Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 11:06 PM JST

PDB ID	:	7VBN
EMDB ID	:	EMD-31883
Title	:	Matrix arm of deactive state CI from DQ-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-08-31
Resolution	:	2.40 Å(reported)

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

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

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

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

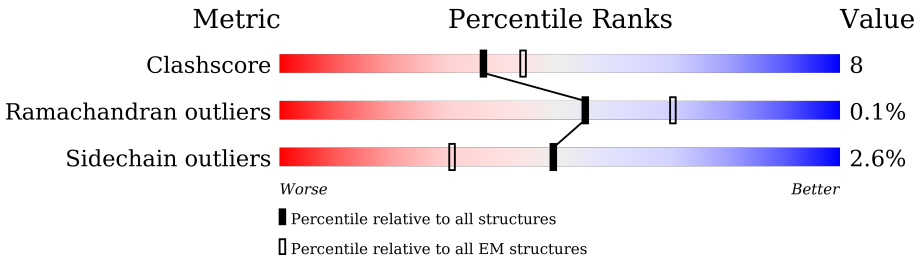
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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	431	5% 77% 21%
2	B	176	81% 19%
3	C	156	80% 17%
4	E	115	82% 18%
5	F	86	8% 83% 17%
6	G	88	55% 70% 30%
7	H	112	86% 14%
8	I	112	21% 71% 14% 13%

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Mol	Chain	Length	Quality of chain
9	J	341	7% 72% 23%
10	K	42	24% 67% 29% 5%
11	L	125	6% 82% 18%
12	M	690	82% 17%
13	N	144	18% 81% 19%
14	O	217	13% 86% 13%
15	P	208	85% 15%
16	Q	385	77% 22%
17	T	96	15% 91% 7%
18	W	29	24% 83% 14%

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	-
19	SF4	C	301	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 29042 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	431	3318	2095	591	612	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	691	434	129	126	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
			693	447	102	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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	331	Total	C	N	O	S	0	0
			2651	1719	466	458	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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	379	Total	C	N	O	S	0	0
			3044	1945	522	554	23		

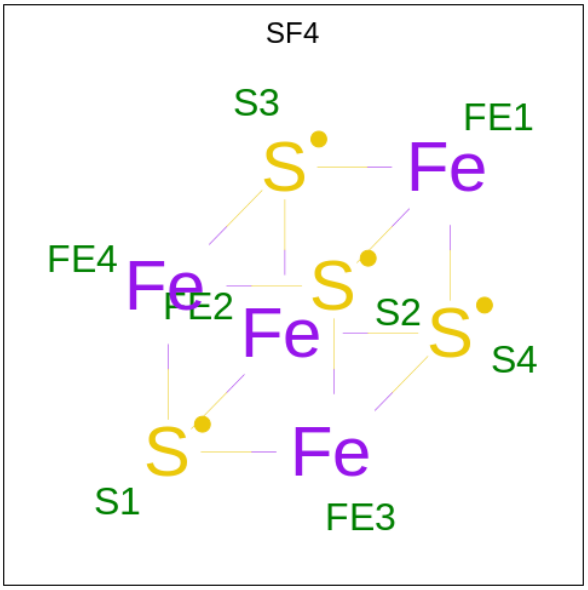
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

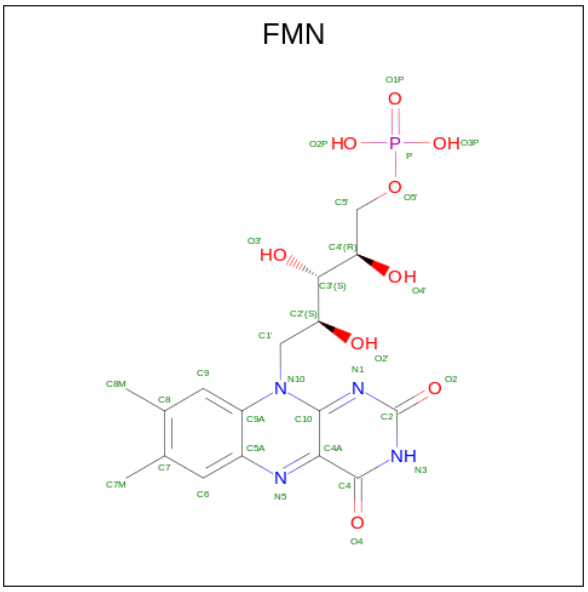
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	29	Total	C	N	O	S	0	0
			224	141	43	39	1		

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



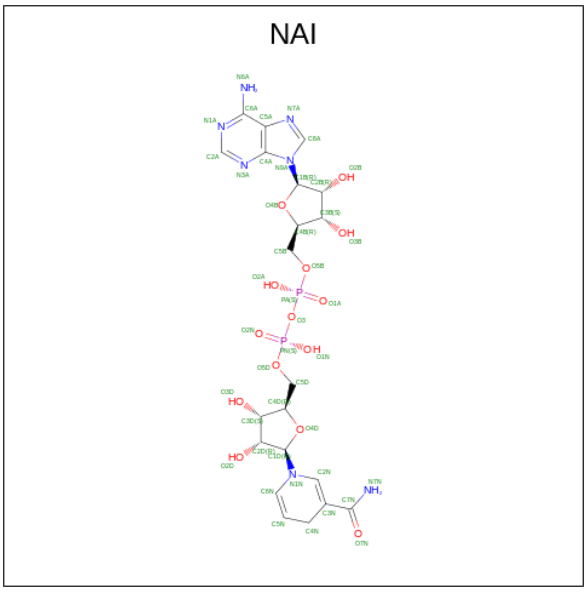
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	Fe	S		0
			8	4	4		
19	B	1	Total	Fe	S		0
			16	8	8		
19	B	1	Total	Fe	S		0
			16	8	8		
19	C	1	Total	Fe	S		0
			8	4	4		
19	M	1	Total	Fe	S		0
			16	8	8		
19	M	1	Total	Fe	S		0
			16	8	8		

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



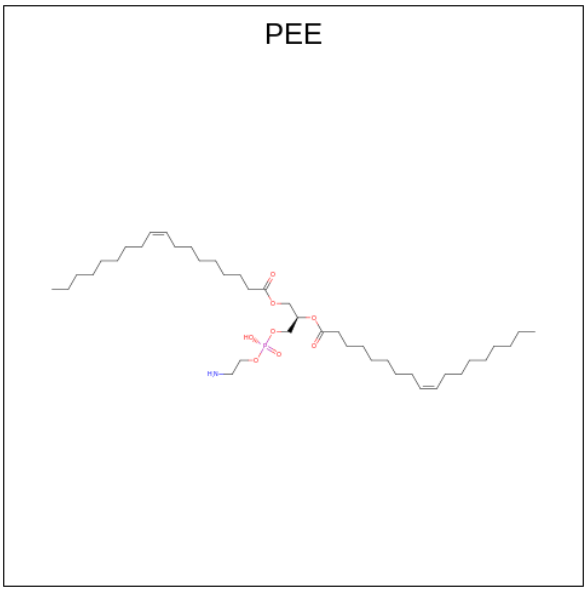
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 21 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



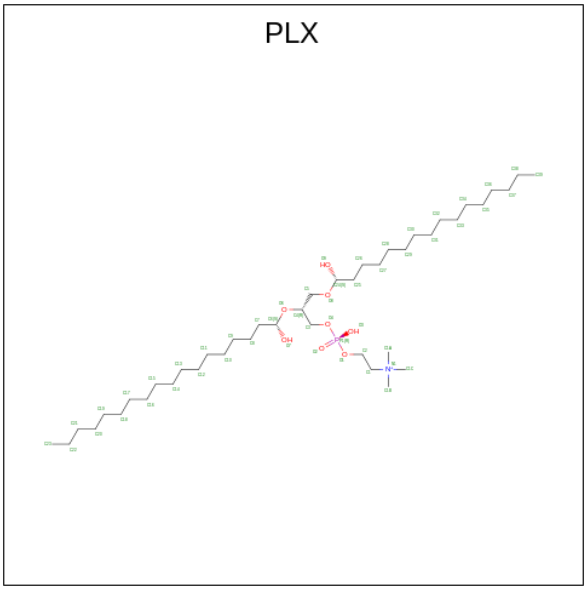
Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 22 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).



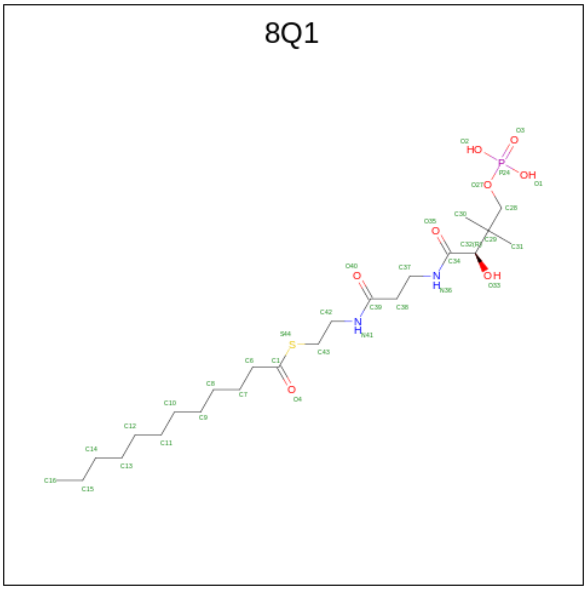
Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 23 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: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



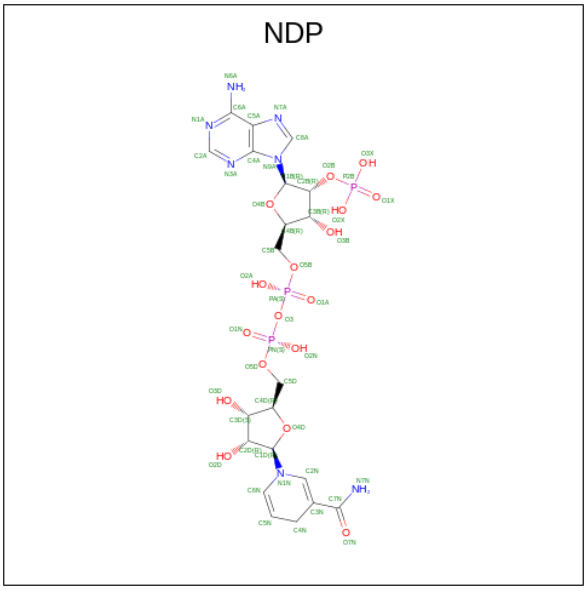
Mol	Chain	Residues	Atoms					AltConf
23	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 24 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).



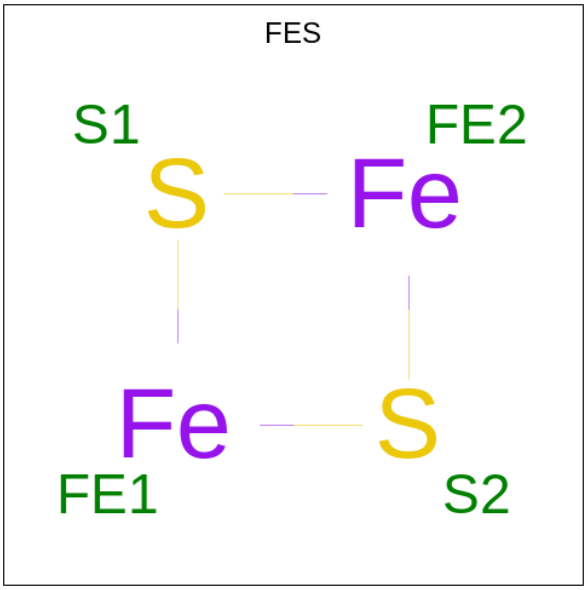
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
24	G	1	35	23	2	8	1	1	0

- Molecule 25 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
25	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

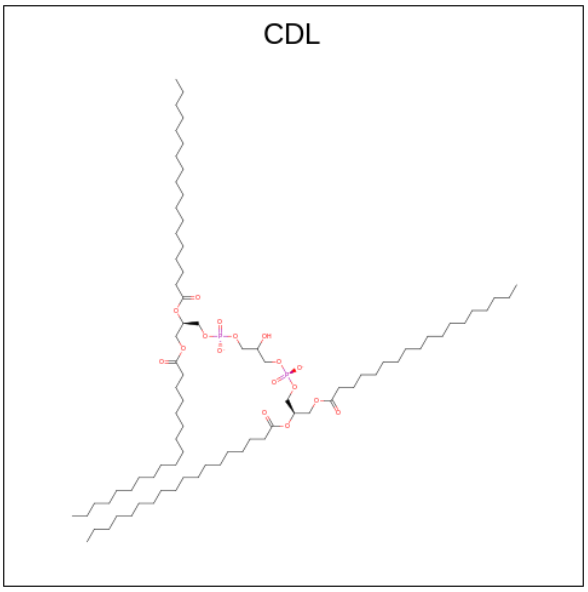


Mol	Chain	Residues	Atoms			AltConf
26	M	1	Total	Fe	S	0
			4	2	2	
26	O	1	Total	Fe	S	0
			4	2	2	

- 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	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	50	Total	O	0
			50	50	
30	B	77	Total	O	0
			77	77	
30	C	55	Total	O	0
			55	55	
30	E	2	Total	O	0
			2	2	
30	F	1	Total	O	0
			1	1	
30	H	4	Total	O	0
			4	4	
30	I	10	Total	O	0
			10	10	

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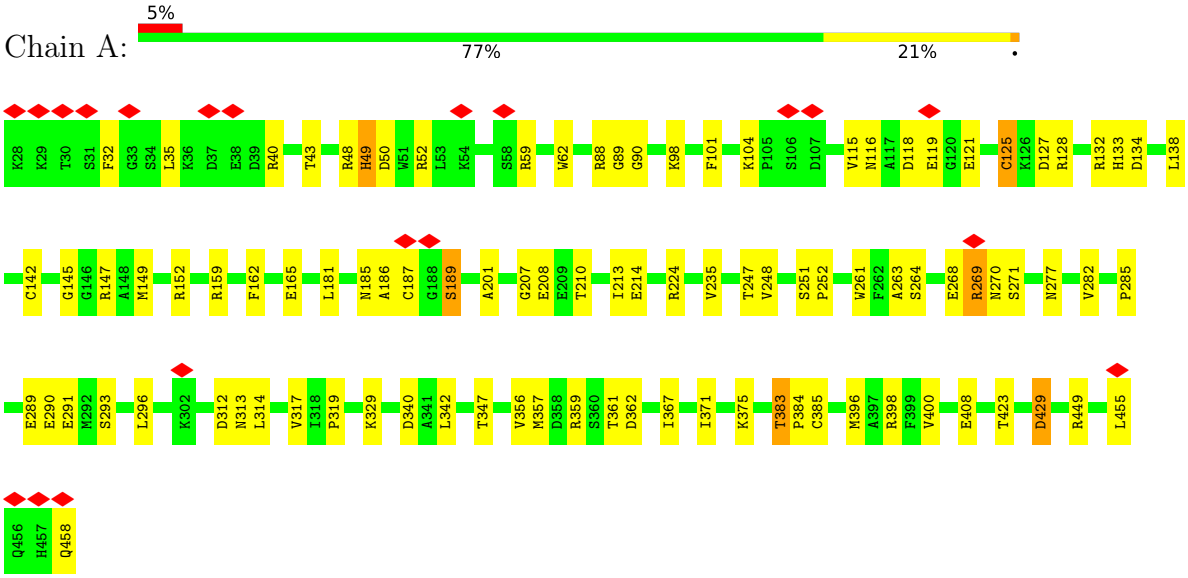
Mol	Chain	Residues	Atoms	AltConf
30	J	7	Total O 7 7	0
30	K	4	Total O 4 4	0
30	L	21	Total O 21 21	0
30	M	193	Total O 193 193	0
30	N	6	Total O 6 6	0
30	O	15	Total O 15 15	0
30	P	75	Total O 75 75	0
30	Q	181	Total O 181 181	0
30	T	10	Total O 10 10	0
30	W	2	Total O 2 2	0

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.

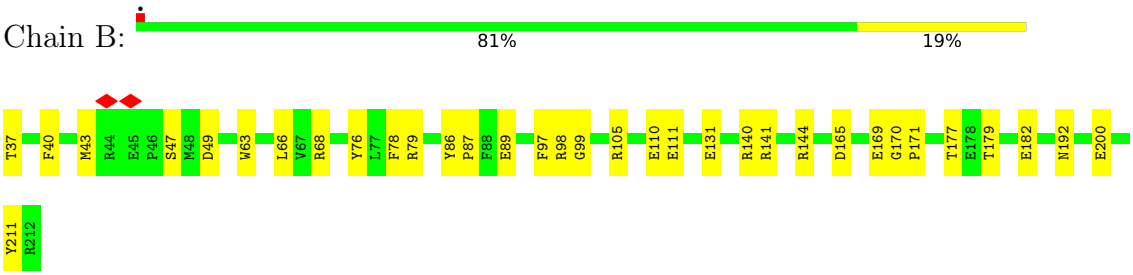
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A:



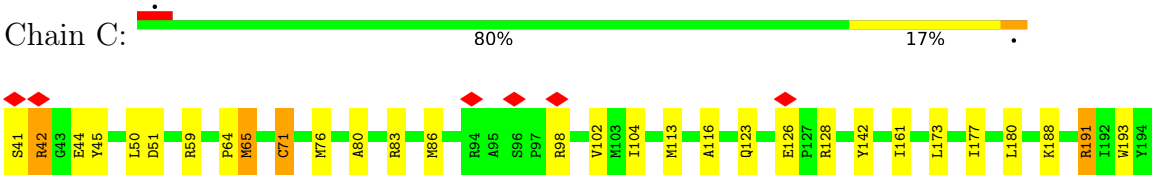
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B:



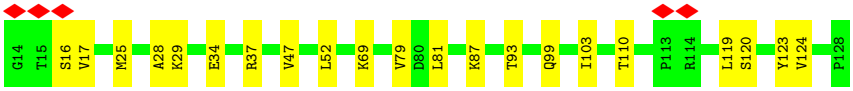
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:



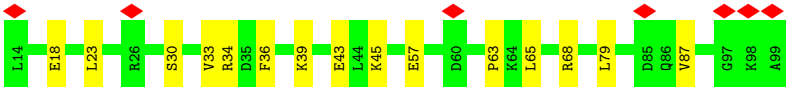
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



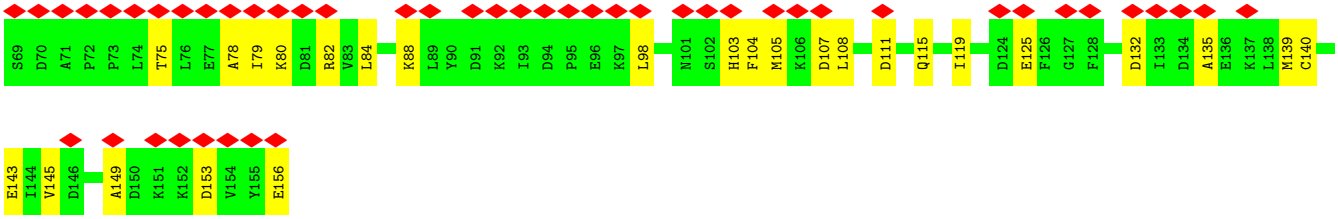
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



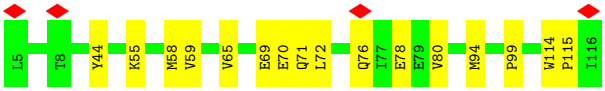
• Molecule 6: Acyl carrier protein, mitochondrial

Chain G:



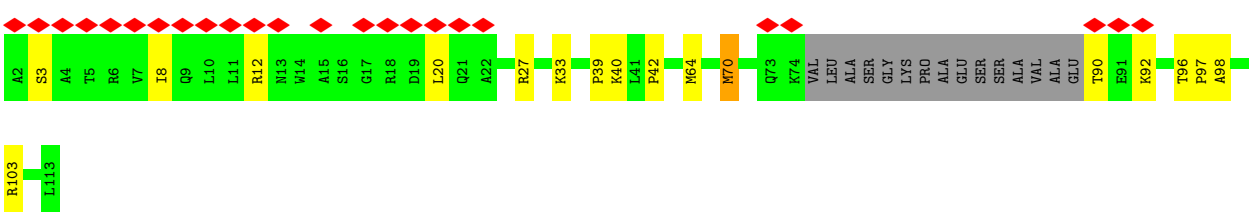
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain H:

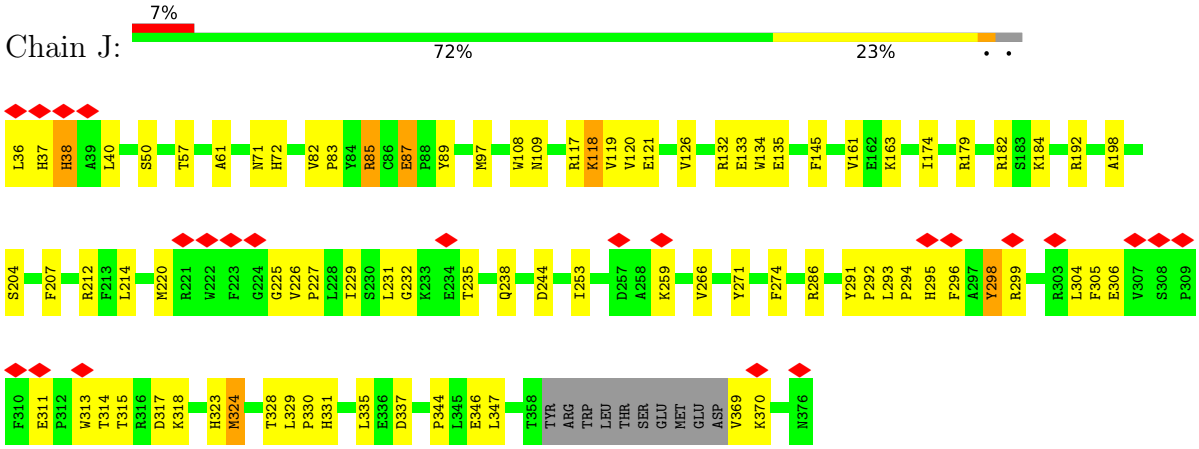


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

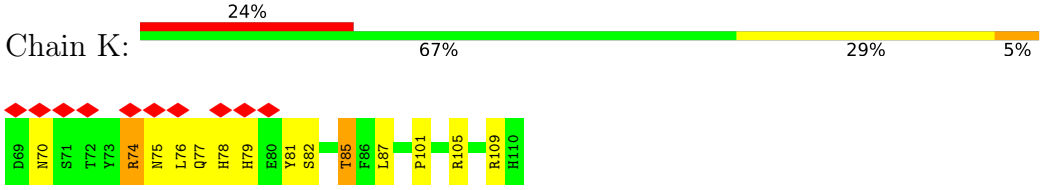
Chain I:



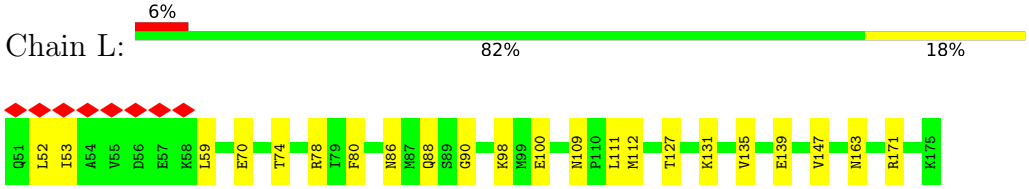
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



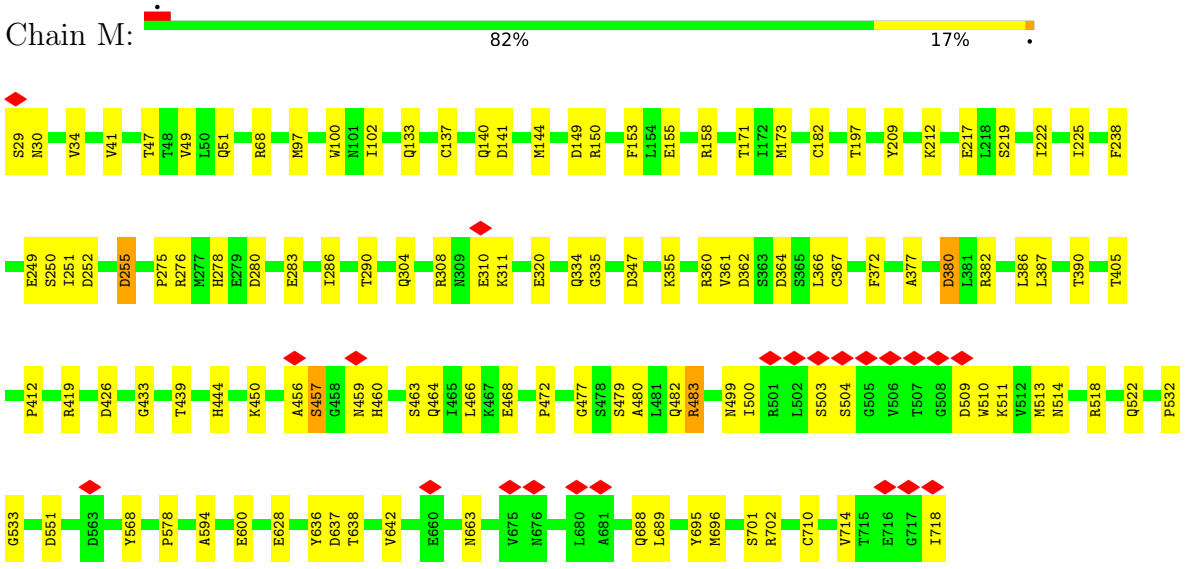
• Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



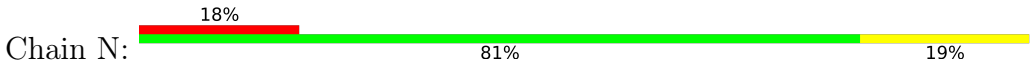
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

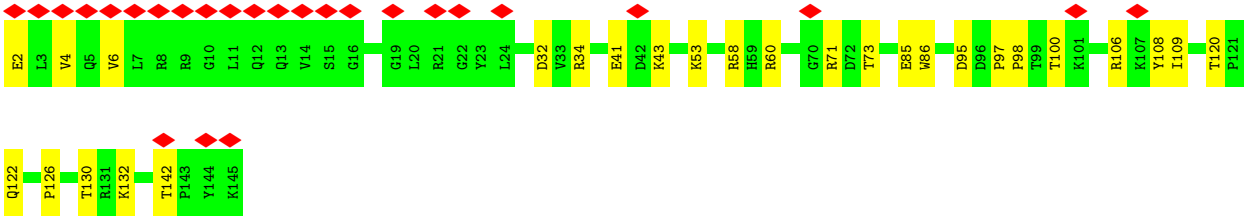


• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

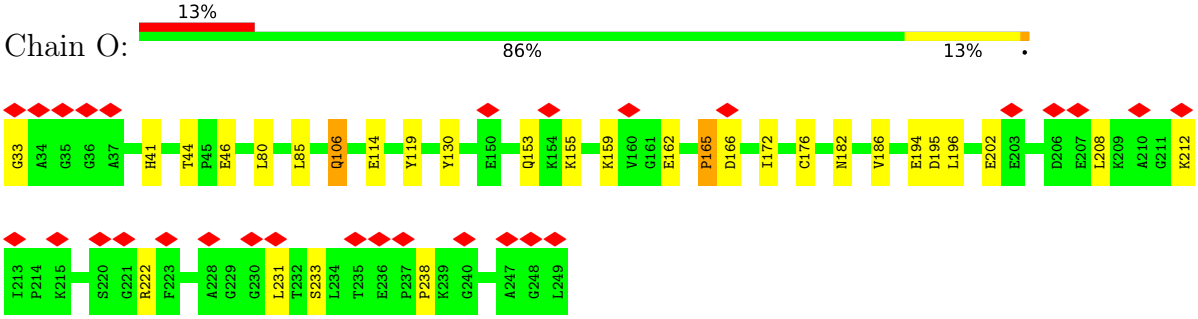


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

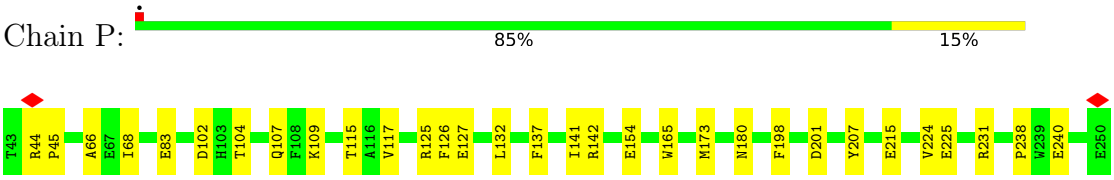




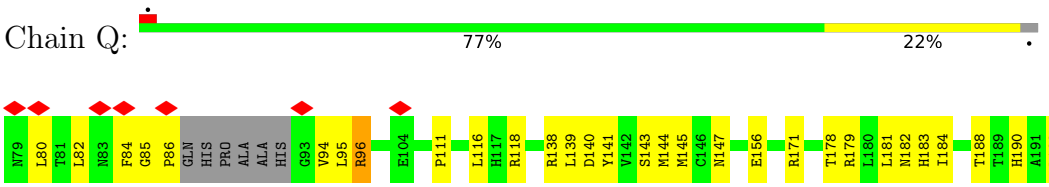
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



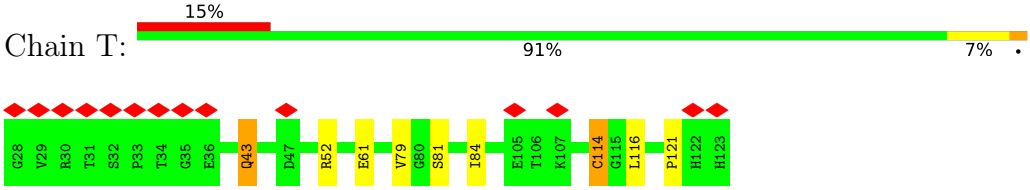
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



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

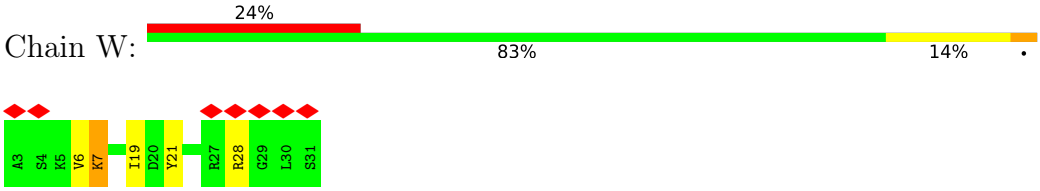


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• 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	387112	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	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	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: 2MR, NAI, 8Q1, NDP, FMN, FES, PEE, MG, SF4, ZN, CDL, PLX

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	0/3393	0.49	0/4584
2	B	0.26	0/1443	0.50	0/1952
3	C	0.26	0/1279	0.54	0/1730
4	E	0.25	0/995	0.52	0/1340
5	F	0.27	0/702	0.54	0/945
6	G	0.26	0/705	0.49	0/956
7	H	0.24	0/929	0.43	0/1258
8	I	0.25	0/798	0.55	0/1079
9	J	0.25	0/2724	0.49	0/3691
10	K	0.24	0/365	0.48	0/493
11	L	0.25	0/1039	0.51	0/1403
12	M	0.25	0/5384	0.50	0/7295
13	N	0.25	0/1245	0.51	0/1694
14	O	0.30	1/1711 (0.1%)	0.55	3/2328 (0.1%)
15	P	0.27	0/1789	0.52	0/2436
16	Q	0.27	0/3101	0.52	0/4189
17	T	0.25	0/755	0.52	0/1018
18	W	0.27	0/230	0.52	0/309
All	All	0.26	1/28587 (0.0%)	0.51	3/38700 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	165	PRO	CG-CD	-5.46	1.32	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	165	PRO	N-CD-CG	-9.27	89.30	103.20
14	O	165	PRO	CA-CB-CG	-7.11	90.50	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	165	PRO	N-CA-CB	-5.58	96.46	102.60

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	3318	0	3280	63	0
2	B	1412	0	1363	25	0
3	C	1248	0	1254	32	0
4	E	971	0	975	12	0
5	F	691	0	704	11	0
6	G	693	0	671	16	0
7	H	910	0	950	9	0
8	I	780	0	808	14	0
9	J	2651	0	2681	78	0
10	K	355	0	329	10	0
11	L	1016	0	1016	15	0
12	M	5296	0	5326	74	0
13	N	1204	0	1162	19	0
14	O	1671	0	1673	22	0
15	P	1738	0	1693	23	0
16	Q	3044	0	3018	81	0
17	T	741	0	702	6	0
18	W	224	0	230	5	0
19	A	8	0	0	2	0
19	B	16	0	0	0	0
19	C	8	0	0	2	0
19	M	16	0	0	0	0
20	A	31	0	19	2	0
21	A	44	0	27	5	0
22	C	47	0	71	20	0
23	C	52	0	88	10	0
24	G	35	0	0	0	0
25	J	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
29	T	1	0	0	0	0
30	A	50	0	0	0	0
30	B	77	0	0	1	0
30	C	55	0	0	3	0
30	E	2	0	0	1	0
30	F	1	0	0	0	0
30	H	4	0	0	0	0
30	I	10	0	0	0	0
30	J	7	0	0	1	0
30	K	4	0	0	0	0
30	L	21	0	0	0	0
30	M	193	0	0	3	0
30	N	6	0	0	0	0
30	O	15	0	0	0	0
30	P	75	0	0	3	0
30	Q	181	0	0	10	0
30	T	10	0	0	0	0
30	W	2	0	0	0	0
All	All	29042	0	28112	472	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 8.

All (472) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LEU:CD1	22:C:302:PEE:H25	1.19	1.57
3:C:50:LEU:HD13	22:C:302:PEE:C17	1.52	1.37
3:C:50:LEU:CD1	22:C:302:PEE:C17	1.99	1.36
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.21
3:C:50:LEU:HD11	22:C:302:PEE:H25	1.28	1.12
9:J:231:LEU:HD21	9:J:292:PRO:HD3	1.30	1.08
16:Q:404:LYS:HE2	16:Q:457:VAL:CG2	1.84	1.06
16:Q:404:LYS:HE2	16:Q:457:VAL:HG23	1.30	1.06
9:J:305:PHE:CE1	9:J:313:TRP:CE3	2.43	1.06
16:Q:141:TYR:O	16:Q:144:MET:SD	2.17	1.02
16:Q:404:LYS:CE	16:Q:457:VAL:HG23	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:305:PHE:CD1	9:J:313:TRP:HE3	1.86	0.94
3:C:50:LEU:HD13	22:C:302:PEE:H25	0.91	0.91
9:J:305:PHE:CE1	9:J:313:TRP:HE3	1.85	0.91
19:C:301:SF4:S4	16:Q:223:HIS:CD2	2.65	0.90
22:C:302:PEE:H58	22:C:302:PEE:H27	1.51	0.89
3:C:50:LEU:HD12	22:C:302:PEE:C17	2.03	0.89
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.56	0.88
9:J:133:GLU:OE2	9:J:212:ARG:HD2	1.75	0.87
3:C:42:ARG:HB3	3:C:42:ARG:HH11	1.40	0.86
3:C:188:LYS:N	9:J:87:GLU:OE2	2.09	0.84
3:C:42:ARG:HB3	3:C:42:ARG:NH1	1.92	0.84
9:J:305:PHE:CD1	9:J:313:TRP:CE3	2.64	0.84
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.60	0.84
9:J:231:LEU:CD2	9:J:292:PRO:HD3	2.09	0.82
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.16	0.81
3:C:50:LEU:CD1	22:C:302:PEE:H26	2.10	0.80
9:J:231:LEU:HG	9:J:292:PRO:HB3	1.63	0.80
16:Q:281:GLU:OE2	30:Q:501:HOH:O	2.00	0.79
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.66	0.77
16:Q:145:MET:CG	16:Q:214:TYR:OH	2.34	0.76
16:Q:139:LEU:CD1	16:Q:424:ILE:HD13	2.16	0.75
11:L:59:LEU:HD21	30:P:309:HOH:O	1.86	0.75
22:C:302:PEE:H27	22:C:302:PEE:C36	2.17	0.74
22:C:302:PEE:H49	30:C:455:HOH:O	1.87	0.74
9:J:293:LEU:HD12	9:J:294:PRO:HD2	1.69	0.73
9:J:305:PHE:HE1	9:J:313:TRP:CE3	2.05	0.73
1:A:89:GLY:O	21:A:503:NAI:H2N	1.87	0.73
9:J:305:PHE:CE1	9:J:313:TRP:CZ3	2.77	0.73
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.22	0.73
9:J:305:PHE:HE1	9:J:313:TRP:CZ3	2.07	0.73
3:C:50:LEU:HD13	22:C:302:PEE:H26	1.65	0.72
16:Q:145:MET:HG2	16:Q:214:TYR:OH	1.89	0.72
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.23	0.72
16:Q:426:ALA:O	30:Q:502:HOH:O	2.07	0.71
16:Q:145:MET:HB2	16:Q:178:THR:OG1	1.90	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.70
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.25	0.70
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.25	0.70
11:L:109:ASN:ND2	11:L:111:LEU:O	2.23	0.69
3:C:126:GLU:O	9:J:89:TYR:OH	2.11	0.69
12:M:460:HIS:O	12:M:463:SER:OG	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:40:LYS:HB3	18:W:7:LYS:H	1.58	0.69
9:J:295:HIS:O	9:J:299:ARG:HG3	1.92	0.69
9:J:192:ARG:NH1	9:J:198:ALA:O	2.25	0.68
3:C:59:ARG:NH1	23:C:303:PLX:O3	2.26	0.68
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.75	0.68
1:A:383:THR:HG23	1:A:384:PRO:HD3	1.75	0.67
16:Q:402:ALA:O	30:Q:503:HOH:O	2.10	0.67
22:C:302:PEE:H75	23:C:303:PLX:H172	1.76	0.67
9:J:134:TRP:CH2	9:J:311:GLU:HG3	2.29	0.67
3:C:42:ARG:HH11	3:C:42:ARG:CB	2.07	0.66
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.29	0.66
1:A:88:ARG:HB2	1:A:247:THR:OG1	1.96	0.66
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.76	0.66
2:B:177:THR:HG22	2:B:179:THR:H	1.61	0.66
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.78	0.66
9:J:304:LEU:HD13	9:J:304:LEU:O	1.95	0.66
9:J:305:PHE:CD2	9:J:314:THR:HG22	2.32	0.65
16:Q:145:MET:HG2	16:Q:214:TYR:CZ	2.31	0.65
9:J:231:LEU:HD21	9:J:292:PRO:CD	2.17	0.65
9:J:293:LEU:HD12	9:J:294:PRO:CD	2.26	0.65
9:J:304:LEU:HD13	9:J:304:LEU:C	2.17	0.65
15:P:102:ASP:OD2	30:P:301:HOH:O	2.14	0.65
9:J:244:ASP:HB3	9:J:335:LEU:HD21	1.77	0.65
10:K:81:TYR:HB3	10:K:85:THR:HG21	1.77	0.65
9:J:71:ASN:ND2	30:J:501:HOH:O	2.30	0.64
13:N:120:THR:HG22	13:N:122:GLN:H	1.62	0.64
1:A:40:ARG:NH1	1:A:289:GLU:O	2.30	0.64
15:P:104:THR:O	15:P:107:GLN:NE2	2.30	0.64
12:M:419:ARG:NH1	12:M:439:THR:O	2.30	0.64
28:N:201:CDL:C53	28:N:201:CDL:H742	2.27	0.64
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.80	0.63
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.80	0.63
9:J:232:GLY:O	9:J:274:PHE:N	2.31	0.63
16:Q:147:ASN:ND2	30:Q:508:HOH:O	2.28	0.63
9:J:229:ILE:HB	9:J:323:HIS:CD2	2.33	0.63
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.32	0.63
1:A:375:LYS:NZ	14:O:33:GLY:O	2.32	0.62
1:A:455:LEU:O	1:A:458:GLN:NE2	2.32	0.62
22:C:302:PEE:C44	23:C:303:PLX:H172	2.29	0.62
1:A:159:ARG:NH2	14:O:176:CYS:O	2.28	0.62
1:A:357:MET:HB3	1:A:361:THR:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:149:ALA:O	6:G:153:ASP:N	2.32	0.62
28:N:201:CDL:H742	28:N:201:CDL:H531	1.83	0.61
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.81	0.61
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.81	0.61
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.33	0.61
9:J:50:SER:OG	15:P:225:GLU:OE2	2.16	0.61
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.83	0.61
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.83	0.61
20:A:502:FMN:N5	21:A:503:NAI:H4N	2.15	0.60
16:Q:144:MET:HG2	16:Q:222:MET:O	2.01	0.60
16:Q:404:LYS:HE2	16:Q:457:VAL:HG21	1.82	0.60
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.83	0.60
3:C:65:MET:O	30:C:401:HOH:O	2.17	0.60
1:A:214:GLU:OE1	1:A:224:ARG:NH2	2.28	0.59
8:I:98:ALA:HB3	15:P:137:PHE:O	2.01	0.59
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.84	0.59
9:J:133:GLU:OE2	9:J:212:ARG:CD	2.48	0.59
9:J:225:GLY:O	9:J:291:TYR:HE1	1.86	0.59
4:E:120:SER:O	4:E:124:VAL:HG13	2.03	0.59
12:M:695:TYR:O	12:M:701:SER:OG	2.19	0.59
15:P:107:GLN:HB2	15:P:109:LYS:HE2	1.84	0.59
16:Q:145:MET:CG	16:Q:214:TYR:CZ	2.86	0.59
6:G:104:PHE:HA	6:G:108:LEU:HD12	1.85	0.58
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.85	0.58
9:J:38:HIS:CE1	13:N:132:LYS:HE3	2.38	0.58
6:G:75:THR:HG23	6:G:78:ALA:H	1.69	0.58
3:C:50:LEU:HD13	22:C:302:PEE:C18	2.32	0.58
9:J:37:HIS:HB3	9:J:40:LEU:HD12	1.84	0.58
4:E:25:MET:O	4:E:29:LYS:HG3	2.03	0.58
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.86	0.58
16:Q:192:LEU:O	16:Q:192:LEU:HD23	2.04	0.58
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.36	0.57
7:H:55:LYS:O	7:H:59:VAL:HG13	2.03	0.57
15:P:142:ARG:NH1	30:P:305:HOH:O	2.34	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.86	0.57
1:A:319:PRO:HG2	1:A:347:THR:HG21	1.87	0.57
11:L:98:LYS:NZ	11:L:127:THR:OG1	2.34	0.57
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.85	0.57
8:I:3:SER:O	28:N:201:CDL:HA22	2.05	0.57
16:Q:404:LYS:CE	16:Q:457:VAL:CG2	2.64	0.57
1:A:210:THR:HB	1:A:224:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.37	0.57
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.37	0.56
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.86	0.56
1:A:50:ASP:O	1:A:59:ARG:NH2	2.38	0.56
9:J:293:LEU:CD1	9:J:294:PRO:HD2	2.34	0.56
16:Q:190:HIS:O	16:Q:194:ILE:HG12	2.05	0.56
8:I:8:ILE:HD11	28:N:201:CDL:H142	1.88	0.55
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.06	0.55
1:A:90:GLY:HA3	21:A:503:NAI:H1D	1.89	0.55
9:J:204:SER:OG	9:J:238:GLN:O	2.25	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.88	0.55
3:C:191:ARG:HG2	3:C:191:ARG:HH11	1.72	0.55
1:A:313:ASN:HA	1:A:359:ARG:NH1	2.22	0.55
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.42	0.55
12:M:310:GLU:H	12:M:310:GLU:CD	2.10	0.55
16:Q:182:ASN:HD21	16:Q:404:LYS:NZ	2.04	0.55
1:A:145:GLY:O	1:A:149:MET:HG3	2.07	0.55
4:E:69:LYS:HB2	4:E:69:LYS:NZ	2.21	0.55
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.55
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.47	0.55
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.31	0.55
10:K:109:ARG:NH2	14:O:106:GLN:O	2.40	0.54
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.90	0.54
9:J:132:ARG:NH2	25:J:401:NDP:O2X	2.40	0.54
12:M:372:PHE:H	12:M:532:PRO:HB2	1.72	0.54
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.36	0.54
16:Q:222:MET:CE	30:Q:641:HOH:O	2.55	0.54
12:M:29:SER:HG	12:M:30:ASN:H	1.54	0.54
14:O:195:ASP:OD2	14:O:222:ARG:HD3	2.08	0.54
9:J:207:PHE:HB2	9:J:214:LEU:HD13	1.90	0.54
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.89	0.54
16:Q:139:LEU:HD11	16:Q:424:ILE:CD1	2.36	0.54
9:J:329:LEU:HD12	9:J:331:HIS:HE1	1.72	0.53
9:J:231:LEU:HG	9:J:292:PRO:CB	2.36	0.53
12:M:308:ARG:NH2	12:M:578:PRO:O	2.41	0.53
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.90	0.53
16:Q:198:THR:CG2	16:Q:202:TRP:CE2	2.91	0.53
9:J:305:PHE:CD2	9:J:314:THR:CG2	2.91	0.53
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.43	0.53
11:L:135:VAL:O	11:L:139:GLU:HG3	2.09	0.53
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:112:MET:SD	13:N:126:PRO:HB2	2.50	0.52
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.28	0.52
12:M:638:THR:O	12:M:642:VAL:HG23	2.10	0.52
6:G:84:LEU:O	6:G:88:LYS:HG2	2.10	0.52
13:N:6:VAL:HB	28:N:201:CDL:OB7	2.10	0.52
2:B:97:PHE:HB2	16:Q:215:GLU:OE2	2.10	0.52
11:L:163:ASN:O	11:L:171:ARG:HA	2.10	0.52
12:M:249:GLU:HG2	12:M:276:ARG:CD	2.40	0.52
16:Q:140:ASP:OD2	16:Q:404:LYS:HD2	2.10	0.52
12:M:133:GLN:O	12:M:137:CYS:HB2	2.10	0.51
12:M:334:GLN:HA	12:M:361:VAL:HG13	1.92	0.51
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.93	0.51
2:B:40:PHE:HB3	2:B:43:MET:HB2	1.93	0.51
9:J:229:ILE:HD13	9:J:295:HIS:ND1	2.25	0.51
11:L:70:GLU:O	11:L:74:THR:OG1	2.25	0.51
12:M:511:LYS:HE3	12:M:663:ASN:HB2	1.92	0.51
16:Q:145:MET:HG3	16:Q:214:TYR:OH	2.11	0.51
3:C:104:ILE:N	30:C:401:HOH:O	2.43	0.51
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.93	0.51
12:M:278:HIS:HD2	12:M:280:ASP:H	1.58	0.51
16:Q:308:TYR:OH	30:Q:504:HOH:O	2.19	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.44	0.51
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.93	0.51
9:J:295:HIS:CD2	9:J:299:ARG:HD2	2.46	0.51
12:M:522:GLN:NE2	30:M:920:HOH:O	2.37	0.51
12:M:433:GLY:O	12:M:444:HIS:NE2	2.38	0.50
10:K:75:ASN:O	10:K:78:HIS:ND1	2.41	0.50
1:A:116:ASN:ND2	1:A:207:GLY:O	2.37	0.50
2:B:192:ASN:ND2	17:T:61:GLU:OE2	2.39	0.50
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.35	0.50
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.92	0.50
12:M:457:SER:OG	12:M:459:ASN:OD1	2.27	0.50
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.50
9:J:315:THR:H	9:J:318:LYS:HB3	1.77	0.50
12:M:252:ASP:OD2	12:M:290:THR:OG1	2.25	0.50
15:P:201:ASP:OD1	15:P:201:ASP:N	2.41	0.50
16:Q:192:LEU:HD23	16:Q:192:LEU:C	2.31	0.50
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.47	0.50
2:B:47:SER:OG	2:B:49:ASP:OD1	2.25	0.49
6:G:79:ILE:HG22	6:G:145:VAL:HG22	1.94	0.49
9:J:117:ARG:O	9:J:121:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:335:GLY:HA2	12:M:362:ASP:O	2.11	0.49
16:Q:198:THR:HG21	16:Q:202:TRP:CZ2	2.46	0.49
17:T:79:VAL:HG21	17:T:84:ILE:HG21	1.95	0.49
5:F:33:VAL:O	5:F:36:PHE:HB3	2.12	0.49
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.35	0.49
16:Q:198:THR:CG2	16:Q:202:TRP:CZ2	2.96	0.49
16:Q:182:ASN:HD21	16:Q:404:LYS:HZ2	1.60	0.49
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	1.95	0.49
16:Q:182:ASN:ND2	16:Q:404:LYS:NZ	2.61	0.49
9:J:134:TRP:CZ3	9:J:311:GLU:HG3	2.47	0.48
17:T:52:ARG:HG2	17:T:52:ARG:HH11	1.78	0.48
16:Q:95:LEU:HB2	16:Q:458:PHE:HZ	1.72	0.48
2:B:110:GLU:OE1	30:B:401:HOH:O	2.19	0.48
3:C:50:LEU:HD12	22:C:302:PEE:H26	1.83	0.48
8:I:96:THR:HB	8:I:97:PRO:HD2	1.94	0.48
9:J:204:SER:OG	9:J:204:SER:O	2.31	0.48
16:Q:116:LEU:HD23	16:Q:459:GLY:HA2	1.95	0.48
9:J:344:PRO:HG2	9:J:347:LEU:HG	1.94	0.48
16:Q:194:ILE:HG22	16:Q:194:ILE:O	2.12	0.48
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.44	0.48
5:F:45:LYS:HE2	12:M:380:ASP:OD2	2.13	0.48
6:G:115:GLN:O	6:G:119:ILE:HG12	2.14	0.48
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.43	0.48
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.47	0.48
1:A:132:ARG:HG3	1:A:133:HIS:CD2	2.48	0.48
1:A:248:VAL:O	1:A:251:SER:OG	2.28	0.48
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.96	0.48
9:J:163:LYS:HG2	9:J:259:LYS:HZ3	1.79	0.48
9:J:294:PRO:HB3	9:J:296:PHE:CE1	2.48	0.48
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.44	0.48
6:G:80:LYS:HG2	6:G:145:VAL:HG21	1.95	0.48
12:M:464:GLN:O	12:M:468:GLU:HG3	2.13	0.48
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.44	0.47
19:C:301:SF4:S2	16:Q:138:ARG:HG2	2.54	0.47
4:E:28:ALA:HB1	4:E:79:VAL:HG11	1.96	0.47
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.97	0.47
12:M:450:LYS:NZ	12:M:450:LYS:HB3	2.29	0.47
1:A:187:CYS:HB2	1:A:189:SER:HB3	1.96	0.47
7:H:70:GLU:OE2	8:I:103:ARG:NH1	2.48	0.47
9:J:220:MET:SD	9:J:226:VAL:HG13	2.54	0.47
12:M:171:THR:HG23	12:M:173:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.95	0.47
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.50	0.47
10:K:78:HIS:HA	10:K:81:TYR:CE2	2.49	0.47
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.46	0.47
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.50	0.47
16:Q:143:SER:HB2	16:Q:178:THR:HG22	1.96	0.47
4:E:110:THR:OG1	30:E:201:HOH:O	2.20	0.47
5:F:43:GLU:OE2	5:F:43:GLU:HA	2.14	0.47
9:J:163:LYS:NZ	9:J:253:ILE:O	2.46	0.47
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.80	0.47
13:N:53:LYS:HA	13:N:53:LYS:HD3	1.76	0.46
13:N:71:ARG:HG3	13:N:73:THR:HG23	1.96	0.46
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.23	0.46
22:C:302:PEE:H73	23:C:303:PLX:H192	1.96	0.46
9:J:118:LYS:HA	9:J:121:GLU:OE1	2.15	0.46
12:M:710:CYS:O	12:M:714:VAL:HG22	2.15	0.46
1:A:263:ALA:HA	1:A:271:SER:HB2	1.97	0.46
10:K:87:LEU:HD12	14:O:85:LEU:HD13	1.97	0.46
6:G:75:THR:OG1	6:G:156:GLU:O	2.32	0.46
12:M:250:SER:OG	12:M:251:ILE:N	2.48	0.46
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.97	0.46
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.98	0.46
16:Q:338:ARG:HD3	18:W:21:TYR:O	2.16	0.46
1:A:48:ARG:HD3	10:K:70:ASN:O	2.15	0.46
16:Q:80:LEU:HD12	16:Q:82:LEU:HD21	1.96	0.46
3:C:80:ALA:HA	3:C:86:MET:HG2	1.97	0.46
4:E:16:SER:HB3	11:L:52:LEU:HB3	1.97	0.46
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.80	0.46
22:C:302:PEE:H58	22:C:302:PEE:C18	2.36	0.46
12:M:182:CYS:HA	12:M:225:ILE:HD11	1.98	0.46
9:J:61:ALA:HB3	9:J:82:VAL:HG13	1.97	0.46
16:Q:300:TRP:CE3	16:Q:305:THR:HG21	2.51	0.46
12:M:390:THR:HA	12:M:600:GLU:HG2	1.97	0.45
14:O:159:LYS:HB2	14:O:162:GLU:HG3	1.96	0.45
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.98	0.45
28:N:201:CDL:H742	28:N:201:CDL:H532	1.98	0.45
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.31	0.45
12:M:509:ASP:OD1	12:M:509:ASP:N	2.42	0.45
16:Q:144:MET:SD	16:Q:144:MET:N	2.90	0.45
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.52	0.45
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:CYS:H	1:A:277:ASN:ND2	2.15	0.45
12:M:149:ASP:HA	16:Q:380:HIS:CE1	2.51	0.45
3:C:98:ARG:HH22	3:C:123:GLN:HG2	1.82	0.45
3:C:195:ARG:HG3	3:C:195:ARG:HH11	1.81	0.45
22:C:302:PEE:H68	23:C:303:PLX:H191	1.99	0.45
6:G:82:ARG:NH2	6:G:125:GLU:O	2.49	0.45
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.51	0.45
16:Q:179:ARG:NH1	30:Q:524:HOH:O	2.45	0.45
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.99	0.45
8:I:42:PRO:HB3	18:W:6:VAL:HG21	1.99	0.45
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.82	0.45
15:P:115:THR:HB	16:Q:423:LYS:HE3	1.99	0.45
12:M:377:ALA:O	12:M:380:ASP:HB2	2.17	0.44
2:B:78:PHE:O	8:I:12:ARG:NH2	2.51	0.44
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.99	0.44
12:M:456:ALA:O	12:M:499:ASN:ND2	2.50	0.44
9:J:304:LEU:C	9:J:304:LEU:CD1	2.86	0.44
10:K:76:LEU:O	10:K:79:HIS:HB2	2.17	0.44
16:Q:85:GLY:HA2	16:Q:96:ARG:HG3	1.99	0.44
16:Q:335:GLU:OE1	16:Q:335:GLU:HA	2.18	0.44
4:E:37:ARG:NH1	6:G:132:ASP:OD2	2.43	0.44
9:J:126:VAL:HG23	9:J:161:VAL:HG11	2.00	0.44
9:J:231:LEU:CD2	9:J:292:PRO:CD	2.87	0.44
12:M:696:MET:SD	12:M:702:ARG:HA	2.57	0.44
17:T:114:CYS:SG	17:T:116:LEU:HG	2.58	0.44
15:P:117:VAL:HB	15:P:127:GLU:HG2	1.99	0.44
2:B:99:GLY:O	2:B:169:GLU:CG	2.66	0.44
14:O:186:VAL:HG22	14:O:196:LEU:HD11	2.00	0.44
16:Q:86:PRO:HB3	16:Q:94:VAL:HG23	2.00	0.44
7:H:76:GLN:O	7:H:78:GLU:N	2.50	0.44
2:B:68:ARG:HH11	18:W:28:ARG:HG2	1.82	0.44
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.53	0.44
9:J:36:LEU:N	12:M:304:GLN:HE22	2.16	0.44
9:J:145:PHE:CE1	9:J:184:LYS:HE2	2.52	0.44
12:M:29:SER:OG	12:M:30:ASN:N	2.49	0.44
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.53	0.44
1:A:35:LEU:HD23	1:A:40:ARG:NH1	2.32	0.43
1:A:119:GLU:OE1	1:A:128:ARG:N	2.50	0.43
5:F:23:LEU:O	5:F:57:GLU:HA	2.18	0.43
6:G:140:CYS:HB2	6:G:143:GLU:HG2	2.00	0.43
9:J:179:ARG:HG3	9:J:182:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:225:GLY:O	9:J:291:TYR:CE1	2.67	0.43
9:J:305:PHE:CD1	9:J:313:TRP:CZ3	3.05	0.43
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.00	0.43
3:C:193:TRP:HB2	22:C:302:PEE:H3	2.00	0.43
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.98	0.43
1:A:49:HIS:HA	10:K:74:ARG:CZ	2.48	0.43
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.98	0.43
1:A:367:ILE:O	1:A:371:ILE:HG12	2.19	0.43
1:A:118:ASP:HB3	20:A:502:FMN:O4	2.19	0.43
4:E:17:VAL:O	11:L:53:ILE:HD12	2.18	0.43
6:G:80:LYS:O	6:G:84:LEU:HD23	2.18	0.43
12:M:551:ASP:OD2	12:M:568:TYR:OH	2.35	0.43
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.43
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.18	0.43
9:J:71:ASN:HD22	9:J:97:MET:HG2	1.84	0.43
16:Q:425:LYS:HB2	30:Q:671:HOH:O	2.17	0.43
7:H:94:MET:SD	7:H:99:PRO:HG3	2.58	0.43
12:M:209:TYR:O	14:O:41:HIS:HB3	2.19	0.43
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.00	0.43
9:J:38:HIS:NE2	13:N:132:LYS:HE3	2.34	0.43
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.83	0.43
9:J:83:PRO:HG3	9:J:119:VAL:CG1	2.46	0.43
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.01	0.43
14:O:159:LYS:HA	14:O:159:LYS:HD2	1.63	0.43
1:A:208:GLU:OE2	1:A:210:THR:OG1	2.29	0.42
1:A:362:ASP:CG	1:A:449:ARG:HH12	2.21	0.42
2:B:99:GLY:HA3	2:B:170:GLY:O	2.18	0.42
16:Q:84:PHE:HE2	16:Q:444:LEU:HD11	1.83	0.42
5:F:30:SER:OG	5:F:63:PRO:HG3	2.18	0.42
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.54	0.42
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.01	0.42
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.49	0.42
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.99	0.42
17:T:43:GLN:HE21	17:T:43:GLN:HB2	1.66	0.42
16:Q:198:THR:HB	16:Q:199:PRO:HD3	2.01	0.42
1:A:185:ASN:C	1:A:187:CYS:H	2.22	0.42
4:E:47:VAL:HA	4:E:52:LEU:HD12	2.02	0.42
12:M:405:THR:HB	12:M:477:GLY:HA3	2.00	0.42
16:Q:337:MET:HG2	30:Q:661:HOH:O	2.19	0.42
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.20	0.42
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:58:MET:HE3	7:H:71:GLN:HG2	2.02	0.42
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.52	0.42
16:Q:324:GLY:O	16:Q:329:ARG:NH2	2.52	0.42
3:C:126:GLU:O	3:C:128:ARG:N	2.52	0.42
6:G:119:ILE:HG21	6:G:135:ALA:HB1	2.01	0.42
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.55	0.42
1:A:213:ILE:HG23	1:A:235:VAL:HA	2.02	0.42
1:A:314:LEU:HD23	1:A:329:LYS:HG3	2.02	0.42
12:M:503:SER:OG	12:M:504:SER:N	2.53	0.42
12:M:718:ILE:HD12	12:M:718:ILE:HA	1.93	0.42
1:A:49:HIS:N	1:A:49:HIS:HD1	2.17	0.42
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.89	0.42
1:A:270:ASN:ND2	1:A:340:ASP:OD2	2.49	0.42
23:C:303:PLX:H181	23:C:303:PLX:H212	1.84	0.42
12:M:97:MET:HB2	12:M:100:TRP:CE2	2.55	0.42
14:O:172:ILE:HD13	14:O:172:ILE:HA	1.95	0.42
1:A:268:GLU:HB3	1:A:269:ARG:HH11	1.85	0.41
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.02	0.41
1:A:201:ALA:O	14:O:119:TYR:HB3	2.19	0.41
1:A:261:TRP:O	1:A:264:SER:OG	2.29	0.41
15:P:207:TYR:C	15:P:224:VAL:HG23	2.41	0.41
4:E:93:THR:HG23	4:E:103:ILE:HD11	2.01	0.41
9:J:293:LEU:HD23	9:J:298:TYR:CD2	2.55	0.41
9:J:324:MET:HE2	9:J:324:MET:HB3	1.83	0.41
1:A:43:THR:HB	14:O:238:PRO:HB3	2.02	0.41
9:J:179:ARG:HG2	9:J:179:ARG:HH11	1.84	0.41
14:O:44:THR:HG22	14:O:46:GLU:H	1.86	0.41
14:O:80:LEU:HD21	14:O:119:TYR:CZ	2.56	0.41
16:Q:235:ASP:N	16:Q:356:ILE:HD13	2.35	0.41
23:C:303:PLX:H251	23:C:303:PLX:H52	1.84	0.41
9:J:85:ARG:HD3	25:J:401:NDP:C2A	2.50	0.41
12:M:197:THR:O	14:O:114:GLU:HG2	2.20	0.41
3:C:45:TYR:CD1	3:C:45:TYR:C	2.94	0.41
3:C:173:LEU:O	3:C:177:ILE:HG12	2.20	0.41
23:C:303:PLX:H281	23:C:303:PLX:H311	1.83	0.41
8:I:70:MET:O	8:I:70:MET:SD	2.79	0.41
9:J:132:ARG:HD3	9:J:132:ARG:HA	1.65	0.41
9:J:174:ILE:H	9:J:174:ILE:HG12	1.70	0.41
12:M:212:LYS:HB2	12:M:212:LYS:HE3	1.85	0.41
14:O:208:LEU:HD12	14:O:208:LEU:HA	1.92	0.41
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:303:PLX:H91	23:C:303:PLX:H271	2.01	0.41
12:M:34:VAL:HG23	12:M:41:VAL:HG13	2.03	0.41
16:Q:402:ALA:HB3	16:Q:405:GLY:O	2.21	0.41
1:A:32:PHE:HB2	1:A:293:SER:O	2.20	0.41
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.55	0.41
1:A:251:SER:OG	1:A:252:PRO:HD3	2.20	0.41
1:A:285:PRO:O	14:O:222:ARG:NH2	2.53	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.88	0.41
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.60	0.41
9:J:294:PRO:HB3	9:J:296:PHE:CZ	2.56	0.41
12:M:51:GLN:NE2	30:M:917:HOH:O	2.36	0.41
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.03	0.41
16:Q:182:ASN:ND2	16:Q:404:LYS:HZ3	2.18	0.41
16:Q:278:VAL:HG12	16:Q:329:ARG:HH21	1.86	0.41
1:A:162:PHE:HB3	1:A:165:GLU:HB2	2.02	0.41
2:B:111:GLU:O	2:B:141:ARG:NH1	2.54	0.41
5:F:18:GLU:OE1	5:F:68:ARG:NH1	2.53	0.41
9:J:57:THR:HG21	9:J:120:VAL:HG12	2.02	0.41
9:J:328:THR:HG22	9:J:330:PRO:HD3	2.02	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.53	0.41
16:Q:345:SER:HB2	18:W:19:ILE:HD12	2.03	0.41
8:I:90:THR:HG22	8:I:92:LYS:HG2	2.03	0.40
13:N:85:GLU:HG2	13:N:86:TRP:N	2.36	0.40
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.01	0.40
3:C:41:SER:N	3:C:44:GLU:HG2	2.36	0.40
5:F:33:VAL:HG22	5:F:87:VAL:HG11	2.03	0.40
14:O:166:ASP:OD1	14:O:166:ASP:N	2.54	0.40
16:Q:208:GLU:OE1	30:Q:505:HOH:O	2.22	0.40
17:T:79:VAL:O	17:T:121:PRO:HD3	2.21	0.40
1:A:396:MET:O	1:A:400:VAL:HG23	2.22	0.40
2:B:131:GLU:OE2	13:N:130:THR:HG21	2.21	0.40
3:C:113:MET:HE3	3:C:116:ALA:HB3	2.04	0.40
12:M:472:PRO:O	12:M:510:TRP:NE1	2.45	0.40
12:M:479:SER:HA	12:M:482:GLN:HG2	2.04	0.40
14:O:130:TYR:CE2	14:O:208:LEU:HG	2.56	0.40
1:A:429:ASP:N	1:A:429:ASP:OD1	2.55	0.40
6:G:103:HIS:CD2	6:G:139:MET:HB3	2.56	0.40
12:M:249:GLU:HG2	12:M:276:ARG:HD3	2.03	0.40
12:M:255:ASP:O	30:M:901:HOH:O	2.22	0.40
15:P:165:TRP:HZ2	16:Q:111:PRO:HG2	1.87	0.40
1:A:290:GLU:HG3	1:A:291:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLY:CA	2:B:170:GLY:O	2.70	0.40
22:C:302:PEE:H68	23:C:303:PLX:C19	2.50	0.40
5:F:39:LYS:HD2	5:F:39:LYS:HA	1.93	0.40
7:H:65:VAL:O	7:H:69:GLU:HG3	2.21	0.40
9:J:271:TYR:OH	9:J:346:GLU:OE2	2.37	0.40
12:M:367:CYS:HB3	12:M:533:GLY:O	2.20	0.40
12:M:387:LEU:HD12	12:M:514:ASN:HB3	2.04	0.40
12:M:480:ALA:O	12:M:483:ARG:HG2	2.20	0.40
14:O:155:LYS:HD3	14:O:202:GLU:HG2	2.02	0.40
14:O:231:LEU:HD13	14:O:231:LEU:HA	1.94	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	429/431 (100%)	417 (97%)	11 (3%)	1 (0%)	47 62
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100 100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100 100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100 100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100 100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100 100
7	H	110/112 (98%)	104 (94%)	6 (6%)	0	100 100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100 100
9	J	327/341 (96%)	315 (96%)	10 (3%)	2 (1%)	25 36
10	K	40/42 (95%)	39 (98%)	1 (2%)	0	100 100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100 100
12	M	688/690 (100%)	669 (97%)	18 (3%)	1 (0%)	51 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
15	P	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
16	Q	374/385 (97%)	366 (98%)	8 (2%)	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	3479/3553 (98%)	3366 (97%)	109 (3%)	4 (0%)	54	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
9	J	38	HIS
9	J	227	PRO
12	M	283	GLU

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	345/345 (100%)	335 (97%)	10 (3%)	42	62
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	84
3	C	132/132 (100%)	125 (95%)	7 (5%)	22	37
4	E	107/107 (100%)	103 (96%)	4 (4%)	34	53
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	73 (96%)	3 (4%)	32	50
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	83 (95%)	4 (5%)	27	43
9	J	285/295 (97%)	274 (96%)	11 (4%)	32	50
10	K	41/41 (100%)	37 (90%)	4 (10%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	L	113/113 (100%)	112 (99%)	1 (1%)	78 90
12	M	580/580 (100%)	566 (98%)	14 (2%)	49 68
13	N	130/130 (100%)	127 (98%)	3 (2%)	50 70
14	O	183/183 (100%)	178 (97%)	5 (3%)	44 65
15	P	190/190 (100%)	188 (99%)	2 (1%)	73 87
16	Q	327/331 (99%)	323 (99%)	4 (1%)	71 85
17	T	79/79 (100%)	76 (96%)	3 (4%)	33 51
18	W	24/24 (100%)	23 (96%)	1 (4%)	30 47
All	All	3025/3054 (99%)	2947 (97%)	78 (3%)	49 66

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	52	ARG
1	A	104	LYS
1	A	125	CYS
1	A	134	ASP
1	A	189	SER
1	A	269	ARG
1	A	312	ASP
1	A	383	THR
1	A	429	ASP
2	B	76	TYR
2	B	98	ARG
3	C	42	ARG
3	C	51	ASP
3	C	65	MET
3	C	71	CYS
3	C	76	MET
3	C	142	TYR
3	C	191	ARG
4	E	34	GLU
4	E	81	LEU
4	E	87	LYS
4	E	99	GLN
6	G	105	MET
6	G	107	ASP
6	G	111	ASP

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Mol	Chain	Res	Type
8	I	27	ARG
8	I	33	LYS
8	I	64	MET
8	I	70	MET
9	J	85	ARG
9	J	87	GLU
9	J	108	TRP
9	J	109	ASN
9	J	118	LYS
9	J	235	THR
9	J	286	ARG
9	J	298	TYR
9	J	317	ASP
9	J	324	MET
9	J	337	ASP
10	K	74	ARG
10	K	77	GLN
10	K	82	SER
10	K	85	THR
11	L	86	ASN
12	M	68	ARG
12	M	158	ARG
12	M	219	SER
12	M	255	ASP
12	M	311	LYS
12	M	360	ARG
12	M	380	ASP
12	M	457	SER
12	M	483	ARG
12	M	513	MET
12	M	518	ARG
12	M	636	TYR
12	M	637	ASP
12	M	688	GLN
13	N	41	GLU
13	N	43	LYS
13	N	142	THR
14	O	106	GLN
14	O	153	GLN
14	O	165	PRO
14	O	212	LYS
14	O	233	SER

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Mol	Chain	Res	Type
15	P	231	ARG
15	P	240	GLU
16	Q	96	ARG
16	Q	183	HIS
16	Q	217	VAL
16	Q	249	LYS
17	T	43	GLN
17	T	81	SER
17	T	114	CYS
18	W	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	J	323	HIS
15	P	82	ASN
16	Q	182	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.01	1 (10%)	5,13,15	6.09	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	5.69	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	12.46	130.90	119.48
16	Q	118	2MR	CD-NE-CZ	3.99	130.87	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.36	131.29	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	16,3	0,12,12	-	-	-		
19	SF4	A	501	1	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		
26	FES	M	803	12	0,4,4	-	-	-		
23	PLX	C	303	-	51,51,51	1.15	5 (9%)	55,59,59	0.62	1 (1%)
21	NAI	A	503	-	42,48,48	4.94	18 (42%)	47,73,73	1.30	7 (14%)
25	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.14	3 (5%)
26	FES	O	301	14	0,4,4	-	-	-		
24	8Q1	G	201	-	31,34,34	2.04	6 (19%)	40,43,43	1.77	10 (25%)
19	SF4	B	301	2	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.23	8 (16%)
28	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.26	5 (8%)
22	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)
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
19	SF4	C	301	16,3	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
26	FES	M	803	12	-	-	0/1/1/1
23	PLX	C	303	-	-	28/55/55/55	-
21	NAI	A	503	-	-	7/25/72/72	0/5/5/5
25	NDP	J	401	-	-	6/30/77/77	0/5/5/5
26	FES	O	301	14	-	-	0/1/1/1
24	8Q1	G	201	-	-	12/41/41/41	-
19	SF4	B	301	2	-	-	0/6/5/5
20	FMN	A	502	-	-	10/18/18/18	0/3/3/3
28	CDL	N	201	-	-	22/61/61/110	-
22	PEE	C	302	-	-	31/50/50/54	-
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	503	NAI	O4B-C1B	16.29	1.63	1.41
21	A	503	NAI	C2B-C1B	-15.29	1.30	1.53
21	A	503	NAI	C3D-C4D	-10.32	1.26	1.53
21	A	503	NAI	O4B-C4B	-8.19	1.26	1.45
21	A	503	NAI	C2D-C1D	-7.59	1.29	1.53
24	G	201	8Q1	P24-O27	7.58	1.84	1.60
21	A	503	NAI	O4D-C4D	6.90	1.60	1.45
21	A	503	NAI	C2D-C3D	5.89	1.69	1.53
21	A	503	NAI	C7N-N7N	5.70	1.48	1.33
21	A	503	NAI	O4D-C1D	5.45	1.54	1.42
21	A	503	NAI	C4N-C3N	-5.03	1.40	1.49
21	A	503	NAI	O2B-C2B	4.57	1.53	1.43
28	N	201	CDL	OB8-CB7	4.32	1.46	1.33
28	N	201	CDL	OA8-CA7	4.26	1.45	1.33
28	N	201	CDL	OA6-CA5	4.17	1.46	1.34
21	A	503	NAI	C6N-C5N	4.09	1.40	1.33
28	N	201	CDL	OB6-CB5	4.02	1.45	1.34
24	G	201	8Q1	C1-S44	3.99	1.85	1.76
20	A	502	FMN	C4A-N5	3.82	1.38	1.30
22	C	302	PEE	C18-C19	3.74	1.53	1.31
22	C	302	PEE	C39-C38	3.66	1.53	1.31
21	A	503	NAI	C6A-N6A	3.58	1.47	1.34
21	A	503	NAI	C7N-C3N	3.56	1.56	1.48
24	G	201	8Q1	C34-N36	3.39	1.41	1.33
25	J	401	NDP	C6N-C5N	3.31	1.39	1.33
24	G	201	8Q1	O27-C28	-3.31	1.33	1.43
21	A	503	NAI	C4N-C5N	-3.27	1.40	1.48
24	G	201	8Q1	C6-C1	2.84	1.53	1.50
24	G	201	8Q1	C39-N41	2.80	1.39	1.33
23	C	303	PLX	O6-C4	-2.74	1.40	1.44
22	C	302	PEE	O3-C30	2.49	1.40	1.33
21	A	503	NAI	O3B-C3B	-2.48	1.37	1.43
20	A	502	FMN	C10-N1	2.46	1.38	1.33
25	J	401	NDP	C5A-C4A	2.40	1.47	1.40
21	A	503	NAI	PN-O5D	2.40	1.69	1.59
22	C	302	PEE	O2-C2	-2.36	1.40	1.46
22	C	302	PEE	O2-C10	2.29	1.40	1.34
21	A	503	NAI	C5B-C4B	2.29	1.58	1.51
23	C	303	PLX	C7-C6	2.27	1.55	1.50
23	C	303	PLX	P1-O4	2.12	1.67	1.59
22	C	302	PEE	O3-C3	-2.05	1.40	1.45
23	C	303	PLX	P1-O1	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	303	PLX	C25-C24	2.01	1.55	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	201	8Q1	C6-C1-S44	5.28	119.61	113.46
21	A	503	NAI	N3A-C2A-N1A	-4.30	121.96	128.68
28	N	201	CDL	OB6-CB5-C51	4.01	120.15	111.50
28	N	201	CDL	OA6-CA5-C11	3.97	120.06	111.50
22	C	302	PEE	O2-C10-C11	3.94	120.00	111.50
24	G	201	8Q1	C43-S44-C1	3.72	113.45	101.87
24	G	201	8Q1	O35-C34-N36	-3.30	115.90	122.99
21	A	503	NAI	C3D-C2D-C1D	3.25	107.61	101.43
25	J	401	NDP	PN-O3-PA	-3.25	121.67	132.83
25	J	401	NDP	N3A-C2A-N1A	-3.23	123.63	128.68
20	A	502	FMN	C4-N3-C2	-3.09	119.93	125.64
21	A	503	NAI	C2D-C3D-C4D	2.84	108.16	102.64
25	J	401	NDP	C4A-C5A-N7A	-2.75	106.53	109.40
20	A	502	FMN	C4A-C4-N3	2.70	120.03	113.19
21	A	503	NAI	C4A-C5A-N7A	-2.67	106.61	109.40
24	G	201	8Q1	O2-P24-O27	-2.67	99.64	106.73
24	G	201	8Q1	O40-C39-N41	-2.66	118.00	123.01
24	G	201	8Q1	O4-C1-C6	-2.62	120.90	123.99
20	A	502	FMN	O4-C4-C4A	-2.62	119.66	126.60
28	N	201	CDL	OB8-CB7-C71	2.59	120.05	111.91
28	N	201	CDL	OA8-CA7-C31	2.59	120.04	111.91
22	C	302	PEE	O3-C30-C31	2.59	120.03	111.91
21	A	503	NAI	C4D-O4D-C1D	-2.57	103.80	109.47
24	G	201	8Q1	C32-C34-N36	2.51	121.58	116.58
24	G	201	8Q1	C38-C39-N41	2.48	120.59	116.42
24	G	201	8Q1	O1-P24-O2	2.42	116.89	107.64
24	G	201	8Q1	O4-C1-S44	-2.40	119.50	122.61
20	A	502	FMN	C9A-C5A-N5	-2.39	119.83	122.43
20	A	502	FMN	C4A-C10-N10	2.34	119.90	116.48
23	C	303	PLX	C1A-N1-C1	2.33	119.45	109.92
21	A	503	NAI	PN-O3-PA	-2.29	124.95	132.83
21	A	503	NAI	C3B-C2B-C1B	2.27	104.39	100.98
20	A	502	FMN	C10-C4A-N5	-2.22	120.15	124.86
20	A	502	FMN	C4A-C10-N1	-2.14	119.77	124.73
20	A	502	FMN	C5A-C9A-N10	2.06	120.08	117.95
28	N	201	CDL	CB4-OB6-CB5	-2.04	112.77	117.79

There are no chirality outliers.

All (116) 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	C3'-C4'-C5'-O5'
20	A	502	FMN	O4'-C4'-C5'-O5'
20	A	502	FMN	C5'-O5'-P-O1P
21	A	503	NAI	PN-O3-PA-O5B
22	C	302	PEE	C11-C10-O2-C2
22	C	302	PEE	O4-C10-O2-C2
22	C	302	PEE	C1-O3P-P-O2P
22	C	302	PEE	C1-O3P-P-O1P
22	C	302	PEE	C1-O3P-P-O4P
23	C	303	PLX	C2-O1-P1-O2
23	C	303	PLX	N1-C1-C2-O1
24	G	201	8Q1	O4-C1-S44-C43
24	G	201	8Q1	C6-C1-S44-C43
24	G	201	8Q1	N36-C37-C38-C39
24	G	201	8Q1	C42-C43-S44-C1
25	J	401	NDP	C2B-O2B-P2B-O3X
28	N	201	CDL	O1-C1-CB2-OB2
28	N	201	CDL	CA2-C1-CB2-OB2
28	N	201	CDL	CA2-OA2-PA1-OA4
28	N	201	CDL	CA3-OA5-PA1-OA2
28	N	201	CDL	CA6-CA4-OA6-CA5
28	N	201	CDL	C11-CA5-OA6-CA4
28	N	201	CDL	CB2-OB2-PB2-OB4
28	N	201	CDL	OA7-CA5-OA6-CA4
28	N	201	CDL	OB7-CB5-OB6-CB4
28	N	201	CDL	C51-CB5-OB6-CB4
28	N	201	CDL	O1-C1-CA2-OA2
20	A	502	FMN	O2'-C2'-C3'-O3'
25	J	401	NDP	O4B-C4B-C5B-O5B
20	A	502	FMN	O2'-C2'-C3'-C4'
23	C	303	PLX	C28-C29-C30-C31
22	C	302	PEE	C4-O4P-P-O3P
23	C	303	PLX	C2-O1-P1-O4
28	N	201	CDL	CA2-OA2-PA1-OA5
28	N	201	CDL	CB2-OB2-PB2-OB5
23	C	303	PLX	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	C	303	PLX	C7-C8-C9-C10
23	C	303	PLX	C10-C11-C12-C13
24	G	201	8Q1	C11-C12-C13-C14
24	G	201	8Q1	N41-C42-C43-S44
23	C	303	PLX	C11-C12-C13-C14
23	C	303	PLX	C25-C26-C27-C28
23	C	303	PLX	O7-C6-C7-C8
23	C	303	PLX	C12-C13-C14-C15
24	G	201	8Q1	C10-C11-C12-C13
22	C	302	PEE	C11-C12-C13-C14
23	C	303	PLX	C13-C14-C15-C16
23	C	303	PLX	C33-C34-C35-C36
22	C	302	PEE	C15-C16-C17-C18
21	A	503	NAI	C3D-C4D-C5D-O5D
24	G	201	8Q1	C9-C10-C11-C12
24	G	201	8Q1	C12-C13-C14-C15
22	C	302	PEE	C42-C43-C44-C45
28	N	201	CDL	CB5-C51-C52-C53
22	C	302	PEE	C1-C2-C3-O3
22	C	302	PEE	C19-C20-C21-C22
22	C	302	PEE	O3P-C1-C2-C3
23	C	303	PLX	C17-C18-C19-C20
23	C	303	PLX	C3-C4-C5-O8
23	C	303	PLX	C3-C4-O6-C6
28	N	201	CDL	CB3-OB5-PB2-OB2
21	A	503	NAI	C2D-C1D-N1N-C2N
23	C	303	PLX	C11-C10-C9-C8
22	C	302	PEE	C31-C30-O3-C3
23	C	303	PLX	C29-C30-C31-C32
22	C	302	PEE	O5-C30-O3-C3
25	J	401	NDP	PN-O3-PA-O2A
23	C	303	PLX	C3-O4-P1-O1
25	J	401	NDP	O4D-C1D-N1N-C6N
22	C	302	PEE	C4-O4P-P-O2P
22	C	302	PEE	C4-O4P-P-O1P
23	C	303	PLX	C2-O1-P1-O3
28	N	201	CDL	CA3-OA5-PA1-OA4
23	C	303	PLX	C30-C31-C32-C33
22	C	302	PEE	O3P-C1-C2-O2
22	C	302	PEE	C33-C34-C35-C36
22	C	302	PEE	O2-C2-C3-O3
23	C	303	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
23	C	303	PLX	C27-C28-C29-C30
21	A	503	NAI	O4D-C1D-N1N-C2N
28	N	201	CDL	C11-C12-C13-C14
28	N	201	CDL	OA9-CA7-OA8-CA6
22	C	302	PEE	C16-C17-C18-C19
28	N	201	CDL	C31-CA7-OA8-CA6
21	A	503	NAI	C2D-C1D-N1N-C6N
22	C	302	PEE	C38-C39-C40-C41
23	C	303	PLX	C14-C15-C16-C17
22	C	302	PEE	C18-C19-C20-C21
22	C	302	PEE	C14-C15-C16-C17
23	C	303	PLX	C9-C10-C11-C12
23	C	303	PLX	C6-C7-C8-C9
28	N	201	CDL	OB6-CB4-CB6-OB8
23	C	303	PLX	C18-C19-C20-C21
21	A	503	NAI	O4D-C1D-N1N-C6N
28	N	201	CDL	CB2-C1-CA2-OA2
24	G	201	8Q1	C6-C7-C8-C9
22	C	302	PEE	C41-C42-C43-C44
21	A	503	NAI	O4D-C4D-C5D-O5D
22	C	302	PEE	C20-C21-C22-C23
20	A	502	FMN	C5'-O5'-P-O2P
22	C	302	PEE	C1-C2-O2-C10
24	G	201	8Q1	C31-C29-C32-C34
25	J	401	NDP	PN-O3-PA-O1A
23	C	303	PLX	C31-C32-C33-C34
22	C	302	PEE	O3-C30-C31-C32
22	C	302	PEE	C13-C14-C15-C16
25	J	401	NDP	C5B-O5B-PA-O1A
28	N	201	CDL	CB3-OB5-PB2-OB4
22	C	302	PEE	C3-C2-O2-C10
24	G	201	8Q1	C28-C29-C32-C34
22	C	302	PEE	O5-C30-C31-C32
22	C	302	PEE	C43-C44-C45-C46

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	301	SF4	2	0
19	A	501	SF4	2	0
23	C	303	PLX	10	0

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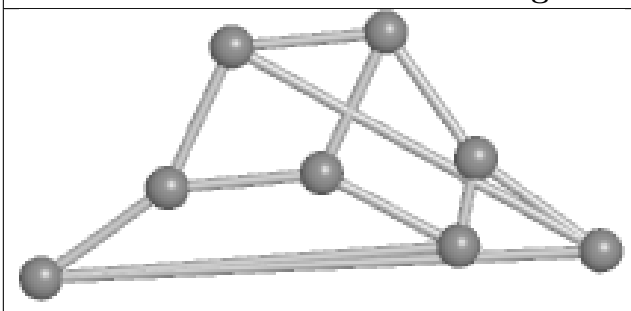
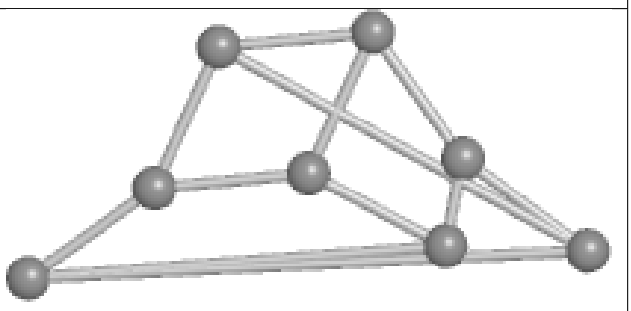
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	503	NAI	5	0
25	J	401	NDP	2	0
20	A	502	FMN	2	0
28	N	201	CDL	6	0
22	C	302	PEE	20	0

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.

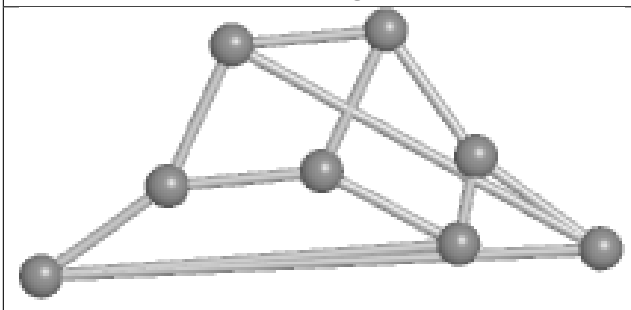
Ligand SF4 C 301



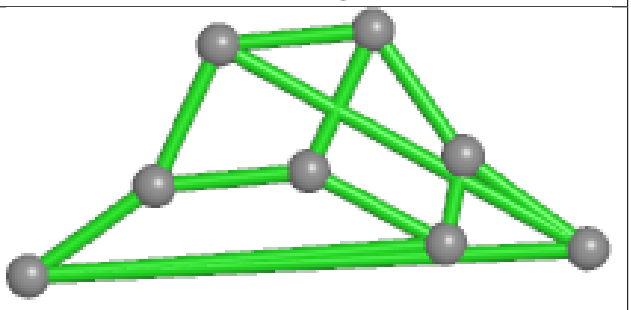
Bond lengths



Bond angles

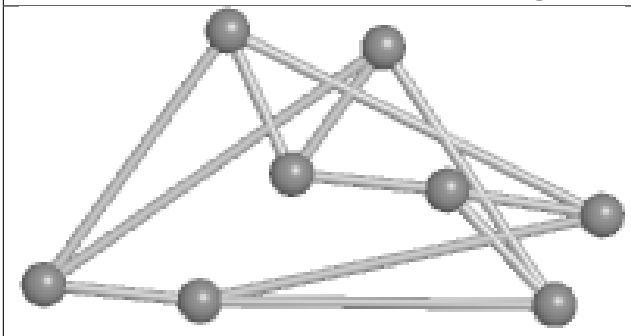


Torsions

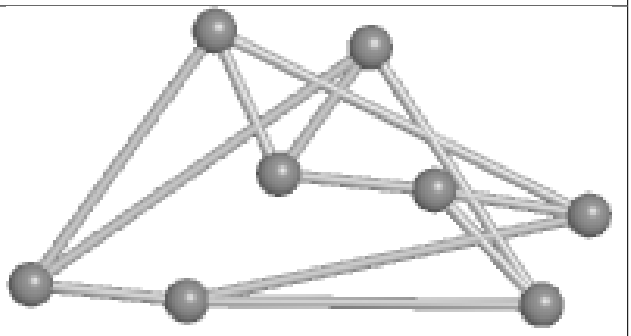


Rings

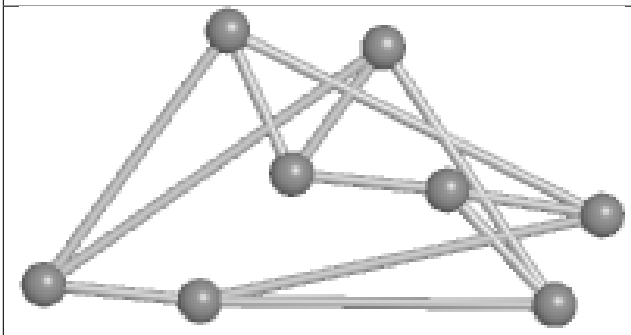
Ligand SF4 A 501



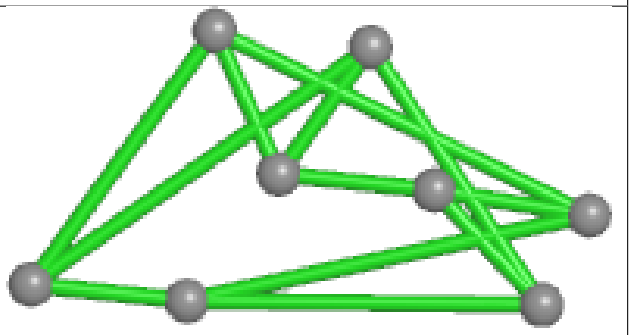
Bond lengths



Bond angles

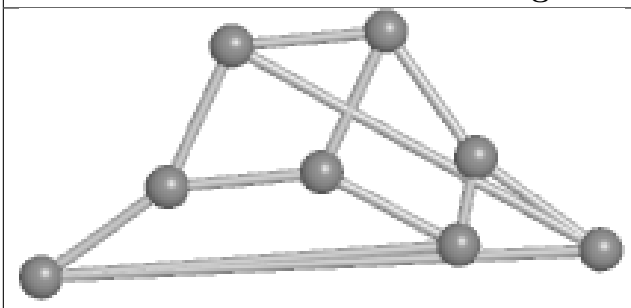


Torsions

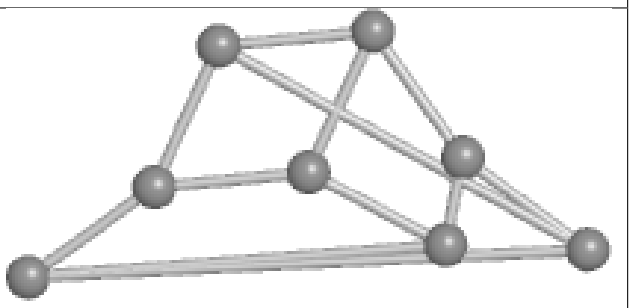


Rings

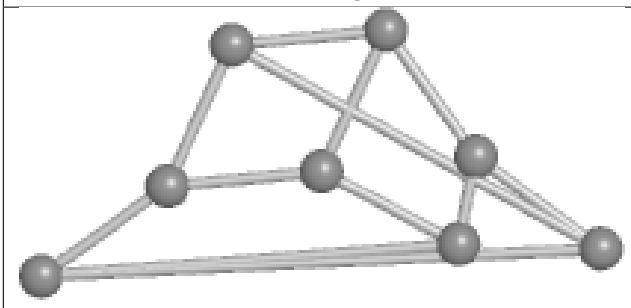
Ligand SF4 B 302



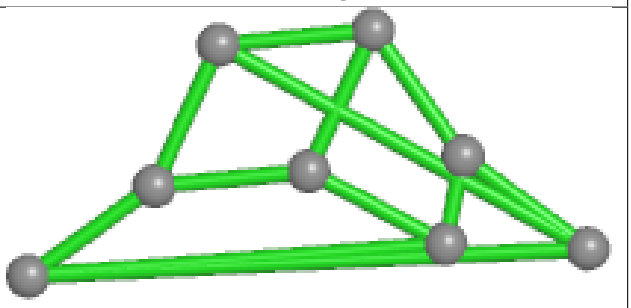
Bond lengths



Bond angles

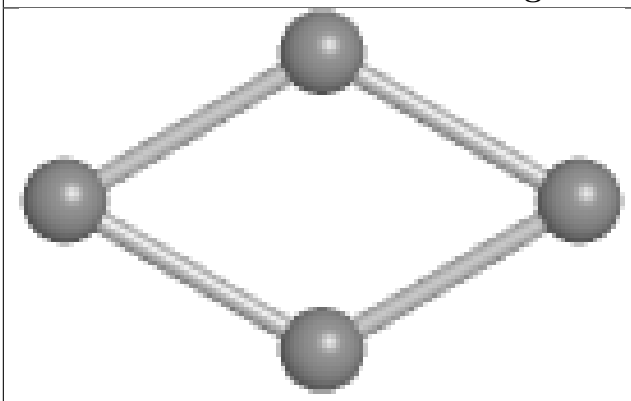


Torsions

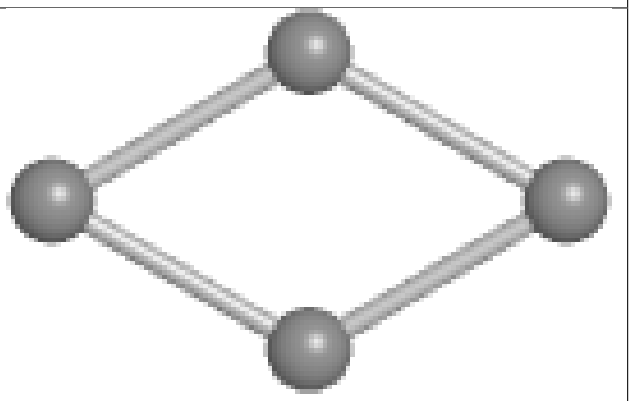


Rings

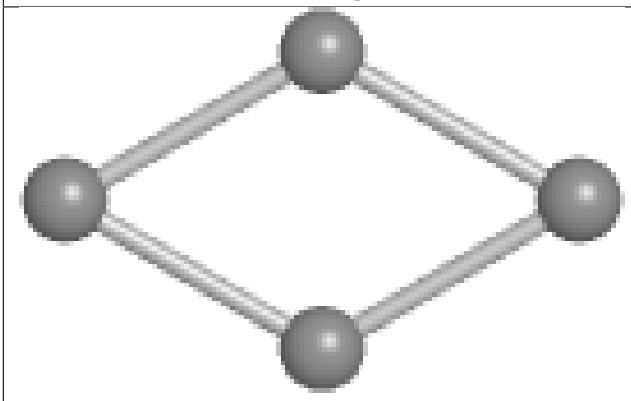
Ligand FES M 803



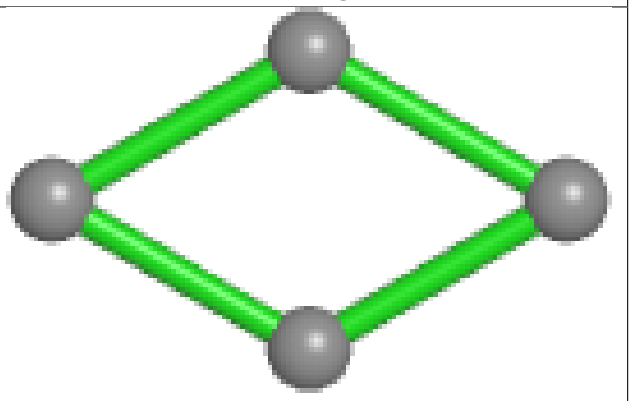
Bond lengths



Bond angles

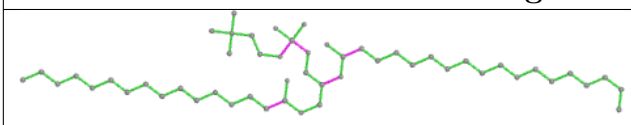


Torsions

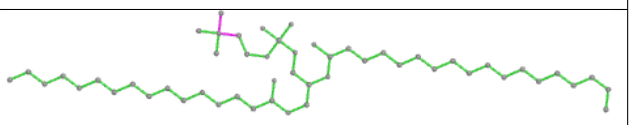


Rings

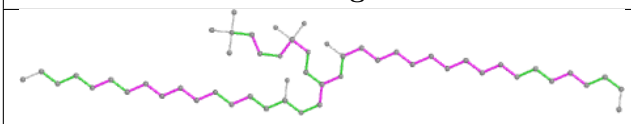
Ligand PLX C 303



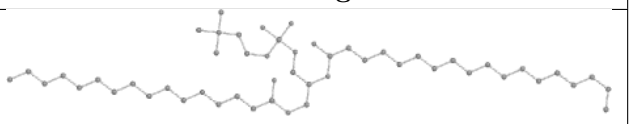
Bond lengths



Bond angles

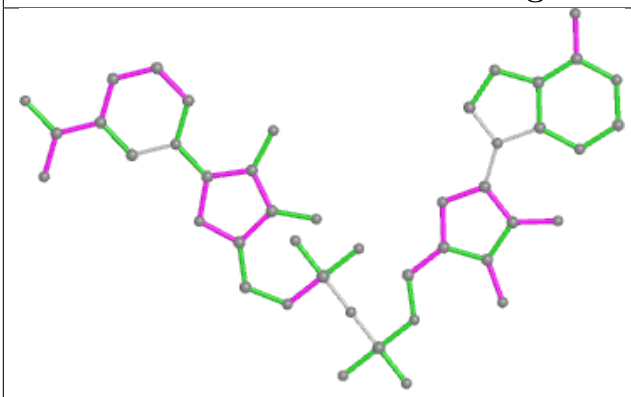


Torsions

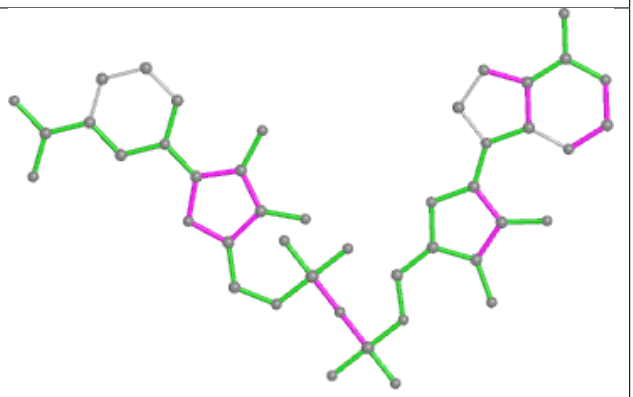


Rings

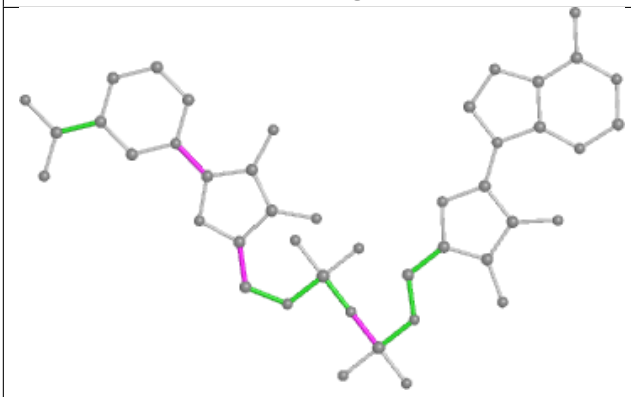
Ligand NAI A 503



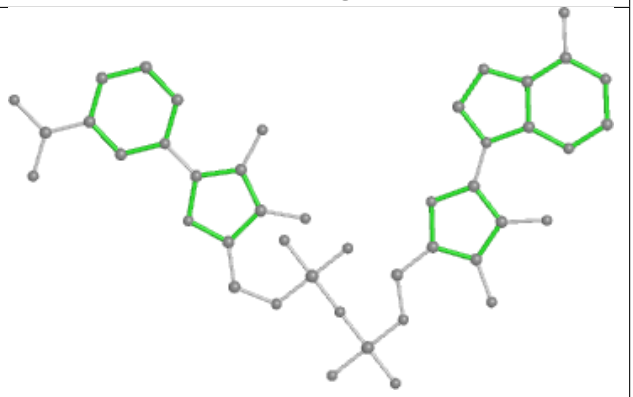
Bond lengths



Bond angles

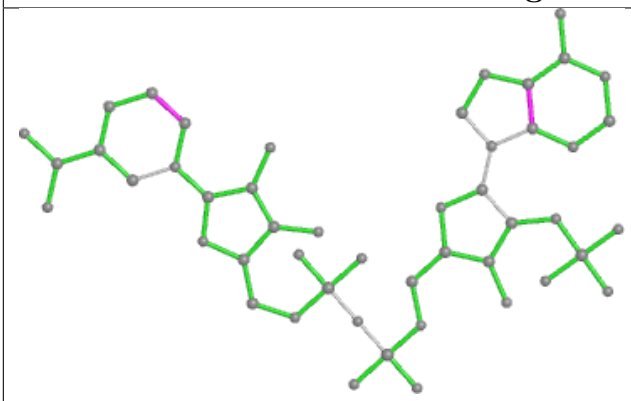


Torsions

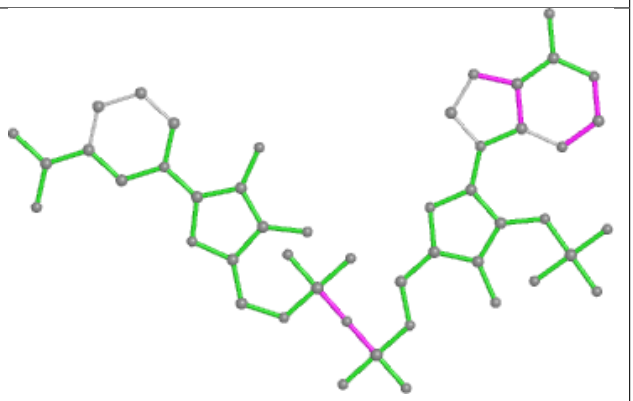


Rings

Ligand NDP J 401



Bond lengths



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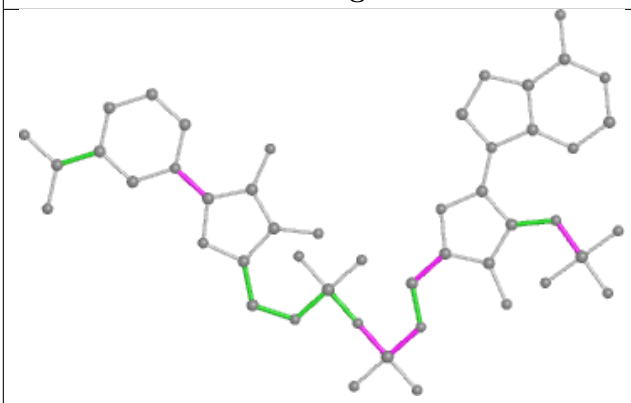
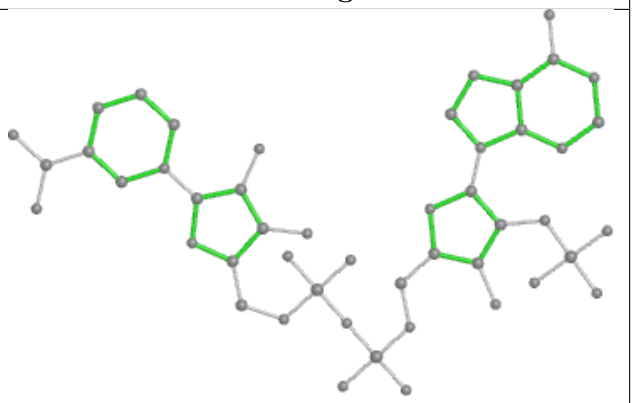
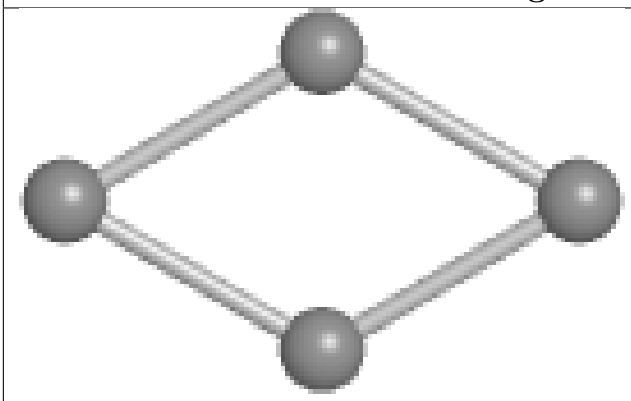


Torsions

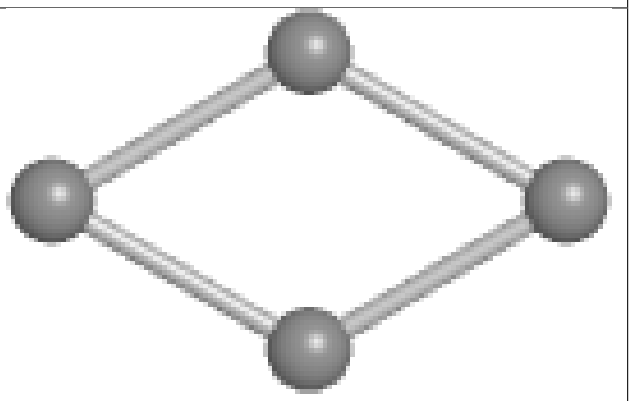


Rings

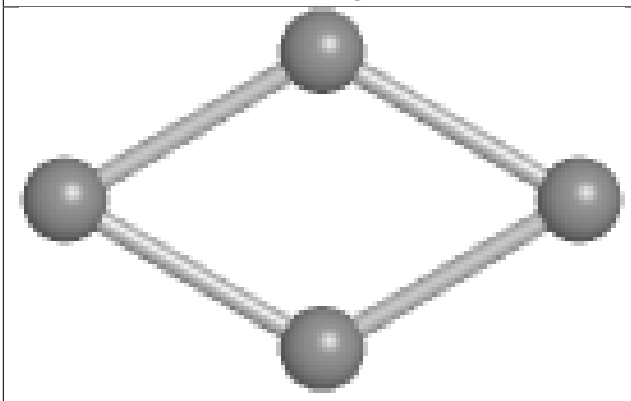
Ligand FES O 301



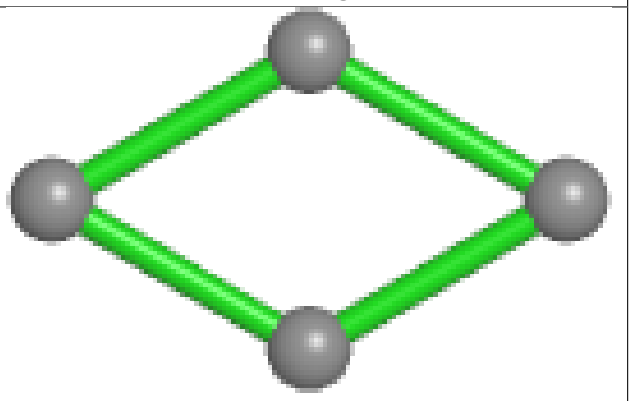
Bond lengths



Bond angles

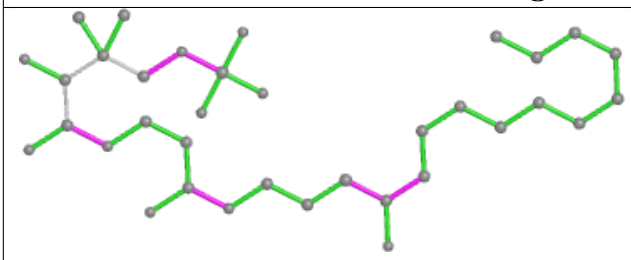


Torsions

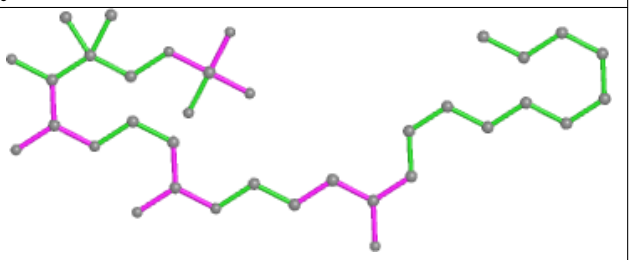


Rings

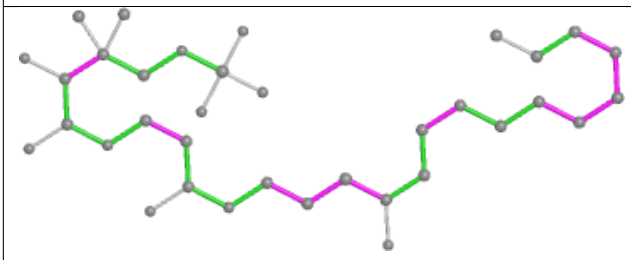
Ligand 8Q1 G 201



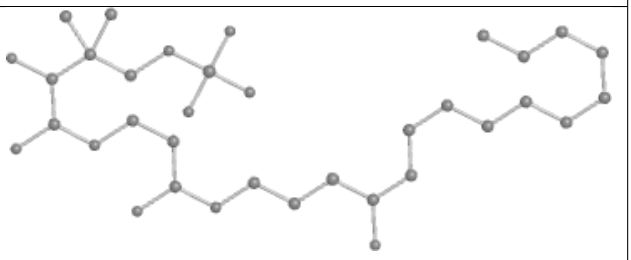
Bond lengths



Bond angles

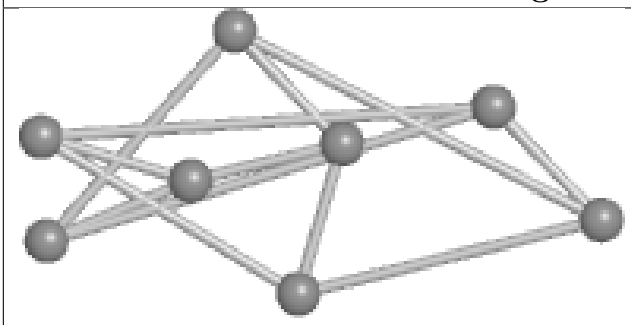


Torsions

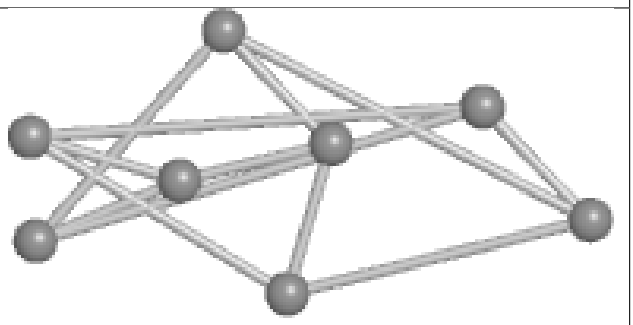


Rings

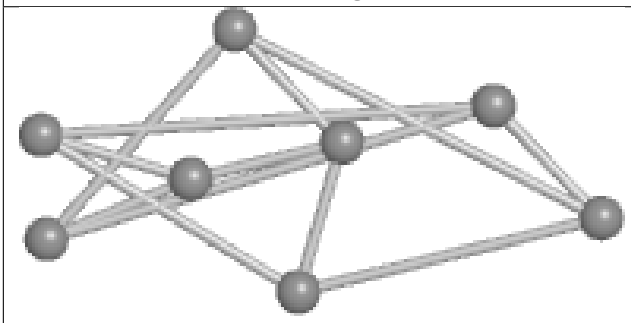
Ligand SF4 B 301



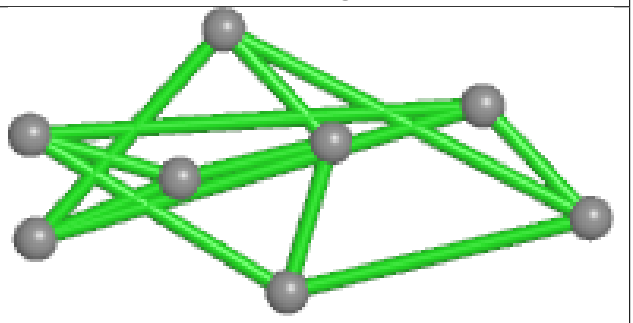
Bond lengths



Bond angles

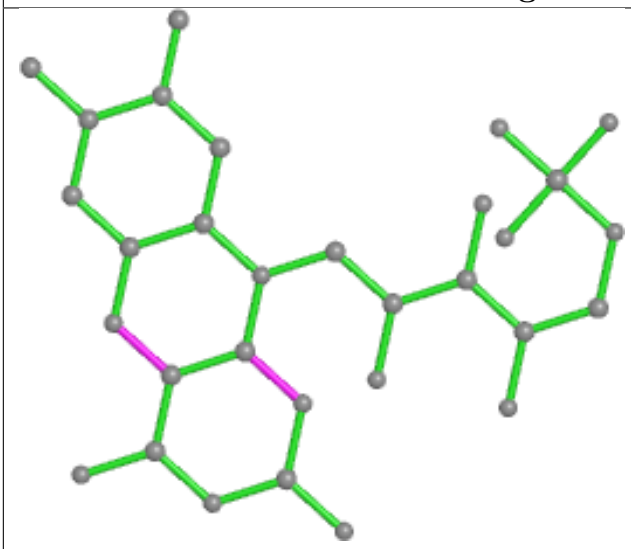


Torsions

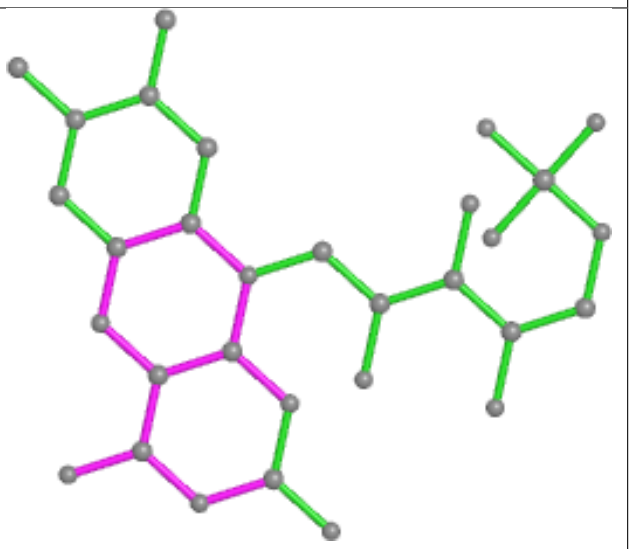


Rings

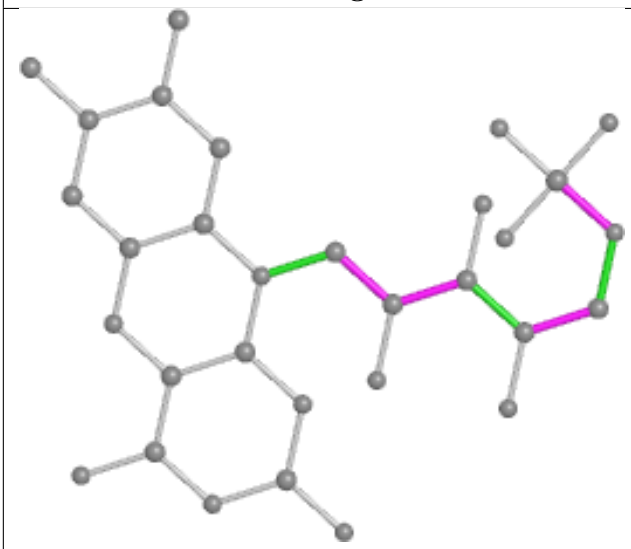
Ligand FMN A 502



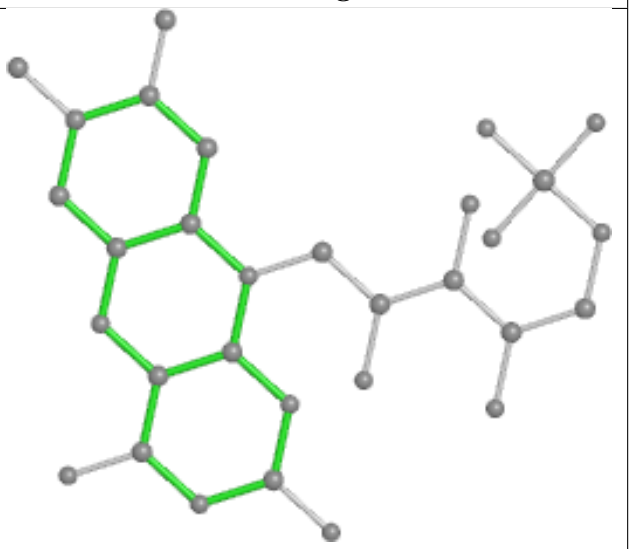
Bond lengths



Bond angles

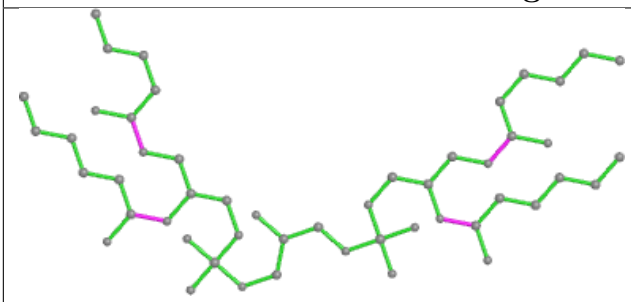


Torsions

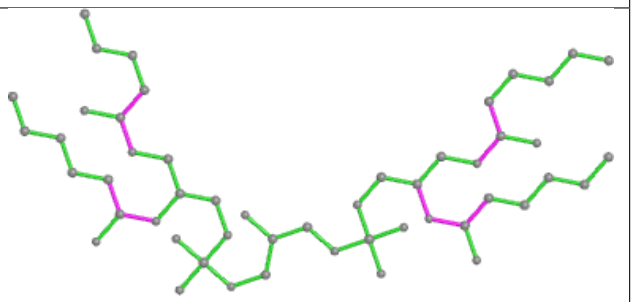


Rings

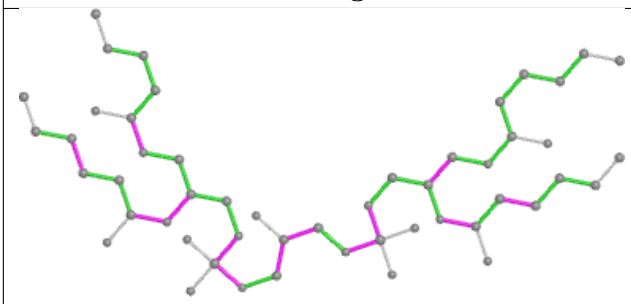
Ligand CDL N 201



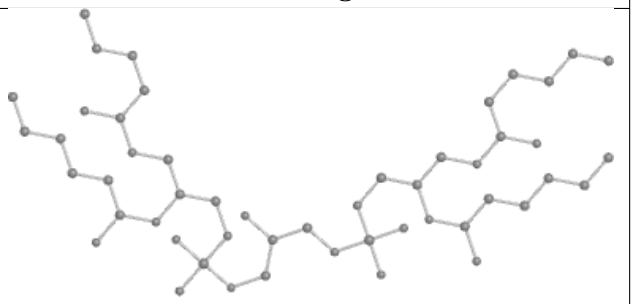
Bond lengths



Bond angles

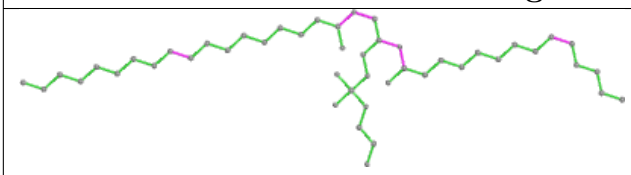


Torsions

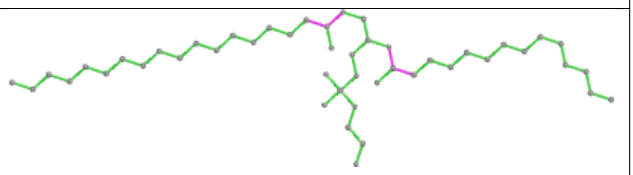


Rings

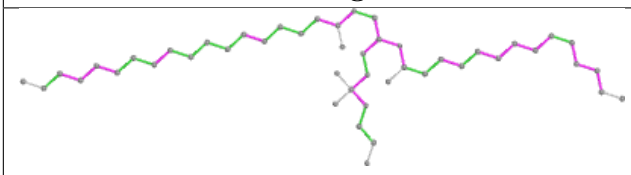
Ligand PEE C 302



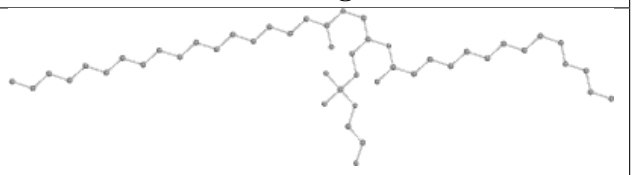
Bond lengths



Bond angles

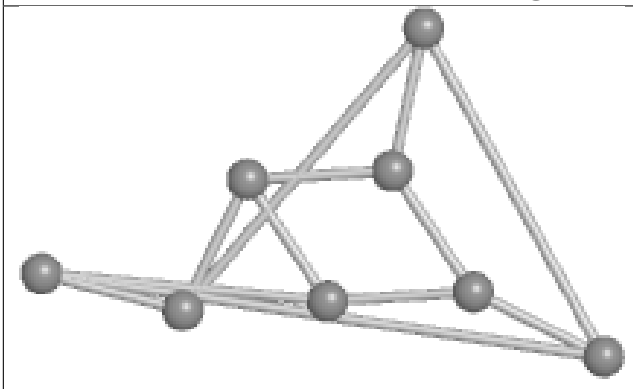


Torsions

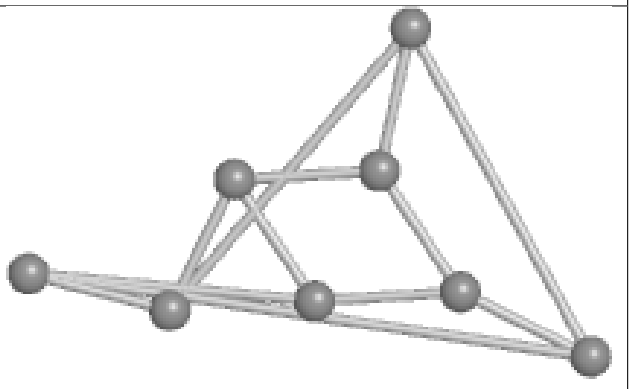


Rings

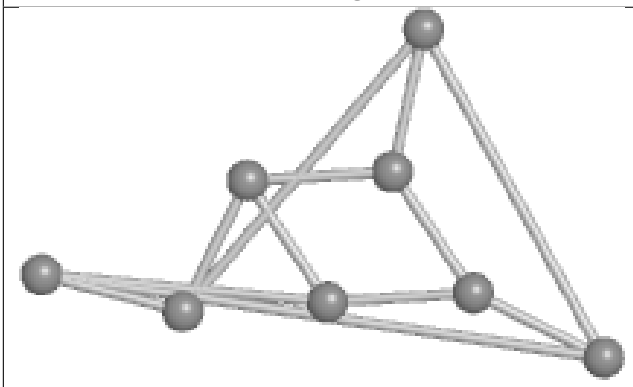
Ligand SF4 M 801



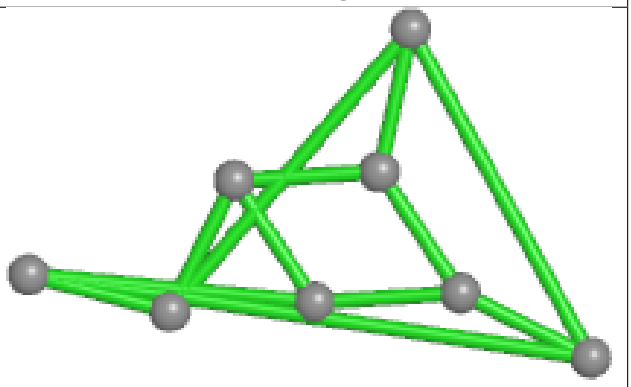
Bond lengths



Bond angles

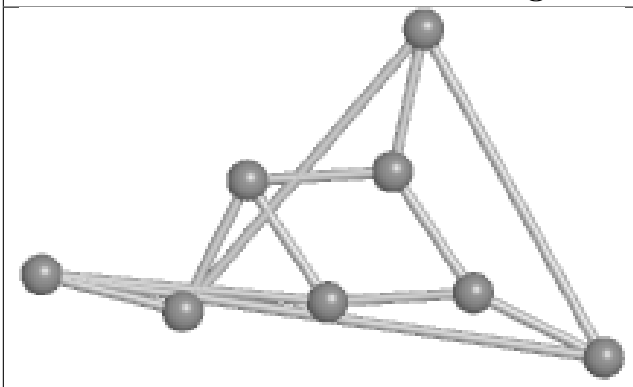


Torsions

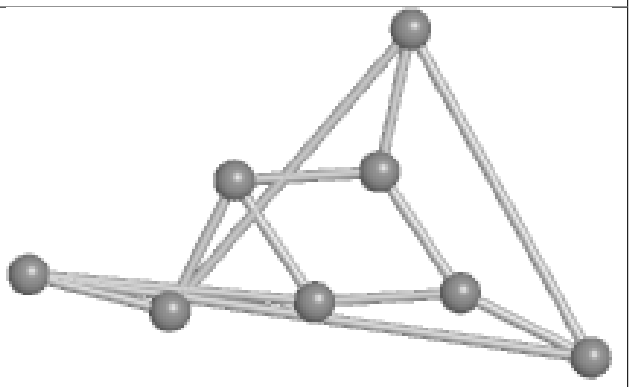


Rings

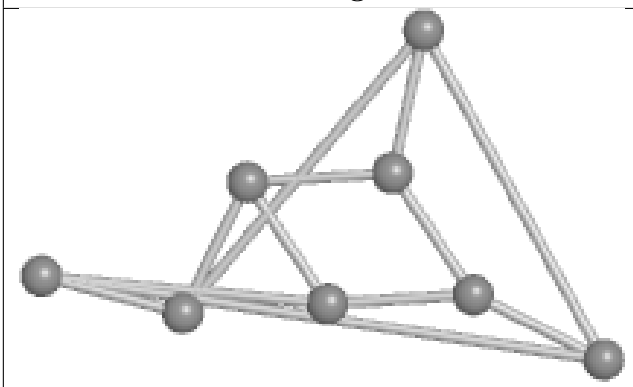
Ligand SF4 M 802



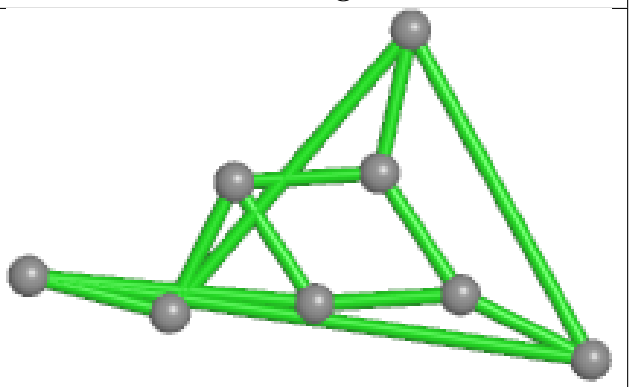
Bond lengths



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.

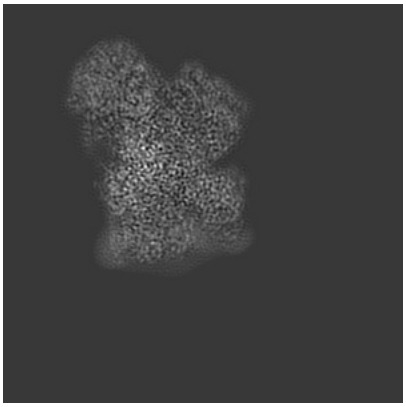
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31883. These allow visual inspection of the internal detail of the map and identification of artifacts.

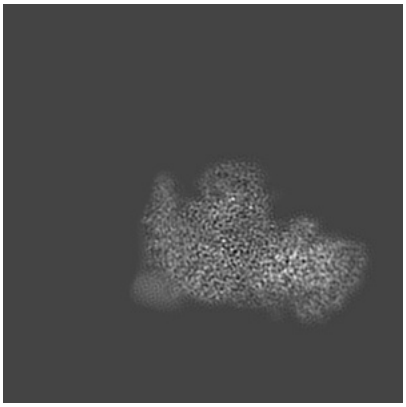
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

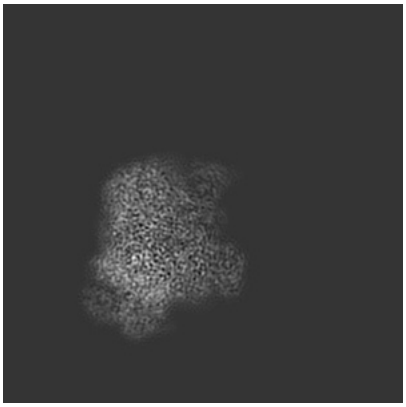
6.1.1 Primary map



X



Y



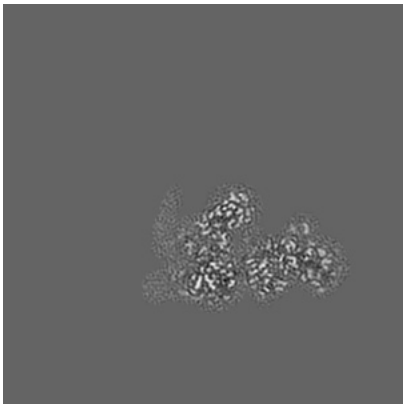
Z

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

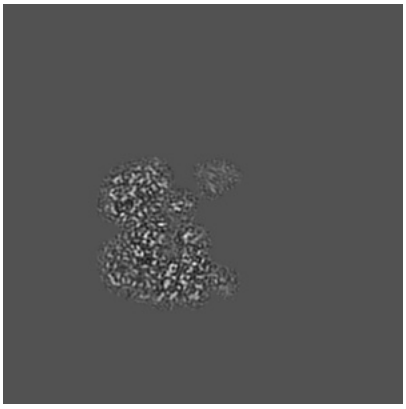
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

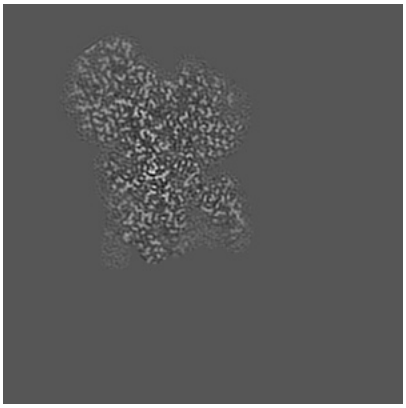


Z Index: 256

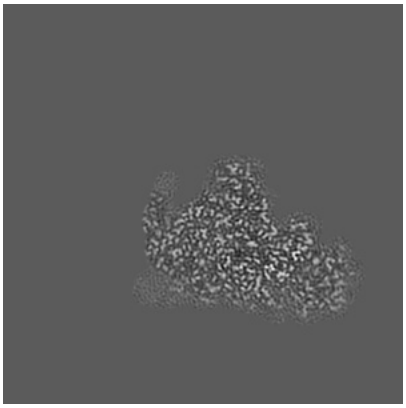
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 184



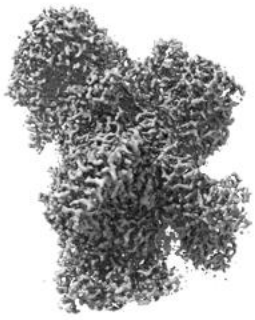
Y Index: 176

Z Index: 290

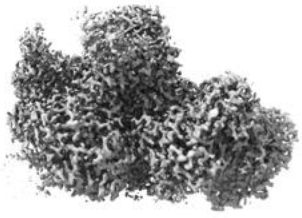
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

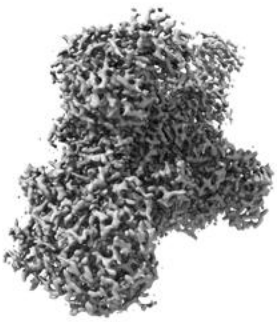
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

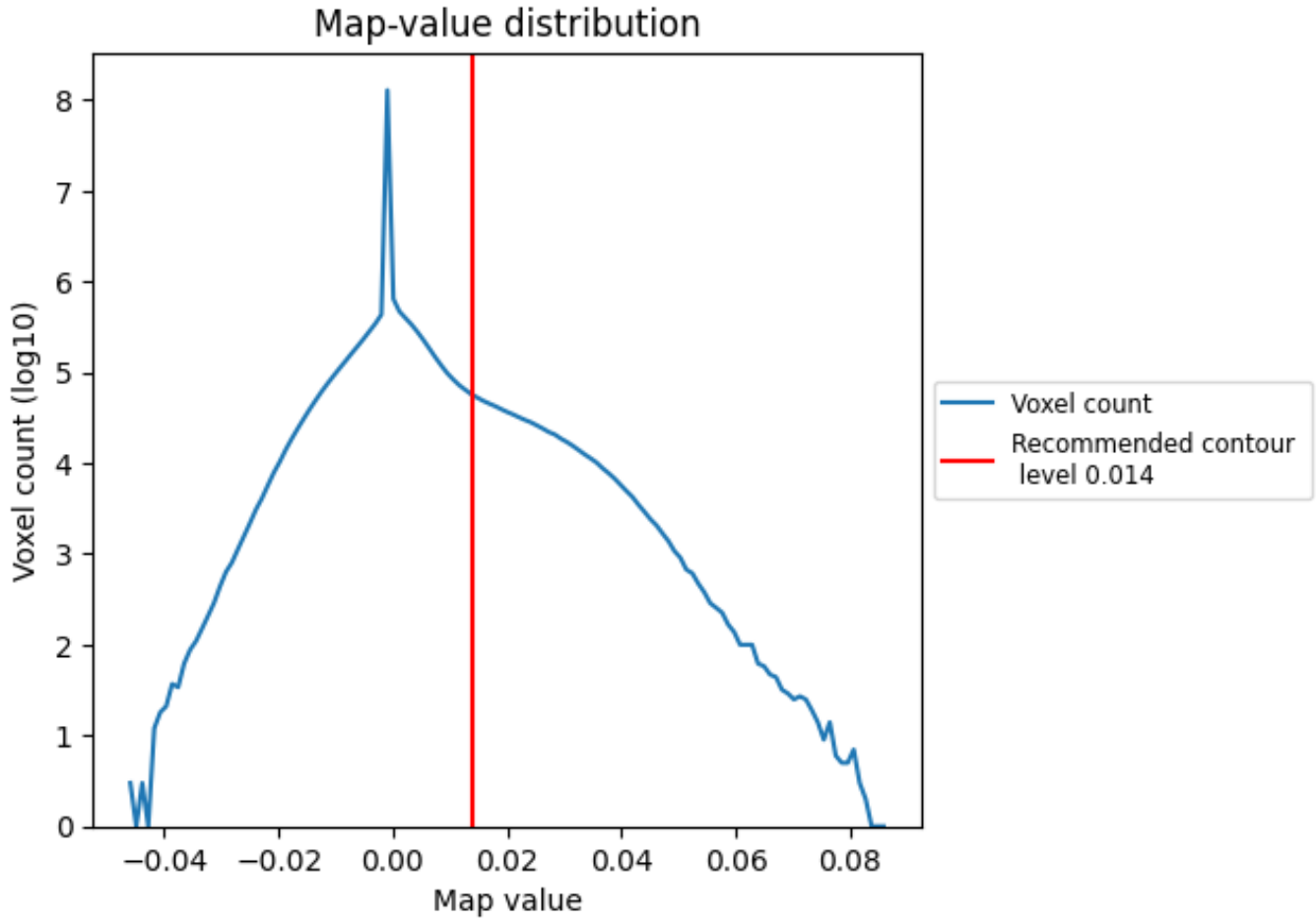
6.5 Mask visualisation (i)

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

7 Map analysis

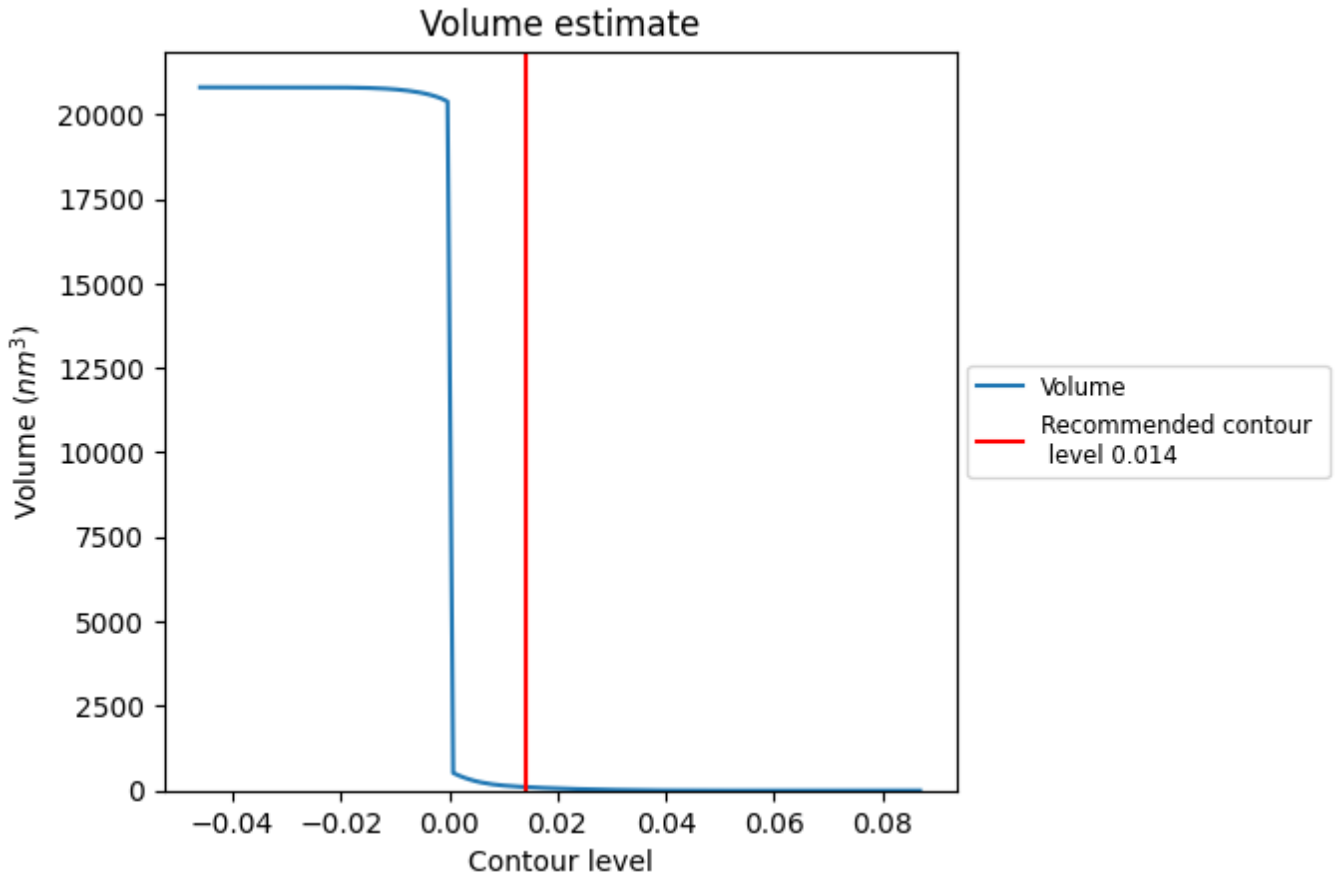
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

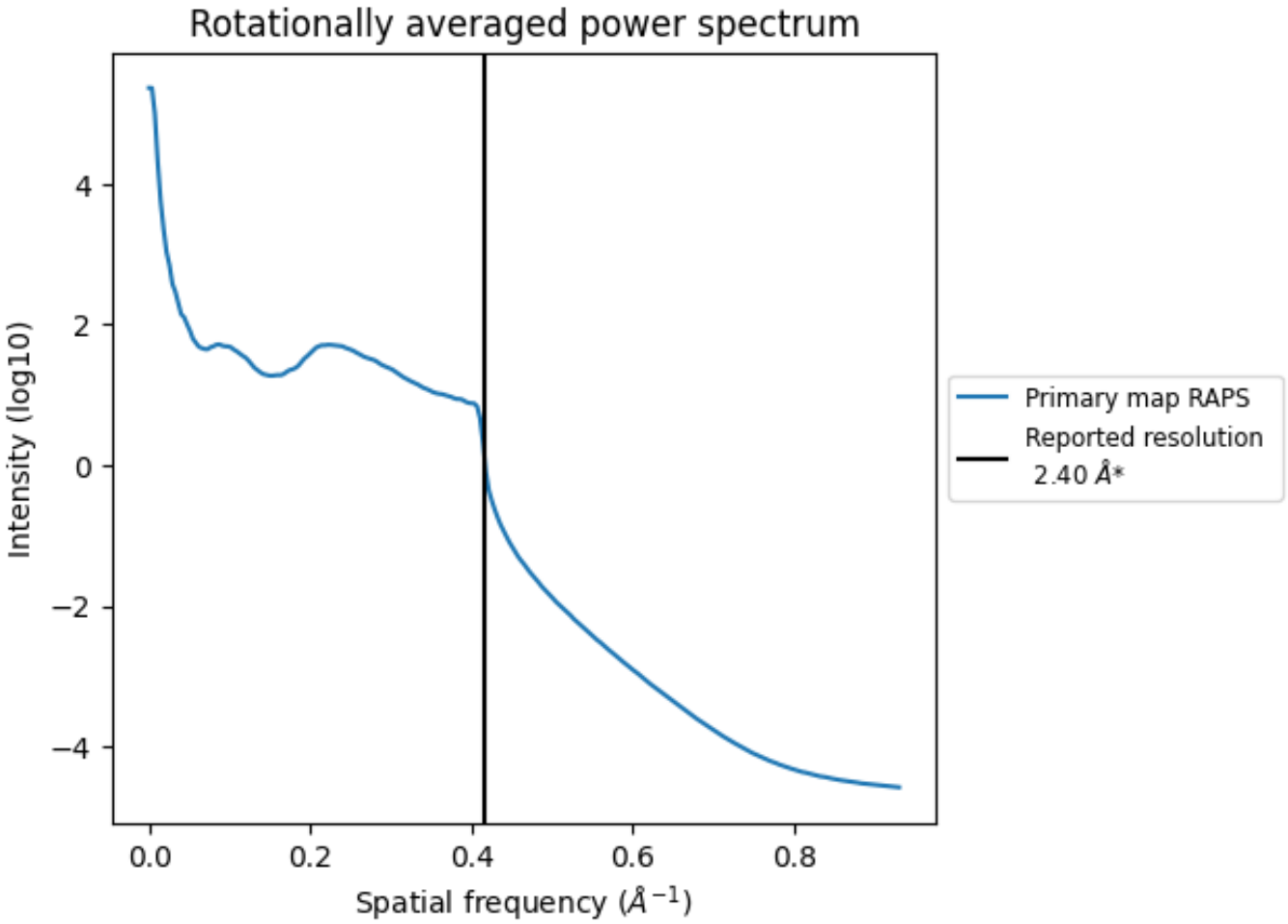
7.2 Volume estimate



The volume at the recommended contour level is 105 nm^3; this corresponds to an approximate mass of 95 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 0.417 $Å^{-1}$

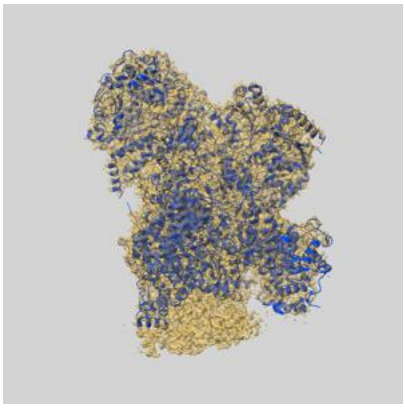
8 Fourier-Shell correlation

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

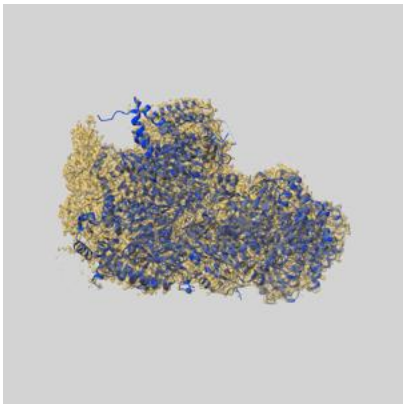
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31883 and PDB model 7VBN. Per-residue inclusion information can be found in section 3 on page 14.

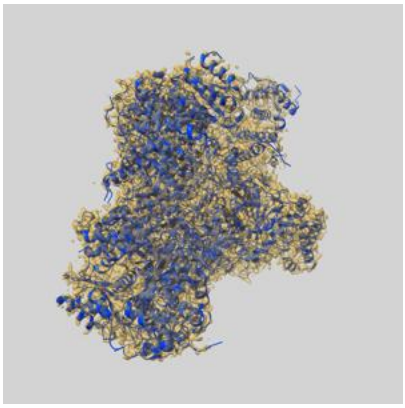
9.1 Map-model overlay



X



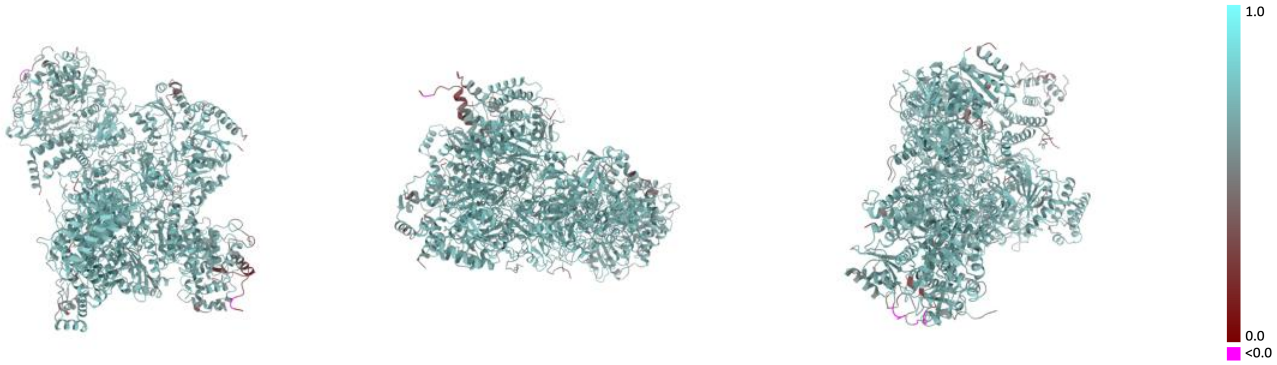
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

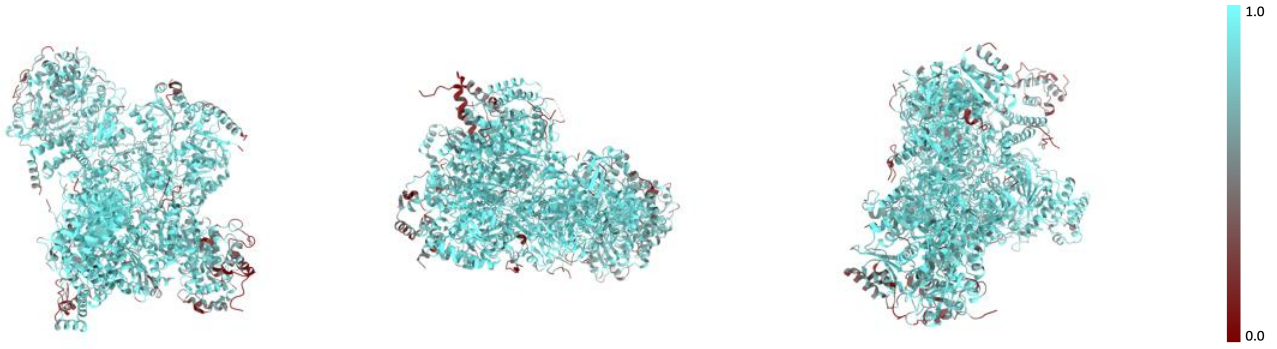
9.2 Q-score mapped to coordinate model (i)



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.

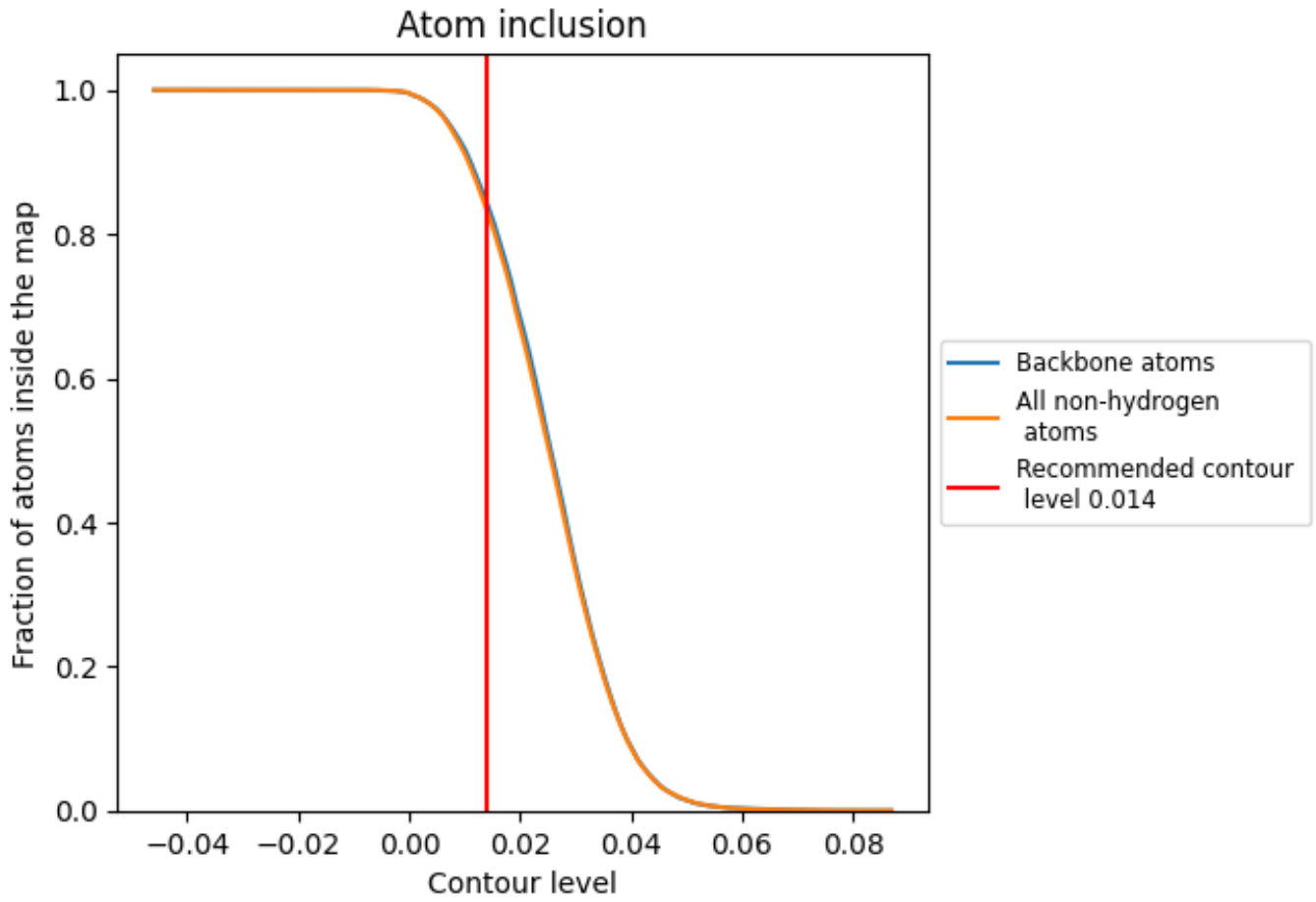
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8337	0.6650
A	0.8278	0.6600
B	0.9294	0.7020
C	0.8607	0.6740
E	0.8482	0.6730
F	0.7649	0.6300
G	0.4294	0.5020
H	0.8514	0.6590
I	0.6918	0.6270
J	0.8162	0.6580
K	0.6570	0.5810
L	0.8753	0.6840
M	0.8944	0.6840
N	0.6743	0.6360
O	0.7412	0.6290
P	0.9497	0.7050
Q	0.9384	0.7010
T	0.7590	0.6540
W	0.6852	0.6120