Full wwPDB EM Validation Report ⓘ

May 31, 2023 – 10:25 PM JST

PDB ID	:	7VXP
EMDB ID	:	EMD-32186
Title	:	Matrix arm of active state CI from Q10 dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-13
Resolution	:	2.70 Å(reported)

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

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

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

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

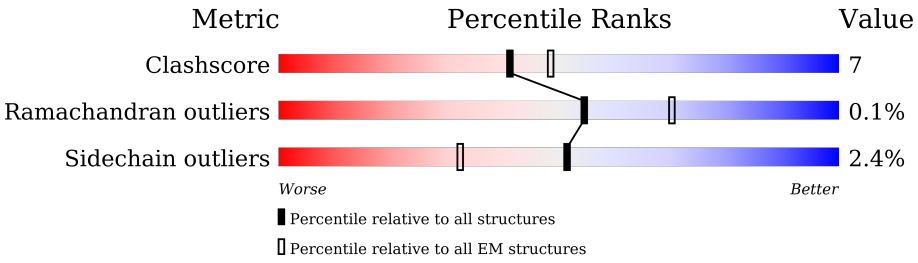
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	79% 21%
2	B	176	81% 19%
3	C	156	86% 13%
4	E	115	85% 14%
5	F	86	6% 74% 24%
6	G	88	18% 78% 19%
7	H	112	85% 15%
8	I	112	12% 68% 16% 13%

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Mol	Chain	Length	Quality of chain
9	J	342	82% 18%
10	K	43	5% 67% 33%
11	L	125	6% 83% 16%
12	M	690	84% 15%
13	N	144	10% 83% 17%
14	O	217	82% 17%
15	P	208	88% 12%
16	Q	386	78% 21%
17	T	96	7% 86% 14%
18	W	29	10% 79% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	A	501	-	-	X	-
25	UQ	Q	501	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 28589 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	687	432	129	124	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	386	Total	C	N	O	S	0	0
			3096	1976	534	563	23		

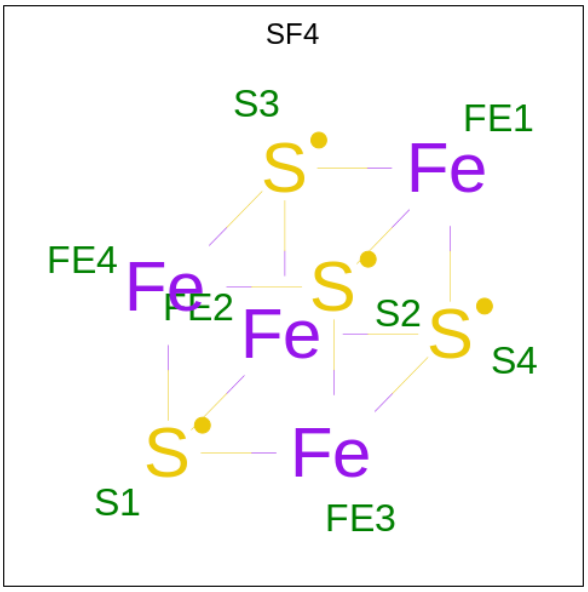
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

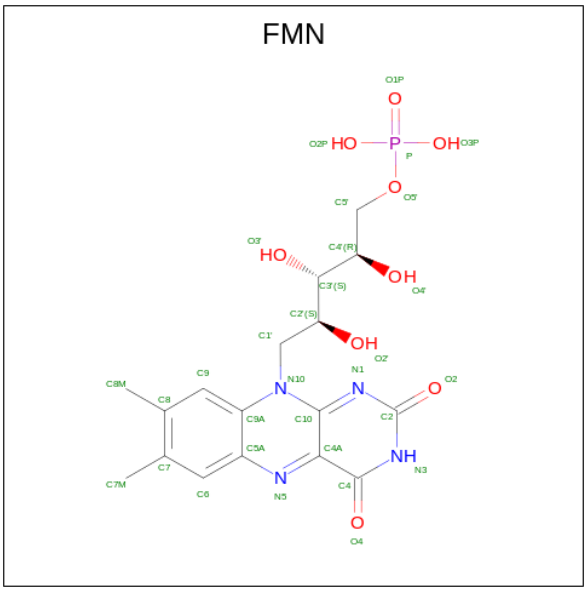
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			212	135	37	39	1		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



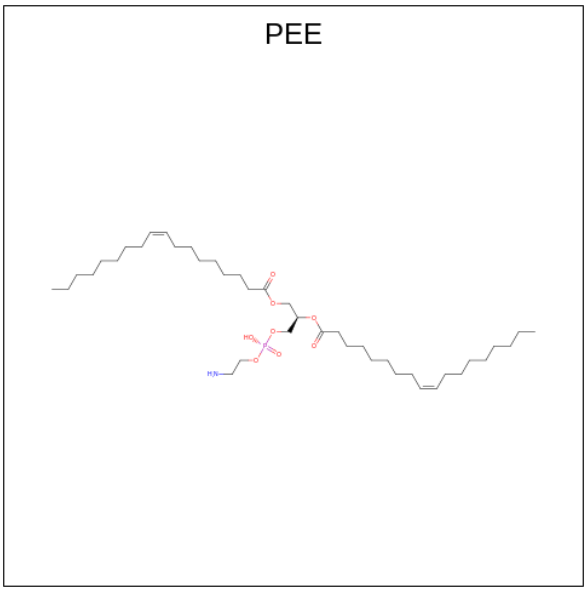
Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total Fe S 8 4 4	0
19	B	1	Total Fe S 8 4 4	0
19	B	1	Total Fe S 8 4 4	0
19	C	1	Total Fe S 8 4 4	0
19	M	1	Total Fe S 8 4 4	0
19	M	1	Total Fe S 8 4 4	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

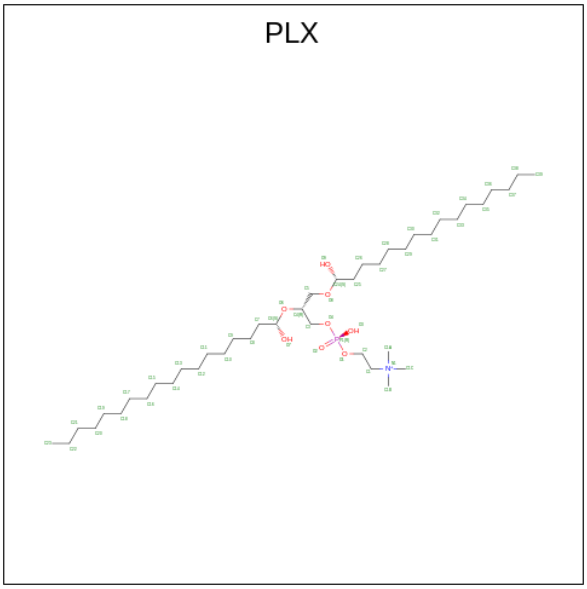
- Molecule 21 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	C	1	Total	C	N	O	P	0
			47	37	1	8	1	

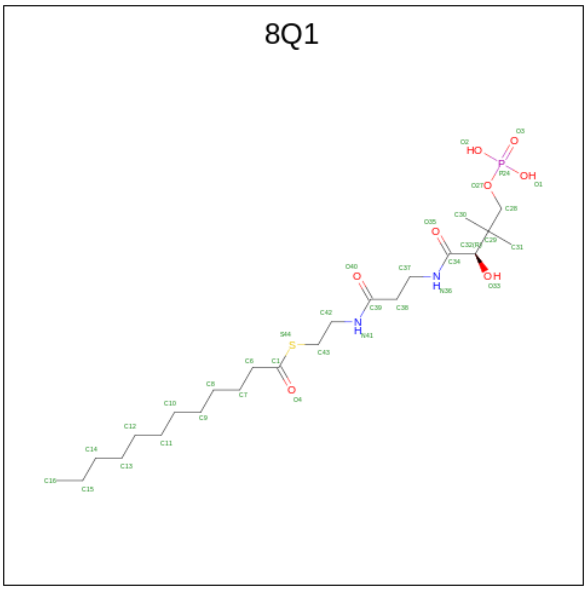
- Molecule 22 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DI METHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSA

NE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



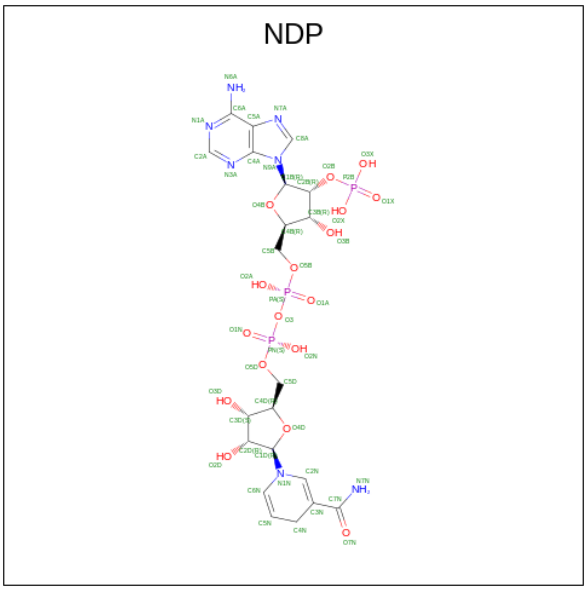
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
22	N	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 23 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



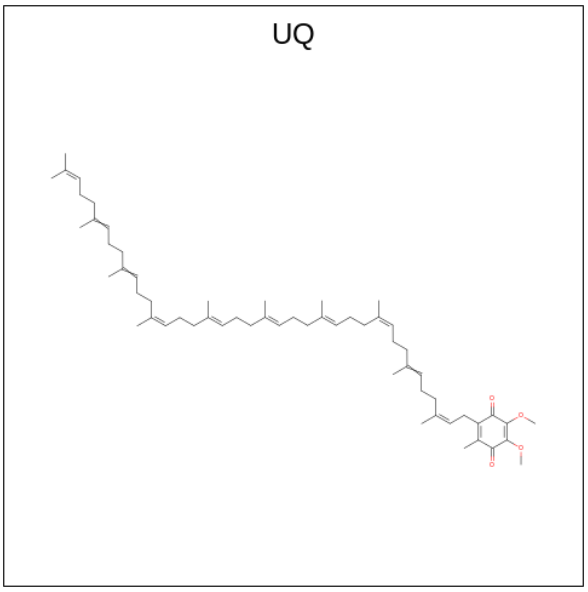
Mol	Chain	Residues	Atoms						AltConf
23	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 24 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



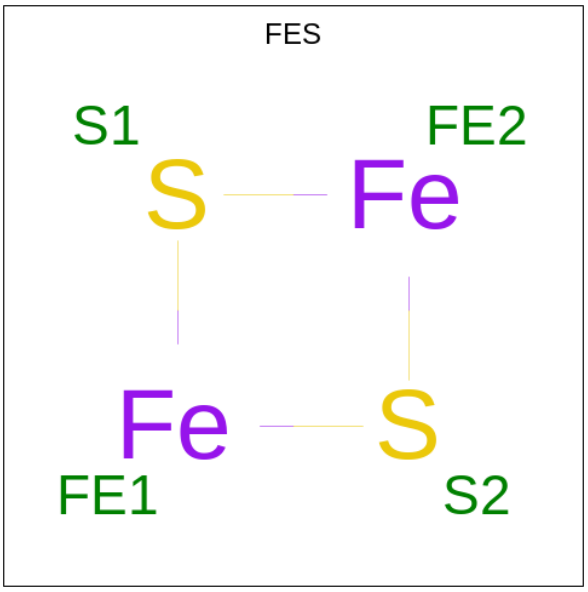
Mol	Chain	Residues	Atoms					AltConf
24	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 25 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	J	1	Total C O 33 29 4	0
25	Q	1	Total C O 63 59 4	0

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	M	1	Total Fe S 4 2 2	0

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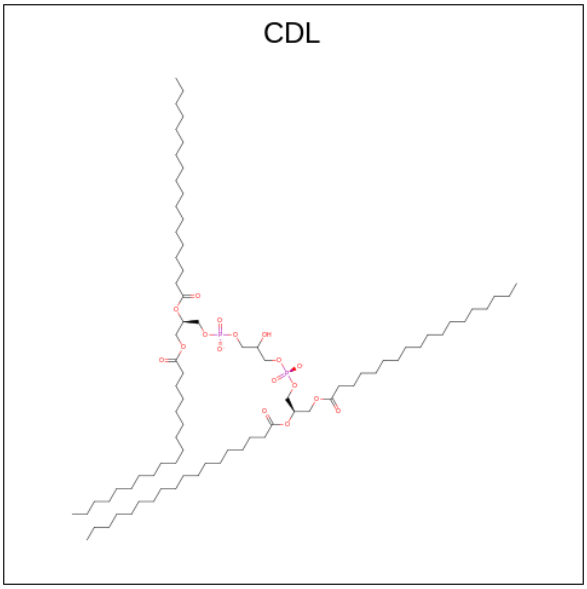
Mol	Chain	Residues	Atoms			AltConf
26	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	M	1	Total	Mg	0
			1	1	

- Molecule 28 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	N	1	Total	C	O	P	0
			51	32	17	2	

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

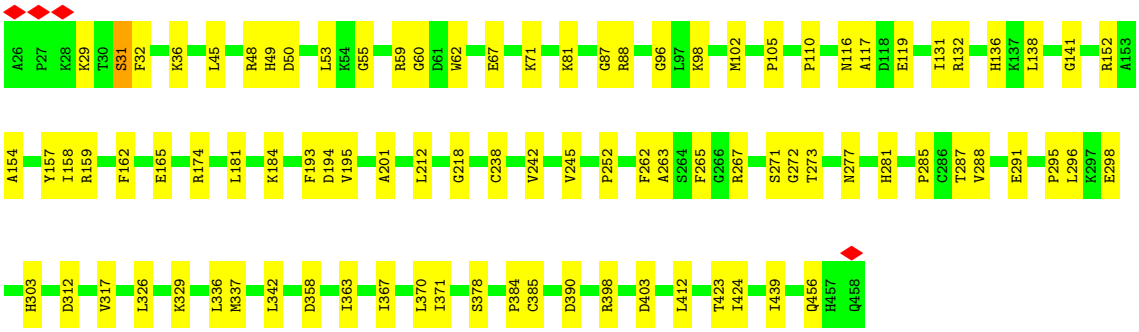
Mol	Chain	Residues	Atoms		AltConf
29	T	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

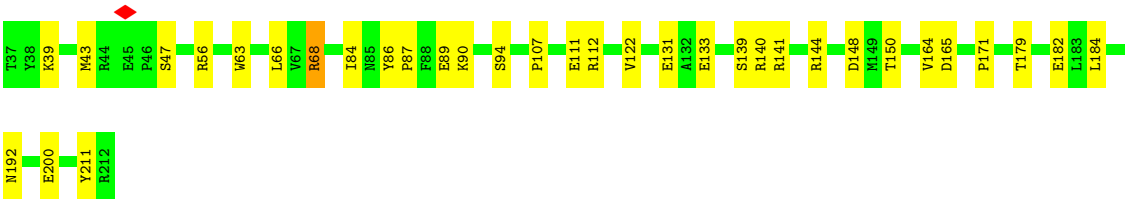
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A:



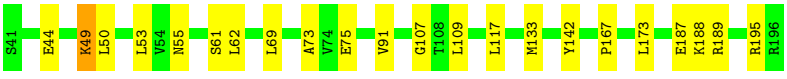
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B:



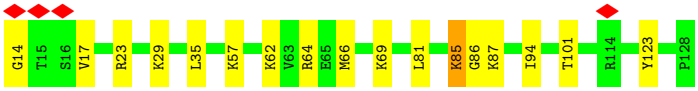
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:

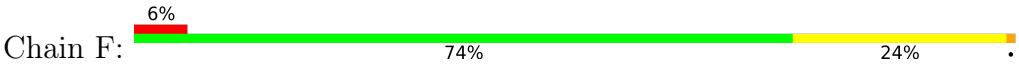


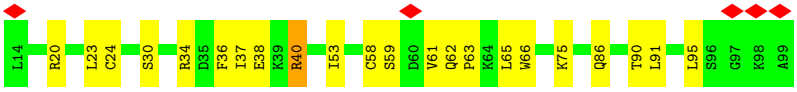
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:

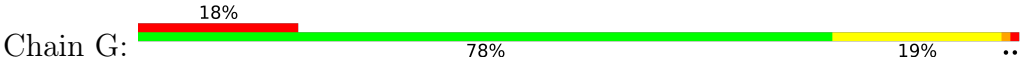


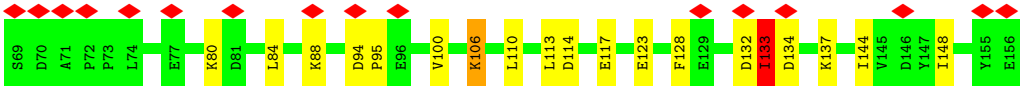
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



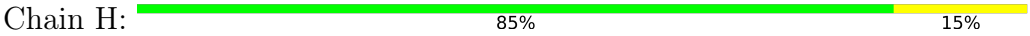


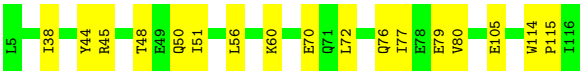
• Molecule 6: Acyl carrier protein, mitochondrial



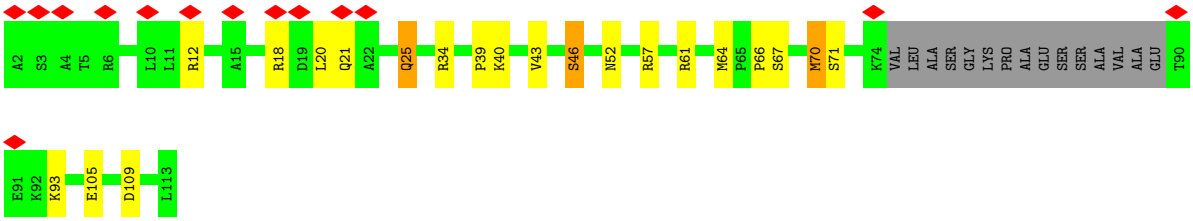


• Molecule 7: Complex I subunit B13

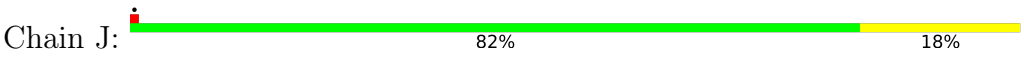


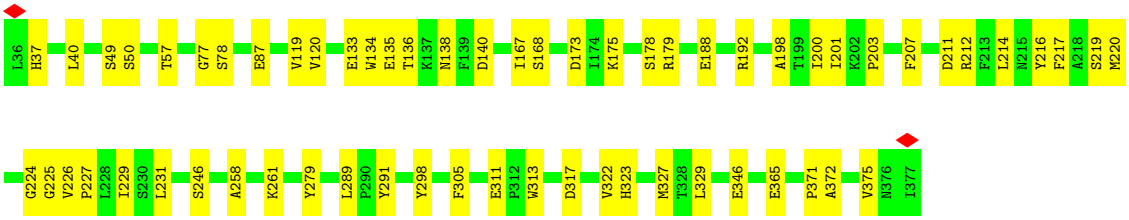


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



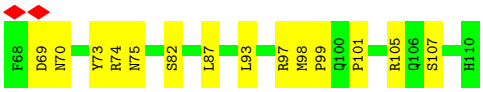
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial





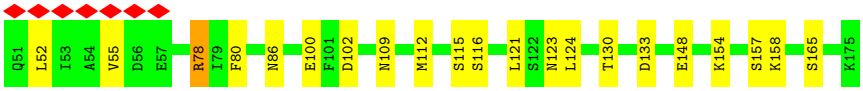
• Molecule 10: Complex I-9kD

Chain K:



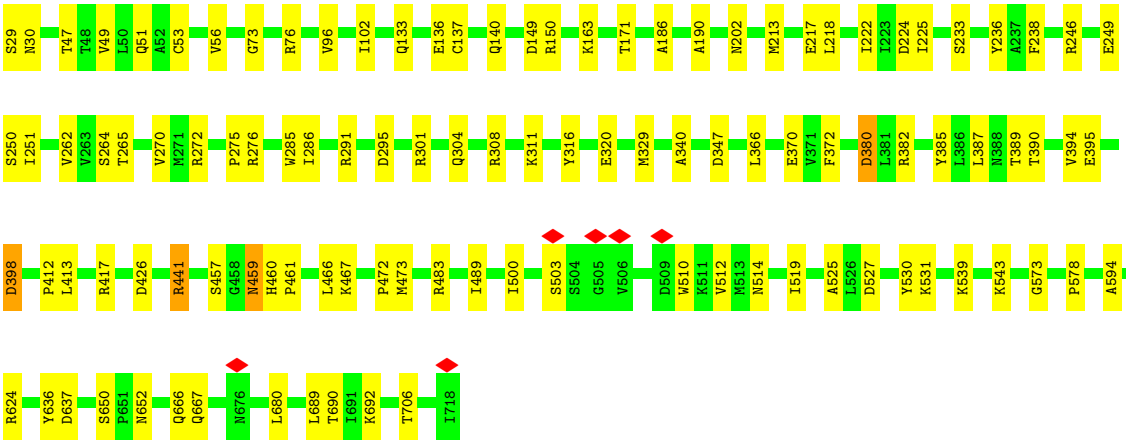
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



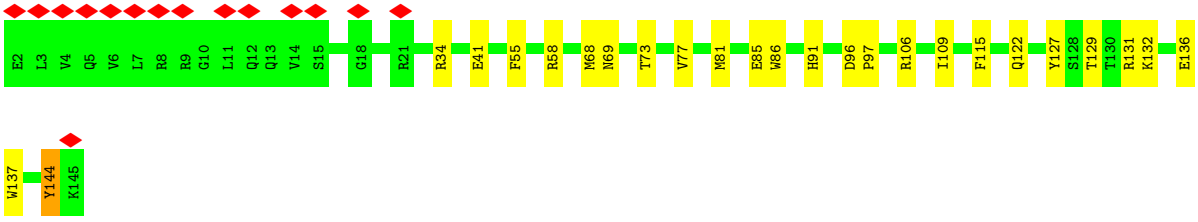
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



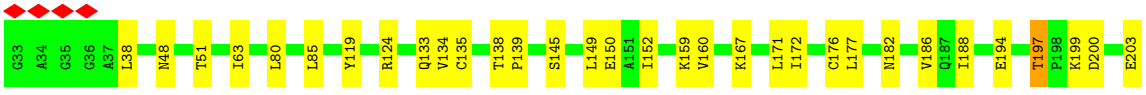
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

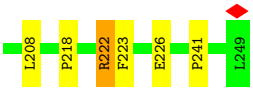
Chain N:



• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:



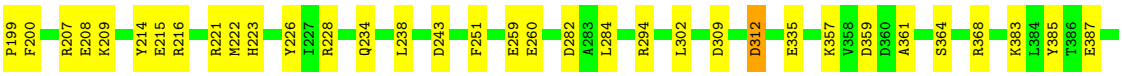


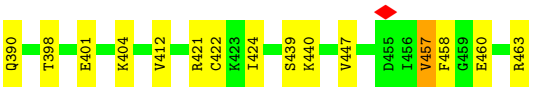
• Molecule 15: Complex I-30kD

Chain P:

• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

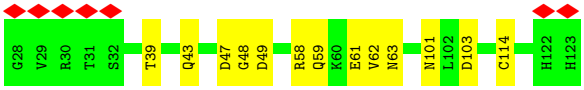
Chain Q:





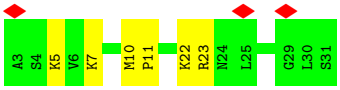
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:



• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252573	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)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.199	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0248	Depositor
Map size (Å)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, UQ, 8Q1, ZN, CDL, SF4, MG, NDP, PLX, FES, FMN, 2MR

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	0.26	0/3406	0.49	0/4603
2	B	0.27	0/1443	0.50	0/1952
3	C	0.27	0/1279	0.52	0/1730
4	E	0.26	0/995	0.51	0/1340
5	F	0.26	0/698	0.54	0/940
6	G	0.27	0/702	0.55	1/952 (0.1%)
7	H	0.25	0/929	0.43	0/1258
8	I	0.26	0/798	0.53	0/1079
9	J	0.26	0/2828	0.48	0/3834
10	K	0.25	0/377	0.48	0/509
11	L	0.25	0/1039	0.51	0/1403
12	M	0.26	0/5384	0.50	0/7295
13	N	0.26	0/1245	0.51	0/1694
14	O	0.26	0/1711	0.48	0/2328
15	P	0.27	0/1789	0.50	0/2436
16	Q	0.28	0/3157	0.51	0/4268
17	T	0.26	0/755	0.51	0/1018
18	W	0.28	0/218	0.46	0/295
All	All	0.26	0/28753	0.50	1/38934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	133	ILE	CG1-CB-CG2	-5.81	98.61	111.40

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	3330	0	3292	63	0
2	B	1412	0	1363	25	0
3	C	1248	0	1254	19	0
4	E	971	0	975	9	0
5	F	687	0	700	13	0
6	G	690	0	669	13	0
7	H	910	0	950	9	0
8	I	780	0	808	15	0
9	J	2751	0	2773	43	0
10	K	366	0	338	12	0
11	L	1016	0	1016	13	0
12	M	5296	0	5326	69	0
13	N	1204	0	1162	20	0
14	O	1671	0	1673	22	0
15	P	1738	0	1693	17	0
16	Q	3096	0	3063	85	0
17	T	741	0	702	9	0
18	W	212	0	208	4	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	0	0
19	M	16	0	0	0	0
20	A	31	0	19	5	0
21	C	47	0	71	1	0
22	C	52	0	88	5	0
22	N	52	0	88	2	0
23	G	35	0	0	0	0
24	J	48	0	25	3	0
25	J	33	0	39	5	0
25	Q	63	0	90	29	0
26	M	4	0	0	0	0
26	O	4	0	0	0	0
27	M	1	0	0	0	0
28	N	51	0	46	0	0
29	T	1	0	0	0	0
All	All	28589	0	28431	419	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 (419) 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)
24:J:401:NDP:O4D	24:J:401:NDP:C4D	1.68	1.19
16:Q:197:MET:CE	25:Q:501:UQ:H23	1.79	1.11
16:Q:197:MET:HE3	25:Q:501:UQ:H23	1.33	1.10
16:Q:197:MET:CE	25:Q:501:UQ:H252	1.85	1.07
16:Q:197:MET:HE1	25:Q:501:UQ:C25	1.87	1.03
16:Q:197:MET:HE2	25:Q:501:UQ:H252	1.49	0.91
16:Q:197:MET:CE	25:Q:501:UQ:C23	2.49	0.91
16:Q:144:MET:CE	16:Q:144:MET:H	1.87	0.87
16:Q:197:MET:CE	25:Q:501:UQ:C25	2.50	0.85
13:N:68:MET:HG3	13:N:69:ASN:H	1.44	0.81
25:Q:501:UQ:C33	25:Q:501:UQ:H301	2.11	0.81
16:Q:197:MET:HE1	25:Q:501:UQ:H23	1.64	0.80
18:W:10:MET:HE3	18:W:11:PRO:HD2	1.64	0.78
16:Q:197:MET:HE1	25:Q:501:UQ:C23	2.15	0.75
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.21	0.73
1:A:138:LEU:HD13	1:A:245:VAL:HG23	1.72	0.71
16:Q:189:THR:HG21	25:Q:501:UQ:HM23	1.71	0.71
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.23	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.73	0.70
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.25	0.69
3:C:73:ALA:HB3	25:Q:501:UQ:HM53	1.73	0.69
6:G:144:ILE:O	6:G:148:ILE:HG13	1.92	0.69
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.26	0.68
8:I:18:ARG:NH2	16:Q:260:GLU:OE1	2.23	0.68
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.29	0.68
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.26	0.67
16:Q:144:MET:H	16:Q:144:MET:HE2	1.58	0.67
2:B:47:SER:O	2:B:56:ARG:NH2	2.27	0.67
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.78	0.66
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.31	0.65
16:Q:189:THR:HG21	25:Q:501:UQ:CM2	2.26	0.65
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.29	0.65
22:C:303:PLX:H211	25:Q:501:UQ:H551	1.78	0.65
1:A:98:LYS:NZ	20:A:502:FMN:O3P	2.30	0.65
5:F:24:CYS:N	5:F:58:CYS:SG	2.71	0.64
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.80	0.64
16:Q:197:MET:HE1	25:Q:501:UQ:H253	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.79	0.64
9:J:212:ARG:O	9:J:216:TYR:HB2	1.97	0.64
15:P:43:THR:HA	15:P:47:ILE:HD12	1.79	0.63
3:C:73:ALA:CB	25:Q:501:UQ:HM53	2.28	0.63
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.80	0.63
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.32	0.63
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.34	0.63
1:A:152:ARG:NH2	10:K:99:PRO:O	2.33	0.62
16:Q:145:MET:HG3	16:Q:214:TYR:CE2	2.35	0.62
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.82	0.61
5:F:86:GLN:O	5:F:90:THR:HG23	2.00	0.61
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.83	0.61
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.29	0.61
2:B:192:ASN:OD1	17:T:63:ASN:ND2	2.32	0.61
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.34	0.61
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.83	0.61
12:M:398:ASP:N	12:M:398:ASP:OD1	2.33	0.60
16:Q:94:VAL:O	16:Q:94:VAL:HG23	2.01	0.60
11:L:78:ARG:NE	11:L:148:GLU:OE2	2.32	0.60
1:A:159:ARG:NH2	14:O:176:CYS:O	2.34	0.60
9:J:212:ARG:O	9:J:216:TYR:CB	2.50	0.60
16:Q:133:LEU:HB3	16:Q:134:PRO:HD3	1.83	0.60
16:Q:144:MET:H	16:Q:144:MET:HE3	1.65	0.60
25:Q:501:UQ:H301	25:Q:501:UQ:H33	1.82	0.59
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.35	0.59
12:M:265:THR:HG22	12:M:270:VAL:HA	1.84	0.59
14:O:188:ILE:HG21	14:O:208:LEU:HD21	1.83	0.59
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.84	0.59
1:A:49:HIS:O	1:A:59:ARG:NH1	2.36	0.59
6:G:132:ASP:O	6:G:133:ILE:HG22	2.03	0.59
12:M:441:ARG:HB3	12:M:441:ARG:NH1	2.17	0.59
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.36	0.59
8:I:40:LYS:HB3	18:W:7:LYS:H	1.68	0.59
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.84	0.58
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.36	0.58
3:C:167:PRO:HD3	16:Q:223:HIS:HD2	1.68	0.58
12:M:650:SER:OG	12:M:652:ASN:ND2	2.36	0.58
1:A:263:ALA:HA	1:A:271:SER:HB3	1.84	0.58
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.86	0.57
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.44	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:134:ASP:HA	6:G:137:LYS:HD3	1.85	0.57
1:A:45:LEU:HD21	1:A:287:THR:HG22	1.86	0.57
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.85	0.57
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.24	0.57
25:Q:501:UQ:HM22	25:Q:501:UQ:O1	2.02	0.57
9:J:217:PHE:HA	9:J:220:MET:HE2	1.85	0.57
16:Q:139:LEU:O	16:Q:460:GLU:N	2.37	0.57
16:Q:95:LEU:HB2	16:Q:458:PHE:CE2	2.39	0.57
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.86	0.56
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.86	0.56
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.87	0.56
9:J:192:ARG:NH1	9:J:198:ALA:O	2.39	0.56
9:J:220:MET:HE3	9:J:226:VAL:HG13	1.87	0.56
12:M:29:SER:OG	12:M:30:ASN:N	2.39	0.56
14:O:38:LEU:O	14:O:124:ARG:NH2	2.39	0.56
16:Q:189:THR:HB	25:Q:501:UQ:HM21	1.87	0.56
6:G:133:ILE:HD12	6:G:134:ASP:H	1.71	0.55
9:J:225:GLY:O	9:J:227:PRO:HD3	2.07	0.55
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.39	0.55
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.42	0.55
3:C:44:GLU:OE2	3:C:195:ARG:NH1	2.39	0.55
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.88	0.55
1:A:184:LYS:HB2	10:K:98:MET:SD	2.46	0.55
7:H:44:TYR:O	7:H:48:THR:HG22	2.06	0.55
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.23	0.55
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.90	0.54
9:J:258:ALA:HA	9:J:261:LYS:HG3	1.89	0.54
16:Q:144:MET:SD	16:Q:222:MET:HB2	2.48	0.54
1:A:116:ASN:ND2	20:A:502:FMN:O3'	2.40	0.54
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.89	0.54
9:J:219:SER:CB	25:J:402:UQ:HM52	2.37	0.54
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.88	0.54
1:A:262:PHE:CE2	1:A:272:GLY:HA3	2.43	0.54
1:A:285:PRO:O	14:O:222:ARG:NH2	2.40	0.54
16:Q:136:PHE:CE1	16:Q:151:TYR:CD1	2.96	0.54
16:Q:197:MET:HE3	25:Q:501:UQ:C23	2.20	0.54
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.89	0.54
5:F:24:CYS:O	5:F:34:ARG:NH1	2.41	0.54
6:G:113:LEU:O	6:G:117:GLU:HG3	2.08	0.54
4:E:17:VAL:HG21	11:L:55:VAL:HG12	1.89	0.53
9:J:119:VAL:HG23	9:J:120:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.43	0.53
9:J:178:SER:OG	9:J:317:ASP:OD1	2.25	0.53
16:Q:142:VAL:C	16:Q:144:MET:HE2	2.29	0.53
16:Q:198:THR:N	16:Q:199:PRO:HD2	2.23	0.53
16:Q:95:LEU:HD22	16:Q:458:PHE:HZ	1.73	0.53
9:J:37:HIS:NE2	17:T:48:GLY:O	2.42	0.53
15:P:211:ARG:NE	15:P:222:GLU:OE2	2.36	0.53
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.90	0.52
1:A:98:LYS:NZ	1:A:242:VAL:O	2.28	0.52
12:M:472:PRO:O	12:M:510:TRP:NE1	2.36	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.91	0.52
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.90	0.52
9:J:305:PHE:CE1	9:J:313:TRP:CE3	2.98	0.52
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.30	0.52
4:E:35:LEU:HD21	4:E:86:GLY:HA3	1.91	0.52
1:A:117:ALA:HB1	1:A:131:ILE:HD11	1.92	0.52
5:F:36:PHE:CD1	5:F:40:ARG:HG3	2.44	0.52
3:C:55:ASN:ND2	3:C:187:GLU:O	2.41	0.52
13:N:144:TYR:HD1	13:N:144:TYR:H	1.56	0.52
7:H:38:ILE:O	7:H:45:ARG:NH1	2.42	0.52
16:Q:197:MET:HE1	25:Q:501:UQ:C24	2.39	0.52
1:A:277:ASN:ND2	1:A:287:THR:OG1	2.43	0.51
16:Q:189:THR:CB	25:Q:501:UQ:HM21	2.41	0.51
1:A:110:PRO:O	1:A:238:CYS:HB3	2.09	0.51
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.92	0.51
2:B:39:LYS:NZ	16:Q:335:GLU:OE2	2.43	0.51
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.92	0.51
14:O:138:THR:HG22	14:O:139:PRO:HD3	1.92	0.51
9:J:37:HIS:O	9:J:40:LEU:N	2.40	0.51
9:J:211:ASP:OD2	9:J:214:LEU:N	2.26	0.51
17:T:39:THR:HG22	17:T:62:VAL:HG22	1.92	0.51
3:C:189:ARG:HG2	9:J:87:GLU:HG3	1.92	0.51
1:A:119:GLU:O	1:A:159:ARG:NH1	2.44	0.50
2:B:43:MET:O	2:B:43:MET:HG3	2.11	0.50
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.93	0.50
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.92	0.50
9:J:229:ILE:HB	9:J:323:HIS:CD2	2.47	0.50
17:T:101:ASN:ND2	17:T:103:ASP:OD2	2.41	0.50
14:O:197:THR:OG1	14:O:200:ASP:OD2	2.29	0.50
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.20	0.50
7:H:48:THR:HA	7:H:51:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:68:MET:HG3	13:N:69:ASN:N	2.21	0.50
16:Q:197:MET:CE	25:Q:501:UQ:C24	2.90	0.50
9:J:305:PHE:CE1	9:J:313:TRP:HE3	2.30	0.50
12:M:250:SER:OG	12:M:251:ILE:N	2.43	0.50
12:M:395:GLU:OE2	12:M:417:ARG:HD2	2.12	0.50
16:Q:136:PHE:CZ	16:Q:151:TYR:CD1	3.00	0.50
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.45	0.50
9:J:201:ILE:HG22	9:J:203:PRO:HD3	1.93	0.50
9:J:50:SER:O	9:J:77:GLY:HA3	2.12	0.49
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.30	0.49
4:E:62:LYS:O	4:E:66:MET:HG2	2.12	0.49
14:O:199:LYS:O	14:O:203:GLU:HG3	2.13	0.49
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.19	0.49
3:C:61:SER:O	3:C:61:SER:OG	2.30	0.49
12:M:295:ASP:OD2	12:M:706:THR:OG1	2.17	0.49
12:M:467:LYS:HG2	12:M:503:SER:OG	2.13	0.49
12:M:512:VAL:O	12:M:514:ASN:ND2	2.46	0.49
12:M:394:VAL:HA	12:M:473:MET:HE1	1.94	0.49
16:Q:121:GLU:HG2	16:Q:422:CYS:O	2.13	0.49
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.13	0.49
1:A:194:ASP:OD2	10:K:98:MET:HG2	2.12	0.49
1:A:412:LEU:HD23	1:A:439:ILE:HD11	1.95	0.49
6:G:84:LEU:HD21	6:G:100:VAL:HG22	1.95	0.49
16:Q:189:THR:CG2	25:Q:501:UQ:CM2	2.90	0.49
11:L:109:ASN:HB2	11:L:116:SER:OG	2.13	0.48
12:M:467:LYS:HE3	12:M:503:SER:HB3	1.95	0.48
5:F:59:SER:O	5:F:61:VAL:N	2.46	0.48
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.94	0.48
6:G:110:LEU:HB3	6:G:114:ASP:HB2	1.95	0.48
4:E:69:LYS:HB3	4:E:69:LYS:HE3	1.67	0.48
8:I:109:ASP:OD1	18:W:22:LYS:NZ	2.45	0.48
12:M:525:ALA:O	12:M:530:TYR:HB2	2.14	0.48
16:Q:133:LEU:N	16:Q:134:PRO:CD	2.77	0.48
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.79	0.48
14:O:135:CYS:HB2	14:O:177:LEU:HD12	1.95	0.48
1:A:81:LYS:HG2	1:A:96:GLY:HA3	1.95	0.48
1:A:265:PHE:HB3	1:A:291:GLU:HG3	1.96	0.48
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.54	0.48
9:J:365:GLU:OE2	9:J:365:GLU:N	2.42	0.48
12:M:389:THR:O	12:M:390:THR:OG1	2.29	0.47
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.49	0.47
9:J:224:GLY:O	9:J:289:LEU:HD12	2.14	0.47
16:Q:88:HIS:HB3	16:Q:91:ALA:HB2	1.95	0.47
16:Q:440:LYS:HA	16:Q:440:LYS:HD3	1.69	0.47
1:A:195:VAL:O	10:K:97:ARG:NH1	2.47	0.47
2:B:68:ARG:NE	16:Q:260:GLU:OE2	2.47	0.47
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.47	0.47
5:F:61:VAL:HG23	5:F:62:GLN:N	2.28	0.47
25:J:402:UQ:H221	25:J:402:UQ:H201	1.60	0.47
16:Q:80:LEU:C	16:Q:80:LEU:HD23	2.35	0.47
9:J:219:SER:HB2	25:J:402:UQ:HM52	1.96	0.47
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.97	0.47
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.48	0.47
12:M:308:ARG:NH2	12:M:578:PRO:O	2.48	0.47
16:Q:154:ALA:HA	16:Q:398:THR:HG21	1.96	0.47
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.50	0.47
13:N:132:LYS:NZ	13:N:136:GLU:OE2	2.48	0.47
16:Q:357:LYS:HD3	16:Q:364:SER:HB2	1.97	0.47
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.50	0.46
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.48	0.46
3:C:53:LEU:HD22	22:C:303:PLX:H322	1.96	0.46
22:C:303:PLX:H92	22:C:303:PLX:H122	1.60	0.46
4:E:23:ARG:HB3	4:E:23:ARG:NH1	2.30	0.46
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.47	0.46
9:J:327:MET:HE2	9:J:329:LEU:HD21	1.97	0.46
12:M:29:SER:HG	12:M:30:ASN:H	1.63	0.46
1:A:48:ARG:NH1	10:K:70:ASN:O	2.48	0.46
3:C:188:LYS:N	9:J:87:GLU:OE2	2.42	0.46
4:E:81:LEU:O	4:E:85:LYS:HG3	2.16	0.46
5:F:23:LEU:HD13	5:F:37:ILE:HD12	1.97	0.46
10:K:69:ASP:N	10:K:69:ASP:OD1	2.49	0.46
11:L:102:ASP:OD1	11:L:102:ASP:N	2.49	0.46
12:M:690:THR:HG22	12:M:692:LYS:H	1.79	0.46
1:A:312:ASP:HA	1:A:329:LYS:NZ	2.30	0.46
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.97	0.46
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.45	0.46
2:B:139:SER:HB3	2:B:141:ARG:HE	1.81	0.46
3:C:133:MET:SD	3:C:173:LEU:HD22	2.55	0.46
9:J:225:GLY:HA3	9:J:291:TYR:HE2	1.78	0.46
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.33	0.46
13:N:129:THR:HA	17:T:43:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:175:LYS:HB2	9:J:175:LYS:HE3	1.86	0.46
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.51	0.46
12:M:213:MET:HE2	12:M:213:MET:HB2	1.84	0.46
12:M:466:LEU:HD22	12:M:500:ILE:HD11	1.98	0.46
5:F:91:LEU:O	5:F:95:LEU:HD12	2.16	0.46
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.79	0.46
1:A:390:ASP:OD2	12:M:202:ASN:ND2	2.49	0.46
2:B:133:GLU:OE2	13:N:131:ARG:NH1	2.38	0.46
5:F:53:ILE:O	12:M:380:ASP:HB3	2.16	0.46
12:M:53:CYS:O	12:M:56:VAL:HG22	2.16	0.46
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.97	0.46
1:A:378:SER:OG	1:A:385:CYS:SG	2.67	0.45
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.97	0.45
1:A:50:ASP:HB3	1:A:55:GLY:HA3	1.97	0.45
1:A:424:ILE:HG12	12:M:76:ARG:NH2	2.30	0.45
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.98	0.45
8:I:12:ARG:NH2	8:I:21:GLN:OE1	2.49	0.45
12:M:163:LYS:O	12:M:171:THR:OG1	2.34	0.45
1:A:131:ILE:HD13	1:A:158:ILE:HD13	1.98	0.45
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.96	0.45
7:H:56:LEU:HG	7:H:60:LYS:HE2	1.97	0.45
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.76	0.45
9:J:192:ARG:HA	9:J:192:ARG:HD3	1.86	0.45
1:A:154:ALA:HB2	1:A:193:PHE:CZ	2.51	0.45
6:G:94:ASP:OD1	6:G:94:ASP:N	2.46	0.45
22:N:201:PLX:H312	22:N:201:PLX:H342	1.67	0.45
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.99	0.45
7:H:76:GLN:O	7:H:79:GLU:N	2.40	0.45
8:I:105:GLU:OE2	8:I:105:GLU:HA	2.17	0.45
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.74	0.45
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.48	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.17	0.45
9:J:219:SER:HB3	25:J:402:UQ:HM52	1.98	0.45
25:Q:501:UQ:C33	25:Q:501:UQ:C30	2.86	0.45
1:A:154:ALA:HB2	1:A:193:PHE:HZ	1.82	0.45
11:L:121:LEU:HD22	11:L:124:LEU:HD22	1.99	0.45
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.50	0.45
13:N:73:THR:HG21	13:N:81:MET:CE	2.47	0.45
1:A:87:GLY:HA3	20:A:502:FMN:O2P	2.17	0.44
22:C:303:PLX:H252	22:C:303:PLX:H101	1.99	0.44
16:Q:259:GLU:OE1	18:W:23:ARG:NE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:MET:SD	1:A:342:LEU:HD11	2.56	0.44
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.36	0.44
16:Q:95:LEU:HD22	16:Q:458:PHE:CZ	2.53	0.44
17:T:47:ASP:OD1	17:T:48:GLY:N	2.48	0.44
14:O:152:ILE:HG21	14:O:171:LEU:HD13	2.00	0.44
1:A:31:SER:O	1:A:31:SER:OG	2.33	0.44
1:A:48:ARG:HH11	10:K:70:ASN:HB3	1.82	0.44
9:J:140:ASP:N	9:J:140:ASP:OD1	2.51	0.44
16:Q:137:ASP:OD1	16:Q:148:GLU:OE1	2.35	0.44
9:J:207:PHE:HB2	9:J:214:LEU:HG	1.99	0.44
25:Q:501:UQ:H261	25:Q:501:UQ:H222	1.62	0.44
8:I:93:LYS:HD2	8:I:93:LYS:HA	1.68	0.44
11:L:78:ARG:HE	11:L:148:GLU:CD	2.21	0.44
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.83	0.44
12:M:380:ASP:OD1	12:M:380:ASP:N	2.51	0.44
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.47	0.44
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.99	0.44
12:M:543:LYS:HE3	12:M:543:LYS:HB3	1.82	0.44
12:M:667:GLN:OE1	12:M:667:GLN:N	2.51	0.44
8:I:46:SER:O	8:I:46:SER:OG	2.36	0.44
9:J:135:GLU:HG3	9:J:140:ASP:HA	2.00	0.44
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.81	0.44
24:J:401:NDP:O2N	24:J:401:NDP:N7N	2.51	0.43
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	1.99	0.43
1:A:60:GLY:HA2	14:O:241:PRO:HA	2.00	0.43
1:A:201:ALA:O	14:O:119:TYR:HB3	2.18	0.43
6:G:106:LYS:HB2	6:G:106:LYS:HE2	1.64	0.43
9:J:375:VAL:O	9:J:375:VAL:HG13	2.18	0.43
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.00	0.43
22:N:201:PLX:H1C3	22:N:201:PLX:H22	1.75	0.43
1:A:32:PHE:CE1	1:A:267:ARG:HG3	2.53	0.43
2:B:184:LEU:HD23	11:L:112:MET:HG3	2.00	0.43
8:I:34:ARG:HD2	8:I:34:ARG:HA	1.66	0.43
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.99	0.43
13:N:85:GLU:HG2	13:N:86:TRP:H	1.84	0.43
13:N:106:ARG:HB2	13:N:109:ILE:HG13	2.00	0.43
16:Q:85:GLY:HA3	16:Q:95:LEU:O	2.18	0.43
10:K:87:LEU:HD12	14:O:85:LEU:HD13	2.00	0.43
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.01	0.43
3:C:188:LYS:HB3	3:C:188:LYS:HE3	1.73	0.43
4:E:14:GLY:O	11:L:52:LEU:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:O	1:A:71:LYS:HG2	2.18	0.43
2:B:90:LYS:HG2	13:N:91:HIS:NE2	2.33	0.43
12:M:366:LEU:O	12:M:531:LYS:HB3	2.18	0.43
9:J:37:HIS:NE2	17:T:49:ASP:HA	2.33	0.43
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.53	0.43
16:Q:383:LYS:HD2	16:Q:383:LYS:HA	1.86	0.43
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.48	0.43
16:Q:140:ASP:HB3	16:Q:147:ASN:OD1	2.19	0.43
3:C:62:LEU:O	3:C:91:VAL:HA	2.19	0.43
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.00	0.43
1:A:267:ARG:HH11	1:A:336:LEU:HD12	1.83	0.42
4:E:64:ARG:NH1	6:G:117:GLU:OE2	2.52	0.42
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.54	0.42
12:M:483:ARG:HH11	12:M:489:ILE:HD11	1.84	0.42
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.54	0.42
14:O:134:VAL:HG22	14:O:186:VAL:HG22	2.00	0.42
25:Q:501:UQ:H13	25:Q:501:UQ:H171	1.95	0.42
20:A:502:FMN:O3'	20:A:502:FMN:N1	2.45	0.42
9:J:136:THR:HG23	9:J:138:ASN:H	1.84	0.42
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.54	0.42
25:J:402:UQ:H71	25:J:402:UQ:HM51	1.67	0.42
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.54	0.42
15:P:197:PRO:HA	15:P:202:PHE:CD2	2.55	0.42
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.54	0.42
12:M:285:TRP:HB2	12:M:413:LEU:HD11	2.01	0.42
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.01	0.42
16:Q:457:VAL:HG12	16:Q:460:GLU:HG2	2.01	0.42
1:A:88:ARG:NH2	1:A:273:THR:O	2.53	0.42
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.01	0.42
13:N:122:GLN:HA	17:T:59:GLN:HG2	2.02	0.42
3:C:49:LYS:HG3	22:C:303:PLX:H291	2.02	0.42
11:L:78:ARG:HH22	12:M:249:GLU:HG3	1.85	0.42
16:Q:88:HIS:ND1	16:Q:89:PRO:HD2	2.35	0.42
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.89	0.41
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.88	0.41
14:O:63:ILE:HG13	14:O:85:LEU:HD23	2.02	0.41
15:P:128:ILE:HB	15:P:145:THR:HG22	2.02	0.41
16:Q:439:SER:HB2	16:Q:447:VAL:HG22	2.02	0.41
25:Q:501:UQ:H251	25:Q:501:UQ:H272	1.83	0.41
1:A:29:LYS:H	1:A:29:LYS:HG3	1.71	0.41
12:M:186:ALA:HA	12:M:190:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:284:LEU:HD23	16:Q:284:LEU:HA	1.95	0.41
1:A:157:TYR:HB2	1:A:212:LEU:HD21	2.02	0.41
1:A:281:HIS:ND1	1:A:358:ASP:OD1	2.53	0.41
9:J:134:TRP:CZ2	9:J:311:GLU:HB3	2.55	0.41
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.01	0.41
12:M:73:GLY:O	12:M:76:ARG:NH2	2.51	0.41
12:M:311:LYS:HB2	12:M:311:LYS:HE3	1.79	0.41
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.02	0.41
1:A:358:ASP:OD1	1:A:358:ASP:N	2.50	0.41
8:I:66:PRO:HB3	15:P:79:SER:HA	2.02	0.41
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.24	0.41
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.56	0.41
8:I:12:ARG:HB3	8:I:20:LEU:HD12	2.03	0.41
12:M:457:SER:HB3	12:M:459:ASN:OD1	2.21	0.41
13:N:127:TYR:OH	17:T:61:GLU:O	2.30	0.41
14:O:149:LEU:HD11	14:O:160:VAL:HG23	2.02	0.41
15:P:68:ILE:HG22	15:P:69:LEU:HG	2.02	0.41
2:B:107:PRO:HB3	13:N:106:ARG:NH1	2.36	0.41
9:J:231:LEU:HD23	9:J:231:LEU:HA	1.89	0.41
12:M:264:SER:HB2	12:M:272:ARG:HG2	2.03	0.41
25:Q:501:UQ:H353	25:Q:501:UQ:H371	1.93	0.41
12:M:133:GLN:O	12:M:137:CYS:HB2	2.20	0.41
13:N:96:ASP:HA	13:N:97:PRO:HD3	1.95	0.41
12:M:47:THR:HG23	12:M:51:GLN:HB2	2.01	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.02	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
2:B:148:ASP:OD1	2:B:150:THR:OG1	2.32	0.41
6:G:123:GLU:HB2	6:G:128:PHE:O	2.20	0.41
8:I:70:MET:HG3	15:P:66:ALA:HB1	2.02	0.41
12:M:47:THR:O	12:M:96:VAL:HG22	2.21	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.56	0.41
8:I:25:GLN:H	8:I:25:GLN:NE2	2.19	0.41
12:M:233:SER:HB3	12:M:236:TYR:HB3	2.02	0.41
16:Q:194:ILE:O	16:Q:194:ILE:HG22	2.20	0.41
2:B:111:GLU:O	2:B:141:ARG:NH1	2.54	0.40
2:B:112:ARG:HD3	2:B:164:VAL:O	2.21	0.40
3:C:50:LEU:HD23	3:C:50:LEU:HA	1.90	0.40
5:F:30:SER:OG	5:F:63:PRO:HG3	2.21	0.40
6:G:94:ASP:HA	6:G:95:PRO:HD3	1.95	0.40
15:P:51:ASN:HB3	15:P:82:ASN:ND2	2.36	0.40
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:LEU:HD13	3:C:117:LEU:HD13	2.02	0.40
21:C:302:PEE:H82	21:C:302:PEE:H74	1.86	0.40
12:M:370:GLU:HG3	12:M:519:ILE:HG13	2.03	0.40
12:M:382:ARG:HE	12:M:527:ASP:CG	2.24	0.40
14:O:133:GLN:HG2	14:O:172:ILE:HD11	2.03	0.40
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.56	0.40
16:Q:162:GLN:HA	16:Q:163:PRO:HD3	1.95	0.40
1:A:218:GLY:HA2	14:O:80:LEU:HD23	2.04	0.40
3:C:75:GLU:HG3	3:C:167:PRO:HB2	2.04	0.40
24:J:401:NDP:H2D	24:J:401:NDP:H2N	1.74	0.40
12:M:372:PHE:CZ	12:M:385:TYR:HB3	2.56	0.40
5:F:61:VAL:HG23	5:F:62:GLN:H	1.86	0.40
11:L:158:LYS:HB3	11:L:158:LYS:HE3	1.97	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	431/433 (100%)	418 (97%)	13 (3%)	0	100	100
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	78 (91%)	7 (8%)	1 (1%)	13	32
7	H	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	17	40
8	I	93/112 (83%)	79 (85%)	14 (15%)	0	100	100
9	J	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
10	K	41/43 (95%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	667 (97%)	21 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	383/386 (99%)	368 (96%)	15 (4%)	0	100	100
17	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
18	W	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
All	All	3504/3558 (98%)	3377 (96%)	125 (4%)	2 (0%)	54	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
7	H	77	ILE

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	346/346 (100%)	341 (99%)	5 (1%)	67	86
2	B	151/151 (100%)	150 (99%)	1 (1%)	84	94
3	C	132/132 (100%)	130 (98%)	2 (2%)	65	86
4	E	107/107 (100%)	101 (94%)	6 (6%)	21	45
5	F	75/76 (99%)	72 (96%)	3 (4%)	31	60
6	G	75/81 (93%)	73 (97%)	2 (3%)	44	74
7	H	99/99 (100%)	97 (98%)	2 (2%)	55	81
8	I	87/97 (90%)	79 (91%)	8 (9%)	9	21
9	J	296/296 (100%)	289 (98%)	7 (2%)	49	77
10	K	42/42 (100%)	39 (93%)	3 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	L	113/113 (100%)	107 (95%)	6 (5%)	22 48
12	M	580/580 (100%)	571 (98%)	9 (2%)	62 85
13	N	130/130 (100%)	128 (98%)	2 (2%)	65 86
14	O	183/183 (100%)	177 (97%)	6 (3%)	38 67
15	P	190/190 (100%)	188 (99%)	2 (1%)	73 90
16	Q	332/332 (100%)	327 (98%)	5 (2%)	65 86
17	T	79/79 (100%)	77 (98%)	2 (2%)	47 76
18	W	22/24 (92%)	21 (96%)	1 (4%)	27 55
All	All	3039/3058 (99%)	2967 (98%)	72 (2%)	51 77

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	36	LYS
1	A	102	MET
1	A	105	PRO
1	A	456	GLN
2	B	68	ARG
3	C	49	LYS
3	C	142	TYR
4	E	29	LYS
4	E	57	LYS
4	E	85	LYS
4	E	87	LYS
4	E	94	ILE
4	E	101	THR
5	F	38	GLU
5	F	40	ARG
5	F	75	LYS
6	G	88	LYS
6	G	106	LYS
7	H	50	GLN
7	H	70	GLU
8	I	25	GLN
8	I	43	VAL
8	I	46	SER
8	I	61	ARG
8	I	64	MET

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Mol	Chain	Res	Type
8	I	67	SER
8	I	70	MET
8	I	71	SER
9	J	78	SER
9	J	133	GLU
9	J	173	ASP
9	J	179	ARG
9	J	246	SER
9	J	298	TYR
9	J	322	VAL
10	K	74	ARG
10	K	82	SER
10	K	107	SER
11	L	78	ARG
11	L	86	ASN
11	L	115	SER
11	L	154	LYS
11	L	157	SER
11	L	165	SER
12	M	329	MET
12	M	380	ASP
12	M	398	ASP
12	M	441	ARG
12	M	459	ASN
12	M	539	LYS
12	M	636	TYR
12	M	666	GLN
12	M	680	LEU
13	N	41	GLU
13	N	144	TYR
14	O	145	SER
14	O	150	GLU
14	O	159	LYS
14	O	167	LYS
14	O	197	THR
14	O	222	ARG
15	P	110	SER
15	P	161	LYS
16	Q	144	MET
16	Q	148	GLU
16	Q	282	ASP
16	Q	312	ASP

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Mol	Chain	Res	Type
16	Q	457	VAL
17	T	58	ARG
17	T	114	CYS
18	W	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	303	HIS
12	M	652	ASN
16	Q	223	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	5.95	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.66	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.20	130.67	119.48
16	Q	118	2MR	CD-NE-CZ	4.00	130.89	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.20	130.94	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	O-C-CA-CB
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	NDP	J	401	-	45,52,52	4.55	20 (44%)	53,80,80	1.93	6 (11%)
26	FES	O	301	14	0,4,4	-	-	-		
22	PLX	N	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
22	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.58	1 (1%)
23	8Q1	G	201	6	31,34,34	1.70	6 (19%)	40,43,43	1.57	6 (15%)
25	UQ	J	402	-	33,33,63	3.45	10 (30%)	40,43,79	2.78	13 (32%)
25	UQ	Q	501	-	63,63,63	3.63	15 (23%)	76,79,79	3.21	31 (40%)
21	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
19	SF4	A	501	1	0,12,12	-	-	-		
19	SF4	B	301	2	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.22	8 (16%)
26	FES	M	803	12	0,4,4	-	-	-		
28	CDL	N	202	-	50,50,99	1.41	8 (16%)	56,62,111	1.12	4 (7%)
19	SF4	M	801	12	0,12,12	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		

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
24	NDP	J	401	-	-	10/30/77/77	0/4/5/5
19	SF4	B	302	2	-	-	0/6/5/5
19	SF4	C	301	3	-	-	0/6/5/5
26	FES	O	301	14	-	-	0/1/1/1
22	PLX	N	201	-	-	26/55/55/55	-
22	PLX	C	303	-	-	27/55/55/55	-
23	8Q1	G	201	6	-	10/41/41/41	-
25	UQ	J	402	-	-	16/27/51/87	0/1/1/1
25	UQ	Q	501	-	-	32/63/87/87	0/1/1/1
21	PEE	C	302	-	-	30/50/50/54	-
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	B	301	2	-	-	0/6/5/5
20	FMN	A	502	-	-	9/18/18/18	0/3/3/3
26	FES	M	803	12	-	-	0/1/1/1
28	CDL	N	202	-	-	29/61/61/110	-
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	401	NDP	C3B-C2B	-12.98	1.24	1.52
24	J	401	NDP	C6N-C5N	12.42	1.55	1.33
24	J	401	NDP	O4D-C4D	10.53	1.68	1.45
24	J	401	NDP	C3D-C4D	-9.93	1.27	1.53
25	J	402	UQ	C18-C19	9.57	1.55	1.33
25	Q	501	UQ	C18-C19	9.56	1.55	1.33
25	Q	501	UQ	C13-C14	9.24	1.55	1.33
25	J	402	UQ	C13-C14	9.16	1.54	1.33
25	Q	501	UQ	C23-C24	9.10	1.54	1.33
25	J	402	UQ	C8-C9	9.06	1.54	1.33
25	Q	501	UQ	C28-C29	8.90	1.54	1.33
25	Q	501	UQ	C8-C9	8.89	1.54	1.33
24	J	401	NDP	O4B-C1B	8.50	1.52	1.41
25	Q	501	UQ	C33-C34	8.50	1.53	1.33
25	Q	501	UQ	C43-C44	8.25	1.52	1.33
25	Q	501	UQ	C38-C39	8.22	1.52	1.33
25	Q	501	UQ	C48-C49	7.92	1.52	1.33
24	J	401	NDP	O4B-C4B	-7.85	1.27	1.45
25	J	402	UQ	C23-C24	7.79	1.54	1.32
25	Q	501	UQ	C53-C54	7.36	1.53	1.32
24	J	401	NDP	C2N-C3N	7.30	1.55	1.34
24	J	401	NDP	P2B-O2B	5.53	1.69	1.59
23	G	201	8Q1	C34-N36	5.37	1.45	1.33
23	G	201	8Q1	C39-N41	5.36	1.45	1.33
24	J	401	NDP	C3B-C4B	5.28	1.66	1.53
24	J	401	NDP	O4D-C1D	-4.87	1.30	1.42
24	J	401	NDP	C6N-N1N	4.77	1.49	1.37
24	J	401	NDP	O2D-C2D	-4.16	1.33	1.43
24	J	401	NDP	C7N-N7N	4.12	1.44	1.33
24	J	401	NDP	C6A-N6A	4.07	1.48	1.34
21	C	302	PEE	C18-C19	3.72	1.53	1.31
20	A	502	FMN	C4A-N5	3.67	1.37	1.30
21	C	302	PEE	C39-C38	3.63	1.52	1.31
28	N	202	CDL	OA8-CA7	3.41	1.43	1.33
28	N	202	CDL	OB6-CB5	3.05	1.42	1.34
24	J	401	NDP	O3D-C3D	3.04	1.50	1.43
24	J	401	NDP	C7N-C3N	3.00	1.55	1.48
28	N	202	CDL	OB8-CB7	2.99	1.42	1.33
28	N	202	CDL	OA6-CA5	2.93	1.42	1.34
22	N	201	PLX	O6-C4	-2.67	1.41	1.44
25	Q	501	UQ	C6-C1	2.65	1.54	1.46
25	J	402	UQ	C6-C1	2.64	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	303	PLX	O6-C4	-2.58	1.41	1.44
25	J	402	UQ	C7-C8	2.48	1.54	1.50
20	A	502	FMN	C10-N1	2.48	1.38	1.33
21	C	302	PEE	O2-C2	-2.46	1.40	1.46
21	C	302	PEE	O3-C30	2.45	1.40	1.33
28	N	202	CDL	OA6-CA4	-2.39	1.40	1.46
23	G	201	8Q1	C1-S44	2.39	1.81	1.76
25	Q	501	UQ	C7-C8	2.38	1.54	1.50
22	N	201	PLX	C7-C6	2.33	1.55	1.50
23	G	201	8Q1	O35-C34	-2.31	1.18	1.23
24	J	401	NDP	O2B-C2B	2.30	1.52	1.44
23	G	201	8Q1	O40-C39	-2.30	1.18	1.23
25	Q	501	UQ	O4-C4	-2.29	1.18	1.23
22	C	303	PLX	C7-C6	2.26	1.55	1.50
23	G	201	8Q1	C6-C1	2.26	1.53	1.50
21	C	302	PEE	O2-C10	2.24	1.40	1.34
24	J	401	NDP	C2D-C3D	2.24	1.59	1.53
28	N	202	CDL	PB2-OB2	2.21	1.68	1.59
28	N	202	CDL	PB2-OB5	2.20	1.68	1.59
25	J	402	UQ	O4-C4	-2.19	1.18	1.23
24	J	401	NDP	O7N-C7N	-2.18	1.19	1.24
22	N	201	PLX	P1-O4	2.17	1.68	1.59
28	N	202	CDL	OB6-CB4	-2.17	1.41	1.46
22	C	303	PLX	P1-O4	2.13	1.67	1.59
22	N	201	PLX	P1-O1	2.07	1.67	1.59
25	J	402	UQ	O1-C1	-2.07	1.18	1.23
24	J	401	NDP	PA-O5B	2.06	1.67	1.59
21	C	302	PEE	O3-C3	-2.06	1.40	1.45
25	Q	501	UQ	O1-C1	-2.06	1.18	1.23
25	J	402	UQ	C21-C19	2.06	1.55	1.51
25	J	402	UQ	O3-CM3	-2.03	1.40	1.45
22	C	303	PLX	P1-O1	2.03	1.67	1.59
25	Q	501	UQ	O3-CM3	-2.02	1.40	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	401	NDP	C3N-C2N-N1N	-9.20	109.97	123.10
25	J	402	UQ	C7-C8-C9	-7.89	113.66	126.79
25	Q	501	UQ	C7-C8-C9	-7.84	113.75	126.79
25	Q	501	UQ	C42-C43-C44	-6.49	112.04	127.66
25	J	402	UQ	C12-C13-C14	-6.39	112.27	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	501	UQ	C12-C13-C14	-6.39	112.27	127.66
25	Q	501	UQ	C47-C48-C49	-6.19	112.77	127.66
25	Q	501	UQ	C32-C33-C34	-6.19	112.77	127.66
25	Q	501	UQ	C37-C38-C39	-6.11	112.94	127.66
25	Q	501	UQ	C17-C18-C19	-6.06	113.07	127.66
25	Q	501	UQ	C22-C23-C24	-6.02	113.16	127.66
25	Q	501	UQ	C27-C28-C29	-5.99	113.25	127.66
25	J	402	UQ	C17-C18-C19	-5.94	113.35	127.66
23	G	201	8Q1	C6-C1-S44	5.94	120.37	113.46
24	J	401	NDP	C1D-N1N-C2N	-5.94	111.23	121.11
24	J	401	NDP	C1D-N1N-C6N	-4.52	111.09	120.83
25	Q	501	UQ	C30-C29-C28	-4.47	112.21	123.68
25	J	402	UQ	C21-C19-C18	-4.45	112.12	121.12
25	Q	501	UQ	C45-C44-C43	-4.37	112.46	123.68
25	Q	501	UQ	C15-C14-C13	-4.37	112.47	123.68
25	Q	501	UQ	C52-C53-C54	-4.35	112.89	127.75
25	J	402	UQ	C22-C23-C24	-4.35	112.89	127.75
25	Q	501	UQ	C11-C9-C8	-4.34	112.34	121.12
25	Q	501	UQ	C20-C19-C18	-4.33	112.58	123.68
25	Q	501	UQ	C35-C34-C33	-4.29	112.67	123.68
25	Q	501	UQ	C31-C29-C28	-4.26	112.50	121.12
25	Q	501	UQ	C10-C9-C8	-4.24	112.80	123.68
25	Q	501	UQ	C21-C19-C18	-4.24	112.53	121.12
25	J	402	UQ	C20-C19-C18	-4.24	112.80	123.68
25	Q	501	UQ	C50-C49-C48	-4.22	112.85	123.68
25	Q	501	UQ	C51-C49-C48	-4.21	112.59	121.12
25	J	402	UQ	C11-C9-C8	-4.20	112.62	121.12
25	Q	501	UQ	C25-C24-C23	-4.19	112.92	123.68
24	J	401	NDP	N3A-C2A-N1A	-4.17	122.16	128.68
25	J	402	UQ	C15-C14-C13	-4.13	113.08	123.68
25	Q	501	UQ	C46-C44-C43	-4.12	112.77	121.12
25	Q	501	UQ	C40-C39-C38	-4.06	113.27	123.68
25	J	402	UQ	C10-C9-C8	-4.05	113.28	123.68
25	Q	501	UQ	C41-C39-C38	-4.01	113.01	121.12
25	J	402	UQ	C16-C14-C13	-4.00	113.02	121.12
21	C	302	PEE	O2-C10-C11	3.99	120.11	111.50
28	N	202	CDL	OA6-CA5-C11	3.97	120.05	111.50
25	Q	501	UQ	C36-C34-C33	-3.96	113.11	121.12
25	Q	501	UQ	C16-C14-C13	-3.90	113.22	121.12
28	N	202	CDL	OB6-CB5-C51	3.85	119.79	111.50
25	Q	501	UQ	C26-C24-C23	-3.73	113.57	121.12
25	J	402	UQ	C26-C24-C23	-3.46	112.64	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	501	UQ	C56-C54-C53	-3.40	112.83	122.65
25	J	402	UQ	C25-C24-C23	-3.40	112.83	122.65
25	Q	501	UQ	C55-C54-C53	-3.39	112.85	122.65
23	G	201	8Q1	O4-C1-C6	-3.36	120.02	123.99
23	G	201	8Q1	C37-C38-C39	3.25	117.78	112.36
20	A	502	FMN	C4-N3-C2	-3.11	119.90	125.64
20	A	502	FMN	C4A-C4-N3	2.70	120.03	113.19
25	Q	501	UQ	CM5-C5-C6	-2.69	120.01	124.40
28	N	202	CDL	OB8-CB7-C71	2.61	120.09	111.91
21	C	302	PEE	O3-C30-C31	2.60	120.07	111.91
28	N	202	CDL	OA8-CA7-C31	2.60	120.06	111.91
24	J	401	NDP	PN-O3-PA	-2.59	123.94	132.83
20	A	502	FMN	O4-C4-C4A	-2.53	119.88	126.60
25	J	402	UQ	CM5-C5-C6	-2.47	120.37	124.40
20	A	502	FMN	C4A-C10-N10	2.40	119.99	116.48
20	A	502	FMN	C4A-C10-N1	-2.35	119.28	124.73
22	N	201	PLX	C1A-N1-C1	2.34	119.51	109.92
23	G	201	8Q1	O4-C1-S44	-2.32	119.61	122.61
23	G	201	8Q1	C38-C39-N41	2.31	120.31	116.42
22	C	303	PLX	C1A-N1-C1	2.30	119.34	109.92
24	J	401	NDP	C4A-C5A-N7A	-2.29	107.01	109.40
23	G	201	8Q1	C43-S44-C1	2.17	108.62	101.87
20	A	502	FMN	C5A-C9A-N10	2.16	120.19	117.95
20	A	502	FMN	C9A-C5A-N5	-2.07	120.18	122.43
20	A	502	FMN	C10-C4A-N5	-2.07	120.47	124.86

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	N10-C1'-C2'-O2'
20	A	502	FMN	N10-C1'-C2'-C3'
20	A	502	FMN	C1'-C2'-C3'-O3'
20	A	502	FMN	C1'-C2'-C3'-C4'
20	A	502	FMN	C5'-O5'-P-O2P
20	A	502	FMN	C5'-O5'-P-O3P
21	C	302	PEE	C11-C10-O2-C2
21	C	302	PEE	C1-O3P-P-O2P
21	C	302	PEE	C1-O3P-P-O1P
21	C	302	PEE	C4-O4P-P-O1P
22	C	303	PLX	O6-C4-C5-O8
22	C	303	PLX	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
22	C	303	PLX	O9-C24-C25-C26
22	N	201	PLX	O7-C6-O6-C4
22	N	201	PLX	C2-O1-P1-O2
22	N	201	PLX	C2-O1-P1-O3
22	N	201	PLX	O9-C24-O8-C5
23	G	201	8Q1	C42-C43-S44-C1
23	G	201	8Q1	C28-O27-P24-O1
24	J	401	NDP	O4B-C4B-C5B-O5B
24	J	401	NDP	O4D-C1D-N1N-C6N
25	J	402	UQ	C7-C8-C9-C10
25	J	402	UQ	C7-C8-C9-C11
25	J	402	UQ	C11-C12-C13-C14
25	J	402	UQ	C12-C13-C14-C15
25	J	402	UQ	C12-C13-C14-C16
25	J	402	UQ	C14-C16-C17-C18
25	J	402	UQ	C17-C18-C19-C21
25	J	402	UQ	C18-C19-C21-C22
25	J	402	UQ	C19-C21-C22-C23
25	J	402	UQ	C22-C23-C24-C26
25	Q	501	UQ	C7-C8-C9-C10
25	Q	501	UQ	C16-C17-C18-C19
25	Q	501	UQ	C17-C18-C19-C20
25	Q	501	UQ	C20-C19-C21-C22
25	Q	501	UQ	C25-C24-C26-C27
25	Q	501	UQ	C27-C28-C29-C31
25	Q	501	UQ	C28-C29-C31-C32
25	Q	501	UQ	C32-C33-C34-C36
25	Q	501	UQ	C42-C43-C44-C45
25	Q	501	UQ	C42-C43-C44-C46
25	Q	501	UQ	C47-C48-C49-C51
28	N	202	CDL	O1-C1-CA2-OA2
28	N	202	CDL	CA2-OA2-PA1-OA3
28	N	202	CDL	CA2-OA2-PA1-OA4
28	N	202	CDL	OA5-CA3-CA4-OA6
28	N	202	CDL	CB2-OB2-PB2-OB3
28	N	202	CDL	CB2-OB2-PB2-OB4
28	N	202	CDL	CB2-OB2-PB2-OB5
28	N	202	CDL	CB3-OB5-PB2-OB3
21	C	302	PEE	O4-C10-O2-C2
25	Q	501	UQ	C52-C53-C54-C55
25	J	402	UQ	C15-C14-C16-C17
25	J	402	UQ	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
25	Q	501	UQ	C43-C44-C46-C47
25	Q	501	UQ	C27-C28-C29-C30
25	Q	501	UQ	C37-C38-C39-C40
25	Q	501	UQ	C47-C48-C49-C50
25	Q	501	UQ	C12-C13-C14-C16
25	Q	501	UQ	C17-C18-C19-C21
25	Q	501	UQ	C22-C23-C24-C26
22	C	303	PLX	C9-C10-C11-C12
22	C	303	PLX	C33-C34-C35-C36
25	J	402	UQ	C12-C11-C9-C10
25	Q	501	UQ	C48-C49-C51-C52
25	J	402	UQ	C9-C11-C12-C13
25	Q	501	UQ	C14-C16-C17-C18
25	Q	501	UQ	C34-C36-C37-C38
22	N	201	PLX	C31-C32-C33-C34
25	Q	501	UQ	C22-C23-C24-C25
28	N	202	CDL	CB2-C1-CA2-OA2
21	C	302	PEE	C11-C12-C13-C14
25	J	402	UQ	C17-C18-C19-C20
24	J	401	NDP	C3B-C4B-C5B-O5B
21	C	302	PEE	C1-O3P-P-O4P
21	C	302	PEE	C4-O4P-P-O3P
28	N	202	CDL	CA2-OA2-PA1-OA5
22	N	201	PLX	C29-C30-C31-C32
22	N	201	PLX	C14-C15-C16-C17
28	N	202	CDL	O1-C1-CB2-OB2
22	N	201	PLX	C27-C28-C29-C30
22	C	303	PLX	C30-C31-C32-C33
22	C	303	PLX	C17-C18-C19-C20
22	N	201	PLX	C7-C8-C9-C10
22	N	201	PLX	C33-C34-C35-C36
28	N	202	CDL	CB7-C71-C72-C73
21	C	302	PEE	C42-C43-C44-C45
23	G	201	8Q1	C12-C13-C14-C15
28	N	202	CDL	C11-C12-C13-C14
22	C	303	PLX	C11-C12-C13-C14
22	C	303	PLX	C7-C8-C9-C10
22	C	303	PLX	O7-C6-C7-C8
22	N	201	PLX	C25-C26-C27-C28
22	N	201	PLX	C12-C13-C14-C15
28	N	202	CDL	C71-C72-C73-C74
28	N	202	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
28	N	202	CDL	OA7-CA5-OA6-CA4
22	N	201	PLX	C28-C29-C30-C31
20	A	502	FMN	O2'-C2'-C3'-C4'
22	C	303	PLX	C2-O1-P1-O4
22	N	201	PLX	C2-O1-P1-O4
28	N	202	CDL	CB3-OB5-PB2-OB2
22	C	303	PLX	C14-C15-C16-C17
22	C	303	PLX	C3-C4-C5-O8
21	C	302	PEE	C32-C33-C34-C35
22	C	303	PLX	C10-C11-C12-C13
21	C	302	PEE	C15-C16-C17-C18
20	A	502	FMN	C5'-O5'-P-O1P
28	N	202	CDL	OB5-CB3-CB4-OB6
22	N	201	PLX	C16-C17-C18-C19
28	N	202	CDL	C52-C53-C54-C55
25	Q	501	UQ	C3-C2-O2-CM2
22	N	201	PLX	C30-C31-C32-C33
21	C	302	PEE	O3P-C1-C2-C3
28	N	202	CDL	OB5-CB3-CB4-CB6
25	Q	501	UQ	C45-C44-C46-C47
25	Q	501	UQ	C13-C14-C16-C17
25	J	402	UQ	C21-C22-C23-C24
28	N	202	CDL	C31-C32-C33-C34
21	C	302	PEE	C1-C2-C3-O3
22	C	303	PLX	C35-C36-C37-C38
22	C	303	PLX	O4-C3-C4-O6
22	N	201	PLX	C13-C14-C15-C16
28	N	202	CDL	C51-C52-C53-C54
22	C	303	PLX	C36-C37-C38-C39
22	C	303	PLX	O8-C24-C25-C26
28	N	202	CDL	OA5-CA3-CA4-CA6
21	C	302	PEE	C43-C44-C45-C46
23	G	201	8Q1	C28-O27-P24-O2
28	N	202	CDL	CA7-C31-C32-C33
24	J	401	NDP	C2D-C1D-N1N-C2N
24	J	401	NDP	C5B-O5B-PA-O3
20	A	502	FMN	O2'-C2'-C3'-O3'
24	J	401	NDP	O4D-C4D-C5D-O5D
21	C	302	PEE	C4-O4P-P-O2P
22	C	303	PLX	C2-O1-P1-O3
24	J	401	NDP	C5B-O5B-PA-O2A
28	N	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
22	C	303	PLX	C25-C24-O8-C5
21	C	302	PEE	O3P-C1-C2-O2
22	C	303	PLX	N1-C1-C2-O1
28	N	202	CDL	CA3-CA4-CA6-OA8
22	N	201	PLX	O6-C4-C5-O8
28	N	202	CDL	OA6-CA4-CA6-OA8
25	Q	501	UQ	C9-C11-C12-C13
22	N	201	PLX	O9-C24-C25-C26
22	N	201	PLX	O4-C3-C4-C5
23	G	201	8Q1	C28-O27-P24-O3
22	N	201	PLX	O4-C3-C4-O6
25	Q	501	UQ	C52-C53-C54-C56
21	C	302	PEE	O2-C2-C3-O3
22	C	303	PLX	C3-O4-P1-O1
22	N	201	PLX	C10-C11-C12-C13
22	C	303	PLX	O4-C3-C4-C5
25	Q	501	UQ	C4-C3-O3-CM3
21	C	302	PEE	C44-C45-C46-C47
22	C	303	PLX	C5-C4-O6-C6
23	G	201	8Q1	C10-C11-C12-C13
21	C	302	PEE	C13-C14-C15-C16
22	C	303	PLX	C20-C21-C22-C23
22	C	303	PLX	C6-C7-C8-C9
21	C	302	PEE	C33-C34-C35-C36
24	J	401	NDP	O4D-C1D-N1N-C2N
28	N	202	CDL	CA2-C1-CB2-OB2
25	Q	501	UQ	C12-C11-C9-C8
25	Q	501	UQ	C40-C39-C41-C42
22	N	201	PLX	C26-C27-C28-C29
22	N	201	PLX	O8-C24-C25-C26
22	C	303	PLX	C13-C14-C15-C16
23	G	201	8Q1	C1-C6-C7-C8
24	J	401	NDP	C3D-C4D-C5D-O5D
21	C	302	PEE	C38-C39-C40-C41
21	C	302	PEE	O3-C30-C31-C32
21	C	302	PEE	C18-C19-C20-C21
21	C	302	PEE	C16-C17-C18-C19
22	N	201	PLX	C3-C4-C5-O8
21	C	302	PEE	C14-C15-C16-C17
21	C	302	PEE	O2-C10-C11-C12
23	G	201	8Q1	C30-C29-C32-O33
24	J	401	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
21	C	302	PEE	C34-C35-C36-C37
25	Q	501	UQ	C2-C3-O3-CM3
21	C	302	PEE	C37-C38-C39-C40
28	N	202	CDL	C12-C13-C14-C15
21	C	302	PEE	O5-C30-C31-C32
22	N	201	PLX	C1-C2-O1-P1
21	C	302	PEE	O4-C10-C11-C12
23	G	201	8Q1	C28-C29-C32-C34
23	G	201	8Q1	C43-C42-N41-C39

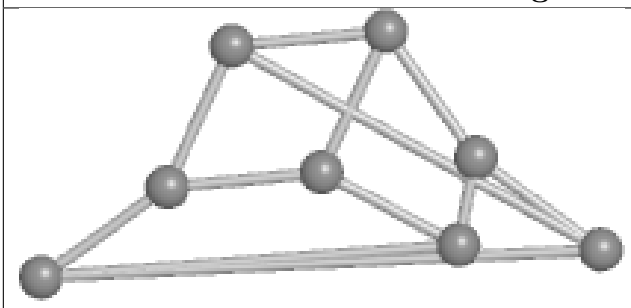
There are no ring outliers.

8 monomers are involved in 51 short contacts:

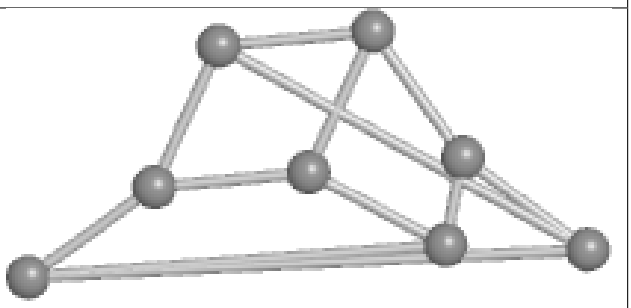
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	J	401	NDP	3	0
22	N	201	PLX	2	0
22	C	303	PLX	5	0
25	J	402	UQ	5	0
25	Q	501	UQ	29	0
21	C	302	PEE	1	0
19	A	501	SF4	2	0
20	A	502	FMN	5	0

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.

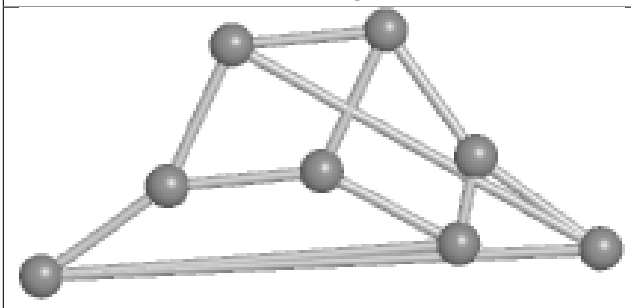
Ligand SF4 C 301



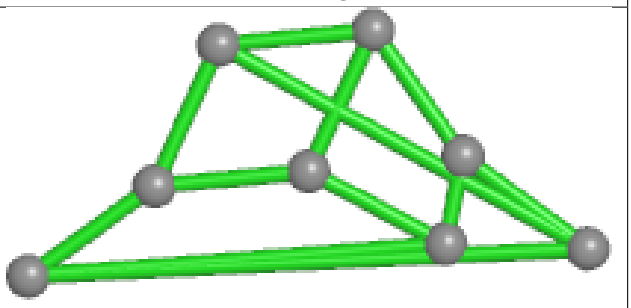
Bond lengths



Bond angles

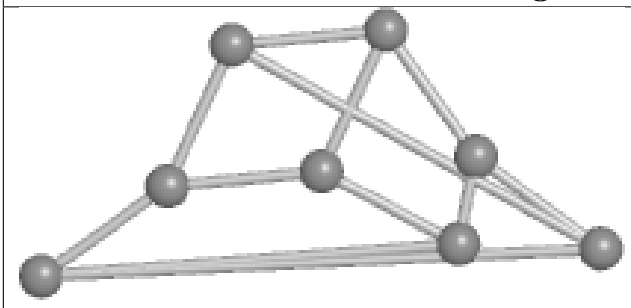


Torsions

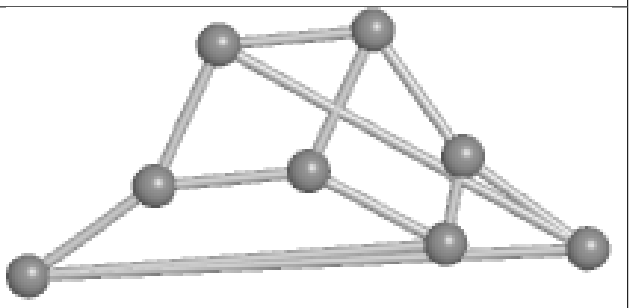


Rings

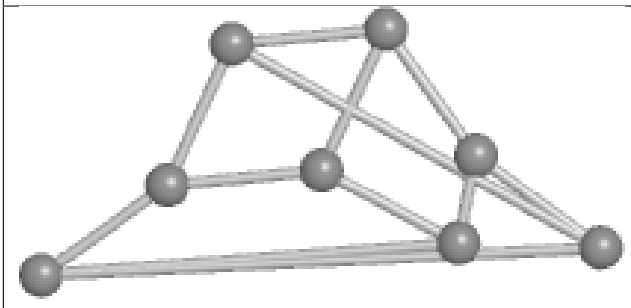
Ligand SF4 B 302



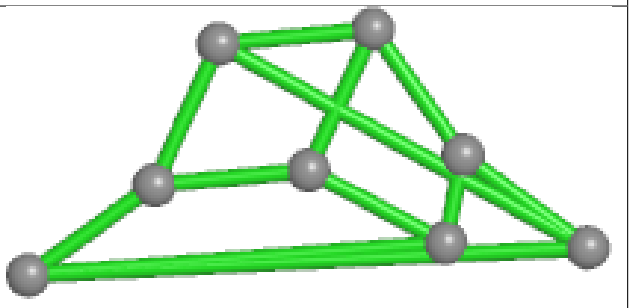
Bond lengths



Bond angles

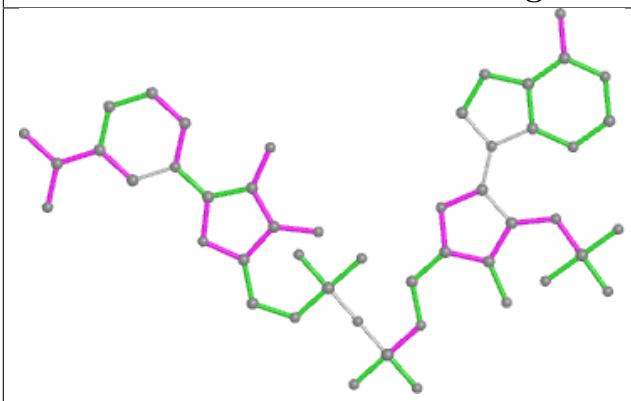


Torsions

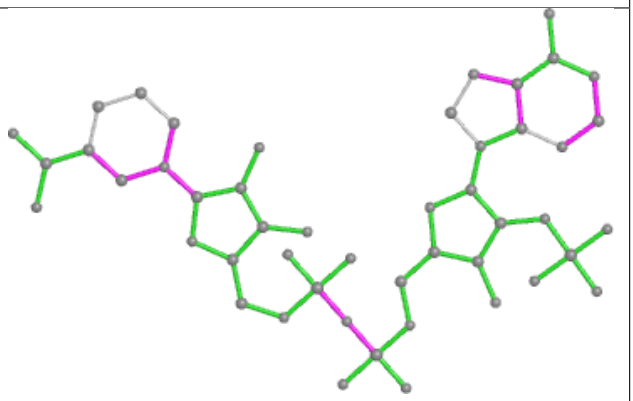


Rings

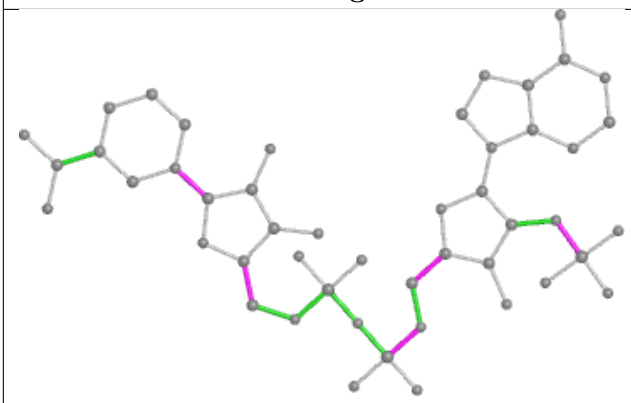
Ligand NDP J 401



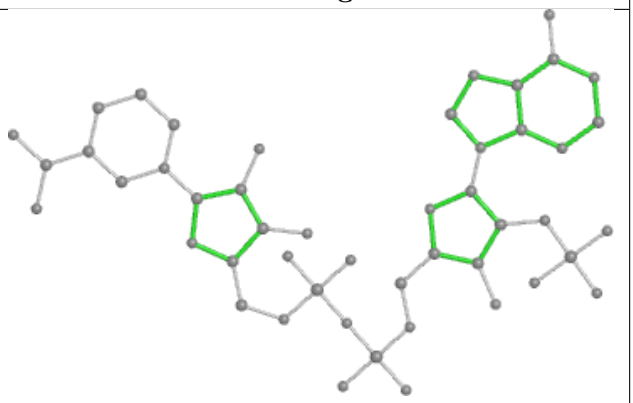
Bond lengths



Bond angles

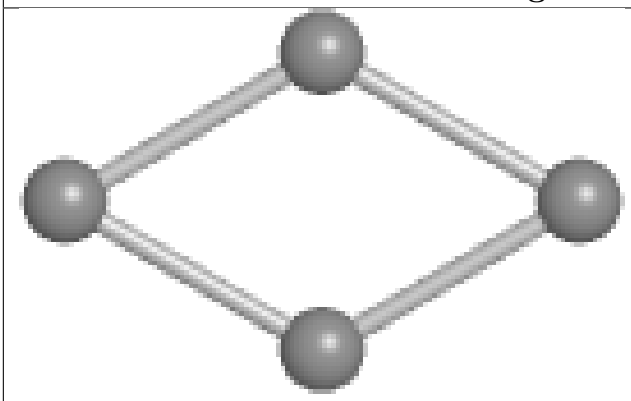


Torsions

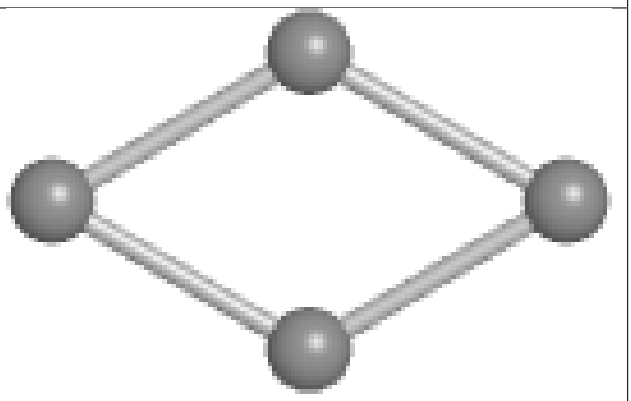


Rings

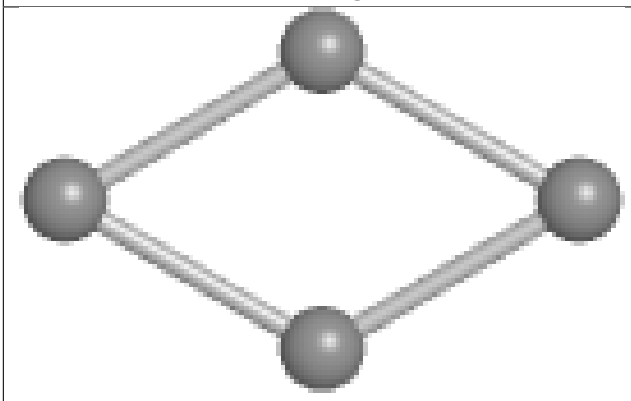
Ligand FES O 301



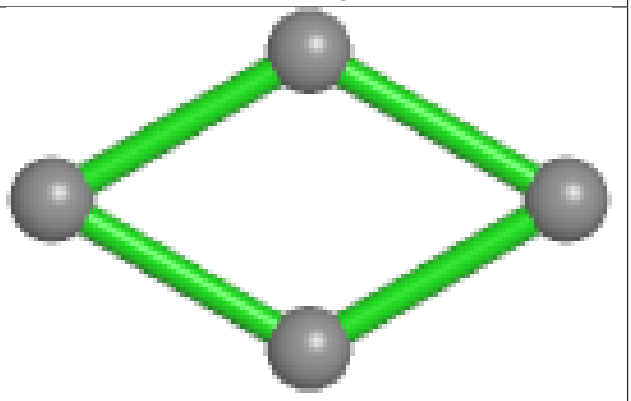
Bond lengths



Bond angles

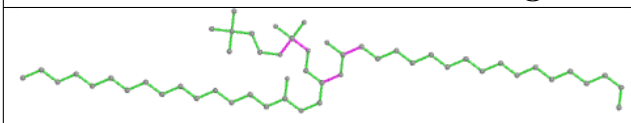


Torsions

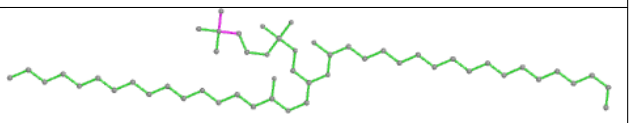


Rings

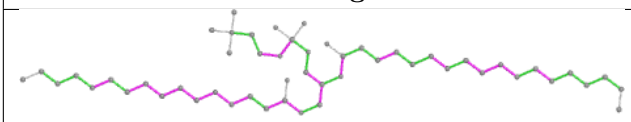
Ligand PLX N 201



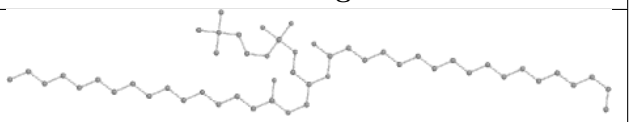
Bond lengths



Bond angles

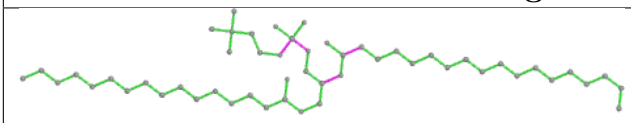


Torsions

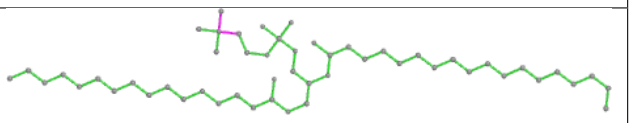


Rings

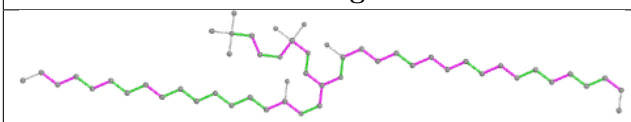
Ligand PLX C 303



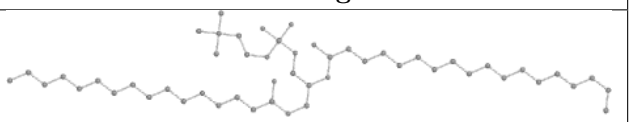
Bond lengths



Bond angles

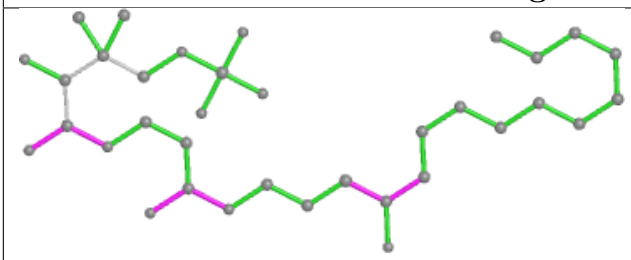


Torsions

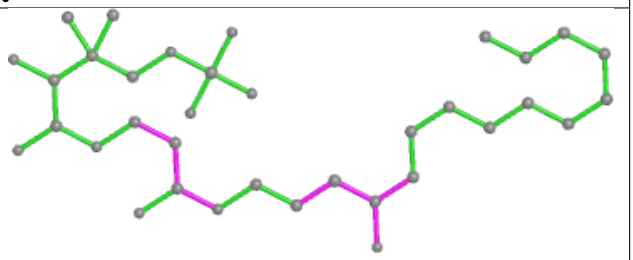


Rings

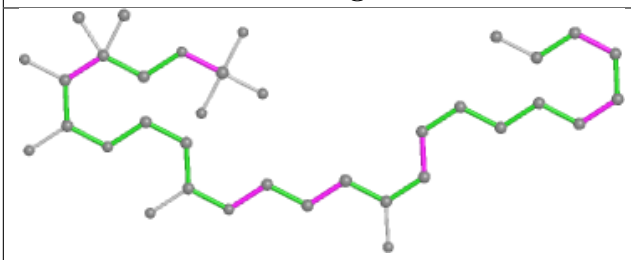
Ligand 8Q1 G 201



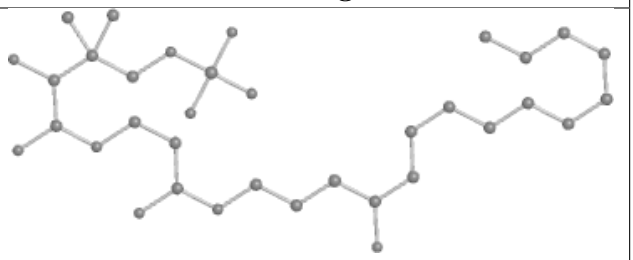
Bond lengths



Bond angles

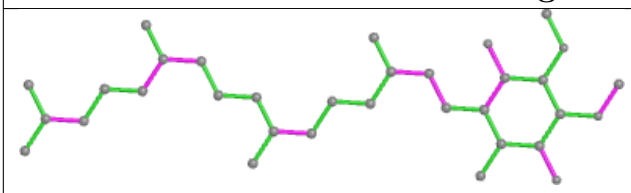


Torsions

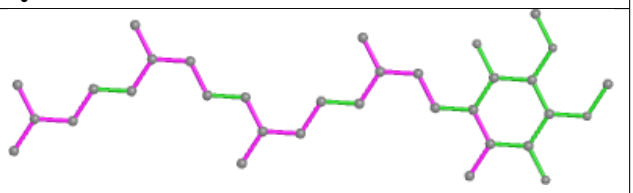


Rings

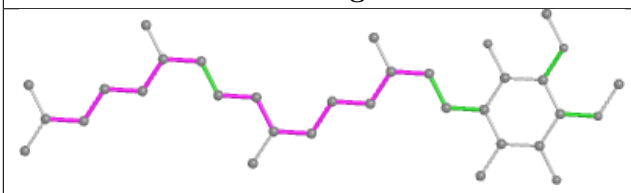
Ligand UQ J 402



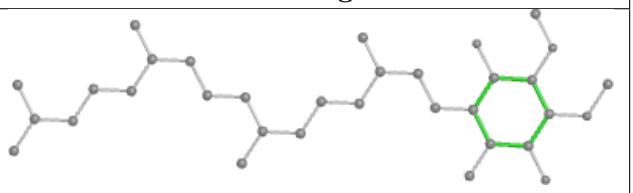
Bond lengths



Bond angles



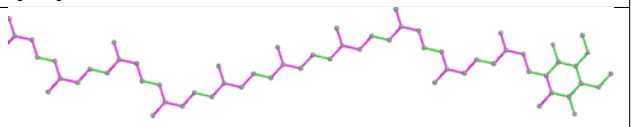
Torsions



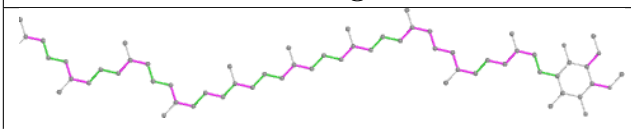
Rings

Ligand UQ Q 501

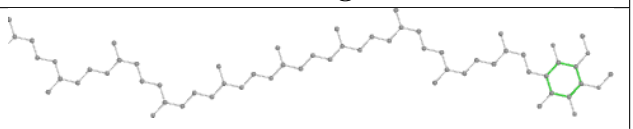
Bond lengths



Bond angles

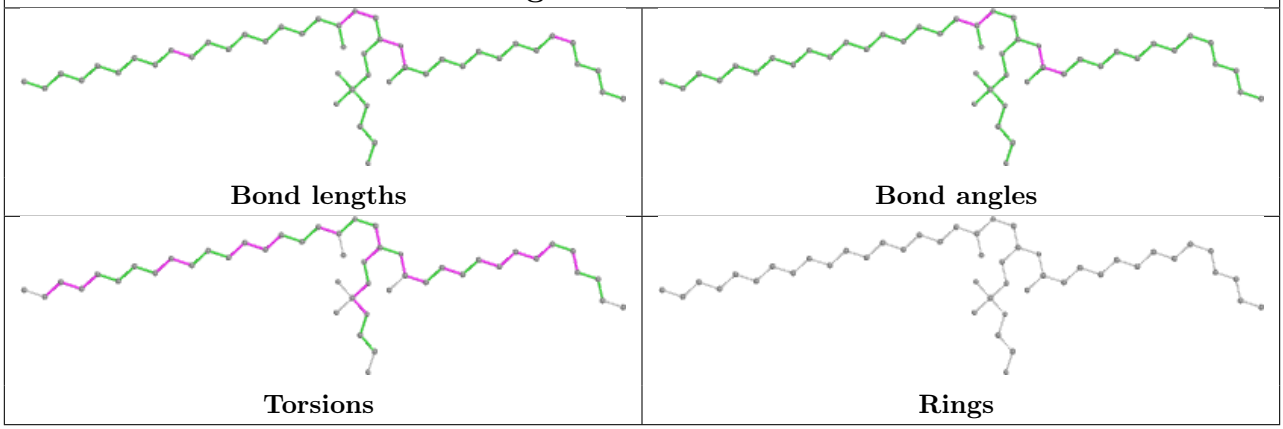


Torsions

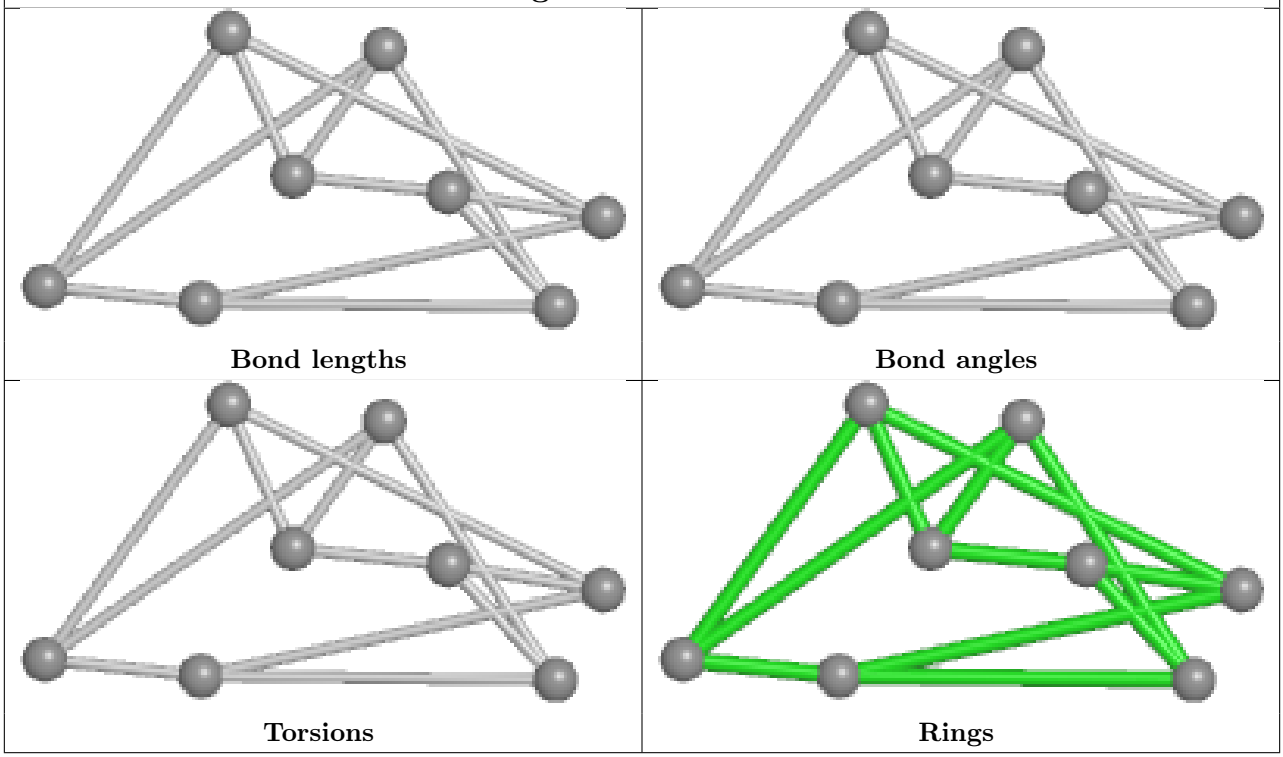


Rings

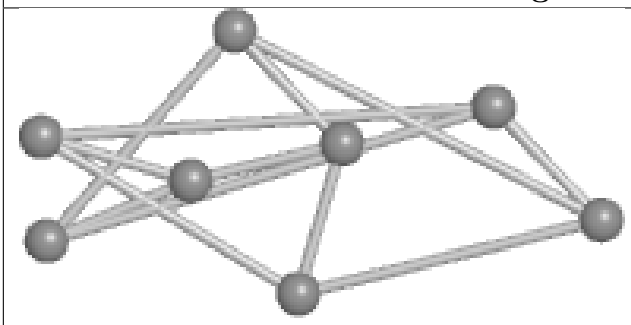
Ligand PEE C 302



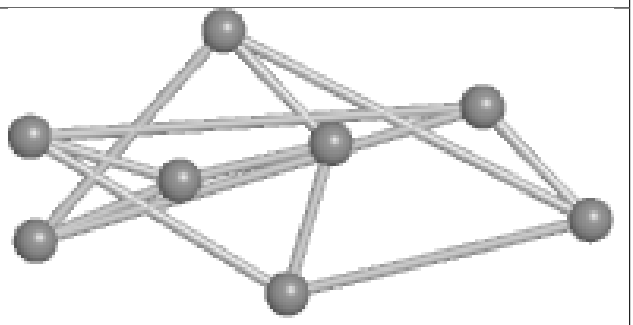
Ligand SF4 A 501



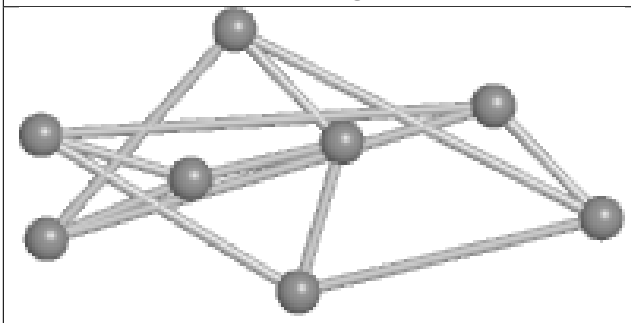
Ligand SF4 B 301



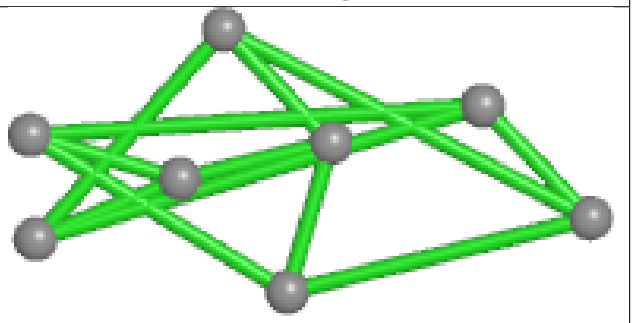
Bond lengths



Bond angles

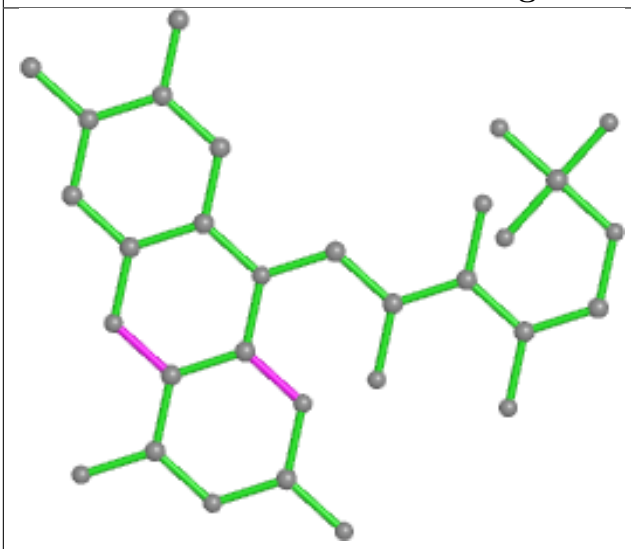


Torsions

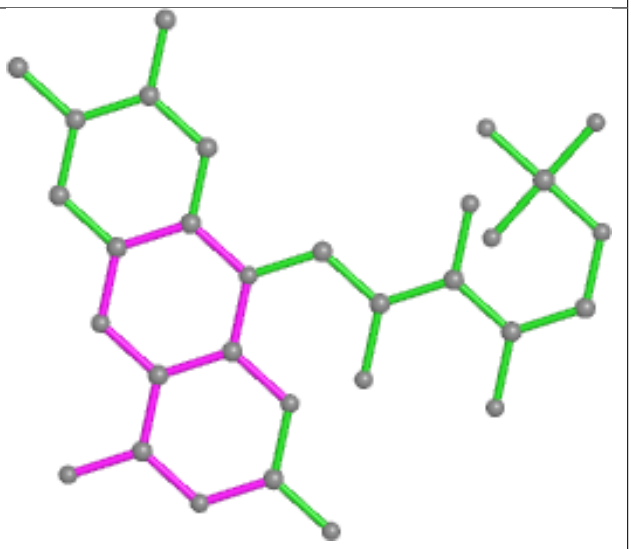


Rings

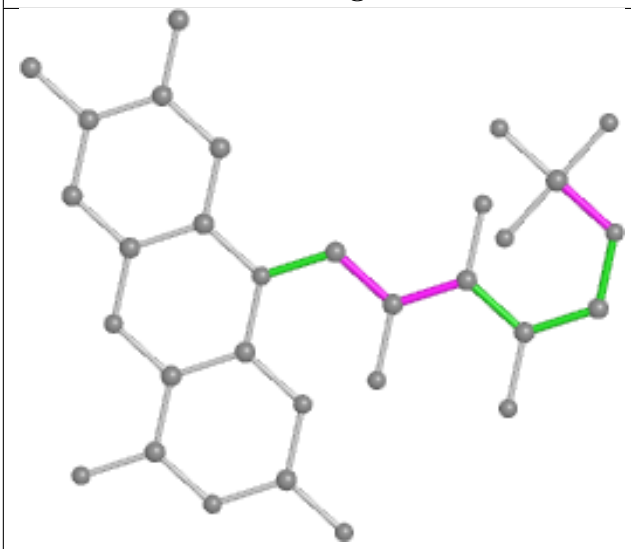
Ligand FMN A 502



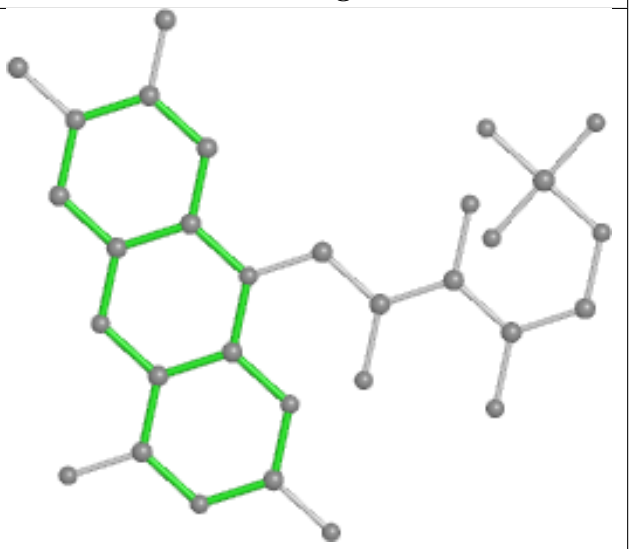
Bond lengths



Bond angles

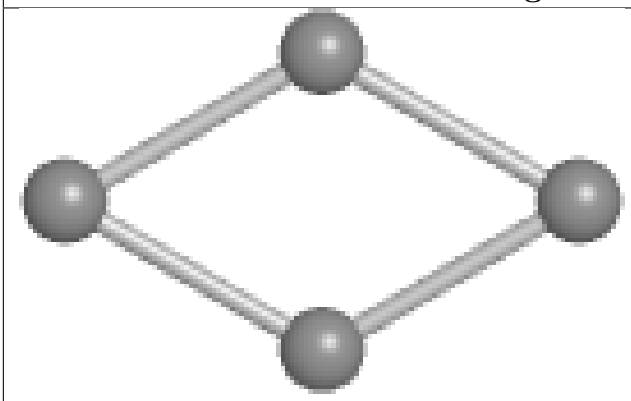


Torsions

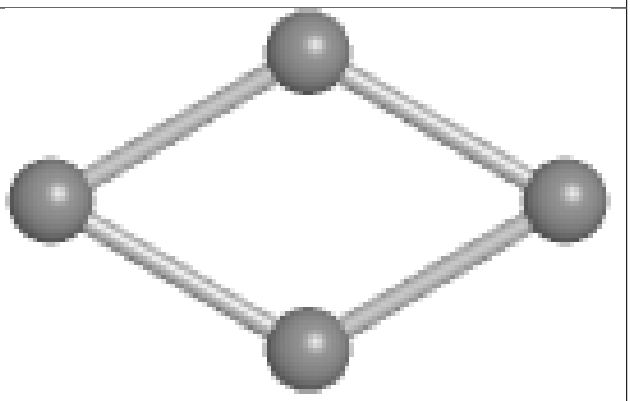


Rings

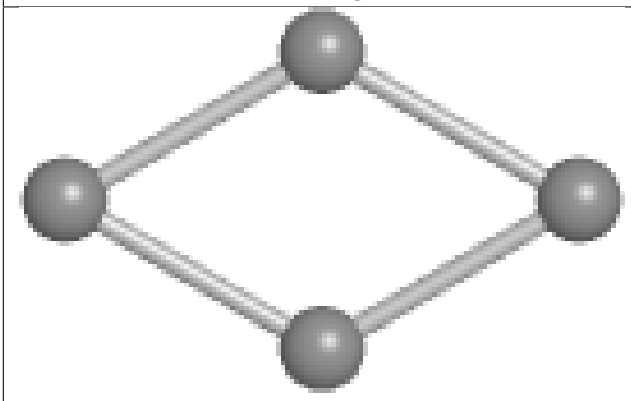
Ligand FES M 803



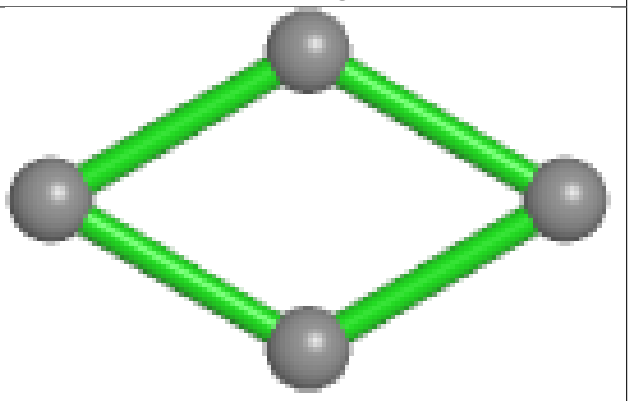
Bond lengths



Bond angles

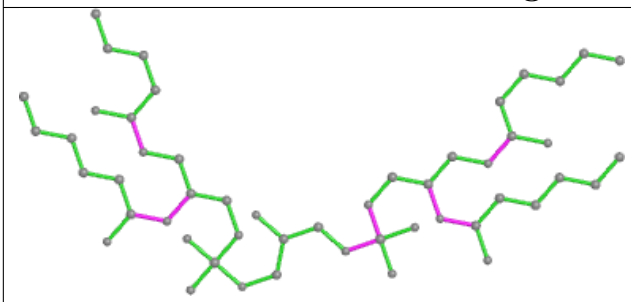


Torsions

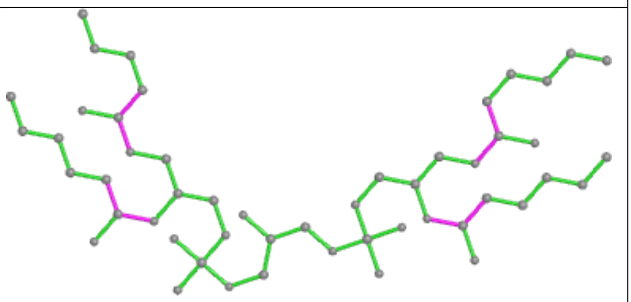


Rings

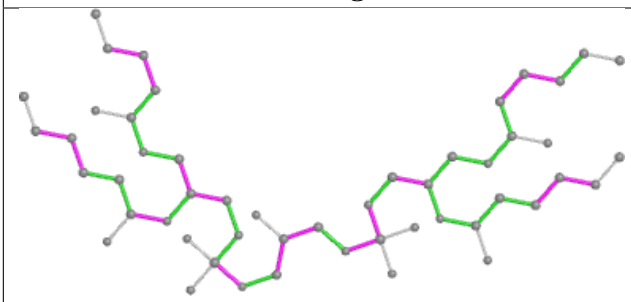
Ligand CDL N 202



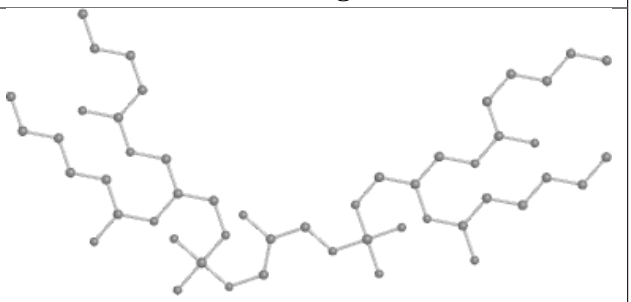
Bond lengths



Bond angles

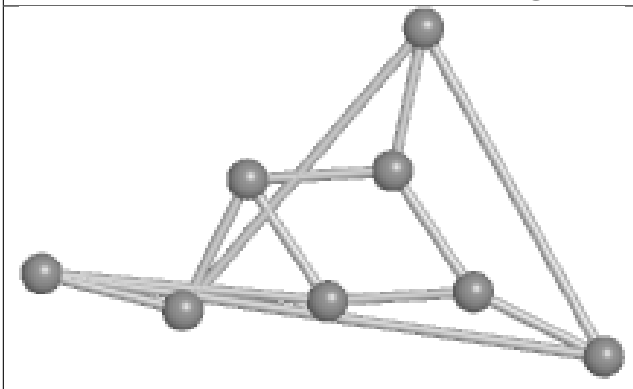


Torsions

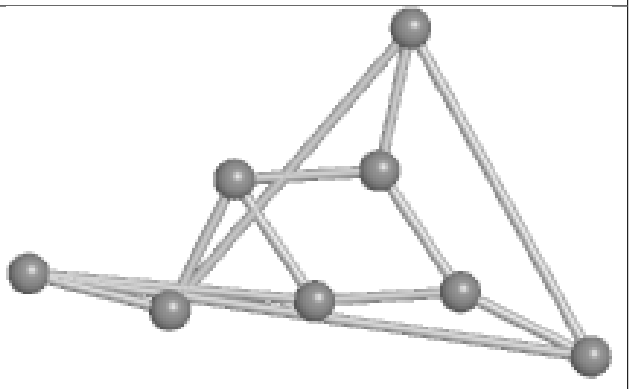


Rings

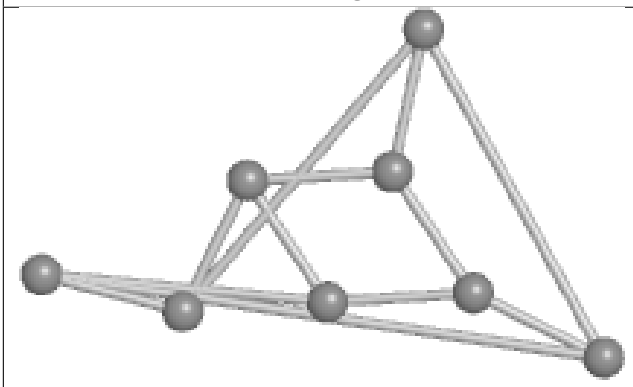
Ligand SF4 M 801



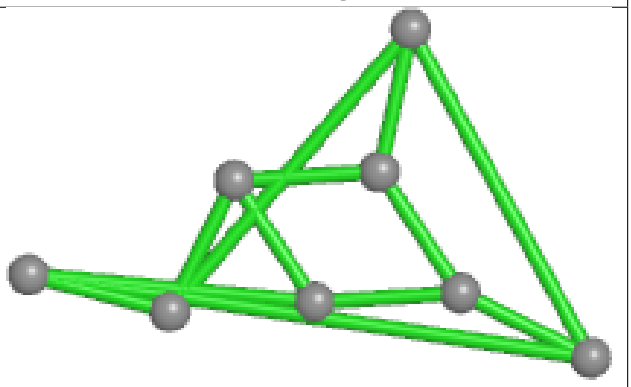
Bond lengths



Bond angles

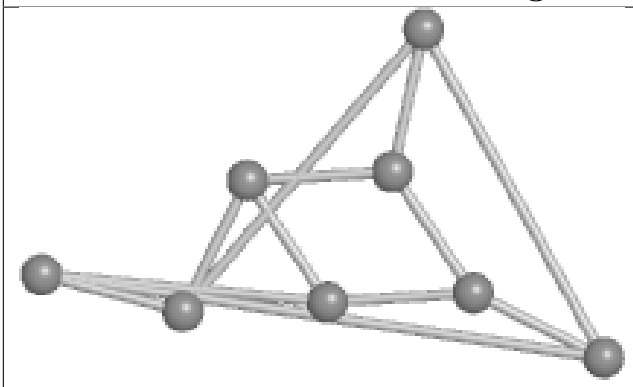


Torsions

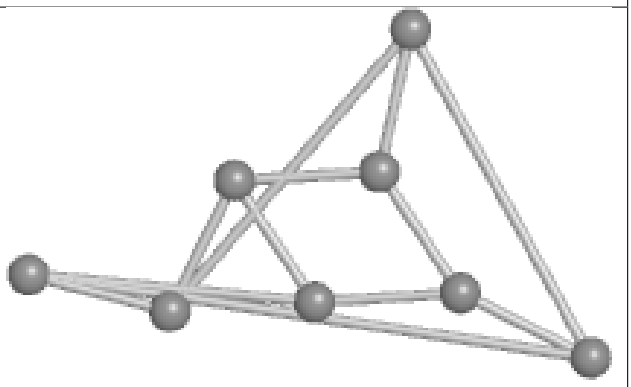


Rings

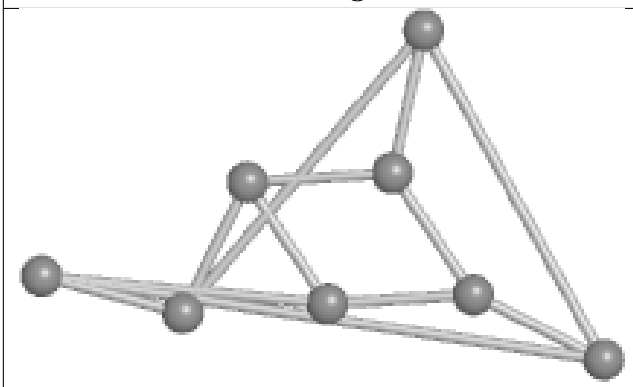
Ligand SF4 M 802



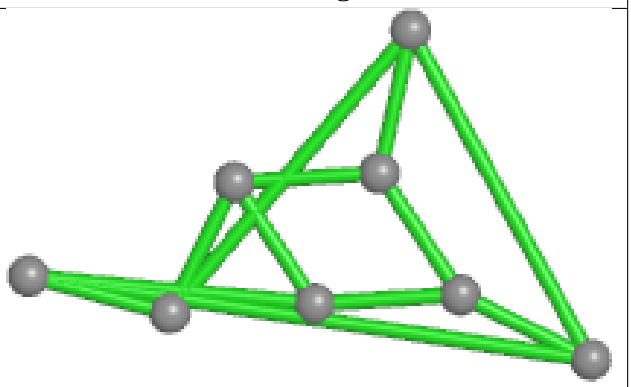
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

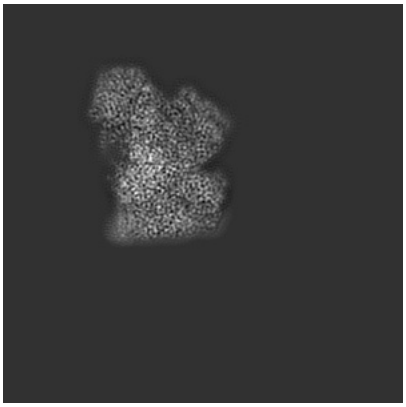
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32186. These allow visual inspection of the internal detail of the map and identification of artifacts.

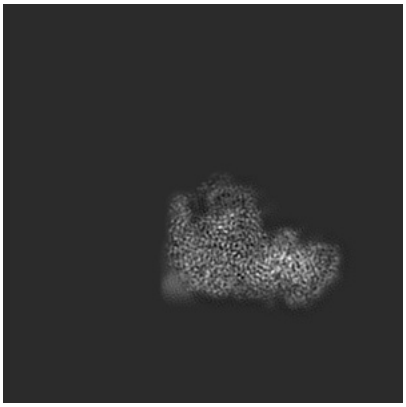
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

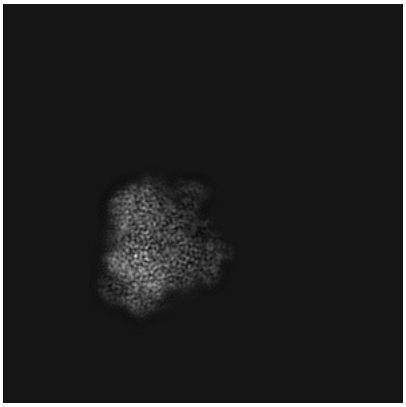
6.1.1 Primary map



X



Y

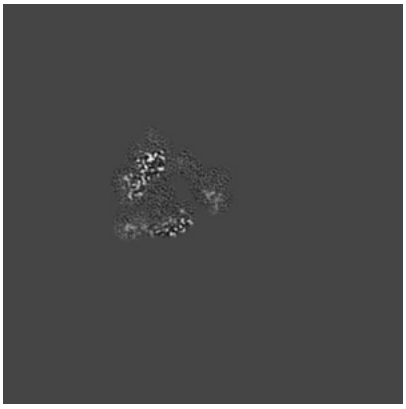


Z

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

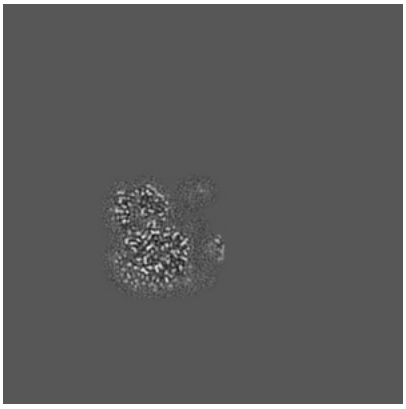
6.2 Central slices

6.2.1 Primary map



X Index: 165

Y Index: 165

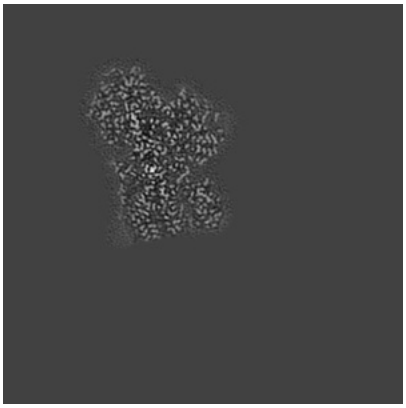


Z Index: 165

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

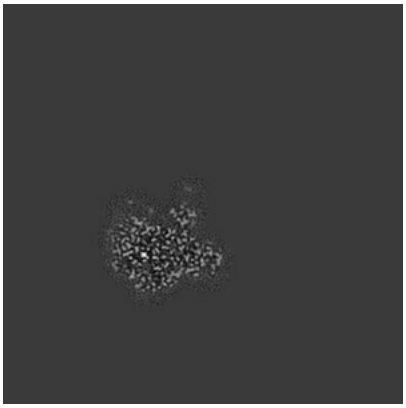
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 116

Y Index: 118

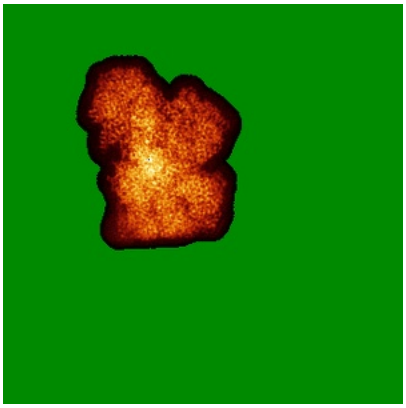


Z Index: 192

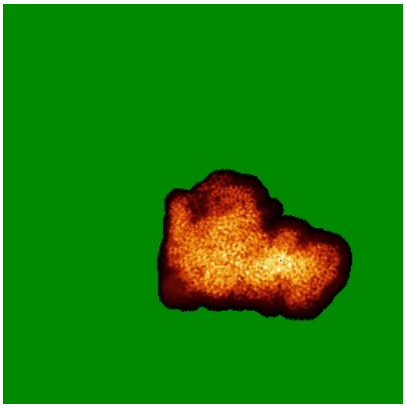
The images above show the largest variance slices of the map in three orthogonal directions.

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

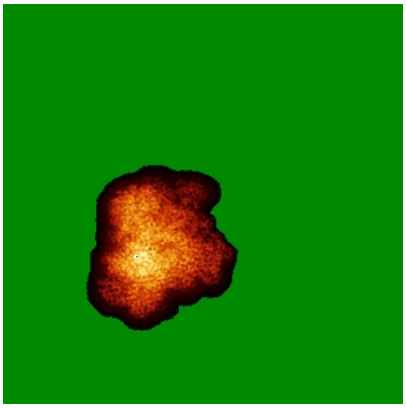
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0248. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

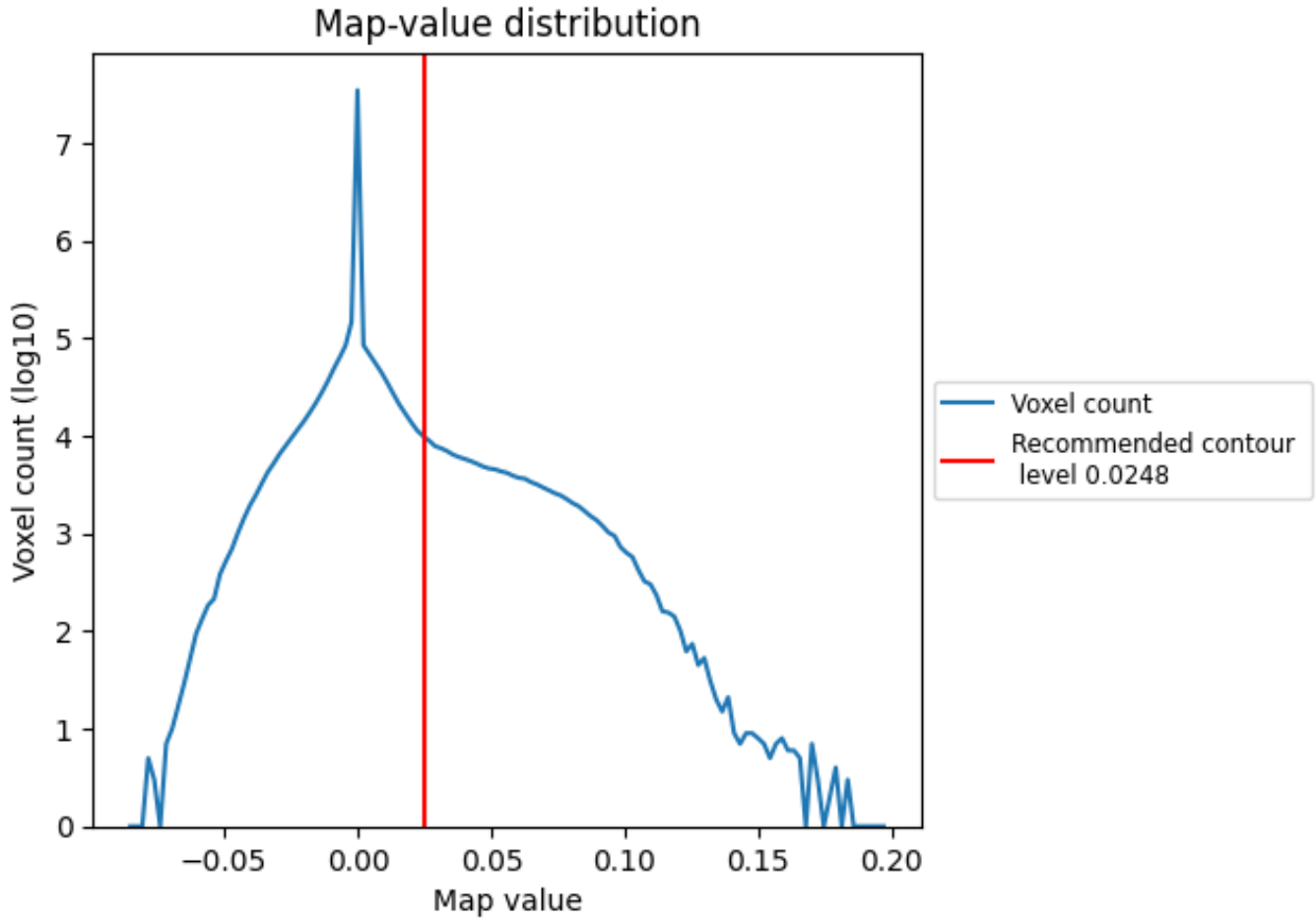
6.6 Mask visualisation (i)

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

7 Map analysis

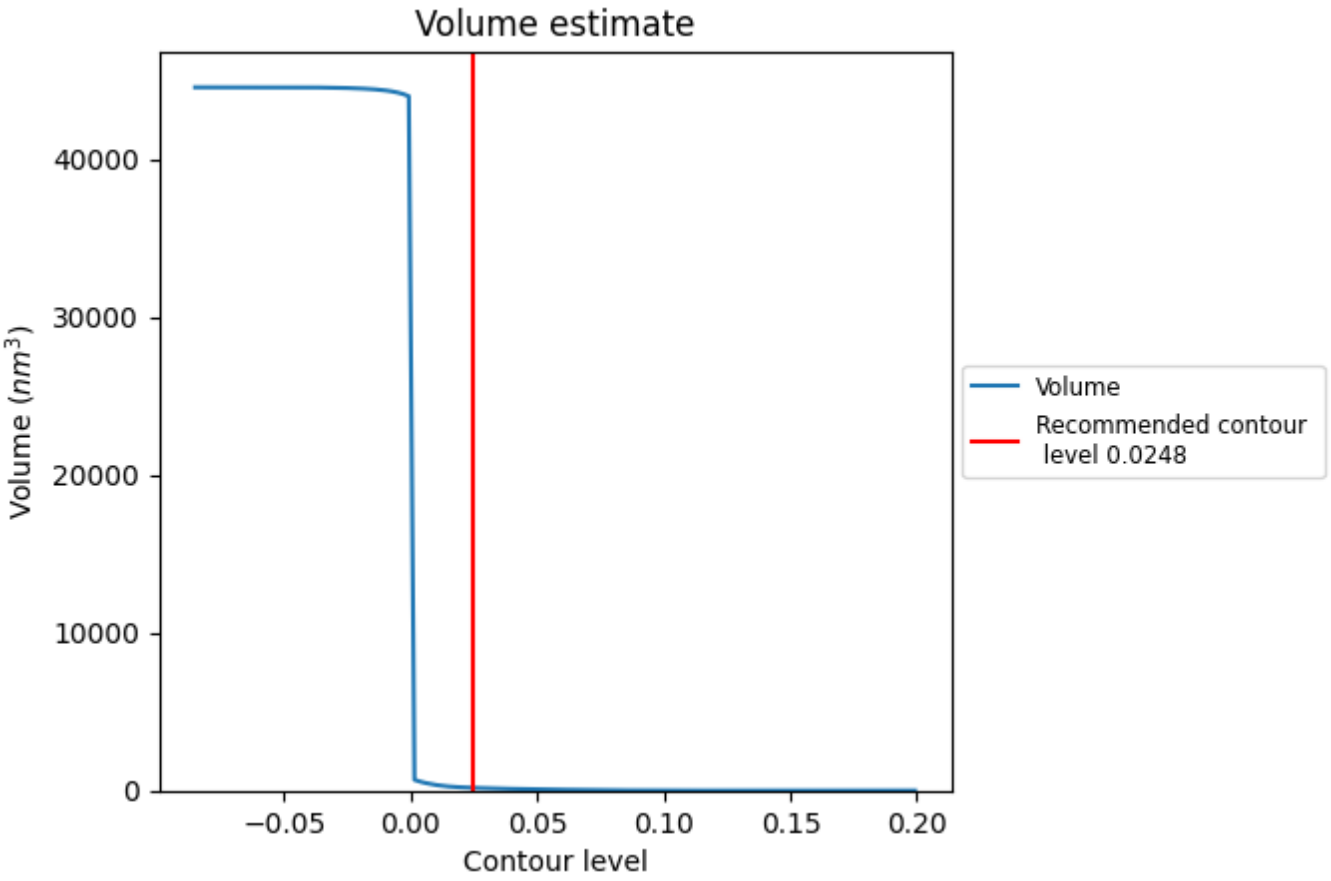
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

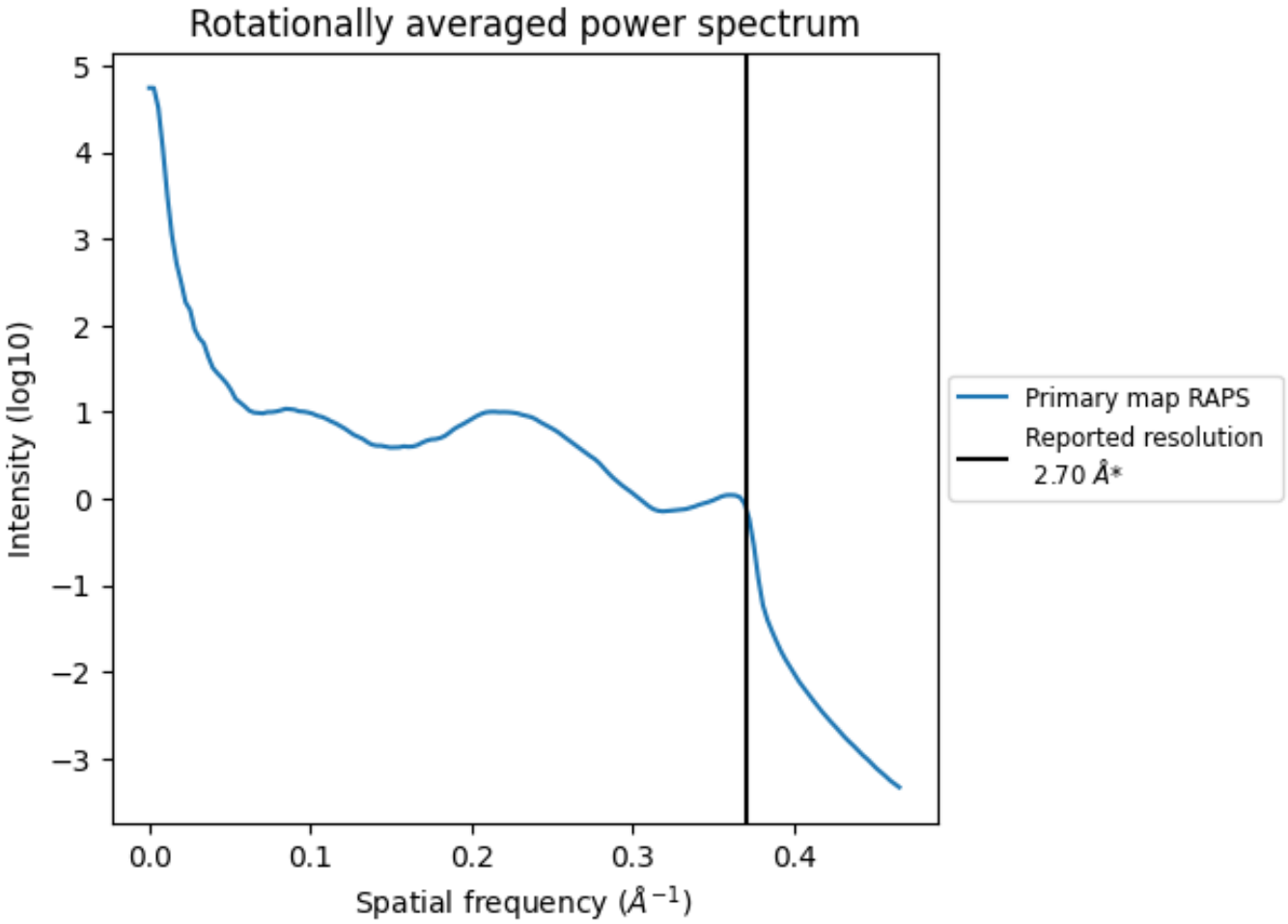
7.2 Volume estimate



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

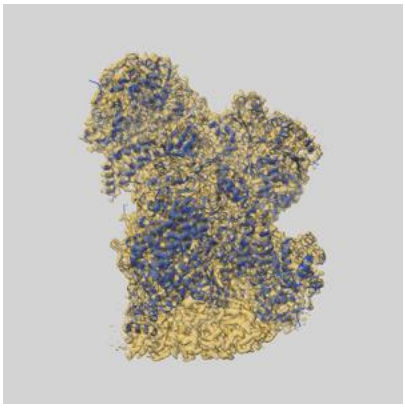
8 Fourier-Shell correlation (i)

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

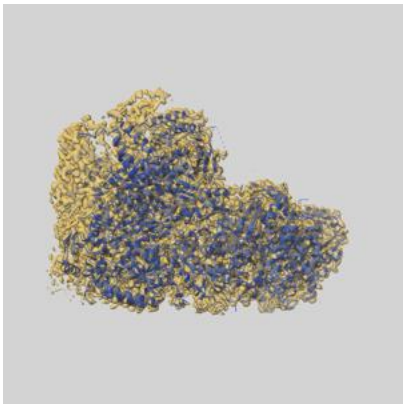
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32186 and PDB model 7VXP. Per-residue inclusion information can be found in section 3 on page 13.

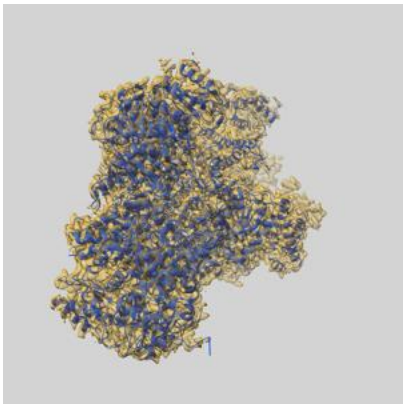
9.1 Map-model overlay



X



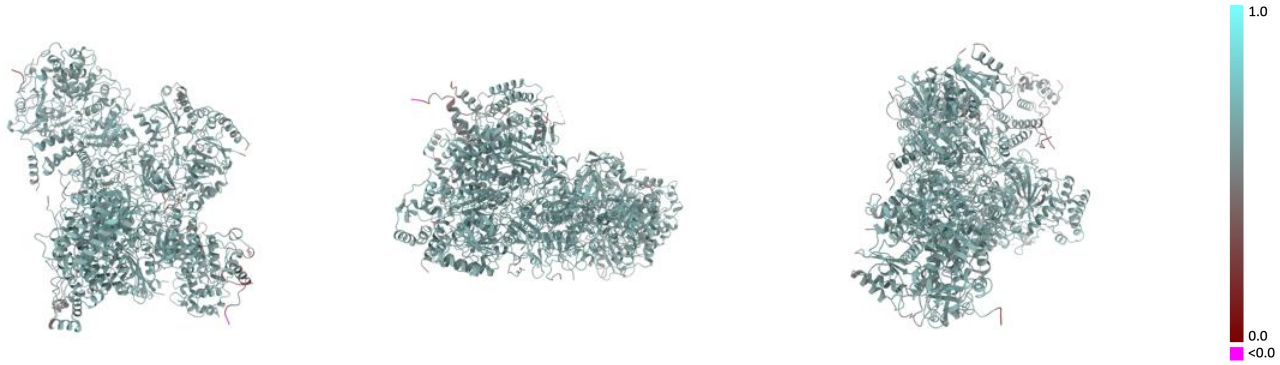
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

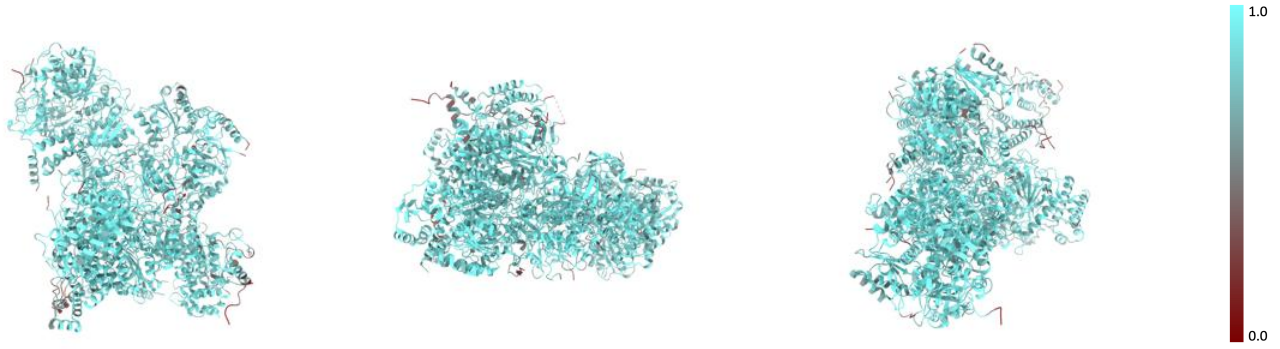
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

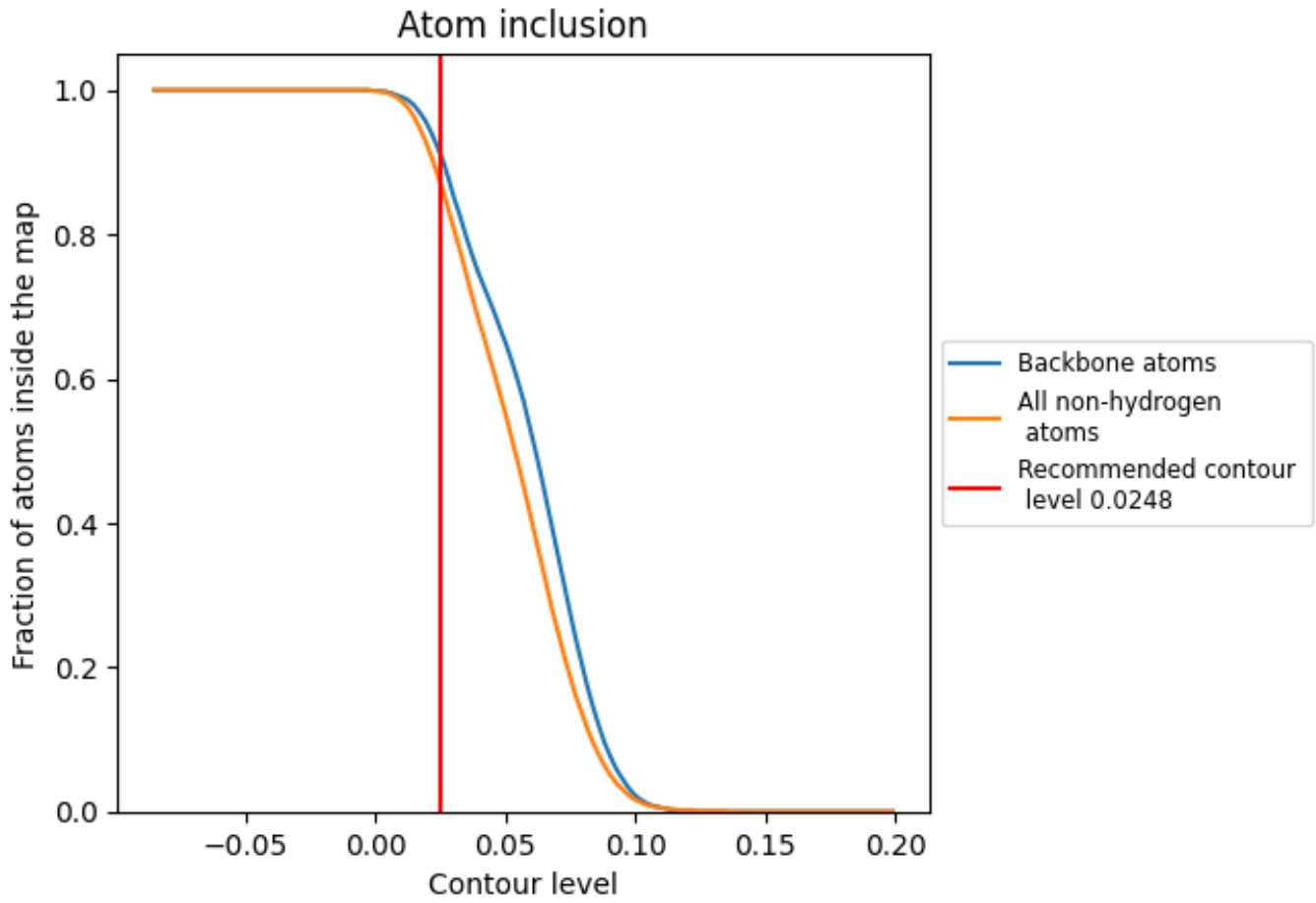
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0248).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.6150
A	0.8810	0.6100
B	0.9280	0.6370
C	0.9130	0.6390
E	0.8580	0.6150
F	0.8080	0.5850
G	0.6560	0.5110
H	0.8560	0.6050
I	0.7510	0.5760
J	0.8860	0.6190
K	0.8390	0.5980
L	0.8810	0.6200
M	0.8970	0.6210
N	0.7470	0.5870
O	0.8580	0.6000
P	0.9240	0.6430
Q	0.9200	0.6340
T	0.8240	0.6150
W	0.7980	0.5760