



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 10:51 PM UTC

PDB ID : 7VB7 / pdb_00007vb7
EMDB ID : EMD-31874
Title : Matrix arm of active state CI from DQ-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-30
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:

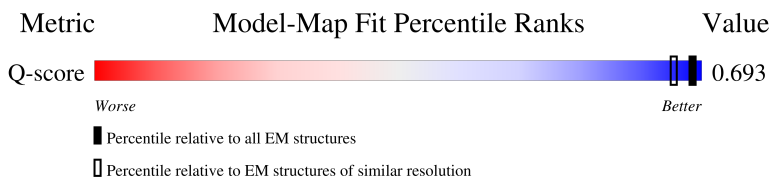
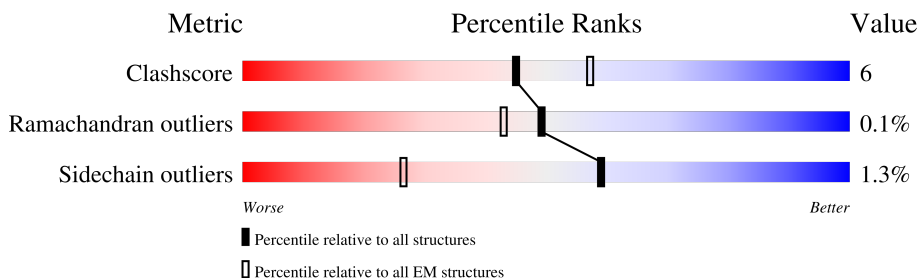
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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 $\leq 5\%$. 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	
2	B	176	
3	C	156	
4	E	115	

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	386	
17	T	96	
18	W	29	

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	-
19	SF4	M	802	-	-	X	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 29279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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 dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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 dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

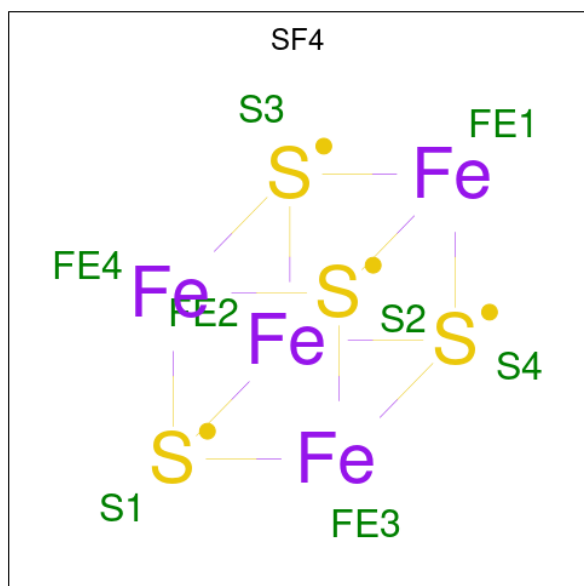
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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.

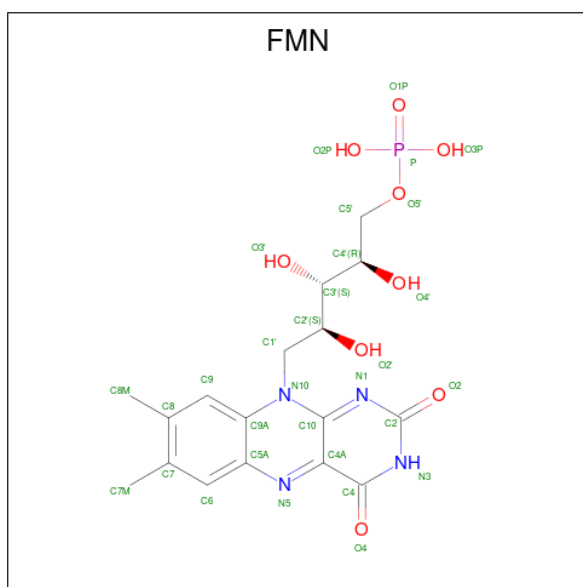
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	W	29	212	135	37	39	1	0	0

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



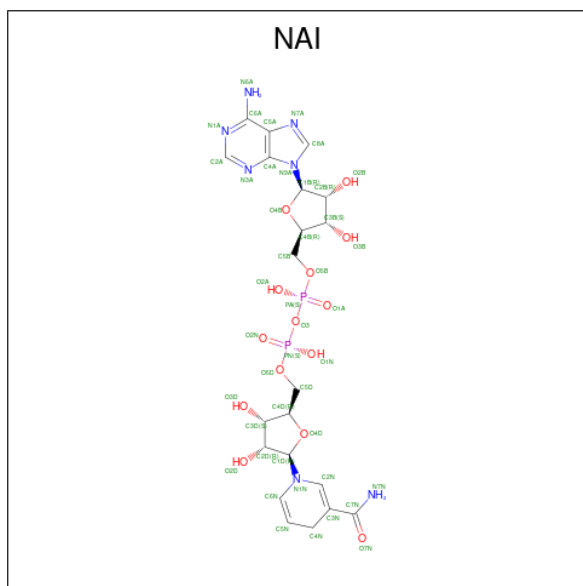
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
19	A	1	8	4	4	0
19	B	1	8	4	4	0
19	B	1	8	4	4	0
19	C	1	8	4	4	0
19	M	1	8	4	4	0
19	M	1	8	4	4	0

- Molecule 20 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



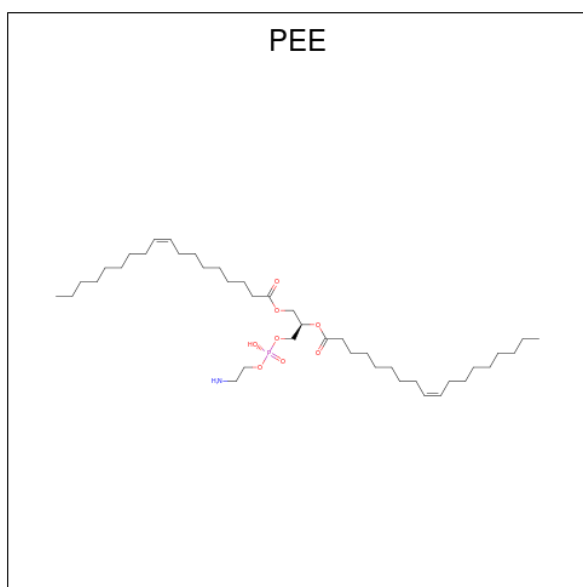
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	A	1	31	17	4	9	1	0

- 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).



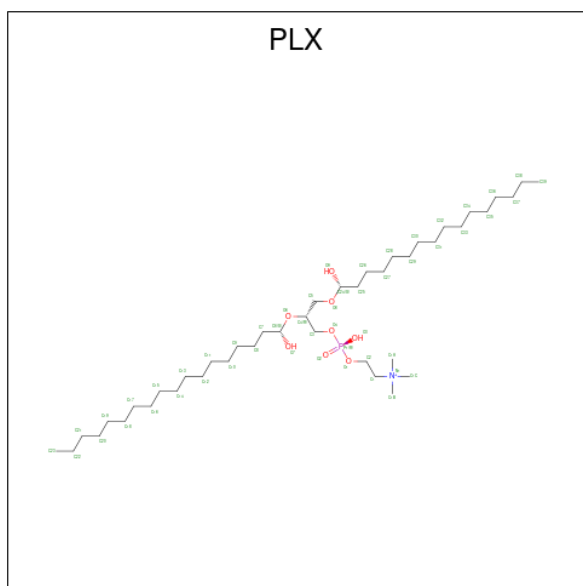
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
21	A	1	44	21	7	14	2	0

- Molecule 22 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



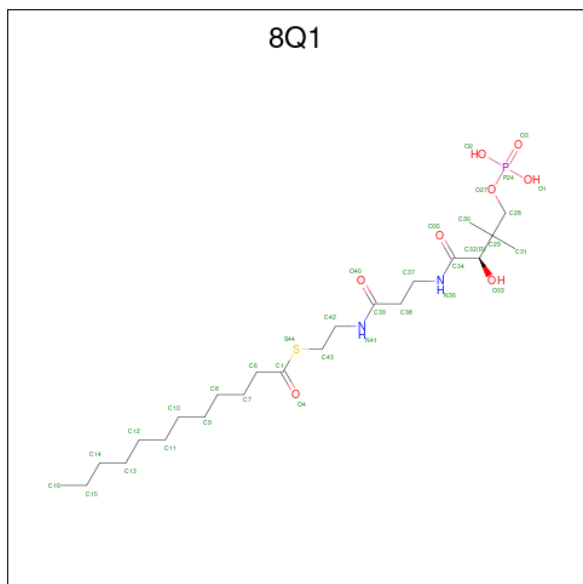
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
22	C	1	47	37	1	8	1	0

- 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-TRIOXOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



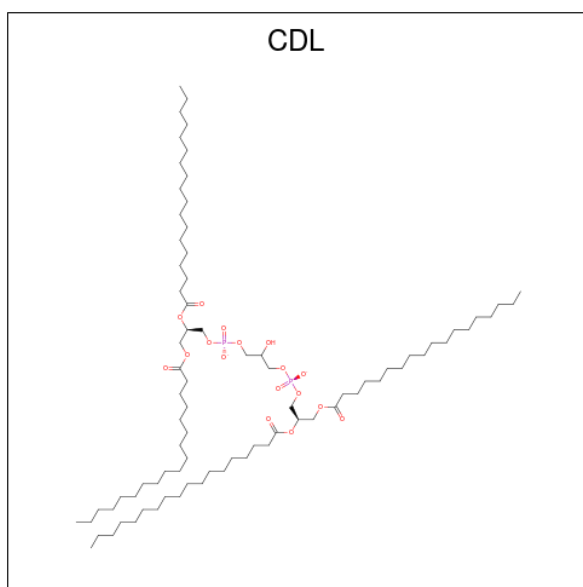
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	C	1	52	42	1	8	1	0

- Molecule 24 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



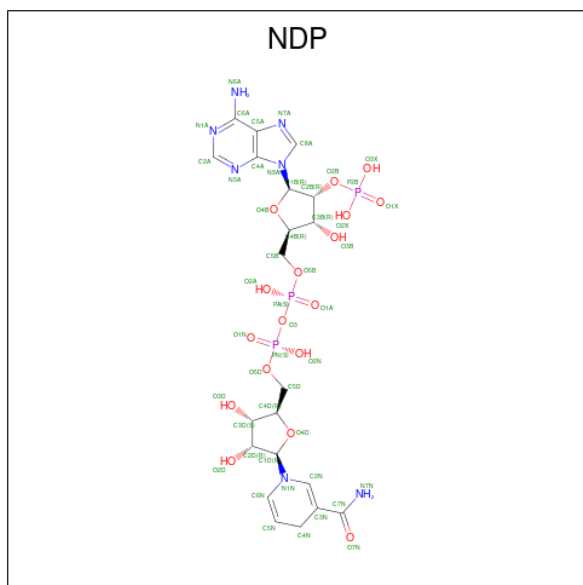
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
24	E	1	35	23	2	8	1	1	0

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



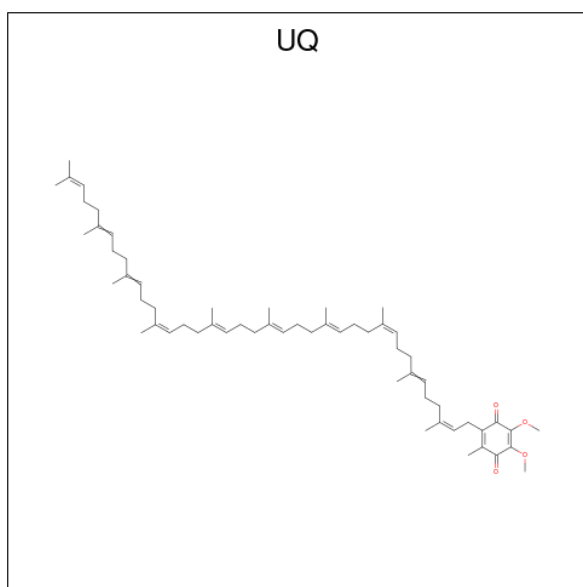
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	I	1	50	31	17	2	0

- 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).



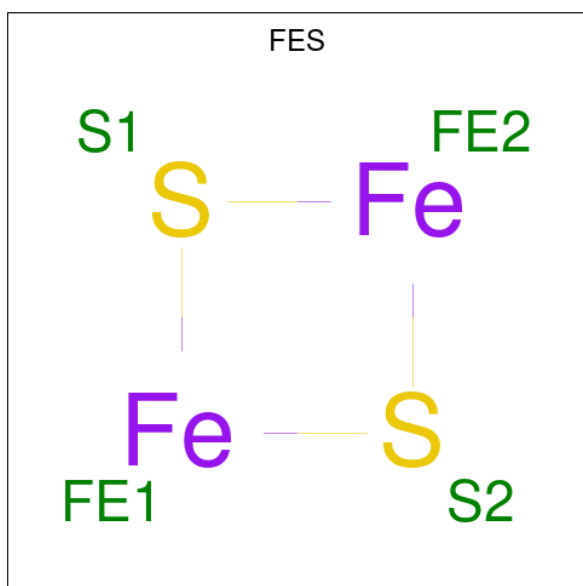
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
26	J	1	48	21	7	17	3	0

- 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) (labeled as "Ligand of Interest" by depositor).

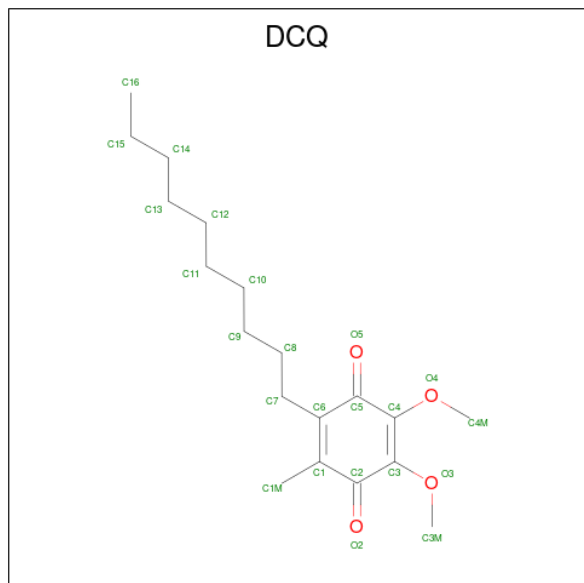


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	M	1	4	2	2	0
28	O	1	4	2	2	0

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 30 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	Q	1	Total	C	O	0
			23	19	4	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	A	53	Total	O	0
			53	53	
32	B	80	Total	O	0
			80	80	

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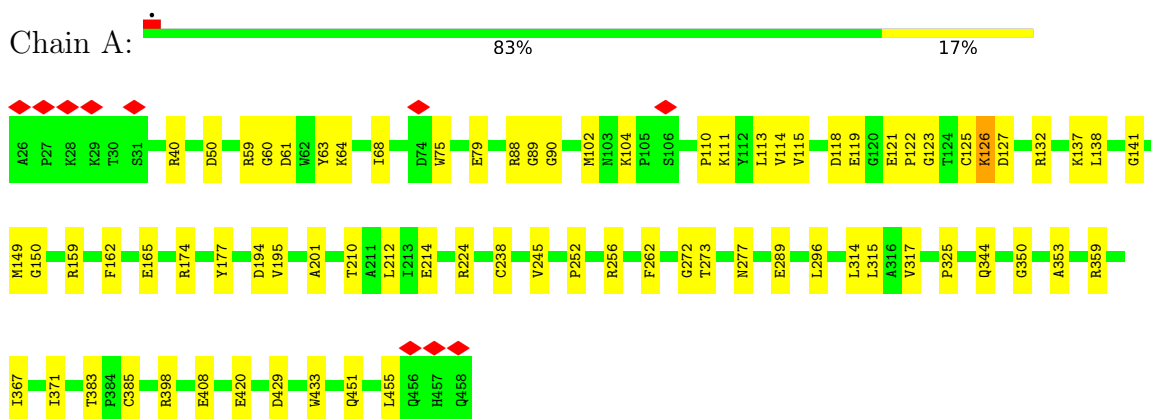
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Mol	Chain	Residues	Atoms		AltConf
32	C	58	Total 58	O 58	0
32	E	3	Total 3	O 3	0
32	F	1	Total 1	O 1	0
32	H	4	Total 4	O 4	0
32	I	13	Total 13	O 13	0
32	J	5	Total 5	O 5	0
32	K	4	Total 4	O 4	0
32	L	24	Total 24	O 24	0
32	M	196	Total 196	O 196	0
32	N	5	Total 5	O 5	0
32	O	17	Total 17	O 17	0
32	P	74	Total 74	O 74	0
32	Q	189	Total 189	O 189	0
32	T	8	Total 8	O 8	0
32	W	2	Total 2	O 2	0

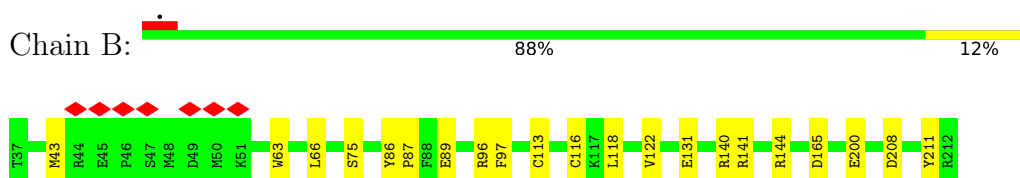
3 Residue-property plots [i](#)

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.

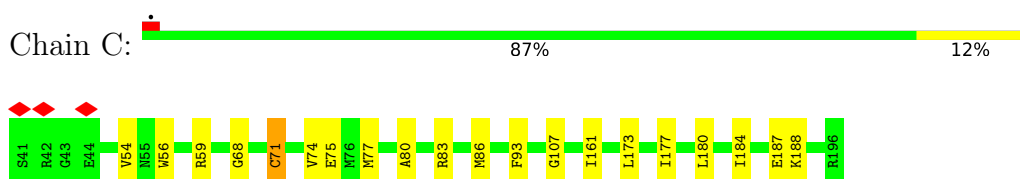
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



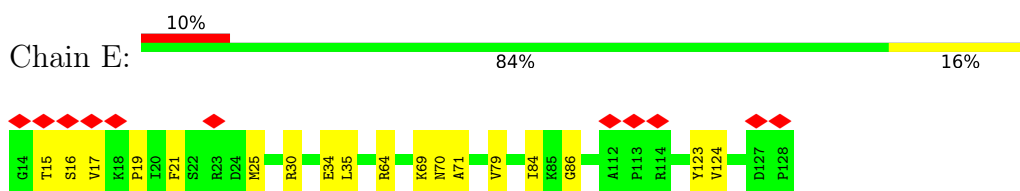
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



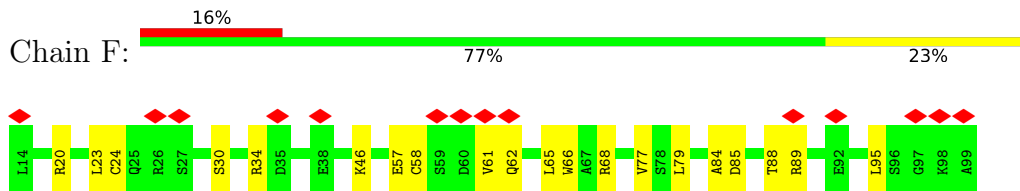
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



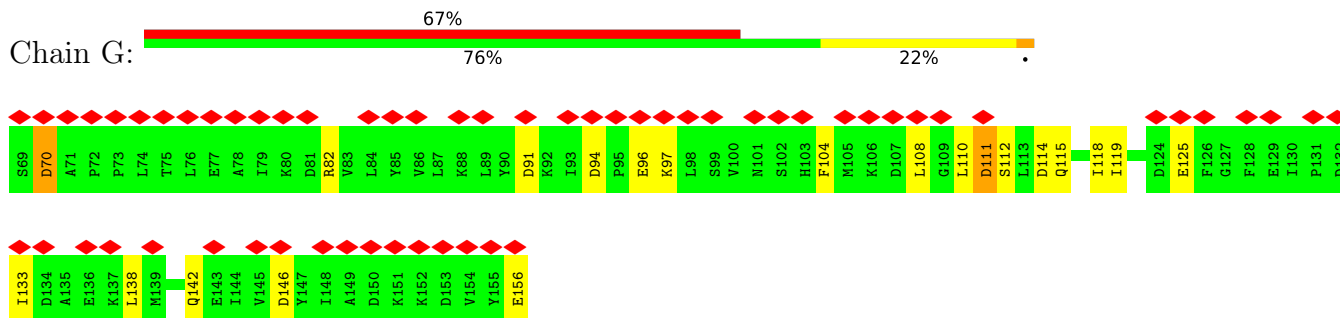
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



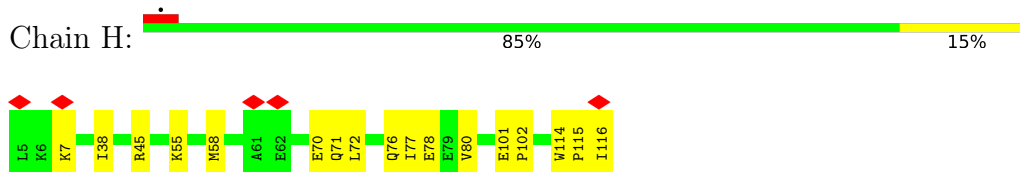
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



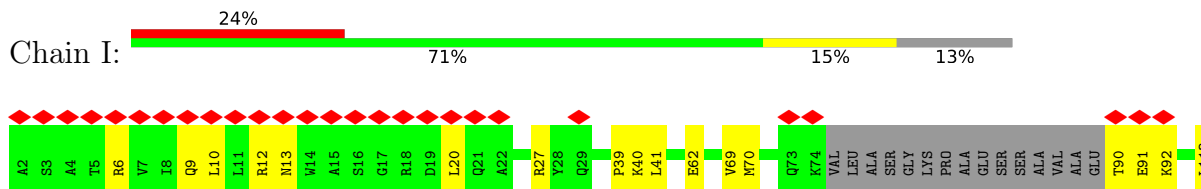
- Molecule 6: Acyl carrier protein, mitochondrial



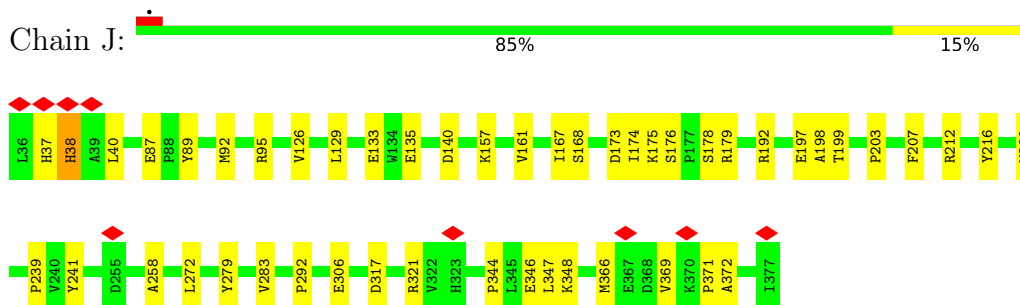
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



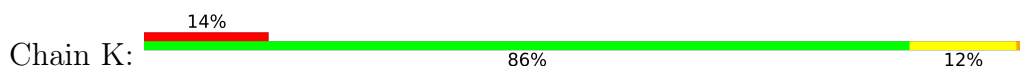
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

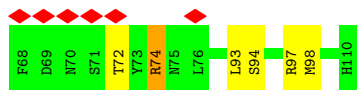


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

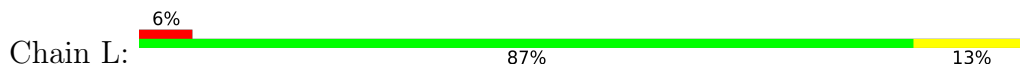


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

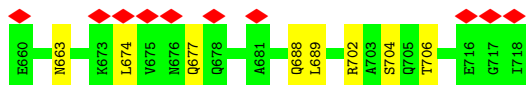
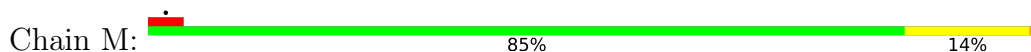




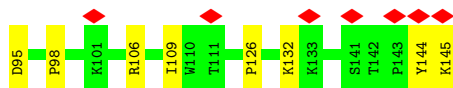
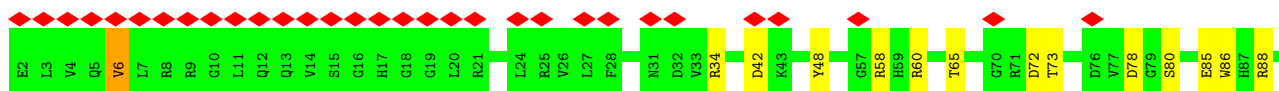
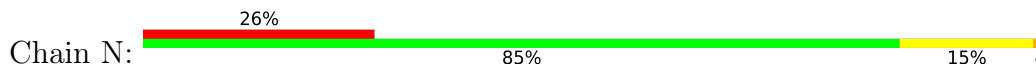
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



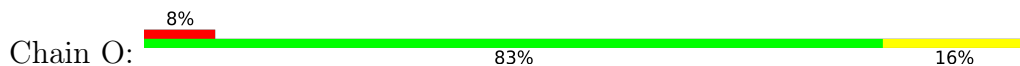
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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

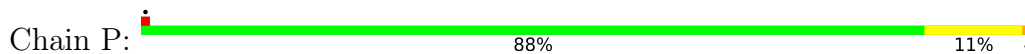


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

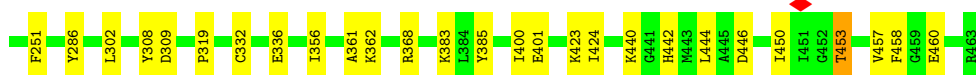
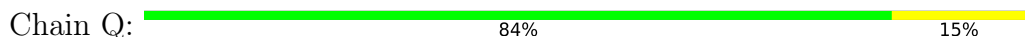




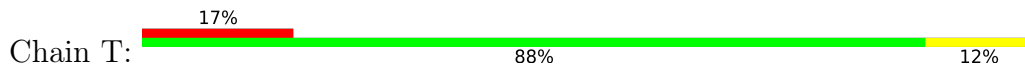
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



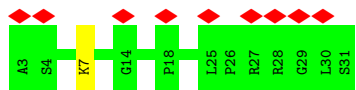
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	462013	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 ($e^-/\text{\AA}^2$)	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	0.100	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0167	Depositor
Map size (Å)	257.808, 257.808, 257.808	wwPDB
Map dimensions	480, 480, 480	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: CDL, MG, FES, PEE, 2MR, DCQ, UQ, NAI, ZN, PLX, FMN, NDP, 8Q1, SF4

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	0.43	1/4603 (0.0%)
2	B	0.16	0/1443	0.36	0/1952
3	C	0.17	0/1279	0.39	0/1730
4	E	0.17	0/995	0.38	0/1340
5	F	0.17	0/698	0.40	0/940
6	G	0.15	0/705	0.38	0/956
7	H	0.18	0/929	0.49	0/1258
8	I	0.20	0/798	0.49	0/1079
9	J	0.16	0/2828	0.37	0/3834
10	K	0.14	0/377	0.37	0/509
11	L	0.15	0/1039	0.37	0/1403
12	M	0.19	0/5384	0.47	6/7295 (0.1%)
13	N	0.14	0/1245	0.34	0/1694
14	O	0.17	0/1711	0.41	0/2328
15	P	0.17	0/1789	0.45	1/2436 (0.0%)
16	Q	0.34	3/3157 (0.1%)	0.44	1/4268 (0.0%)
17	T	0.14	0/755	0.35	0/1018
18	W	0.27	0/218	0.76	0/295
All	All	0.20	3/28756 (0.0%)	0.42	9/38938 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	192	LEU	C-N	10.17	1.47	1.33
16	Q	141	TYR	C-N	-7.79	1.23	1.33
16	Q	92	HIS	C-N	-6.82	1.23	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	94	VAL	N-CA-C	7.62	119.45	112.29
12	M	576	GLY	N-CA-C	6.50	121.08	112.77
12	M	397	ALA	N-CA-C	5.90	118.81	109.96
12	M	396	GLU	N-CA-C	5.79	117.67	111.36
15	P	47	ILE	N-CA-C	5.39	116.00	108.89
12	M	612	PRO	CA-C-N	5.34	125.10	119.76
12	M	612	PRO	C-N-CA	5.34	125.10	119.76
1	A	126	LYS	N-CA-C	5.19	116.94	111.28
12	M	406	ASN	N-CA-C	-5.18	99.82	108.94

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	50	0
2	B	1412	0	1363	15	0
3	C	1248	0	1254	16	0
4	E	971	0	975	13	0
5	F	687	0	700	11	0
6	G	693	0	671	17	0
7	H	910	0	950	10	0
8	I	780	0	808	14	0
9	J	2751	0	2773	29	0
10	K	366	0	338	4	0
11	L	1016	0	1016	13	0
12	M	5296	0	5327	75	0
13	N	1204	0	1162	16	0
14	O	1671	0	1673	22	0
15	P	1738	0	1693	28	0
16	Q	3096	0	3063	49	0
17	T	741	0	702	9	0
18	W	212	0	208	1	0
19	A	8	0	0	1	0
19	B	16	0	0	0	0
19	C	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	16	0	0	4	0
20	A	31	0	19	1	0
21	A	44	0	27	5	0
22	C	47	0	71	5	0
23	C	52	0	88	2	0
24	E	35	0	0	5	0
25	I	50	0	44	2	0
26	J	48	0	26	0	0
27	J	33	0	39	7	0
28	M	4	0	0	0	0
28	O	4	0	0	0	0
29	M	1	0	0	0	0
30	Q	23	0	30	7	0
31	T	1	0	0	0	0
32	A	53	0	0	1	0
32	B	80	0	0	0	0
32	C	58	0	0	0	0
32	E	3	0	0	0	0
32	F	1	0	0	0	0
32	H	4	0	0	0	0
32	I	13	0	0	0	0
32	J	5	0	0	0	0
32	K	4	0	0	0	0
32	L	24	0	0	0	0
32	M	196	0	0	2	0
32	N	5	0	0	0	0
32	O	17	0	0	1	0
32	P	74	0	0	2	0
32	Q	189	0	0	5	0
32	T	8	0	0	0	0
32	W	2	0	0	0	0
All	All	29279	0	28312	360	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 (360) 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)
15:P:44:ARG:HB3	15:P:45:PRO:CD	1.66	1.26
24:E:201:8Q1:O2	6:G:112:SER:CB	1.83	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:503:NAI:C1B	21:A:503:NAI:O4B	1.63	1.16
16:Q:92:HIS:ND1	30:Q:501:DCQ:H3MB	1.61	1.15
15:P:44:ARG:HB3	15:P:45:PRO:HD2	1.36	1.07
27:J:402:UQ:C26	27:J:402:UQ:H202	1.95	0.96
12:M:179:CYS:HG	19:M:802:SF4:FE1	0.81	0.96
24:E:201:8Q1:P24	6:G:112:SER:CB	2.53	0.96
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.46	0.96
15:P:44:ARG:CB	15:P:45:PRO:CD	2.44	0.95
8:I:27:ARG:NH2	16:Q:212:GLU:OE1	1.99	0.94
27:J:402:UQ:H111	27:J:402:UQ:H152	1.48	0.93
12:M:306:MET:HE2	12:M:314:LEU:HB3	1.50	0.91
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.09	0.86
12:M:307:ILE:HD12	12:M:307:ILE:O	1.79	0.83
11:L:109:ASN:ND2	11:L:111:LEU:O	2.11	0.83
9:J:220:MET:HE2	9:J:226:VAL:HG13	1.62	0.81
12:M:309:ASN:OD1	12:M:312:GLY:N	2.13	0.81
3:C:74:VAL:HA	3:C:77:MET:HE3	1.61	0.81
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.62	0.80
12:M:179:CYS:SG	19:M:802:SF4:FE1	1.74	0.79
8:I:62:GLU:OE1	15:P:47:ILE:HD13	1.83	0.79
16:Q:141:TYR:CE1	30:Q:501:DCQ:H4M	2.17	0.78
8:I:40:LYS:HB3	18:W:7:LYS:H	1.50	0.76
27:J:402:UQ:H152	27:J:402:UQ:C11	2.16	0.74
12:M:308:ARG:NH2	12:M:578:PRO:O	2.20	0.74
12:M:398:ASP:OD2	12:M:471:LYS:N	2.19	0.74
16:Q:99:MET:HE1	16:Q:444:LEU:HD21	1.69	0.74
1:A:50:ASP:O	1:A:59:ARG:NH2	2.21	0.73
15:P:44:ARG:CB	15:P:45:PRO:HD3	2.15	0.73
24:E:201:8Q1:O3	6:G:112:SER:CB	2.37	0.71
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.73	0.71
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.72	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.24	0.71
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.26	0.71
12:M:179:CYS:SG	19:M:802:SF4:S4	2.89	0.71
14:O:44:THR:HG22	14:O:46:GLU:H	1.56	0.71
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.74	0.70
16:Q:141:TYR:HE1	30:Q:501:DCQ:H4M	1.56	0.69
1:A:121:GLU:HB2	21:A:503:NAI:H42N	1.75	0.69
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.68
12:M:307:ILE:HD12	12:M:307:ILE:C	2.18	0.68
11:L:151:LYS:HE3	32:M:946:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:147:ASN:OD1	32:Q:601:HOH:O	2.11	0.68
16:Q:89:PRO:O	32:Q:602:HOH:O	2.12	0.68
1:A:89:GLY:O	21:A:503:NAI:H2N	1.94	0.67
15:P:85:GLU:HG3	32:P:309:HOH:O	1.93	0.67
12:M:166:GLY:HA2	12:M:213:MET:HE2	1.77	0.67
9:J:178:SER:OG	9:J:317:ASP:OD1	2.13	0.66
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.77	0.66
3:C:59:ARG:HH22	23:C:303:PLX:H32	1.59	0.66
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.77	0.65
22:C:302:PEE:C41	22:C:302:PEE:H76	2.28	0.64
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.31	0.64
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.80	0.64
1:A:210:THR:HB	1:A:224:ARG:HG3	1.78	0.64
3:C:80:ALA:HB2	3:C:86:MET:HE2	1.80	0.64
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.80	0.64
12:M:485:ASP:O	12:M:487:THR:N	2.31	0.63
7:H:58:MET:HE2	7:H:71:GLN:HB3	1.80	0.63
1:A:123:GLY:O	1:A:353:ALA:HB1	1.98	0.62
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.80	0.62
9:J:135:GLU:OE2	9:J:179:ARG:NH2	2.32	0.62
12:M:557:ARG:HG3	12:M:579:MET:HE3	1.81	0.62
16:Q:92:HIS:ND1	30:Q:501:DCQ:C3M	2.51	0.62
22:C:302:PEE:H76	22:C:302:PEE:H68	1.82	0.62
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.32	0.61
17:T:51:ARG:HG2	17:T:54:ARG:HH21	1.64	0.61
3:C:75:GLU:OE1	3:C:75:GLU:HA	1.99	0.61
12:M:456:ALA:O	12:M:499:ASN:ND2	2.34	0.61
17:T:47:ASP:O	17:T:52:ARG:NH2	2.34	0.60
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.81	0.60
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.16	0.60
12:M:485:ASP:O	12:M:488:ALA:N	2.34	0.60
20:A:502:FMN:N5	21:A:503:NAI:H4N	2.16	0.60
17:T:78:GLU:OE2	17:T:119:ARG:NH1	2.31	0.60
27:J:402:UQ:HM23	27:J:402:UQ:O1	2.02	0.60
27:J:402:UQ:O4	27:J:402:UQ:HM33	2.02	0.59
6:G:94:ASP:OD2	6:G:97:LYS:NZ	2.25	0.59
15:P:43:THR:HA	15:P:47:ILE:HD12	1.85	0.58
16:Q:88:HIS:HD2	16:Q:90:ALA:H	1.51	0.58
12:M:598:ASN:C	12:M:598:ASN:HD22	2.12	0.58
12:M:577:ALA:N	12:M:578:PRO:HD2	2.19	0.58
12:M:485:ASP:HA	12:M:677:GLN:OE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:372:PHE:H	12:M:532:PRO:HB2	1.70	0.57
14:O:38:LEU:O	14:O:124:ARG:NH2	2.37	0.57
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.86	0.57
17:T:49:ASP:OD2	17:T:51:ARG:NH2	2.38	0.57
15:P:44:ARG:CG	15:P:45:PRO:HD3	2.36	0.56
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.42	0.55
2:B:43:MET:HA	2:B:43:MET:HE2	1.89	0.55
1:A:385:CYS:HB3	19:A:501:SF4:S2	2.46	0.55
12:M:397:ALA:HB2	12:M:510:TRP:CZ2	2.42	0.55
1:A:102:MET:O	1:A:111:LYS:NZ	2.39	0.55
6:G:111:ASP:OD1	6:G:111:ASP:N	2.40	0.54
1:A:122:PRO:HA	14:O:176:CYS:SG	2.47	0.54
5:F:46:LYS:HD2	12:M:674:LEU:HD11	1.89	0.54
6:G:82:ARG:NH1	6:G:125:GLU:OE2	2.35	0.54
1:A:119:GLU:OE2	1:A:125:CYS:HA	2.08	0.54
6:G:142:GLN:NE2	6:G:146:ASP:OD2	2.31	0.54
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.40	0.54
12:M:256:ALA:O	12:M:598:ASN:HB2	2.08	0.54
16:Q:88:HIS:CD2	16:Q:89:PRO:HD2	2.43	0.54
12:M:406:ASN:ND2	12:M:688:GLN:O	2.36	0.54
5:F:61:VAL:HG23	5:F:62:GLN:H	1.73	0.53
1:A:201:ALA:O	14:O:119:TYR:HB3	2.09	0.53
2:B:116:CYS:SG	2:B:118:LEU:HG	2.49	0.53
16:Q:184:ILE:HD12	16:Q:210:MET:HE1	1.91	0.52
9:J:220:MET:HE3	9:J:227:PRO:HD2	1.91	0.52
12:M:144:MET:O	16:Q:362:LYS:HE3	2.09	0.52
7:H:116:ILE:HD13	11:L:96:LYS:HD2	1.91	0.52
22:C:302:PEE:C41	22:C:302:PEE:C45	2.86	0.52
8:I:6:ARG:HH21	8:I:10:LEU:HD11	1.74	0.52
12:M:398:ASP:O	12:M:427:LEU:HD12	2.10	0.52
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.92	0.52
1:A:224:ARG:HD2	11:L:164:PHE:CZ	2.46	0.51
13:N:42:ASP:OD2	13:N:48:TYR:OH	2.24	0.51
12:M:574:ASP:OD2	12:M:702:ARG:NH2	2.35	0.51
3:C:83:ARG:NH2	16:Q:205:GLU:OE2	2.38	0.51
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.92	0.51
4:E:69:LYS:HB2	4:E:69:LYS:NZ	2.26	0.51
6:G:115:GLN:NE2	6:G:119:ILE:HD11	2.26	0.50
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.92	0.50
3:C:86:MET:HE1	3:C:93:PHE:CE2	2.47	0.50
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:308:TYR:OH	32:Q:603:HOH:O	2.19	0.50
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.47	0.50
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.47	0.50
4:E:21:PHE:HE2	4:E:84:ILE:HD11	1.77	0.50
8:I:90:THR:OG1	8:I:91:GLU:N	2.40	0.50
9:J:92:MET:SD	9:J:95:ARG:HD2	2.51	0.50
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.41	0.50
6:G:115:GLN:O	6:G:119:ILE:HG12	2.12	0.50
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.47	0.50
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.49
1:A:40:ARG:NH2	1:A:289:GLU:O	2.45	0.49
27:J:402:UQ:C11	27:J:402:UQ:C15	2.86	0.49
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.94	0.49
6:G:70:ASP:OD1	6:G:70:ASP:N	2.37	0.49
9:J:168:SER:O	9:J:203:PRO:HD2	2.13	0.49
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.78	0.49
16:Q:319:PRO:HG2	16:Q:336:GLU:HG2	1.94	0.49
16:Q:336:GLU:OE1	32:Q:604:HOH:O	2.19	0.49
9:J:38:HIS:CE1	13:N:132:LYS:HE3	2.47	0.49
13:N:144:TYR:CZ	13:N:145:LYS:HD2	2.47	0.49
15:P:127:GLU:OE1	15:P:144:LYS:HE3	2.12	0.49
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.94	0.49
1:A:195:VAL:O	10:K:97:ARG:NH1	2.41	0.49
12:M:485:ASP:O	12:M:486:GLY:C	2.54	0.49
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.46	0.49
1:A:88:ARG:NH2	1:A:273:THR:O	2.45	0.48
3:C:68:GLY:HA3	30:Q:501:DCQ:H8	1.95	0.48
5:F:30:SER:HB2	5:F:34:ARG:NH1	2.28	0.48
12:M:219:SER:O	12:M:222:ILE:HG12	2.12	0.48
16:Q:232:VAL:HG23	16:Q:356:ILE:HD13	1.94	0.48
1:A:127:ASP:OD2	32:A:601:HOH:O	2.20	0.48
12:M:307:ILE:C	12:M:307:ILE:CD1	2.86	0.48
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.44	0.48
4:E:70:ASN:O	24:E:201:8Q1:O40	2.31	0.48
9:J:344:PRO:HG2	9:J:347:LEU:HG	1.95	0.48
13:N:65:THR:O	13:N:73:THR:OG1	2.30	0.48
4:E:19:PRO:HB3	11:L:53:ILE:HG21	1.96	0.48
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.78	0.48
1:A:90:GLY:HA3	21:A:503:NAI:H1D	1.95	0.48
3:C:107:GLY:HA2	19:C:301:SF4:S1	2.54	0.48
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:CG1	1:A:245:VAL:HG22	2.44	0.47
5:F:85:ASP:O	5:F:89:ARG:HG2	2.14	0.47
7:H:70:GLU:OE1	7:H:70:GLU:HA	2.13	0.47
12:M:309:ASN:ND2	12:M:313:LEU:HB2	2.29	0.47
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.95	0.47
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.94	0.47
1:A:110:PRO:O	1:A:238:CYS:HB3	2.15	0.47
5:F:24:CYS:N	5:F:58:CYS:SG	2.87	0.47
15:P:144:LYS:NZ	32:P:303:HOH:O	2.26	0.47
5:F:23:LEU:O	5:F:57:GLU:HA	2.15	0.47
8:I:9:GLN:O	8:I:13:ASN:ND2	2.48	0.47
1:A:126:LYS:HB3	1:A:277:ASN:HD21	1.79	0.47
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.50	0.47
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.96	0.47
3:C:71:CYS:HB2	19:C:301:SF4:S4	2.54	0.47
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.96	0.47
12:M:398:ASP:OD1	12:M:469:ALA:HB1	2.14	0.47
15:P:44:ARG:HG2	15:P:45:PRO:HD3	1.97	0.47
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.47	0.47
12:M:397:ALA:HB2	12:M:510:TRP:CH2	2.49	0.47
6:G:96:GLU:OE2	6:G:97:LYS:HD3	2.14	0.47
9:J:241:TYR:CZ	9:J:348:LYS:HG2	2.50	0.47
12:M:638:THR:O	12:M:642:VAL:HG23	2.15	0.47
11:L:105:GLU:HA	12:M:611:THR:HG21	1.96	0.47
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.97	0.47
12:M:419:ARG:NH1	12:M:439:THR:O	2.47	0.47
1:A:118:ASP:O	1:A:159:ARG:HD2	2.15	0.46
9:J:135:GLU:HG2	9:J:140:ASP:HA	1.97	0.46
6:G:119:ILE:HD12	6:G:138:LEU:HD12	1.98	0.46
9:J:37:HIS:CE1	17:T:49:ASP:HA	2.50	0.46
15:P:43:THR:CB	15:P:47:ILE:HD12	2.45	0.46
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.97	0.46
3:C:54:VAL:HG21	22:C:302:PEE:H55	1.96	0.46
16:Q:144:MET:H	16:Q:144:MET:HE2	1.80	0.46
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.97	0.46
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.98	0.46
13:N:78:ASP:OD2	13:N:80:SER:OG	2.27	0.46
13:N:85:GLU:HG2	13:N:86:TRP:H	1.81	0.46
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.98	0.46
4:E:30:ARG:NE	4:E:34:GLU:OE1	2.42	0.46
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:306:MET:CE	12:M:314:LEU:HB3	2.35	0.46
12:M:347:ASP:HB2	12:M:594:ALA:HB1	1.97	0.46
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.96	0.46
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.16	0.46
12:M:295:ASP:OD1	12:M:704:SER:OG	2.27	0.46
6:G:110:LEU:CD1	6:G:118:ILE:HD11	2.46	0.46
8:I:69:VAL:O	15:P:76:VAL:HB	2.15	0.46
9:J:133:GLU:OE1	9:J:321:ARG:NH2	2.42	0.46
3:C:173:LEU:O	3:C:177:ILE:HG12	2.16	0.46
12:M:206:VAL:HG21	19:M:802:SF4:S2	2.56	0.46
1:A:398:ARG:HH22	1:A:408:GLU:CD	2.24	0.45
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.51	0.45
1:A:63:TYR:CD1	14:O:241:PRO:HB2	2.52	0.45
11:L:165:SER:OG	11:L:168:LYS:HB2	2.15	0.45
10:K:72:THR:OG1	10:K:74:ARG:HD3	2.16	0.45
14:O:137:THR:HG22	14:O:138:THR:H	1.81	0.45
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.99	0.45
11:L:112:MET:SD	13:N:126:PRO:HB2	2.57	0.45
12:M:428:LYS:HE3	12:M:465:ILE:HD13	1.99	0.45
3:C:184:ILE:O	3:C:187:GLU:HG3	2.17	0.45
1:A:115:VAL:HG12	1:A:245:VAL:HG22	1.99	0.45
5:F:84:ALA:O	5:F:88:THR:OG1	2.33	0.45
27:J:402:UQ:H102	27:J:402:UQ:H72	1.73	0.45
12:M:647:GLU:HG3	12:M:654:VAL:HG21	2.00	0.44
1:A:63:TYR:CE2	1:A:64:LYS:HE2	2.53	0.44
4:E:35:LEU:HD21	4:E:86:GLY:HA3	1.99	0.44
16:Q:440:LYS:HA	16:Q:440:LYS:HD3	1.72	0.44
16:Q:457:VAL:HG13	16:Q:460:GLU:HG2	1.99	0.44
2:B:96:ARG:HG2	2:B:208:ASP:OD2	2.18	0.44
15:P:51:ASN:HB3	15:P:82:ASN:ND2	2.32	0.44
25:I:201:CDL:HA61	13:N:6:VAL:HG21	2.00	0.44
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.99	0.44
17:T:43:GLN:C	17:T:43:GLN:CD	2.86	0.44
12:M:598:ASN:C	12:M:598:ASN:ND2	2.73	0.44
12:M:625:ALA:O	12:M:629:ILE:HD12	2.18	0.44
9:J:87:GLU:HG3	9:J:89:TYR:H	1.83	0.44
11:L:151:LYS:CE	32:M:946:HOH:O	2.56	0.44
14:O:149:LEU:O	14:O:153:GLN:HG3	2.17	0.44
15:P:204:LEU:HD11	16:Q:123:LEU:HD23	1.99	0.44
22:C:302:PEE:H76	22:C:302:PEE:H69	1.99	0.44
9:J:126:VAL:HG23	9:J:161:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:44:GLU:H	12:M:44:GLU:CD	2.23	0.44
16:Q:116:LEU:O	16:Q:118:2MR:HD3	2.18	0.44
1:A:60:GLY:HA2	14:O:241:PRO:HA	2.00	0.44
8:I:27:ARG:HH22	16:Q:212:GLU:CD	2.26	0.44
8:I:113:LEU:HA	8:I:113:LEU:HD12	1.81	0.44
12:M:171:THR:HG23	12:M:173:MET:HG2	2.00	0.44
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.99	0.44
4:E:64:ARG:NH2	6:G:114:ASP:OD1	2.27	0.43
14:O:35:GLY:O	17:T:82:ARG:NH1	2.48	0.43
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.99	0.43
9:J:174:ILE:HG23	9:J:175:LYS:HG2	2.00	0.43
14:O:222:ARG:HD2	14:O:226:GLU:O	2.18	0.43
1:A:59:ARG:HG2	14:O:238:PRO:HB2	2.00	0.43
12:M:162:ASP:O	17:T:104:LYS:NZ	2.52	0.43
15:P:87:PHE:CE2	15:P:144:LYS:HE2	2.52	0.43
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.17	0.43
6:G:97:LYS:HE2	6:G:97:LYS:HB2	1.64	0.43
12:M:197:THR:O	14:O:114:GLU:HG2	2.19	0.43
12:M:335:GLY:HA2	12:M:362:ASP:O	2.19	0.43
14:O:149:LEU:HD11	14:O:160:VAL:HG12	2.00	0.43
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	2.00	0.43
1:A:90:GLY:HA2	1:A:350:GLY:O	2.18	0.43
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.00	0.43
7:H:7:LYS:HA	7:H:7:LYS:HD3	1.62	0.43
9:J:228:LEU:O	9:J:292:PRO:HA	2.18	0.43
16:Q:141:TYR:HE1	30:Q:501:DCQ:C4M	2.27	0.43
1:A:61:ASP:OD1	1:A:137:LYS:NZ	2.50	0.43
12:M:307:ILE:HG23	12:M:317:THR:HG21	2.01	0.43
2:B:113:CYS:O	2:B:141:ARG:NH1	2.49	0.43
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.83	0.43
12:M:511:LYS:HE2	12:M:663:ASN:HB2	2.00	0.43
9:J:212:ARG:O	9:J:216:TYR:CB	2.67	0.42
11:L:111:LEU:HD11	13:N:126:PRO:HG2	2.01	0.42
12:M:222:ILE:HA	12:M:225:ILE:HG12	2.00	0.42
16:Q:193:ASP:HB2	32:Q:677:HOH:O	2.18	0.42
12:M:250:SER:OG	12:M:251:ILE:N	2.49	0.42
12:M:84:LYS:HB2	12:M:84:LYS:HE2	1.61	0.42
12:M:338:VAL:O	12:M:363:SER:OG	2.35	0.42
1:A:75:TRP:O	1:A:79:GLU:HG2	2.18	0.42
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.01	0.42
25:I:201:CDL:H531	25:I:201:CDL:H712	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:HB3	1:A:165:GLU:HB2	2.02	0.42
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.54	0.42
16:Q:207:ARG:HA	16:Q:210:MET:HE3	2.02	0.42
1:A:314:LEU:HD11	1:A:317:VAL:HG23	2.00	0.42
1:A:367:ILE:O	1:A:371:ILE:HG12	2.20	0.42
6:G:104:PHE:HA	6:G:108:LEU:HD12	2.02	0.42
15:P:113:ASP:CG	16:Q:423:LYS:HZ2	2.27	0.42
9:J:212:ARG:O	9:J:216:TYR:HB2	2.19	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.42
12:M:402:LEU:HD23	12:M:475:VAL:HB	2.02	0.42
12:M:535:GLU:OE2	12:M:535:GLU:HA	2.20	0.42
12:M:577:ALA:N	12:M:578:PRO:CD	2.83	0.42
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.45	0.42
3:C:188:LYS:HB2	3:C:188:LYS:HE2	1.92	0.42
8:I:92:LYS:HD3	8:I:92:LYS:HA	1.93	0.42
12:M:399:VAL:HG12	12:M:400:ILE:N	2.34	0.42
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.54	0.42
14:O:134:VAL:HG22	14:O:186:VAL:HG22	2.01	0.42
17:T:69:ASP:O	17:T:73:GLU:HG3	2.20	0.42
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.02	0.41
4:E:17:VAL:HG21	11:L:55:VAL:HG22	2.01	0.41
9:J:283:VAL:HG22	9:J:369:VAL:HG11	2.01	0.41
1:A:104:LYS:H	1:A:104:LYS:HG2	1.66	0.41
1:A:111:LYS:HE3	1:A:150:GLY:O	2.19	0.41
9:J:366:MET:HE2	9:J:366:MET:HB3	1.92	0.41
12:M:309:ASN:CG	12:M:313:LEU:H	2.26	0.41
14:O:43:ASP:OD1	14:O:49:PRO:HD3	2.20	0.41
1:A:68:ILE:HD11	1:A:256:ARG:HG3	2.02	0.41
4:E:71:ALA:HB1	24:E:201:8Q1:O33	2.21	0.41
10:K:98:MET:HE3	10:K:98:MET:HB3	1.94	0.41
14:O:195:ASP:HB3	14:O:220:SER:OG	2.19	0.41
1:A:113:LEU:HD13	1:A:149:MET:HE1	2.01	0.41
7:H:72:LEU:HD13	7:H:80:VAL:HG11	2.02	0.41
12:M:485:ASP:C	12:M:487:THR:N	2.78	0.41
1:A:296:LEU:HD21	1:A:317:VAL:HG11	2.01	0.41
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.20	0.41
2:B:97:PHE:HB2	16:Q:215:GLU:OE2	2.20	0.41
15:P:43:THR:CA	15:P:47:ILE:HD12	2.49	0.41
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	2.00	0.41
7:H:38:ILE:O	7:H:45:ARG:NH1	2.45	0.41
7:H:76:GLN:O	7:H:78:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.20	0.41
1:A:315:LEU:HB2	1:A:359:ARG:HA	2.02	0.41
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.54	0.41
12:M:421:SER:OG	12:M:427:LEU:HD22	2.20	0.41
1:A:214:GLU:CD	1:A:224:ARG:HD3	2.46	0.41
3:C:56:TRP:CE2	23:C:303:PLX:H91	2.56	0.41
12:M:556:THR:HA	12:M:579:MET:HE1	2.02	0.41
13:N:85:GLU:HG2	13:N:86:TRP:N	2.35	0.41
15:P:90:PRO:O	15:P:93:VAL:HG23	2.20	0.41
15:P:128:ILE:HB	15:P:145:THR:HG22	2.03	0.41
30:Q:501:DCQ:H1MB	30:Q:501:DCQ:H7	1.84	0.41
2:B:200:GLU:HG2	13:N:88:ARG:HD3	2.02	0.41
8:I:70:MET:O	8:I:70:MET:SD	2.78	0.41
12:M:292:PHE:HB3	12:M:706:THR:HG21	2.02	0.41
1:A:114:VAL:HG11	1:A:212:LEU:HD22	2.03	0.40
3:C:86:MET:HE1	3:C:93:PHE:CD2	2.56	0.40
9:J:199:THR:OG1	9:J:258:ALA:O	2.30	0.40
4:E:15:THR:HG22	4:E:17:VAL:HG13	2.03	0.40
5:F:23:LEU:C	5:F:58:CYS:SG	3.04	0.40
6:G:133:ILE:HD12	6:G:133:ILE:HA	1.87	0.40
12:M:372:PHE:N	12:M:532:PRO:HB2	2.35	0.40
14:O:57:PRO:O	14:O:61:LYS:HG2	2.22	0.40
1:A:383:THR:HG21	12:M:120:LEU:HG	2.03	0.40
8:I:70:MET:HG3	15:P:66:ALA:HB1	2.04	0.40
9:J:40:LEU:HD23	9:J:40:LEU:HA	1.89	0.40
16:Q:94:VAL:O	16:Q:115:LEU:HD12	2.20	0.40
14:O:124:ARG:NH1	32:O:401:HOH:O	2.37	0.40
14:O:155:LYS:HG3	14:O:202:GLU:HG2	2.03	0.40
4:E:16:SER:O	4:E:16:SER:OG	2.27	0.40
9:J:207:PHE:HD2	9:J:239:PRO:HB2	1.86	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%)	421 (98%)	10 (2%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	106 (96%)	3 (3%)	1 (1%)	14	22
8	I	93/112 (83%)	87 (94%)	6 (6%)	0	100	100
9	J	340/342 (99%)	326 (96%)	13 (4%)	1 (0%)	36	50
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%)	669 (97%)	18 (3%)	1 (0%)	48	64
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	202 (94%)	13 (6%)	0	100	100
15	P	206/208 (99%)	198 (96%)	7 (3%)	1 (0%)	24	37
16	Q	383/386 (99%)	376 (98%)	7 (2%)	0	100	100
17	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
18	W	27/29 (93%)	24 (89%)	3 (11%)	0	100	100
All	All	3504/3558 (98%)	3395 (97%)	105 (3%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	44	ARG
7	H	77	ILE
12	M	486	GLY
9	J	38	HIS

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%)	343 (99%)	3 (1%)	70	85
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	88
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	86
4	E	107/107 (100%)	106 (99%)	1 (1%)	70	85
5	F	75/76 (99%)	73 (97%)	2 (3%)	39	62
6	G	76/81 (94%)	72 (95%)	4 (5%)	20	36
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	82
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	88
10	K	42/42 (100%)	40 (95%)	2 (5%)	23	40
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	85
12	M	580/580 (100%)	570 (98%)	10 (2%)	53	74
13	N	130/130 (100%)	128 (98%)	2 (2%)	57	77
14	O	183/183 (100%)	177 (97%)	6 (3%)	33	55
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	91
16	Q	332/332 (100%)	330 (99%)	2 (1%)	78	89
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	22/24 (92%)	22 (100%)	0	100	100
All	All	3040/3058 (99%)	3001 (99%)	39 (1%)	59	80

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	A	451	GLN
1	A	455	LEU
2	B	75	SER
3	C	71	CYS
4	E	124	VAL
5	F	77	VAL
5	F	95	LEU
6	G	70	ASP
6	G	91	ASP
6	G	111	ASP

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Mol	Chain	Res	Type
6	G	156	GLU
8	I	41	LEU
9	J	272	LEU
9	J	306	GLU
10	K	74	ARG
10	K	94	SER
11	L	124	LEU
12	M	171	THR
12	M	361	VAL
12	M	364	ASP
12	M	405	THR
12	M	463	SER
12	M	470	LYS
12	M	507	THR
12	M	598	ASN
12	M	636	TYR
12	M	689	LEU
13	N	6	VAL
13	N	72	ASP
14	O	40	VAL
14	O	50	ASP
14	O	150	GLU
14	O	181	VAL
14	O	186	VAL
14	O	235	THR
15	P	248	PRO
16	Q	217	VAL
16	Q	453	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
4	E	126	HIS
5	F	48	ASN
8	I	13	ASN
8	I	29	GLN
12	M	123	ASN
12	M	178	GLN
12	M	202	ASN
12	M	425	ASN
12	M	495	ASN

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Mol	Chain	Res	Type
12	M	540	ASN
12	M	598	ASN
12	M	604	GLN
12	M	652	ASN
12	M	669	ASN
13	N	5	GLN
13	N	12	GLN
13	N	123	GLN
14	O	90	ASN
14	O	131	HIS
14	O	182	ASN
15	P	51	ASN
15	P	82	ASN
15	P	124	ASN
15	P	196	HIS
15	P	228	GLN
16	Q	88	HIS
16	Q	250	ASN
17	T	74	GLN
17	T	120	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	2.03	1 (10%)	5,13,15	6.08	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.33	130.78	119.48
16	Q	118	2MR	CQ2-NH2-CZ	3.97	132.19	123.65
16	Q	118	2MR	CD-NE-CZ	3.50	129.95	123.36

There are no chirality outliers.

All (2) 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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	SF4	C	301	3	0,12,12	-	-	-		
19	SF4	B	301	2	0,12,12	-	-	-		
30	DCQ	Q	501	-	23,23,23	1.34	5 (21%)	27,29,29	1.08	2 (7%)
26	NDP	J	401	-	51,52,52	2.39	6 (11%)	71,80,80	1.50	15 (21%)
23	PLX	C	303	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
19	SF4	B	302	2	0,12,12	-	-	-		
19	SF4	M	801	12	0,12,12	-	-	-		
19	SF4	M	802	12	0,12,12	-	-	-		
25	CDL	I	201	-	49,49,99	1.43	8 (16%)	55,61,111	1.17	5 (9%)
19	SF4	A	501	1	0,12,12	-	-	-		
28	FES	M	803	12	0,4,4	-	-	-		
22	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
20	FMN	A	502	-	33,33,33	1.45	5 (15%)	48,50,50	1.24	7 (14%)
27	UQ	J	402	-	33,33,63	3.52	9 (27%)	42,43,79	2.77	14 (33%)
28	FES	O	301	14	0,4,4	-	-	-		
24	8Q1	E	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.51	6 (15%)
21	NAI	A	503	-	47,48,48	3.99	22 (46%)	64,73,73	1.70	11 (17%)

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
30	DCQ	Q	501	-	-	4/14/38/38	0/1/1/1
19	SF4	C	301	3	-	-	0/6/5/5
26	NDP	J	401	-	-	6/34/77/77	0/5/5/5
23	PLX	C	303	-	-	29/55/55/55	-
19	SF4	B	302	2	-	-	0/6/5/5
25	CDL	I	201	-	-	29/60/60/110	-
19	SF4	M	801	12	-	-	0/6/5/5
19	SF4	M	802	12	-	-	0/6/5/5
19	SF4	A	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	FES	M	803	12	-	-	0/1/1/1
22	PEE	C	302	-	-	27/50/50/54	-
20	FMN	A	502	-	-	1/18/18/18	0/3/3/3
27	UQ	J	402	-	-	14/27/51/87	0/1/1/1
28	FES	O	301	14	-	-	0/1/1/1
24	8Q1	E	201	-	-	10/41/41/41	-
21	NAI	A	503	-	-	5/29/72/72	0/5/5/5

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	P2B-O2B	13.69	1.83	1.59
21	A	503	NAI	C3D-C4D	-10.38	1.26	1.53
27	J	402	UQ	C18-C19	9.96	1.56	1.33
27	J	402	UQ	C13-C14	9.61	1.55	1.33
21	A	503	NAI	O4B-C1B	9.41	1.63	1.42
27	J	402	UQ	C8-C9	9.30	1.54	1.33
21	A	503	NAI	O4B-C4B	-8.25	1.26	1.45
21	A	503	NAI	C2D-C1D	-7.73	1.29	1.53
27	J	402	UQ	C23-C24	7.49	1.54	1.32
21	A	503	NAI	C2B-C1B	-7.33	1.30	1.53
21	A	503	NAI	O4D-C4D	6.88	1.60	1.45
21	A	503	NAI	PA-O3	6.19	1.66	1.59
21	A	503	NAI	C2D-C3D	5.94	1.69	1.53
21	A	503	NAI	O4D-C1D	5.54	1.54	1.42
21	A	503	NAI	PN-O3	5.49	1.65	1.59
21	A	503	NAI	C7N-N7N	5.28	1.48	1.33
20	A	502	FMN	C9A-C5A	5.26	1.49	1.41
21	A	503	NAI	C4N-C3N	-5.19	1.40	1.50
24	E	201	8Q1	C39-N41	5.10	1.45	1.33
24	E	201	8Q1	C34-N36	5.10	1.45	1.33
21	A	503	NAI	C6A-N6A	5.06	1.47	1.34
26	J	401	NDP	PA-O3	4.90	1.64	1.59
21	A	503	NAI	O2B-C2B	4.30	1.53	1.43
26	J	401	NDP	PN-O5D	4.01	1.75	1.59
22	C	302	PEE	C18-C19	3.82	1.53	1.31
22	C	302	PEE	C39-C38	3.75	1.53	1.31
21	A	503	NAI	C7N-C3N	3.54	1.56	1.48
25	I	201	CDL	OA8-CA7	3.41	1.43	1.33
20	A	502	FMN	C8-C7	3.35	1.49	1.40
21	A	503	NAI	C4N-C5N	-3.32	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	401	NDP	O2B-C2B	-3.13	1.33	1.44
25	I	201	CDL	OB8-CB7	2.94	1.41	1.33
25	I	201	CDL	OB6-CB5	2.90	1.42	1.34
25	I	201	CDL	OA6-CA5	2.85	1.42	1.34
27	J	402	UQ	C6-C1	2.72	1.54	1.46
23	C	303	PLX	O6-C4	-2.72	1.41	1.44
21	A	503	NAI	C8A-N9A	-2.69	1.33	1.37
22	C	302	PEE	O2-C2	-2.61	1.40	1.46
25	I	201	CDL	OA6-CA4	-2.57	1.40	1.46
20	A	502	FMN	C4-N3	-2.56	1.34	1.38
24	E	201	8Q1	C6-C1	2.51	1.53	1.50
21	A	503	NAI	C6N-C5N	2.46	1.40	1.33
21	A	503	NAI	PN-O5D	2.45	1.69	1.59
24	E	201	8Q1	C1-S44	2.40	1.81	1.76
24	E	201	8Q1	O35-C34	-2.40	1.18	1.23
21	A	503	NAI	C5B-C4B	2.38	1.58	1.51
25	I	201	CDL	OB6-CB4	-2.36	1.41	1.46
21	A	503	NAI	O3B-C3B	-2.35	1.37	1.43
24	E	201	8Q1	O40-C39	-2.35	1.18	1.23
23	C	303	PLX	C7-C6	2.35	1.55	1.50
22	C	302	PEE	O3-C30	2.35	1.40	1.33
25	I	201	CDL	PB2-OB2	2.30	1.68	1.59
30	Q	501	DCQ	O4-C4M	-2.29	1.40	1.45
27	J	402	UQ	C7-C8	2.28	1.54	1.50
30	Q	501	DCQ	C6-C5	2.28	1.52	1.46
25	I	201	CDL	PB2-OB5	2.27	1.68	1.59
30	Q	501	DCQ	O3-C3M	-2.25	1.40	1.45
22	C	302	PEE	O2-C10	2.22	1.40	1.34
22	C	302	PEE	O3-C3	-2.20	1.40	1.45
20	A	502	FMN	C5A-N5	-2.18	1.35	1.39
20	A	502	FMN	C4A-N5	2.14	1.35	1.30
26	J	401	NDP	C5A-C4A	2.13	1.42	1.39
27	J	402	UQ	O4-C4	-2.13	1.18	1.23
23	C	303	PLX	P1-O4	2.12	1.67	1.59
27	J	402	UQ	O3-CM3	-2.12	1.40	1.45
30	Q	501	DCQ	O2-C2	-2.08	1.18	1.23
30	Q	501	DCQ	O5-C5	-2.06	1.18	1.23
21	A	503	NAI	C5A-N7A	-2.04	1.35	1.39
26	J	401	NDP	O5D-C5D	-2.04	1.36	1.44
23	C	303	PLX	P1-O1	2.01	1.67	1.59
27	J	402	UQ	C21-C19	2.01	1.55	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	402	UQ	C7-C8-C9	-8.13	112.83	126.83
27	J	402	UQ	C12-C13-C14	-6.48	112.79	127.62
27	J	402	UQ	C17-C18-C19	-6.46	112.84	127.62
21	A	503	NAI	C5A-C4A-N3A	-5.55	119.07	126.72
24	E	201	8Q1	C6-C1-S44	5.30	119.72	113.40
27	J	402	UQ	C22-C23-C24	-4.42	112.89	127.64
21	A	503	NAI	N3A-C2A-N1A	-4.41	121.91	128.58
25	I	201	CDL	OB6-CB5-C51	4.24	120.66	111.48
27	J	402	UQ	C20-C19-C18	-4.22	112.78	123.63
27	J	402	UQ	C10-C9-C8	-4.19	112.87	123.63
27	J	402	UQ	C15-C14-C13	-4.19	112.88	123.63
21	A	503	NAI	N3A-C4A-N9A	3.92	133.83	127.17
22	C	302	PEE	O2-C10-C11	3.89	119.91	111.48
25	I	201	CDL	OA6-CA5-C11	3.87	119.85	111.48
26	J	401	NDP	P2B-O2B-C2B	-3.77	113.37	123.43
21	A	503	NAI	C2A-N3A-C4A	3.72	120.93	111.83
27	J	402	UQ	C11-C9-C8	-3.71	112.85	121.17
27	J	402	UQ	C16-C14-C13	-3.67	112.92	121.17
27	J	402	UQ	C21-C19-C18	-3.67	112.93	121.17
26	J	401	NDP	O2B-P2B-O1X	-3.55	96.69	109.33
21	A	503	NAI	C4A-C5A-N7A	-3.47	106.62	110.58
26	J	401	NDP	O3-PA-O1A	-3.46	100.31	110.70
21	A	503	NAI	C5A-N7A-C8A	3.41	108.81	103.45
24	E	201	8Q1	C37-C38-C39	3.33	117.95	112.39
21	A	503	NAI	N9A-C8A-N7A	-3.29	109.26	113.94
27	J	402	UQ	C26-C24-C23	-3.26	112.88	122.66
27	J	402	UQ	C25-C24-C23	-3.24	112.93	122.66
21	A	503	NAI	C3D-C2D-C1D	3.19	107.49	101.46
24	E	201	8Q1	O4-C1-C6	-3.15	120.35	123.98
21	A	503	NAI	C4D-O4D-C1D	-3.08	102.66	109.47
30	Q	501	DCQ	C1M-C1-C6	-3.04	119.46	124.45
26	J	401	NDP	PA-O5B-C5B	-3.01	104.09	121.35
20	A	502	FMN	C4-C4A-N5	2.90	122.21	118.21
27	J	402	UQ	C7-C6-C5	-2.85	120.00	124.89
24	E	201	8Q1	C43-S44-C1	2.74	109.93	101.84
27	J	402	UQ	CM5-C5-C6	-2.74	119.95	124.45
25	I	201	CDL	OB8-CB7-C71	2.72	120.13	111.83
22	C	302	PEE	O3-C30-C31	2.66	119.95	111.83
25	I	201	CDL	OA8-CA7-C31	2.64	119.90	111.83
26	J	401	NDP	PN-O5D-C5D	-2.64	106.22	121.35
26	J	401	NDP	O3X-P2B-O2X	2.53	117.29	107.80
20	A	502	FMN	C4A-C10-N1	-2.48	118.52	124.59
26	J	401	NDP	O2N-PN-O3	2.43	113.84	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	303	PLX	C1A-N1-C1	2.42	119.54	109.91
21	A	503	NAI	C2D-C3D-C4D	2.42	107.29	102.61
26	J	401	NDP	O2N-PN-O1N	2.39	123.57	112.44
21	A	503	NAI	C4A-N9A-C8A	2.36	108.21	105.74
26	J	401	NDP	O4B-C4B-C3B	2.35	109.81	105.15
26	J	401	NDP	C2A-N1A-C6A	-2.34	114.88	118.73
26	J	401	NDP	O5D-PN-O1N	-2.30	99.81	108.94
26	J	401	NDP	N3A-C4A-N9A	2.27	131.03	127.17
20	A	502	FMN	O4-C4-C4A	-2.21	120.70	126.53
20	A	502	FMN	C4A-C10-N10	2.19	119.62	116.48
24	E	201	8Q1	O4-C1-S44	-2.16	119.94	122.68
20	A	502	FMN	C10-N1-C2	2.14	121.47	116.85
26	J	401	NDP	C5B-C4B-C3B	-2.11	107.60	115.21
20	A	502	FMN	C4A-C4-N3	2.11	118.61	113.25
24	E	201	8Q1	C38-C39-N41	2.10	120.16	116.34
26	J	401	NDP	C5A-C4A-N3A	-2.09	123.83	126.72
26	J	401	NDP	C2B-C1B-N9A	-2.03	110.41	113.75
30	Q	501	DCQ	C7-C6-C5	2.01	120.27	116.92
20	A	502	FMN	C4-N3-C2	-2.01	122.07	125.64
25	I	201	CDL	OB6-CB5-OB7	-2.01	119.01	123.70

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	C	302	PEE	C1-O3P-P-O1P
22	C	302	PEE	C4-O4P-P-O2P
22	C	302	PEE	C4-O4P-P-O1P
23	C	303	PLX	O6-C4-C5-O8
23	C	303	PLX	C2-O1-P1-O4
23	C	303	PLX	C2-O1-P1-O2
23	C	303	PLX	C2-O1-P1-O3
23	C	303	PLX	O9-C24-C25-C26
24	E	201	8Q1	O27-C28-C29-C30
24	E	201	8Q1	O27-C28-C29-C31
24	E	201	8Q1	O27-C28-C29-C32
24	E	201	8Q1	C28-C29-C32-C34
24	E	201	8Q1	C28-C29-C32-O33
24	E	201	8Q1	C30-C29-C32-C34
24	E	201	8Q1	C30-C29-C32-O33
24	E	201	8Q1	C31-C29-C32-C34
24	E	201	8Q1	C31-C29-C32-O33

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Mol	Chain	Res	Type	Atoms
24	E	201	8Q1	N41-C42-C43-S44
25	I	201	CDL	CA2-OA2-PA1-OA4
25	I	201	CDL	CA2-OA2-PA1-OA5
25	I	201	CDL	CA3-OA5-PA1-OA3
25	I	201	CDL	OA6-CA4-CA6-OA8
25	I	201	CDL	CB2-OB2-PB2-OB3
25	I	201	CDL	CB2-OB2-PB2-OB4
25	I	201	CDL	CB2-OB2-PB2-OB5
25	I	201	CDL	CB3-OB5-PB2-OB2
25	I	201	CDL	CB3-OB5-PB2-OB3
25	I	201	CDL	OB6-CB4-CB6-OB8
26	J	401	NDP	C5B-O5B-PA-O1A
27	J	402	UQ	C12-C13-C14-C15
27	J	402	UQ	C16-C17-C18-C19
27	J	402	UQ	C17-C18-C19-C20
27	J	402	UQ	C17-C18-C19-C21
27	J	402	UQ	C22-C23-C24-C26
27	J	402	UQ	C15-C14-C16-C17
27	J	402	UQ	C13-C14-C16-C17
30	Q	501	DCQ	C6-C7-C8-C9
27	J	402	UQ	C7-C8-C9-C11
25	I	201	CDL	O1-C1-CB2-OB2
27	J	402	UQ	C22-C23-C24-C25
25	I	201	CDL	CA2-C1-CB2-OB2
21	A	503	NAI	O4D-C4D-C5D-O5D
21	A	503	NAI	C3D-C4D-C5D-O5D
26	J	401	NDP	O4D-C4D-C5D-O5D
25	I	201	CDL	CB5-C51-C52-C53
23	C	303	PLX	C25-C26-C27-C28
23	C	303	PLX	O8-C24-C25-C26
22	C	302	PEE	C11-C10-O2-C2
22	C	302	PEE	O4-C10-O2-C2
22	C	302	PEE	C41-C42-C43-C44
22	C	302	PEE	C11-C12-C13-C14
23	C	303	PLX	C26-C27-C28-C29
23	C	303	PLX	O7-C6-C7-C8
23	C	303	PLX	C14-C15-C16-C17
23	C	303	PLX	C9-C10-C11-C12
25	I	201	CDL	CA7-C31-C32-C33
30	Q	501	DCQ	C7-C8-C9-C10
23	C	303	PLX	C11-C12-C13-C14
22	C	302	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
23	C	303	PLX	C11-C10-C9-C8
30	Q	501	DCQ	C10-C11-C12-C13
25	I	201	CDL	C11-C12-C13-C14
22	C	302	PEE	C13-C14-C15-C16
23	C	303	PLX	C13-C14-C15-C16
25	I	201	CDL	C71-CB7-OB8-CB6
23	C	303	PLX	C10-C11-C12-C13
22	C	302	PEE	O5-C30-O3-C3
23	C	303	PLX	C16-C17-C18-C19
23	C	303	PLX	O6-C6-C7-C8
23	C	303	PLX	C27-C28-C29-C30
23	C	303	PLX	C3-C4-C5-O8
25	I	201	CDL	CA3-CA4-CA6-OA8
25	I	201	CDL	CB3-CB4-CB6-OB8
23	C	303	PLX	C33-C34-C35-C36
25	I	201	CDL	OB9-CB7-OB8-CB6
22	C	302	PEE	C15-C16-C17-C18
23	C	303	PLX	C31-C32-C33-C34
27	J	402	UQ	C11-C12-C13-C14
25	I	201	CDL	C1-CB2-OB2-PB2
22	C	302	PEE	C19-C20-C21-C22
25	I	201	CDL	CB7-C71-C72-C73
23	C	303	PLX	C29-C30-C31-C32
23	C	303	PLX	C19-C20-C21-C22
26	J	401	NDP	O4B-C4B-C5B-O5B
23	C	303	PLX	C7-C8-C9-C10
25	I	201	CDL	CA5-C11-C12-C13
23	C	303	PLX	N1-C1-C2-O1
23	C	303	PLX	C25-C24-O8-C5
26	J	401	NDP	O4D-C1D-N1N-C6N
25	I	201	CDL	OB5-CB3-CB4-CB6
22	C	302	PEE	O2-C2-C3-O3
22	C	302	PEE	C1-C2-C3-O3
22	C	302	PEE	C1-O3P-P-O2P
22	C	302	PEE	C1-O3P-P-O4P
22	C	302	PEE	C4-O4P-P-O3P
25	I	201	CDL	CB3-OB5-PB2-OB4
27	J	402	UQ	C3-C2-O2-CM2
27	J	402	UQ	C2-C3-O3-CM3
23	C	303	PLX	C30-C31-C32-C33
27	J	402	UQ	C20-C19-C21-C22
22	C	302	PEE	C44-C45-C46-C47

Continued on next page...

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Mol	Chain	Res	Type	Atoms
22	C	302	PEE	C34-C35-C36-C37
20	A	502	FMN	C5'-O5'-P-O1P
22	C	302	PEE	C36-C37-C38-C39
25	I	201	CDL	OB5-CB3-CB4-OB6
23	C	303	PLX	C15-C16-C17-C18
26	J	401	NDP	C3D-C4D-C5D-O5D
21	A	503	NAI	O4D-C1D-N1N-C2N
26	J	401	NDP	C3B-C4B-C5B-O5B
25	I	201	CDL	C71-C72-C73-C74
22	C	302	PEE	C12-C13-C14-C15
25	I	201	CDL	C12-C11-CA5-OA6
22	C	302	PEE	C38-C39-C40-C41
30	Q	501	DCQ	C13-C14-C15-C16
21	A	503	NAI	C2D-C1D-N1N-C2N
22	C	302	PEE	O3-C30-C31-C32
27	J	402	UQ	C12-C11-C9-C8
22	C	302	PEE	C16-C17-C18-C19
22	C	302	PEE	O5-C30-C31-C32
21	A	503	NAI	C2N-C3N-C7N-O7N
23	C	303	PLX	O9-C24-O8-C5
22	C	302	PEE	C18-C19-C20-C21
25	I	201	CDL	OB7-CB5-OB6-CB4
25	I	201	CDL	C32-C31-CA7-OA8
22	C	302	PEE	C10-C11-C12-C13

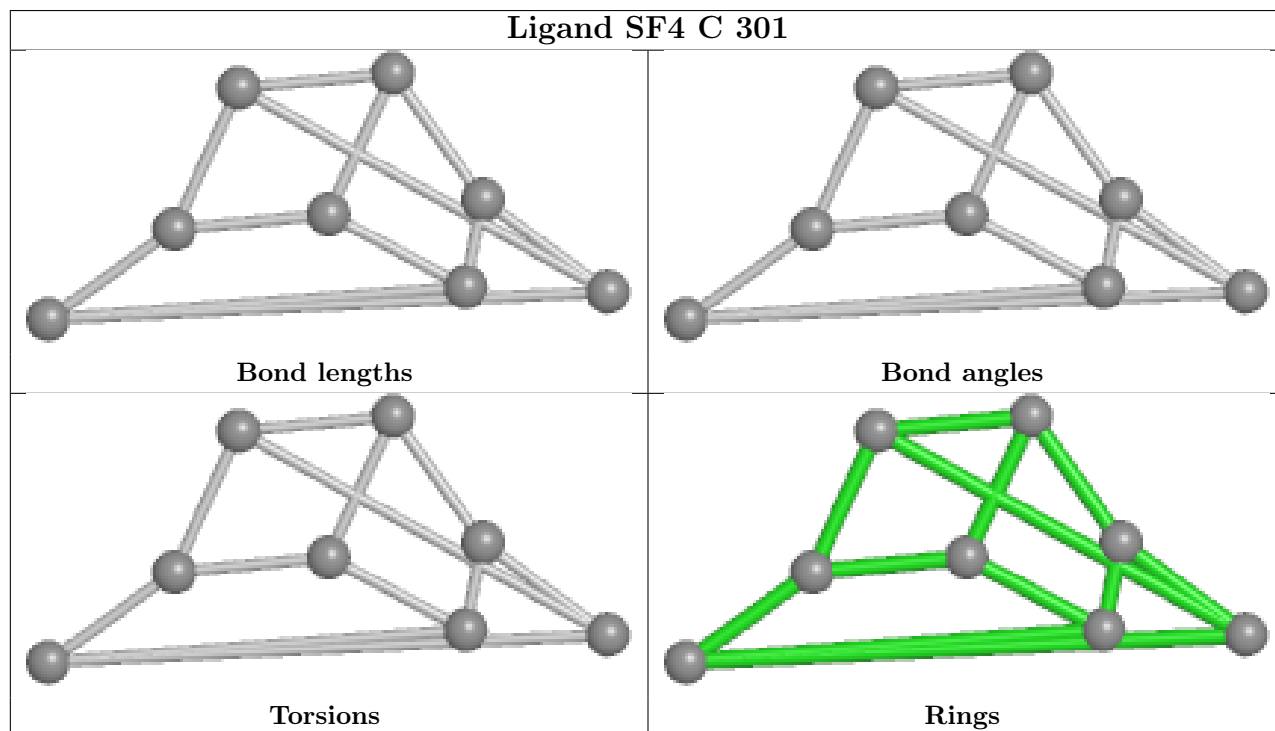
There are no ring outliers.

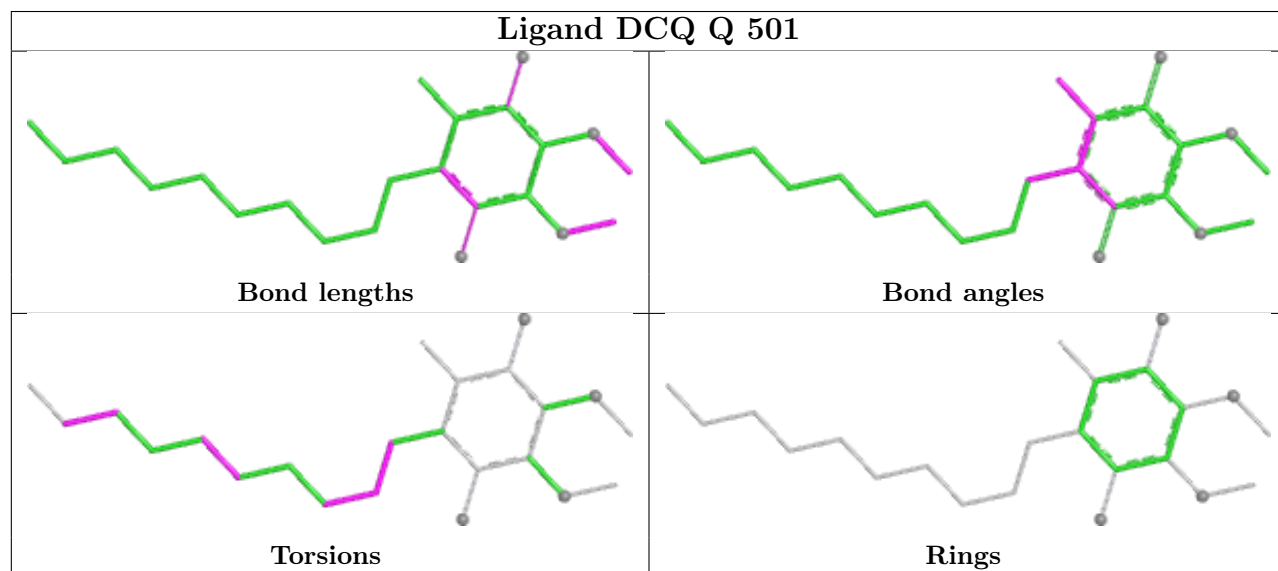
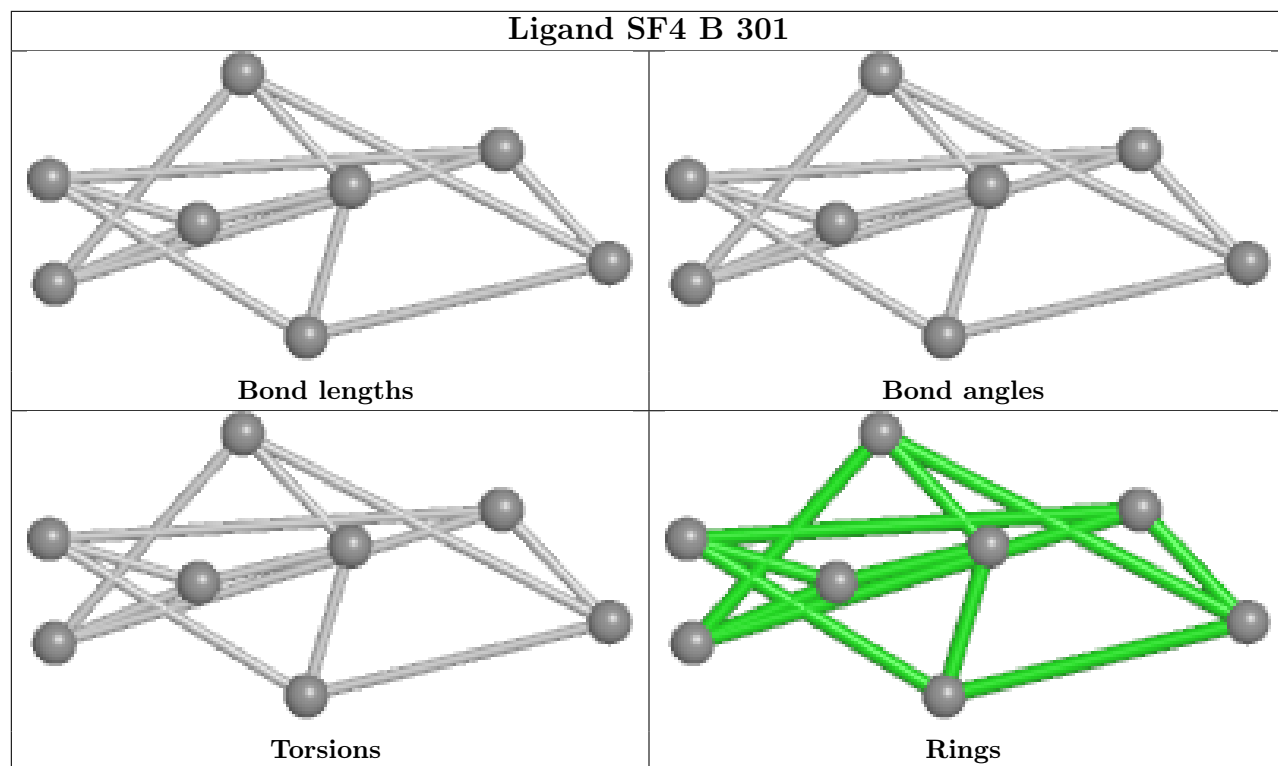
11 monomers are involved in 40 short contacts:

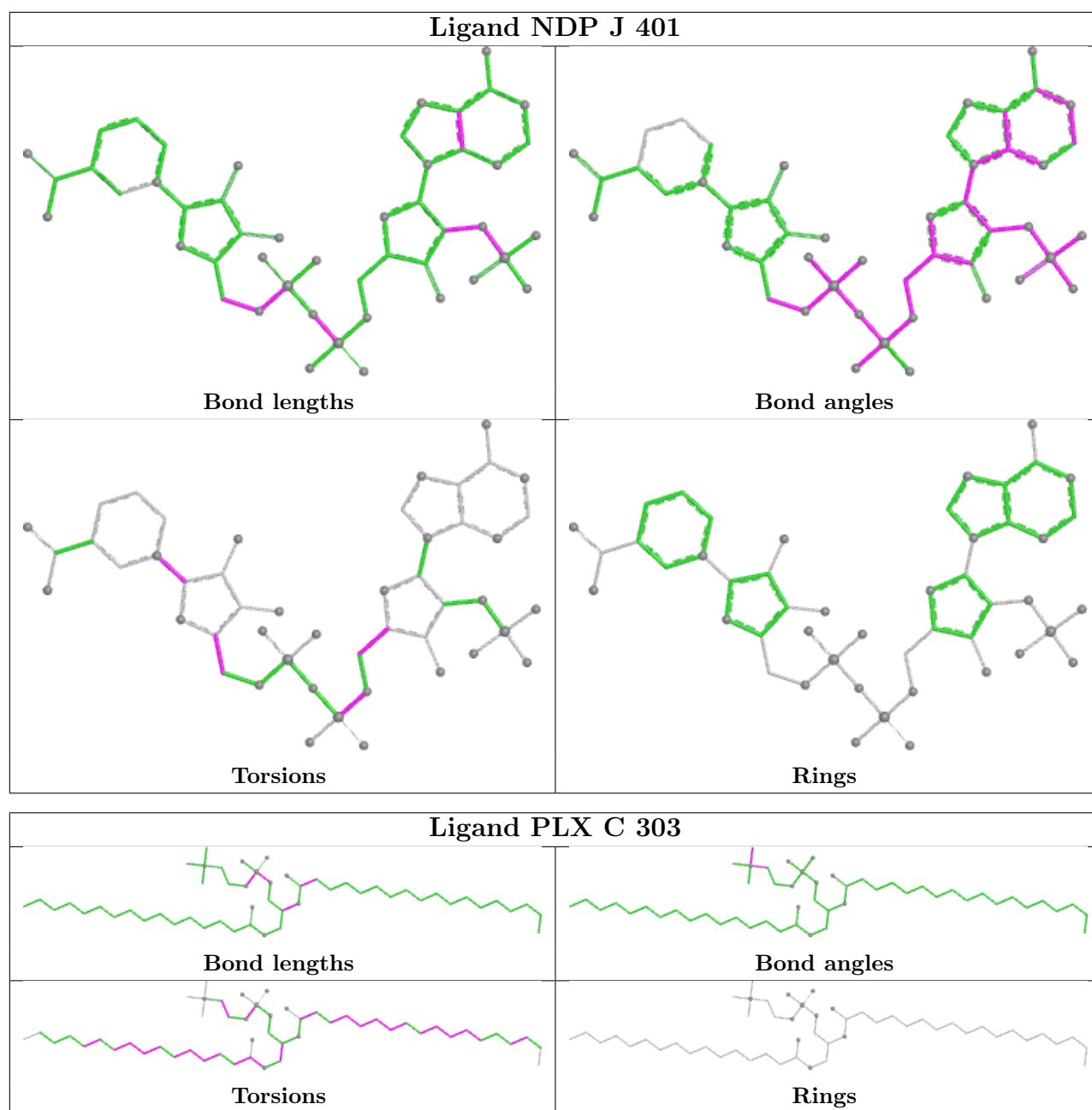
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	301	SF4	2	0
30	Q	501	DCQ	7	0
23	C	303	PLX	2	0
19	M	802	SF4	4	0
25	I	201	CDL	2	0
19	A	501	SF4	1	0
22	C	302	PEE	5	0
20	A	502	FMN	1	0
27	J	402	UQ	7	0
24	E	201	8Q1	5	0
21	A	503	NAI	5	0

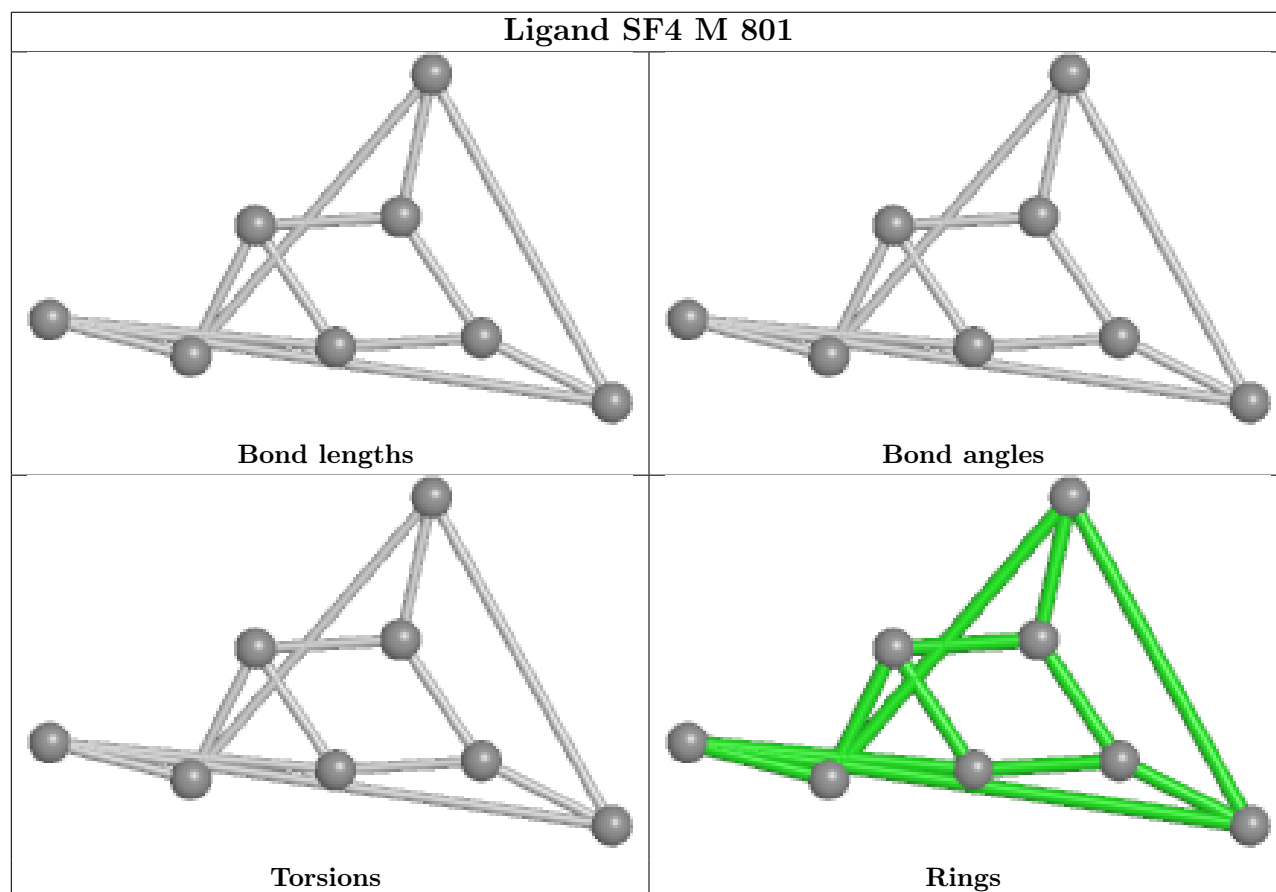
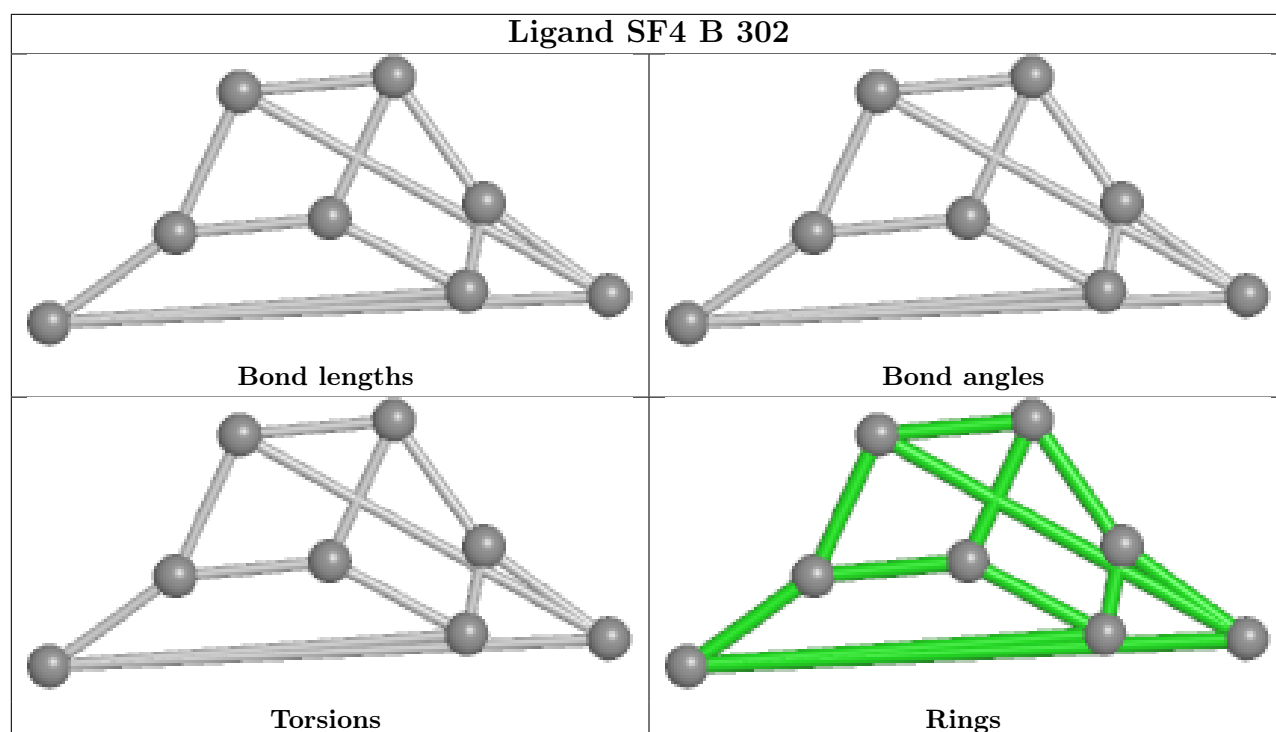
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

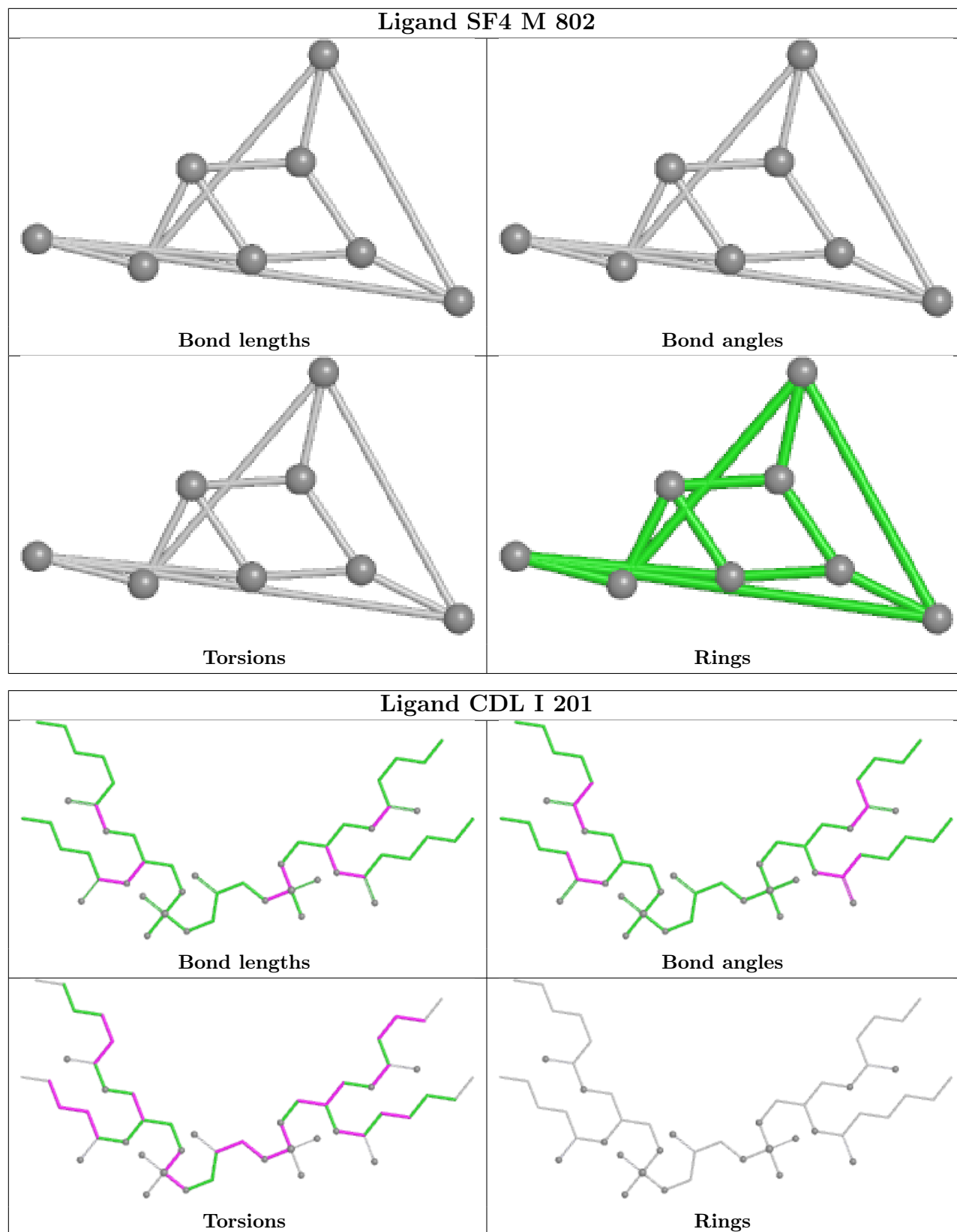
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

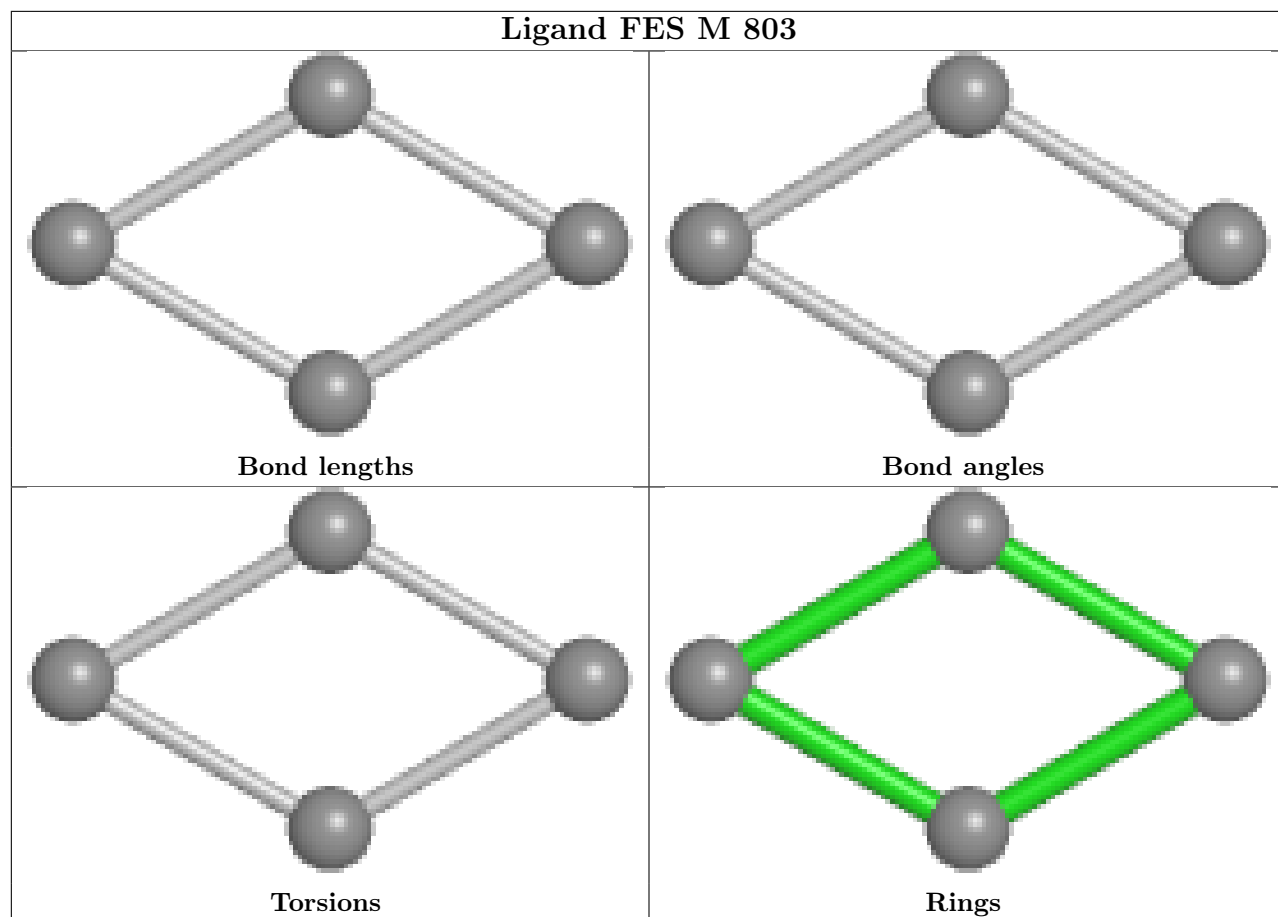
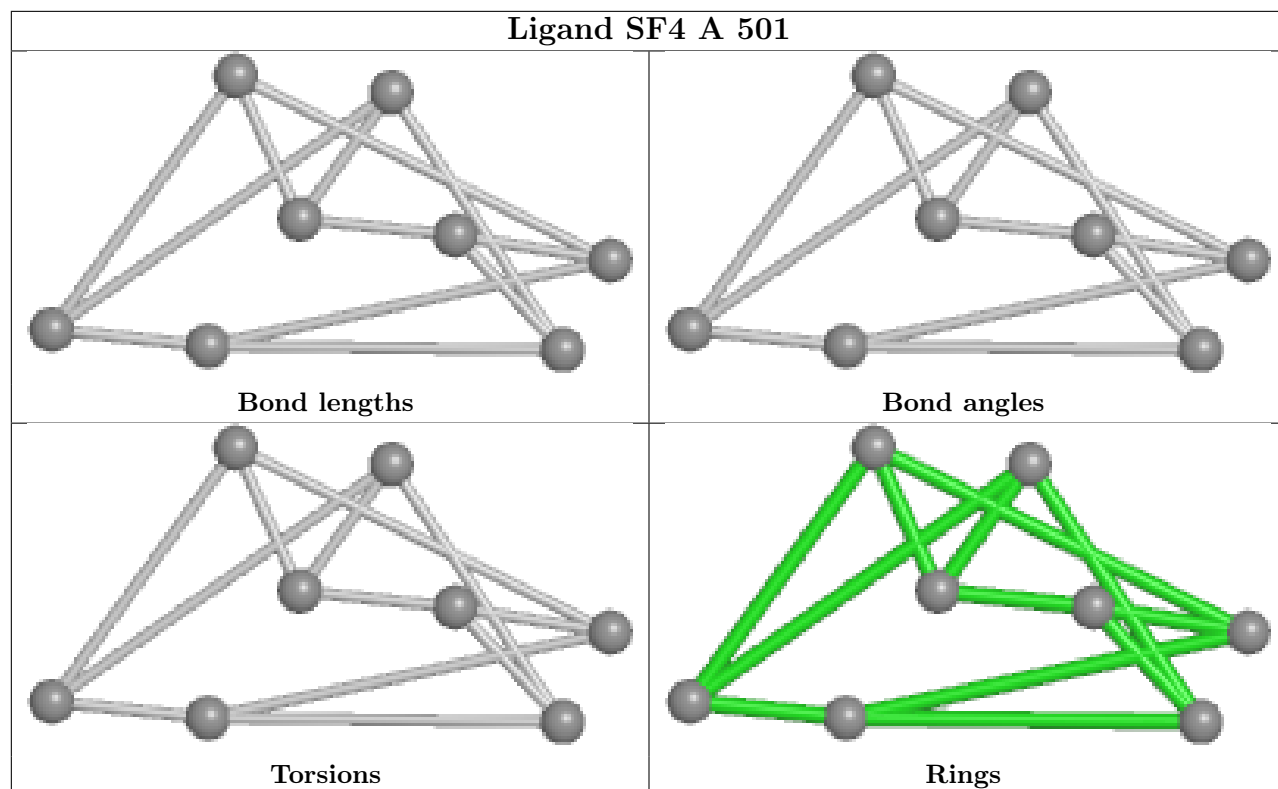


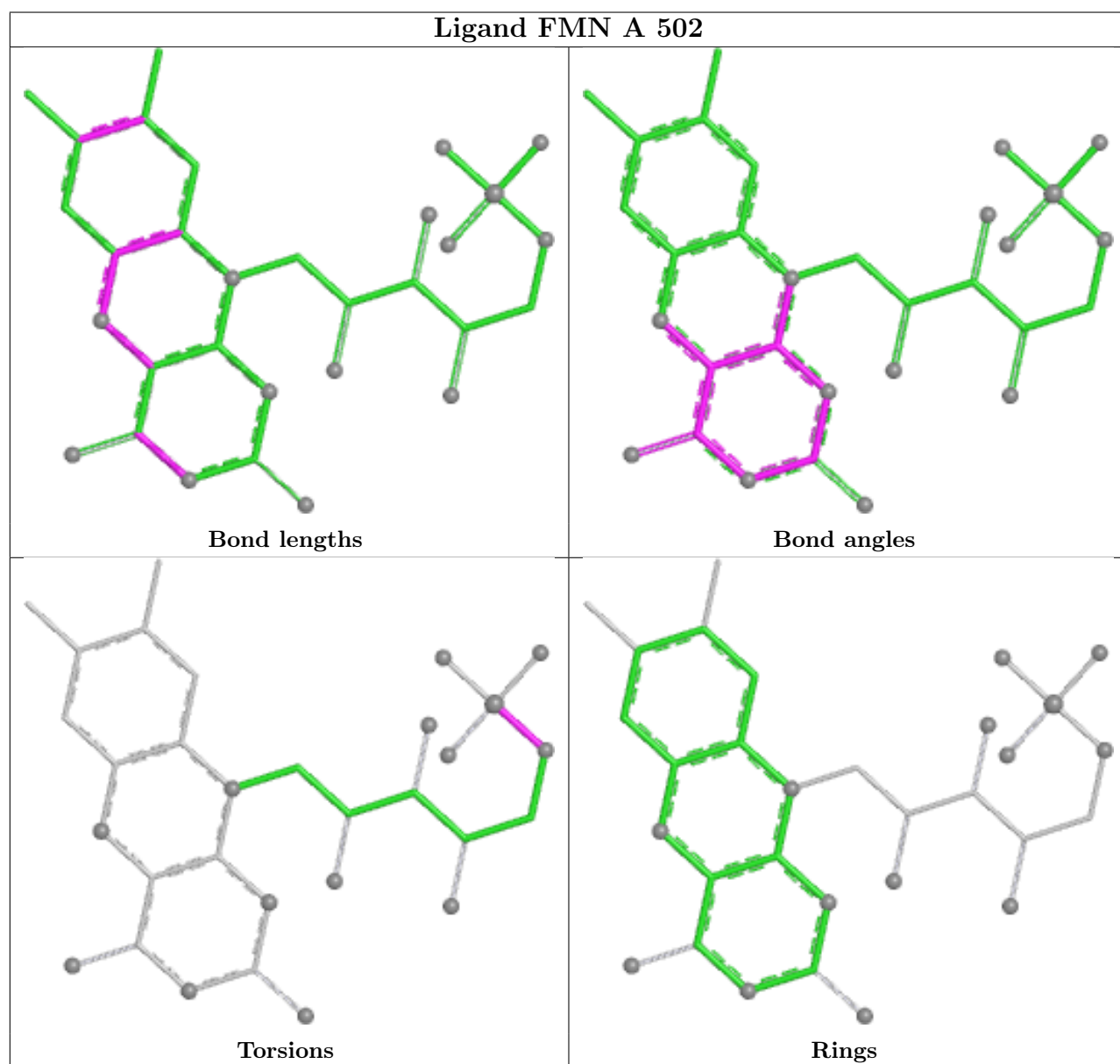
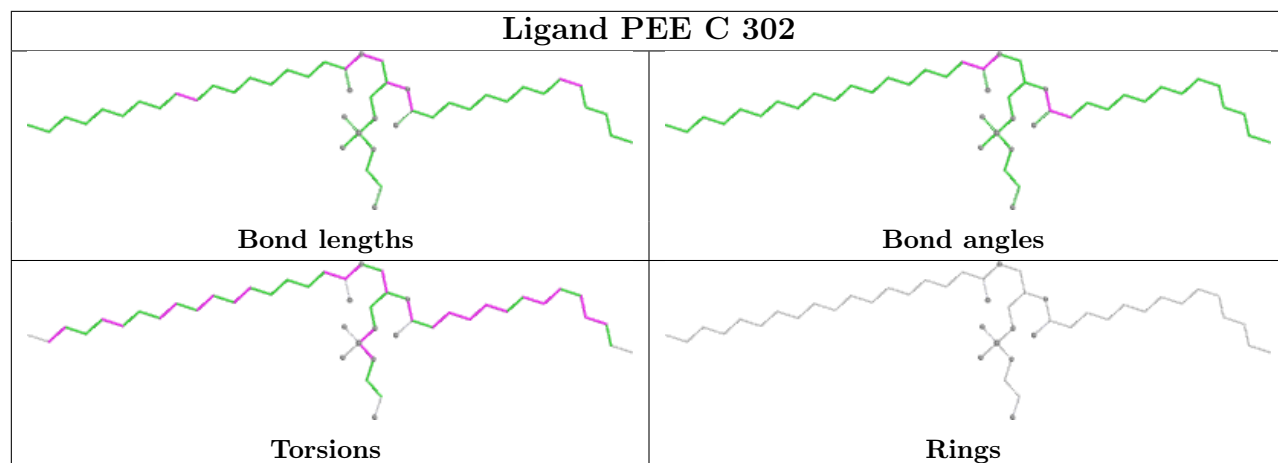


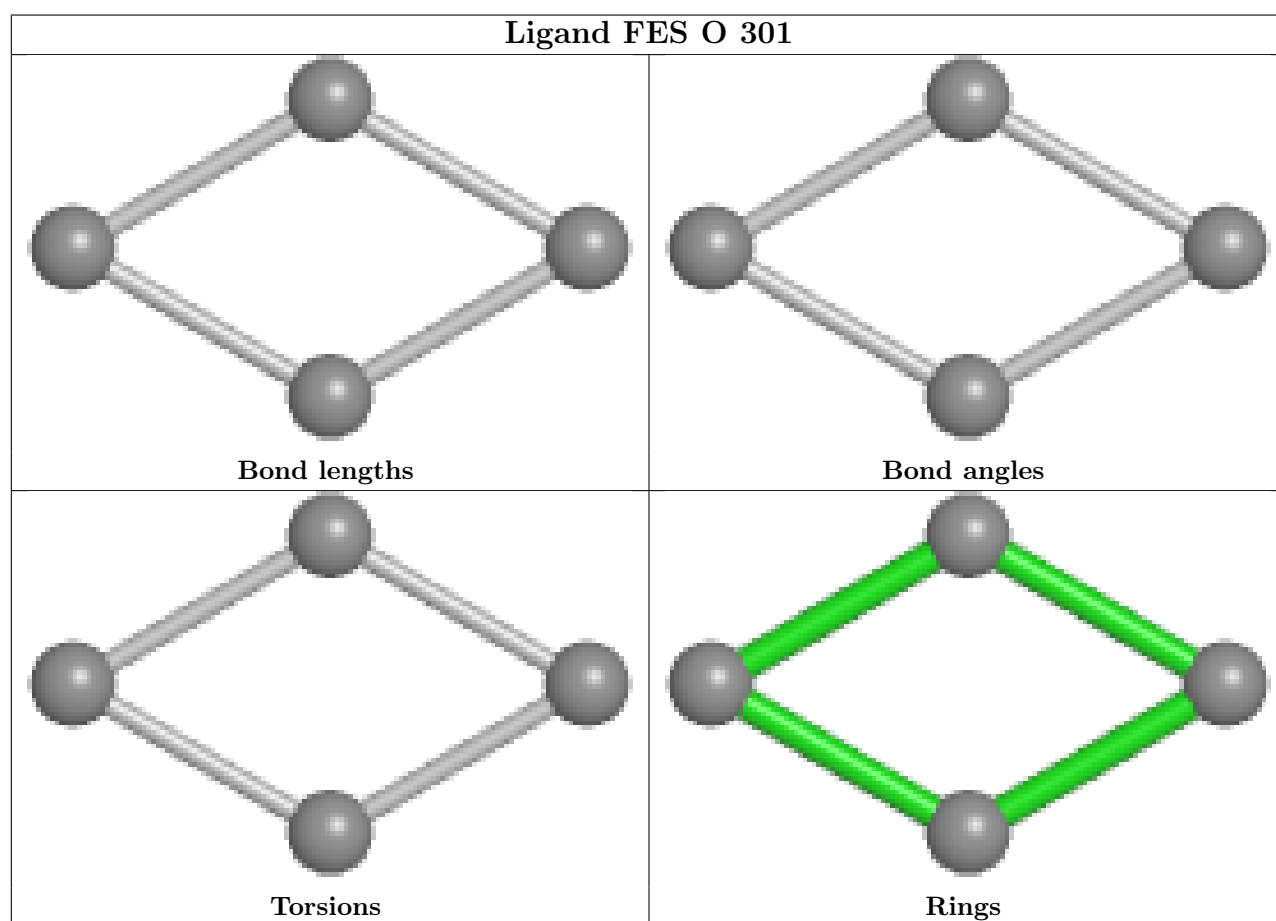
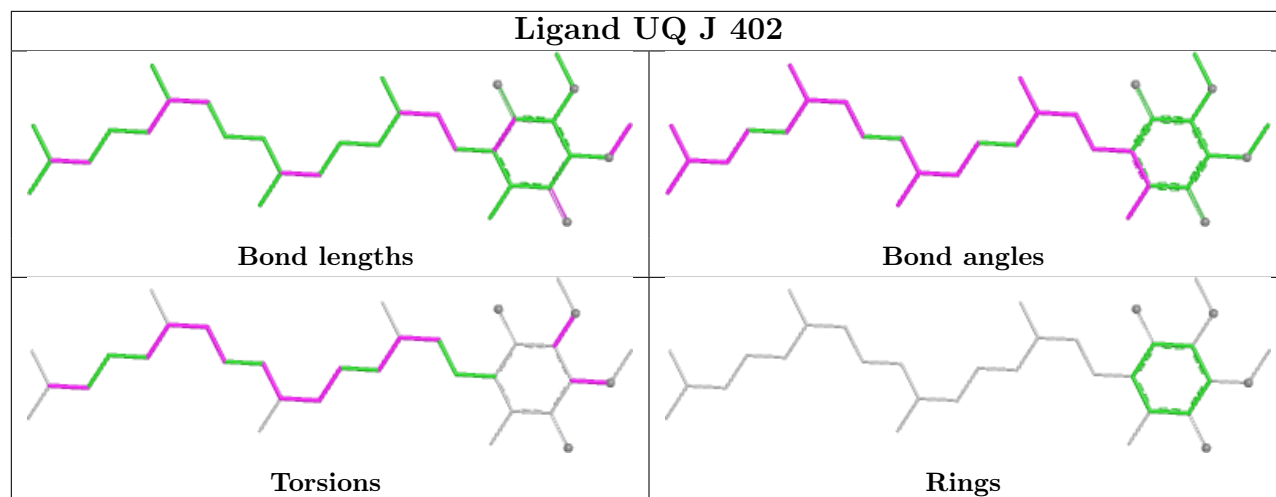


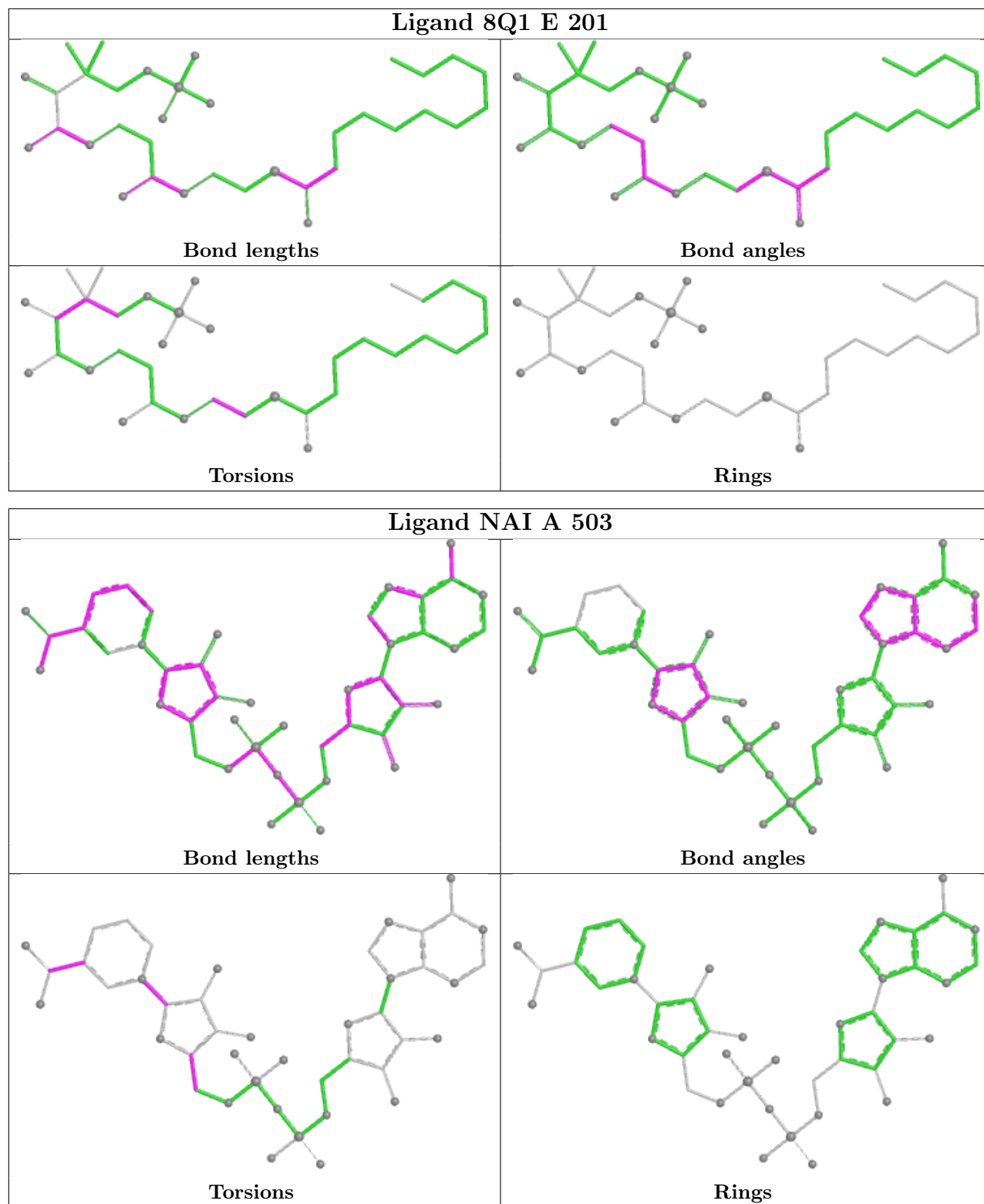












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

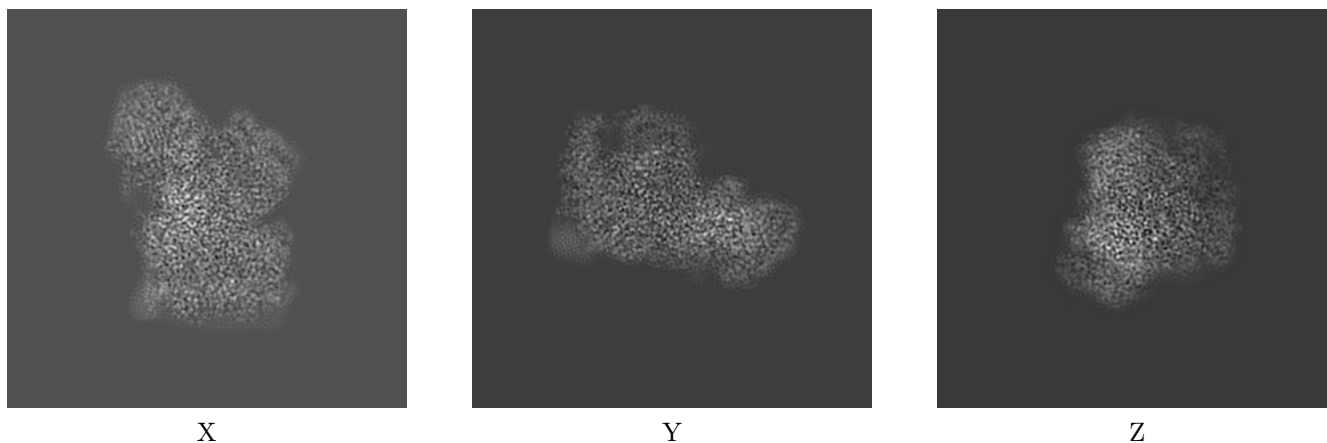
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31874. 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](#)

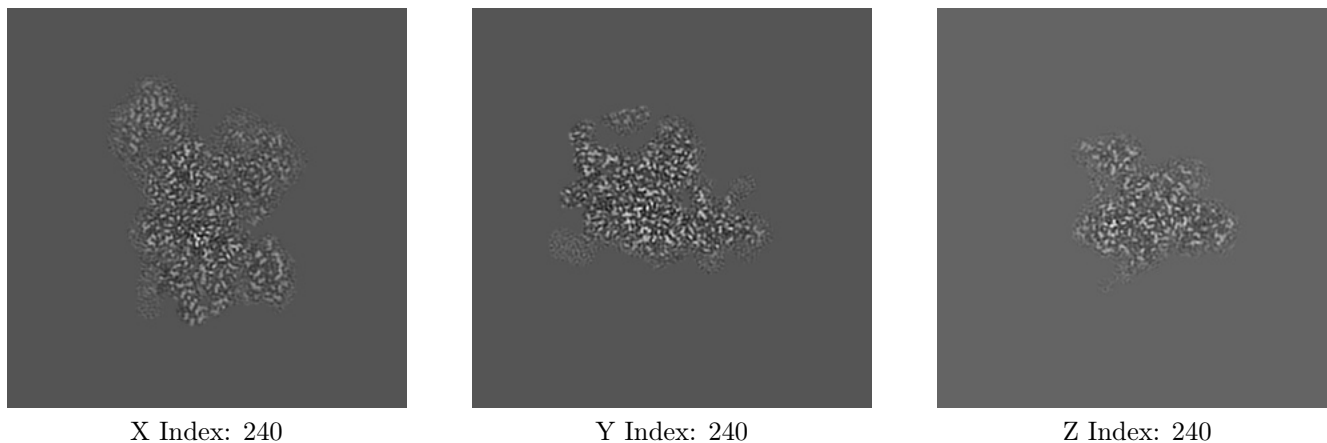
6.1.1 Primary map



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

6.2 Central slices [i](#)

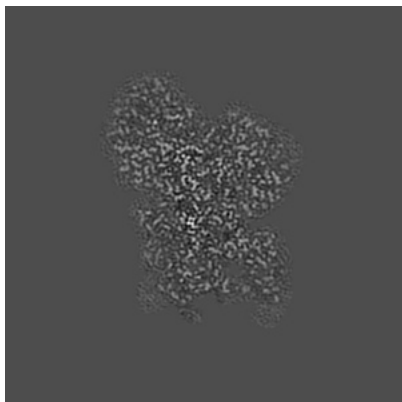
6.2.1 Primary map



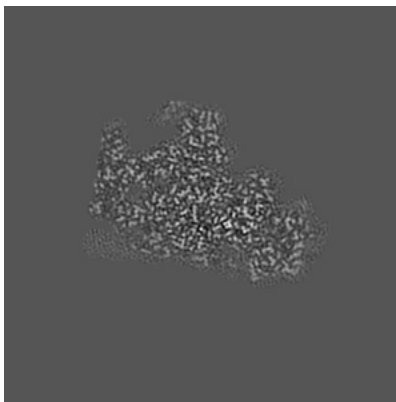
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

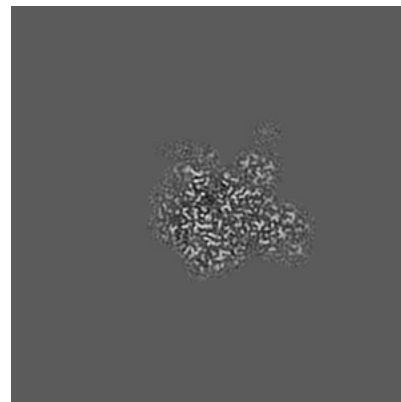
6.3.1 Primary map



X Index: 227



Y Index: 216

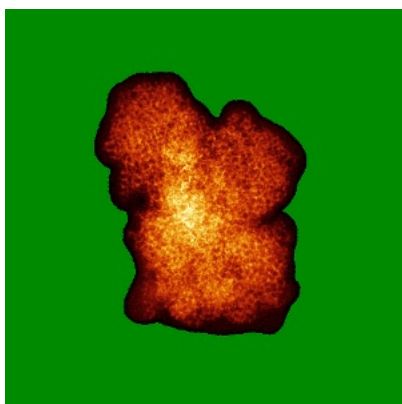


Z Index: 228

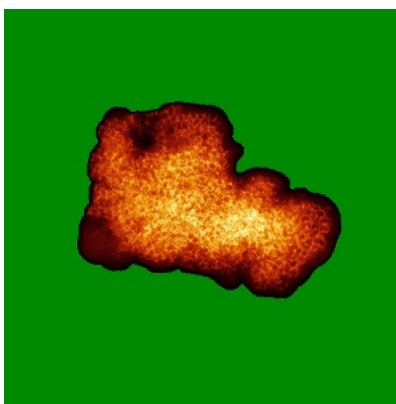
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

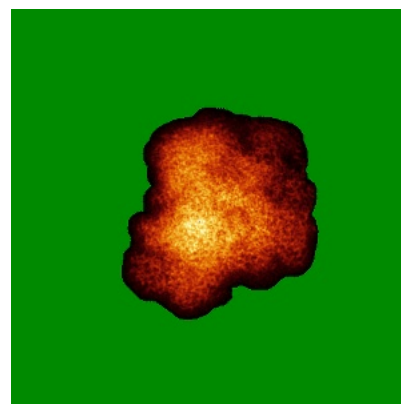
6.4.1 Primary map



X



Y

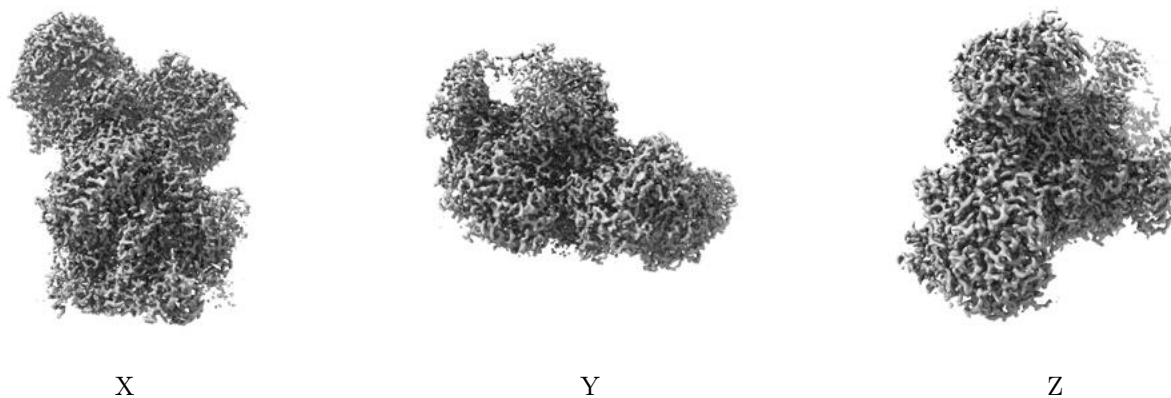


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0167. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

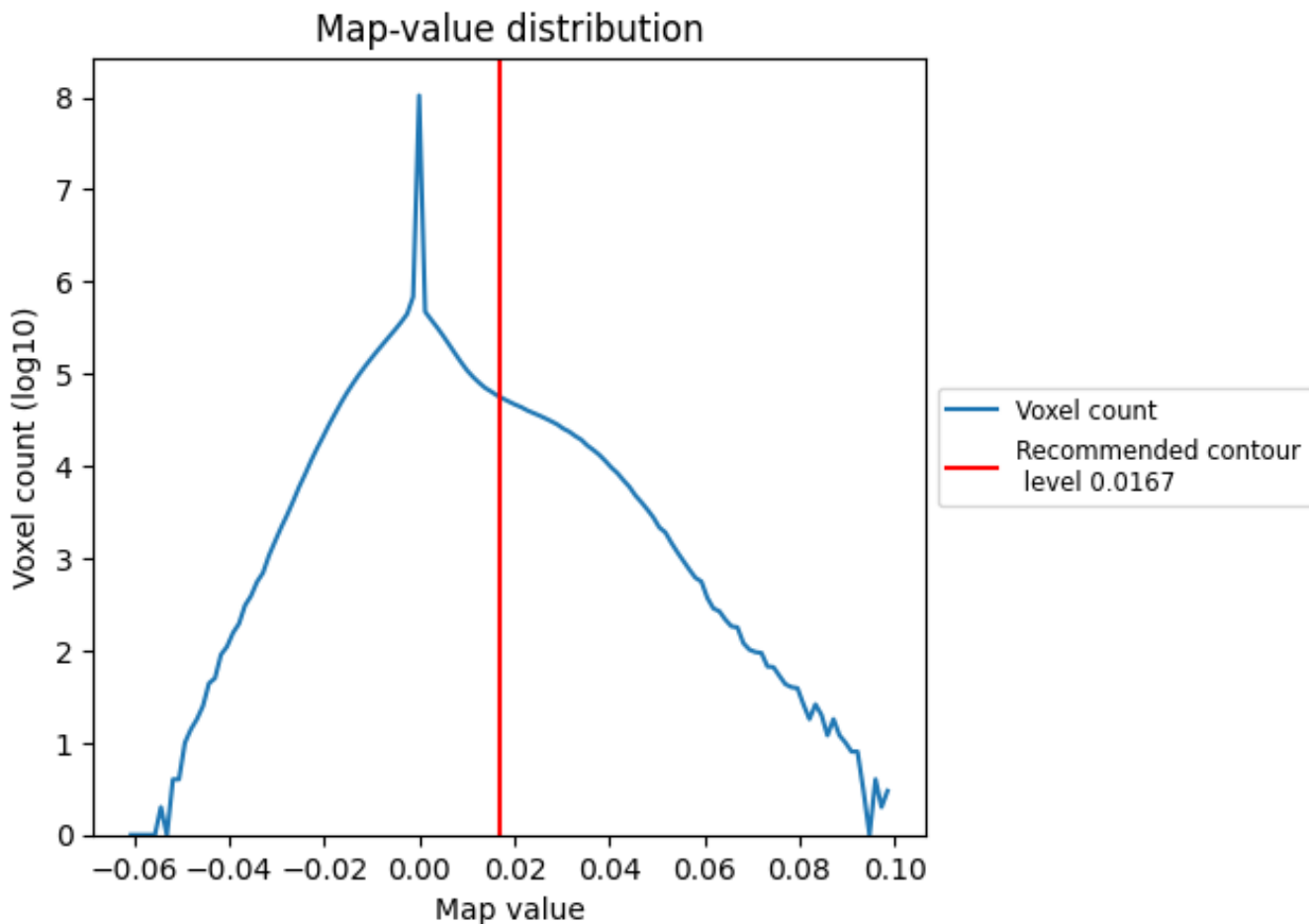
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

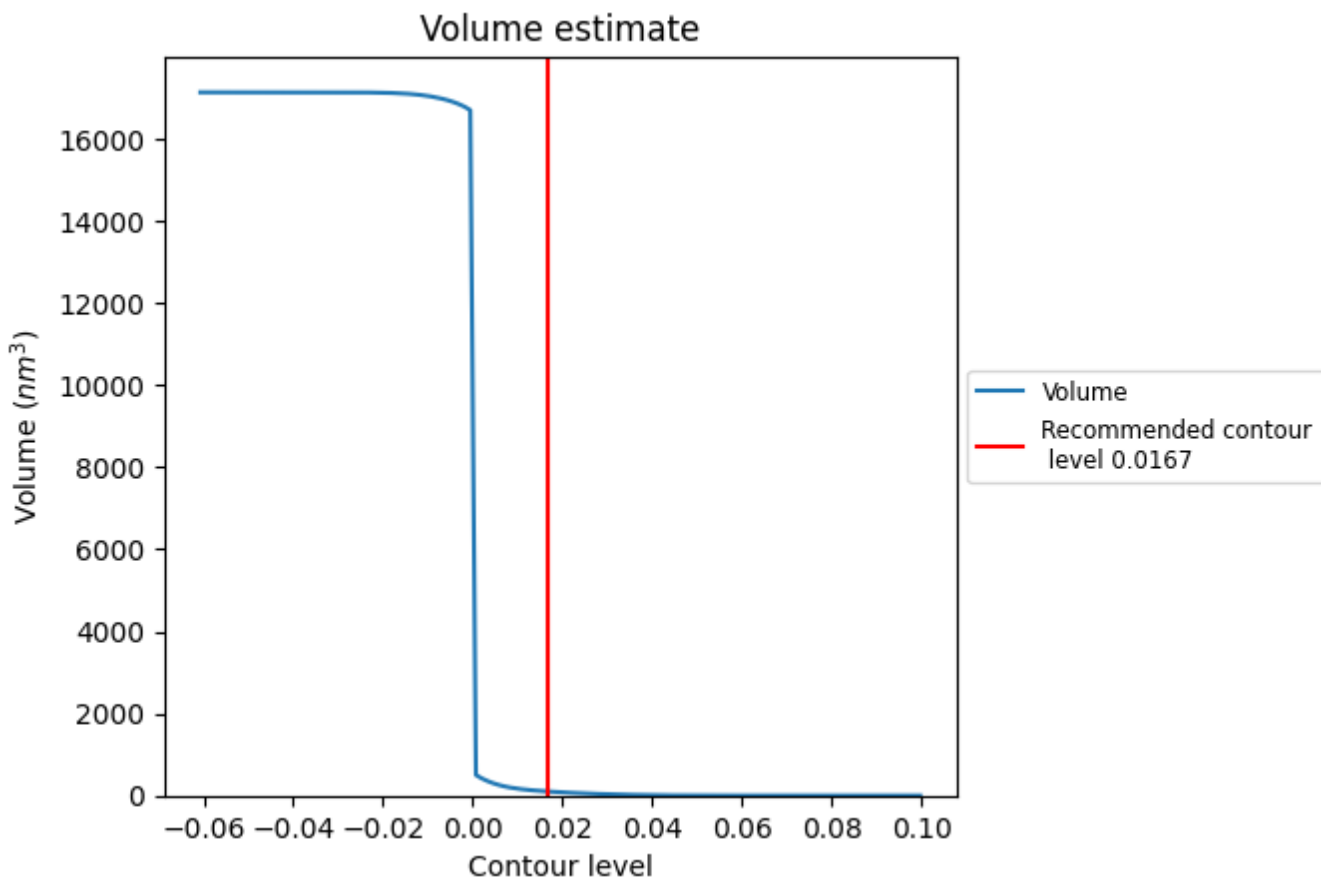
This section contains the results of statistical analysis of the map.

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.

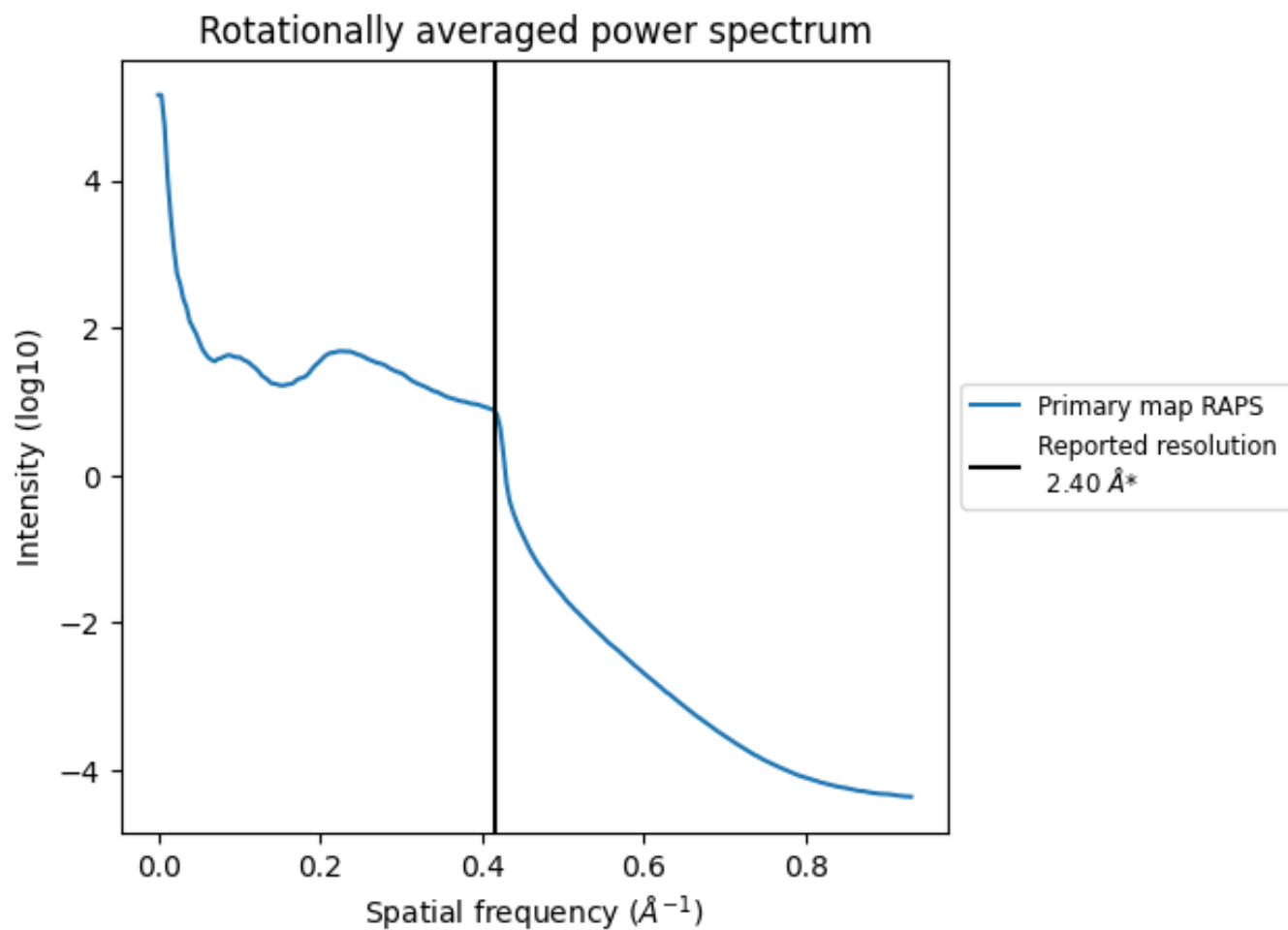
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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\AA^{-1}

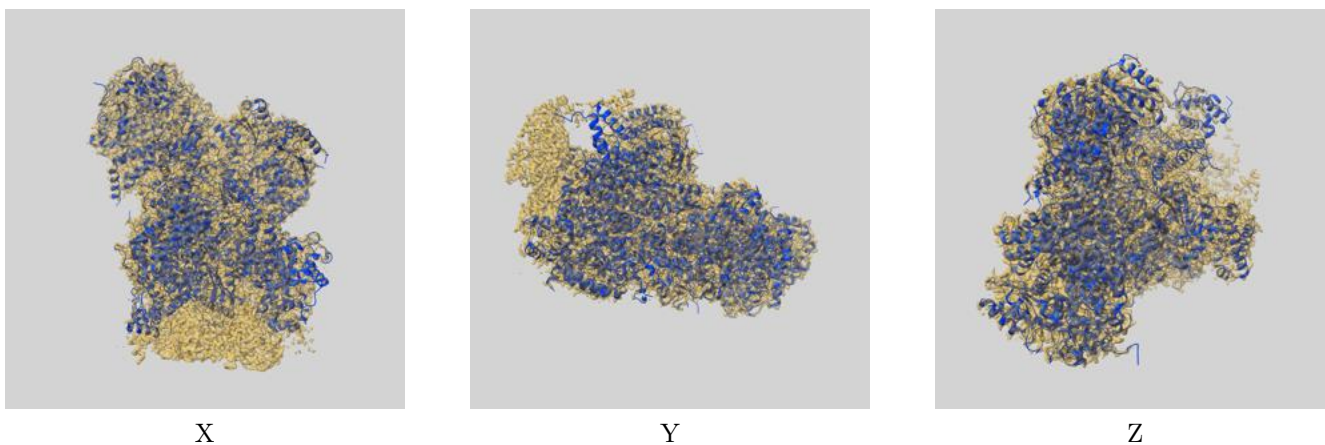
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

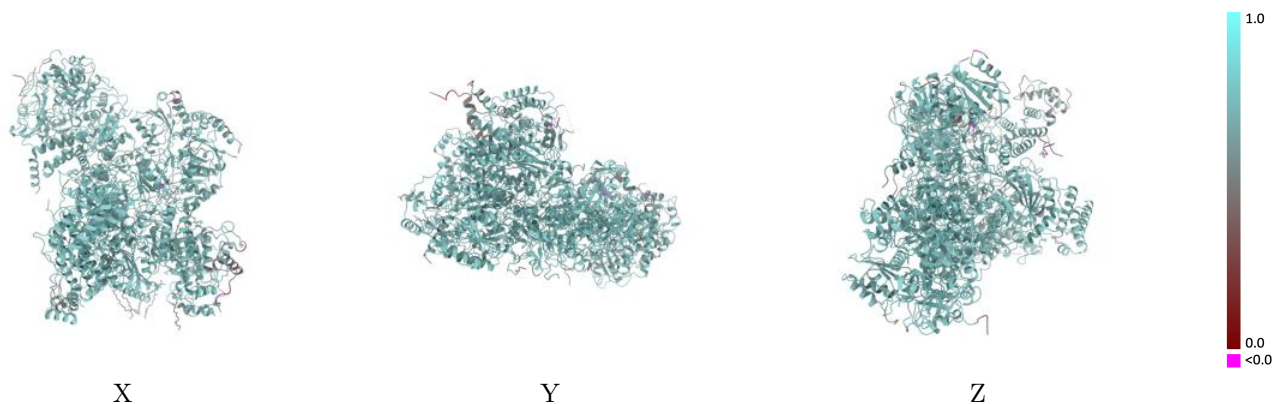
This section contains information regarding the fit between EMDB map EMD-31874 and PDB model 7VB7. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0167 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](#)

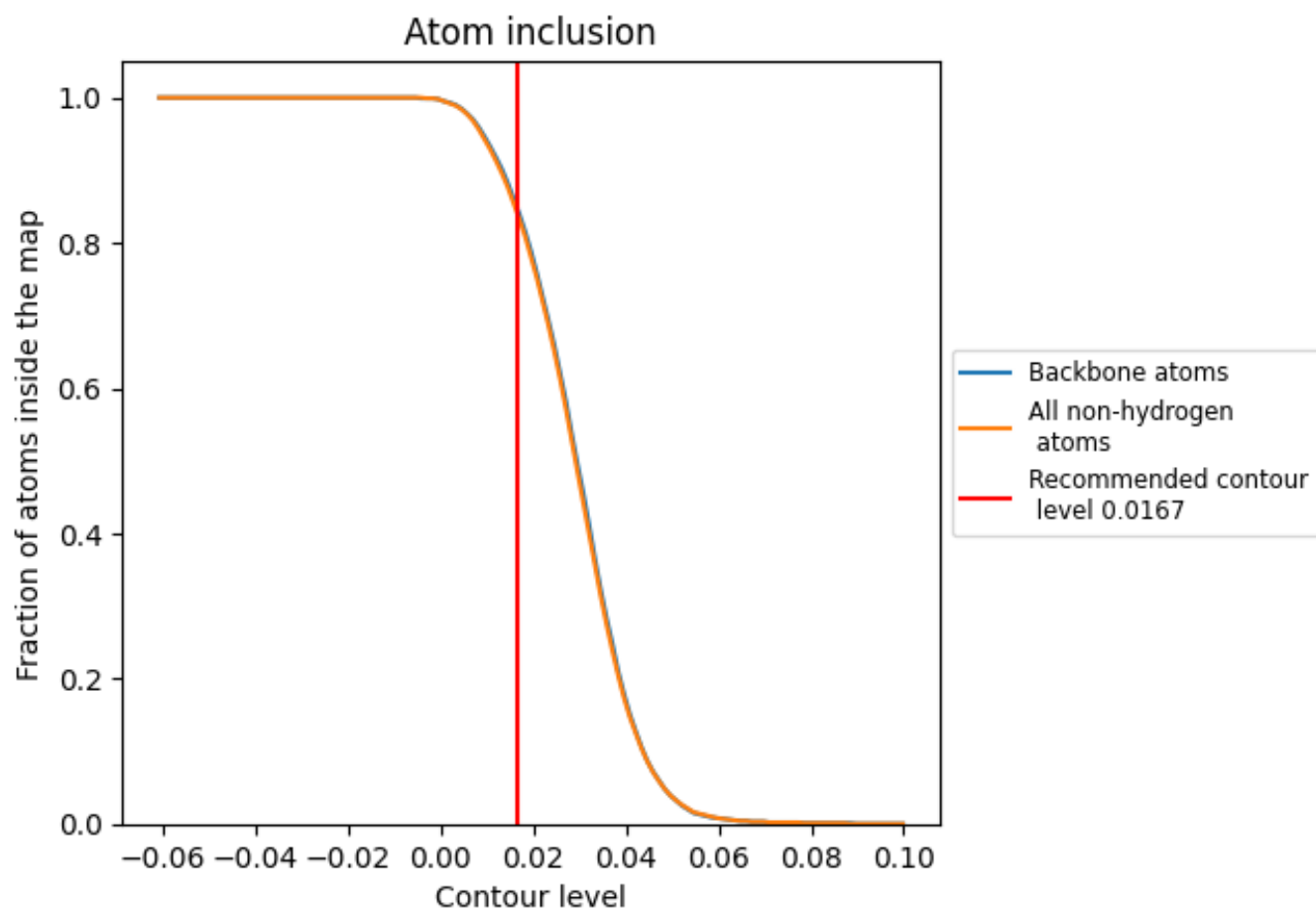


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.







































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.0167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.6930
A	 0.8770	 0.6960
B	 0.9190	 0.7220
C	 0.8870	 0.7130
E	 0.8170	 0.6860
F	 0.6920	 0.6440
G	 0.3410	 0.5290
H	 0.8200	 0.6860
I	 0.6150	 0.6420
J	 0.8470	 0.6930
K	 0.7300	 0.6480
L	 0.8720	 0.7010
M	 0.8850	 0.7040
N	 0.6440	 0.6650
O	 0.8050	 0.6800
P	 0.9430	 0.7230
Q	 0.9510	 0.7270
T	 0.7530	 0.6850
W	 0.6780	 0.6540

