



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 01:40 AM EDT

PDB ID : 7T2R / pdb_00007t2r
EMDB ID : EMD-25633
Title : Structure of electron bifurcating Ni-Fe hydrogenase complex HydABCSL in FMN-free apo state
Authors : Feng, X.; Li, H.
Deposited on : 2021-12-06
Resolution : 3.20 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.dev133
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) : 2.50

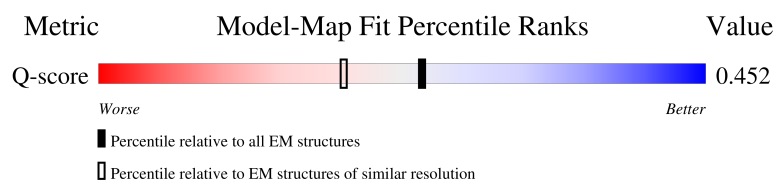
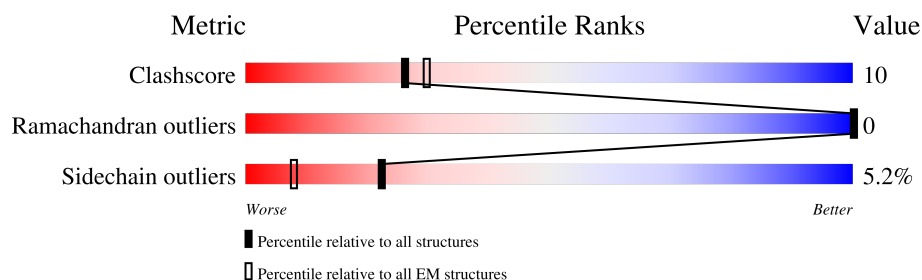
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	692	
1	F	692	
2	B	597	
2	G	597	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	156	
3	H	156	
4	D	475	
4	I	475	
5	E	179	
5	J	179	

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
6	FES	A	701	-	-	X	-
6	FES	B	602	-	-	X	-
6	FES	C	501	-	-	X	-
6	FES	F	701	-	-	X	-
6	FES	G	602	-	-	X	-
6	FES	H	501	-	-	X	-
7	SF4	A	702	-	-	X	-
7	SF4	A	703	-	-	X	-
7	SF4	A	704	-	-	X	-
7	SF4	B	601	-	-	X	-
7	SF4	E	201	-	-	X	-
7	SF4	F	702	-	-	X	-
7	SF4	F	703	-	-	X	-
7	SF4	F	704	-	-	X	-
7	SF4	G	601	-	-	X	-
7	SF4	J	201	-	-	X	-
9	FCO	D	602	-	-	X	-
9	FCO	I	602	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29216 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 NiFe hydrogenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5175	3267	905	960	43		
1	F	665	Total	C	N	O	S	0	0
			5175	3267	905	960	43		

- Molecule 2 is a protein called NiFe hydrogenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	425	Total	C	N	O	S	0	0
			3236	2046	551	609	30		
2	G	425	Total	C	N	O	S	0	0
			3236	2046	551	609	30		

- Molecule 3 is a protein called NiFe hydrogenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	152	Total	C	N	O	S	0	0
			1194	758	208	219	9		
3	H	152	Total	C	N	O	S	0	0
			1194	758	208	219	9		

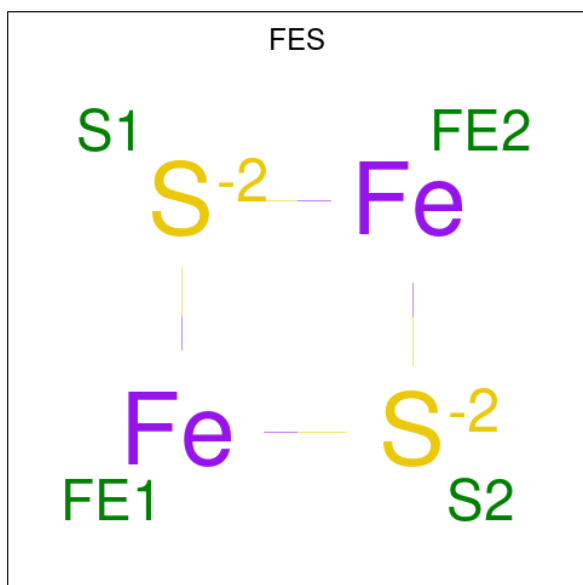
- Molecule 4 is a protein called NiFe hydrogenase large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	447	Total	C	N	O	S	0	0
			3537	2264	615	642	16		
4	I	447	Total	C	N	O	S	0	0
			3537	2264	615	642	16		

- Molecule 5 is a protein called NiFe hydrogenase small subunit.

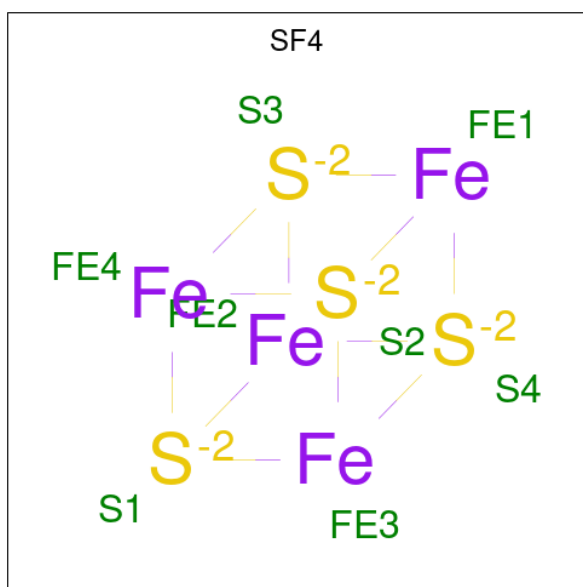
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	179	Total	C	N	O	S	0	0
			1398	900	225	261	12		
5	J	179	Total	C	N	O	S	0	0
			1398	900	225	261	12		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Fe	S	0
			4	2	2	
6	B	1	Total	Fe	S	0
			4	2	2	
6	C	1	Total	Fe	S	0
			4	2	2	
6	F	1	Total	Fe	S	0
			4	2	2	
6	G	1	Total	Fe	S	0
			4	2	2	
6	H	1	Total	Fe	S	0
			4	2	2	

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

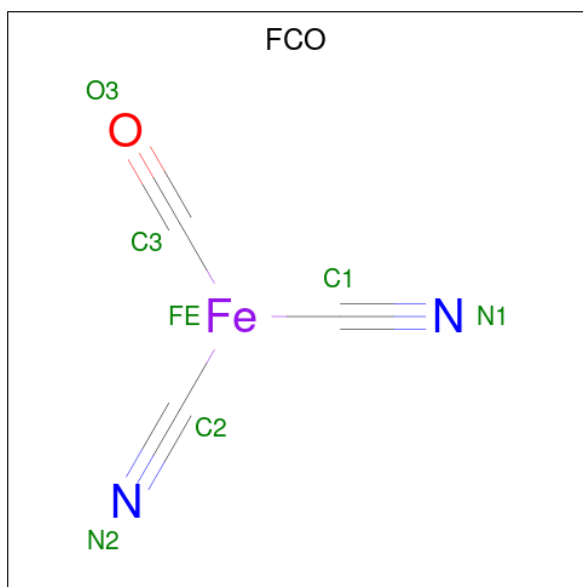


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	A	1	Total	Fe	S	0
			8	4	4	
7	B	1	Total	Fe	S	0
			8	4	4	
7	E	1	Total	Fe	S	0
			8	4	4	
7	F	1	Total	Fe	S	0
			8	4	4	
7	F	1	Total	Fe	S	0
			8	4	4	
7	F	1	Total	Fe	S	0
			8	4	4	
7	F	1	Total	Fe	S	0
			8	4	4	
7	G	1	Total	Fe	S	0
			8	4	4	
7	J	1	Total	Fe	S	0
			8	4	4	

- Molecule 8 is NICKEL (III) ION (CCD ID: 3NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Ni	0
			1	1	
8	I	1	Total	Ni	0
			1	1	

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$) (labeled as "Ligand of Interest" by depositor).

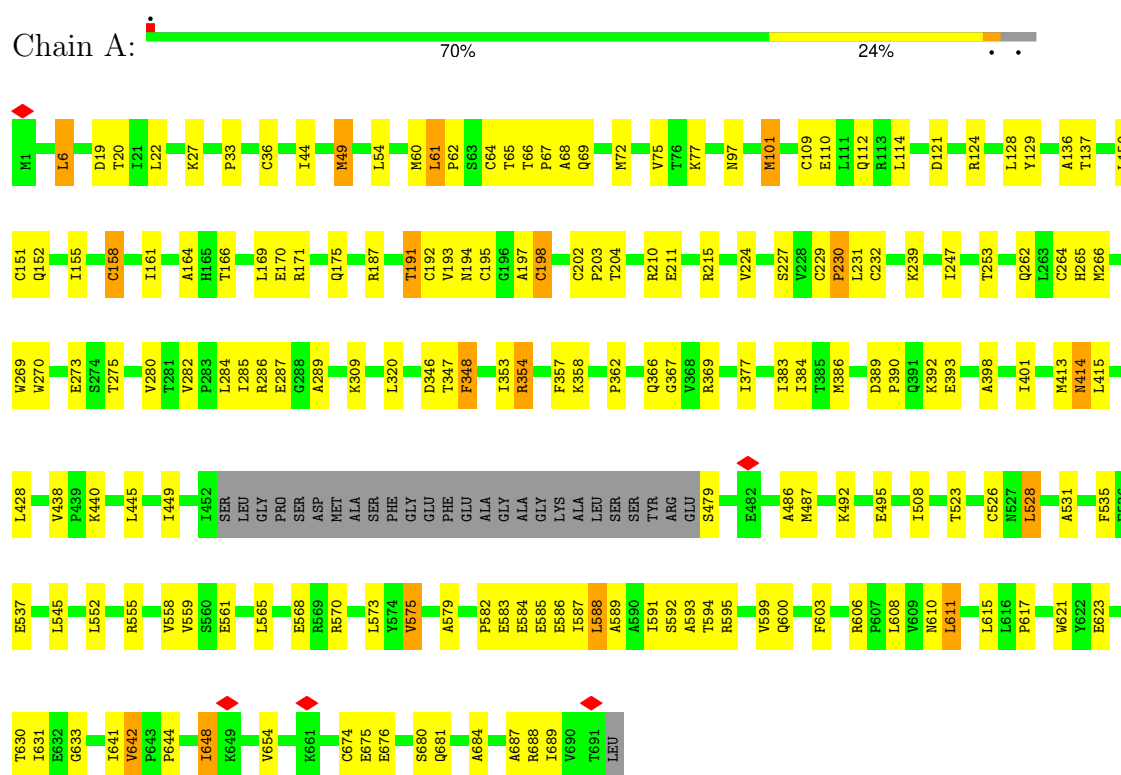


Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	Fe	N	O	0
			7	3	1	2	1	
9	I	1	Total	C	Fe	N	O	0
			7	3	1	2	1	

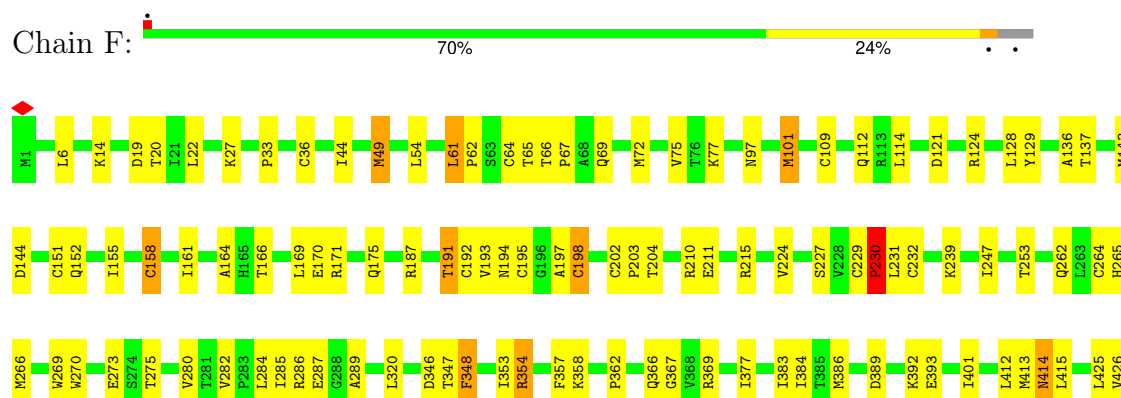
3 Residue-property plots

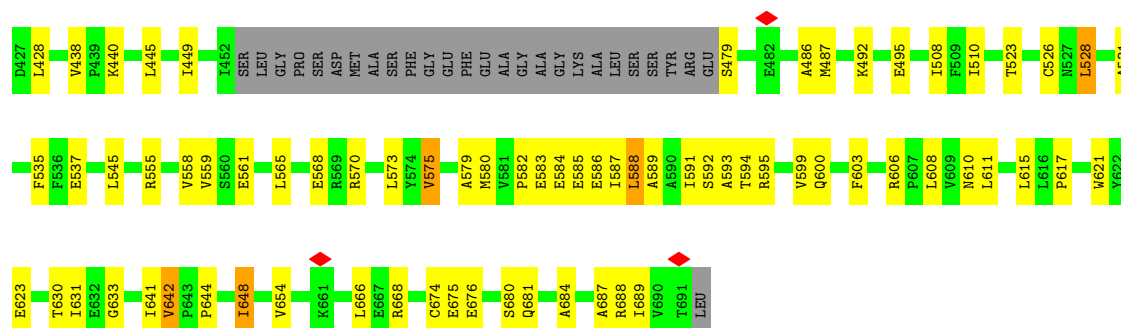
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NiFe hydrogenase subunit A

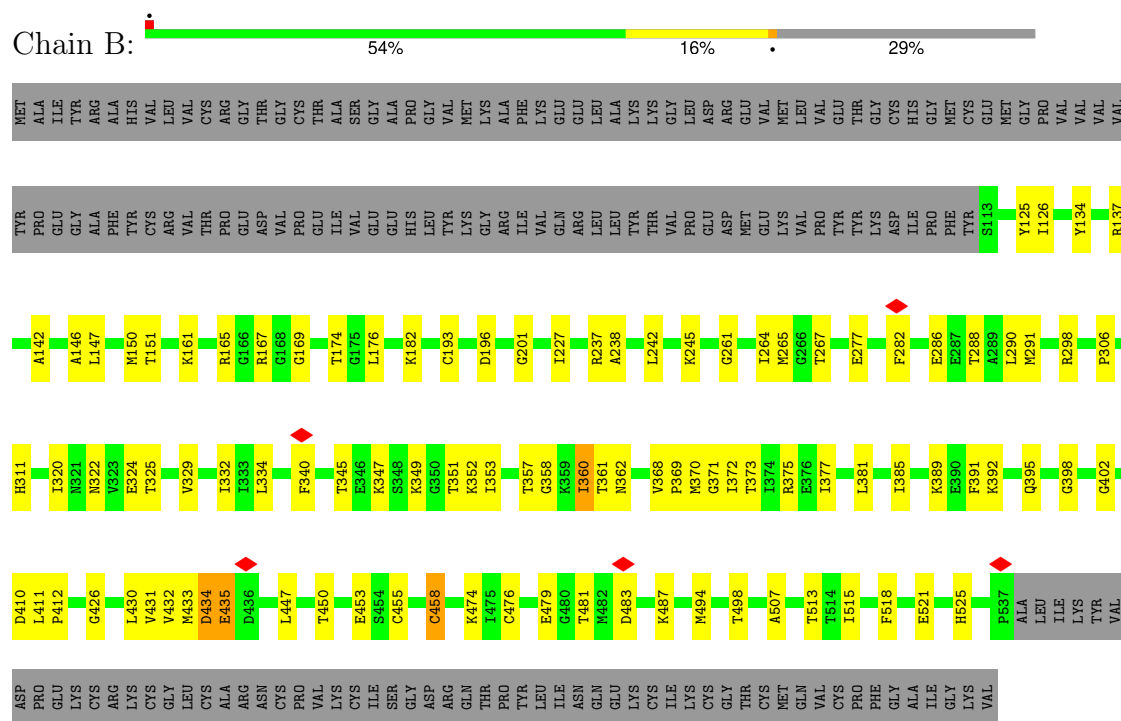


• Molecule 1: NiFe hydrogenase subunit A

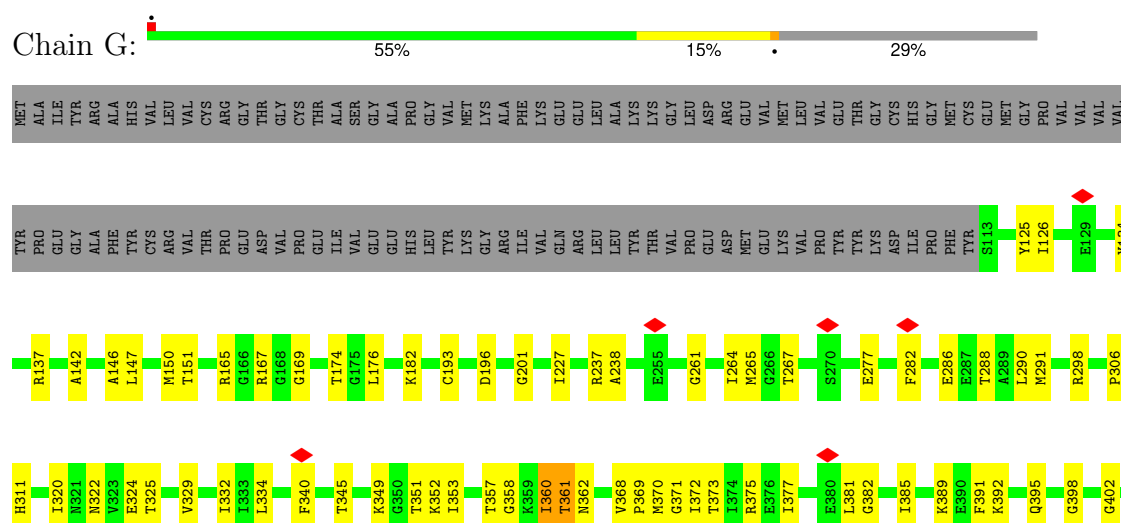


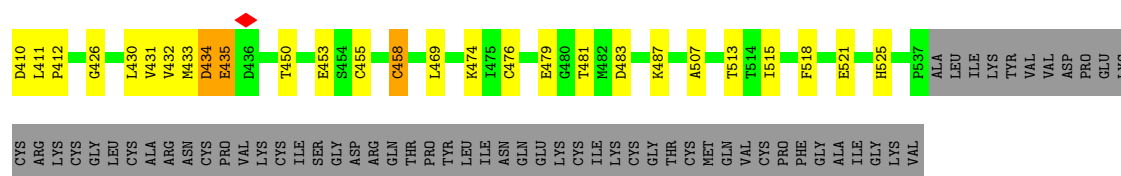


• Molecule 2: NiFe hydrogenase subunit B

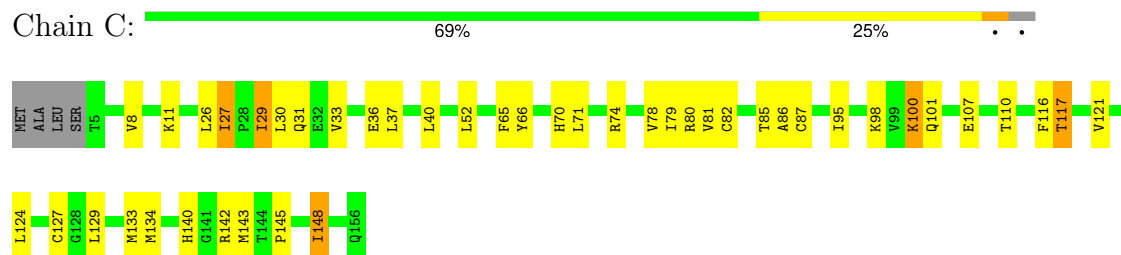


• Molecule 2: NiFe hydrogenase subunit B

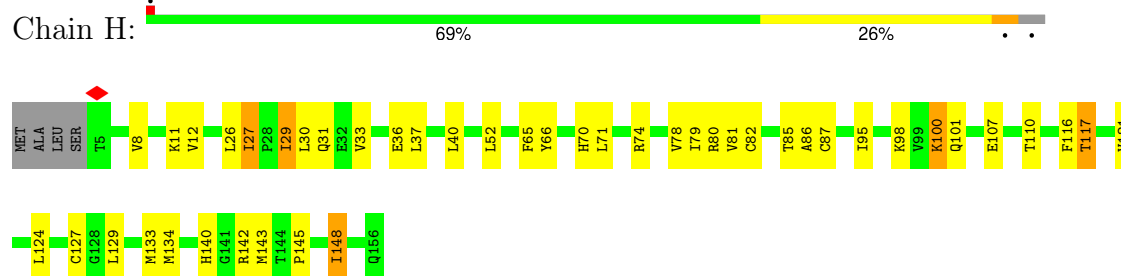




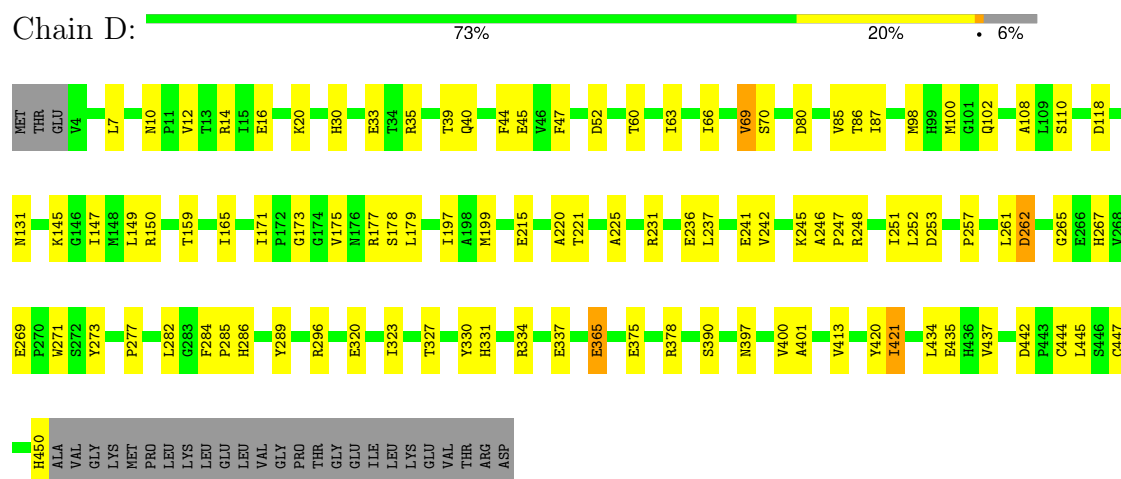
• Molecule 3: NiFe hydrogenase subunit C



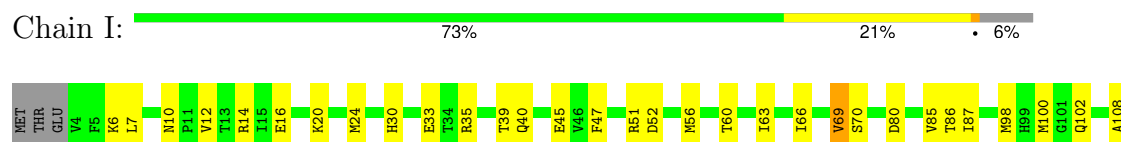
• Molecule 3: NiFe hydrogenase subunit C

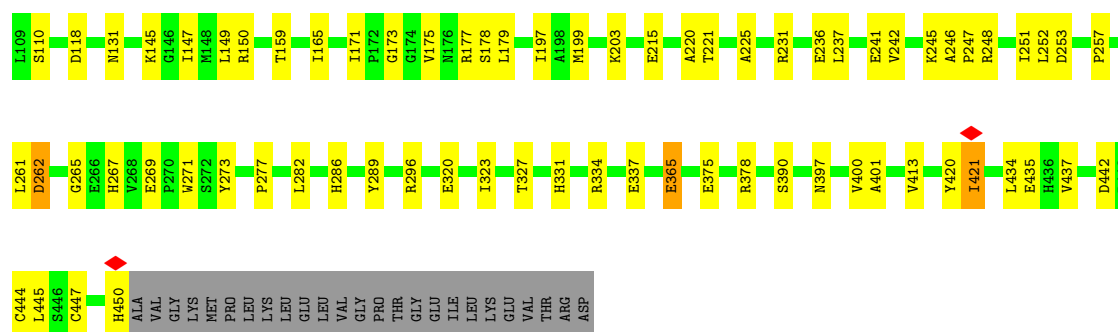


• Molecule 4: NiFe hydrogenase large subunit



• Molecule 4: NiFe hydrogenase large subunit





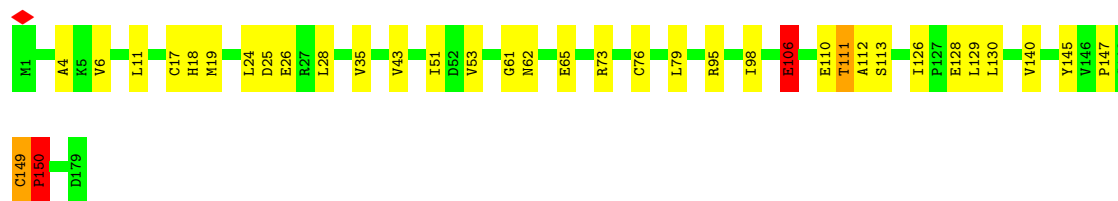
- Molecule 5: NiFe hydrogenase small subunit

Chain E: 78% 20% ..



- Molecule 5: NiFe hydrogenase small subunit

Chain J: 80% 18% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	269151	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.514	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	267.54, 267.54, 267.54	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.029, 1.029, 1.029	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3NI, FCO, SF4, FES

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	0.56	1/5272 (0.0%)	0.92	5/7132 (0.1%)
1	F	0.57	1/5272 (0.0%)	0.92	6/7132 (0.1%)
2	B	0.43	0/3299	0.80	0/4445
2	G	0.43	0/3299	0.80	0/4445
3	C	0.46	0/1214	0.91	3/1638 (0.2%)
3	H	0.46	0/1214	0.91	3/1638 (0.2%)
4	D	0.40	0/3624	0.72	4/4908 (0.1%)
4	I	0.40	0/3624	0.72	4/4908 (0.1%)
5	E	0.43	0/1429	0.82	3/1941 (0.2%)
5	J	0.43	0/1429	0.82	3/1941 (0.2%)
All	All	0.48	2/29676 (0.0%)	0.84	31/40128 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	SER	CA-CB	-7.39	1.48	1.54
1	F	227	SER	CA-CB	-7.39	1.48	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	230	PRO	N-CA-CB	-9.15	93.65	103.25
5	E	150	PRO	N-CA-CB	-8.73	93.00	102.60
5	J	150	PRO	N-CA-CB	-8.73	93.00	102.60
3	C	26	LEU	N-CA-C	-8.58	103.41	114.04
3	H	26	LEU	N-CA-C	-8.58	103.41	114.04
4	D	86	THR	CA-C-N	6.95	134.22	121.70
4	D	86	THR	C-N-CA	6.95	134.22	121.70
4	I	86	THR	CA-C-N	6.95	134.22	121.70
4	I	86	THR	C-N-CA	6.95	134.22	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ILE	N-CA-C	-6.10	104.79	110.53
1	F	155	ILE	N-CA-C	-6.10	104.79	110.53
3	C	124	LEU	N-CA-C	-5.95	105.79	113.16
3	H	124	LEU	N-CA-C	-5.95	105.79	113.16
1	A	648	ILE	CA-C-N	5.79	132.59	121.54
1	A	648	ILE	C-N-CA	5.79	132.59	121.54
1	F	648	ILE	CA-C-N	5.79	132.59	121.54
1	F	648	ILE	C-N-CA	5.79	132.59	121.54
5	E	18	HIS	N-CA-C	-5.48	106.27	113.12
5	J	18	HIS	N-CA-C	-5.48	106.27	113.12
4	D	365	GLU	CA-CB-CG	5.45	124.99	114.10
4	I	365	GLU	CA-CB-CG	5.45	124.99	114.10
3	C	127	CYS	N-CA-C	-5.26	106.84	113.20
3	H	127	CYS	N-CA-C	-5.26	106.84	113.20
4	D	320	GLU	CA-CB-CG	5.12	124.34	114.10
4	I	320	GLU	CA-CB-CG	5.12	124.34	114.10
1	A	62	PRO	CB-CA-C	-5.11	104.86	111.46
1	F	62	PRO	CB-CA-C	-5.11	104.86	111.46
5	E	106	GLU	CB-CG-CD	5.11	121.29	112.60
5	J	106	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	197	ALA	N-CA-C	-5.09	106.33	112.54
1	F	197	ALA	N-CA-C	-5.09	106.33	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5175	0	5216	136	0
1	F	5175	0	5216	137	0
2	B	3236	0	3243	60	0
2	G	3236	0	3243	57	0
3	C	1194	0	1229	29	0
3	H	1194	0	1229	29	0
4	D	3537	0	3534	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	3537	0	3534	74	0
5	E	1398	0	1402	31	0
5	J	1398	0	1402	29	0
6	A	4	0	0	2	0
6	B	4	0	0	2	0
6	C	4	0	0	3	0
6	F	4	0	0	2	0
6	G	4	0	0	2	0
6	H	4	0	0	3	0
7	A	32	0	0	25	0
7	B	8	0	0	5	0
7	E	8	0	0	4	0
7	F	32	0	0	25	0
7	G	8	0	0	6	0
7	J	8	0	0	4	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
9	D	7	0	0	2	0
9	I	7	0	0	3	0
All	All	29216	0	29248	587	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 10.

All (587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:CYS:SG	7:F:703:SF4:FE1	1.20	1.32
1:A:195:CYS:SG	7:A:703:SF4:FE1	1.20	1.30
2:G:458:CYS:SG	7:G:601:SF4:FE1	1.27	1.26
2:B:458:CYS:SG	7:B:601:SF4:FE1	1.27	1.25
1:A:36:CYS:SG	6:A:701:FES:FE1	1.39	1.15
1:F:36:CYS:SG	6:F:701:FES:FE1	1.39	1.14
5:J:149:CYS:SG	7:J:201:SF4:FE3	1.51	1.02
1:F:264:CYS:SG	7:F:704:SF4:FE1	1.51	1.01
5:E:149:CYS:SG	7:E:201:SF4:FE3	1.51	1.00
1:A:264:CYS:SG	7:A:704:SF4:FE1	1.51	1.00
1:F:264:CYS:HG	7:F:704:SF4:FE1	0.70	0.97
1:F:229:CYS:HG	7:F:704:SF4:FE3	0.79	0.96
1:A:229:CYS:HG	7:A:704:SF4:FE3	0.78	0.96
1:A:198:CYS:HG	7:A:703:SF4:FE3	0.69	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:CYS:HG	7:A:704:SF4:FE1	0.71	0.92
1:F:198:CYS:HG	7:F:703:SF4:FE3	0.71	0.91
5:E:149:CYS:HG	7:E:201:SF4:FE3	0.60	0.89
1:F:158:CYS:HG	7:F:703:SF4:FE2	0.83	0.89
2:B:476:CYS:SG	6:B:602:FES:FE2	1.65	0.89
2:G:476:CYS:SG	6:G:602:FES:FE2	1.65	0.89
1:A:158:CYS:SG	7:A:703:SF4:FE2	1.63	0.88
1:F:158:CYS:SG	7:F:703:SF4:FE2	1.63	0.88
1:A:158:CYS:HG	7:A:703:SF4:FE2	0.85	0.87
1:A:36:CYS:HG	6:A:701:FES:FE1	0.90	0.86
3:H:82:CYS:HG	6:H:501:FES:FE2	0.55	0.86
1:A:195:CYS:HG	7:A:703:SF4:FE1	0.93	0.86
1:F:195:CYS:HG	7:F:703:SF4:FE1	0.92	0.85
5:J:149:CYS:HG	7:J:201:SF4:FE3	0.55	0.84
3:C:82:CYS:HG	6:C:501:FES:FE2	0.56	0.83
1:F:36:CYS:HG	6:F:701:FES:FE1	0.95	0.83
2:B:455:CYS:SG	7:B:601:SF4:FE4	1.72	0.82
1:F:192:CYS:HG	7:F:703:SF4:FE4	0.98	0.81
1:A:606:ARG:NH1	4:I:253:ASP:OD1	2.15	0.80
4:D:253:ASP:OD1	1:F:606:ARG:NH1	2.15	0.80
2:G:455:CYS:SG	7:G:601:SF4:FE4	1.72	0.80
1:A:198:CYS:SG	7:A:703:SF4:FE3	1.74	0.79
1:F:151:CYS:SG	7:F:702:SF4:FE4	1.75	0.79
1:A:192:CYS:SG	7:A:703:SF4:FE4	1.76	0.78
1:F:198:CYS:SG	7:F:703:SF4:FE3	1.74	0.78
4:D:282:LEU:O	1:F:585:GLU:HB3	1.83	0.78
1:A:585:GLU:HB3	4:I:282:LEU:O	1.83	0.78
1:A:151:CYS:SG	7:A:702:SF4:FE4	1.75	0.78
1:F:192:CYS:SG	7:F:703:SF4:FE4	1.76	0.77
4:D:265:GLY:O	4:D:277:PRO:HA	1.86	0.76
1:A:192:CYS:HG	7:A:703:SF4:FE4	1.02	0.76
3:C:82:CYS:SG	6:C:501:FES:FE2	1.74	0.75
4:I:265:GLY:O	4:I:277:PRO:HA	1.86	0.75
3:H:82:CYS:SG	6:H:501:FES:FE2	1.74	0.75
1:A:595:ARG:HB2	4:I:248:ARG:HE	1.52	0.75
4:D:248:ARG:HE	1:F:595:ARG:HB2	1.52	0.74
2:B:458:CYS:HG	7:B:601:SF4:FE1	1.02	0.74
4:D:401:ALA:HB3	9:D:602:FCO:N1	2.03	0.74
4:I:401:ALA:HB3	9:I:602:FCO:N1	2.03	0.74
4:D:253:ASP:CG	1:F:606:ARG:HH11	1.97	0.73
1:A:606:ARG:HH11	4:I:253:ASP:CG	1.97	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:ASN:HB2	4:D:20:LYS:HG3	1.73	0.71
4:I:10:ASN:HB2	4:I:20:LYS:HG3	1.73	0.70
2:G:476:CYS:HG	6:G:602:FES:FE2	0.47	0.70
1:A:289:ALA:HB2	4:I:251:ILE:HG21	1.74	0.69
4:I:110:SER:HB2	4:I:378:ARG:HH12	1.57	0.69
2:G:458:CYS:HG	7:G:601:SF4:FE1	1.02	0.69
2:B:476:CYS:HG	6:B:602:FES:FE2	0.47	0.69
4:D:110:SER:HB2	4:D:378:ARG:HH12	1.57	0.69
1:F:195:CYS:SG	7:F:703:SF4:S4	2.91	0.69
1:A:195:CYS:SG	7:A:703:SF4:S4	2.91	0.68
4:D:247:PRO:HG2	1:F:593:ALA:HB2	1.76	0.68
4:D:247:PRO:HG2	1:F:593:ALA:CB	2.24	0.68
4:D:251:ILE:HG21	1:F:289:ALA:HB2	1.74	0.68
1:A:593:ALA:CB	4:I:247:PRO:HG2	2.24	0.67
5:J:149:CYS:SG	7:J:201:SF4:S1	2.93	0.67
1:A:593:ALA:HB2	4:I:247:PRO:HG2	1.76	0.67
2:G:458:CYS:SG	7:G:601:SF4:S4	2.94	0.66
5:E:6:VAL:HG12	5:E:53:VAL:HB	1.77	0.66
5:E:149:CYS:SG	7:E:201:SF4:S1	2.93	0.66
5:J:6:VAL:HG12	5:J:53:VAL:HB	1.77	0.66
5:E:25:ASP:OD1	5:E:25:ASP:N	2.29	0.65
2:B:147:LEU:HB3	2:B:267:THR:HG21	1.78	0.65
2:B:458:CYS:SG	7:B:601:SF4:S4	2.94	0.65
2:G:165:ARG:O	2:G:167:ARG:NH1	2.30	0.65
1:A:61:LEU:HB2	1:A:66:THR:HG21	1.79	0.65
2:G:147:LEU:HB3	2:G:267:THR:HG21	1.78	0.65
1:A:377:ILE:HG22	1:A:508:ILE:HD13	1.78	0.65
4:I:378:ARG:HB2	9:I:602:FCO:N2	2.12	0.65
1:F:151:CYS:HG	7:F:702:SF4:FE4	1.13	0.65
1:F:377:ILE:HG22	1:F:508:ILE:HD13	1.78	0.64
4:D:378:ARG:HB2	9:D:602:FCO:N2	2.12	0.64
2:B:360:ILE:HG23	2:B:432:VAL:HG11	1.80	0.64
5:J:25:ASP:OD1	5:J:25:ASP:N	2.29	0.64
2:G:182:LYS:HG2	2:G:227:ILE:HA	1.79	0.64
1:F:61:LEU:HB2	1:F:66:THR:HG21	1.79	0.63
2:B:165:ARG:O	2:B:167:ARG:NH1	2.30	0.63
4:D:248:ARG:NE	1:F:595:ARG:HB2	2.13	0.63
2:B:182:LYS:HG2	2:B:227:ILE:HA	1.79	0.63
4:I:334:ARG:O	4:I:337:GLU:HB2	1.99	0.63
5:J:111:THR:O	5:J:111:THR:OG1	2.16	0.63
1:A:230:PRO:HG3	1:A:621:TRP:CD1	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:334:ARG:O	4:D:337:GLU:HB2	1.99	0.63
1:A:589:ALA:HA	4:I:282:LEU:HD13	1.81	0.62
1:A:264:CYS:SG	7:A:704:SF4:S4	2.97	0.62
2:G:360:ILE:HG23	2:G:432:VAL:HG11	1.80	0.62
1:A:348:PHE:CE1	1:A:583:GLU:HB3	2.35	0.62
1:A:353:ILE:HG21	1:A:559:VAL:HG21	1.82	0.62
1:A:195:CYS:SG	7:A:703:SF4:S3	2.98	0.62
1:F:195:CYS:SG	7:F:703:SF4:S3	2.98	0.62
1:F:348:PHE:CE1	1:F:583:GLU:HB3	2.35	0.62
1:A:595:ARG:HB2	4:I:248:ARG:NE	2.13	0.62
2:B:411:LEU:HD12	2:B:412:PRO:HD2	1.82	0.61
1:F:264:CYS:SG	7:F:704:SF4:S4	2.97	0.61
1:A:440:LYS:HD2	1:A:486:ALA:HB1	1.81	0.61
4:D:282:LEU:HD13	1:F:589:ALA:HA	1.81	0.61
2:G:411:LEU:HD12	2:G:412:PRO:HD2	1.82	0.61
1:A:393:GLU:HG2	1:A:545:LEU:HB3	1.83	0.60
1:F:440:LYS:HD2	1:F:486:ALA:HB1	1.81	0.60
2:B:142:ALA:HB2	2:B:334:LEU:HG	1.84	0.60
1:F:353:ILE:HG21	1:F:559:VAL:HG21	1.82	0.60
4:I:150:ARG:NH2	5:J:19:MET:SD	2.75	0.60
1:F:22:LEU:HD22	1:F:64:CYS:SG	2.42	0.60
1:F:393:GLU:HG2	1:F:545:LEU:HB3	1.83	0.60
1:A:22:LEU:HD22	1:A:64:CYS:SG	2.42	0.60
4:D:150:ARG:NH2	5:E:19:MET:SD	2.75	0.60
5:E:11:LEU:HB3	5:E:65:GLU:HB2	1.84	0.60
2:B:238:ALA:HB2	2:B:277:GLU:HB2	1.84	0.59
2:G:142:ALA:HB2	2:G:334:LEU:HG	1.84	0.59
4:I:100:MET:HE1	4:I:237:LEU:HB2	1.85	0.59
4:D:100:MET:HE1	4:D:237:LEU:HB2	1.85	0.59
4:D:247:PRO:CG	1:F:593:ALA:HB2	2.33	0.59
2:G:169:GLY:HA2	2:G:426:GLY:HA2	1.85	0.59
3:C:110:THR:HG22	3:C:117:THR:HB	1.85	0.59
1:A:587:ILE:O	1:A:591:ILE:HG13	2.03	0.59
3:H:110:THR:HG22	3:H:117:THR:HB	1.85	0.59
4:D:331:HIS:O	4:D:334:ARG:HB3	2.03	0.59
2:G:238:ALA:HB2	2:G:277:GLU:HB2	1.84	0.58
1:A:593:ALA:HB2	4:I:247:PRO:CG	2.33	0.58
4:D:47:PHE:HE1	5:E:95:ARG:HB3	1.66	0.58
1:A:610:ASN:HB3	4:I:252:LEU:HD12	1.85	0.58
1:F:587:ILE:O	1:F:591:ILE:HG13	2.03	0.58
4:I:47:PHE:HE1	5:J:95:ARG:HB3	1.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:11:LEU:HB3	5:J:65:GLU:HB2	1.84	0.58
4:D:252:LEU:HD12	1:F:610:ASN:HB3	1.85	0.58
1:F:136:ALA:O	1:F:210:ARG:NH1	2.36	0.58
4:I:30:HIS:HA	4:I:421:ILE:HG21	1.86	0.58
3:H:30:LEU:HD22	3:H:40:LEU:HD13	1.87	0.57
4:I:242:VAL:HG23	4:I:257:PRO:HG3	1.86	0.57
4:I:331:HIS:O	4:I:334:ARG:HB3	2.03	0.57
2:B:169:GLY:HA2	2:B:426:GLY:HA2	1.85	0.57
1:F:215:ARG:HD3	4:I:171:ILE:HG21	1.86	0.57
2:B:518:PHE:O	2:B:521:GLU:HB3	2.05	0.57
4:D:30:HIS:HA	4:D:421:ILE:HG21	1.86	0.57
1:F:137:THR:HB	1:F:187:ARG:HE	1.70	0.57
1:A:565:LEU:HD23	1:A:587:ILE:HG12	1.87	0.57
1:F:414:ASN:OD1	1:F:414:ASN:N	2.37	0.57
1:A:151:CYS:HG	7:A:702:SF4:FE4	1.19	0.56
4:D:242:VAL:HG23	4:D:257:PRO:HG3	1.86	0.56
2:G:518:PHE:O	2:G:521:GLU:HB3	2.05	0.56
1:A:136:ALA:O	1:A:210:ARG:NH1	2.36	0.56
3:C:30:LEU:HD22	3:C:40:LEU:HD13	1.87	0.56
1:A:170:GLU:HG2	1:A:171:ARG:HG3	1.87	0.56
1:A:137:THR:HB	1:A:187:ARG:HE	1.70	0.56
3:C:11:LYS:HE3	3:C:36:GLU:HG3	1.86	0.56
1:F:565:LEU:HD23	1:F:587:ILE:HG12	1.87	0.56
1:F:568:GLU:OE2	1:F:570:ARG:NH2	2.38	0.56
1:A:171:ARG:HH11	1:A:175:GLN:HB3	1.70	0.56
3:H:11:LYS:HE3	3:H:36:GLU:HG3	1.86	0.56
1:A:568:GLU:OE2	1:A:570:ARG:NH2	2.38	0.56
5:E:17:CYS:SG	7:E:201:SF4:S4	3.04	0.56
4:I:262:ASP:OD1	4:I:262:ASP:N	2.35	0.56
1:A:449:ILE:HG21	1:A:688:ARG:HD2	1.89	0.55
4:D:39:THR:HG22	5:E:126:ILE:HG22	1.88	0.55
4:I:273:TYR:OH	5:J:128:GLU:O	2.24	0.55
1:A:215:ARG:HD3	4:D:171:ILE:HG21	1.86	0.55
1:F:284:LEU:HD12	1:F:615:LEU:HD23	1.89	0.55
1:F:170:GLU:HG2	1:F:171:ARG:HG3	1.87	0.55
1:F:171:ARG:HH11	1:F:175:GLN:HB3	1.70	0.55
4:D:178:SER:OG	4:D:179:LEU:N	2.39	0.55
4:I:39:THR:HG22	5:J:126:ILE:HG22	1.88	0.55
1:A:383:ILE:HG21	1:A:401:ILE:HG12	1.89	0.55
4:D:33:GLU:OE1	4:D:35:ARG:NH2	2.36	0.55
4:D:165:ILE:HB	5:E:150:PRO:HG3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:CYS:HG	7:F:704:SF4:FE2	1.23	0.54
4:D:273:TYR:OH	5:E:128:GLU:O	2.24	0.54
2:G:345:THR:H	2:G:370:MET:HG2	1.72	0.54
4:I:165:ILE:HB	5:J:150:PRO:HG3	1.89	0.54
4:D:231:ARG:HG2	4:D:236:GLU:HB2	1.89	0.54
1:F:633:GLY:HA2	1:F:676:GLU:HG2	1.88	0.54
5:J:17:CYS:SG	7:J:201:SF4:S4	3.04	0.54
1:F:449:ILE:HG21	1:F:688:ARG:HD2	1.89	0.54
1:A:633:GLY:HA2	1:A:676:GLU:HG2	1.88	0.54
1:F:565:LEU:HD21	1:F:587:ILE:HG23	1.90	0.54
2:G:458:CYS:SG	7:G:601:SF4:S3	3.06	0.54
5:E:24:LEU:O	5:E:28:LEU:N	2.41	0.54
1:A:284:LEU:HD12	1:A:615:LEU:HD23	1.89	0.54
2:B:345:THR:H	2:B:370:MET:HG2	1.72	0.54
4:D:282:LEU:HD22	1:F:588:LEU:HB3	1.90	0.53
5:E:111:THR:O	5:E:111:THR:OG1	2.16	0.53
1:F:19:ASP:OD2	1:F:27:LYS:NZ	2.40	0.53
1:A:265:HIS:O	1:A:269:TRP:HB2	2.08	0.53
1:A:266:MET:O	1:A:270:TRP:HB2	2.09	0.53
1:A:588:LEU:HB3	4:I:282:LEU:HD22	1.90	0.53
4:I:296:ARG:HD3	4:I:375:GLU:HG2	1.90	0.53
2:B:357:THR:OG1	2:B:358:GLY:N	2.42	0.53
1:F:266:MET:O	1:F:270:TRP:HB2	2.09	0.53
1:F:383:ILE:HG21	1:F:401:ILE:HG12	1.89	0.53
1:A:584:GLU:HB2	1:A:587:ILE:HD12	1.91	0.53
2:B:458:CYS:SG	7:B:601:SF4:S3	3.06	0.53
1:F:555:ARG:HA	1:F:559:VAL:HB	1.90	0.53
1:A:358:LYS:NZ	1:A:561:GLU:O	2.42	0.53
3:C:8:VAL:HG23	3:C:37:LEU:HD21	1.91	0.53
5:J:24:LEU:O	5:J:28:LEU:N	2.41	0.53
2:G:357:THR:OG1	2:G:358:GLY:N	2.42	0.53
4:I:231:ARG:HG2	4:I:236:GLU:HB2	1.89	0.53
4:D:12:VAL:HG13	4:D:435:GLU:HG2	1.91	0.53
4:D:296:ARG:HD3	4:D:375:GLU:HG2	1.90	0.53
2:G:126:ILE:HG13	2:G:137:ARG:NH1	2.24	0.53
1:A:565:LEU:HD21	1:A:587:ILE:HG23	1.90	0.52
1:F:584:GLU:HB2	1:F:587:ILE:HD12	1.91	0.52
2:G:392:LYS:HD2	2:G:435:GLU:HA	1.91	0.52
5:E:73:ARG:HB2	5:E:140:VAL:HG13	1.91	0.52
5:E:113:SER:O	5:E:113:SER:OG	2.27	0.52
1:F:623:GLU:HB3	1:F:644:PRO:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:LYS:HD2	2:B:435:GLU:HA	1.91	0.52
1:F:358:LYS:NZ	1:F:561:GLU:O	2.42	0.52
1:A:19:ASP:OD2	1:A:27:LYS:NZ	2.40	0.52
4:D:80:ASP:OD1	4:D:173:GLY:N	2.43	0.52
1:A:555:ARG:HA	1:A:559:VAL:HB	1.90	0.52
2:B:126:ILE:HG13	2:B:137:ARG:NH1	2.24	0.52
3:C:80:ARG:HD3	3:C:121:VAL:HG11	1.92	0.52
1:F:362:PRO:HB3	1:F:689:ILE:HG21	1.91	0.52
3:H:8:VAL:HG23	3:H:37:LEU:HD21	1.91	0.52
3:H:80:ARG:HD3	3:H:121:VAL:HG11	1.92	0.52
1:A:623:GLU:HB3	1:A:644:PRO:HG3	1.90	0.52
1:F:265:HIS:O	1:F:269:TRP:HB2	2.08	0.52
4:I:33:GLU:OE1	4:I:35:ARG:NH2	2.36	0.52
1:A:414:ASN:OD1	1:A:414:ASN:N	2.37	0.51
5:J:73:ARG:HB2	5:J:140:VAL:HG13	1.91	0.51
3:C:81:VAL:HG22	3:C:133:MET:HG2	1.93	0.51
2:G:174:THR:HG21	2:G:325:THR:HG21	1.92	0.51
4:I:12:VAL:HG13	4:I:435:GLU:HG2	1.91	0.51
1:F:366:GLN:HE22	1:F:687:ALA:HB3	1.76	0.51
2:B:351:THR:HG23	2:B:369:PRO:HA	1.92	0.51
4:I:16:GLU:HB3	4:I:444:CYS:HA	1.92	0.51
4:I:80:ASP:OD1	4:I:173:GLY:N	2.43	0.51
1:A:357:PHE:CD2	1:A:555:ARG:HD3	2.46	0.51
4:D:286:HIS:HB3	1:F:589:ALA:HB2	1.92	0.51
3:H:70:HIS:HB3	3:H:74:ARG:HH21	1.76	0.51
1:A:610:ASN:HB3	4:I:252:LEU:CD1	2.40	0.51
4:D:252:LEU:CD1	1:F:610:ASN:HB3	2.40	0.51
2:B:174:THR:HG21	2:B:325:THR:HG21	1.92	0.51
1:A:232:CYS:HG	7:A:704:SF4:FE2	1.28	0.51
4:D:262:ASP:OD1	4:D:262:ASP:N	2.35	0.51
1:F:203:PRO:HG2	1:F:204:THR:HG23	1.93	0.51
4:I:35:ARG:HD3	4:I:271:TRP:CG	2.46	0.51
4:I:85:VAL:HG21	4:I:173:GLY:HA2	1.92	0.51
3:H:81:VAL:HG22	3:H:133:MET:HG2	1.93	0.51
1:A:393:GLU:HB3	1:A:545:LEU:HD13	1.93	0.51
1:F:54:LEU:HD21	1:F:61:LEU:HD11	1.94	0.51
1:F:393:GLU:HB3	1:F:545:LEU:HD13	1.93	0.51
2:G:351:THR:HG23	2:G:369:PRO:HA	1.92	0.51
4:I:245:LYS:HD2	4:I:323:ILE:HD11	1.93	0.51
5:J:61:GLY:O	5:J:130:LEU:N	2.44	0.51
2:B:481:THR:OG1	2:B:483:ASP:OD1	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD21	1:A:61:LEU:HD11	1.94	0.50
1:A:280:VAL:HG23	1:A:617:PRO:HB3	1.93	0.50
4:D:220:ALA:O	4:D:327:THR:OG1	2.25	0.50
2:G:126:ILE:HD13	2:G:134:TYR:HA	1.93	0.50
4:I:178:SER:OG	4:I:179:LEU:N	2.39	0.50
3:C:70:HIS:HB3	3:C:74:ARG:HH21	1.76	0.50
1:F:357:PHE:CD2	1:F:555:ARG:HD3	2.46	0.50
1:A:136:ALA:O	4:D:390:SER:OG	2.30	0.50
1:A:211:GLU:O	1:A:215:ARG:NH2	2.45	0.50
1:A:366:GLN:HE22	1:A:687:ALA:HB3	1.76	0.50
3:C:86:ALA:HB3	6:C:501:FES:S2	2.52	0.50
4:D:35:ARG:HD3	4:D:271:TRP:CG	2.46	0.50
2:B:126:ILE:HD13	2:B:134:TYR:HA	1.93	0.50
4:D:245:LYS:HD2	4:D:323:ILE:HD11	1.93	0.50
1:A:362:PRO:HB3	1:A:689:ILE:HG21	1.91	0.50
4:D:16:GLU:HB3	4:D:444:CYS:HA	1.92	0.50
4:D:85:VAL:HG21	4:D:173:GLY:HA2	1.92	0.50
1:F:136:ALA:O	4:I:390:SER:OG	2.30	0.50
1:F:192:CYS:SG	7:F:703:SF4:S2	3.10	0.50
1:A:203:PRO:HG2	1:A:204:THR:HG23	1.93	0.50
4:D:413:VAL:HG13	4:D:434:LEU:HD22	1.93	0.50
2:G:481:THR:OG1	2:G:483:ASP:OD1	2.29	0.50
1:A:386:MET:HG2	1:A:415:LEU:HD12	1.94	0.50
2:G:282:PHE:HB3	2:G:453:GLU:HB3	1.94	0.50
2:B:282:PHE:HB3	2:B:453:GLU:HB3	1.94	0.50
2:B:494:MET:O	2:B:498:THR:OG1	2.27	0.50
1:F:211:GLU:O	1:F:215:ARG:NH2	2.45	0.50
4:I:413:VAL:HG13	4:I:434:LEU:HD22	1.93	0.50
1:A:192:CYS:SG	7:A:703:SF4:S2	3.10	0.49
1:A:230:PRO:HG2	1:A:231:LEU:HD23	1.94	0.49
1:A:270:TRP:HZ3	1:A:582:PRO:HD3	1.78	0.49
1:F:280:VAL:HG23	1:F:617:PRO:HB3	1.93	0.49
3:H:86:ALA:HB3	6:H:501:FES:S2	2.52	0.49
2:B:264:ILE:HG22	2:B:265:MET:HG2	1.94	0.49
1:A:589:ALA:HB2	4:I:286:HIS:HB3	1.92	0.49
1:F:230:PRO:HG3	1:F:621:TRP:NE1	2.27	0.49
1:F:210:ARG:NH2	4:I:52:ASP:OD1	2.46	0.49
1:F:270:TRP:HZ3	1:F:582:PRO:HD3	1.78	0.49
1:A:413:MET:HG2	1:A:428:LEU:HB3	1.95	0.49
1:F:413:MET:HG2	1:F:428:LEU:HB3	1.95	0.49
4:I:70:SER:OG	4:I:102:GLN:OE1	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:113:SER:O	5:J:113:SER:OG	2.27	0.49
1:F:384:ILE:HD12	1:F:413:MET:HE3	1.95	0.49
1:F:386:MET:HG2	1:F:415:LEU:HD12	1.94	0.49
2:G:264:ILE:HG22	2:G:265:MET:HG2	1.94	0.49
1:A:348:PHE:HE1	1:A:583:GLU:HB3	1.77	0.48
4:I:261:LEU:HD23	5:J:113:SER:HB3	1.95	0.48
2:B:125:TYR:HB2	2:B:137:ARG:HH12	1.78	0.48
1:F:164:ALA:HB1	1:F:191:THR:O	2.13	0.48
1:A:202:CYS:HA	7:A:702:SF4:S2	2.53	0.48
4:D:221:THR:HG22	4:D:327:THR:H	1.77	0.48
1:A:247:ILE:HG13	1:A:275:THR:HG21	1.95	0.48
1:F:239:LYS:HB2	1:F:253:THR:HG23	1.96	0.48
2:G:201:GLY:HA3	3:H:85:THR:HG22	1.95	0.48
1:F:348:PHE:HE1	1:F:583:GLU:HB3	1.77	0.48
1:A:210:ARG:NH2	4:D:52:ASP:OD1	2.46	0.48
4:I:221:THR:HG22	4:I:327:THR:H	1.77	0.48
5:J:106:GLU:HA	5:J:110:GLU:HG2	1.94	0.48
1:A:49:MET:HE3	1:A:49:MET:HB3	1.59	0.48
2:G:288:THR:HA	2:G:291:MET:HE2	1.96	0.48
3:H:29:ILE:HD13	3:H:52:LEU:HD11	1.95	0.48
1:A:69:GLN:H	1:A:72:MET:HE3	1.79	0.48
1:A:384:ILE:HD12	1:A:413:MET:HE3	1.95	0.48
3:C:140:HIS:HB3	3:C:143:MET:HE3	1.96	0.48
4:D:45:GLU:OE1	4:D:450:HIS:NE2	2.47	0.48
5:E:106:GLU:HA	5:E:110:GLU:HG2	1.94	0.48
2:G:125:TYR:HB2	2:G:137:ARG:HH12	1.78	0.48
2:G:455:CYS:HG	7:G:601:SF4:FE4	1.30	0.48
4:I:45:GLU:OE1	4:I:450:HIS:NE2	2.47	0.48
4:I:63:ILE:HG22	4:I:447:CYS:HA	1.95	0.48
1:A:124:ARG:HG3	2:B:487:LYS:HE2	1.96	0.48
1:A:161:ILE:O	1:A:262:GLN:NE2	2.47	0.48
2:B:201:GLY:HA3	3:C:85:THR:HG22	1.95	0.48
1:F:247:ILE:HG13	1:F:275:THR:HG21	1.95	0.48
3:C:29:ILE:HD13	3:C:52:LEU:HD11	1.95	0.48
4:D:70:SER:OG	4:D:102:GLN:OE1	2.31	0.48
3:H:140:HIS:HB3	3:H:143:MET:HE3	1.96	0.47
1:A:49:MET:HE2	1:A:114:LEU:HD13	1.95	0.47
2:B:375:ARG:NH1	2:B:410:ASP:OD1	2.48	0.47
2:B:391:PHE:HA	2:B:434:ASP:HA	1.96	0.47
2:G:375:ARG:NH1	2:G:410:ASP:OD1	2.48	0.47
4:I:56:MET:O	4:I:60:THR:OG1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ALA:HB1	1:A:191:THR:O	2.13	0.47
2:B:474:LYS:HG2	2:B:479:GLU:HB2	1.96	0.47
3:C:74:ARG:HG3	3:C:117:THR:HG21	1.96	0.47
5:E:61:GLY:O	5:E:130:LEU:N	2.44	0.47
1:F:49:MET:HE3	1:F:49:MET:HB3	1.59	0.47
1:F:389:ASP:HB3	1:F:392:LYS:HE3	1.97	0.47
4:D:159:THR:O	4:D:177:ARG:NH1	2.48	0.47
2:G:362:ASN:OD1	2:G:362:ASN:N	2.47	0.47
2:G:434:ASP:OD1	2:G:434:ASP:N	2.36	0.47
5:J:4:ALA:HB3	5:J:35:VAL:HG23	1.97	0.47
2:B:288:THR:HA	2:B:291:MET:HE2	1.96	0.47
1:F:20:THR:HA	1:F:67:PRO:HA	1.96	0.47
2:G:474:LYS:HG2	2:G:479:GLU:HB2	1.96	0.47
3:C:100:LYS:HD3	3:C:107:GLU:HA	1.97	0.47
1:F:202:CYS:HA	7:F:702:SF4:S2	2.53	0.47
1:F:630:THR:OG1	1:F:631:ILE:N	2.48	0.47
2:G:391:PHE:HA	2:G:434:ASP:HA	1.96	0.47
2:B:362:ASN:OD1	2:B:362:ASN:N	2.47	0.47
4:D:261:LEU:HD23	5:E:113:SER:HB3	1.95	0.47
5:E:4:ALA:HB3	5:E:35:VAL:HG23	1.97	0.47
1:F:49:MET:HE2	1:F:114:LEU:HD13	1.95	0.47
1:F:69:GLN:H	1:F:72:MET:HE3	1.79	0.47
1:F:161:ILE:O	1:F:262:GLN:NE2	2.47	0.47
1:F:232:CYS:SG	7:F:704:SF4:S1	3.10	0.47
1:F:445:LEU:HD22	1:F:528:LEU:N	2.30	0.47
1:A:109:CYS:HB3	1:A:112:GLN:HB2	1.97	0.47
1:A:239:LYS:HB2	1:A:253:THR:HG23	1.96	0.47
2:B:434:ASP:OD1	2:B:434:ASP:N	2.36	0.47
1:F:230:PRO:HG2	1:F:231:LEU:HD23	1.95	0.47
1:A:445:LEU:HD22	1:A:528:LEU:N	2.30	0.47
4:I:159:THR:O	4:I:177:ARG:NH1	2.48	0.47
1:A:20:THR:HA	1:A:67:PRO:HA	1.96	0.47
4:D:63:ILE:HG22	4:D:447:CYS:HA	1.95	0.47
3:H:74:ARG:HG3	3:H:117:THR:HG21	1.96	0.47
4:D:85:VAL:HG23	4:D:87:ILE:HG22	1.97	0.46
1:F:124:ARG:HG3	2:G:487:LYS:HE2	1.96	0.46
1:A:630:THR:OG1	1:A:631:ILE:N	2.48	0.46
1:F:600:GLN:HE22	1:F:654:VAL:HG21	1.80	0.46
4:D:225:ALA:HB3	4:D:289:TYR:HB3	1.98	0.46
1:F:101:MET:HB3	1:F:101:MET:HE3	1.62	0.46
3:H:30:LEU:HA	3:H:33:VAL:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:HB2	1:A:77:LYS:HE2	1.73	0.46
1:F:121:ASP:HB3	5:J:145:TYR:HB2	1.98	0.46
4:I:60:THR:O	4:I:63:ILE:HG13	2.16	0.46
3:C:30:LEU:HA	3:C:33:VAL:HG22	1.96	0.46
4:I:390:SER:OG	4:I:390:SER:O	2.33	0.46
1:A:389:ASP:HB3	1:A:392:LYS:HE3	1.97	0.46
4:D:60:THR:O	4:D:63:ILE:HG13	2.16	0.46
1:A:121:ASP:HB3	5:E:145:TYR:HB2	1.98	0.46
3:H:100:LYS:HD3	3:H:107:GLU:HA	1.97	0.46
1:A:600:GLN:HE22	1:A:654:VAL:HG21	1.80	0.45
3:C:79:ILE:HD11	3:C:116:PHE:CD1	2.52	0.45
1:F:109:CYS:HB3	1:F:112:GLN:HB2	1.97	0.45
5:E:6:VAL:HG13	5:E:35:VAL:HG21	1.98	0.45
4:D:241:GLU:HA	4:D:257:PRO:HD3	1.98	0.45
4:I:241:GLU:HA	4:I:257:PRO:HD3	1.98	0.45
1:A:195:CYS:SG	7:A:703:SF4:S2	2.97	0.45
1:A:232:CYS:SG	7:A:704:SF4:S1	3.10	0.45
3:C:98:LYS:HA	3:C:101:GLN:HG3	1.99	0.45
4:D:252:LEU:HD12	1:F:610:ASN:C	2.42	0.45
4:I:225:ALA:HB3	4:I:289:TYR:HB3	1.98	0.45
1:A:210:ARG:NH2	4:D:390:SER:O	2.49	0.45
4:D:40:GLN:HA	5:E:62:ASN:HD21	1.82	0.45
3:H:79:ILE:HD11	3:H:116:PHE:CD1	2.52	0.45
4:I:85:VAL:HG23	4:I:87:ILE:HG22	1.97	0.45
1:A:610:ASN:C	4:I:252:LEU:HD12	2.42	0.45
2:B:261:GLY:H	2:B:264:ILE:HD11	1.80	0.45
2:B:450:THR:HG21	2:B:507:ALA:HB1	1.98	0.45
3:C:82:CYS:SG	3:C:87:CYS:SG	3.15	0.45
2:G:261:GLY:H	2:G:264:ILE:HD11	1.80	0.45
5:J:61:GLY:N	5:J:65:GLU:OE2	2.38	0.45
4:D:215:GLU:OE2	4:D:420:TYR:OH	2.30	0.45
4:D:273:TYR:OH	5:E:127:PRO:O	2.35	0.45
3:H:98:LYS:HA	3:H:101:GLN:HG3	1.99	0.45
1:F:77:LYS:HB2	1:F:77:LYS:HE2	1.73	0.45
3:H:82:CYS:SG	3:H:87:CYS:SG	3.15	0.45
2:B:146:ALA:HA	2:B:150:MET:HB2	1.98	0.44
4:D:14:ARG:HH22	4:D:118:ASP:CG	2.25	0.44
1:F:354:ARG:O	1:F:358:LYS:HB2	2.17	0.44
5:J:6:VAL:HG13	5:J:35:VAL:HG21	1.98	0.44
4:D:131:ASN:HD22	5:E:43:VAL:HG12	1.82	0.44
1:F:14:LYS:HB3	1:F:14:LYS:HE3	1.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:GLY:HA3	1:F:681:GLN:HE21	1.82	0.44
1:F:425:LEU:HD23	1:F:425:LEU:HA	1.84	0.44
1:A:151:CYS:SG	7:A:702:SF4:S2	3.16	0.44
4:I:40:GLN:HA	5:J:62:ASN:HD21	1.82	0.44
1:A:354:ARG:O	1:A:358:LYS:HB2	2.17	0.44
2:B:306:PRO:HB2	2:B:311:HIS:HB3	1.99	0.44
3:C:129:LEU:HA	3:C:142:ARG:HH22	1.83	0.44
2:G:146:ALA:HA	2:G:150:MET:HB2	1.98	0.44
2:G:450:THR:HG21	2:G:507:ALA:HB1	1.98	0.44
1:A:152:GLN:HE21	1:A:169:LEU:HD11	1.83	0.44
4:D:69:VAL:HB	4:D:98:MET:HE3	2.00	0.44
4:I:401:ALA:HB3	9:I:602:FCO:C1	2.48	0.44
1:A:320:LEU:HD12	1:A:558:VAL:CG1	2.48	0.44
4:D:390:SER:OG	4:D:390:SER:O	2.33	0.44
1:F:151:CYS:SG	7:F:702:SF4:S2	3.16	0.44
2:G:167:ARG:HG2	2:G:352:LYS:HD2	2.00	0.44
4:I:397:ASN:HB2	5:J:112:ALA:HB3	1.99	0.44
2:G:306:PRO:HB2	2:G:311:HIS:HB3	1.99	0.44
4:I:220:ALA:O	4:I:327:THR:OG1	2.25	0.44
2:B:167:ARG:HG2	2:B:352:LYS:HD2	2.00	0.44
2:B:196:ASP:HB2	2:B:237:ARG:HH11	1.82	0.44
3:C:98:LYS:NZ	3:C:145:PRO:O	2.39	0.44
4:D:397:ASN:HB2	5:E:112:ALA:HB3	1.99	0.44
1:A:592:SER:O	4:I:246:ALA:HB1	2.18	0.44
2:B:395:GLN:O	2:B:430:LEU:HA	2.18	0.44
4:I:215:GLU:OE2	4:I:420:TYR:OH	2.30	0.44
1:F:320:LEU:HD12	1:F:558:VAL:CG1	2.48	0.43
4:I:131:ASN:HD22	5:J:43:VAL:HG12	1.82	0.43
1:A:575:VAL:HG13	1:A:599:VAL:HG22	2.00	0.43
1:F:617:PRO:HG2	1:F:648:ILE:HG23	1.99	0.43
1:F:641:ILE:HG22	1:F:642:VAL:HG12	2.00	0.43
1:F:97:ASN:HD21	1:F:129:TYR:HA	1.83	0.43
3:H:100:LYS:HE2	3:H:100:LYS:HB3	1.83	0.43
1:A:492:LYS:O	1:A:495:GLU:HG2	2.18	0.43
3:C:27:ILE:HD13	3:C:27:ILE:HA	1.64	0.43
3:C:27:ILE:HD11	3:C:66:TYR:CE2	2.53	0.43
3:C:95:ILE:HD12	3:C:148:ILE:HD11	2.00	0.43
1:F:573:LEU:HB2	1:F:594:THR:HG21	1.99	0.43
1:F:575:VAL:HG13	1:F:599:VAL:HG22	2.00	0.43
2:G:196:ASP:HB2	2:G:237:ARG:HH11	1.82	0.43
2:G:290:LEU:HD23	2:G:320:ILE:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:LEU:HD23	2:B:320:ILE:HD13	2.01	0.43
1:F:27:LYS:HE3	1:F:27:LYS:HB2	1.90	0.43
1:A:617:PRO:HG2	1:A:648:ILE:HG23	1.99	0.43
1:F:143:MET:HE2	1:F:143:MET:HB3	1.91	0.43
3:H:27:ILE:HD11	3:H:66:TYR:CE2	2.53	0.43
4:I:199:MET:HE3	4:I:199:MET:HB3	1.93	0.43
2:B:329:VAL:HA	2:B:332:ILE:HG12	2.01	0.43
2:B:402:GLY:HA3	2:B:513:THR:HG21	2.01	0.43
2:G:329:VAL:HA	2:G:332:ILE:HG12	2.01	0.43
2:G:395:GLN:O	2:G:430:LEU:HA	2.18	0.43
4:I:14:ARG:HH22	4:I:118:ASP:CG	2.25	0.43
1:A:367:GLY:HA3	1:A:681:GLN:HE21	1.82	0.43
1:A:641:ILE:HG22	1:A:642:VAL:HG12	2.00	0.43
1:F:230:PRO:HG3	1:F:621:TRP:CD1	2.53	0.43
4:I:69:VAL:HB	4:I:98:MET:HE3	2.00	0.43
1:A:230:PRO:HG3	1:A:621:TRP:NE1	2.33	0.43
2:B:161:LYS:HB2	2:B:161:LYS:HE3	1.81	0.43
3:H:95:ILE:HD12	3:H:148:ILE:HD11	2.00	0.43
3:H:129:LEU:HA	3:H:142:ARG:HH22	1.83	0.43
2:B:447:LEU:HD23	2:B:447:LEU:HA	1.87	0.43
1:F:369:ARG:HB2	1:F:680:SER:HB3	2.00	0.43
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.78	0.42
4:D:246:ALA:HB1	1:F:592:SER:O	2.18	0.42
4:D:267:HIS:HD2	4:D:269:GLU:HG2	1.84	0.42
1:F:152:GLN:HE21	1:F:169:LEU:HD11	1.83	0.42
1:F:487:MET:HB2	1:F:487:MET:HE2	1.84	0.42
5:J:51:ILE:HG13	5:J:76:CYS:HB3	2.01	0.42
1:A:573:LEU:HB2	1:A:594:THR:HG21	1.99	0.42
4:D:108:ALA:HB2	4:D:149:LEU:HD23	2.01	0.42
1:F:231:LEU:CD2	1:F:580:MET:HB3	2.49	0.42
1:F:492:LYS:O	1:F:495:GLU:HG2	2.18	0.42
1:F:535:PHE:CD1	1:F:684:ALA:HA	2.54	0.42
2:G:402:GLY:HA3	2:G:513:THR:HG21	2.01	0.42
1:A:97:ASN:HD21	1:A:129:TYR:HA	1.83	0.42
1:A:369:ARG:HB2	1:A:680:SER:HB3	2.00	0.42
4:I:267:HIS:HD2	4:I:269:GLU:HG2	1.84	0.42
1:A:449:ILE:HB	1:A:531:ALA:HA	2.01	0.42
1:F:204:THR:OG1	7:F:702:SF4:S3	2.78	0.42
2:B:298:ARG:HH11	3:C:65:PHE:HB2	1.84	0.42
5:E:51:ILE:HG13	5:E:76:CYS:HB3	2.01	0.42
1:F:588:LEU:HD12	1:F:588:LEU:HA	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:62:ASN:HB2	5:J:65:GLU:HG2	2.02	0.42
1:A:193:VAL:HG22	7:A:703:SF4:S3	2.60	0.42
4:D:286:HIS:HB3	1:F:589:ALA:CB	2.50	0.42
5:E:62:ASN:HB2	5:E:65:GLU:HG2	2.02	0.42
2:G:298:ARG:HH11	3:H:65:PHE:HB2	1.84	0.42
2:G:361:THR:OG1	2:G:382:GLY:O	2.33	0.42
1:A:535:PHE:CD1	1:A:684:ALA:HA	2.54	0.42
3:C:80:ARG:HD2	3:C:134:MET:HE2	2.02	0.42
1:F:449:ILE:HB	1:F:531:ALA:HA	2.01	0.42
1:A:204:THR:OG1	7:A:702:SF4:S3	2.78	0.42
1:A:589:ALA:CB	4:I:286:HIS:HB3	2.50	0.42
2:B:324:GLU:HG3	2:B:353:ILE:HG12	2.02	0.42
1:F:668:ARG:HD2	1:F:668:ARG:HA	1.84	0.42
2:B:372:ILE:HB	2:B:377:ILE:HD11	2.02	0.41
3:H:27:ILE:HD13	3:H:27:ILE:HA	1.64	0.41
2:B:167:ARG:O	2:B:322:ASN:ND2	2.54	0.41
1:F:347:THR:HG21	1:F:559:VAL:HG22	2.02	0.41
2:B:357:THR:HG23	2:B:431:VAL:HG22	2.02	0.41
4:D:199:MET:HE3	4:D:199:MET:HB3	1.93	0.41
1:F:193:VAL:HG22	7:F:703:SF4:S3	2.60	0.41
1:F:579:ALA:HB3	1:F:603:PHE:HD2	1.85	0.41
2:G:395:GLN:NE2	2:G:398:GLY:O	2.53	0.41
2:G:469:LEU:HD12	2:G:469:LEU:HA	1.93	0.41
1:A:101:MET:HE3	1:A:101:MET:HB3	1.62	0.41
2:B:349:LYS:HA	2:B:370:MET:HE1	2.01	0.41
2:G:167:ARG:HH21	2:G:351:THR:N	2.19	0.41
2:G:349:LYS:HA	2:G:370:MET:HE1	2.01	0.41
2:G:372:ILE:HB	2:G:377:ILE:HD11	2.02	0.41
4:I:203:LYS:HB3	4:I:203:LYS:HE3	1.81	0.41
3:C:11:LYS:HA	3:C:11:LYS:HD2	1.95	0.41
1:F:144:ASP:OD2	4:I:51:ARG:NH2	2.43	0.41
2:G:370:MET:HG3	2:G:371:GLY:H	1.85	0.41
4:I:145:LYS:HB3	4:I:197:ILE:HG23	2.03	0.41
1:A:579:ALA:HB3	1:A:603:PHE:HD2	1.85	0.41
1:A:611:LEU:H	1:A:611:LEU:HG	1.64	0.41
4:D:145:LYS:HB3	4:D:197:ILE:HG23	2.03	0.41
2:G:357:THR:HG23	2:G:431:VAL:HG22	2.02	0.41
3:H:78:VAL:HA	3:H:117:THR:HG23	2.02	0.41
4:I:108:ALA:HB2	4:I:149:LEU:HD23	2.01	0.41
5:J:129:LEU:HD23	5:J:129:LEU:HA	2.00	0.41
1:A:60:MET:HE2	1:A:60:MET:HB3	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HE3	1:A:309:LYS:HB2	1.94	0.41
1:A:390:PRO:HB2	1:A:398:ALA:HB2	2.02	0.41
2:B:370:MET:HG3	2:B:371:GLY:H	1.85	0.41
1:F:195:CYS:SG	7:F:703:SF4:S2	2.97	0.41
1:F:412:LEU:HB3	1:F:426:VAL:HG12	2.02	0.41
2:G:324:GLU:HG3	2:G:353:ILE:HG12	2.02	0.41
1:A:164:ALA:O	1:A:166:THR:N	2.54	0.41
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.74	0.41
2:B:242:LEU:HA	2:B:245:LYS:HZ2	1.84	0.41
3:C:11:LYS:O	3:C:11:LYS:NZ	2.53	0.41
3:C:78:VAL:HA	3:C:117:THR:HG23	2.02	0.41
1:A:6:LEU:HD11	1:A:68:ALA:HB1	2.03	0.41
1:A:229:CYS:SG	7:A:704:SF4:S4	3.19	0.41
2:B:347:LYS:HA	2:B:347:LYS:HD2	1.78	0.41
2:B:395:GLN:NE2	2:B:398:GLY:O	2.53	0.41
1:F:33:PRO:HB3	1:F:114:LEU:HD22	2.03	0.41
3:H:80:ARG:HD2	3:H:134:MET:HE2	2.02	0.41
5:E:170:LYS:HE2	5:E:170:LYS:HB3	1.82	0.40
1:F:164:ALA:O	1:F:166:THR:N	2.54	0.40
1:F:401:ILE:HD11	1:F:510:ILE:HG13	2.03	0.40
3:H:98:LYS:NZ	3:H:145:PRO:O	2.39	0.40
4:I:6:LYS:HB3	4:I:24:MET:HG3	2.03	0.40
2:B:167:ARG:HH21	2:B:351:THR:N	2.19	0.40
4:D:247:PRO:HG2	1:F:593:ALA:CA	2.51	0.40
5:E:10:TRP:HB2	5:E:13:ALA:HB3	2.03	0.40
1:F:666:LEU:HD12	1:F:666:LEU:HA	1.86	0.40
1:A:33:PRO:HB3	1:A:114:LEU:HD22	2.03	0.40
1:A:231:LEU:HD12	1:A:266:MET:HB3	2.02	0.40
4:D:284:PHE:HA	4:D:285:PRO:HA	1.93	0.40
1:F:198:CYS:SG	7:F:703:SF4:S4	3.19	0.40
3:H:12:VAL:HG13	3:H:33:VAL:HG11	2.03	0.40
1:A:347:THR:HG21	1:A:559:VAL:HG22	2.02	0.40
1:A:487:MET:HE2	1:A:487:MET:HB2	1.84	0.40
5:E:100:LYS:HE2	5:E:100:LYS:HB2	1.95	0.40
2:G:167:ARG:O	2:G:322:ASN:ND2	2.54	0.40
1:A:110:GLU:HB2	1:A:203:PRO:HB2	2.03	0.40
1:A:357:PHE:HE2	1:A:552:LEU:HD13	1.86	0.40
2:B:264:ILE:O	2:B:267:THR:OG1	2.30	0.40
4:D:44:PHE:HB2	4:D:450:HIS:HB2	2.04	0.40
4:D:327:THR:O	4:D:330:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	661/692 (96%)	587 (89%)	74 (11%)	0	100	100
1	F	661/692 (96%)	587 (89%)	74 (11%)	0	100	100
2	B	423/597 (71%)	376 (89%)	47 (11%)	0	100	100
2	G	423/597 (71%)	376 (89%)	47 (11%)	0	100	100
3	C	150/156 (96%)	136 (91%)	14 (9%)	0	100	100
3	H	150/156 (96%)	136 (91%)	14 (9%)	0	100	100
4	D	445/475 (94%)	408 (92%)	37 (8%)	0	100	100
4	I	445/475 (94%)	408 (92%)	37 (8%)	0	100	100
5	E	177/179 (99%)	158 (89%)	19 (11%)	0	100	100
5	J	177/179 (99%)	158 (89%)	19 (11%)	0	100	100
All	All	3712/4198 (88%)	3330 (90%)	382 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	564/583 (97%)	527 (93%)	37 (7%)	15	47
1	F	564/583 (97%)	527 (93%)	37 (7%)	15	47
2	B	341/488 (70%)	323 (95%)	18 (5%)	20	53
2	G	341/488 (70%)	323 (95%)	18 (5%)	20	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	130/133 (98%)	123 (95%)	7 (5%)	20	53
3	H	130/133 (98%)	123 (95%)	7 (5%)	20	53
4	D	378/402 (94%)	366 (97%)	12 (3%)	34	65
4	I	378/402 (94%)	366 (97%)	12 (3%)	34	65
5	E	154/154 (100%)	146 (95%)	8 (5%)	21	54
5	J	154/154 (100%)	146 (95%)	8 (5%)	21	54
All	All	3134/3520 (89%)	2970 (95%)	164 (5%)	22	54

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	44	ILE
1	A	49	MET
1	A	61	LEU
1	A	65	THR
1	A	75	VAL
1	A	101	MET
1	A	128	LEU
1	A	158	CYS
1	A	191	THR
1	A	194	ASN
1	A	198	CYS
1	A	224	VAL
1	A	230	PRO
1	A	273	GLU
1	A	282	VAL
1	A	285	ILE
1	A	286	ARG
1	A	287	GLU
1	A	346	ASP
1	A	348	PHE
1	A	354	ARG
1	A	414	ASN
1	A	438	VAL
1	A	479	SER
1	A	523	THR
1	A	526	CYS
1	A	528	LEU
1	A	537	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	575	VAL
1	A	586	GLU
1	A	588	LEU
1	A	608	LEU
1	A	611	LEU
1	A	642	VAL
1	A	674	CYS
1	A	675	GLU
2	B	151	THR
2	B	176	LEU
2	B	193	CYS
2	B	286	GLU
2	B	340	PHE
2	B	360	ILE
2	B	361	THR
2	B	368	VAL
2	B	373	THR
2	B	381	LEU
2	B	385	ILE
2	B	389	LYS
2	B	433	MET
2	B	434	ASP
2	B	435	GLU
2	B	458	CYS
2	B	515	ILE
2	B	525	HIS
3	C	27	ILE
3	C	29	ILE
3	C	31	GLN
3	C	71	LEU
3	C	100	LYS
3	C	117	THR
3	C	148	ILE
4	D	7	LEU
4	D	66	ILE
4	D	69	VAL
4	D	147	ILE
4	D	175	VAL
4	D	262	ASP
4	D	365	GLU
4	D	400	VAL
4	D	421	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	437	VAL
4	D	442	ASP
4	D	445	LEU
5	E	26	GLU
5	E	79	LEU
5	E	98	ILE
5	E	106	GLU
5	E	111	THR
5	E	147	PRO
5	E	149	CYS
5	E	150	PRO
1	F	6	LEU
1	F	44	ILE
1	F	49	MET
1	F	61	LEU
1	F	65	THR
1	F	75	VAL
1	F	101	MET
1	F	128	LEU
1	F	158	CYS
1	F	191	THR
1	F	194	ASN
1	F	198	CYS
1	F	224	VAL
1	F	230	PRO
1	F	273	GLU
1	F	282	VAL
1	F	285	ILE
1	F	286	ARG
1	F	287	GLU
1	F	346	ASP
1	F	348	PHE
1	F	354	ARG
1	F	414	ASN
1	F	438	VAL
1	F	479	SER
1	F	523	THR
1	F	526	CYS
1	F	528	LEU
1	F	537	GLU
1	F	575	VAL
1	F	586	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	588	LEU
1	F	608	LEU
1	F	611	LEU
1	F	642	VAL
1	F	674	CYS
1	F	675	GLU
2	G	151	THR
2	G	176	LEU
2	G	193	CYS
2	G	286	GLU
2	G	340	PHE
2	G	360	ILE
2	G	361	THR
2	G	368	VAL
2	G	373	THR
2	G	381	LEU
2	G	385	ILE
2	G	389	LYS
2	G	433	MET
2	G	434	ASP
2	G	435	GLU
2	G	458	CYS
2	G	515	ILE
2	G	525	HIS
3	H	27	ILE
3	H	29	ILE
3	H	31	GLN
3	H	71	LEU
3	H	100	LYS
3	H	117	THR
3	H	148	ILE
4	I	7	LEU
4	I	66	ILE
4	I	69	VAL
4	I	147	ILE
4	I	175	VAL
4	I	262	ASP
4	I	365	GLU
4	I	400	VAL
4	I	421	ILE
4	I	437	VAL
4	I	442	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	445	LEU
5	J	26	GLU
5	J	79	LEU
5	J	98	ILE
5	J	106	GLU
5	J	111	THR
5	J	147	PRO
5	J	149	CYS
5	J	150	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	28	ASN
1	A	69	GLN
1	A	87	GLN
1	A	97	ASN
1	A	140	ASN
1	A	146	ASN
1	A	152	GLN
1	A	194	ASN
1	A	366	GLN
1	A	375	HIS
1	A	391	GLN
1	A	407	HIS
1	A	409	ASN
1	A	436	GLN
1	A	652	HIS
2	B	467	GLN
2	B	509	ASN
3	C	34	GLN
3	C	88	HIS
3	C	149	GLN
4	D	267	HIS
4	D	397	ASN
4	D	410	ASN
5	E	62	ASN
1	F	28	ASN
1	F	69	GLN
1	F	87	GLN
1	F	97	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	140	ASN
1	F	152	GLN
1	F	194	ASN
1	F	366	GLN
1	F	375	HIS
1	F	391	GLN
1	F	407	HIS
1	F	409	ASN
1	F	436	GLN
1	F	444	ASN
1	F	652	HIS
2	G	467	GLN
2	G	509	ASN
3	H	34	GLN
3	H	88	HIS
3	H	149	GLN
4	I	267	HIS
4	I	397	ASN
4	I	410	ASN
5	J	62	ASN
5	J	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	SF4	E	201	5	0,12,12	-	-	-		
6	FES	H	501	3	0,4,4	-	-	-		
7	SF4	A	703	-	0,12,12	-	-	-		
7	SF4	F	704	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
6	FES	A	701	1	0,4,4	-	-	-		
7	SF4	J	201	5	0,12,12	-	-	-		
6	FES	B	602	2	0,4,4	-	-	-		
7	SF4	F	703	-	0,12,12	-	-	-		
6	FES	G	602	2	0,4,4	-	-	-		
9	FCO	D	602	4	3,6,6	0.71	0	-		
6	FES	C	501	3	0,4,4	-	-	-		
7	SF4	B	601	2	0,12,12	-	-	-		
6	FES	F	701	1	0,4,4	-	-	-		
7	SF4	G	601	2	0,12,12	-	-	-		
7	SF4	F	705	1	0,12,12	-	-	-		
7	SF4	F	702	1	0,12,12	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
9	FCO	I	602	4	3,6,6	0.71	0	-		
7	SF4	A	702	1	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
6	FES	B	602	2	-	-	0/1/1/1
6	FES	H	501	3	-	-	0/1/1/1
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	E	201	5	-	-	0/6/5/5
7	SF4	F	703	-	-	-	0/6/5/5
7	SF4	G	601	2	-	-	0/6/5/5
6	FES	G	602	2	-	-	0/1/1/1
7	SF4	A	703	-	-	-	0/6/5/5
7	SF4	A	702	1	-	-	0/6/5/5
7	SF4	F	702	1	-	-	0/6/5/5
7	SF4	J	201	5	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	F	704	1	-	-	0/6/5/5
7	SF4	F	705	1	-	-	0/6/5/5
6	FES	C	501	3	-	-	0/1/1/1
6	FES	A	701	1	-	-	0/1/1/1
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	B	601	2	-	-	0/6/5/5
6	FES	F	701	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

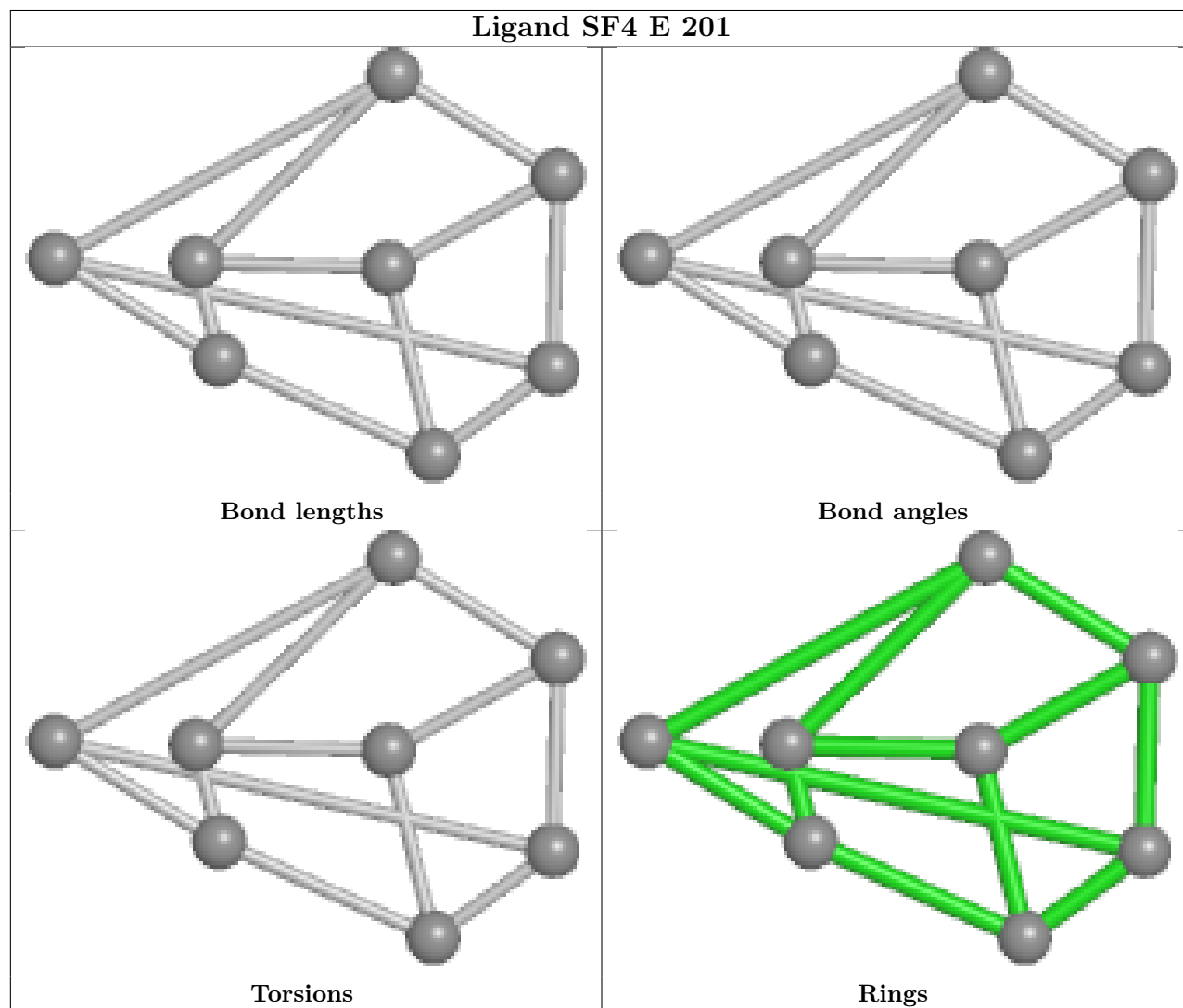
There are no ring outliers.

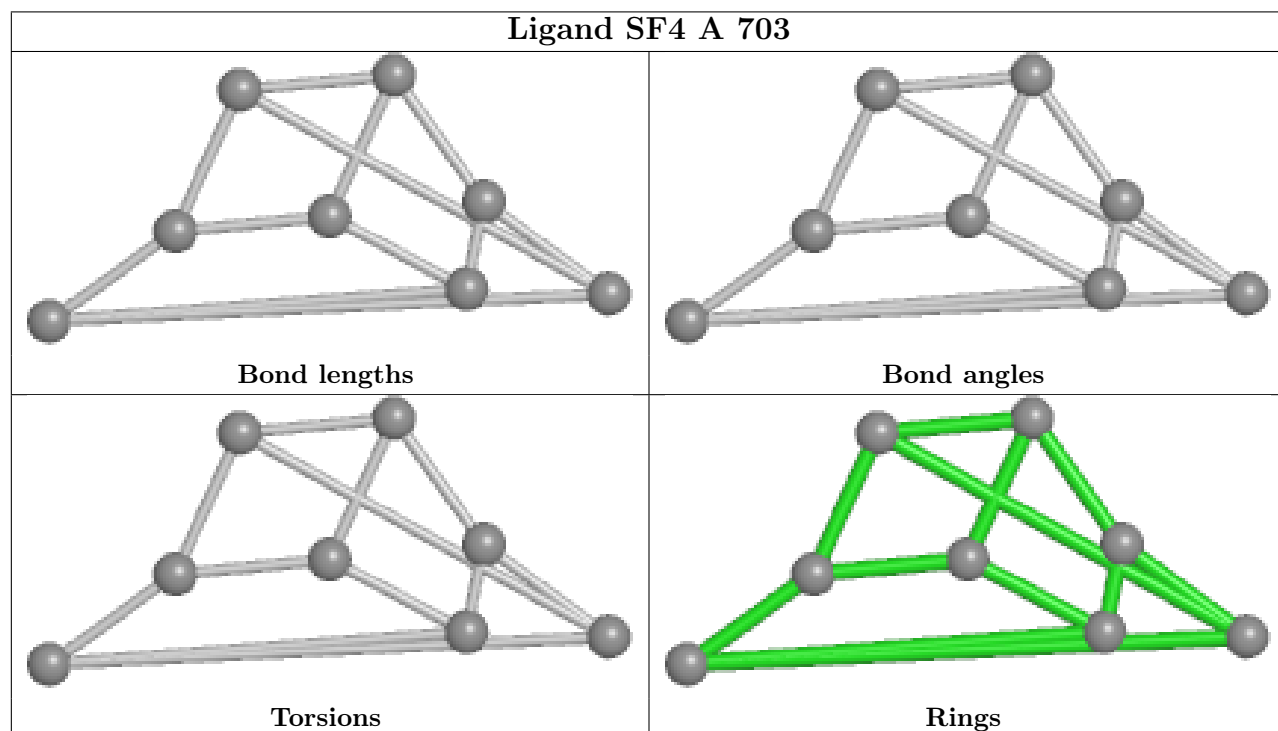
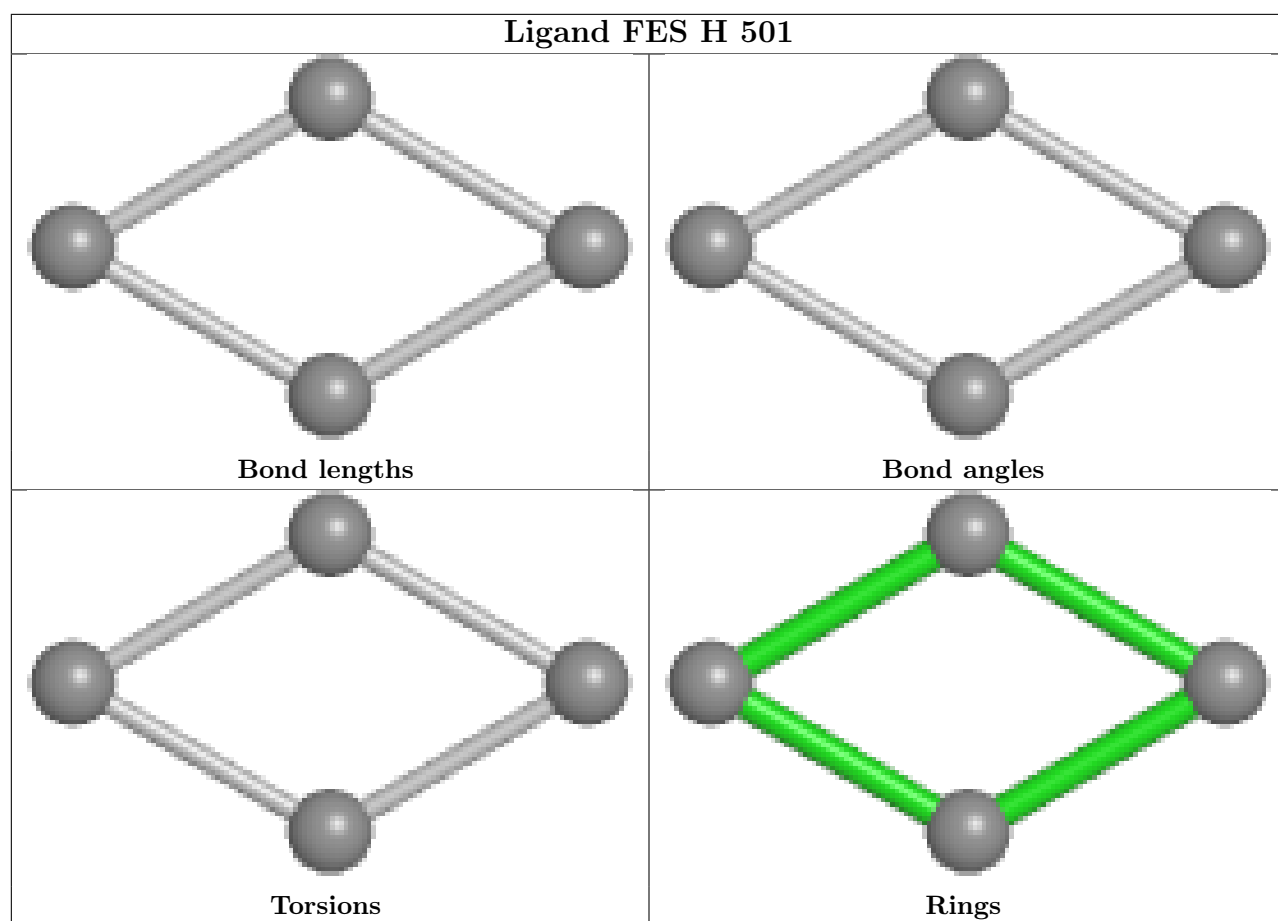
18 monomers are involved in 88 short contacts:

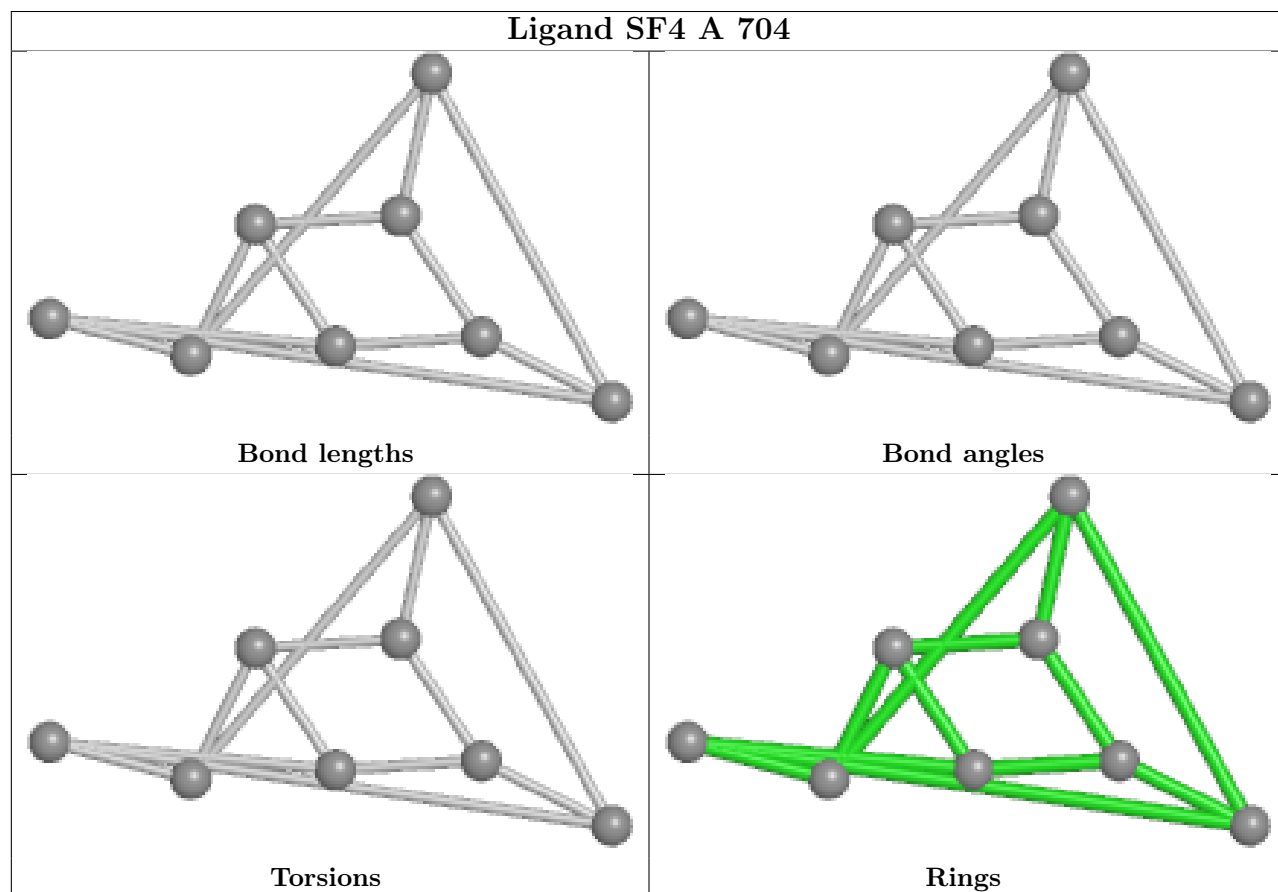
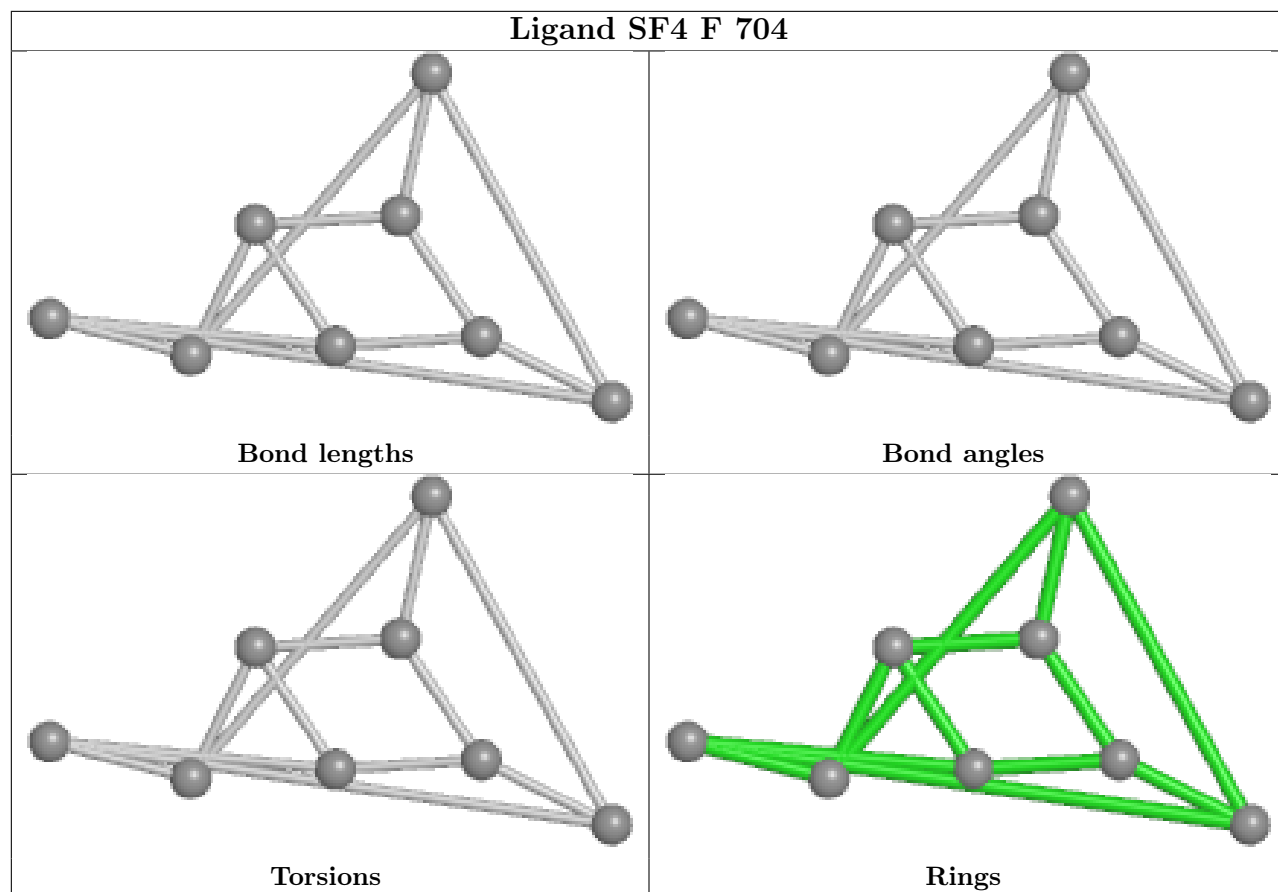
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	201	SF4	4	0
6	H	501	FES	3	0
7	A	703	SF4	13	0
7	F	704	SF4	6	0
7	A	704	SF4	7	0
6	A	701	FES	2	0
7	J	201	SF4	4	0
6	B	602	FES	2	0
7	F	703	SF4	14	0
6	G	602	FES	2	0
9	D	602	FCO	2	0
6	C	501	FES	3	0
7	B	601	SF4	5	0
6	F	701	FES	2	0
7	G	601	SF4	6	0
7	F	702	SF4	5	0
9	I	602	FCO	3	0
7	A	702	SF4	5	0

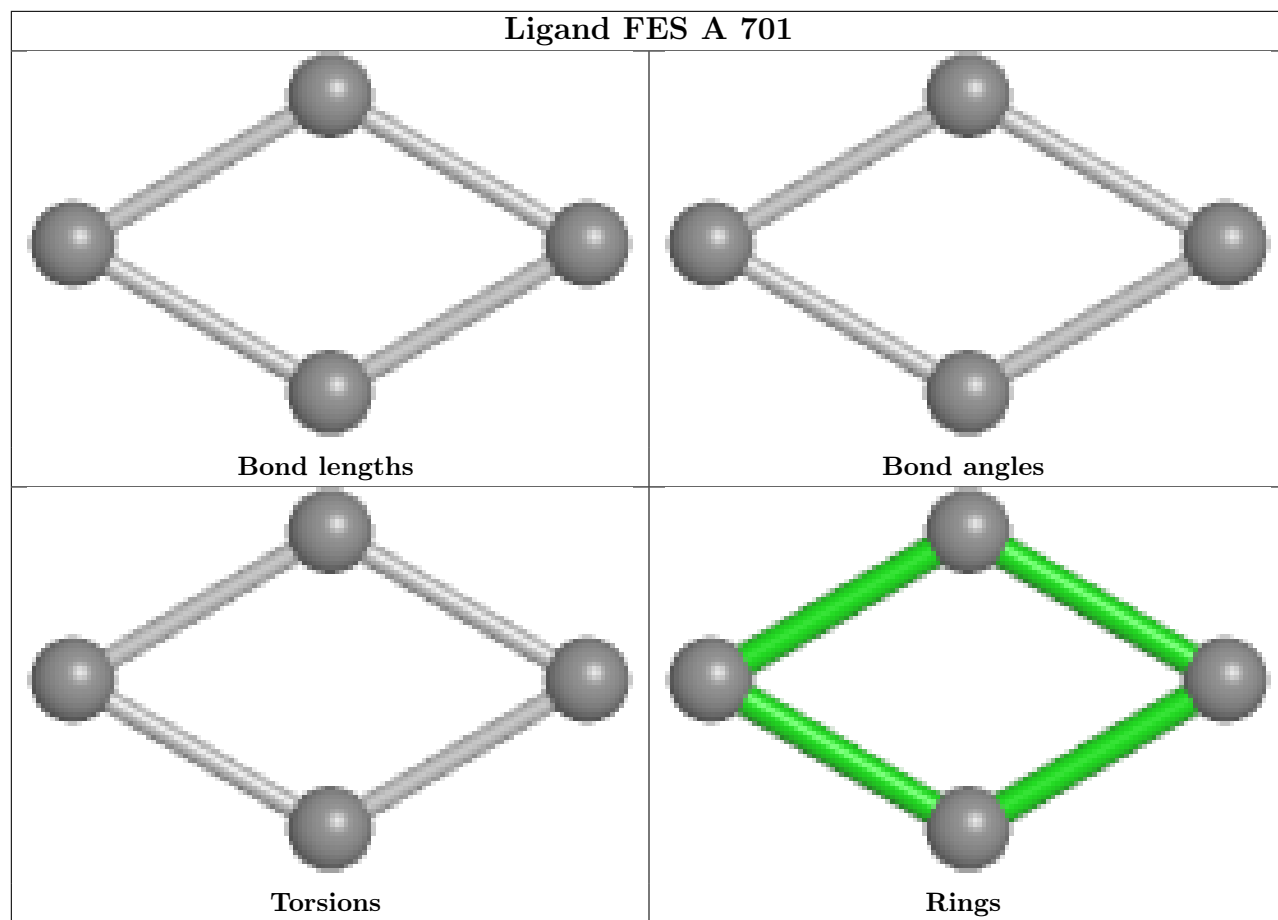
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

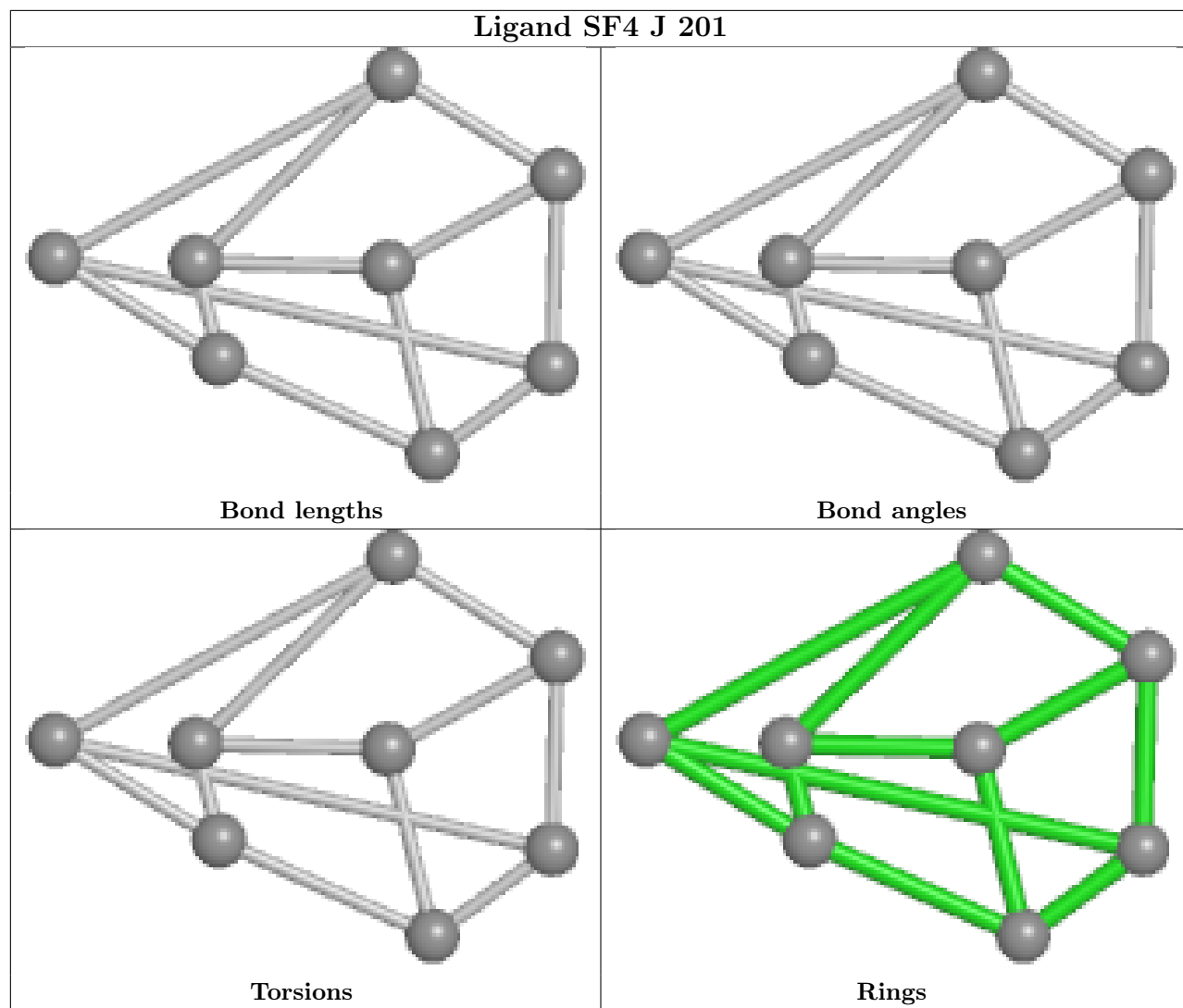
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

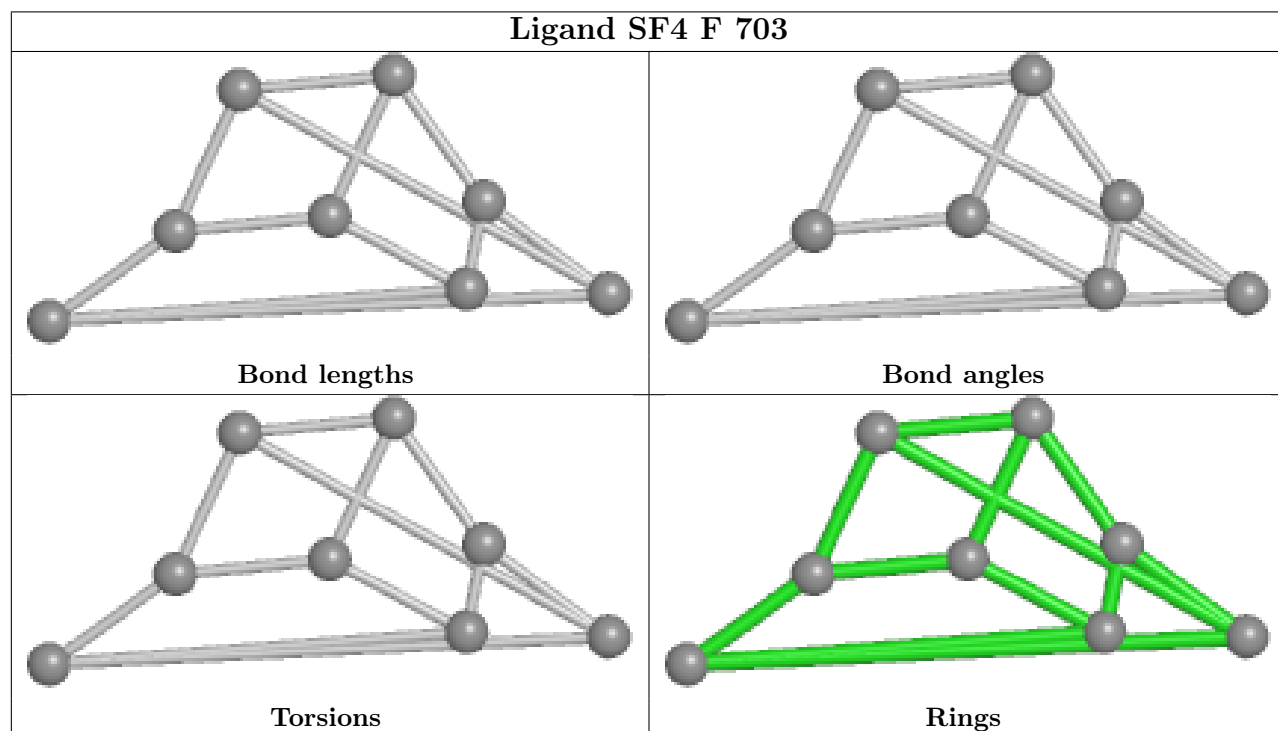
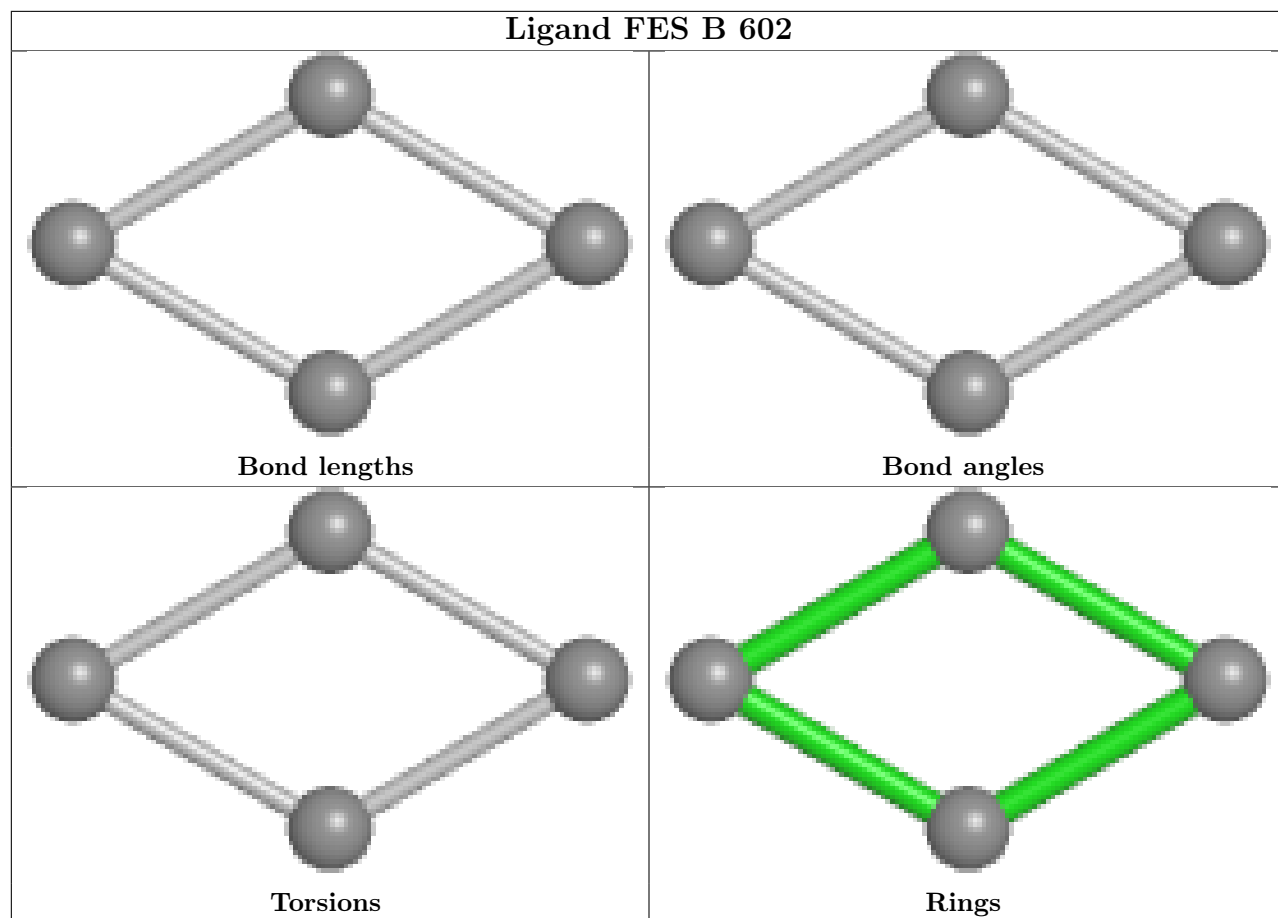


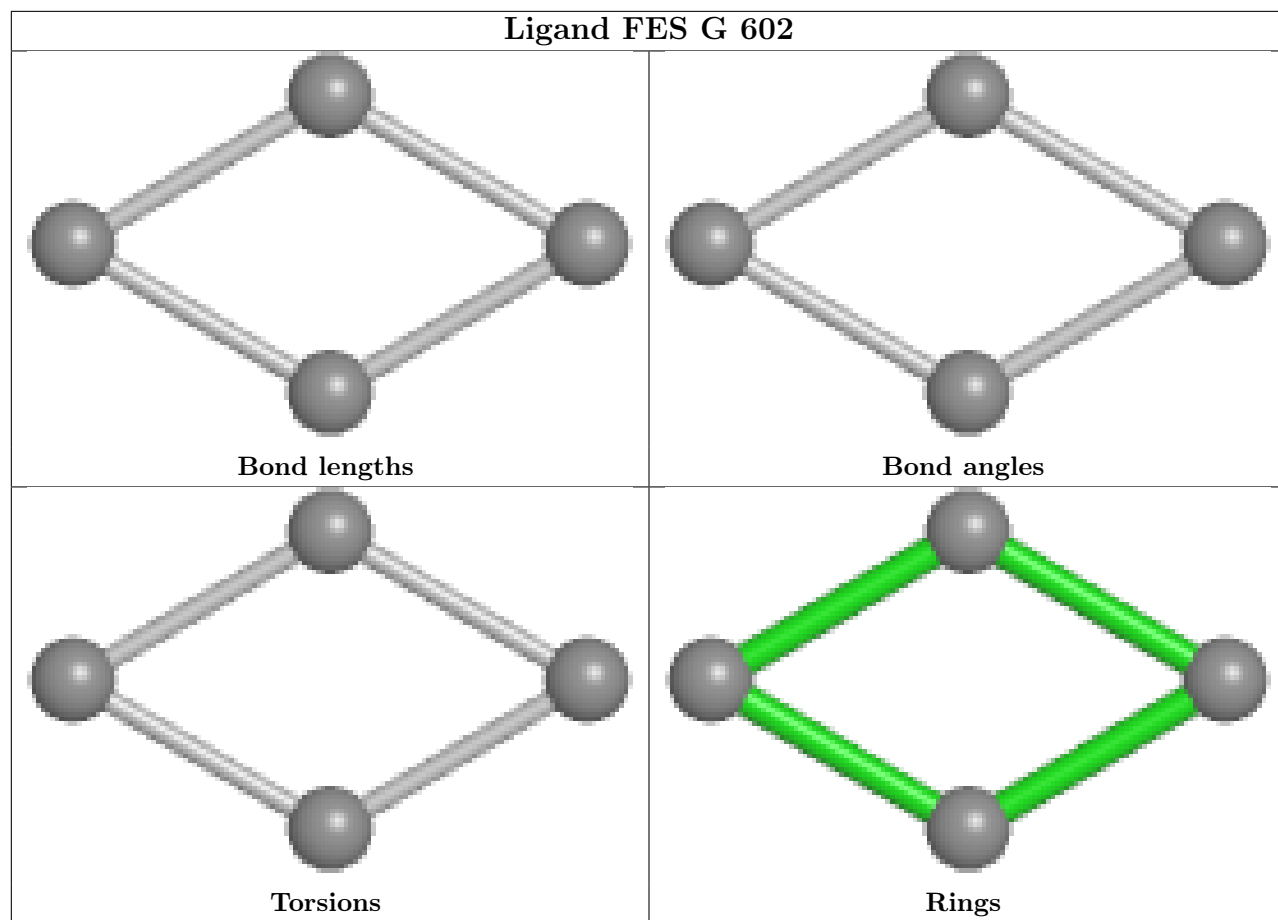


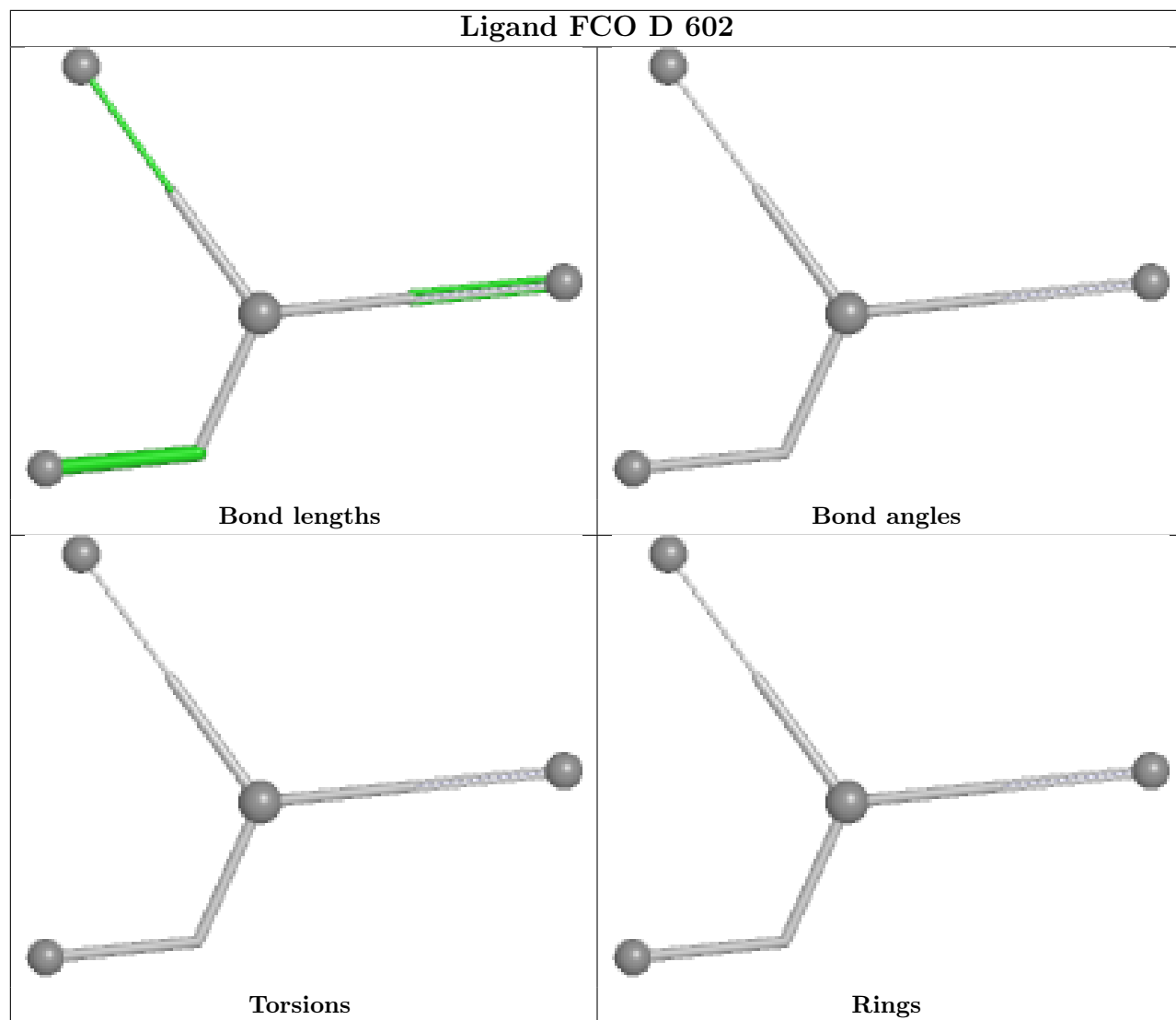


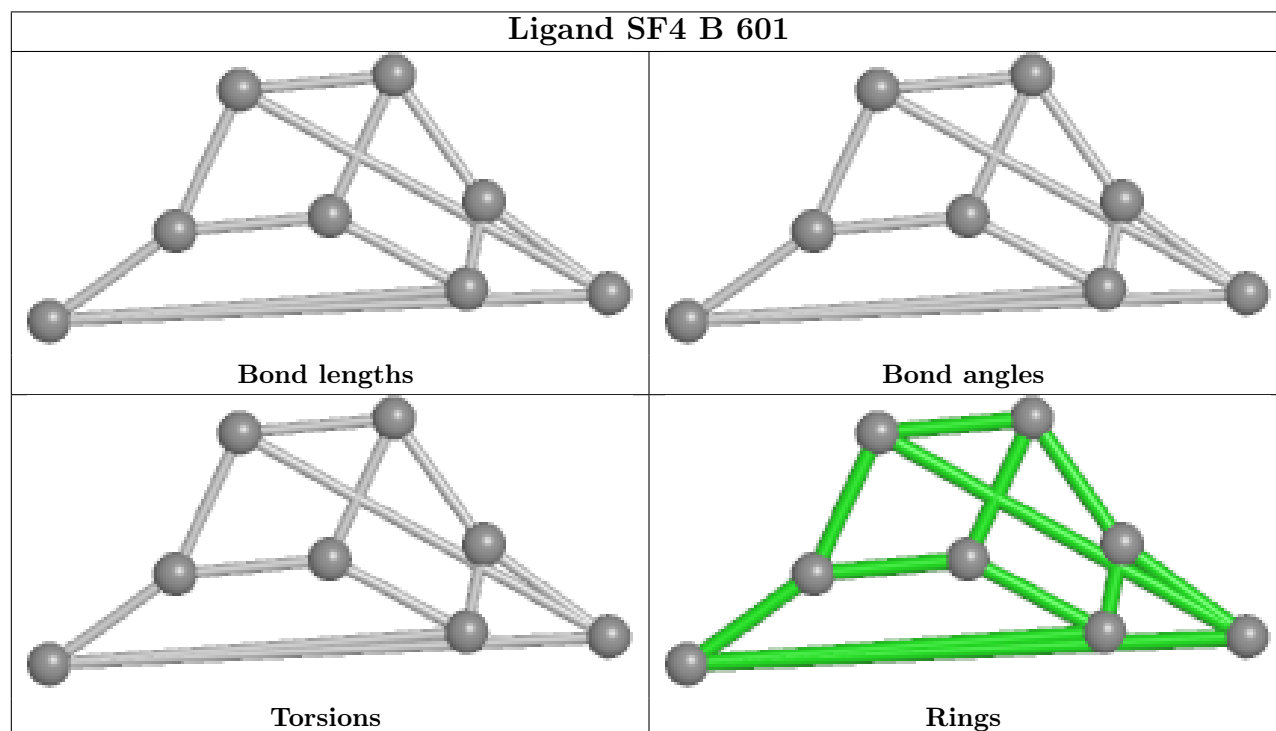
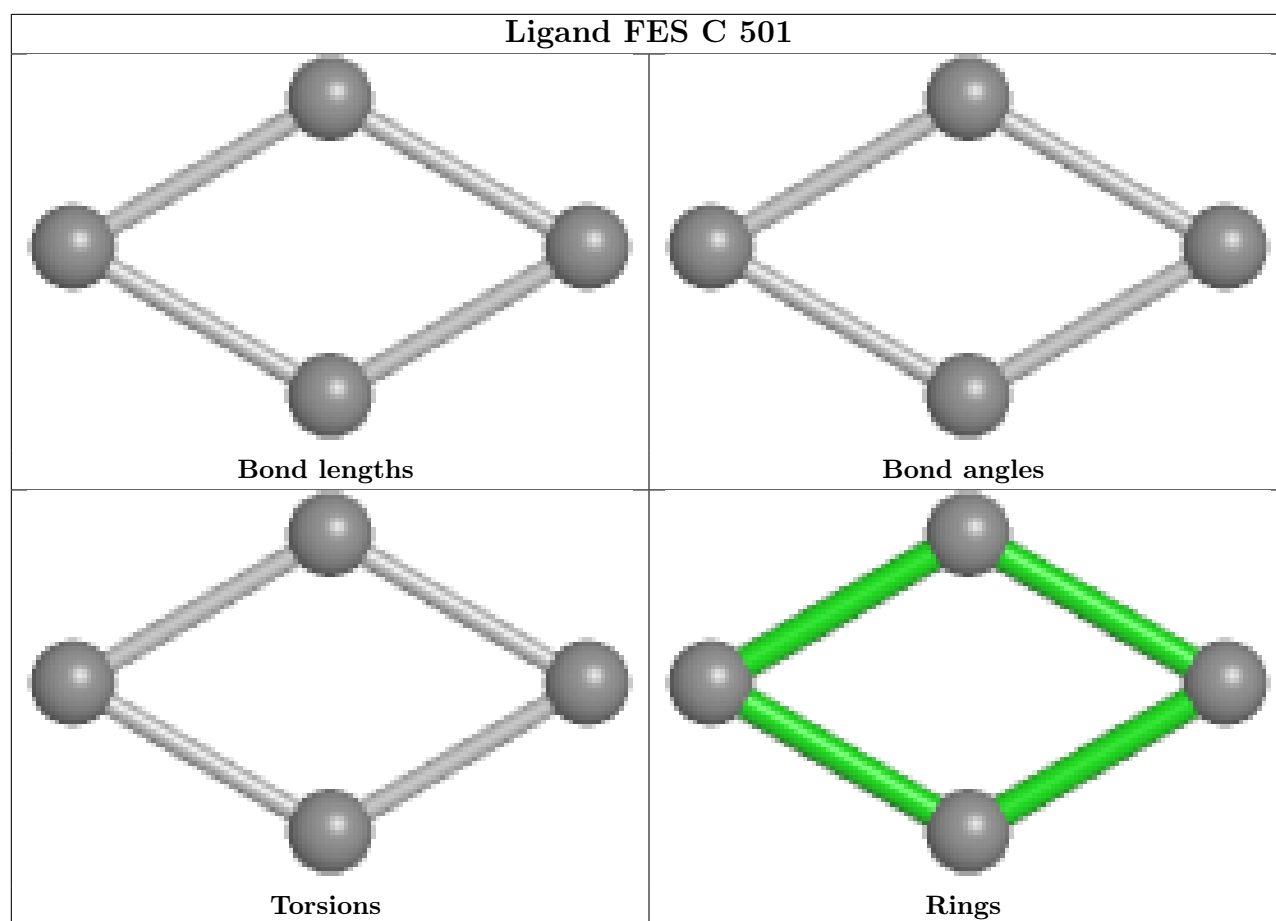


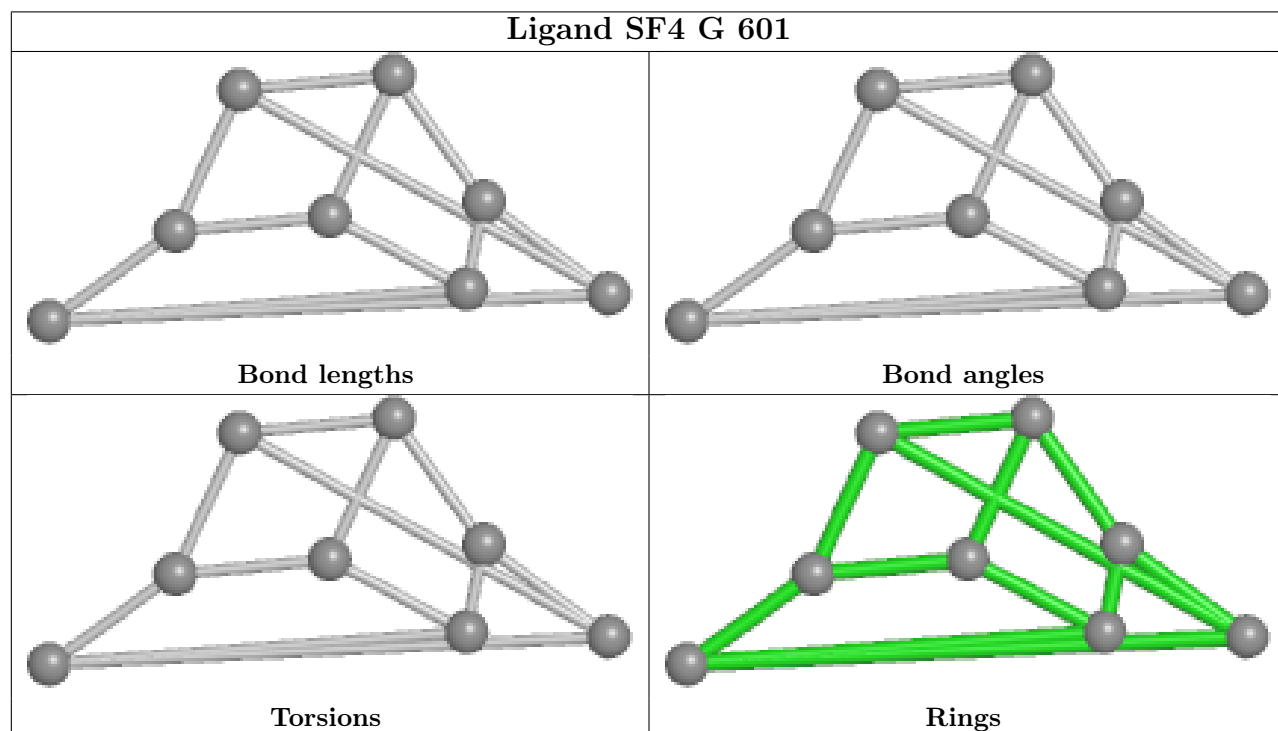
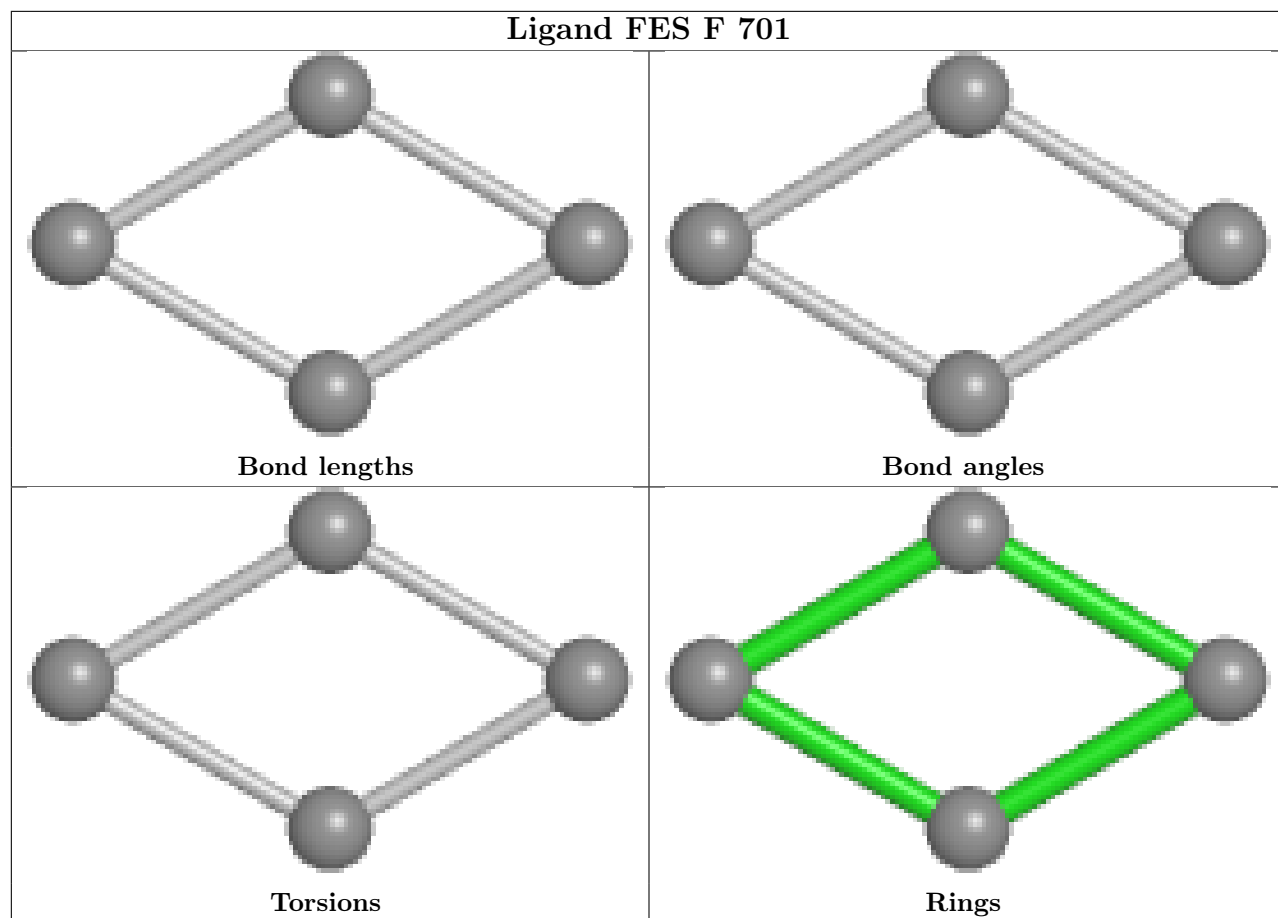


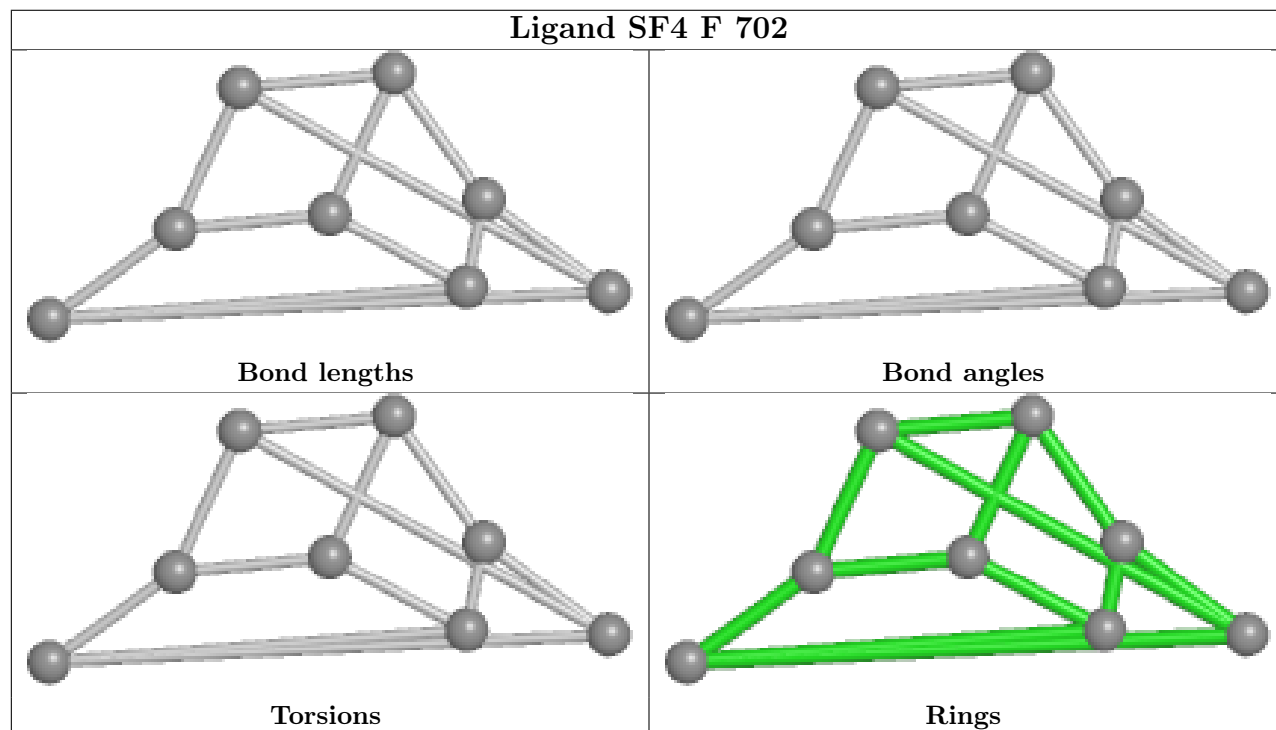
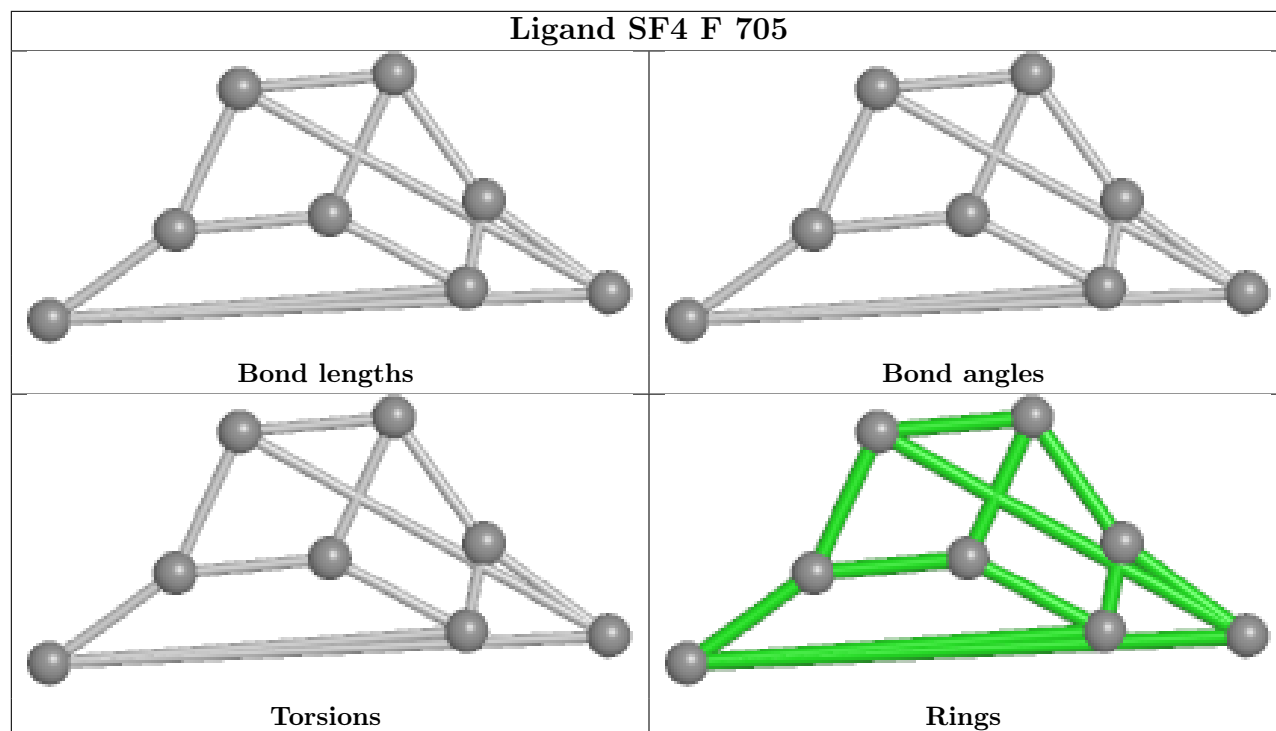


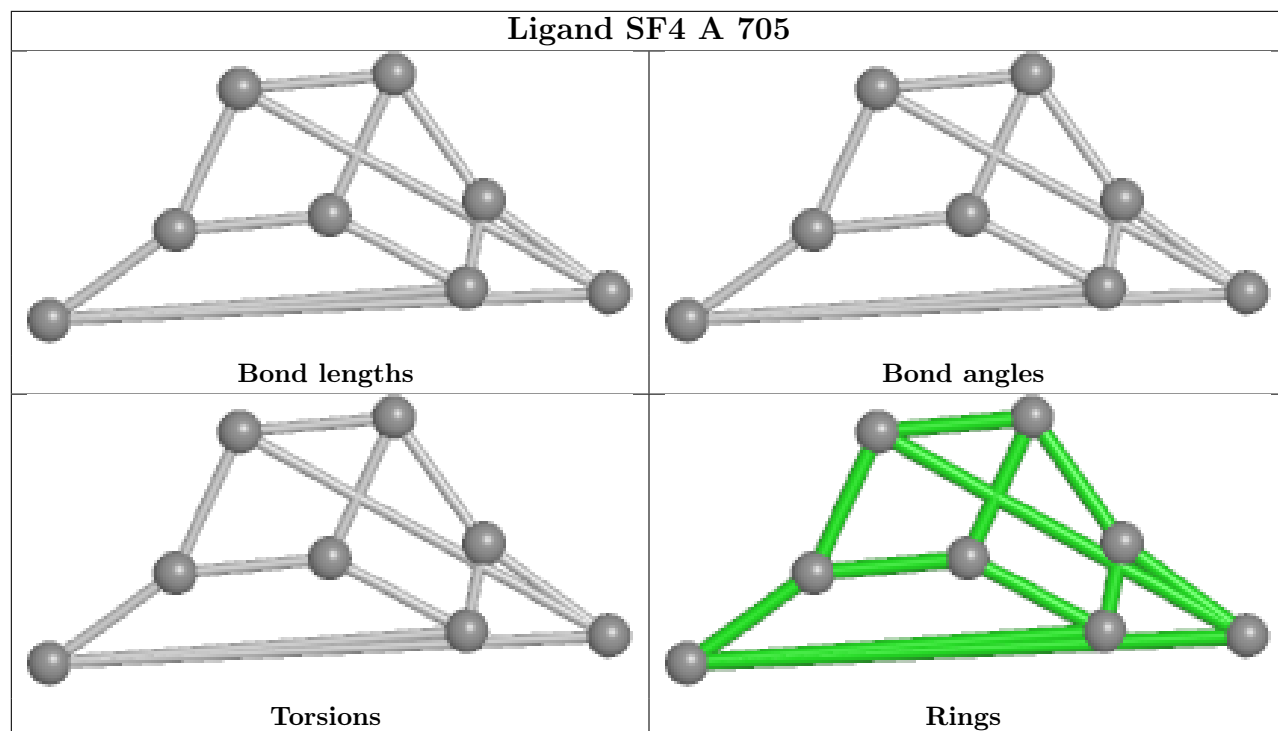


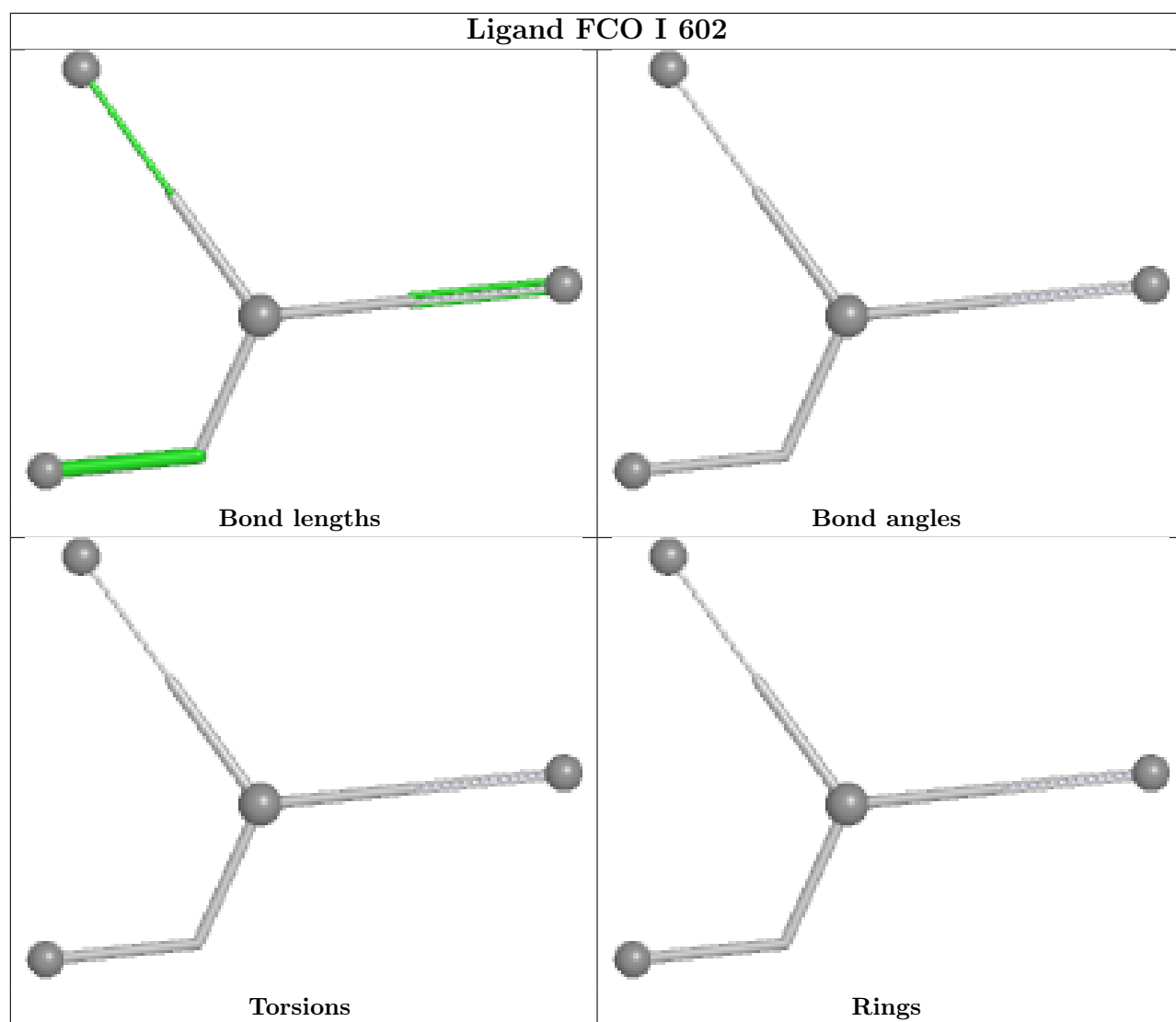


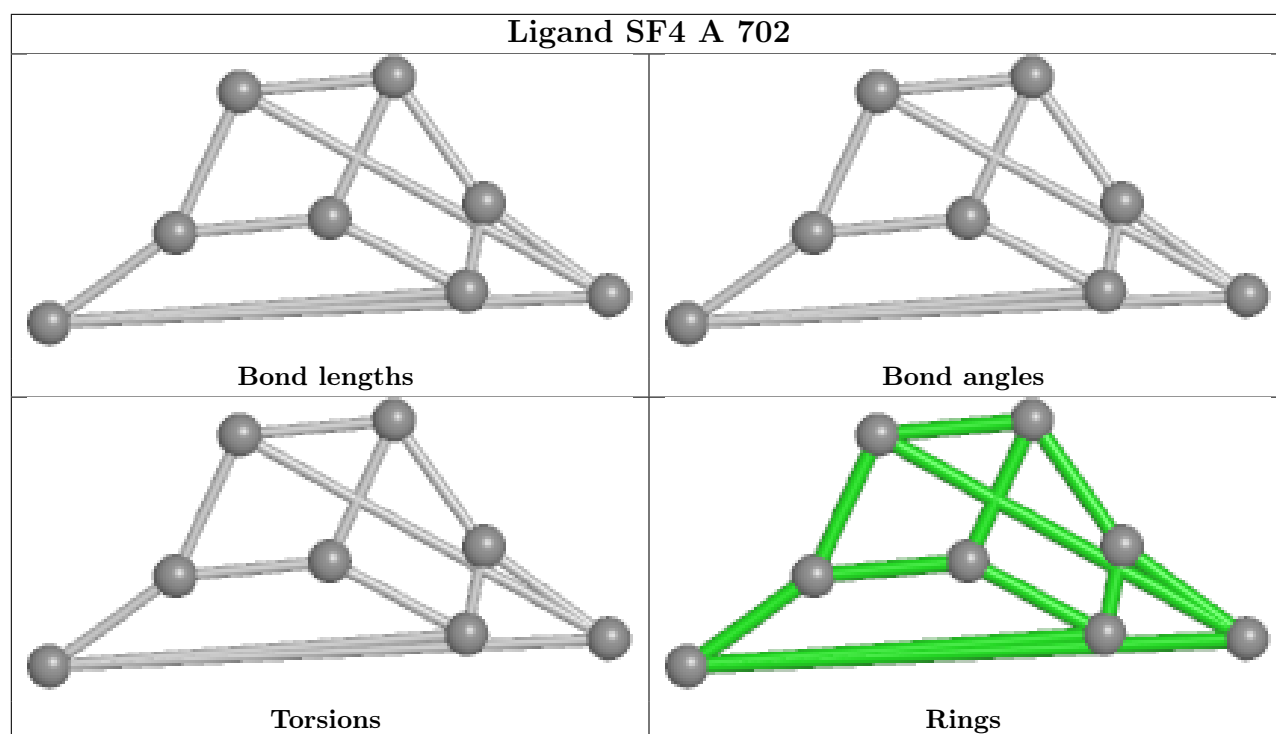












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

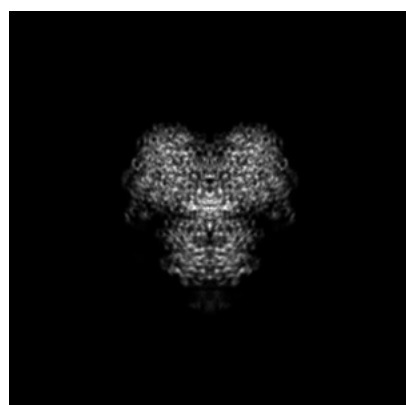
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25633. These allow visual inspection of the internal detail of the map and identification of artifacts.

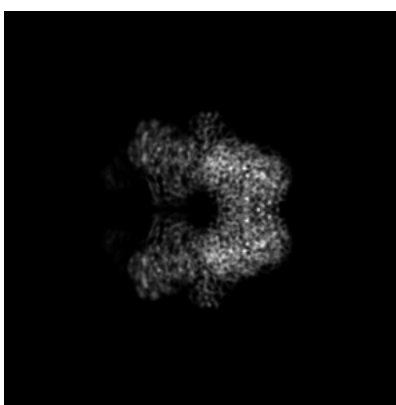
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

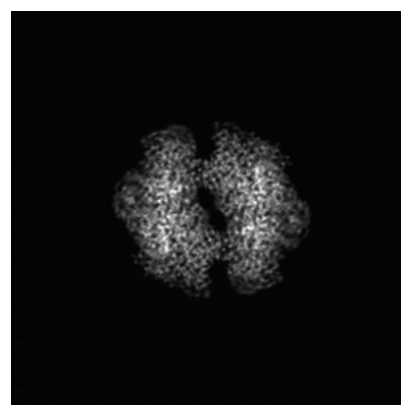
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

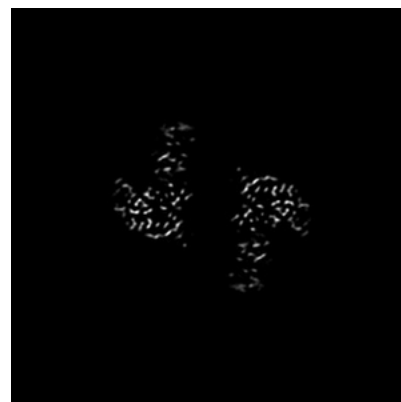
6.2.1 Primary map



X Index: 130



Y Index: 130



Z Index: 130

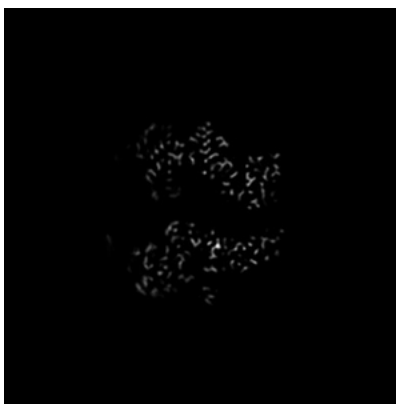
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 99



Y Index: 142

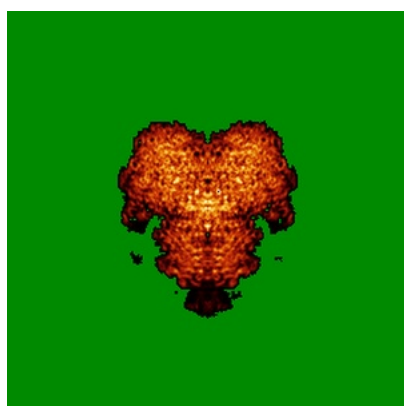


Z Index: 157

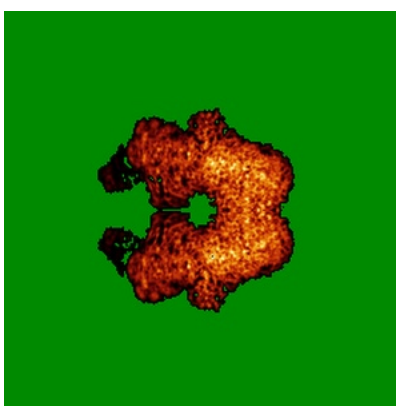
The images above show the largest variance slices of the map in three orthogonal directions.

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

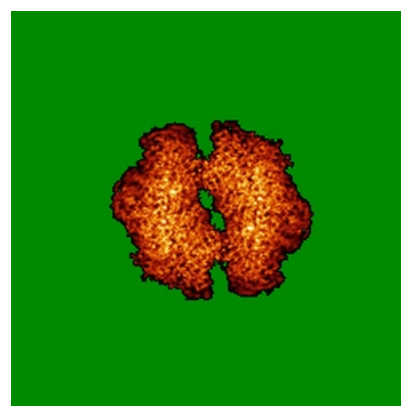
6.4.1 Primary map



X



Y

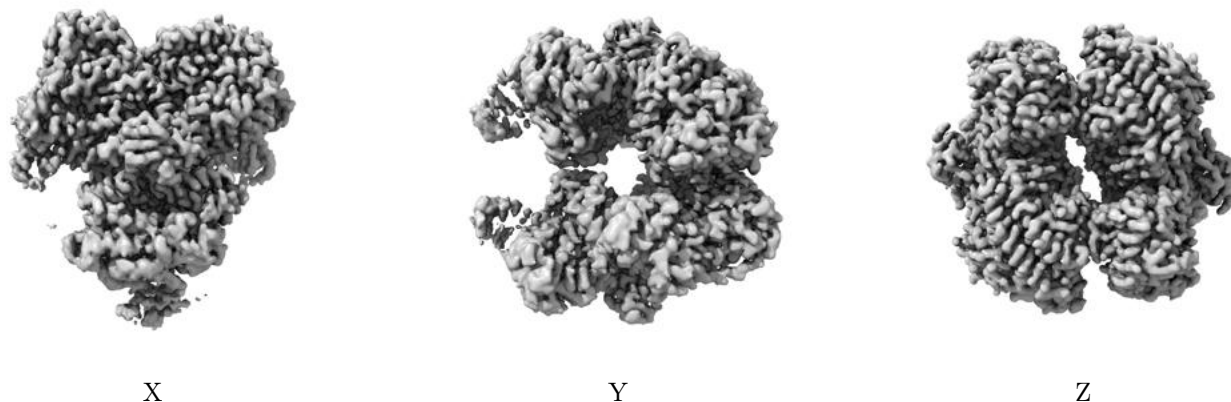


Z

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

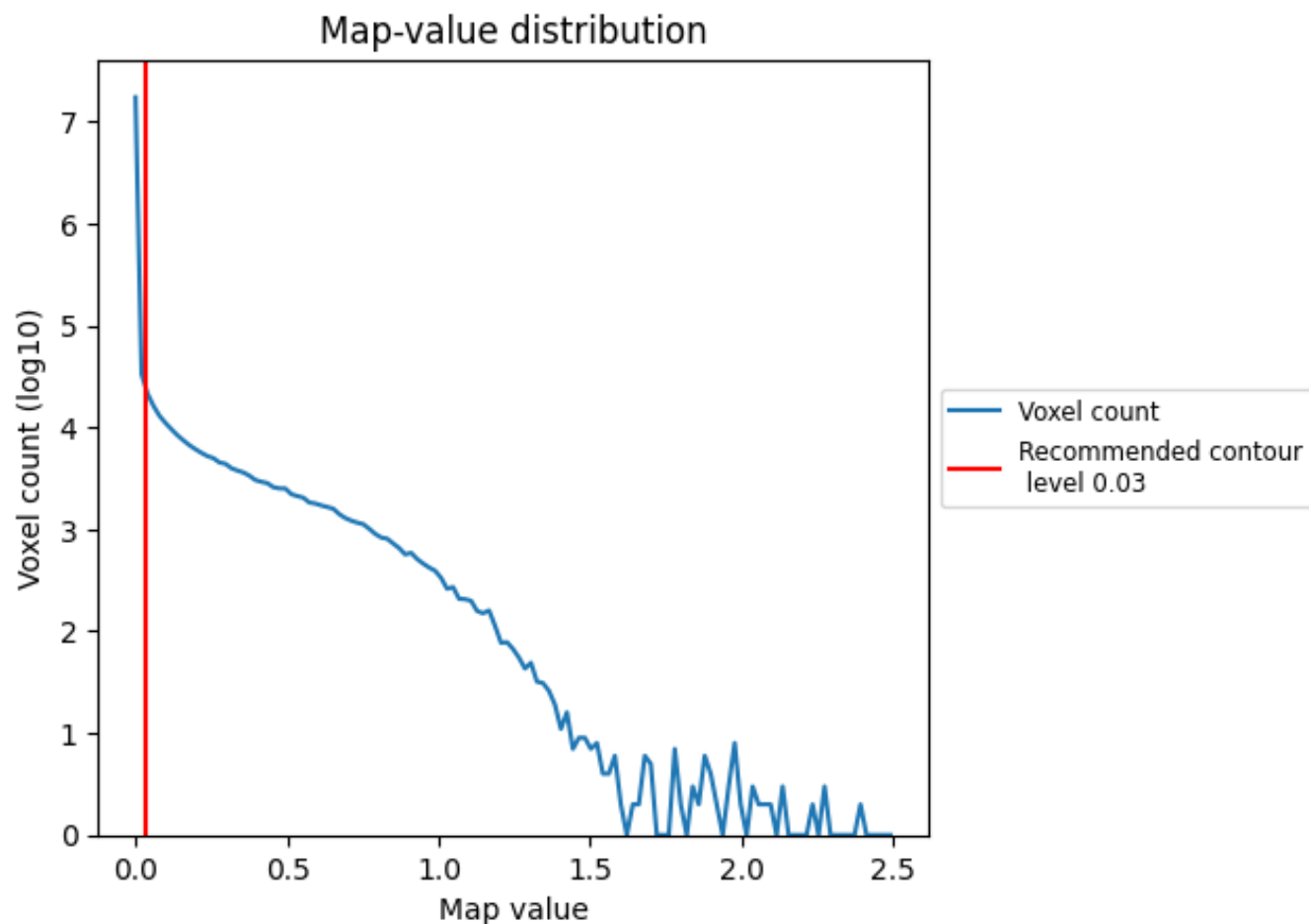
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

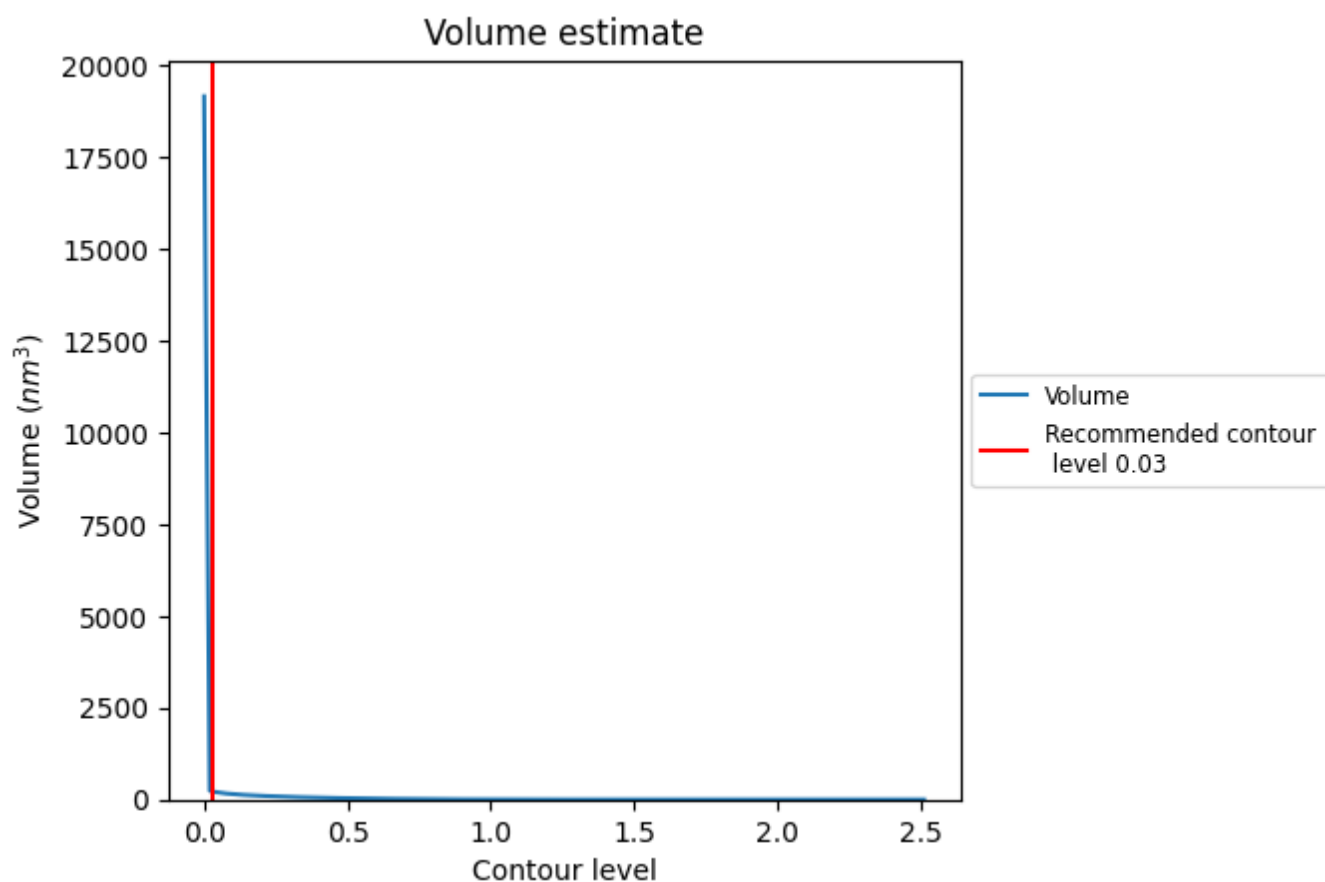
This section contains the results of statistical analysis of the map.

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.

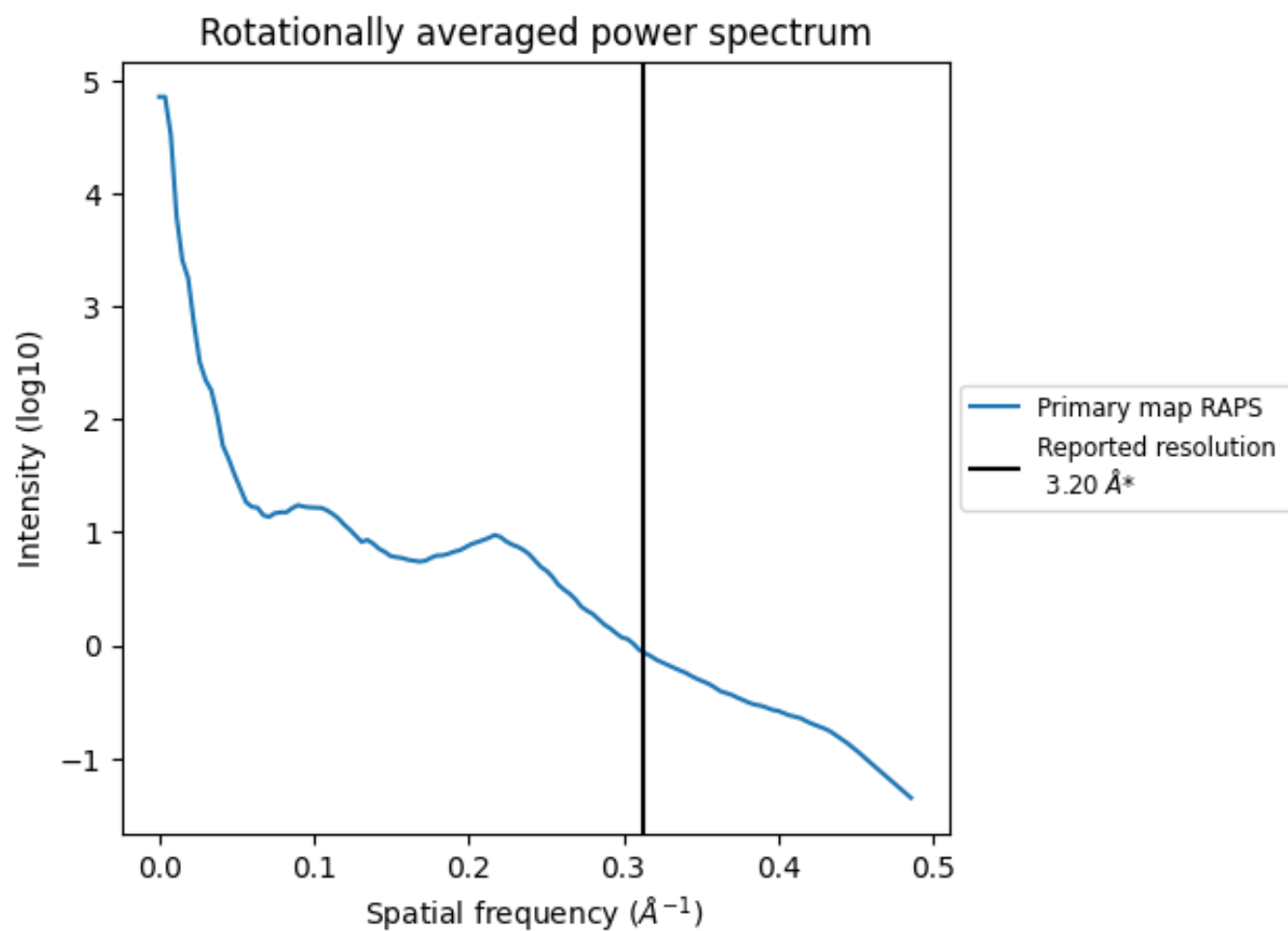
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 198 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 ⓘ

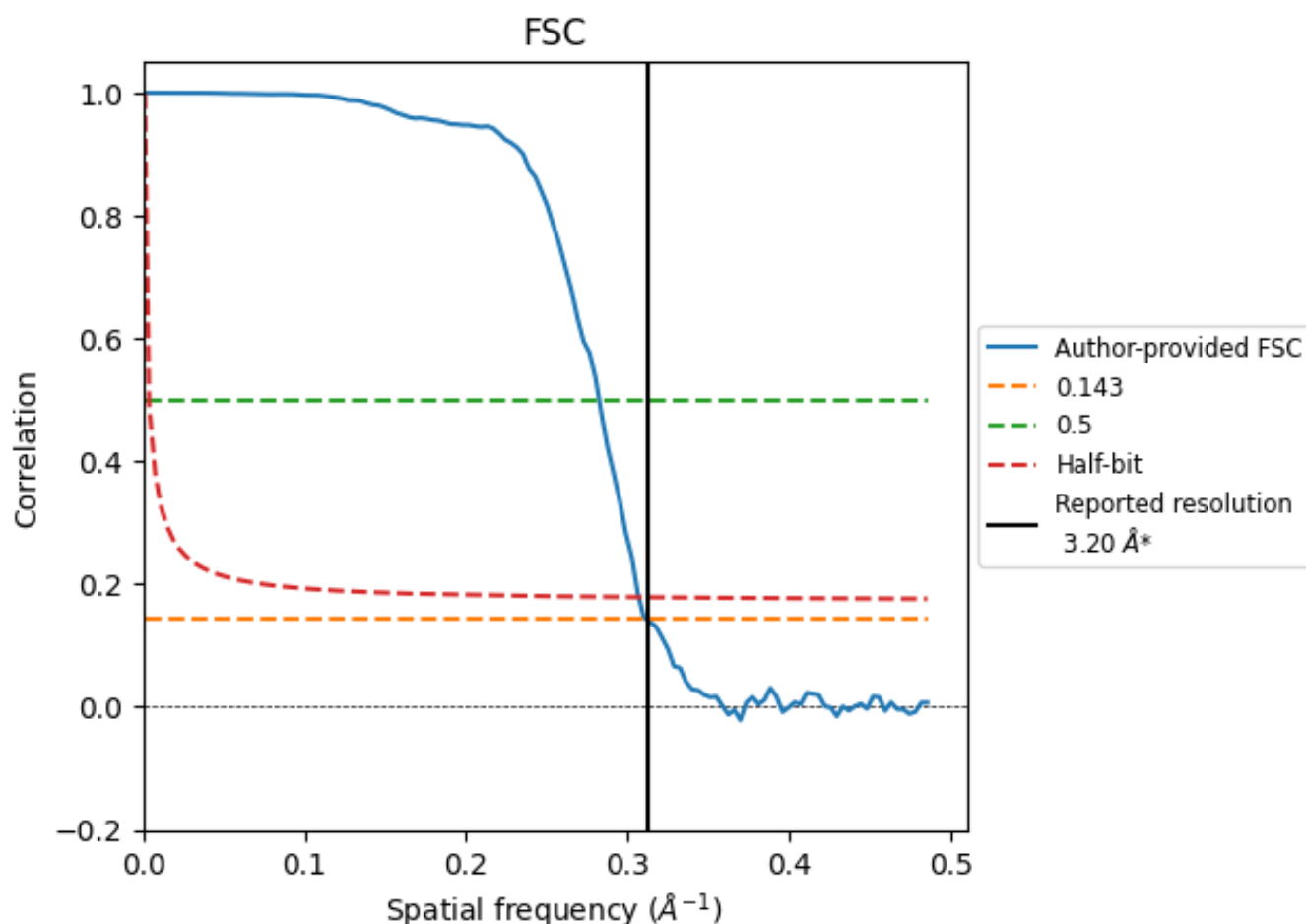


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

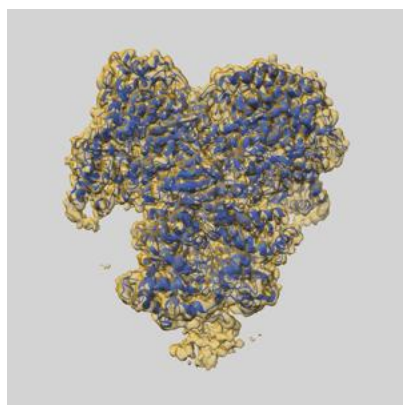
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.54	3.26
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

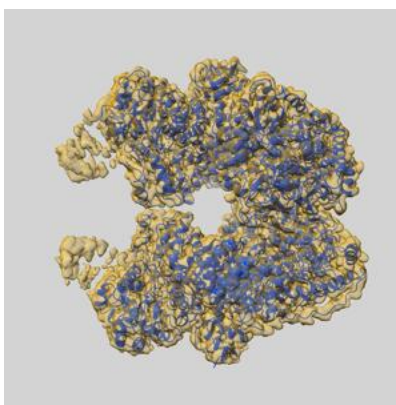
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25633 and PDB model 7T2R. Per-residue inclusion information can be found in section [3](#) on page [8](#).

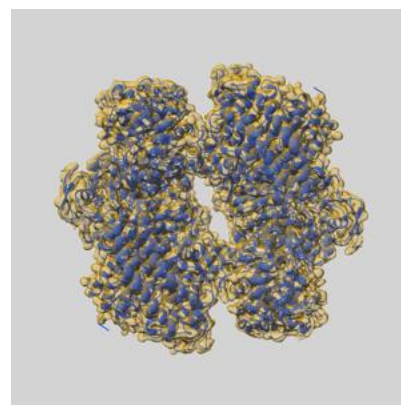
9.1 Map-model overlay [i](#)



X



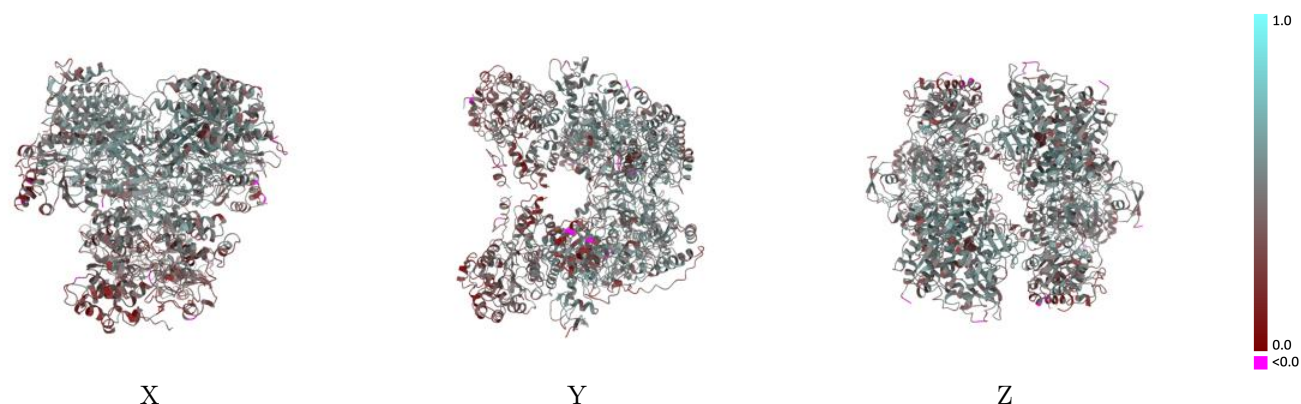
Y



Z

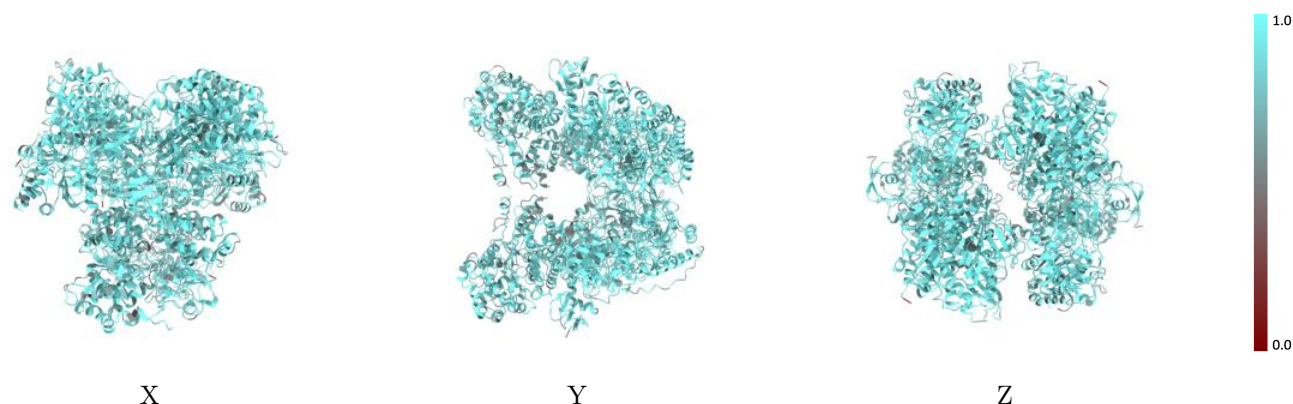
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



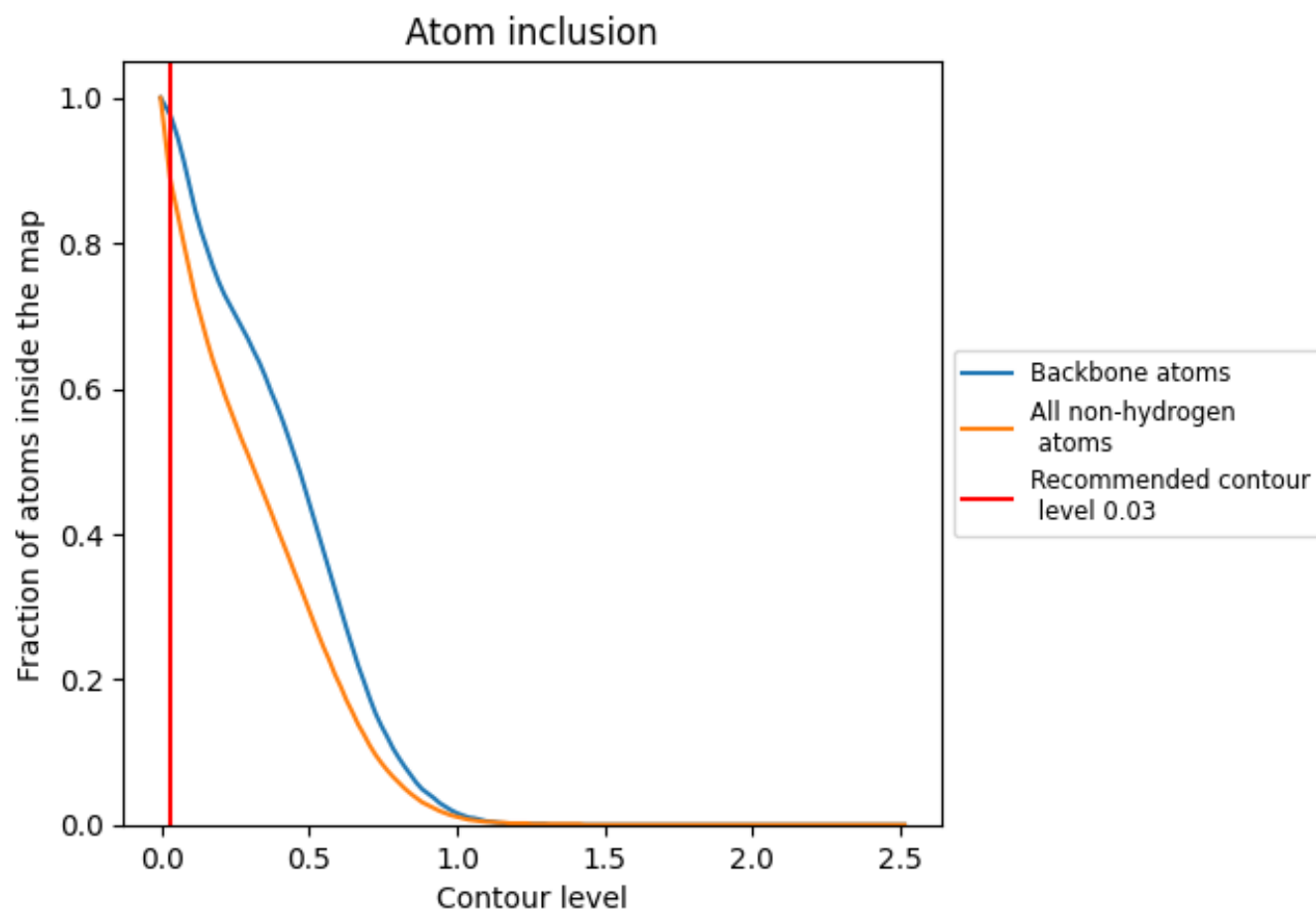
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.4520
A	0.8980	0.4640
B	0.8530	0.3840
C	0.8430	0.3850
D	0.9260	0.5100
E	0.9090	0.4900
F	0.8960	0.4630
G	0.8450	0.3810
H	0.8470	0.3830
I	0.9270	0.5050
J	0.9060	0.4870

1.0

0.0

<0.0