Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 11:25 AM JST

PDB ID	:	7VY8 / pdb_00007vy8
EMDB ID	:	EMD-32196
Title	:	Matrix arm of active state CI from Q10-NADH dataset
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-13
Resolution	:	2.60 Å(reported)

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

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

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

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

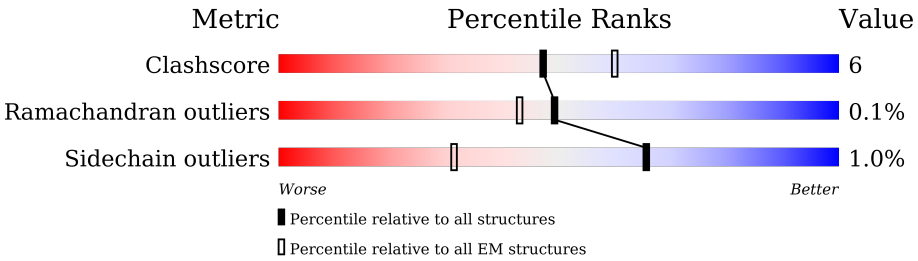
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

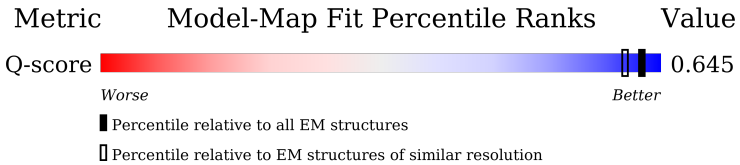
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	81% 19%
2	B	176	89% 11%
3	C	156	86% 14%
4	E	115	6% 87% 11%

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Mol	Chain	Length	Quality of chain
5	F	86	10% 77% 19% 5%
6	G	88	60% 82% 16%
7	H	112	81% 19%
8	I	112	12% 71% 15% 13%
9	J	342	84% 15%
10	K	43	7% 79% 19%
11	L	125	7% 89% 11%
12	M	690	84% 16%
13	N	144	15% 81% 19%
14	O	217	6% 89% 11%
15	P	208	84% 16%
16	Q	386	86% 14%
17	T	96	9% 95% 5%
18	W	29	21% 86% 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	C	301	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 28527 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 13 kDa-B subunit.

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

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

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

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

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

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase 9 kDa subunit.

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase 30 kDa subunit.

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

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

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

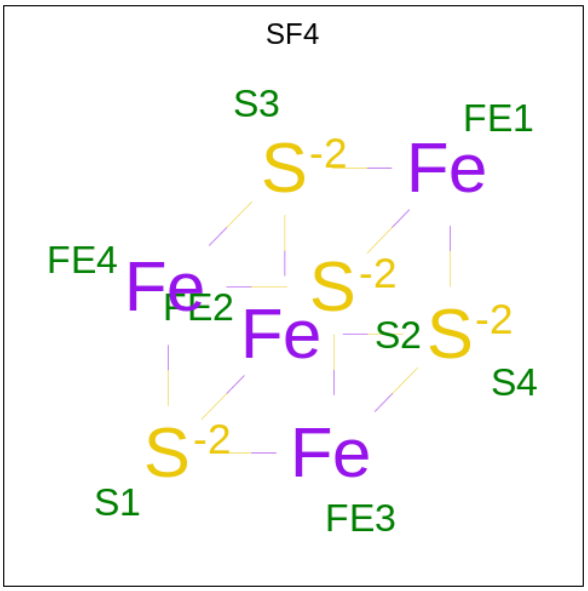
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

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

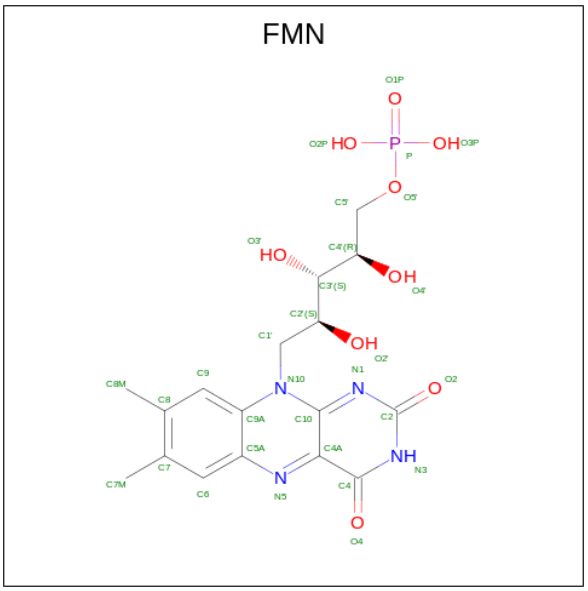
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	29	218	138	40	39	1	0	0

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



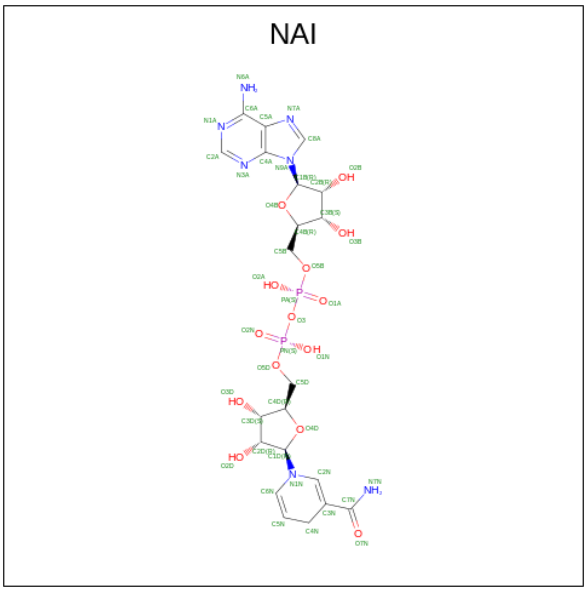
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	A	1	8	4	4	0
19	B	1	8	4	4	0
19	B	1	8	4	4	0
19	C	1	8	4	4	0
19	M	1	8	4	4	0
19	M	1	8	4	4	0

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



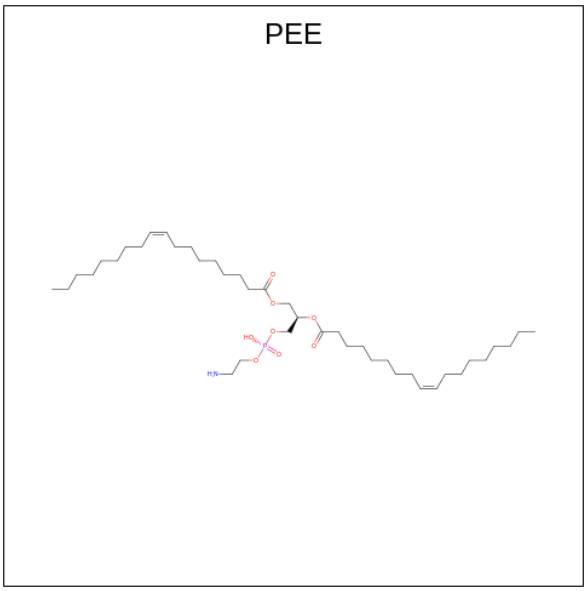
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	A	1	31	17	4	9	1	0

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



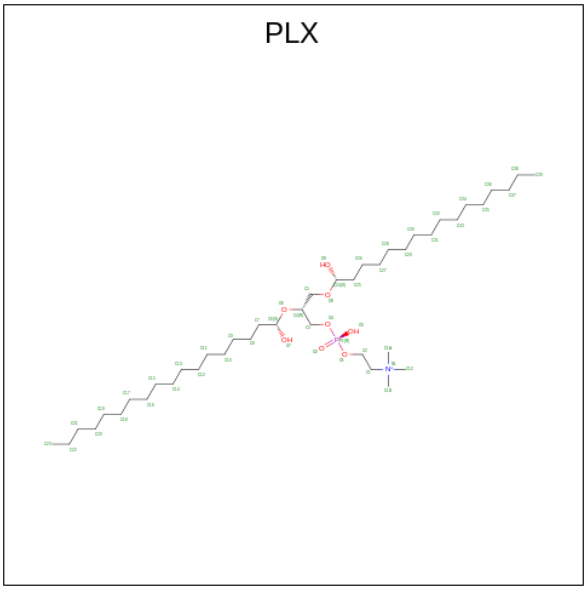
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
21	A	1	44	21	7	14	2	0

- Molecule 22 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



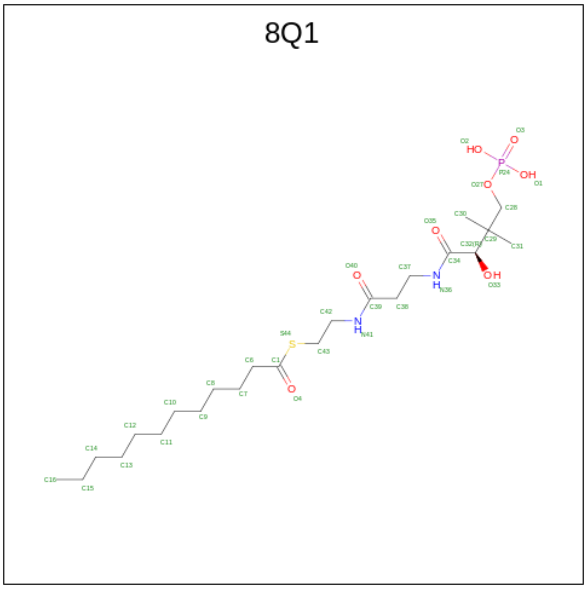
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	C	1	47	37	1	8	1	0

- 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 (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$) (labeled as "Ligand of Interest" by depositor).



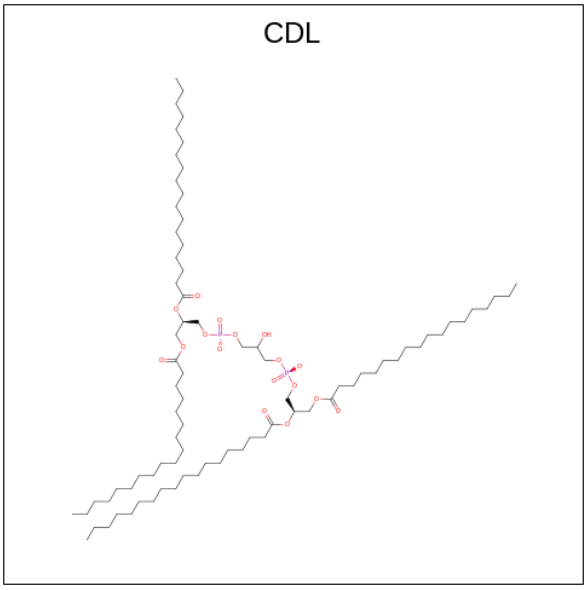
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	C	1	52	42	1	8	1	0

- Molecule 24 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



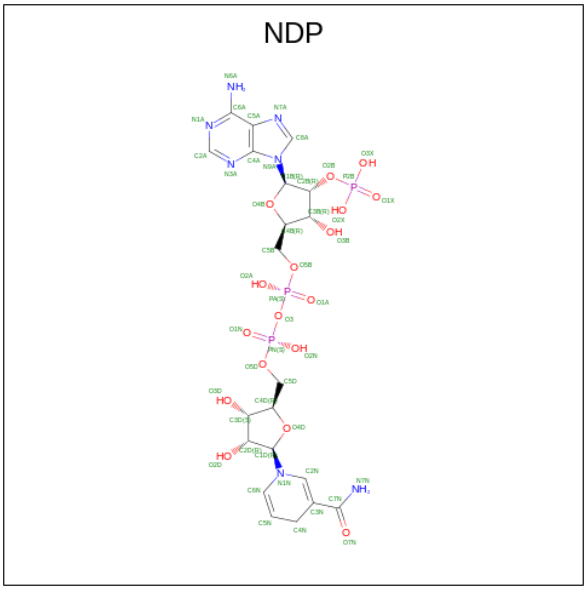
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
24	G	1	35	23	2	8	1	1	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



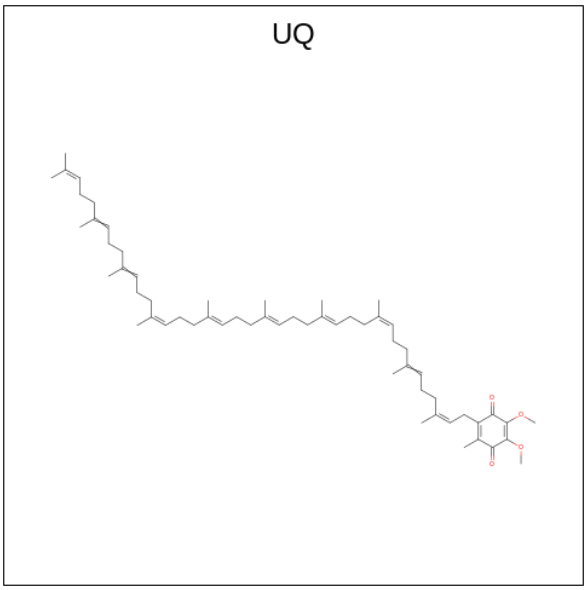
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	I	1	51	32	17	2	0

- Molecule 26 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



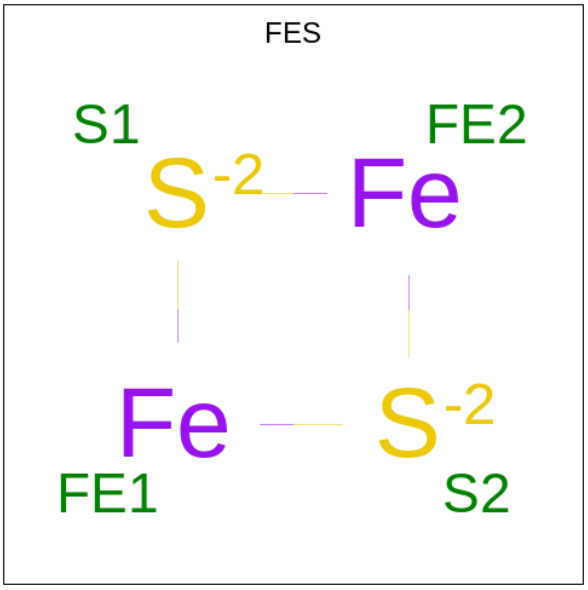
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	J	1	48	21	7	17	3	0

- Molecule 27 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	J	1	33	29	4	0

- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

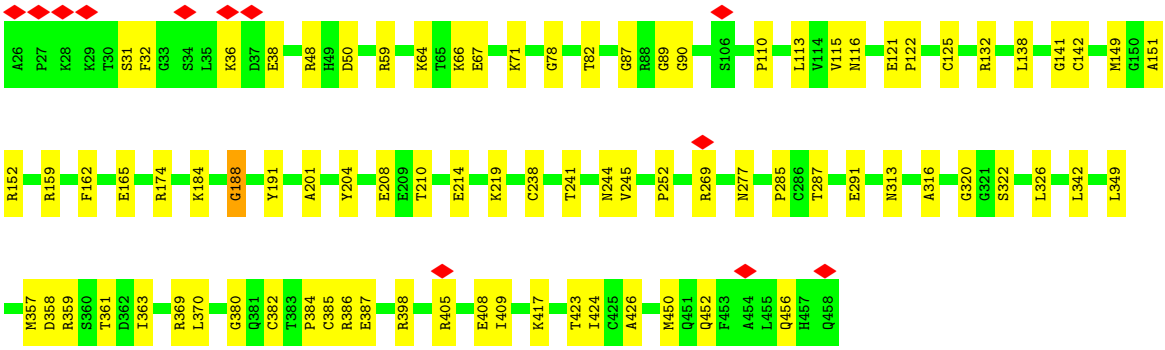
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
30	T	1	1	1	0

3 Residue-property plots (i)

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

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

Chain A:



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

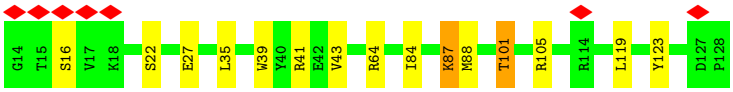
Chain B:

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

Chain C:

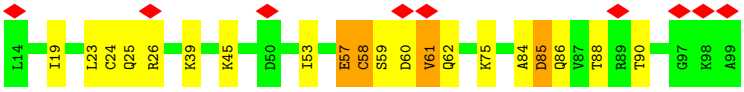
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



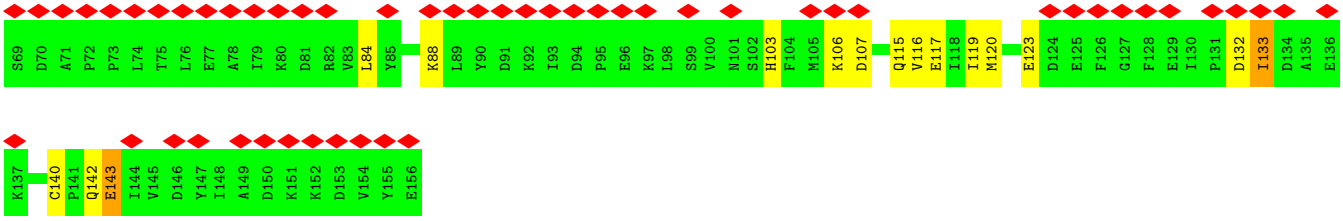
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:



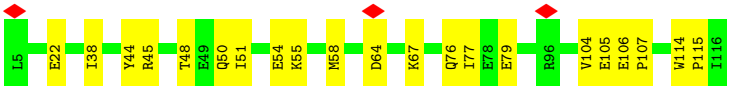
• Molecule 6: Acyl carrier protein

Chain G:



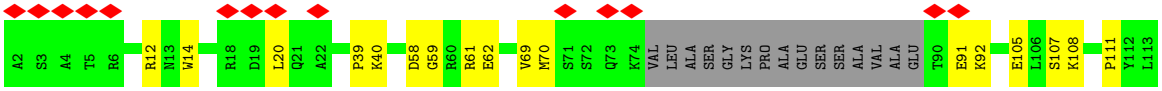
• Molecule 7: NADH-ubiquinone oxidoreductase 13 kDa-B subunit

Chain H:



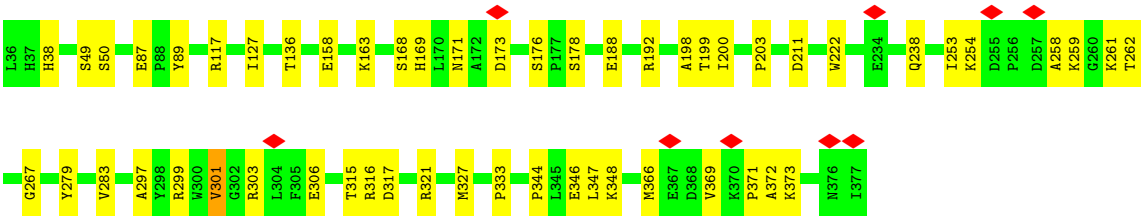
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I:



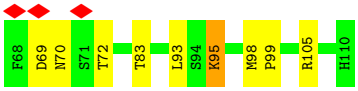
• Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

Chain J:

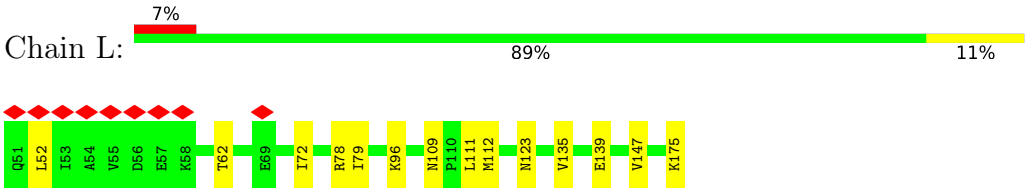


• Molecule 10: NADH-ubiquinone oxidoreductase 9 kDa subunit

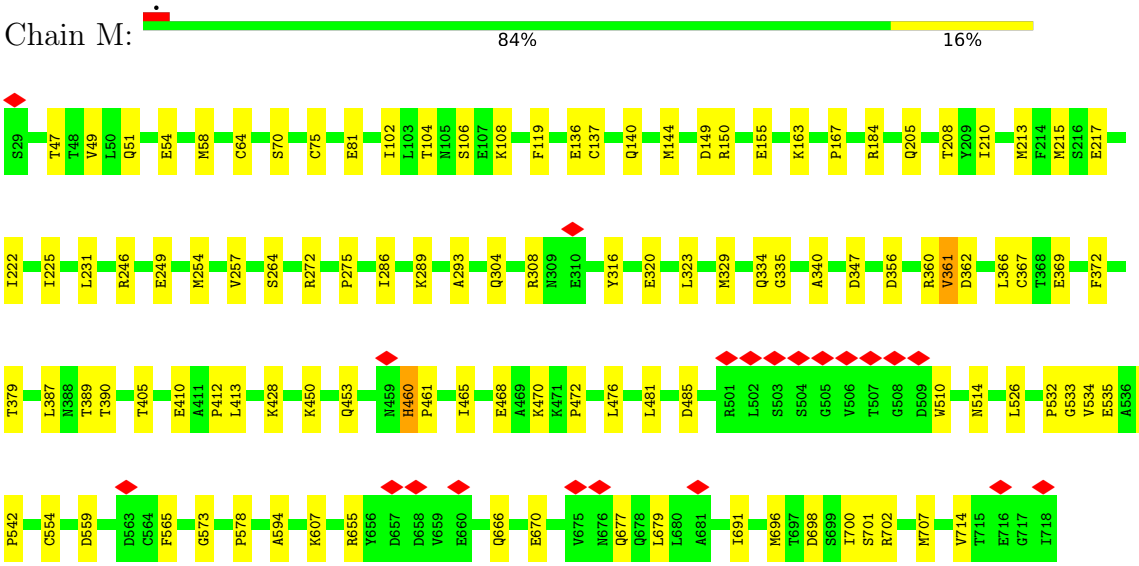
Chain K:



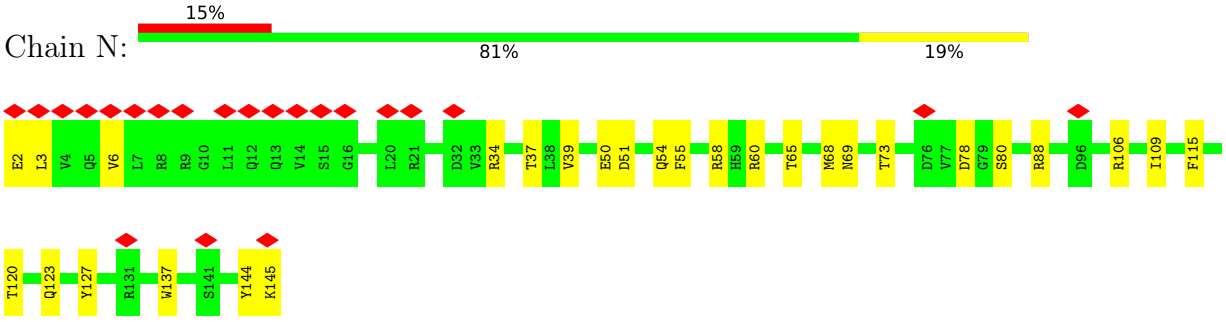
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



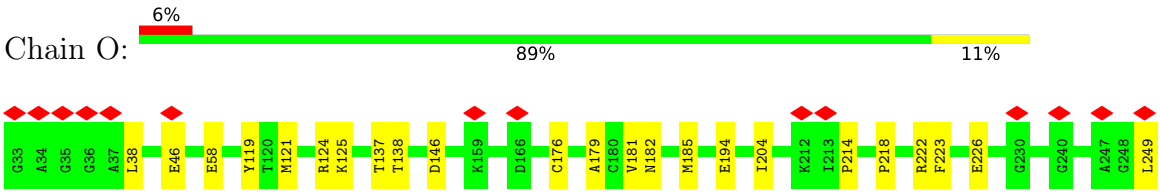
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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

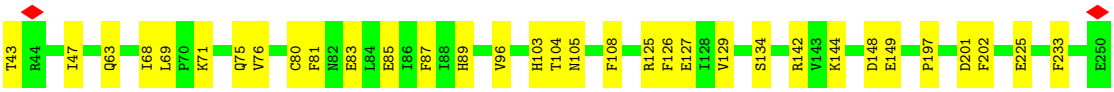


• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



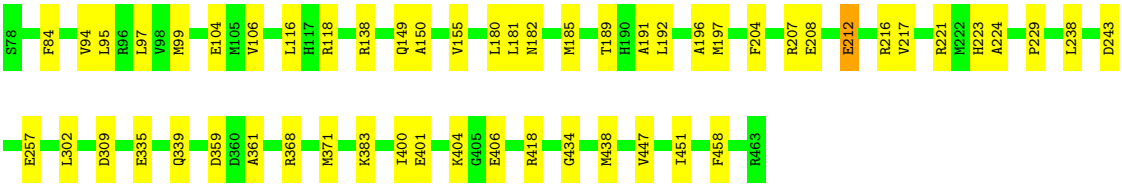
• Molecule 15: NADH-ubiquinone oxidoreductase 30 kDa subunit

Chain P: 84% 16%



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

Chain Q: 86% 14%

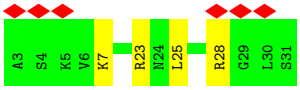


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 9% 95% 5%

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

Chain W: 21% 86% 14%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152604	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	0.216	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0372	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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: NDP, SF4, 2MR, NAI, MG, ZN, PEE, FMN, PLX, UQ, CDL, FES, 8Q1

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	0.18	0/3406	0.37	0/4603
2	B	0.18	0/1443	0.35	0/1952
3	C	0.17	0/1279	0.33	0/1730
4	E	0.15	0/995	0.29	0/1340
5	F	0.17	0/698	0.43	0/940
6	G	0.17	0/705	0.44	0/956
7	H	0.18	0/929	0.39	0/1258
8	I	0.16	0/798	0.38	0/1079
9	J	0.16	0/2828	0.32	0/3834
10	K	0.13	0/377	0.27	0/509
11	L	0.16	0/1039	0.30	0/1403
12	M	0.18	0/5384	0.38	2/7295 (0.0%)
13	N	0.15	0/1245	0.31	0/1694
14	O	0.15	0/1711	0.34	0/2328
15	P	0.18	0/1789	0.37	0/2436
16	Q	0.18	0/3157	0.34	0/4268
17	T	0.14	0/755	0.28	0/1018
18	W	0.14	0/224	0.30	0/302
All	All	0.17	0/28762	0.35	2/38945 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	460	HIS	CA-C-N	7.15	126.99	119.05
12	M	460	HIS	C-N-CA	7.15	126.99	119.05

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	65	0
2	B	1412	0	1363	15	0
3	C	1248	0	1254	15	0
4	E	971	0	975	10	0
5	F	687	0	700	13	0
6	G	693	0	671	9	0
7	H	910	0	950	14	0
8	I	780	0	808	14	0
9	J	2751	0	2773	33	0
10	K	366	0	338	8	0
11	L	1016	0	1016	11	0
12	M	5296	0	5326	66	0
13	N	1204	0	1162	19	0
14	O	1671	0	1673	18	0
15	P	1738	0	1693	23	0
16	Q	3096	0	3063	34	0
17	T	741	0	702	3	0
18	W	218	0	219	5	0
19	A	8	0	0	1	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	8	0
21	A	44	0	27	6	0
22	C	47	0	71	2	0
23	C	52	0	88	6	0
24	G	35	0	0	0	0
25	I	51	0	46	1	0
26	J	48	0	25	1	0
27	J	33	0	39	3	0
28	M	4	0	0	0	0
28	O	4	0	0	0	0
29	M	1	0	0	0	0
30	T	1	0	0	0	0
All	All	28527	0	28293	340	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 6.

All (340) 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)
26:J:401:NDP:O4D	26:J:401:NDP:C4D	1.68	1.19
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.16
1:A:66:LYS:HE3	1:A:188:GLY:O	1.77	0.84
12:M:213:MET:HB3	12:M:215:MET:HE2	1.62	0.81
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.61	0.80
20:A:502:FMN:N1	20:A:502:FMN:O3'	2.13	0.79
1:A:50:ASP:O	1:A:59:ARG:NH2	2.22	0.73
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.21	0.73
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.71	0.72
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.70	0.72
9:J:192:ARG:NH1	9:J:198:ALA:O	2.24	0.71
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.25	0.70
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.24	0.70
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.25	0.69
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.25	0.69
12:M:485:ASP:HA	12:M:677:GLN:HE22	1.58	0.68
20:A:502:FMN:HO3'	20:A:502:FMN:C2	2.05	0.68
10:K:69:ASP:OD1	10:K:70:ASN:N	2.27	0.68
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.27	0.68
6:G:103:HIS:HB2	6:G:106:LYS:HE3	1.76	0.67
1:A:36:LYS:HG3	1:A:38:GLU:HG2	1.76	0.67
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.25	0.67
12:M:468:GLU:O	12:M:470:LYS:NZ	2.27	0.66
4:E:16:SER:HA	11:L:52:LEU:HD13	1.76	0.66
8:I:40:LYS:HB3	18:W:7:LYS:H	1.60	0.66
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.78	0.66
7:H:22:GLU:OE1	7:H:22:GLU:N	2.26	0.66
1:A:152:ARG:NH2	10:K:99:PRO:O	2.31	0.64
1:A:285:PRO:O	14:O:222:ARG:NH2	2.31	0.63
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.80	0.63
1:A:87:GLY:HA3	20:A:502:FMN:O2P	1.98	0.63
11:L:109:ASN:ND2	11:L:111:LEU:O	2.32	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.79	0.63
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.80	0.63
1:A:184:LYS:HB2	10:K:98:MET:SD	2.38	0.63
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.31	0.63
9:J:222:TRP:HB3	27:J:402:UQ:H152	1.81	0.62
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HB3	1:A:361:THR:HG21	1.82	0.61
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.33	0.61
23:C:303:PLX:H381	23:C:303:PLX:H211	1.82	0.60
1:A:48:ARG:NH1	10:K:70:ASN:O	2.35	0.60
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.28	0.60
13:N:120:THR:O	13:N:123:GLN:HG2	2.01	0.60
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.83	0.60
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.84	0.59
3:C:86:MET:HE3	3:C:91:VAL:HG12	1.83	0.59
8:I:107:SER:HB3	8:I:111:PRO:HA	1.84	0.59
12:M:308:ARG:NH2	12:M:578:PRO:O	2.35	0.59
12:M:535:GLU:H	12:M:535:GLU:CD	2.11	0.59
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.84	0.59
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.26	0.58
9:J:178:SER:OG	9:J:317:ASP:OD2	2.21	0.58
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.35	0.57
13:N:68:MET:HG3	13:N:69:ASN:H	1.68	0.57
5:F:57:GLU:O	12:M:655:ARG:NH2	2.36	0.57
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.87	0.57
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.34	0.57
12:M:379:THR:HG21	12:M:526:LEU:HD22	1.87	0.57
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.86	0.57
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.87	0.57
6:G:140:CYS:HB2	6:G:143:GLU:OE2	2.05	0.57
1:A:385:CYS:HB2	19:A:501:SF4:S4	2.44	0.57
5:F:84:ALA:O	5:F:88:THR:HG22	2.05	0.56
7:H:44:TYR:O	7:H:48:THR:HG22	2.05	0.56
9:J:117:ARG:HH12	9:J:158:GLU:HG3	1.68	0.56
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.40	0.56
1:A:244:ASN:ND2	20:A:502:FMN:O2	2.38	0.56
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.88	0.56
1:A:405:ARG:HG3	1:A:408:GLU:HG3	1.86	0.56
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.87	0.56
14:O:38:LEU:O	14:O:124:ARG:NH2	2.39	0.55
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.37	0.55
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.88	0.55
22:C:302:PEE:H67	23:C:303:PLX:H212	1.89	0.55
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.88	0.55
2:B:43:MET:HA	2:B:43:MET:HE2	1.89	0.55
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.87	0.55
12:M:472:PRO:O	12:M:510:TRP:NE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:O	21:A:503:NAI:H2N	2.06	0.55
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.40	0.55
2:B:72:MET:HE2	16:Q:257:GLU:HG2	1.88	0.55
13:N:34:ARG:HH11	13:N:54:GLN:HG2	1.71	0.54
9:J:344:PRO:HG2	9:J:347:LEU:HG	1.88	0.54
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.90	0.54
13:N:51:ASP:OD1	13:N:54:GLN:NE2	2.41	0.54
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.89	0.54
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.89	0.53
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.90	0.53
1:A:214:GLU:OE2	11:L:175:LYS:NZ	2.37	0.53
9:J:163:LYS:NZ	9:J:253:ILE:O	2.31	0.53
14:O:204:ILE:HG23	14:O:214:PRO:HG3	1.90	0.53
8:I:14:TRP:O	18:W:28:ARG:NH2	2.41	0.53
12:M:334:GLN:HA	12:M:361:VAL:HG13	1.91	0.53
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.90	0.53
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.91	0.53
2:B:113:CYS:O	2:B:141:ARG:NH1	2.41	0.52
7:H:48:THR:HA	7:H:51:ILE:HG12	1.92	0.52
14:O:46:GLU:N	14:O:46:GLU:OE2	2.41	0.52
17:T:82:ARG:NH2	17:T:103:ASP:OD2	2.42	0.52
6:G:115:GLN:O	6:G:119:ILE:HG12	2.10	0.52
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.90	0.52
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.52
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.91	0.52
1:A:244:ASN:HB2	20:A:502:FMN:O1P	2.10	0.52
12:M:289:LYS:HA	12:M:707:MET:HE1	1.91	0.52
12:M:405:THR:OG1	12:M:410:GLU:OE2	2.25	0.52
9:J:297:ALA:O	9:J:301:VAL:HG13	2.10	0.51
15:P:127:GLU:OE1	15:P:144:LYS:HE3	2.09	0.51
1:A:204:TYR:OH	21:A:503:NAI:H5N	2.11	0.51
12:M:293:ALA:HB2	12:M:707:MET:HE2	1.93	0.51
1:A:125:CYS:H	1:A:277:ASN:ND2	2.07	0.51
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.44	0.51
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.33	0.51
6:G:132:ASP:C	6:G:133:ILE:HD12	2.36	0.51
12:M:460:HIS:CG	12:M:461:PRO:HD2	2.45	0.51
6:G:106:LYS:HD2	6:G:106:LYS:C	2.36	0.51
9:J:87:GLU:HG3	9:J:89:TYR:H	1.76	0.51
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.93	0.50
1:A:122:PRO:HG2	1:A:322:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:O	1:A:191:TYR:OH	2.22	0.50
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.94	0.50
9:J:199:THR:OG1	9:J:258:ALA:O	2.24	0.50
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.94	0.49
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.94	0.49
20:A:502:FMN:N5	21:A:503:NAI:H4N	2.27	0.49
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.94	0.49
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.46	0.49
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.93	0.49
12:M:167:PRO:HD2	12:M:215:MET:HE1	1.93	0.49
1:A:32:PHE:HB3	1:A:291:GLU:HG2	1.95	0.49
2:B:68:ARG:HH12	18:W:28:ARG:HB3	1.77	0.49
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.94	0.49
5:F:59:SER:OG	5:F:60:ASP:N	2.46	0.49
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.94	0.49
1:A:116:ASN:O	1:A:245:VAL:HG23	2.13	0.49
12:M:163:LYS:HZ1	12:M:205:GLN:HB3	1.78	0.49
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.94	0.49
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.94	0.49
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.95	0.49
7:H:54:GLU:O	7:H:58:MET:HG3	2.12	0.49
12:M:696:MET:HB3	12:M:702:ARG:HG2	1.94	0.49
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.95	0.48
4:E:101:THR:O	4:E:105:ARG:HG3	2.12	0.48
1:A:426:ALA:HB3	20:A:502:FMN:HM82	1.94	0.48
7:H:38:ILE:O	7:H:45:ARG:NH1	2.40	0.48
1:A:326:LEU:H	1:A:326:LEU:HD23	1.78	0.48
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.94	0.48
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.46	0.48
7:H:76:GLN:O	7:H:79:GLU:N	2.41	0.48
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.96	0.48
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.96	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.78	0.48
3:C:53:LEU:HD22	23:C:303:PLX:H322	1.96	0.48
5:F:86:GLN:O	5:F:90:THR:HG22	2.14	0.48
12:M:335:GLY:HA2	12:M:362:ASP:O	2.13	0.48
13:N:39:VAL:CG2	13:N:50:GLU:HB2	2.43	0.48
1:A:214:GLU:OE1	1:A:219:LYS:NZ	2.42	0.47
8:I:14:TRP:CD1	18:W:28:ARG:HH22	2.32	0.47
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.96	0.47
12:M:367:CYS:HB3	12:M:533:GLY:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:68:MET:HG2	13:N:115:PHE:CD2	2.49	0.47
13:N:144:TYR:CZ	13:N:145:LYS:HD3	2.49	0.47
3:C:41:SER:N	3:C:44:GLU:OE2	2.47	0.47
9:J:168:SER:O	9:J:203:PRO:HD2	2.14	0.47
15:P:129:VAL:HG22	15:P:144:LYS:HG2	1.95	0.47
16:Q:192:LEU:HD12	16:Q:197:MET:HA	1.96	0.47
3:C:116:ALA:O	3:C:120:VAL:HG22	2.15	0.47
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.97	0.47
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.97	0.47
1:A:269:ARG:HG3	1:A:269:ARG:HH11	1.80	0.47
15:P:201:ASP:OD1	15:P:201:ASP:N	2.41	0.47
1:A:387:GLU:HG2	12:M:119:PHE:O	2.15	0.47
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.96	0.47
1:A:90:GLY:HA3	21:A:503:NAI:H1D	1.97	0.47
8:I:91:GLU:HG2	8:I:92:LYS:H	1.80	0.47
1:A:67:GLU:O	1:A:71:LYS:HG2	2.15	0.46
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.77	0.46
12:M:329:MET:HG2	12:M:565:PHE:CG	2.50	0.46
12:M:369:GLU:HB3	12:M:554:CYS:SG	2.55	0.46
9:J:262:THR:O	9:J:333:PRO:HD2	2.15	0.46
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.50	0.46
3:C:103:MET:HE1	3:C:121:TYR:HB2	1.97	0.46
10:K:95:LYS:O	10:K:95:LYS:HG2	2.15	0.46
11:L:135:VAL:O	11:L:139:GLU:HG3	2.15	0.46
17:T:79:VAL:O	17:T:121:PRO:HD3	2.15	0.46
19:C:301:SF4:S2	16:Q:138:ARG:HG2	2.56	0.46
9:J:168:SER:OG	9:J:169:HIS:N	2.49	0.46
13:N:65:THR:O	13:N:73:THR:OG1	2.33	0.46
16:Q:447:VAL:O	16:Q:451:ILE:HG13	2.16	0.46
1:A:409:ILE:HG13	1:A:450:MET:HE1	1.98	0.46
1:A:452:GLN:O	1:A:456:GLN:HB2	2.15	0.46
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.46	0.46
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.97	0.45
12:M:58:MET:HE2	12:M:104:THR:HB	1.97	0.45
20:A:502:FMN:H9	20:A:502:FMN:H1'1	1.70	0.45
3:C:98:ARG:HA	3:C:125:PRO:HD3	1.98	0.45
12:M:372:PHE:H	12:M:532:PRO:HB2	1.82	0.45
13:N:144:TYR:HD1	13:N:144:TYR:H	1.62	0.45
9:J:317:ASP:OD1	9:J:321:ARG:NH1	2.46	0.45
1:A:78:GLY:O	1:A:82:THR:HG23	2.16	0.45
5:F:39:LYS:HE2	5:F:39:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:70:MET:O	8:I:70:MET:SD	2.75	0.45
12:M:698:ASP:OD1	12:M:701:SER:OG	2.29	0.45
16:Q:335:GLU:OE2	16:Q:339:GLN:NE2	2.45	0.45
1:A:277:ASN:OD1	1:A:287:THR:OG1	2.21	0.45
7:H:50:GLN:O	7:H:54:GLU:HG3	2.15	0.45
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.97	0.45
9:J:283:VAL:HG22	9:J:369:VAL:HG11	1.99	0.45
9:J:373:LYS:HB3	9:J:373:LYS:HE2	1.76	0.45
12:M:450:LYS:HE2	12:M:450:LYS:HB2	1.72	0.45
3:C:107:GLY:HA2	19:C:301:SF4:S1	2.57	0.45
15:P:148:ASP:N	15:P:148:ASP:OD1	2.49	0.45
1:A:122:PRO:HA	14:O:176:CYS:SG	2.57	0.45
12:M:537:ILE:HG23	12:M:542:PRO:HD3	1.97	0.45
2:B:211:TYR:CE1	8:I:39:PRO:HG3	2.52	0.45
14:O:58:GLU:OE1	14:O:58:GLU:N	2.40	0.45
8:I:69:VAL:O	15:P:76:VAL:HB	2.16	0.44
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.84	0.44
3:C:44:GLU:HA	3:C:47:VAL:HG22	1.99	0.44
23:C:303:PLX:H1A2	23:C:303:PLX:H22	1.85	0.44
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.53	0.44
12:M:222:ILE:HD12	12:M:231:LEU:HD13	1.98	0.44
16:Q:434:GLY:O	16:Q:438:MET:HG3	2.16	0.44
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.99	0.44
1:A:201:ALA:O	14:O:119:TYR:HB3	2.17	0.44
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.52	0.44
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.98	0.44
11:L:78:ARG:HD2	12:M:607:LYS:HE2	2.00	0.44
27:J:402:UQ:H202	27:J:402:UQ:H172	1.77	0.44
8:I:58:ASP:OD2	8:I:61:ARG:HB2	2.18	0.44
1:A:149:MET:HE3	1:A:241:THR:HB	1.98	0.44
14:O:125:LYS:HE3	14:O:125:LYS:HB2	1.63	0.44
1:A:110:PRO:O	1:A:238:CYS:HB3	2.17	0.44
9:J:211:ASP:OD1	9:J:211:ASP:C	2.61	0.44
12:M:81:GLU:OE1	12:M:106:SER:OG	2.21	0.44
25:I:201:CDL:H511	25:I:201:CDL:H542	1.57	0.44
14:O:179:ALA:HB3	14:O:185:MET:HE3	2.00	0.44
1:A:159:ARG:NH2	14:O:176:CYS:O	2.41	0.43
5:F:25:GLN:HG2	5:F:26:ARG:HG3	1.99	0.43
5:F:58:CYS:SG	5:F:59:SER:N	2.91	0.43
9:J:254:LYS:HB3	9:J:254:LYS:HE2	1.85	0.43
16:Q:371:MET:HE3	16:Q:371:MET:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:HE2	10:K:98:MET:SD	2.58	0.43
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.81	0.43
15:P:126:PHE:HE2	15:P:149:GLU:HG3	1.84	0.43
1:A:64:LYS:HD3	14:O:249:LEU:HD23	2.01	0.43
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.99	0.43
1:A:208:GLU:OE2	1:A:210:THR:OG1	2.35	0.43
1:A:269:ARG:HG3	1:A:269:ARG:NH1	2.32	0.43
1:A:320:GLY:HA3	1:A:349:LEU:O	2.19	0.43
12:M:356:ASP:O	12:M:360:ARG:HG2	2.19	0.43
1:A:326:LEU:CD1	1:A:363:ILE:HD11	2.49	0.43
12:M:573:GLY:HA3	13:N:137:TRP:CG	2.54	0.43
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.54	0.43
5:F:19:ILE:HD11	5:F:53:ILE:HG12	2.00	0.43
12:M:320:GLU:OE1	12:M:320:GLU:N	2.48	0.43
3:C:59:ARG:NH2	23:C:303:PLX:O3	2.42	0.43
9:J:50:SER:OG	15:P:225:GLU:OE2	2.34	0.43
7:H:106:GLU:HG3	7:H:107:PRO:HD2	2.00	0.42
12:M:691:ILE:HG23	12:M:714:VAL:HG11	2.01	0.42
16:Q:185:MET:O	16:Q:189:THR:OG1	2.32	0.42
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.55	0.42
11:L:62:THR:HG23	11:L:72:ILE:HD13	2.02	0.42
12:M:666:GLN:O	12:M:670:GLU:HG3	2.19	0.42
5:F:85:ASP:OD1	5:F:85:ASP:N	2.51	0.42
6:G:106:LYS:HD2	6:G:107:ASP:N	2.35	0.42
12:M:264:SER:OG	12:M:272:ARG:HG2	2.20	0.42
4:E:39:TRP:O	4:E:43:VAL:HG23	2.20	0.42
7:H:104:VAL:HG23	15:P:71:LYS:HG2	2.01	0.42
9:J:303:ARG:HB2	9:J:316:ARG:HD3	2.01	0.42
9:J:173:ASP:OD1	9:J:176:SER:HB3	2.20	0.42
9:J:366:MET:HE2	9:J:366:MET:HB3	1.95	0.42
27:J:402:UQ:H103	27:J:402:UQ:H121	1.87	0.42
12:M:289:LYS:HA	12:M:707:MET:CE	2.50	0.42
13:N:2:GLU:HG2	13:N:3:LEU:N	2.35	0.42
1:A:369:ARG:HA	1:A:369:ARG:HD2	1.79	0.42
4:E:35:LEU:HD13	4:E:87:LYS:HG3	2.02	0.42
18:W:23:ARG:HD3	18:W:25:LEU:HD12	2.02	0.42
7:H:64:ASP:HB3	7:H:67:LYS:HB2	2.00	0.42
14:O:146:ASP:OD1	14:O:146:ASP:N	2.52	0.42
1:A:316:ALA:HB1	1:A:326:LEU:HD12	2.01	0.42
1:A:358:ASP:O	1:A:361:THR:HG22	2.20	0.42
9:J:299:ARG:NH1	9:J:316:ARG:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:127:TYR:OH	17:T:61:GLU:O	2.35	0.42
14:O:121:MET:HE3	14:O:121:MET:HB3	1.96	0.42
16:Q:84:PHE:HB2	16:Q:99:MET:HE2	2.01	0.42
1:A:382:CYS:HB3	1:A:424:ILE:HD12	2.02	0.41
3:C:173:LEU:O	3:C:177:ILE:HG12	2.20	0.41
9:J:238:GLN:NE2	9:J:267:GLY:O	2.46	0.41
6:G:116:VAL:HG12	6:G:120:MET:HE2	2.01	0.41
8:I:59:GLY:HA2	8:I:62:GLU:HG3	2.02	0.41
9:J:171:ASN:HA	9:J:327:MET:HE3	2.01	0.41
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.01	0.41
5:F:23:LEU:HD23	5:F:23:LEU:H	1.85	0.41
2:B:200:GLU:HG3	13:N:88:ARG:HD3	2.03	0.41
3:C:41:SER:OG	3:C:42:ARG:N	2.52	0.41
12:M:453:GLN:NE2	12:M:679:LEU:HD12	2.35	0.41
13:N:3:LEU:O	13:N:6:VAL:HG22	2.19	0.41
1:A:313:ASN:O	1:A:359:ARG:HG3	2.20	0.41
4:E:119:LEU:HD23	4:E:119:LEU:HA	1.96	0.41
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.56	0.41
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.89	0.41
12:M:428:LYS:HE2	12:M:465:ILE:HD13	2.03	0.41
16:Q:180:LEU:HD23	16:Q:180:LEU:HA	1.92	0.41
12:M:208:THR:C	12:M:210:ILE:H	2.27	0.41
13:N:50:GLU:HG3	13:N:60:ARG:HG2	2.03	0.41
13:N:55:PHE:CE1	13:N:58:ARG:HG3	2.56	0.41
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.61	0.41
22:C:302:PEE:H75	22:C:302:PEE:H68	1.89	0.41
4:E:41:ARG:HA	4:E:41:ARG:HD2	1.87	0.41
12:M:254:MET:HE1	12:M:700:ILE:HB	2.02	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.93	0.41
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.35	0.41
8:I:105:GLU:OE1	8:I:105:GLU:HA	2.20	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.56	0.41
15:P:43:THR:O	15:P:47:ILE:HB	2.21	0.41
15:P:197:PRO:HA	15:P:202:PHE:CD2	2.56	0.41
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.53	0.41
5:F:61:VAL:HG13	5:F:62:GLN:H	1.86	0.41
5:F:75:LYS:HE2	5:F:75:LYS:HB3	1.90	0.41
13:N:106:ARG:HB2	13:N:109:ILE:HG13	2.03	0.41
11:L:79:ILE:HB	11:L:147:VAL:HG22	2.03	0.40
12:M:323:LEU:HD23	12:M:323:LEU:HA	1.94	0.40
15:P:81:PHE:CD1	15:P:83:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:98:MET:HE3	10:K:98:MET:HB3	1.80	0.40
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.03	0.40
3:C:62:LEU:O	3:C:91:VAL:HA	2.21	0.40
8:I:108:LYS:HZ2	8:I:108:LYS:HG2	1.79	0.40
1:A:149:MET:HE2	1:A:149:MET:HB2	1.86	0.40
1:A:201:ALA:HB1	14:O:121:MET:HB2	2.02	0.40
1:A:322:SER:HB2	1:A:370:LEU:HD22	2.04	0.40
6:G:84:LEU:HD23	6:G:84:LEU:HA	1.82	0.40
12:M:257:VAL:HG11	12:M:413:LEU:HB2	2.02	0.40
13:N:78:ASP:OD1	13:N:80:SER:HB2	2.21	0.40
15:P:108:PHE:CD1	15:P:134:SER:HB2	2.57	0.40
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.92	0.40
23:C:303:PLX:H102	23:C:303:PLX:H261	2.03	0.40
9:J:348:LYS:HD3	9:J:348:LYS:HA	1.94	0.40
12:M:70:SER:O	12:M:184:ARG:NH1	2.53	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%)	419 (97%)	11 (3%)	1 (0%)	43	66
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	10	23
7	H	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	14	30
8	I	93/112 (83%)	84 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	340/342 (99%)	323 (95%)	16 (5%)	1 (0%)	36	58
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	664 (96%)	24 (4%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	383/386 (99%)	371 (97%)	12 (3%)	0	100	100
17	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
18	W	27/29 (93%)	24 (89%)	3 (11%)	0	100	100
All	All	3504/3558 (98%)	3371 (96%)	129 (4%)	4 (0%)	49	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
1	A	188	GLY
9	J	38	HIS
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%)	345 (100%)	1 (0%)	86	94
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	88
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	75
5	F	75/76 (99%)	70 (93%)	5 (7%)	15	33
6	G	76/81 (94%)	72 (95%)	4 (5%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	89
10	K	42/42 (100%)	38 (90%)	4 (10%)	8	18
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	576 (99%)	4 (1%)	76	89
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	88
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	92
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	84
16	Q	332/332 (100%)	329 (99%)	3 (1%)	70	87
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	23/24 (96%)	23 (100%)	0	100	100
All	All	3041/3058 (99%)	3011 (99%)	30 (1%)	65	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
3	C	71	CYS
4	E	87	LYS
4	E	101	THR
5	F	24	CYS
5	F	57	GLU
5	F	58	CYS
5	F	61	VAL
5	F	85	ASP
6	G	88	LYS
6	G	123	GLU
6	G	142	GLN
6	G	143	GLU
9	J	136	THR
9	J	301	VAL
10	K	72	THR
10	K	83	THR
10	K	95	LYS
10	K	105	ARG
12	M	108	LYS
12	M	361	VAL

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Mol	Chain	Res	Type
12	M	534	VAL
12	M	559	ASP
13	N	37	THR
14	O	181	VAL
15	P	63	GLN
15	P	80	CYS
16	Q	104	GLU
16	Q	212	GLU
16	Q	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	393	ASN
1	A	452	GLN
2	B	59	GLN
2	B	206	GLN
3	C	111	ASN
4	E	51	GLN
4	E	70	ASN
6	G	142	GLN
7	H	76	GLN
8	I	13	ASN
8	I	25	GLN
8	I	47	HIS
9	J	138	ASN
10	K	106	GLN
11	L	71	HIS
12	M	304	GLN
12	M	453	GLN
12	M	677	GLN
13	N	123	GLN
14	O	133	GLN
15	P	55	HIS
15	P	82	ASN
15	P	196	HIS
15	P	228	GLN
16	Q	250	ASN
16	Q	264	ASN
17	T	117	GLN
17	T	122	HIS

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	6.42	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	5.61	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	13.14	131.53	119.48
16	Q	118	2MR	CD-NE-CZ	4.76	132.32	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.87	130.21	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	B	301	2	0,12,12	-	-	-		
21	NAI	A	503	-	45,48,48	3.88	19 (42%)	60,73,73	1.77	11 (18%)
23	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.64	1 (1%)
24	8Q1	G	201	6	31,34,34	1.68	6 (19%)	40,43,43	1.63	6 (15%)
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	B	302	2	0,12,12	-	-	-		
20	FMN	A	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.32	7 (14%)
19	SF4	A	501	1	0,12,12	-	-	-		
27	UQ	J	402	-	33,33,63	3.47	8 (24%)	40,43,79	2.70	13 (32%)
28	FES	M	803	12	0,4,4	-	-	-		
22	PEE	C	302	-	46,46,50	1.21	6 (13%)	49,51,55	1.00	2 (4%)
25	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.14	4 (7%)
26	NDP	J	401	-	49,52,52	4.38	23 (46%)	66,80,80	2.19	13 (19%)
28	FES	O	301	14	0,4,4	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		
19	SF4	M	801	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	B	301	2	-	-	0/6/5/5
21	NAI	A	503	-	-	8/29/72/72	0/5/5/5
24	8Q1	G	201	6	-	11/41/41/41	-
19	SF4	C	301	3	-	-	0/6/5/5
19	SF4	B	302	2	-	-	0/6/5/5
20	FMN	A	502	-	-	9/18/18/18	0/3/3/3
19	SF4	A	501	1	-	-	0/6/5/5
27	UQ	J	402	-	-	9/27/51/87	0/1/1/1
28	FES	M	803	12	-	-	0/1/1/1
22	PEE	C	302	-	-	19/50/50/54	-
25	CDL	I	201	-	-	31/61/61/110	-
19	SF4	M	801	12	-	-	0/6/5/5
26	NDP	J	401	-	-	6/34/77/77	0/4/5/5
28	FES	O	301	14	-	-	0/1/1/1
19	SF4	M	802	12	-	-	0/6/5/5
23	PLX	C	303	-	-	30/55/55/55	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	C3B-C2B	-13.01	1.23	1.52
26	J	401	NDP	C6N-C5N	12.34	1.55	1.33
26	J	401	NDP	O4D-C4D	10.65	1.68	1.45
21	A	503	NAI	C3D-C4D	-10.33	1.26	1.53
26	J	401	NDP	C3D-C4D	-9.92	1.27	1.53
27	J	402	UQ	C18-C19	9.60	1.56	1.33
27	J	402	UQ	C13-C14	9.37	1.55	1.33
21	A	503	NAI	O4B-C1B	9.13	1.63	1.42
27	J	402	UQ	C8-C9	9.10	1.54	1.33
21	A	503	NAI	O4B-C4B	-8.24	1.26	1.45
26	J	401	NDP	O4B-C4B	-7.93	1.27	1.45
27	J	402	UQ	C23-C24	7.82	1.54	1.32
21	A	503	NAI	C2D-C1D	-7.54	1.29	1.53
26	J	401	NDP	C2N-C3N	7.37	1.55	1.34
21	A	503	NAI	C2B-C1B	-7.17	1.30	1.53
21	A	503	NAI	O4D-C4D	6.71	1.60	1.45
21	A	503	NAI	C2D-C3D	5.93	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	C6A-N6A	5.80	1.48	1.34
21	A	503	NAI	C7N-N7N	5.71	1.48	1.33
26	J	401	NDP	P2B-O2B	5.49	1.69	1.59
21	A	503	NAI	O4D-C1D	5.35	1.54	1.42
26	J	401	NDP	C3B-C4B	5.31	1.66	1.53
24	G	201	8Q1	C34-N36	5.28	1.45	1.33
21	A	503	NAI	C4N-C3N	-5.14	1.39	1.49
24	G	201	8Q1	C39-N41	5.13	1.45	1.33
21	A	503	NAI	C6A-N6A	5.09	1.46	1.34
26	J	401	NDP	O4D-C1D	-4.92	1.30	1.42
26	J	401	NDP	C6N-N1N	4.90	1.49	1.37
20	A	502	FMN	C9A-C5A	4.66	1.49	1.41
26	J	401	NDP	O4B-C1B	4.54	1.52	1.42
26	J	401	NDP	C1B-N9A	-4.51	1.33	1.46
21	A	503	NAI	O2B-C2B	4.51	1.53	1.43
26	J	401	NDP	O2D-C2D	-4.26	1.32	1.43
26	J	401	NDP	C7N-N7N	4.11	1.44	1.33
21	A	503	NAI	C6N-C5N	3.90	1.40	1.33
22	C	302	PEE	C18-C19	3.73	1.53	1.31
22	C	302	PEE	C39-C38	3.66	1.53	1.31
25	I	201	CDL	OA8-CA7	3.46	1.43	1.33
21	A	503	NAI	C7N-C3N	3.44	1.56	1.48
21	A	503	NAI	C4N-C5N	-3.34	1.40	1.48
26	J	401	NDP	C8A-N9A	-3.18	1.31	1.37
20	A	502	FMN	C8-C7	3.12	1.48	1.40
25	I	201	CDL	OB8-CB7	3.03	1.42	1.33
26	J	401	NDP	O3D-C3D	3.02	1.50	1.43
25	I	201	CDL	OB6-CB5	2.96	1.42	1.34
26	J	401	NDP	C5A-N7A	-2.94	1.33	1.39
25	I	201	CDL	OA6-CA5	2.91	1.42	1.34
26	J	401	NDP	C7N-C3N	2.91	1.54	1.48
23	C	303	PLX	O6-C4	-2.77	1.40	1.44
27	J	402	UQ	C6-C1	2.68	1.54	1.46
20	A	502	FMN	C4-N3	-2.63	1.34	1.38
21	A	503	NAI	C8A-N9A	-2.58	1.32	1.37
21	A	503	NAI	O3B-C3B	-2.57	1.36	1.43
27	J	402	UQ	C7-C8	2.53	1.54	1.50
24	G	201	8Q1	O35-C34	-2.47	1.18	1.23
25	I	201	CDL	OA6-CA4	-2.47	1.40	1.46
22	C	302	PEE	O2-C2	-2.46	1.40	1.46
22	C	302	PEE	O3-C30	2.44	1.40	1.33
21	A	503	NAI	PN-O5D	2.39	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	201	8Q1	C1-S44	2.39	1.81	1.76
24	G	201	8Q1	O40-C39	-2.38	1.18	1.23
20	A	502	FMN	C4A-N5	2.37	1.35	1.30
24	G	201	8Q1	C6-C1	2.36	1.53	1.50
26	J	401	NDP	O2B-C2B	2.31	1.52	1.44
23	C	303	PLX	C7-C6	2.30	1.55	1.50
21	A	503	NAI	C5B-C4B	2.29	1.58	1.51
26	J	401	NDP	O7N-C7N	-2.23	1.19	1.24
25	I	201	CDL	OB6-CB4	-2.23	1.41	1.46
22	C	302	PEE	O2-C10	2.21	1.40	1.34
27	J	402	UQ	O4-C4	-2.20	1.18	1.23
26	J	401	NDP	C2D-C3D	2.20	1.59	1.53
25	I	201	CDL	PB2-OB5	2.16	1.68	1.59
25	I	201	CDL	PB2-OB2	2.14	1.68	1.59
22	C	302	PEE	O3-C3	-2.11	1.40	1.45
23	C	303	PLX	P1-O1	2.10	1.67	1.59
23	C	303	PLX	P1-O4	2.06	1.67	1.59
20	A	502	FMN	C5A-N5	-2.05	1.35	1.39
27	J	402	UQ	O1-C1	-2.03	1.19	1.23
20	A	502	FMN	C2-N3	-2.03	1.34	1.39
26	J	401	NDP	PA-O5B	2.02	1.67	1.59

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	402	UQ	C7-C8-C9	-7.94	113.58	126.79
26	J	401	NDP	C3N-C2N-N1N	-7.71	112.09	123.10
26	J	401	NDP	C1D-N1N-C2N	-7.35	108.88	121.11
24	G	201	8Q1	C6-C1-S44	6.50	121.02	113.46
27	J	402	UQ	C17-C18-C19	-5.98	113.27	127.66
21	A	503	NAI	C5A-C4A-N3A	-5.89	119.07	126.75
26	J	401	NDP	C5A-C4A-N3A	-5.88	119.08	126.75
27	J	402	UQ	C12-C13-C14	-5.66	114.04	127.66
26	J	401	NDP	C1D-N1N-C6N	-5.37	109.26	120.83
21	A	503	NAI	N3A-C2A-N1A	-4.31	121.87	128.60
27	J	402	UQ	C22-C23-C24	-4.31	113.04	127.75
27	J	402	UQ	C10-C9-C8	-4.18	112.96	123.68
21	A	503	NAI	N3A-C4A-N9A	4.16	133.93	127.08
26	J	401	NDP	N3A-C4A-N9A	4.10	133.83	127.08
27	J	402	UQ	C20-C19-C18	-4.09	113.19	123.68
26	J	401	NDP	N3A-C2A-N1A	-4.01	122.33	128.60
22	C	302	PEE	O2-C10-C11	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	503	NAI	C2A-N3A-C4A	3.91	120.99	111.75
25	I	201	CDL	OA6-CA5-C11	3.91	119.93	111.50
25	I	201	CDL	OB6-CB5-C51	3.91	119.92	111.50
27	J	402	UQ	C16-C14-C13	-3.89	113.24	121.12
26	J	401	NDP	C2A-N3A-C4A	3.74	120.59	111.75
27	J	402	UQ	C21-C19-C18	-3.74	113.54	121.12
27	J	402	UQ	C11-C9-C8	-3.72	113.59	121.12
27	J	402	UQ	C15-C14-C13	-3.71	114.17	123.68
21	A	503	NAI	C5A-N7A-C8A	3.68	108.74	103.51
24	G	201	8Q1	O4-C1-C6	-3.43	119.94	123.99
27	J	402	UQ	C25-C24-C23	-3.37	112.90	122.65
21	A	503	NAI	N9A-C8A-N7A	-3.35	109.33	113.91
26	J	401	NDP	C5A-N7A-C8A	3.32	108.23	103.51
27	J	402	UQ	C26-C24-C23	-3.29	113.14	122.65
21	A	503	NAI	C4A-C5A-N7A	-3.20	106.73	110.62
21	A	503	NAI	C3D-C2D-C1D	3.19	107.49	101.43
26	J	401	NDP	N9A-C8A-N7A	-3.19	109.55	113.91
26	J	401	NDP	C4A-C5A-N7A	-3.09	106.85	110.62
21	A	503	NAI	C4D-O4D-C1D	-3.05	102.74	109.47
24	G	201	8Q1	O4-C1-S44	-2.76	119.03	122.61
25	I	201	CDL	OA8-CA7-C31	2.71	120.42	111.91
25	I	201	CDL	OB8-CB7-C71	2.68	120.32	111.91
22	C	302	PEE	O3-C30-C31	2.68	120.32	111.91
20	A	502	FMN	C4-C4A-N5	2.63	121.97	118.23
24	G	201	8Q1	C38-C39-N41	2.62	120.84	116.42
20	A	502	FMN	C4A-C10-N1	-2.62	118.65	124.73
26	J	401	NDP	PN-O3-PA	-2.50	124.25	132.83
23	C	303	PLX	C1A-N1-C1	2.37	119.62	109.92
26	J	401	NDP	C4A-N9A-C8A	2.35	108.28	105.73
27	J	402	UQ	CM5-C5-C6	-2.35	120.57	124.40
20	A	502	FMN	O4-C4-C4A	-2.34	120.38	126.60
20	A	502	FMN	O2-C2-N1	-2.32	117.99	121.83
21	A	503	NAI	C4A-N9A-C8A	2.29	108.20	105.73
21	A	503	NAI	C2D-C3D-C4D	2.25	107.01	102.64
24	G	201	8Q1	C37-C38-C39	2.24	116.08	112.36
20	A	502	FMN	C4A-C4-N3	2.18	118.72	113.19
26	J	401	NDP	C2B-C1B-N9A	-2.15	109.91	113.53
20	A	502	FMN	C10-N1-C2	2.13	121.17	116.90
20	A	502	FMN	C4-N3-C2	-2.07	121.81	125.64
24	G	201	8Q1	C32-C34-N36	2.00	120.57	116.58

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	502	FMN	C2'-C1'-N10-C10
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'
21	A	503	NAI	C5B-O5B-PA-O3
22	C	302	PEE	C11-C10-O2-C2
22	C	302	PEE	O4P-C4-C5-N
23	C	303	PLX	N1-C1-C2-O1
23	C	303	PLX	O9-C24-O8-C5
24	G	201	8Q1	C42-C43-S44-C1
24	G	201	8Q1	C28-O27-P24-O3
24	G	201	8Q1	C28-O27-P24-O2
24	G	201	8Q1	C28-O27-P24-O1
25	I	201	CDL	CB2-C1-CA2-OA2
25	I	201	CDL	CA2-OA2-PA1-OA4
25	I	201	CDL	OA5-CA3-CA4-OA6
25	I	201	CDL	CB2-OB2-PB2-OB3
25	I	201	CDL	CB2-OB2-PB2-OB4
25	I	201	CDL	CB3-OB5-PB2-OB3
25	I	201	CDL	CB3-OB5-PB2-OB4
27	J	402	UQ	C7-C8-C9-C10
27	J	402	UQ	C19-C21-C22-C23
22	C	302	PEE	O4-C10-O2-C2
27	J	402	UQ	C7-C8-C9-C11
27	J	402	UQ	C12-C13-C14-C16
25	I	201	CDL	O1-C1-CA2-OA2
27	J	402	UQ	C22-C23-C24-C26
23	C	303	PLX	C27-C28-C29-C30
20	A	502	FMN	O2'-C2'-C3'-O3'
27	J	402	UQ	C13-C14-C16-C17
27	J	402	UQ	C18-C19-C21-C22
23	C	303	PLX	C25-C26-C27-C28
25	I	201	CDL	C51-C52-C53-C54
23	C	303	PLX	C2-C1-N1-C1A
25	I	201	CDL	CA2-OA2-PA1-OA5
25	I	201	CDL	CB2-OB2-PB2-OB5
25	I	201	CDL	CB3-OB5-PB2-OB2
26	J	401	NDP	C2D-C1D-N1N-C6N
23	C	303	PLX	O6-C6-C7-C8
25	I	201	CDL	C51-CB5-OB6-CB4
25	I	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	A	502	FMN	O2'-C2'-C3'-C4'
23	C	303	PLX	C10-C11-C12-C13
23	C	303	PLX	C28-C29-C30-C31
22	C	302	PEE	C43-C44-C45-C46
23	C	303	PLX	C13-C14-C15-C16
23	C	303	PLX	C2-C1-N1-C1C
25	I	201	CDL	C11-C12-C13-C14
23	C	303	PLX	O7-C6-C7-C8
21	A	503	NAI	C3D-C4D-C5D-O5D
23	C	303	PLX	C14-C15-C16-C17
23	C	303	PLX	C7-C8-C9-C10
23	C	303	PLX	C2-C1-N1-C1B
23	C	303	PLX	C11-C12-C13-C14
22	C	302	PEE	C35-C36-C37-C38
22	C	302	PEE	C42-C43-C44-C45
25	I	201	CDL	C71-C72-C73-C74
23	C	303	PLX	C33-C34-C35-C36
25	I	201	CDL	O1-C1-CB2-OB2
22	C	302	PEE	C13-C14-C15-C16
22	C	302	PEE	C32-C33-C34-C35
23	C	303	PLX	C11-C10-C9-C8
23	C	303	PLX	C3-C4-C5-O8
22	C	302	PEE	C15-C16-C17-C18
22	C	302	PEE	C34-C35-C36-C37
23	C	303	PLX	C31-C32-C33-C34
27	J	402	UQ	C17-C18-C19-C20
22	C	302	PEE	C1-C2-C3-O3
22	C	302	PEE	C12-C13-C14-C15
23	C	303	PLX	O4-C3-C4-O6
25	I	201	CDL	CA7-C31-C32-C33
26	J	401	NDP	O4D-C4D-C5D-O5D
23	C	303	PLX	O6-C4-C5-O8
27	J	402	UQ	C9-C11-C12-C13
25	I	201	CDL	OA5-CA3-CA4-CA6
26	J	401	NDP	O4D-C1D-N1N-C6N
22	C	302	PEE	O2-C2-C3-O3
22	C	302	PEE	C19-C20-C21-C22
25	I	201	CDL	C52-C53-C54-C55
21	A	503	NAI	C5B-O5B-PA-O1A
21	A	503	NAI	C5B-O5B-PA-O2A
23	C	303	PLX	O4-C3-C4-C5
23	C	303	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	C	303	PLX	C1-C2-O1-P1
23	C	303	PLX	C15-C16-C17-C18
24	G	201	8Q1	C11-C12-C13-C14
23	C	303	PLX	C19-C20-C21-C22
25	I	201	CDL	OB9-CB7-OB8-CB6
24	G	201	8Q1	O27-C28-C29-C30
20	A	502	FMN	C5'-O5'-P-O1P
25	I	201	CDL	C71-CB7-OB8-CB6
23	C	303	PLX	C3-O4-P1-O1
26	J	401	NDP	PN-O3-PA-O1A
25	I	201	CDL	C31-CA7-OA8-CA6
25	I	201	CDL	OA9-CA7-OA8-CA6
21	A	503	NAI	O4D-C1D-N1N-C2N
21	A	503	NAI	C2D-C1D-N1N-C2N
25	I	201	CDL	C12-C13-C14-C15
24	G	201	8Q1	C10-C11-C12-C13
24	G	201	8Q1	O27-C28-C29-C31
23	C	303	PLX	C34-C35-C36-C37
21	A	503	NAI	O4D-C4D-C5D-O5D
22	C	302	PEE	C38-C39-C40-C41
24	G	201	8Q1	O4-C1-S44-C43
23	C	303	PLX	O8-C24-C25-C26
26	J	401	NDP	C3D-C4D-C5D-O5D
22	C	302	PEE	O3-C30-C31-C32
24	G	201	8Q1	C12-C13-C14-C15
25	I	201	CDL	C72-C71-CB7-OB8
25	I	201	CDL	C12-C11-CA5-OA6
25	I	201	CDL	C52-C51-CB5-OB6
24	G	201	8Q1	C11-C10-C9-C8
22	C	302	PEE	C18-C19-C20-C21
26	J	401	NDP	O4B-C4B-C5B-O5B
22	C	302	PEE	O5-C30-C31-C32
25	I	201	CDL	C52-C51-CB5-OB7
21	A	503	NAI	C2N-C3N-C7N-N7N
23	C	303	PLX	C3-O4-P1-O2
25	I	201	CDL	C12-C11-CA5-OA7
25	I	201	CDL	C72-C71-CB7-OB9
20	A	502	FMN	O4'-C4'-C5'-O5'
22	C	302	PEE	C11-C12-C13-C14

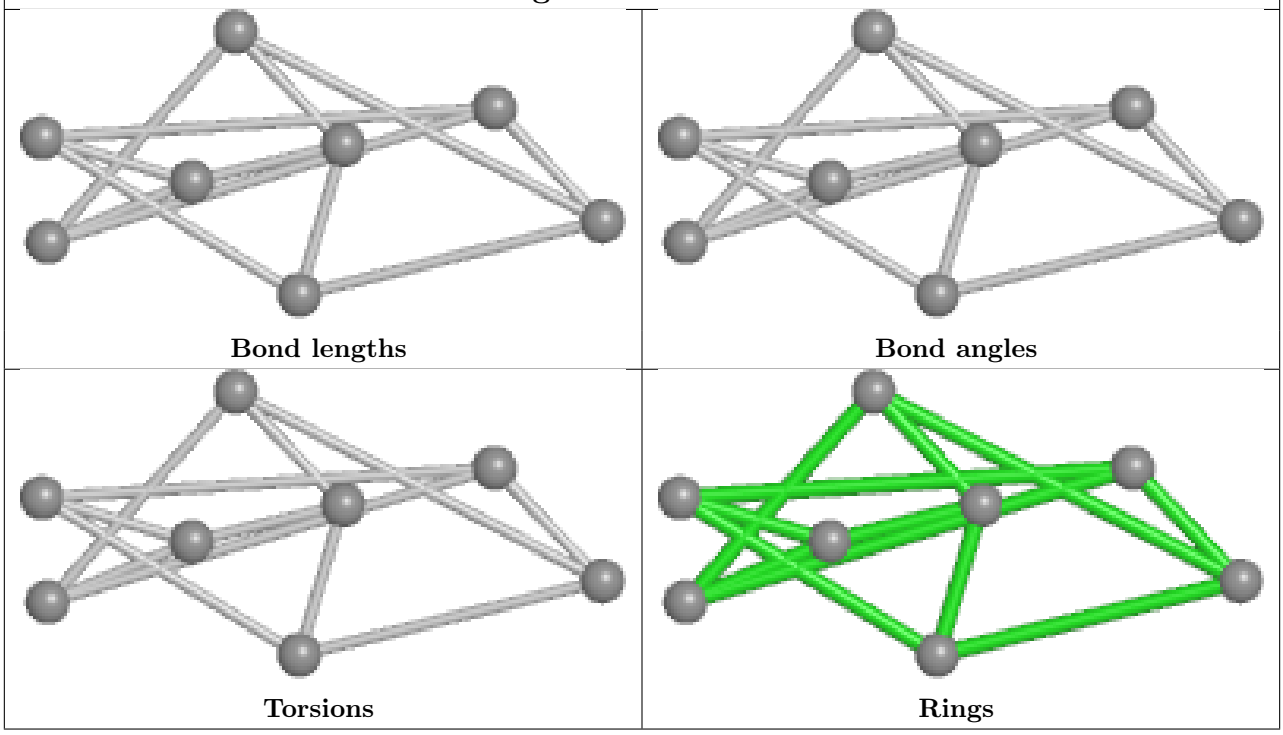
There are no ring outliers.

9 monomers are involved in 28 short contacts:

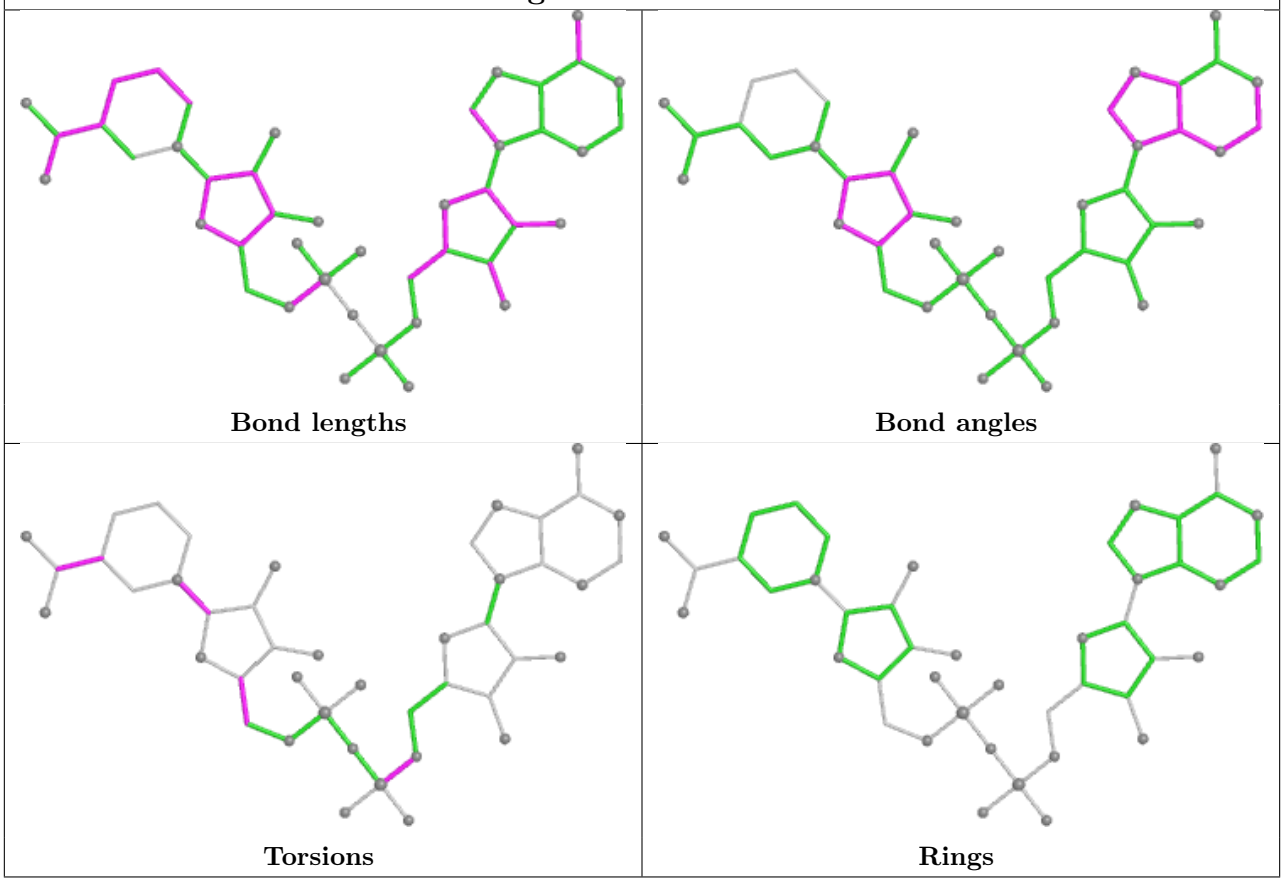
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	503	NAI	6	0
23	C	303	PLX	6	0
19	C	301	SF4	2	0
20	A	502	FMN	8	0
19	A	501	SF4	1	0
27	J	402	UQ	3	0
22	C	302	PEE	2	0
25	I	201	CDL	1	0
26	J	401	NDP	1	0

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.

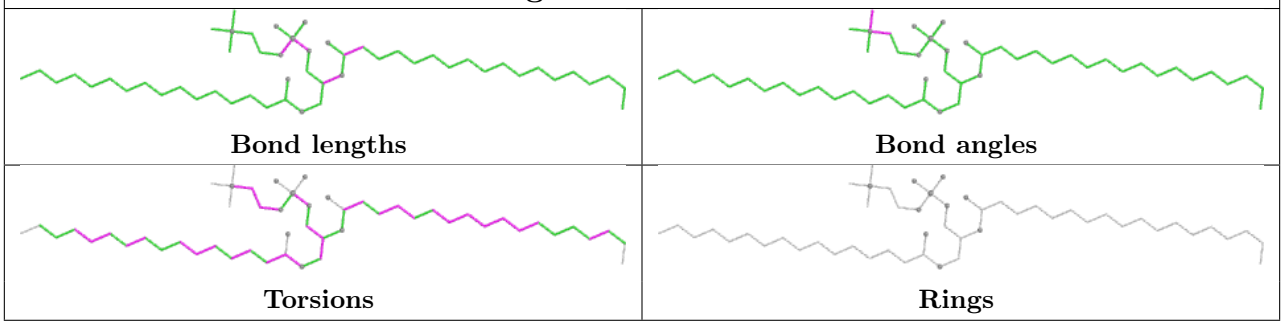
Ligand SF4 B 301



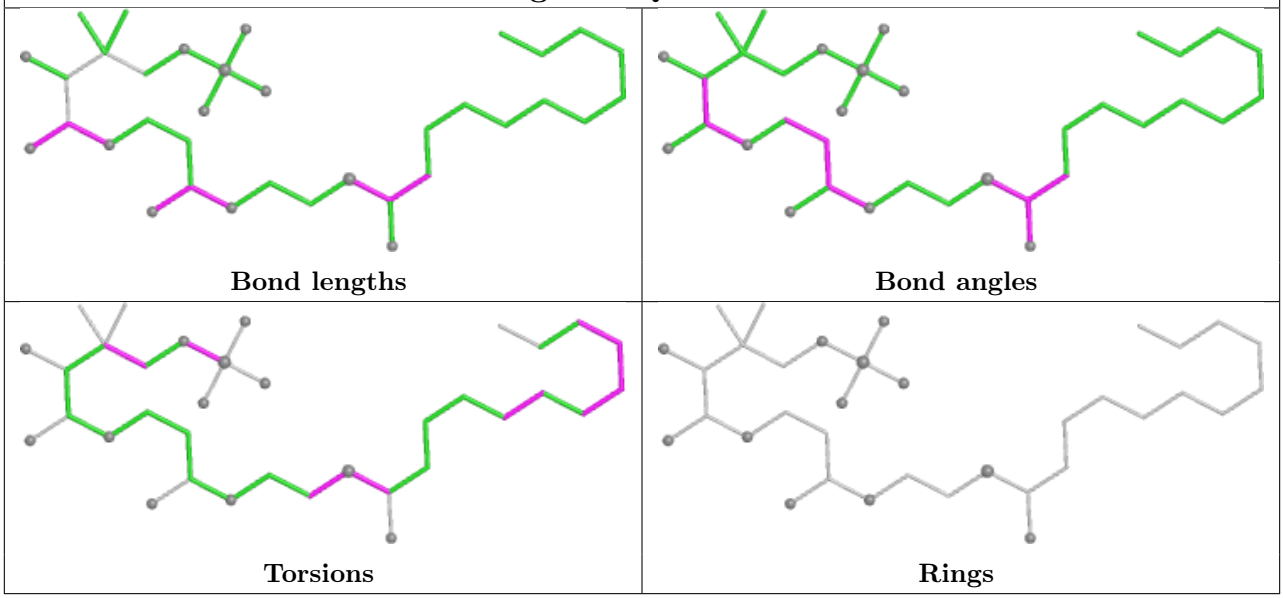
Ligand NAI A 503



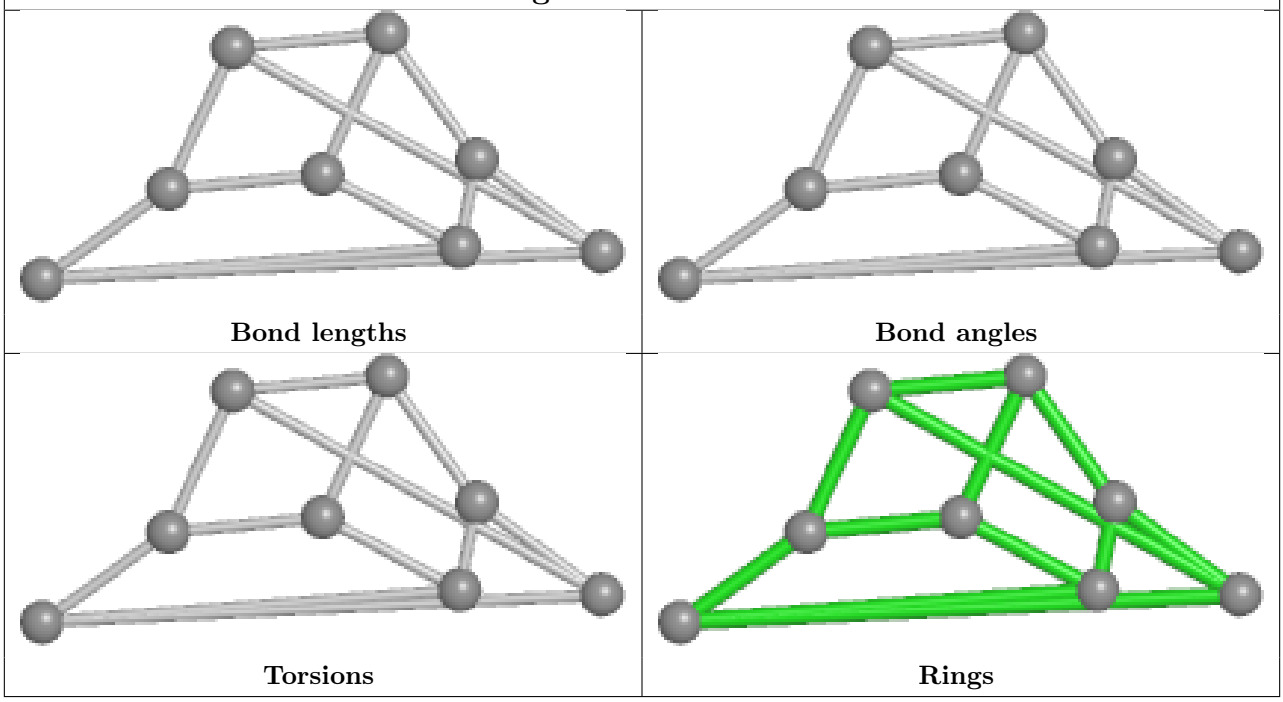
Ligand PLX C 303



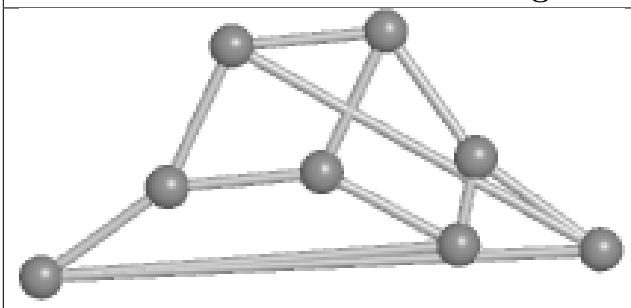
Ligand 8Q1 G 201



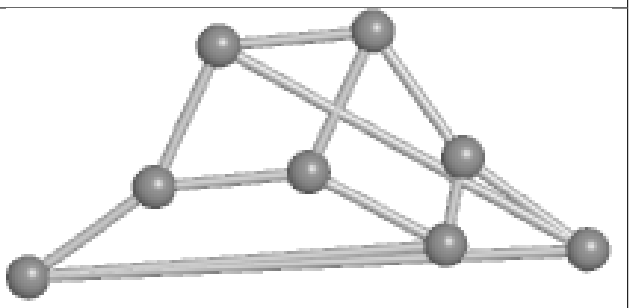
Ligand SF4 C 301



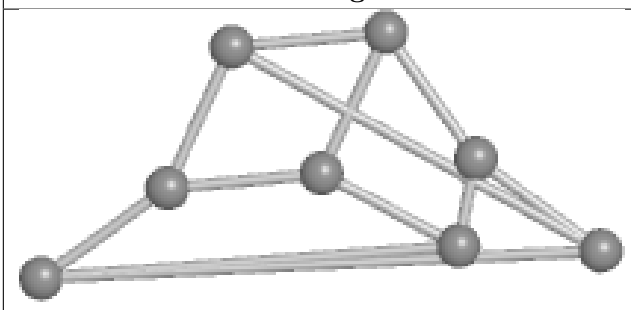
Ligand SF4 B 302



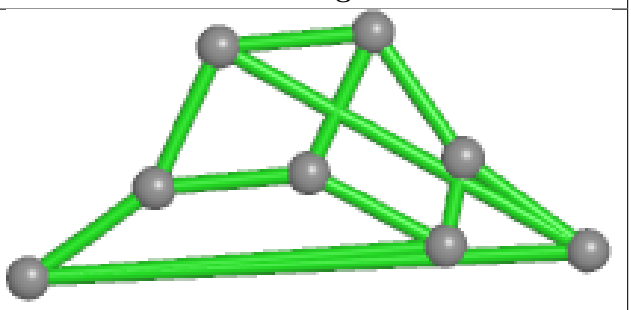
Bond lengths



Bond angles

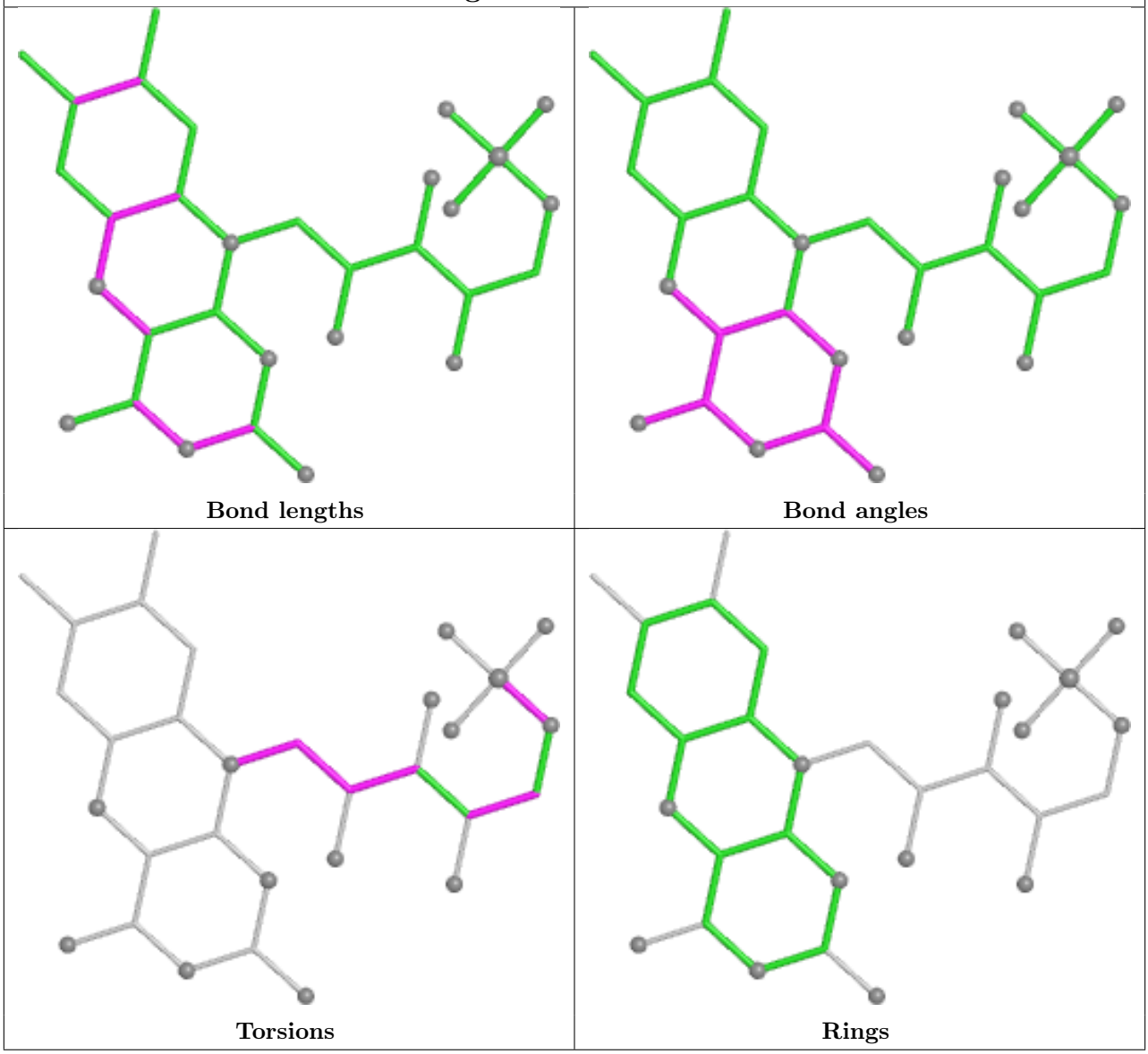


Torsions

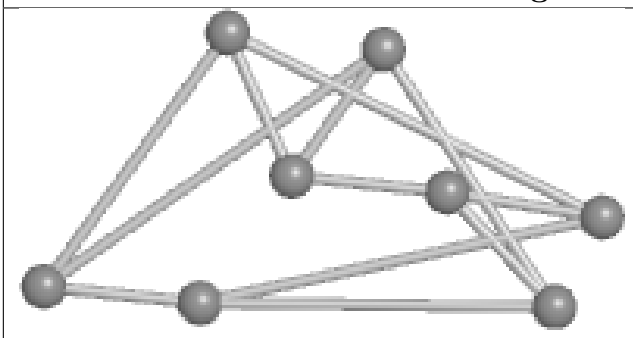


Rings

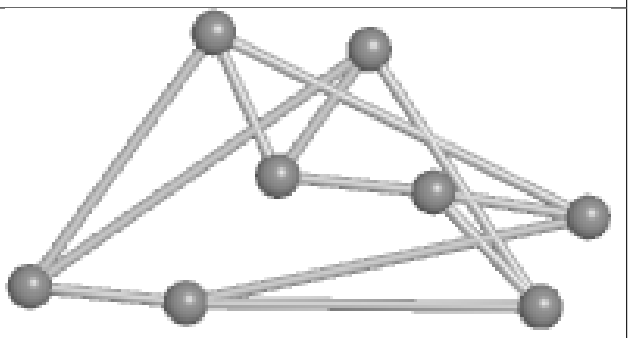
Ligand FMN A 502



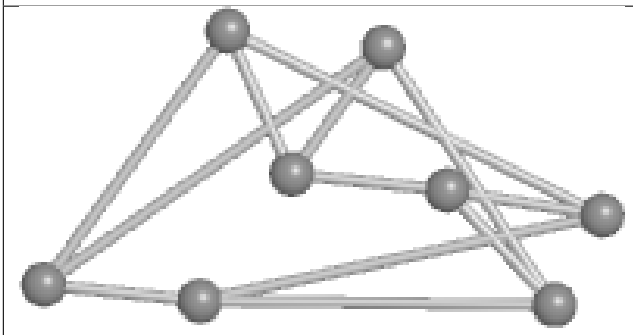
Ligand SF4 A 501



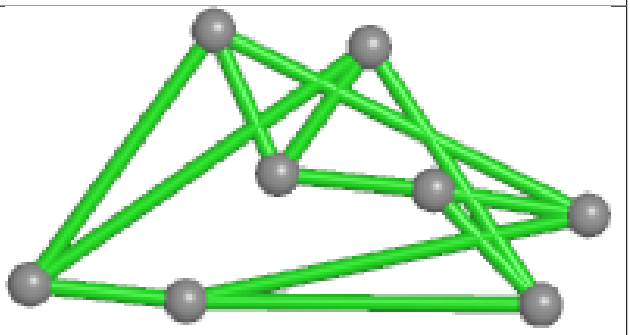
Bond lengths



Bond angles

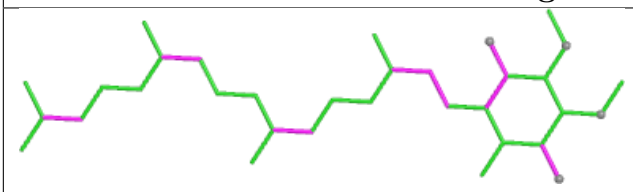


Torsions

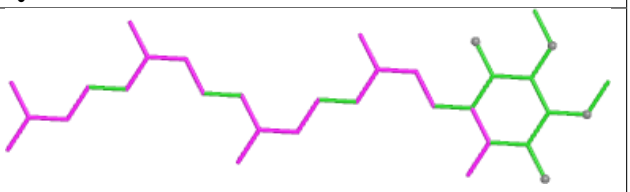


Rings

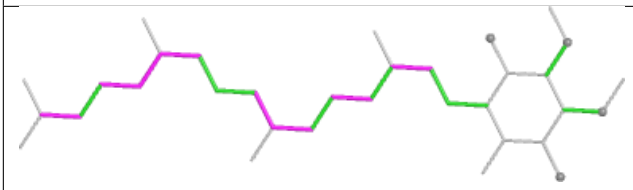
Ligand UQ J 402



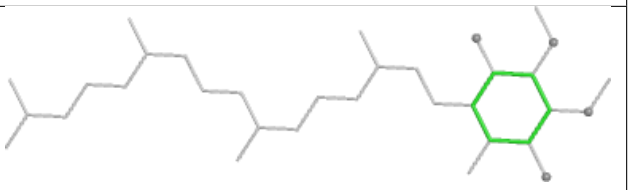
Bond lengths



Bond angles

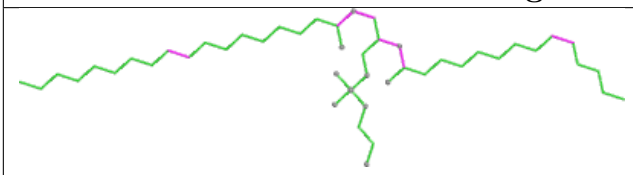


Torsions

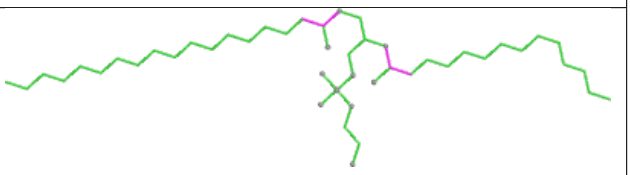


Rings

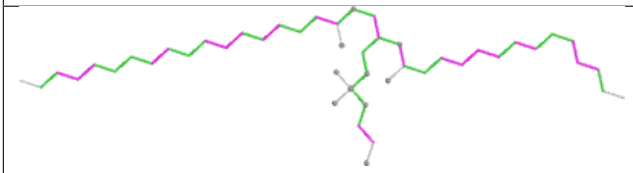
Ligand PEE C 302



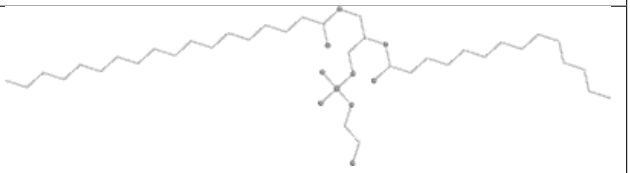
Bond lengths



Bond angles

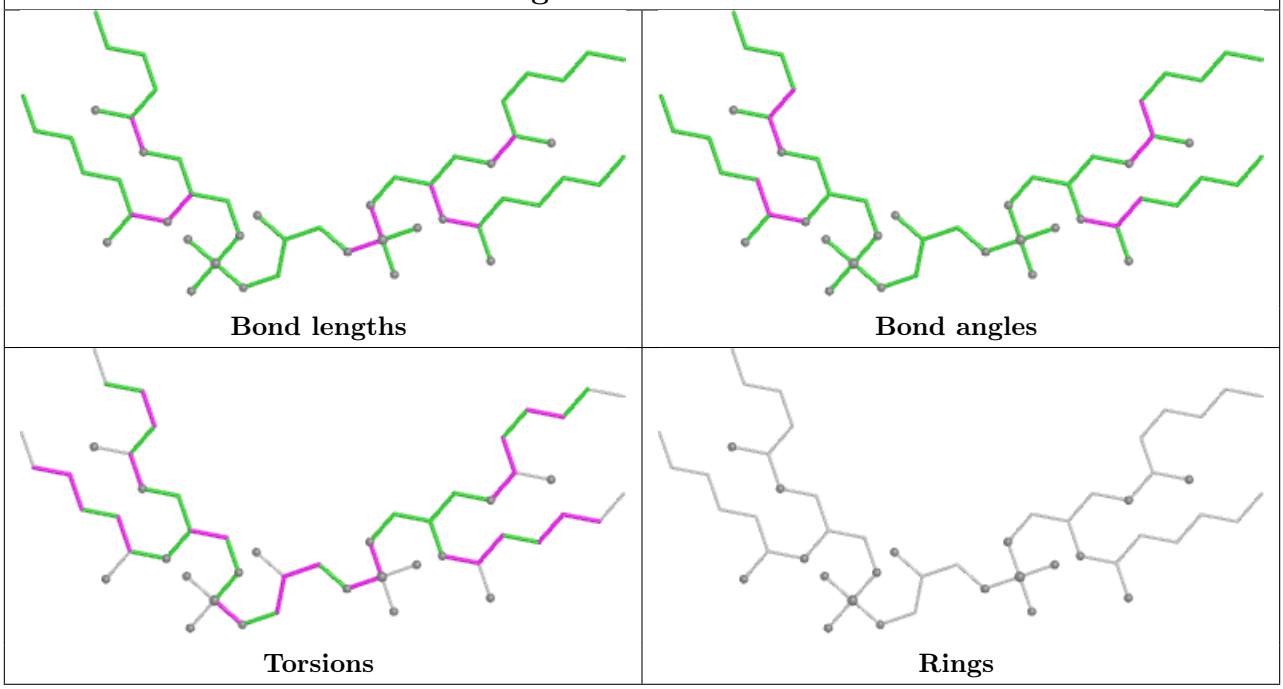


Torsions

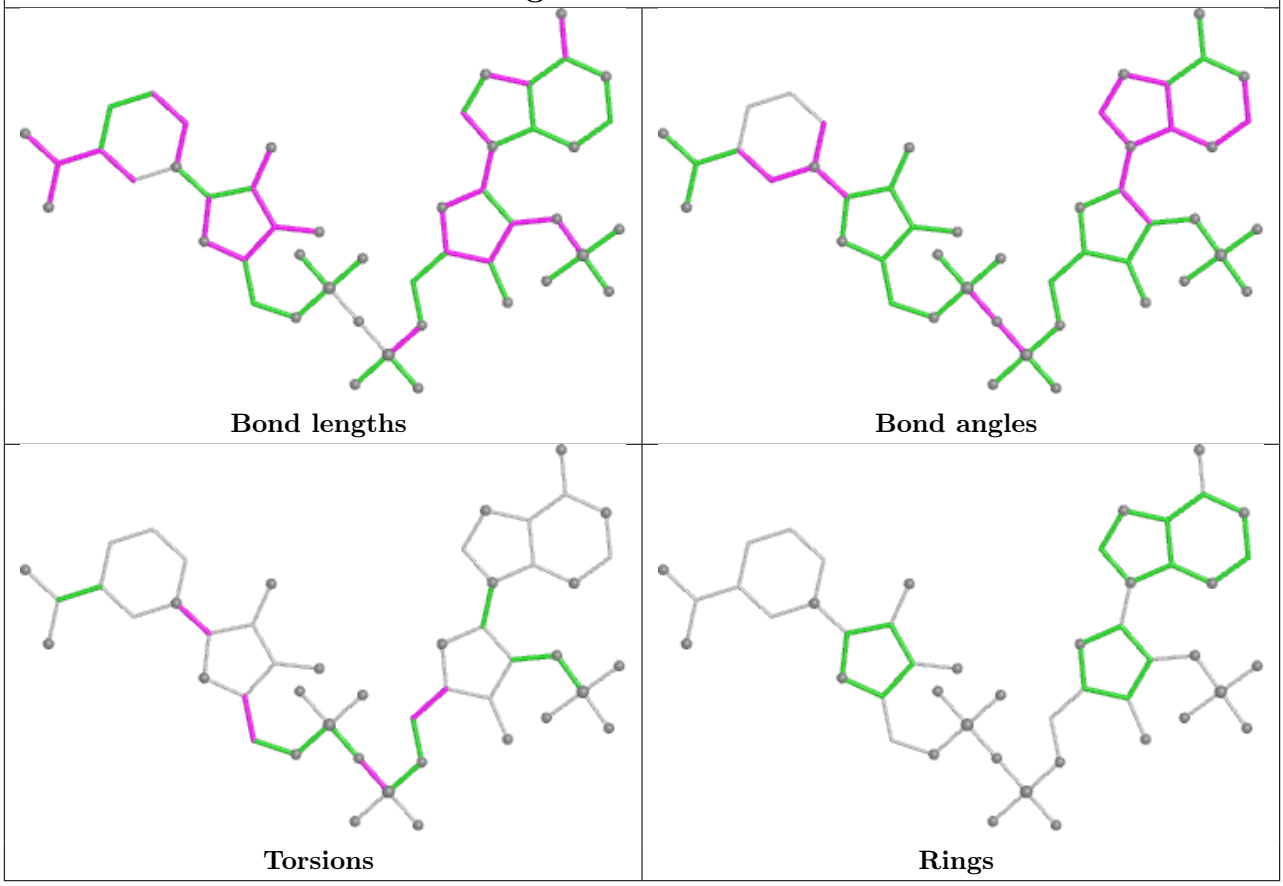


Rings

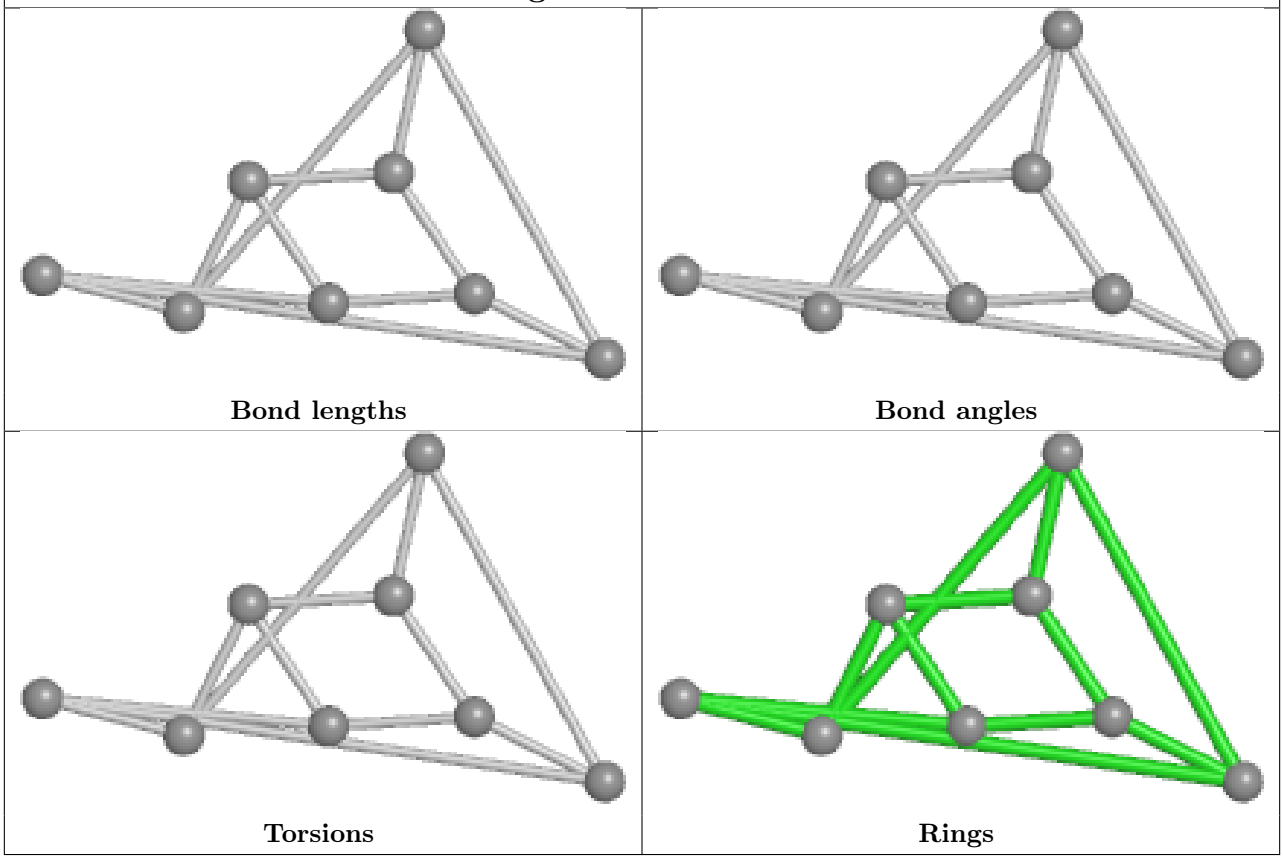
Ligand CDL I 201



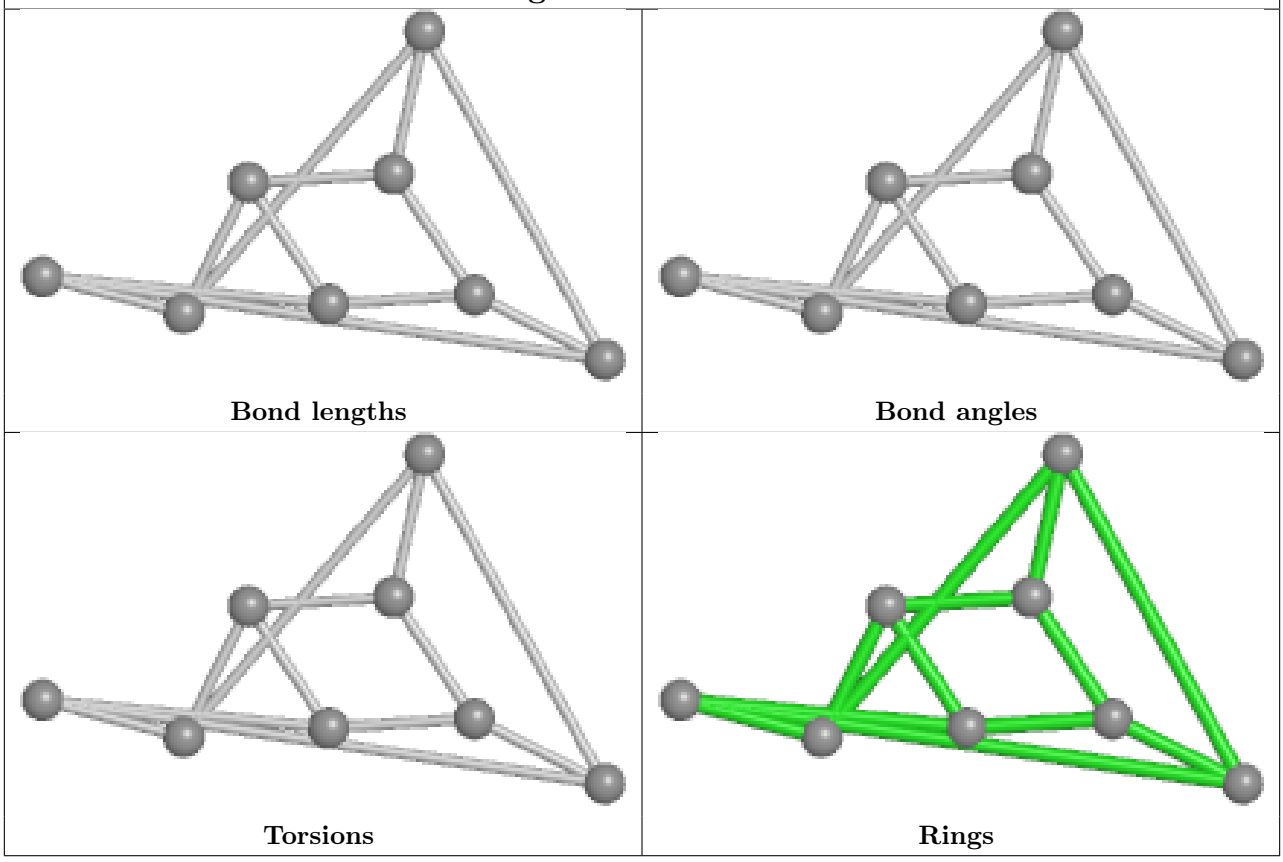
Ligand NDP J 401



Ligand SF4 M 802



Ligand SF4 M 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

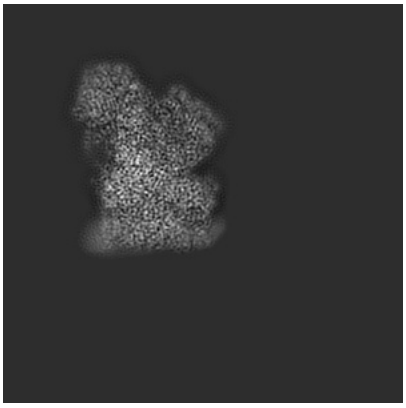
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32196. These allow visual inspection of the internal detail of the map and identification of artifacts.

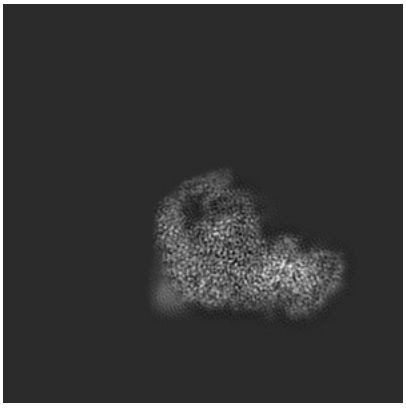
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

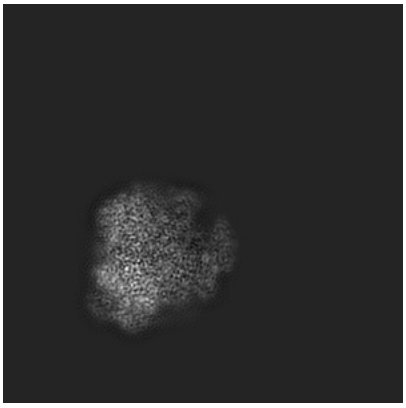
6.1.1 Primary map



X



Y

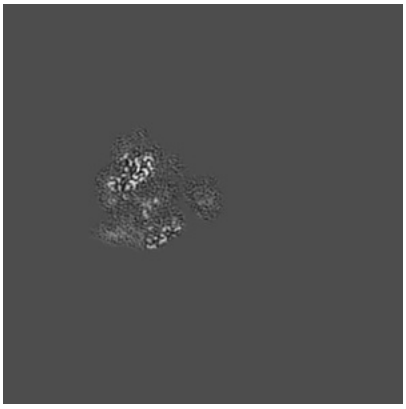


Z

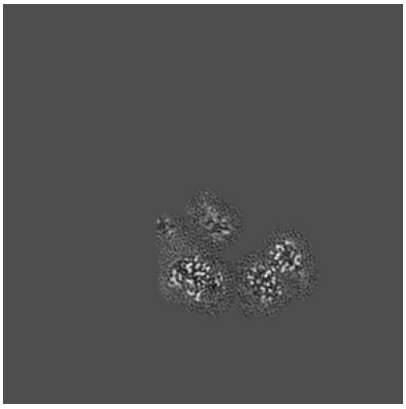
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 155



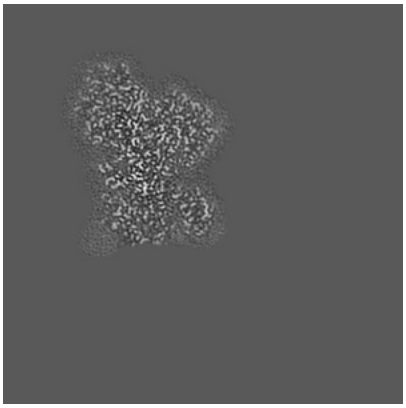
Y Index: 155

Z Index: 155

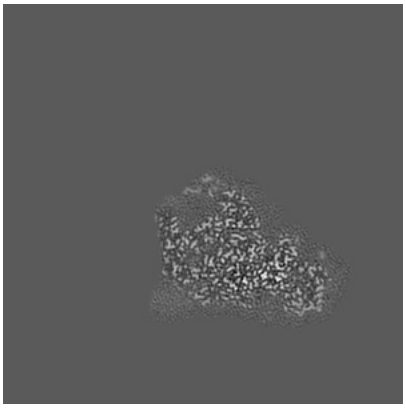
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 104



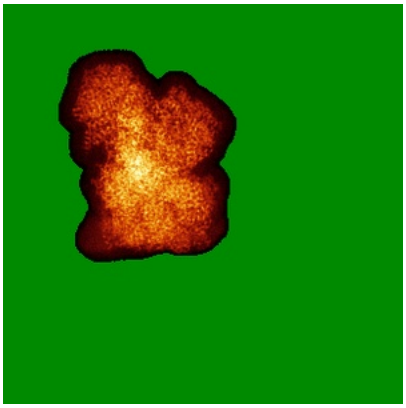
Y Index: 102

Z Index: 168

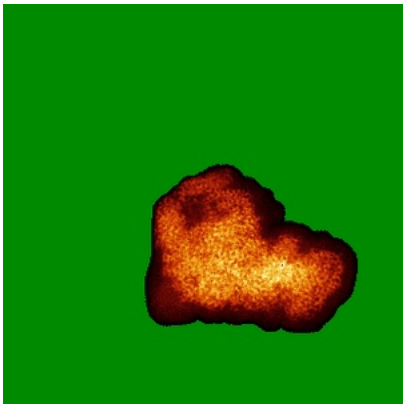
The images above show the largest variance slices of the map in three orthogonal directions.

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

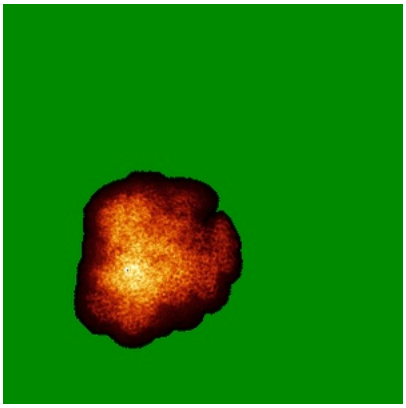
6.4.1 Primary map



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 0.0372. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

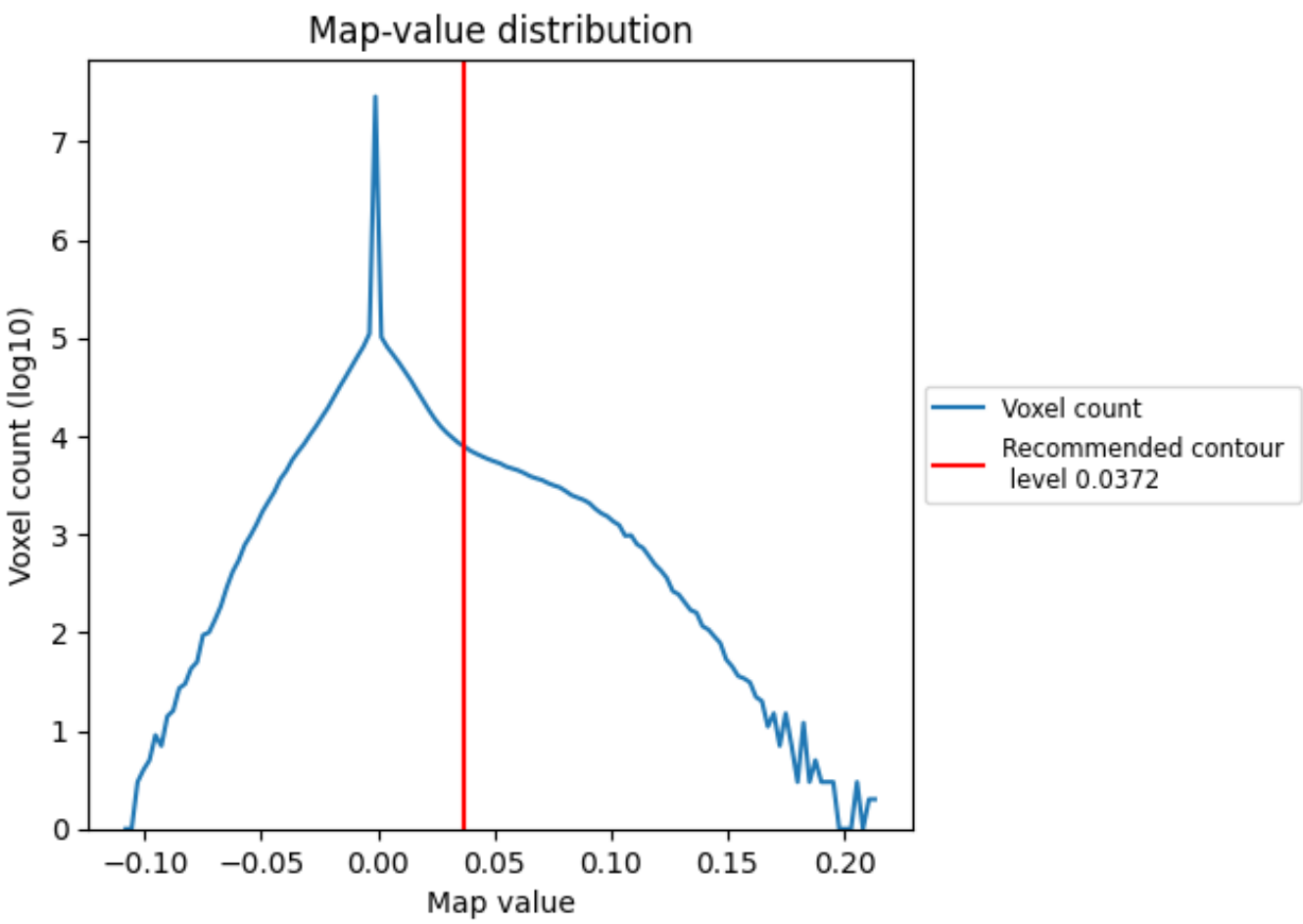
6.6 Mask visualisation (i)

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

7 Map analysis (i)

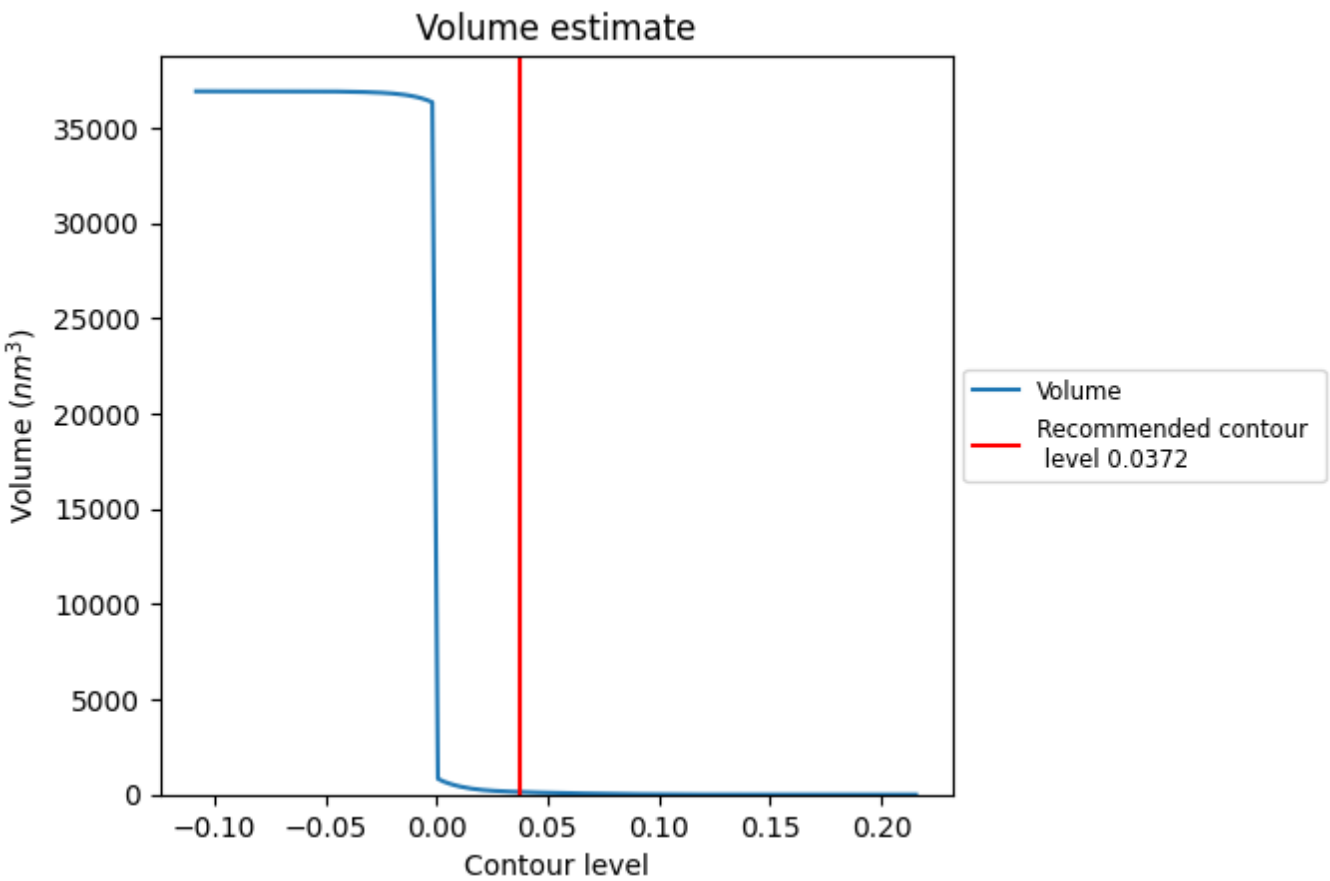
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

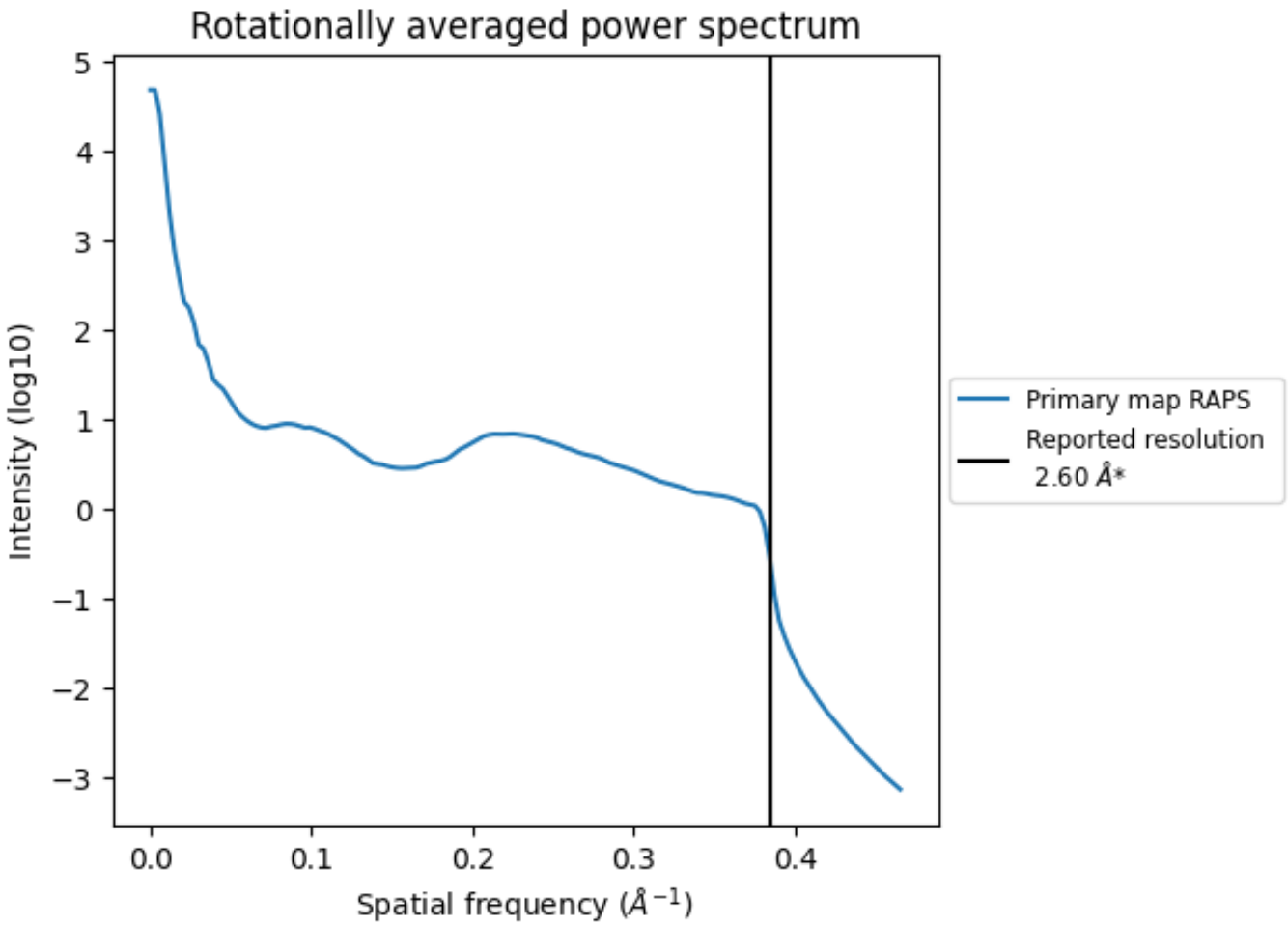
7.2 Volume estimate (i)



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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 0.385 Å^{-1}

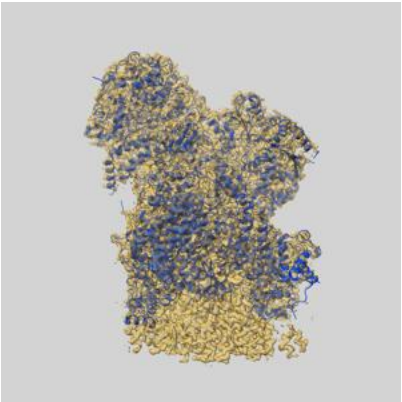
8 Fourier-Shell correlation (i)

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

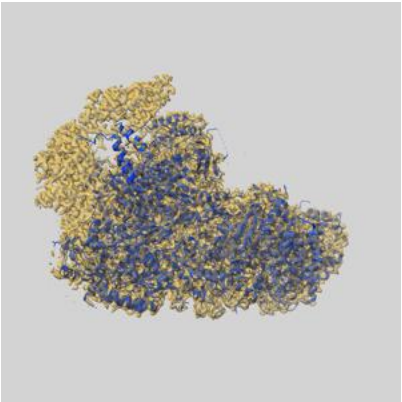
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32196 and PDB model 7VY8. Per-residue inclusion information can be found in section 3 on page 13.

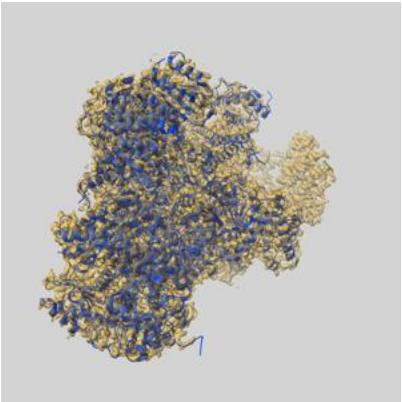
9.1 Map-model overlay (i)



X



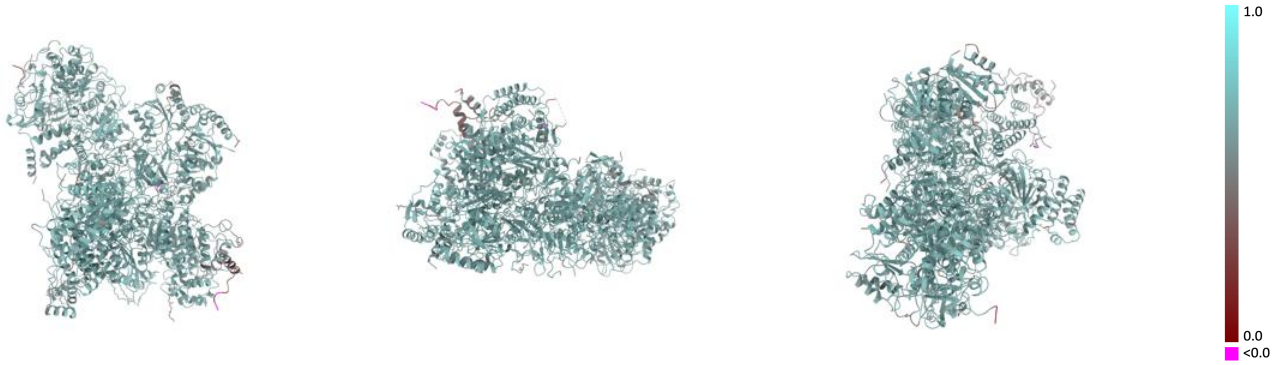
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0372 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.

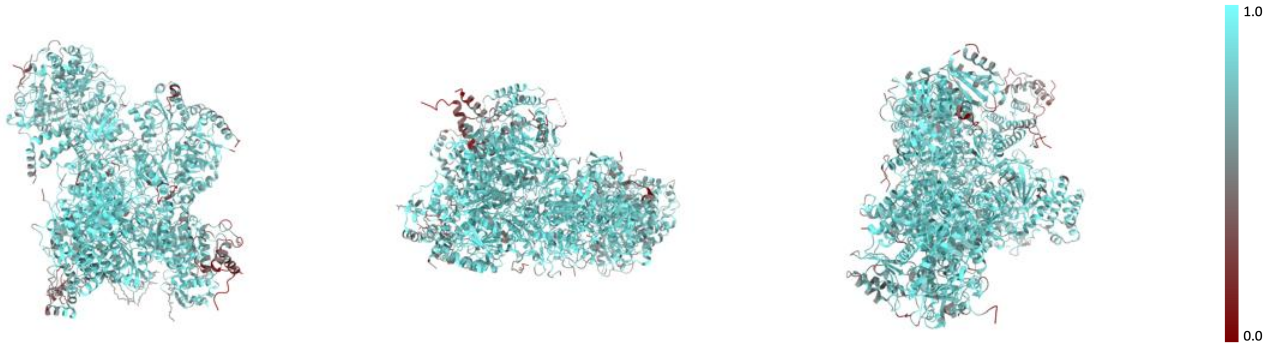
9.2 Q-score mapped to coordinate model (i)



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.

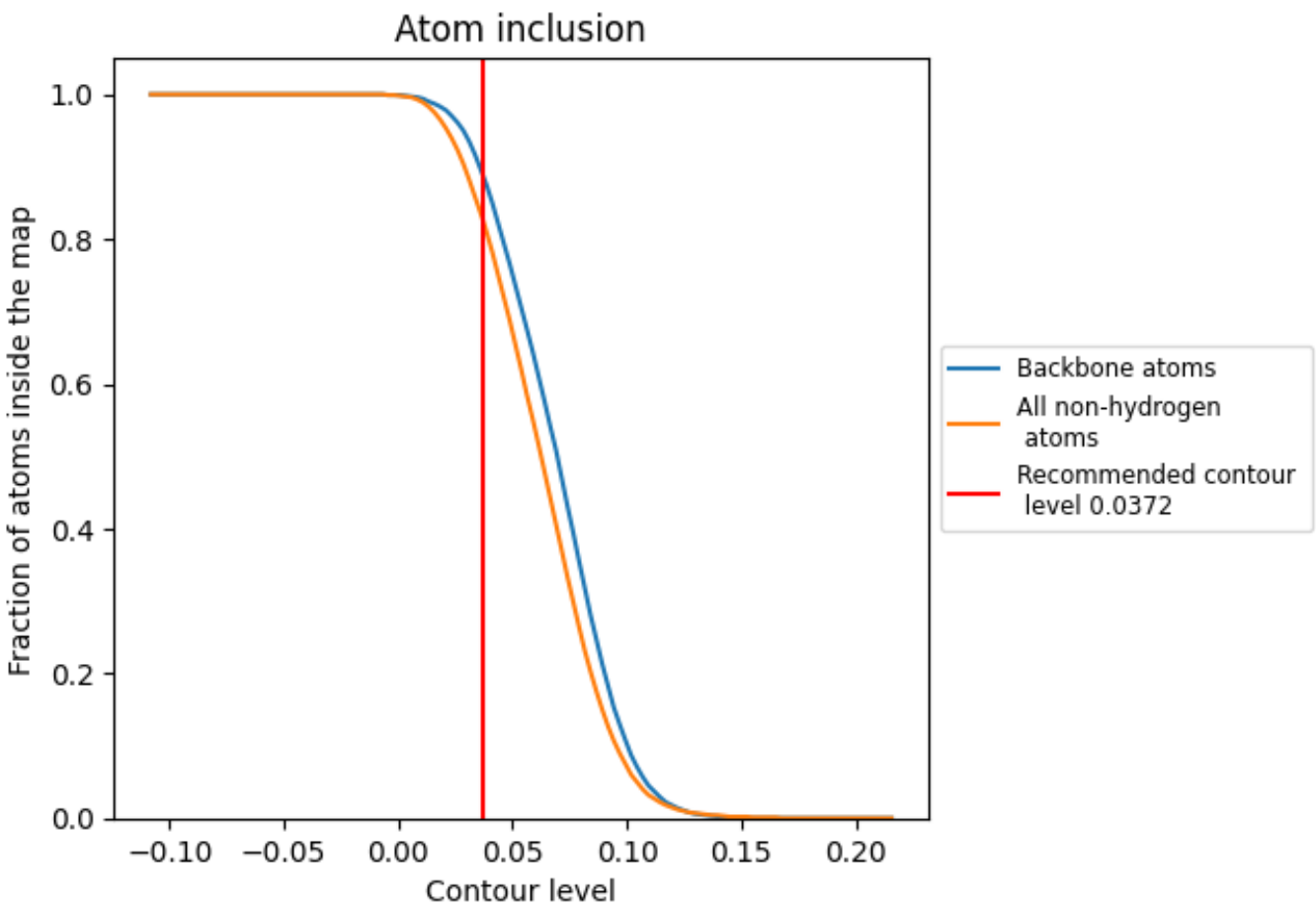
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0372).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0372) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.6450
A	0.8170	0.6430
B	0.9040	0.6670
C	0.8780	0.6650
E	0.8070	0.6470
F	0.7110	0.5960
G	0.3920	0.4900
H	0.7980	0.6330
I	0.6990	0.6200
J	0.8330	0.6450
K	0.7350	0.6320
L	0.8330	0.6540
M	0.8600	0.6540
N	0.7540	0.6340
O	0.7620	0.6250
P	0.9070	0.6720
Q	0.9170	0.6720
T	0.8020	0.6460
W	0.6980	0.6120