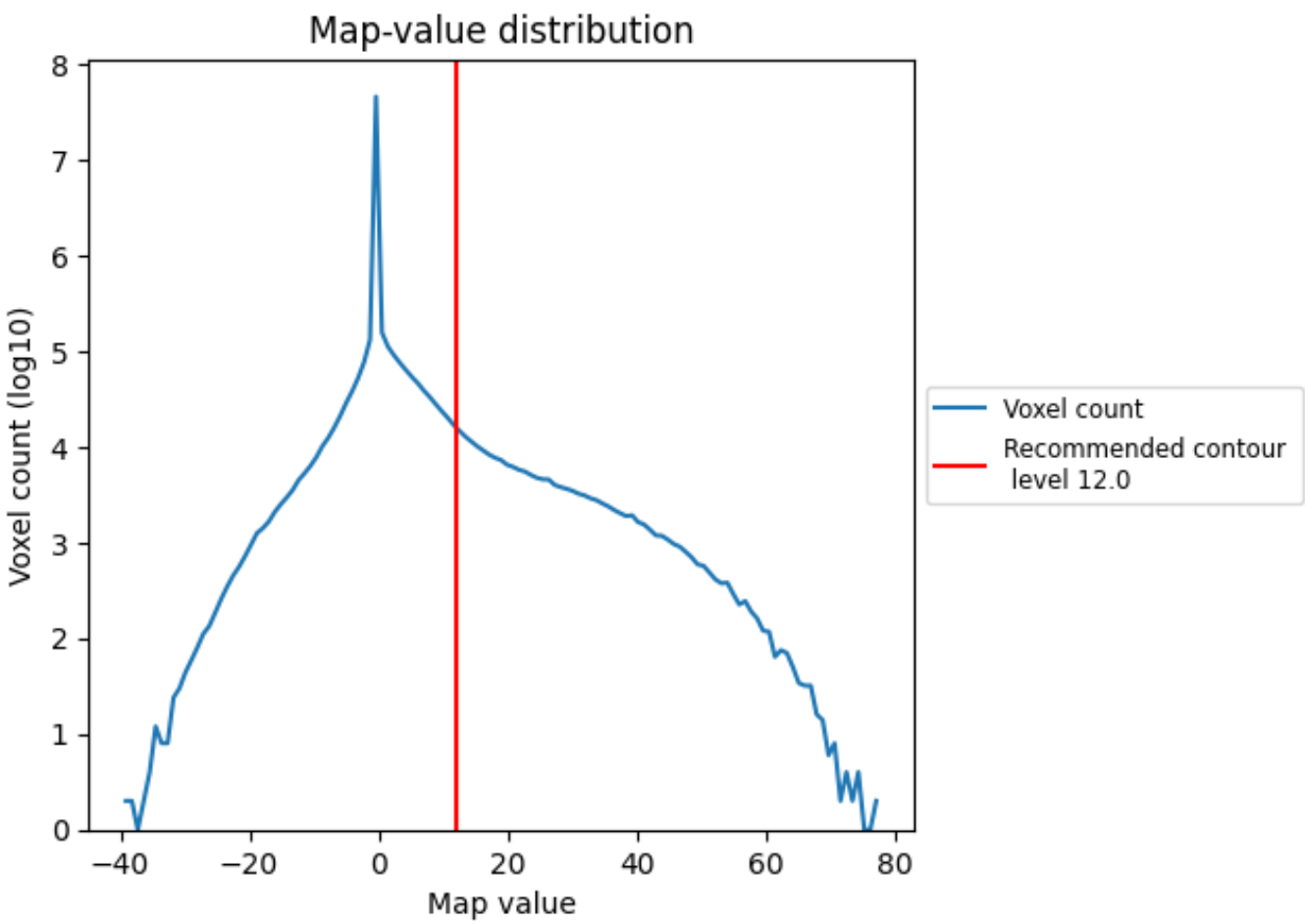
6.6 Mask visualisation (i)

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

7 Map analysis (i)

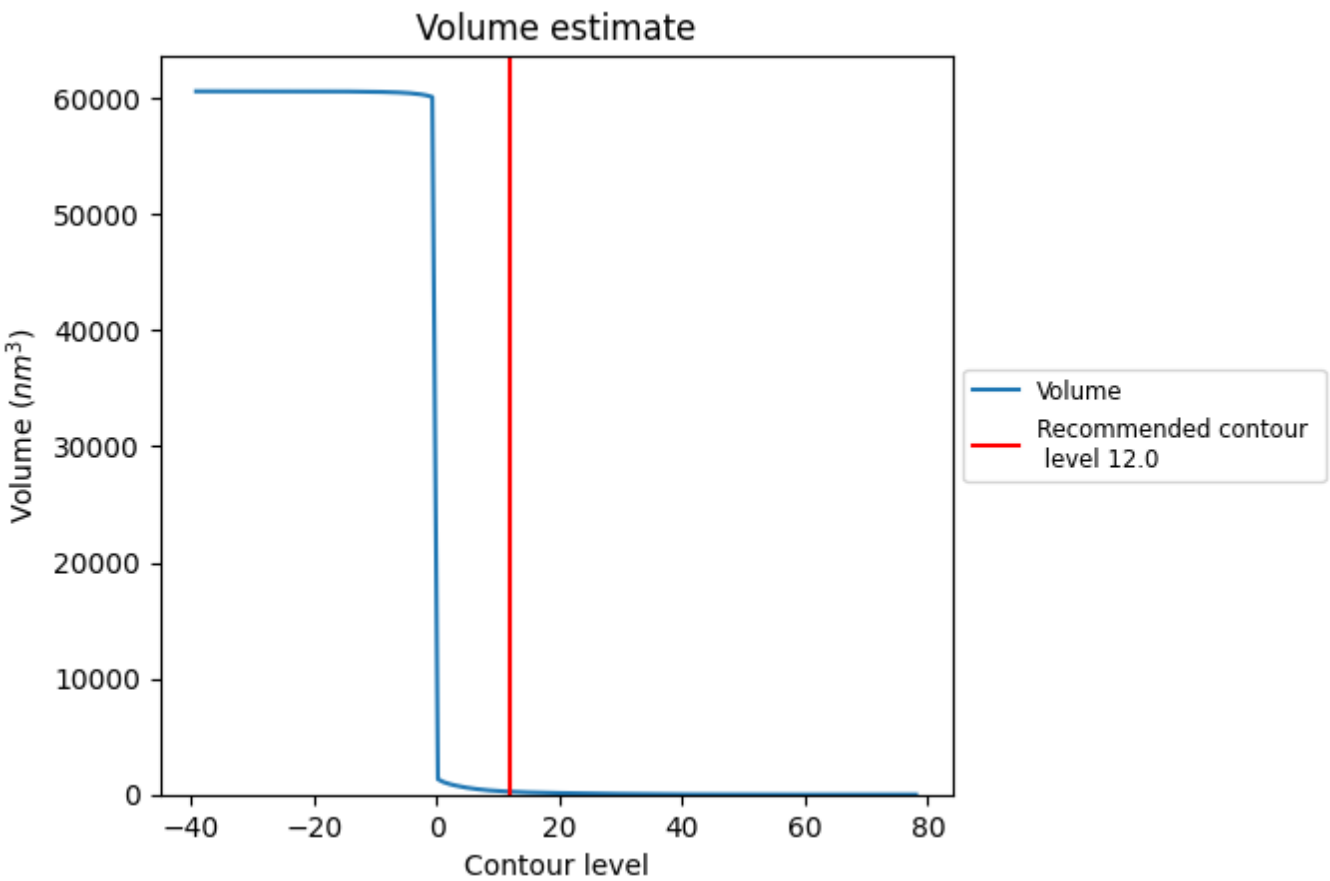
This section contains the results of statistical analysis of the map.

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.

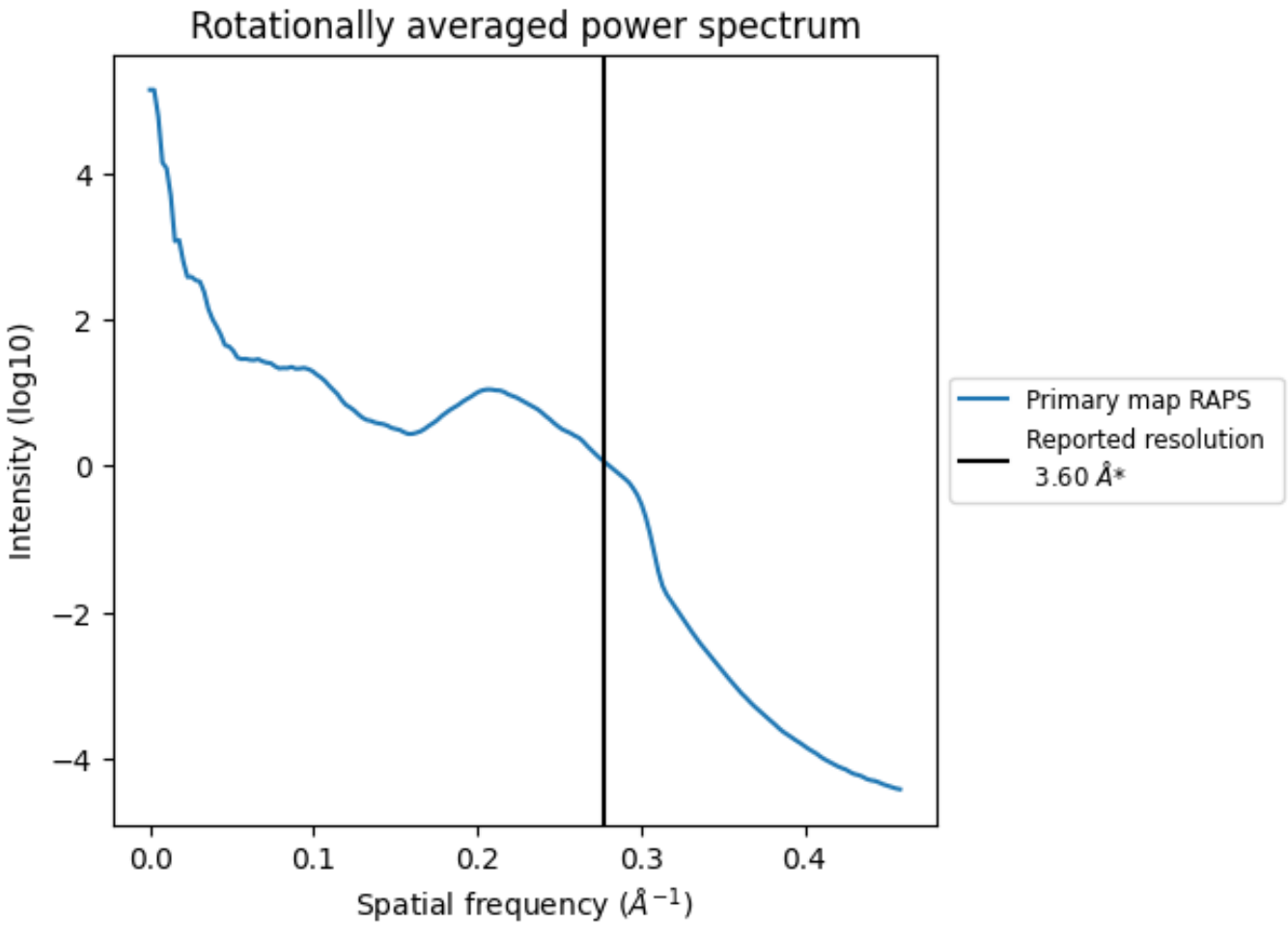
7.2 Volume estimate (i)



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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 0.278 Å^{-1}

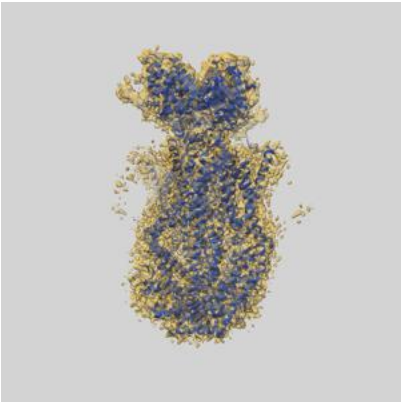
8 Fourier-Shell correlation (i)

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

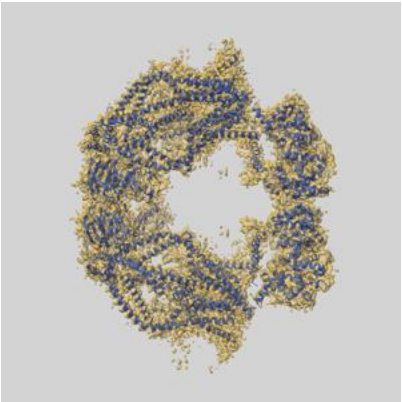
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9945 and PDB model 6K7Y. Per-residue inclusion information can be found in section 3 on page 9.

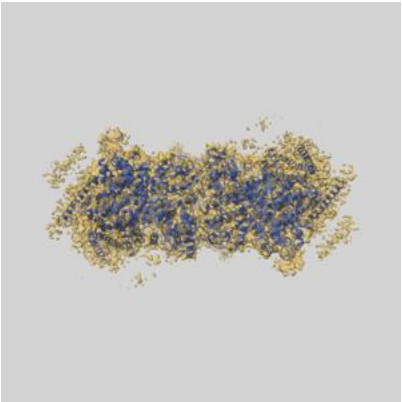
9.1 Map-model overlay (i)



X



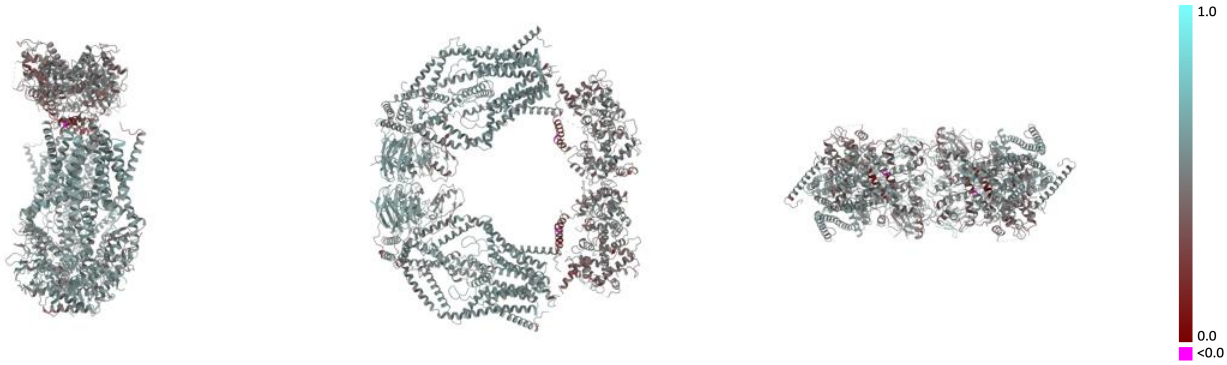
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 12.0 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.

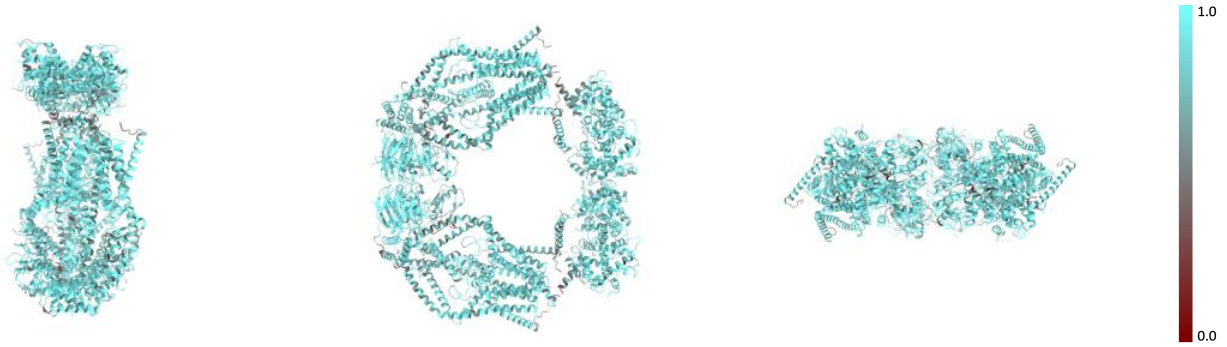
9.2 Q-score mapped to coordinate model (i)



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.

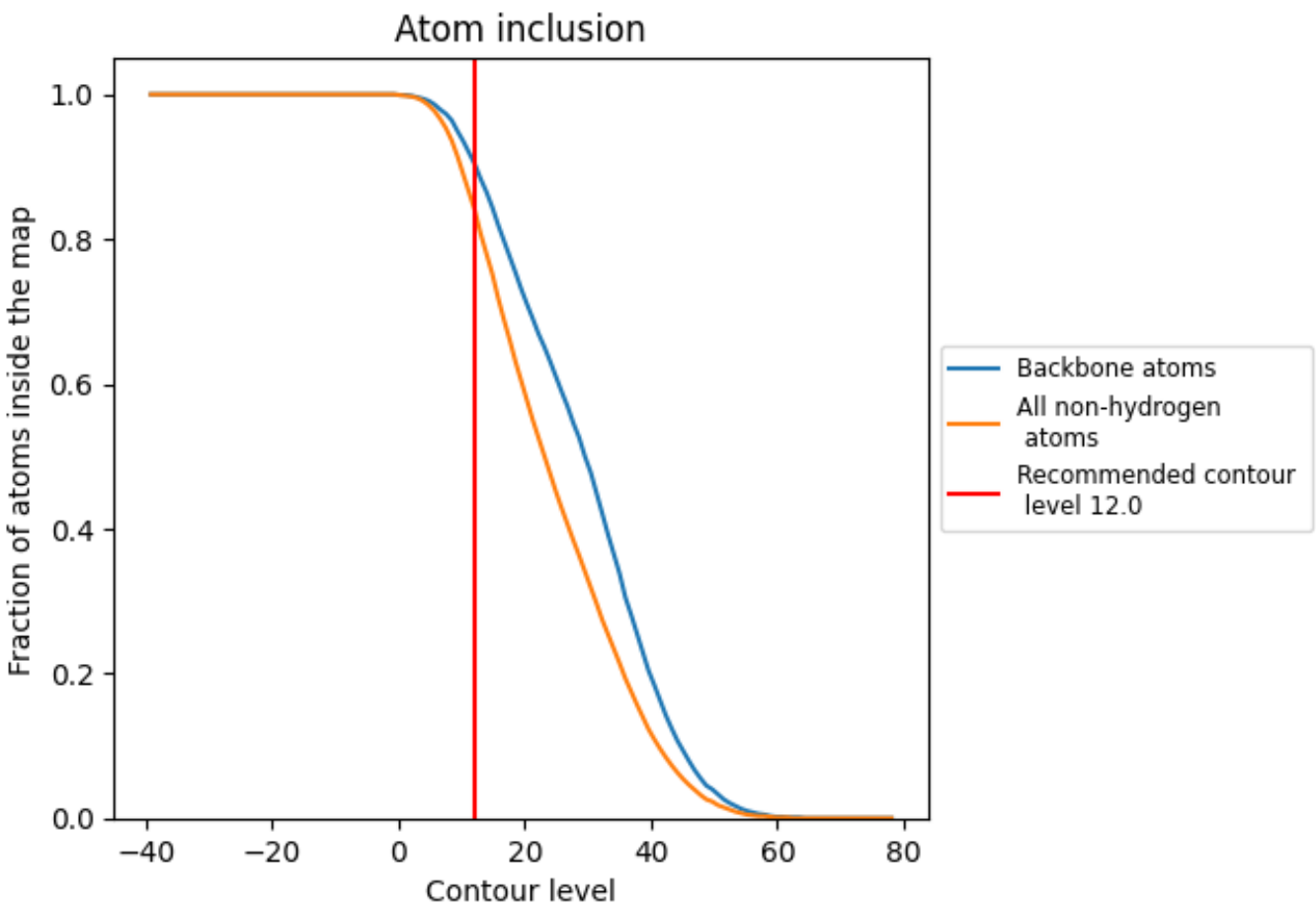
9.3 Atom inclusion mapped to coordinate model (i)



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 (12.0).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (12.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.5110
A	0.8600	0.5450
B	0.8010	0.5120
C	0.8370	0.5440
D	0.8820	0.5510
E	0.8110	0.5330
F	0.7870	0.5210
G	0.7970	0.5290
H	0.7640	0.5220
I	0.8420	0.4380
J	0.8720	0.4630
N	0.8620	0.5480
O	0.8000	0.5140
P	0.8390	0.5450
Q	0.8680	0.5510
R	0.8110	0.5380
S	0.7870	0.5210
T	0.7920	0.5240
U	0.8250	0.5270
V	0.8400	0.4380
W	0.8710	0.4620