Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2024 – 12:16 pm GMT

PDB ID	:	8CP4
Title	:	[4Fe-4S] cluster containing LarE in complex with AMP
Authors	:	Zecchin, P.; Pecqueur, L.; Golinelli-Pimpaneau, B.
Deposited on	:	2023-03-01
Resolution	:	3.19 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

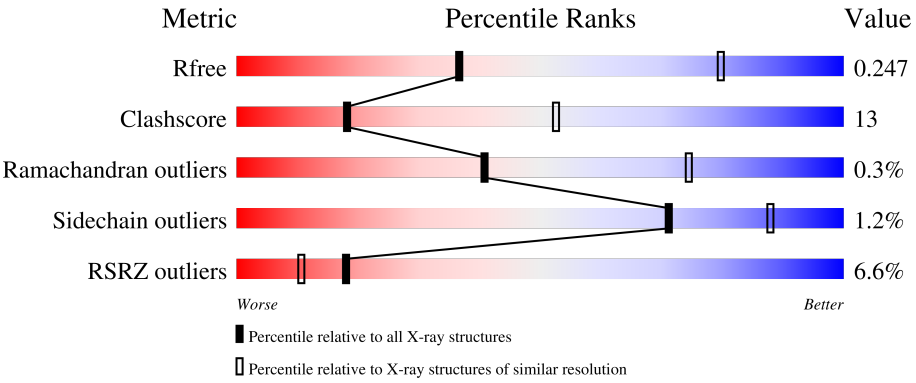
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	271	4% 70% 24% 6%
1	B	271	4% 68% 26% 6%
1	C	271	2% 66% 27% 6%
1	D	271	4% 70% 24%
1	E	271	11% 63% 29% 7%

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Mol	Chain	Length	Quality of chain
1	F	271	7% 58% 34% 7%
1	G	271	11% 61% 31% 7%

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
2	SF4	G	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14535 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NAD_synthase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2060	1315	342	398	5			
1	B	254	Total	C	N	O	S	0	0	0
			2050	1309	339	397	5			
1	C	256	Total	C	N	O	S	0	0	0
			2076	1325	344	401	6			
1	D	261	Total	C	N	O	S	0	0	0
			2111	1349	349	406	7			
1	E	253	Total	C	N	O	S	0	0	0
			2050	1309	340	396	5			
1	F	253	Total	C	N	O	S	0	0	0
			2044	1306	337	396	5			
1	G	253	Total	C	N	O	S	0	0	0
			2050	1309	340	396	5			

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q6LXV7
A	-9	PRO	-	expression tag	UNP Q6LXV7
A	-8	MET	-	expression tag	UNP Q6LXV7
A	-7	LEU	-	expression tag	UNP Q6LXV7
A	-6	GLU	-	expression tag	UNP Q6LXV7
A	-5	VAL	-	expression tag	UNP Q6LXV7
A	-4	LEU	-	expression tag	UNP Q6LXV7
A	-3	PHE	-	expression tag	UNP Q6LXV7
A	-2	GLN	-	expression tag	UNP Q6LXV7
A	-1	GLY	-	expression tag	UNP Q6LXV7
A	0	PRO	-	expression tag	UNP Q6LXV7
A	259	GLY	-	expression tag	UNP Q6LXV7
A	260	SER	-	expression tag	UNP Q6LXV7
B	-10	GLY	-	expression tag	UNP Q6LXV7
B	-9	PRO	-	expression tag	UNP Q6LXV7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q6LXV7
B	-7	LEU	-	expression tag	UNP Q6LXV7
B	-6	GLU	-	expression tag	UNP Q6LXV7
B	-5	VAL	-	expression tag	UNP Q6LXV7
B	-4	LEU	-	expression tag	UNP Q6LXV7
B	-3	PHE	-	expression tag	UNP Q6LXV7
B	-2	GLN	-	expression tag	UNP Q6LXV7
B	-1	GLY	-	expression tag	UNP Q6LXV7
B	0	PRO	-	expression tag	UNP Q6LXV7
B	259	GLY	-	expression tag	UNP Q6LXV7
B	260	SER	-	expression tag	UNP Q6LXV7
C	-10	GLY	-	expression tag	UNP Q6LXV7
C	-9	PRO	-	expression tag	UNP Q6LXV7
C	-8	MET	-	expression tag	UNP Q6LXV7
C	-7	LEU	-	expression tag	UNP Q6LXV7
C	-6	GLU	-	expression tag	UNP Q6LXV7
C	-5	VAL	-	expression tag	UNP Q6LXV7
C	-4	LEU	-	expression tag	UNP Q6LXV7
C	-3	PHE	-	expression tag	UNP Q6LXV7
C	-2	GLN	-	expression tag	UNP Q6LXV7
C	-1	GLY	-	expression tag	UNP Q6LXV7
C	0	PRO	-	expression tag	UNP Q6LXV7
C	259	GLY	-	expression tag	UNP Q6LXV7
C	260	SER	-	expression tag	UNP Q6LXV7
D	-10	GLY	-	expression tag	UNP Q6LXV7
D	-9	PRO	-	expression tag	UNP Q6LXV7
D	-8	MET	-	expression tag	UNP Q6LXV7
D	-7	LEU	-	expression tag	UNP Q6LXV7
D	-6	GLU	-	expression tag	UNP Q6LXV7
D	-5	VAL	-	expression tag	UNP Q6LXV7
D	-4	LEU	-	expression tag	UNP Q6LXV7
D	-3	PHE	-	expression tag	UNP Q6LXV7
D	-2	GLN	-	expression tag	UNP Q6LXV7
D	-1	GLY	-	expression tag	UNP Q6LXV7
D	0	PRO	-	expression tag	UNP Q6LXV7
D	259	GLY	-	expression tag	UNP Q6LXV7
D	260	SER	-	expression tag	UNP Q6LXV7
E	-10	GLY	-	expression tag	UNP Q6LXV7
E	-9	PRO	-	expression tag	UNP Q6LXV7
E	-8	MET	-	expression tag	UNP Q6LXV7
E	-7	LEU	-	expression tag	UNP Q6LXV7
E	-6	GLU	-	expression tag	UNP Q6LXV7

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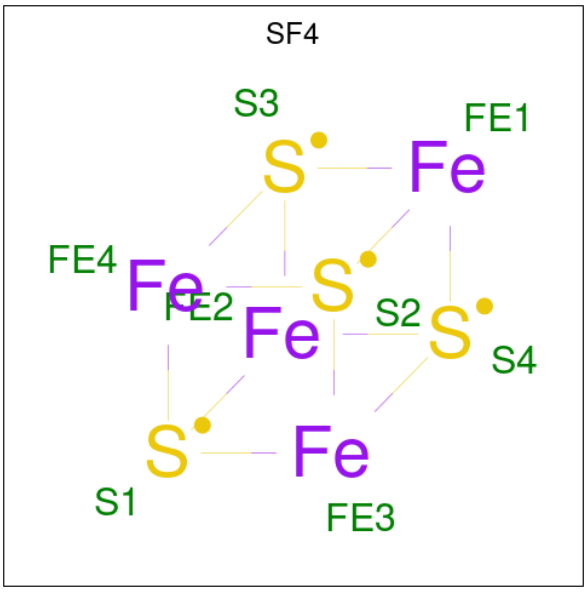
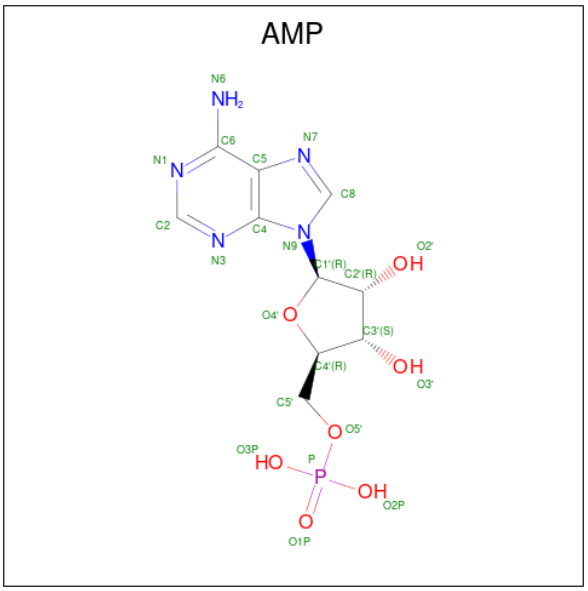
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	expression tag	UNP Q6LXV7
E	-4	LEU	-	expression tag	UNP Q6LXV7
E	-3	PHE	-	expression tag	UNP Q6LXV7
E	-2	GLN	-	expression tag	UNP Q6LXV7
E	-1	GLY	-	expression tag	UNP Q6LXV7
E	0	PRO	-	expression tag	UNP Q6LXV7
E	259	GLY	-	expression tag	UNP Q6LXV7
E	260	SER	-	expression tag	UNP Q6LXV7
F	-10	GLY	-	expression tag	UNP Q6LXV7
F	-9	PRO	-	expression tag	UNP Q6LXV7
F	-8	MET	-	expression tag	UNP Q6LXV7
F	-7	LEU	-	expression tag	UNP Q6LXV7
F	-6	GLU	-	expression tag	UNP Q6LXV7
F	-5	VAL	-	expression tag	UNP Q6LXV7
F	-4	LEU	-	expression tag	UNP Q6LXV7
F	-3	PHE	-	expression tag	UNP Q6LXV7
F	-2	GLN	-	expression tag	UNP Q6LXV7
F	-1	GLY	-	expression tag	UNP Q6LXV7
F	0	PRO	-	expression tag	UNP Q6LXV7
F	259	GLY	-	expression tag	UNP Q6LXV7
F	260	SER	-	expression tag	UNP Q6LXV7
G	-10	GLY	-	expression tag	UNP Q6LXV7
G	-9	PRO	-	expression tag	UNP Q6LXV7
G	-8	MET	-	expression tag	UNP Q6LXV7
G	-7	LEU	-	expression tag	UNP Q6LXV7
G	-6	GLU	-	expression tag	UNP Q6LXV7
G	-5	VAL	-	expression tag	UNP Q6LXV7
G	-4	LEU	-	expression tag	UNP Q6LXV7
G	-3	PHE	-	expression tag	UNP Q6LXV7
G	-2	GLN	-	expression tag	UNP Q6LXV7
G	-1	GLY	-	expression tag	UNP Q6LXV7
G	0	PRO	-	expression tag	UNP Q6LXV7
G	259	GLY	-	expression tag	UNP Q6LXV7
G	260	SER	-	expression tag	UNP Q6LXV7

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0
2	G	1	Total Fe S 8 4 4	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	3	Total	Cl	0	0
			3	3		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	O	0	0
			2	2		

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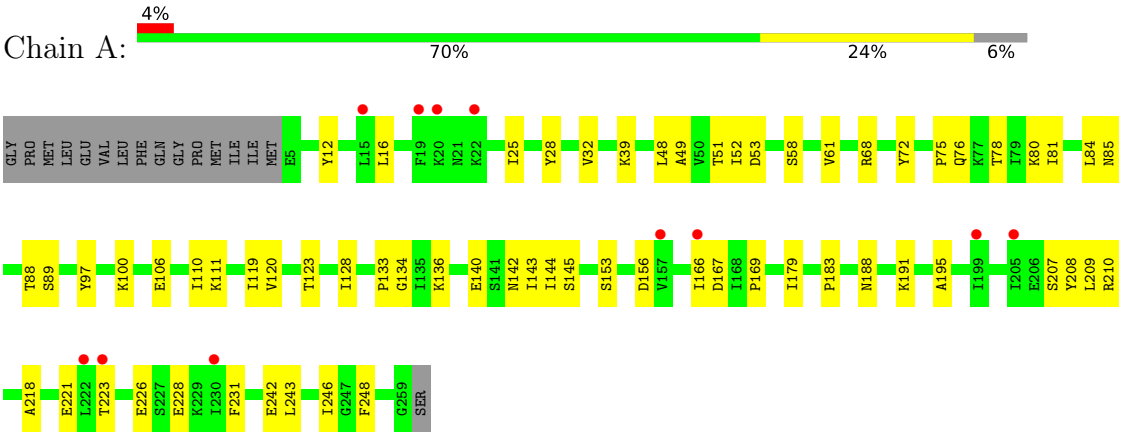
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

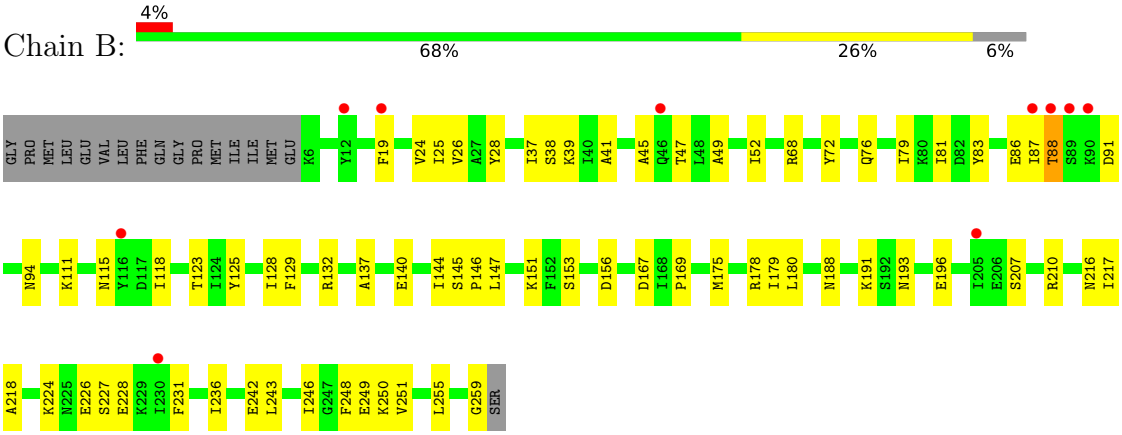
• Molecule 1: NAD_synthase domain-containing protein

Chain A:



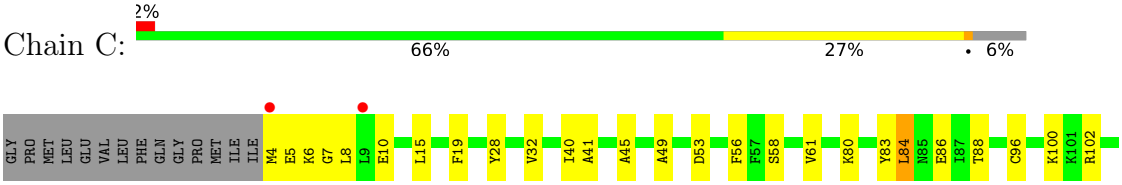
• Molecule 1: NAD_synthase domain-containing protein

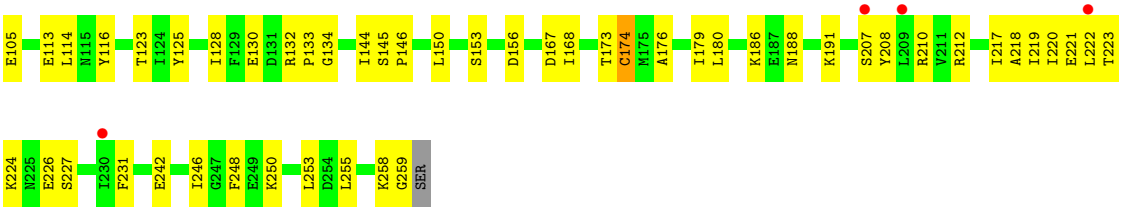
Chain B:



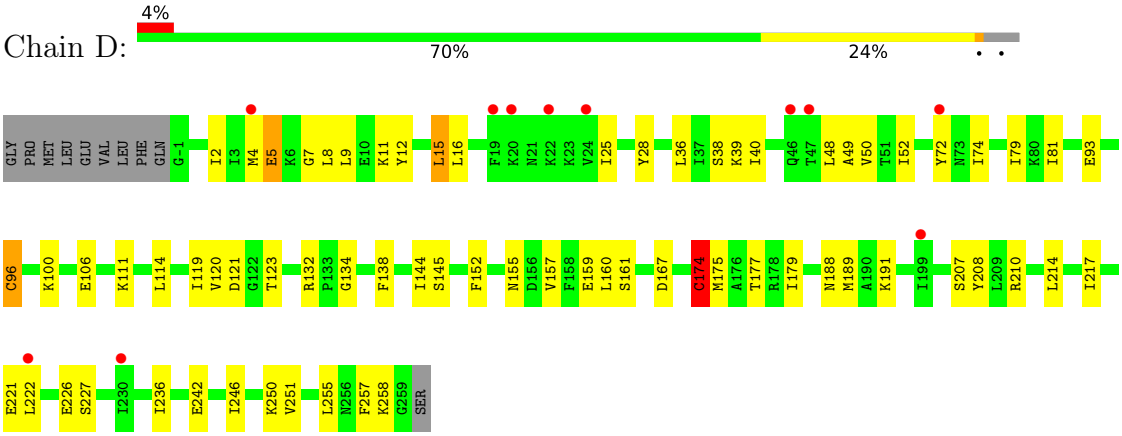
• Molecule 1: NAD_synthase domain-containing protein

Chain C:

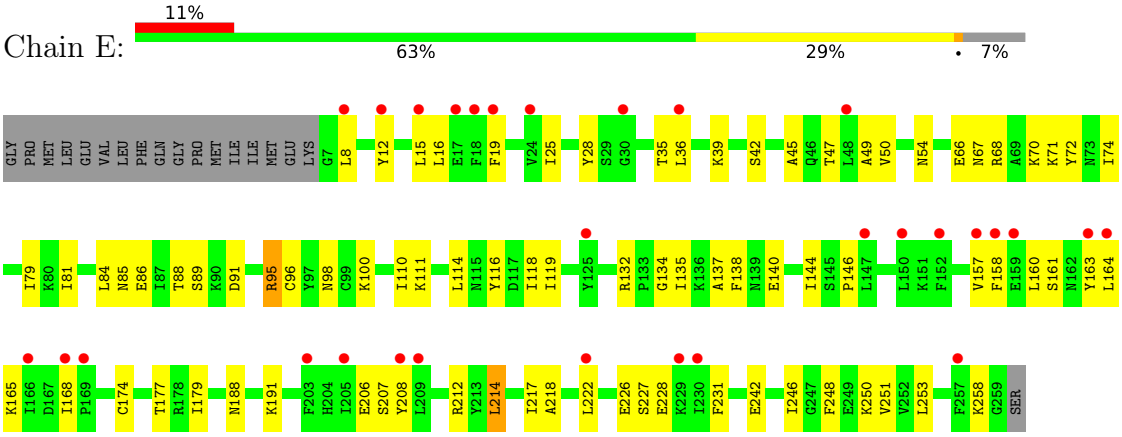




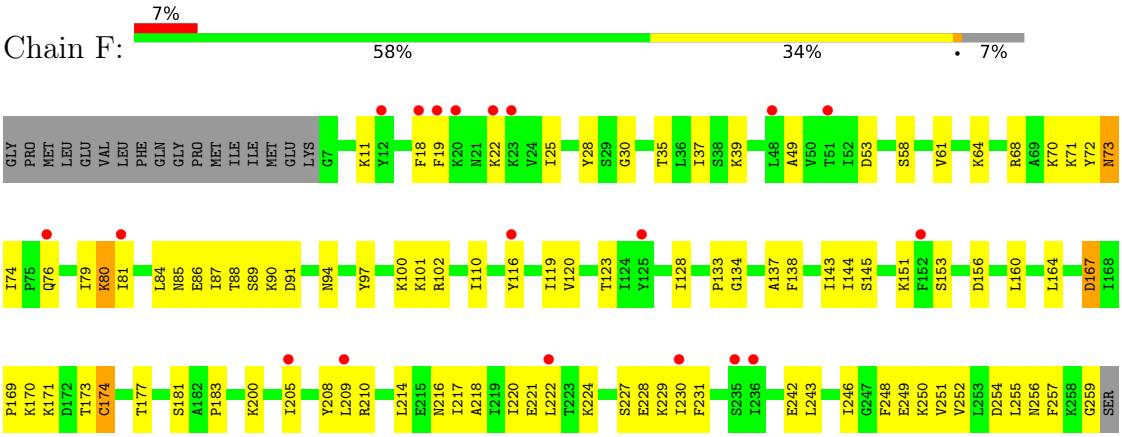
• Molecule 1: NAD_synthase domain-containing protein



• Molecule 1: NAD_synthase domain-containing protein

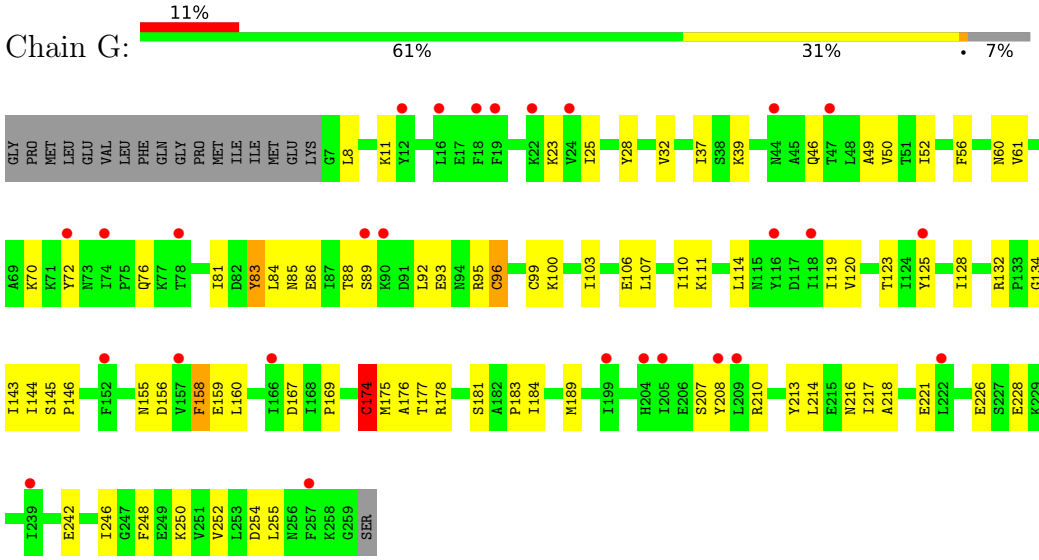


• Molecule 1: NAD_synthase domain-containing protein



• Molecule 1: NAD_synthase domain-containing protein

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	186.17Å 212.69Å 196.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 3.19 49.19 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.87-3.19) 90.1 (49.19-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.47 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.216 , 0.253 0.216 , 0.247	Depositor DCC
R_{free} test set	3230 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	111.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 107.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14535	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, CL, 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	0.57	0/2088	0.76	0/2805
1	B	0.65	0/2078	0.83	1/2792 (0.0%)
1	C	0.65	0/2104	0.84	2/2824 (0.1%)
1	D	0.66	2/2140 (0.1%)	0.85	1/2873 (0.0%)
1	E	0.58	1/2078 (0.0%)	0.79	3/2791 (0.1%)
1	F	0.55	0/2072	0.73	0/2784
1	G	0.56	2/2078 (0.1%)	0.76	0/2791
All	All	0.61	5/14638 (0.0%)	0.80	7/19660 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	174	CYS	CB-SG	-7.60	1.69	1.82
1	E	174	CYS	CB-SG	-7.02	1.70	1.82
1	G	99	CYS	CB-SG	5.92	1.92	1.82
1	D	174	CYS	CB-SG	-5.34	1.73	1.81
1	D	96	CYS	CB-SG	-5.04	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	MET	CA-CB-CG	6.16	123.78	113.30
1	E	164	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	15	LEU	CA-CB-CG	5.45	127.82	115.30
1	E	214	LEU	CA-CB-CG	-5.38	102.94	115.30
1	B	180	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	84	LEU	CA-CB-CG	-5.14	103.47	115.30
1	E	15	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	88	THR	Peptide
1	E	95	ARG	Sidechain
1	G	174	CYS	Peptide

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	2060	0	2103	45	0
1	B	2050	0	2088	54	0
1	C	2076	0	2127	56	0
1	D	2111	0	2171	47	0
1	E	2050	0	2099	50	0
1	F	2044	0	2088	78	0
1	G	2050	0	2099	74	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
2	E	8	0	0	0	0
2	F	8	0	0	1	0
2	G	8	0	0	2	0
3	A	23	0	12	5	0
4	A	2	0	0	1	0
4	B	3	0	0	2	0
4	C	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	14535	0	14787	392	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 13.

All (392) 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:A:81:ILE:HD11	1:A:106:GLU:HG3	1.51	0.91
1:D:111:LYS:HD3	1:D:119:ILE:HG13	1.55	0.89
1:G:95:ARG:NH1	2:G:301:SF4:S2	2.46	0.89
1:A:111:LYS:HD3	1:A:119:ILE:HG13	1.65	0.78
1:G:89:SER:HB2	1:G:183:PRO:HB2	1.64	0.78
1:G:100:LYS:HB3	1:G:138:PHE:CE1	2.20	0.77
1:B:24:VAL:HB	1:B:47:THR:HG22	1.67	0.77
1:C:84:LEU:HD22	1:C:186:LYS:HG3	1.65	0.76
1:G:123:THR:HG22	1:G:145:SER:HB3	1.67	0.75
1:A:53:ASP:HB3	1:A:80:LYS:HA	1.68	0.74
1:G:83:TYR:CZ	1:G:88:THR:HG21	2.21	0.74
1:G:100:LYS:HD2	1:G:134:GLY:HA3	1.69	0.73
1:C:191:LYS:HG2	1:C:246:ILE:HG22	1.71	0.73
1:F:174:CYS:SG	1:F:177:THR:HG23	2.30	0.72
1:A:133:PRO:HD2	4:A:303:CL:CL	2.26	0.72
1:F:68:ARG:HH12	1:F:169:PRO:HB3	1.55	0.72
1:C:222:LEU:HD22	1:C:253:LEU:HD11	1.72	0.71
1:F:68:ARG:NH1	1:F:169:PRO:HB3	2.04	0.71
1:D:81:ILE:HD11	1:D:106:GLU:HG3	1.70	0.71
1:G:111:LYS:HD3	1:G:119:ILE:HG13	1.71	0.70
1:D:4:MET:O	1:D:5:GLU:HG3	1.91	0.70
1:E:36:LEU:HD13	1:E:157:VAL:HG13	1.74	0.68
1:G:25:ILE:HD11	1:G:114:LEU:HD12	1.76	0.68
1:C:100:LYS:HG3	1:C:134:GLY:HA3	1.77	0.67
1:C:132:ARG:HB3	4:C:303:CL:CL	2.32	0.67
1:E:217:ILE:HG23	1:E:250:LYS:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:CYS:HB3	1:G:177:THR:H	1.60	0.66
1:E:191:LYS:HG2	1:E:246:ILE:HG22	1.78	0.66
1:E:84:LEU:O	1:E:86:GLU:N	2.28	0.66
1:D:191:LYS:HG2	1:D:246:ILE:HG22	1.77	0.66
1:G:174:CYS:CB	1:G:177:THR:H	2.08	0.66
1:G:100:LYS:HB3	1:G:138:PHE:HE1	1.61	0.65
1:D:28:TYR:HB2	1:D:49:ALA:HB1	1.78	0.64
1:F:64:LYS:HB3	1:F:68:ARG:NH2	2.13	0.64
1:G:174:CYS:O	1:G:178:ARG:NH1	2.28	0.64
1:F:173:THR:HG21	1:F:210:ARG:HH22	1.61	0.64
1:G:208:TYR:HD2	1:G:210:ARG:NH1	1.96	0.64
1:D:81:ILE:CD1	1:D:106:GLU:HG3	2.27	0.64
1:B:88:THR:HA	1:B:91:ASP:H	1.63	0.63
1:E:179:ILE:HD12	1:E:188:ASN:HB3	1.80	0.63
1:A:228:GLU:HA	1:A:231:PHE:CD2	2.34	0.63
1:B:41:ALA:HB1	1:B:47:THR:HG21	1.81	0.63
1:B:175:MET:HE3	1:B:178:ARG:HD3	1.80	0.63
1:G:155:ASN:O	1:G:159:GLU:HG3	1.99	0.63
1:G:39:LYS:HD3	1:G:72:TYR:HB3	1.81	0.63
1:B:88:THR:HB	1:B:91:ASP:HB3	1.81	0.62
1:D:123:THR:HB	1:D:145:SER:HB3	1.81	0.62
1:F:97:TYR:CE1	1:F:101:LYS:HD3	2.35	0.62
1:A:89:SER:HB3	1:A:183:PRO:HB2	1.82	0.61
1:B:144:ILE:O	1:B:146:PRO:HD3	2.00	0.61
1:C:222:LEU:CD2	1:C:253:LEU:HD11	2.31	0.61
1:C:208:TYR:HB3	1:C:223:THR:HG23	1.81	0.61
1:C:6:LYS:O	1:C:8:LEU:N	2.31	0.61
1:G:100:LYS:HD2	1:G:134:GLY:CA	2.31	0.61
1:D:4:MET:HG2	1:D:9:LEU:HB2	1.83	0.60
1:E:242:GLU:O	1:E:246:ILE:HG13	2.01	0.60
1:F:100:LYS:HD3	1:F:138:PHE:CE1	2.37	0.60
1:F:255:LEU:HB3	1:G:236:ILE:HG23	1.84	0.60
1:E:132:ARG:NH1	1:E:134:GLY:H	1.99	0.60
1:C:212:ARG:HB2	1:C:219:ILE:HB	1.82	0.60
1:G:228:GLU:HA	1:G:231:PHE:CD2	2.37	0.60
1:G:174:CYS:HB3	1:G:176:ALA:N	2.17	0.60
1:B:243:LEU:HA	1:B:246:ILE:HD12	1.84	0.60
1:F:210:ARG:HB2	1:F:221:GLU:HB2	1.84	0.59
1:C:7:GLY:HA2	1:C:10:GLU:HB2	1.84	0.59
1:A:210:ARG:HB2	1:A:221:GLU:HB2	1.83	0.59
1:F:216:ASN:HB3	1:F:249:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:LYS:HG3	1:E:134:GLY:HA3	1.83	0.59
1:A:100:LYS:HD3	3:A:302:AMP:O3'	2.02	0.59
1:G:52:ILE:HG23	1:G:81:ILE:HD12	1.85	0.59
1:F:251:VAL:HG12	1:G:255:LEU:HD12	1.84	0.58
1:F:217:ILE:HG23	1:F:250:LYS:HB3	1.85	0.58
1:B:52:ILE:HD13	1:B:79:ILE:HB	1.84	0.58
1:F:28:TYR:CB	1:F:49:ALA:HB1	2.33	0.58
1:G:68:ARG:NH2	1:G:167:ASP:HB2	2.19	0.58
1:B:179:ILE:HD12	1:B:188:ASN:HB3	1.84	0.58
1:E:39:LYS:HD2	1:E:42:SER:HB2	1.86	0.58
1:D:100:LYS:HG3	1:D:134:GLY:HA3	1.85	0.58
1:E:91:ASP:OD2	1:E:98:ASN:ND2	2.35	0.58
1:G:81:ILE:CD1	1:G:106:GLU:HG3	2.34	0.57
1:F:89:SER:HB3	1:F:183:PRO:HB2	1.87	0.57
1:F:25:ILE:HG13	1:F:116:TYR:CD2	2.39	0.57
1:C:7:GLY:H	1:C:10:GLU:HG3	1.70	0.56
1:C:15:LEU:HD13	1:C:150:LEU:HD12	1.87	0.56
1:A:100:LYS:HE2	3:A:302:AMP:H4'	1.88	0.56
1:A:191:LYS:HG2	1:A:246:ILE:HG22	1.86	0.56
1:F:64:LYS:HB3	1:F:68:ARG:HH21	1.69	0.56
1:E:67:ASN:HA	1:E:70:LYS:HD2	1.87	0.56
1:E:137:ALA:O	1:E:140:GLU:HB2	2.05	0.56
1:G:95:ARG:HG3	1:G:96:CYS:N	2.21	0.56
1:F:28:TYR:HE1	1:F:35:THR:HG22	1.69	0.56
1:B:217:ILE:HG23	1:B:250:LYS:HB3	1.88	0.55
1:D:38:SER:HB3	1:D:74:ILE:HG21	1.88	0.55
1:F:61:VAL:HA	1:F:64:LYS:HD2	1.87	0.55
1:F:181:SER:HB3	1:F:214:LEU:HD12	1.87	0.55
1:A:100:LYS:HE3	1:A:134:GLY:HA3	1.87	0.55
1:C:28:TYR:CB	1:C:49:ALA:HB1	2.37	0.55
1:B:28:TYR:CB	1:B:49:ALA:HB1	2.36	0.55
1:C:15:LEU:HD23	1:C:40:ILE:HD13	1.87	0.55
1:F:153:SER:H	1:F:156:ASP:HB2	1.70	0.55
1:C:15:LEU:HD13	1:C:150:LEU:CD1	2.37	0.55
1:D:179:ILE:HD12	1:D:188:ASN:HB3	1.87	0.55
1:E:95:ARG:HG3	1:E:96:CYS:N	2.22	0.54
1:G:95:ARG:HD3	1:G:184:ILE:HD11	1.88	0.54
1:D:217:ILE:HG23	1:D:250:LYS:HB3	1.88	0.54
1:F:151:LYS:O	1:F:151:LYS:HG2	2.07	0.54
1:F:73:ASN:O	1:F:73:ASN:ND2	2.40	0.54
1:A:28:TYR:CB	1:A:49:ALA:HB1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:TYR:HB2	1:F:74:ILE:HD12	1.89	0.54
1:B:242:GLU:O	1:B:246:ILE:HG13	2.08	0.54
1:D:207:SER:HB2	1:D:226:GLU:HG3	1.90	0.54
1:E:228:GLU:HA	1:E:231:PHE:CD2	2.43	0.54
1:C:113:GLU:OE1	1:F:128:ILE:HD12	2.07	0.54
1:F:28:TYR:CE1	1:F:35:THR:HG22	2.43	0.54
1:G:181:SER:HB3	1:G:214:LEU:HD12	1.90	0.54
1:D:39:LYS:HD3	1:D:72:TYR:HB3	1.90	0.53
1:E:207:SER:HB2	1:E:226:GLU:HG3	1.90	0.53
1:B:91:ASP:OD2	1:B:94:ASN:HB2	2.07	0.53
1:G:84:LEU:HD12	1:G:85:ASN:N	2.24	0.53
1:C:208:TYR:HB3	1:C:223:THR:CG2	2.39	0.53
1:E:12:TYR:CE2	1:E:16:LEU:HD11	2.42	0.53
1:F:73:ASN:C	1:F:73:ASN:HD22	2.12	0.53
1:G:11:LYS:NZ	1:G:156:ASP:OD2	2.35	0.53
1:F:230:ILE:HG22	1:F:230:ILE:O	2.09	0.53
1:C:53:ASP:OD2	1:C:80:LYS:HD3	2.09	0.53
1:F:81:ILE:HD12	1:F:102:ARG:HH21	1.74	0.53
1:D:28:TYR:CB	1:D:49:ALA:HB1	2.38	0.52
1:C:210:ARG:HB2	1:C:221:GLU:HB2	1.90	0.52
1:F:85:ASN:C	1:F:87:ILE:H	2.12	0.52
1:F:53:ASP:HB3	1:F:80:LYS:HD3	1.90	0.52
1:E:39:LYS:HB2	1:E:74:ILE:HD11	1.91	0.52
1:E:86:GLU:HG2	1:E:88:THR:HG23	1.90	0.52
1:B:68:ARG:CZ	1:B:169:PRO:HG3	2.40	0.52
1:F:19:PHE:HZ	1:F:37:ILE:HD11	1.75	0.52
1:F:85:ASN:OD1	1:F:88:THR:N	2.37	0.52
1:C:19:PHE:O	1:C:45:ALA:HB2	2.10	0.52
1:D:132:ARG:NH2	4:D:302:CL:CL	2.80	0.52
1:E:36:LEU:HD12	1:E:161:SER:OG	2.09	0.52
1:A:81:ILE:CD1	1:A:106:GLU:HG3	2.32	0.52
1:E:218:ALA:HB2	1:E:248:PHE:CD1	2.44	0.52
1:A:208:TYR:HB3	1:A:223:THR:HG23	1.92	0.52
1:G:56:PHE:CD1	1:G:176:ALA:HB2	2.45	0.52
1:B:28:TYR:HB2	1:B:49:ALA:HB1	1.92	0.52
1:D:36:LEU:HD22	1:D:157:VAL:HG13	1.91	0.51
1:E:165:LYS:HE2	1:E:165:LYS:HA	1.91	0.51
1:B:175:MET:HE2	1:B:193:ASN:HB2	1.92	0.51
1:F:242:GLU:O	1:F:246:ILE:HG13	2.11	0.51
1:A:153:SER:H	1:A:156:ASP:HB2	1.75	0.51
1:B:123:THR:HB	1:B:145:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:VAL:HG11	1:G:110:ILE:HD13	1.93	0.51
1:F:171:LYS:NZ	1:F:173:THR:HG22	2.25	0.51
1:G:242:GLU:O	1:G:246:ILE:HG13	2.11	0.51
1:A:123:THR:HB	1:A:145:SER:HB3	1.91	0.50
1:C:56:PHE:CD1	1:C:176:ALA:HB2	2.46	0.50
1:C:180:LEU:HD21	1:C:212:ARG:HD2	1.92	0.50
1:C:207:SER:HB3	1:C:226:GLU:HG3	1.92	0.50
1:F:49:ALA:O	1:F:76:GLN:HA	2.11	0.50
1:C:125:TYR:O	1:C:128:ILE:HG12	2.11	0.50
1:E:222:LEU:HD12	1:E:253:LEU:HD11	1.91	0.50
1:G:217:ILE:HG23	1:G:250:LYS:HB3	1.93	0.50
1:B:153:SER:H	1:B:156:ASP:HB2	1.76	0.50
1:C:179:ILE:HD12	1:C:188:ASN:HB3	1.93	0.50
1:A:207:SER:HB3	1:A:226:GLU:HG3	1.93	0.50
1:D:25:ILE:CG2	1:D:119:ILE:HG12	2.42	0.50
1:D:210:ARG:HB2	1:D:221:GLU:HB2	1.92	0.50
1:F:257:PHE:CZ	1:G:236:ILE:HD13	2.46	0.50
1:F:58:SER:OG	1:F:61:VAL:HG23	2.12	0.50
1:F:174:CYS:CB	2:F:301:SF4:S3	2.99	0.50
1:C:130:GLU:HG3	1:C:132:ARG:HG3	1.93	0.50
1:F:68:ARG:O	1:F:71:LYS:HB3	2.11	0.50
1:G:123:THR:CG2	1:G:145:SER:HB3	2.38	0.49
1:B:24:VAL:HG22	1:B:118:ILE:HD11	1.93	0.49
1:F:243:LEU:HA	1:F:246:ILE:HD12	1.94	0.49
1:F:200:LYS:HB2	1:F:209:LEU:HD21	1.93	0.49
1:G:81:ILE:HD13	1:G:106:GLU:HG3	1.95	0.49
1:G:92:LEU:HD23	1:G:95:ARG:HD3	1.93	0.49
1:G:207:SER:HB3	1:G:226:GLU:HG3	1.93	0.49
1:B:207:SER:HB3	1:B:226:GLU:HG3	1.94	0.49
1:B:125:TYR:HB2	1:B:151:LYS:HA	1.94	0.49
1:B:179:ILE:CD1	1:B:188:ASN:HB3	2.43	0.49
1:C:123:THR:HB	1:C:145:SER:HB3	1.94	0.49
1:C:173:THR:HG21	1:C:210:ARG:NH2	2.28	0.49
1:C:208:TYR:CE2	1:C:258:LYS:HG3	2.47	0.49
1:G:125:TYR:O	1:G:128:ILE:HG12	2.13	0.49
1:F:84:LEU:N	1:F:84:LEU:HD22	2.28	0.48
1:G:218:ALA:HB2	1:G:248:PHE:CD1	2.47	0.48
1:A:51:THR:HG23	3:A:302:AMP:HN62	1.78	0.48
1:D:4:MET:CG	1:D:9:LEU:HB2	2.43	0.48
1:C:114:LEU:HB3	1:C:116:TYR:CD1	2.48	0.48
1:D:12:TYR:CE2	1:D:16:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:O	1:B:45:ALA:HB2	2.14	0.48
1:C:86:GLU:HB2	1:C:88:THR:H	1.78	0.48
1:F:91:ASP:OD2	1:F:94:ASN:HB2	2.14	0.48
1:G:83:TYR:CE2	1:G:88:THR:HG21	2.48	0.48
1:C:6:LYS:C	1:C:8:LEU:H	2.15	0.48
1:B:25:ILE:HD12	1:B:111:LYS:HA	1.95	0.48
1:B:125:TYR:O	1:B:128:ILE:HG12	2.13	0.48
1:B:251:VAL:HG12	1:D:255:LEU:HD12	1.95	0.48
1:C:218:ALA:HB2	1:C:248:PHE:CG	2.48	0.48
1:F:72:TYR:HB2	1:F:74:ILE:CD1	2.44	0.48
1:F:100:LYS:HB3	1:F:138:PHE:CD1	2.49	0.48
1:G:28:TYR:CB	1:G:49:ALA:HB1	2.44	0.48
1:B:39:LYS:HD3	1:B:72:TYR:HB3	1.96	0.47
1:C:153:SER:H	1:C:156:ASP:HB2	1.78	0.47
1:G:174:CYS:HB2	1:G:177:THR:HG22	1.96	0.47
1:G:25:ILE:HD12	1:G:111:LYS:HA	1.96	0.47
1:G:221:GLU:HG2	1:G:254:ASP:HB3	1.96	0.47
1:A:133:PRO:O	1:A:136:LYS:HB3	2.15	0.47
1:B:228:GLU:HA	1:B:231:PHE:CD2	2.49	0.47
1:D:120:VAL:HA	1:D:144:ILE:O	2.14	0.47
1:F:79:ILE:CD1	1:F:110:ILE:HD11	2.45	0.47
1:G:132:ARG:HB2	1:G:135:ILE:HD12	1.97	0.47
1:A:97:TYR:OH	1:A:140:GLU:OE2	2.33	0.47
1:C:6:LYS:C	1:C:8:LEU:N	2.68	0.47
1:C:32:VAL:HG11	1:C:168:ILE:HG23	1.97	0.47
1:G:100:LYS:HG3	2:G:301:SF4:S4	2.55	0.47
1:B:37:ILE:HD13	1:B:147:LEU:HG	1.97	0.47
1:B:41:ALA:CB	1:B:47:THR:HG21	2.45	0.47
1:F:160:LEU:O	1:F:164:LEU:HG	2.14	0.47
1:G:89:SER:O	1:G:183:PRO:HA	2.14	0.47
1:A:110:ILE:HD12	1:B:129:PHE:CE1	2.50	0.47
1:A:242:GLU:O	1:A:246:ILE:HG13	2.14	0.46
1:B:132:ARG:HB3	4:B:303:CL:CL	2.51	0.46
1:B:224:LYS:HG3	1:B:259:GLY:HA2	1.97	0.46
1:E:79:ILE:CD1	1:E:110:ILE:HD11	2.45	0.46
1:B:87:ILE:HD12	1:B:87:ILE:H	1.80	0.46
1:B:218:ALA:HB2	1:B:248:PHE:CG	2.50	0.46
1:D:7:GLY:O	1:D:11:LYS:HG3	2.15	0.46
1:F:227:SER:HB2	1:F:231:PHE:CZ	2.50	0.46
1:F:228:GLU:HA	1:F:231:PHE:CD2	2.51	0.46
1:F:254:ASP:HA	1:G:252:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.72	0.46
1:E:66:GLU:HB3	1:E:70:LYS:HE3	1.96	0.46
1:A:76:GLN:NE2	1:A:78:THR:OG1	2.38	0.46
1:C:242:GLU:O	1:C:246:ILE:HG13	2.14	0.46
1:F:28:TYR:HB2	1:F:49:ALA:HB1	1.96	0.46
1:A:12:TYR:CE2	1:A:16:LEU:HD11	2.50	0.46
1:B:218:ALA:HB2	1:B:248:PHE:CD1	2.50	0.46
1:E:54:ASN:HB3	1:E:81:ILE:HD11	1.98	0.46
1:E:177:THR:HG22	1:E:212:ARG:HH12	1.80	0.46
1:G:174:CYS:HB2	1:G:177:THR:H	1.81	0.46
1:C:255:LEU:HD12	1:E:251:VAL:HG12	1.98	0.46
1:C:217:ILE:HG23	1:C:250:LYS:HB3	1.97	0.46
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.63	0.46
1:G:120:VAL:HG13	1:G:146:PRO:CD	2.46	0.46
1:B:52:ILE:CD1	1:B:79:ILE:HB	2.45	0.46
1:F:205:ILE:HD13	1:F:229:LYS:HD2	1.98	0.46
1:C:28:TYR:HB2	1:C:49:ALA:HB1	1.97	0.45
1:E:144:ILE:O	1:E:146:PRO:HD3	2.16	0.45
1:F:205:ILE:HB	1:F:209:LEU:HD23	1.98	0.45
1:G:119:ILE:HG22	1:G:143:ILE:HG23	1.98	0.45
1:E:86:GLU:O	1:E:89:SER:OG	2.33	0.45
1:F:205:ILE:HB	1:F:209:LEU:CD2	2.46	0.45
1:E:214:LEU:HD12	1:E:214:LEU:HA	1.66	0.45
1:F:120:VAL:HA	1:F:144:ILE:O	2.15	0.45
1:C:86:GLU:CB	1:C:88:THR:H	2.29	0.45
1:D:25:ILE:HG23	1:D:119:ILE:HG12	1.97	0.45
1:F:18:PHE:CE1	1:F:22:LYS:HE2	2.51	0.45
1:D:100:LYS:HG3	1:D:134:GLY:CA	2.46	0.45
1:B:49:ALA:O	1:B:76:GLN:HA	2.16	0.45
1:F:170:LYS:HG2	1:F:171:LYS:H	1.81	0.45
1:G:93:GLU:OE2	1:G:93:GLU:N	2.42	0.45
1:C:100:LYS:HG3	1:C:134:GLY:CA	2.46	0.45
1:D:8:LEU:HD11	1:D:160:LEU:HB2	1.99	0.45
1:F:85:ASN:HD21	1:F:88:THR:HG23	1.82	0.45
1:B:255:LEU:HB3	1:D:236:ILE:HG23	1.98	0.45
1:C:83:TYR:OH	1:C:88:THR:HG21	2.17	0.45
1:D:179:ILE:CD1	1:D:188:ASN:HB3	2.47	0.45
1:B:228:GLU:HA	1:B:231:PHE:HD2	1.81	0.45
1:A:28:TYR:HB2	1:A:49:ALA:HB1	1.99	0.44
1:C:58:SER:HB3	1:C:61:VAL:HG23	1.98	0.44
1:G:175:MET:HB3	1:G:189:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:O	1:A:143:ILE:HG12	2.18	0.44
1:A:195:ALA:HB1	1:A:243:LEU:HD21	1.98	0.44
1:G:86:GLU:O	1:G:89:SER:OG	2.32	0.44
1:B:255:LEU:HD12	1:D:251:VAL:HG12	1.99	0.44
1:D:121:ASP:OD2	1:D:123:THR:OG1	2.30	0.44
1:F:252:VAL:HG12	1:G:254:ASP:HA	1.99	0.44
1:G:68:ARG:HH22	1:G:167:ASP:HB2	1.81	0.44
1:B:24:VAL:O	1:B:47:THR:HA	2.17	0.44
1:C:83:TYR:CZ	1:C:88:THR:HG21	2.53	0.44
1:G:107:LEU:HA	1:G:110:ILE:HD12	1.99	0.44
1:D:155:ASN:O	1:D:159:GLU:HG2	2.18	0.44
1:A:218:ALA:HB2	1:A:248:PHE:CD1	2.52	0.44
1:A:48:LEU:HD12	1:A:75:PRO:O	2.18	0.44
1:A:52:ILE:HG23	1:A:81:ILE:HD12	1.99	0.44
1:B:81:ILE:HD12	1:B:83:TYR:HB2	1.99	0.44
1:B:236:ILE:HG21	1:D:257:PHE:CZ	2.53	0.44
1:D:15:LEU:HG	1:D:40:ILE:HG21	2.00	0.44
1:F:70:LYS:HD3	1:F:70:LYS:HA	1.80	0.44
1:E:163:TYR:C	1:E:165:LYS:H	2.21	0.43
1:F:205:ILE:O	1:F:209:LEU:HD23	2.18	0.43
1:E:111:LYS:HB2	1:E:119:ILE:HD11	2.00	0.43
1:G:61:VAL:HA	1:G:64:LYS:NZ	2.33	0.43
1:G:28:TYR:HB2	1:G:49:ALA:HB1	2.00	0.43
1:G:81:ILE:HD11	1:G:106:GLU:HG3	1.99	0.43
1:A:51:THR:CG2	3:A:302:AMP:HN62	2.32	0.43
1:A:100:LYS:CE	3:A:302:AMP:H4'	2.48	0.43
1:A:85:ASN:H	1:A:88:THR:HG1	1.65	0.43
1:E:8:LEU:HD21	1:E:160:LEU:HB2	2.01	0.43
1:E:50:VAL:HG11	1:E:110:ILE:HD13	2.00	0.43
1:E:206:GLU:N	1:E:226:GLU:OE2	2.51	0.43
1:G:52:ILE:HB	1:G:103:ILE:HG23	2.00	0.43
1:A:32:VAL:HG22	1:A:169:PRO:HD2	2.01	0.43
1:B:227:SER:HB2	1:B:231:PHE:CE2	2.54	0.43
1:G:67:ASN:HA	1:G:70:LYS:HD2	1.99	0.43
1:A:120:VAL:HG12	1:A:144:ILE:HB	2.00	0.43
1:B:26:VAL:HG11	1:B:38:SER:OG	2.18	0.43
1:B:83:TYR:O	1:B:86:GLU:HG2	2.19	0.43
1:G:213:TYR:CE1	1:G:216:ASN:HA	2.54	0.43
1:C:144:ILE:O	1:C:146:PRO:HD3	2.18	0.43
1:G:158:PHE:CE1	1:G:159:GLU:HG2	2.54	0.43
1:C:132:ARG:HA	1:C:133:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:MET:HB3	1:D:189:MET:HB3	2.00	0.42
1:G:144:ILE:O	1:G:146:PRO:HD3	2.19	0.42
1:E:19:PHE:O	1:E:45:ALA:HB2	2.19	0.42
1:G:155:ASN:HA	1:G:158:PHE:CE2	2.55	0.42
1:D:222:LEU:HD13	1:D:227:SER:HA	2.01	0.42
1:A:58:SER:OG	1:A:61:VAL:HG23	2.20	0.42
1:B:128:ILE:HG21	1:B:128:ILE:HD13	1.84	0.42
1:F:208:TYR:CE1	1:F:210:ARG:CZ	3.02	0.42
1:D:2:ILE:HG22	1:D:4:MET:HB2	2.01	0.42
1:G:25:ILE:O	1:G:119:ILE:HA	2.20	0.42
1:G:100:LYS:HB3	1:G:138:PHE:CD1	2.54	0.42
1:D:25:ILE:HD11	1:D:50:VAL:HG21	2.01	0.42
1:E:28:TYR:HE1	1:E:35:THR:HG22	1.84	0.42
1:F:39:LYS:HD3	1:F:72:TYR:HB3	2.01	0.42
1:G:61:VAL:HG22	1:G:64:LYS:HZ1	1.84	0.42
1:B:196:GLU:OE2	1:B:210:ARG:HA	2.20	0.42
1:F:28:TYR:OH	1:F:30:GLY:HA2	2.20	0.42
1:A:49:ALA:O	1:A:76:GLN:HG2	2.20	0.42
1:D:52:ILE:HD13	1:D:79:ILE:HB	2.02	0.42
1:D:208:TYR:CD2	1:D:258:LYS:HG3	2.55	0.42
1:D:214:LEU:HD12	1:D:214:LEU:HA	1.82	0.42
1:F:97:TYR:HE1	1:F:101:LYS:HD3	1.85	0.42
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.89	0.42
1:A:209:LEU:HD12	1:A:221:GLU:O	2.19	0.42
1:E:208:TYR:CD2	1:E:258:LYS:HG3	2.55	0.42
1:B:137:ALA:O	1:B:140:GLU:HB2	2.20	0.41
1:D:242:GLU:O	1:D:246:ILE:HG13	2.20	0.41
1:D:174:CYS:SG	1:D:177:THR:HG23	2.60	0.41
1:F:119:ILE:HG22	1:F:143:ILE:HG23	2.01	0.41
1:F:255:LEU:HA	1:F:255:LEU:HD23	1.85	0.41
1:B:115:ASN:ND2	4:B:304:CL:CL	2.83	0.41
1:C:19:PHE:CD2	1:C:41:ALA:HA	2.55	0.41
1:D:25:ILE:HA	1:D:48:LEU:O	2.21	0.41
1:E:50:VAL:HG11	1:E:110:ILE:CD1	2.49	0.41
1:E:218:ALA:HB2	1:E:248:PHE:CG	2.54	0.41
1:G:49:ALA:O	1:G:76:GLN:HG2	2.20	0.41
1:B:191:LYS:HG2	1:B:246:ILE:HG22	2.01	0.41
1:E:132:ARG:O	1:E:135:ILE:HG13	2.21	0.41
1:F:167:ASP:O	1:F:169:PRO:HD3	2.20	0.41
1:F:170:LYS:HG2	1:F:171:LYS:N	2.35	0.41
1:A:25:ILE:CD1	1:A:111:LYS:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HG2	1:A:166:ILE:HD11	2.02	0.41
1:A:128:ILE:HD13	1:A:128:ILE:HG21	1.70	0.41
1:E:28:TYR:CB	1:E:49:ALA:HB1	2.50	0.41
1:E:35:THR:HG21	1:E:68:ARG:HE	1.86	0.41
1:F:218:ALA:HB2	1:F:248:PHE:CG	2.56	0.41
1:D:157:VAL:O	1:D:161:SER:OG	2.26	0.41
1:F:123:THR:HB	1:F:145:SER:HB3	2.02	0.41
1:B:153:SER:N	1:B:156:ASP:HB2	2.35	0.41
1:C:5:GLU:O	1:C:8:LEU:HB3	2.21	0.41
1:E:71:LYS:NZ	1:E:72:TYR:CE1	2.88	0.41
1:C:130:GLU:OE2	1:C:132:ARG:NE	2.54	0.41
1:C:207:SER:HB3	1:C:226:GLU:CG	2.51	0.41
1:C:227:SER:HB2	1:C:231:PHE:CE2	2.56	0.41
1:E:114:LEU:HB3	1:E:116:TYR:CD1	2.56	0.41
1:F:134:GLY:O	1:F:137:ALA:N	2.54	0.41
1:F:222:LEU:HD23	1:F:222:LEU:HA	1.92	0.41
1:G:32:VAL:HG22	1:G:169:PRO:HD2	2.03	0.41
1:B:216:ASN:HB3	1:B:249:GLU:HG2	2.03	0.41
1:E:118:ILE:HB	1:E:144:ILE:HD12	2.03	0.41
1:C:102:ARG:O	1:C:105:GLU:HB2	2.21	0.40
1:C:210:ARG:O	1:C:220:ILE:HA	2.21	0.40
1:E:227:SER:HB2	1:E:231:PHE:CZ	2.56	0.40
1:G:37:ILE:HD12	1:G:37:ILE:HG23	1.87	0.40
1:D:11:LYS:HB3	1:D:152:PHE:CE1	2.56	0.40
1:E:25:ILE:O	1:E:119:ILE:HA	2.22	0.40
1:F:86:GLU:O	1:F:90:LYS:HG3	2.21	0.40
1:G:23:LYS:HD3	1:G:46:GLN:NE2	2.36	0.40
1:A:39:LYS:HD3	1:A:72:TYR:HB3	2.03	0.40
1:A:179:ILE:HD12	1:A:188:ASN:HB3	2.03	0.40
1:F:11:LYS:HD3	1:F:11:LYS:HA	1.88	0.40
1:G:8:LEU:HD21	1:G:160:LEU:HB2	2.03	0.40
1:E:42:SER:HA	1:E:47:THR:HB	2.03	0.40
1:A:68:ARG:NH1	1:A:169:PRO:HD3	2.36	0.40
1:C:224:LYS:HD2	1:C:259:GLY:HA2	2.03	0.40
1:E:86:GLU:HG2	1:E:88:THR:H	1.86	0.40
1:F:210:ARG:O	1:F:220:ILE:HA	2.22	0.40
1:F:224:LYS:CE	1:F:259:GLY:HA2	2.52	0.40
1:F:256:ASN:ND2	1:F:256:ASN:O	2.54	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 X-ray entries followed by that with respect to entries of similar resolution.

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	253/271 (93%)	246 (97%)	7 (3%)	0	100	100
1	B	252/271 (93%)	240 (95%)	12 (5%)	0	100	100
1	C	254/271 (94%)	241 (95%)	12 (5%)	1 (0%)	34	69
1	D	259/271 (96%)	245 (95%)	13 (5%)	1 (0%)	34	69
1	E	251/271 (93%)	239 (95%)	10 (4%)	2 (1%)	19	58
1	F	251/271 (93%)	243 (97%)	7 (3%)	1 (0%)	34	69
1	G	251/271 (93%)	244 (97%)	7 (3%)	0	100	100
All	All	1771/1897 (93%)	1698 (96%)	68 (4%)	5 (0%)	41	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	GLU
1	E	85	ASN
1	E	168	ILE
1	F	133	PRO
1	C	174	CYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	232/248 (94%)	231 (100%)	1 (0%)	91	95
1	B	231/248 (93%)	230 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	235/248 (95%)	232 (99%)	3 (1%)	69 87
1	D	239/248 (96%)	234 (98%)	5 (2%)	53 79
1	E	232/248 (94%)	230 (99%)	2 (1%)	78 91
1	F	231/248 (93%)	227 (98%)	4 (2%)	60 83
1	G	232/248 (94%)	228 (98%)	4 (2%)	60 83
All	All	1632/1736 (94%)	1612 (99%)	20 (1%)	71 88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ASP
1	B	167	ASP
1	C	96	CYS
1	C	167	ASP
1	C	174	CYS
1	D	93	GLU
1	D	96	CYS
1	D	138	PHE
1	D	167	ASP
1	D	174	CYS
1	E	138	PHE
1	E	158	PHE
1	F	73	ASN
1	F	80	LYS
1	F	167	ASP
1	F	174	CYS
1	G	60	ASN
1	G	83	TYR
1	G	96	CYS
1	G	158	PHE

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

Mol	Chain	Res	Type
1	B	46	GLN
1	B	233	ASN
1	F	73	ASN
1	G	46	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	SF4	D	301	1	0,12,12	-	-	-		
2	SF4	C	301	1	0,12,12	-	-	-		
2	SF4	F	301	1	0,12,12	-	-	-		
2	SF4	G	301	1	0,12,12	-	-	-		
3	AMP	A	302	2	22,25,25	0.78	1 (4%)	25,38,38	1.95	5 (20%)
2	SF4	A	301	1,3	0,12,12	-	-	-		
2	SF4	B	301	1	0,12,12	-	-	-		
2	SF4	E	301	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
2	SF4	D	301	1	-	-	0/6/5/5
2	SF4	C	301	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	F	301	1	-	-	0/6/5/5
2	SF4	G	301	1	-	-	0/6/5/5
3	AMP	A	302	2	-	6/6/26/26	0/3/3/3
2	SF4	A	301	1,3	-	-	0/6/5/5
2	SF4	B	301	1	-	-	0/6/5/5
2	SF4	E	301	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	AMP	C5-N7	-2.04	1.32	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	AMP	N3-C2-N1	-5.13	120.65	128.68
3	A	302	AMP	C5-C6-N6	-4.50	113.51	120.35
3	A	302	AMP	N6-C6-N1	4.33	127.57	118.57
3	A	302	AMP	O5'-P-O1P	-2.57	99.25	106.47
3	A	302	AMP	C2-N1-C6	2.24	122.58	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	AMP	C5'-O5'-P-O1P
3	A	302	AMP	C5'-O5'-P-O2P
3	A	302	AMP	C5'-O5'-P-O3P
3	A	302	AMP	O4'-C4'-C5'-O5'
3	A	302	AMP	C3'-C4'-C5'-O5'
3	A	302	AMP	C4'-C5'-O5'-P

There are no ring outliers.

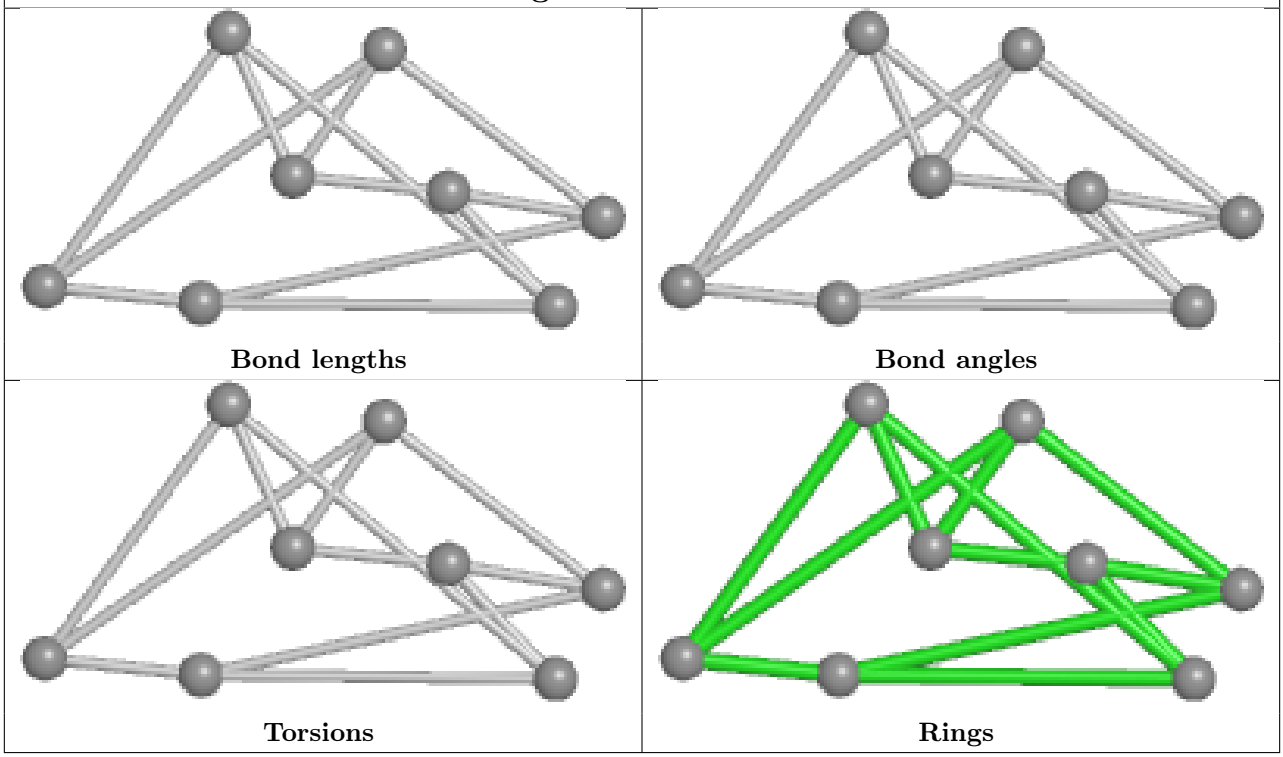
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	SF4	1	0
2	G	301	SF4	2	0
3	A	302	AMP	5	0

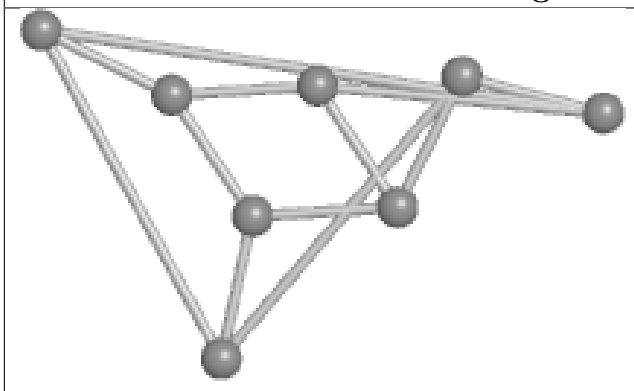
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

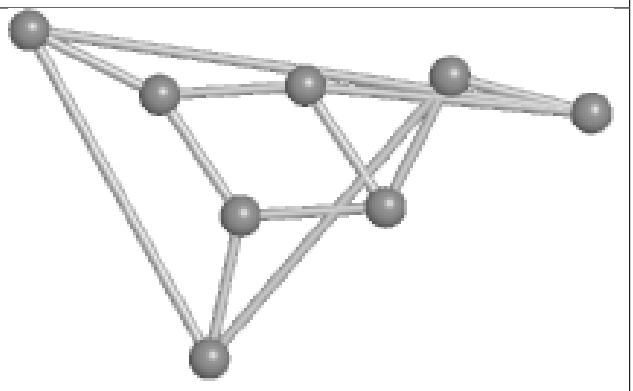
Ligand SF4 D 301



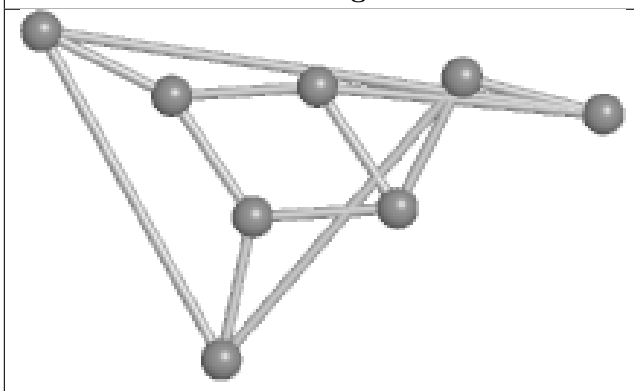
Ligand SF4 C 301



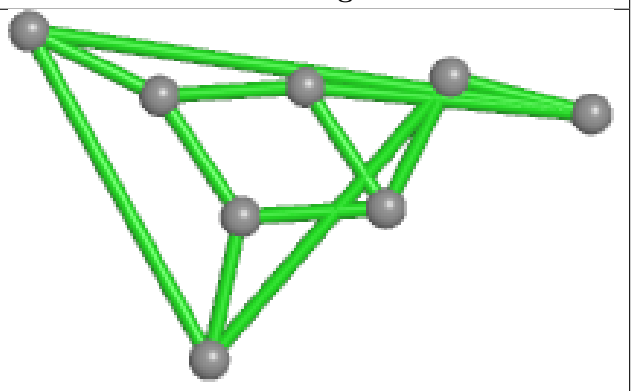
Bond lengths



Bond angles

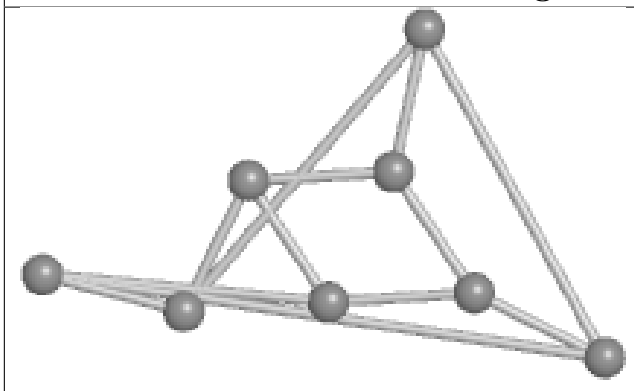


Torsions

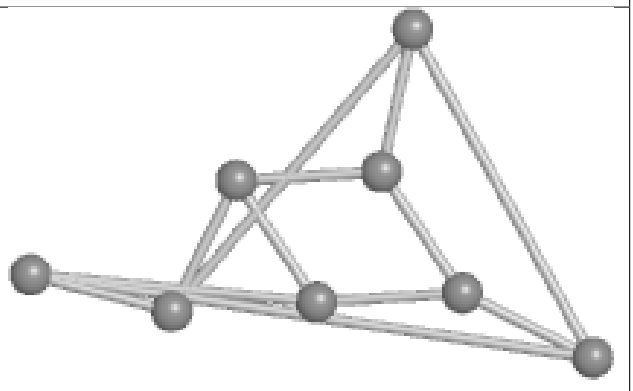


Rings

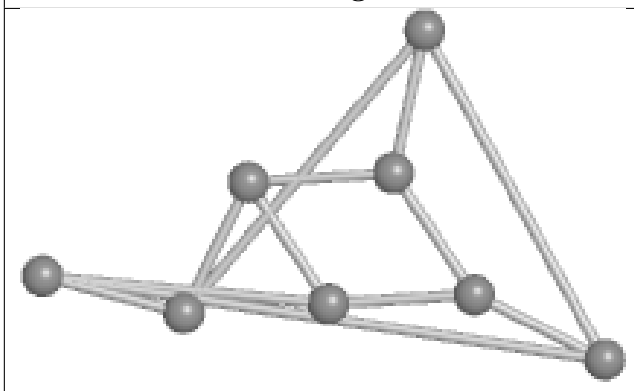
Ligand SF4 F 301



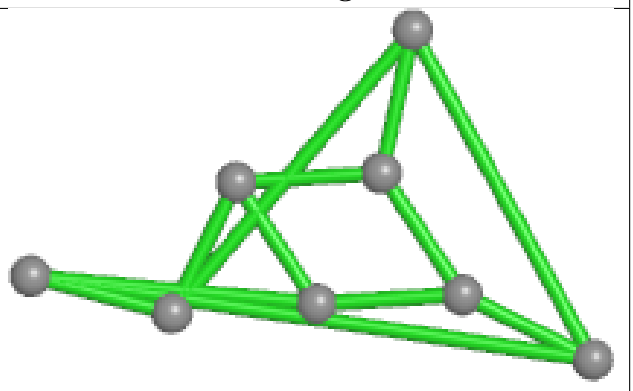
Bond lengths



Bond angles

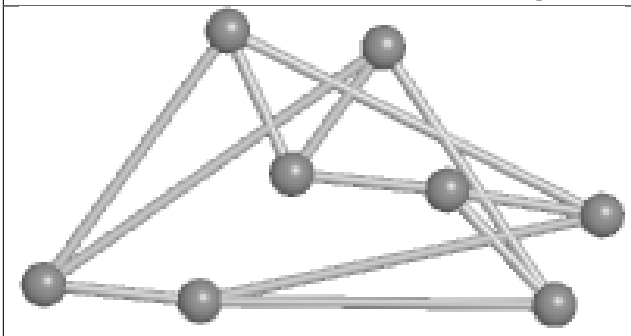


Torsions

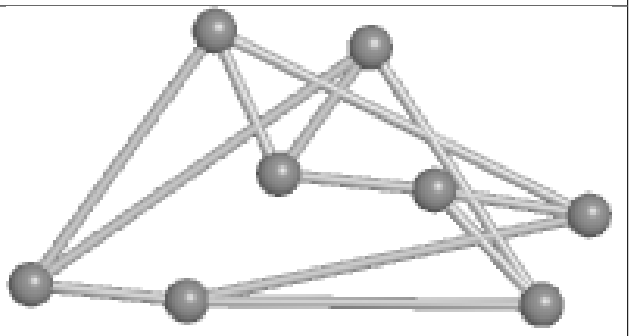


Rings

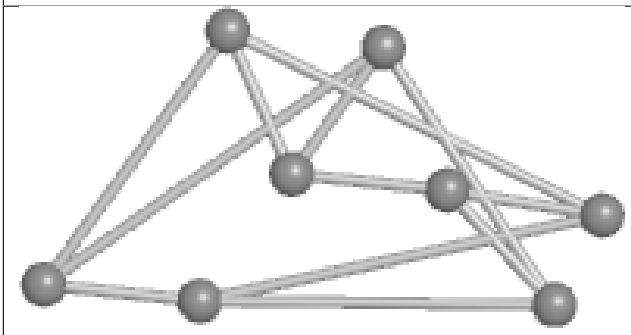
Ligand SF4 G 301



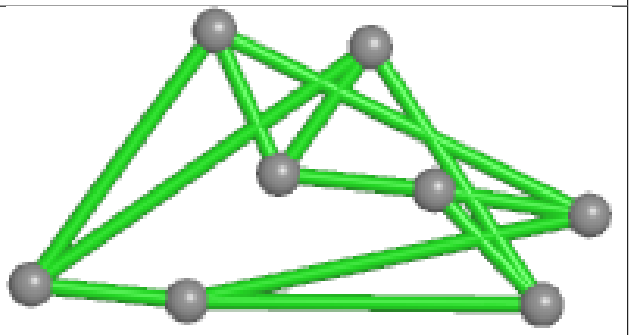
Bond lengths



Bond angles

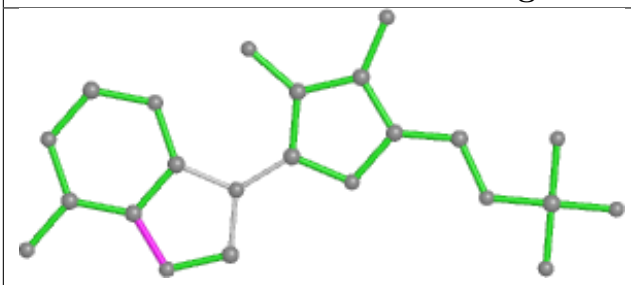


Torsions

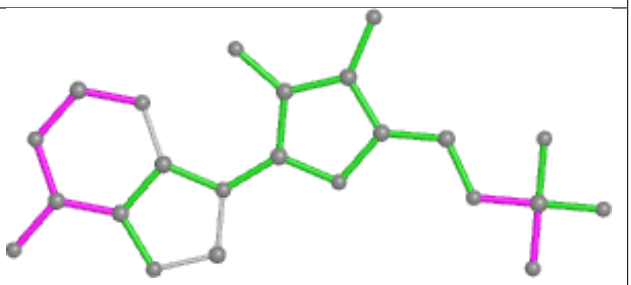


Rings

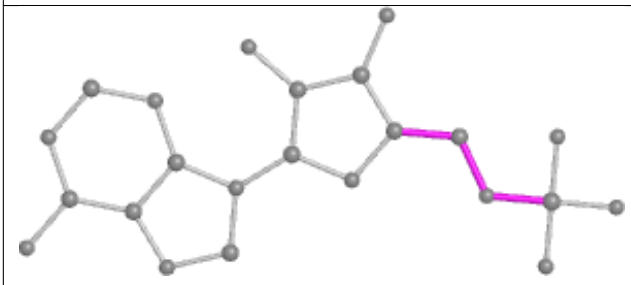
Ligand AMP A 302



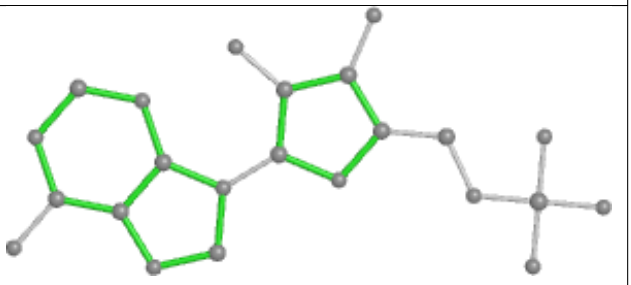
Bond lengths



Bond angles

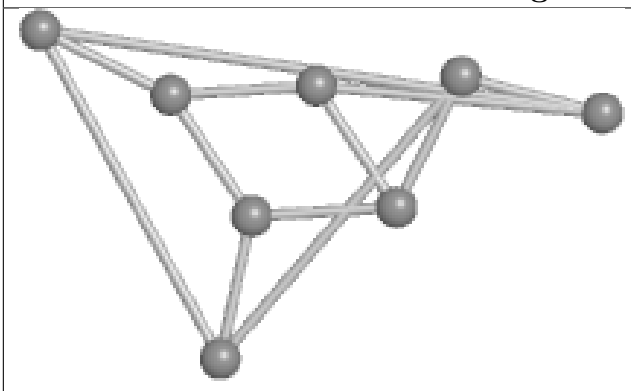


Torsions

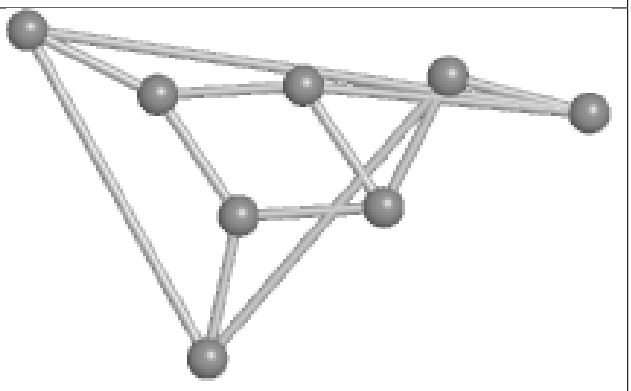


Rings

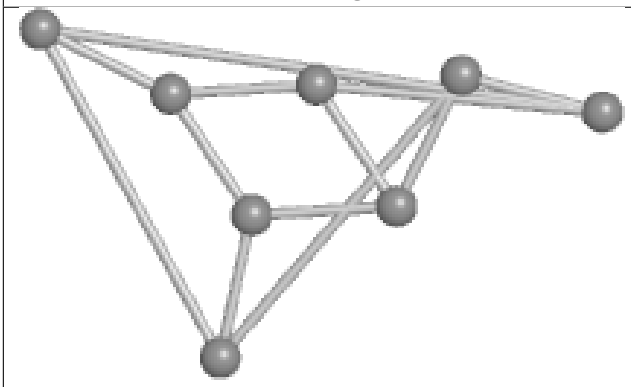
Ligand SF4 A 301



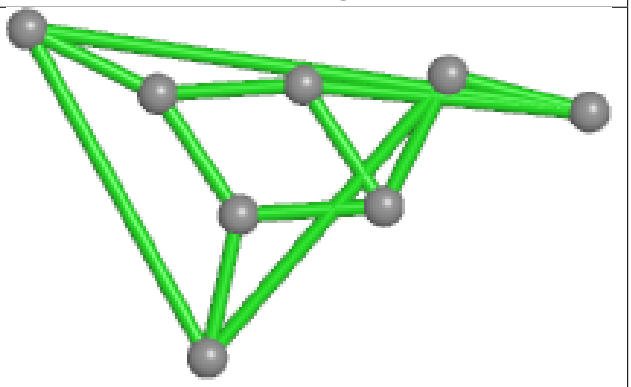
Bond lengths



Bond angles

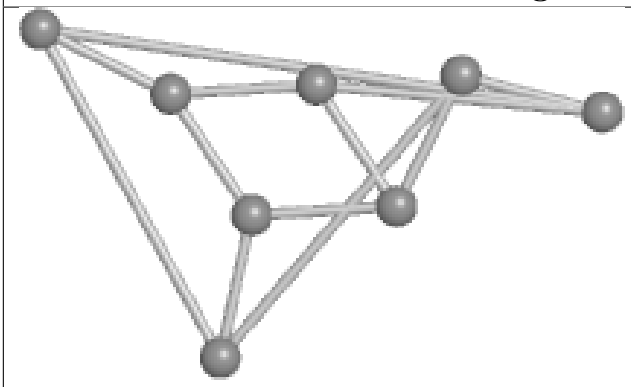


Torsions

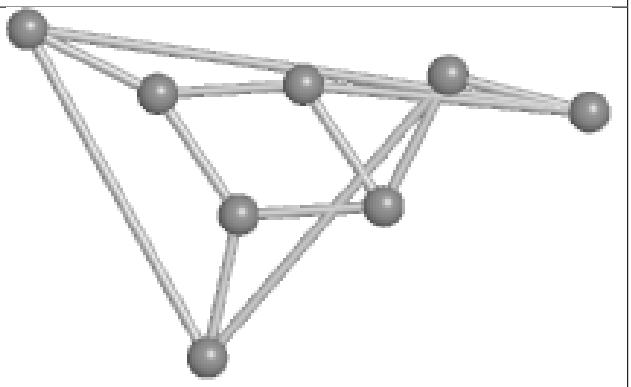


Rings

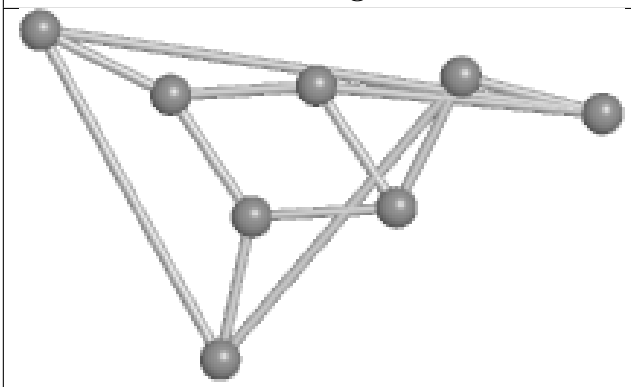
Ligand SF4 B 301



Bond lengths



Bond angles



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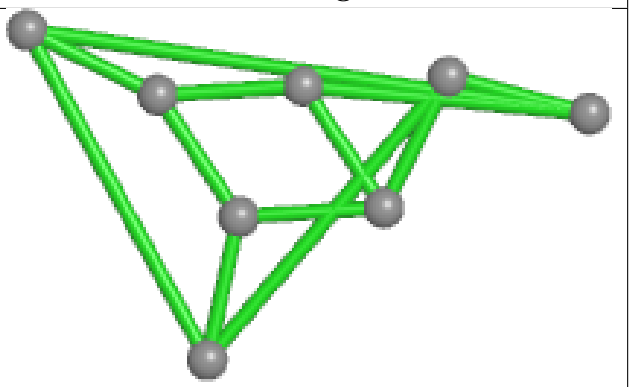
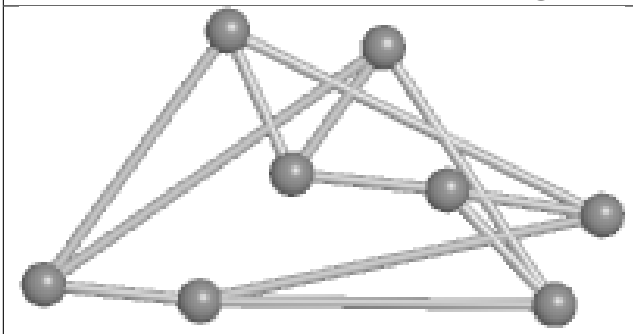
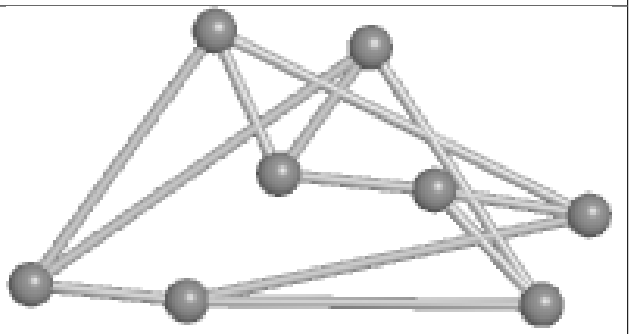


Rings

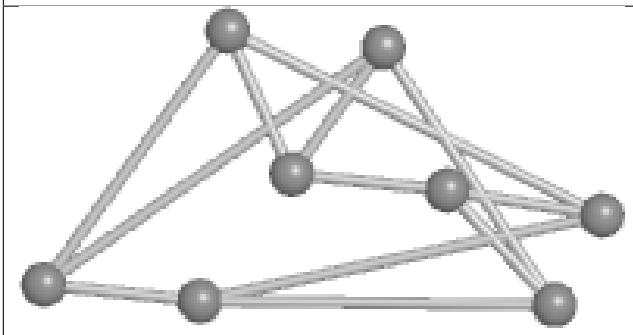
Ligand SF4 E 301



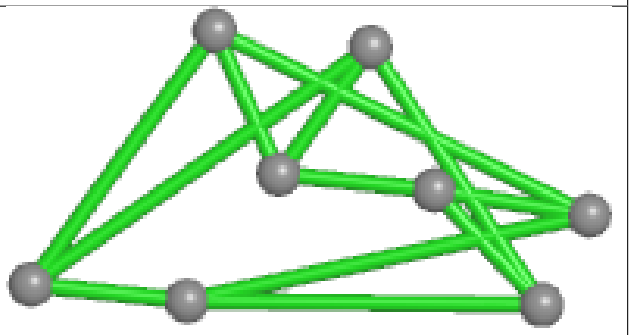
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	255/271 (94%)	0.38	11 (4%) 35 22	85, 127, 161, 184	0
1	B	254/271 (93%)	0.37	10 (3%) 39 25	80, 121, 161, 190	0
1	C	256/271 (94%)	0.38	6 (2%) 60 47	96, 125, 161, 199	0
1	D	261/271 (96%)	0.39	11 (4%) 36 23	82, 128, 158, 177	0
1	E	253/271 (93%)	0.69	30 (11%) 4 2	92, 148, 215, 270	0
1	F	253/271 (93%)	0.46	19 (7%) 14 8	125, 155, 186, 223	0
1	G	253/271 (93%)	0.75	30 (11%) 4 2	121, 165, 205, 229	0
All	All	1785/1897 (94%)	0.49	117 (6%) 18 11	80, 138, 191, 270	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	MET	7.8
1	G	222	LEU	6.1
1	C	230	ILE	5.7
1	E	152	PHE	5.4
1	F	222	LEU	5.3
1	F	236	ILE	4.8
1	E	169	PRO	4.8
1	A	230	ILE	4.7
1	E	163	TYR	4.6
1	G	230	ILE	4.6
1	E	15	LEU	4.5
1	G	152	PHE	4.0
1	E	19	PHE	4.0
1	G	208	TYR	3.9
1	G	209	LEU	3.7
1	A	222	LEU	3.7
1	G	12	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	46	GLN	3.6
1	A	19	PHE	3.6
1	D	4	MET	3.5
1	G	24	VAL	3.5
1	G	199	ILE	3.3
1	G	44	ASN	3.3
1	B	88	THR	3.3
1	E	230	ILE	3.3
1	G	78	THR	3.3
1	D	222	LEU	3.3
1	B	19	PHE	3.3
1	G	19	PHE	3.3
1	G	47	THR	3.2
1	F	12	TYR	3.2
1	G	166	ILE	3.1
1	B	230	ILE	3.1
1	D	22	LYS	3.0
1	F	22	LYS	3.0
1	A	223	THR	2.9
1	G	257	PHE	2.9
1	E	157	VAL	2.8
1	G	239	ILE	2.8
1	G	22	LYS	2.8
1	E	222	LEU	2.8
1	E	166	ILE	2.8
1	D	230	ILE	2.8
1	F	230	ILE	2.8
1	E	8	LEU	2.8
1	E	168	ILE	2.8
1	G	72	TYR	2.8
1	G	157	VAL	2.8
1	F	76	GLN	2.7
1	F	81	ILE	2.7
1	B	12	TYR	2.7
1	A	20	LYS	2.7
1	E	18	PHE	2.7
1	G	118	ILE	2.6
1	E	158	PHE	2.6
1	E	203	PHE	2.6
1	A	199	ILE	2.6
1	F	205	ILE	2.6
1	D	46	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	205	ILE	2.6
1	E	17	GLU	2.6
1	D	24	VAL	2.6
1	F	152	PHE	2.6
1	A	157	VAL	2.6
1	B	90	LYS	2.6
1	F	209	LEU	2.6
1	G	236	ILE	2.6
1	A	15	LEU	2.5
1	A	166	ILE	2.5
1	G	125	TYR	2.4
1	D	47	THR	2.4
1	G	74	ILE	2.4
1	A	205	ILE	2.4
1	D	20	LYS	2.4
1	C	222	LEU	2.4
1	G	18	PHE	2.4
1	G	68	ARG	2.4
1	F	116	TYR	2.4
1	D	199	ILE	2.4
1	F	48	LEU	2.4
1	C	207	SER	2.3
1	E	147	LEU	2.3
1	E	164	LEU	2.3
1	G	16	LEU	2.3
1	G	205	ILE	2.3
1	E	209	LEU	2.3
1	D	19	PHE	2.3
1	E	30	GLY	2.3
1	B	87	ILE	2.3
1	E	24	VAL	2.3
1	E	159	GLU	2.3
1	B	116	TYR	2.3
1	E	125	TYR	2.3
1	B	89	SER	2.3
1	E	257	PHE	2.2
1	C	9	LEU	2.2
1	E	36	LEU	2.2
1	A	22	LYS	2.2
1	G	204	HIS	2.2
1	F	51	THR	2.2
1	F	20	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	209	LEU	2.2
1	E	150	LEU	2.2
1	F	23	LYS	2.2
1	E	229	LYS	2.1
1	F	19	PHE	2.1
1	G	89	SER	2.1
1	F	18	PHE	2.1
1	G	90	LYS	2.1
1	E	208	TYR	2.1
1	E	205	ILE	2.1
1	E	48	LEU	2.1
1	F	125	TYR	2.1
1	F	235	SER	2.1
1	E	12	TYR	2.0
1	G	116	TYR	2.0
1	D	72	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	304	1/1	-0.02	0.35	151,151,151,151	0
4	CL	B	304	1/1	0.57	0.14	159,159,159,159	0
4	CL	B	303	1/1	0.69	0.27	120,120,120,120	0
4	CL	C	303	1/1	0.78	0.35	100,100,100,100	0
3	AMP	A	302	23/23	0.90	0.32	105,129,152,159	23
4	CL	A	303	1/1	0.91	0.27	117,117,117,117	0
4	CL	F	302	1/1	0.96	0.32	174,174,174,174	0

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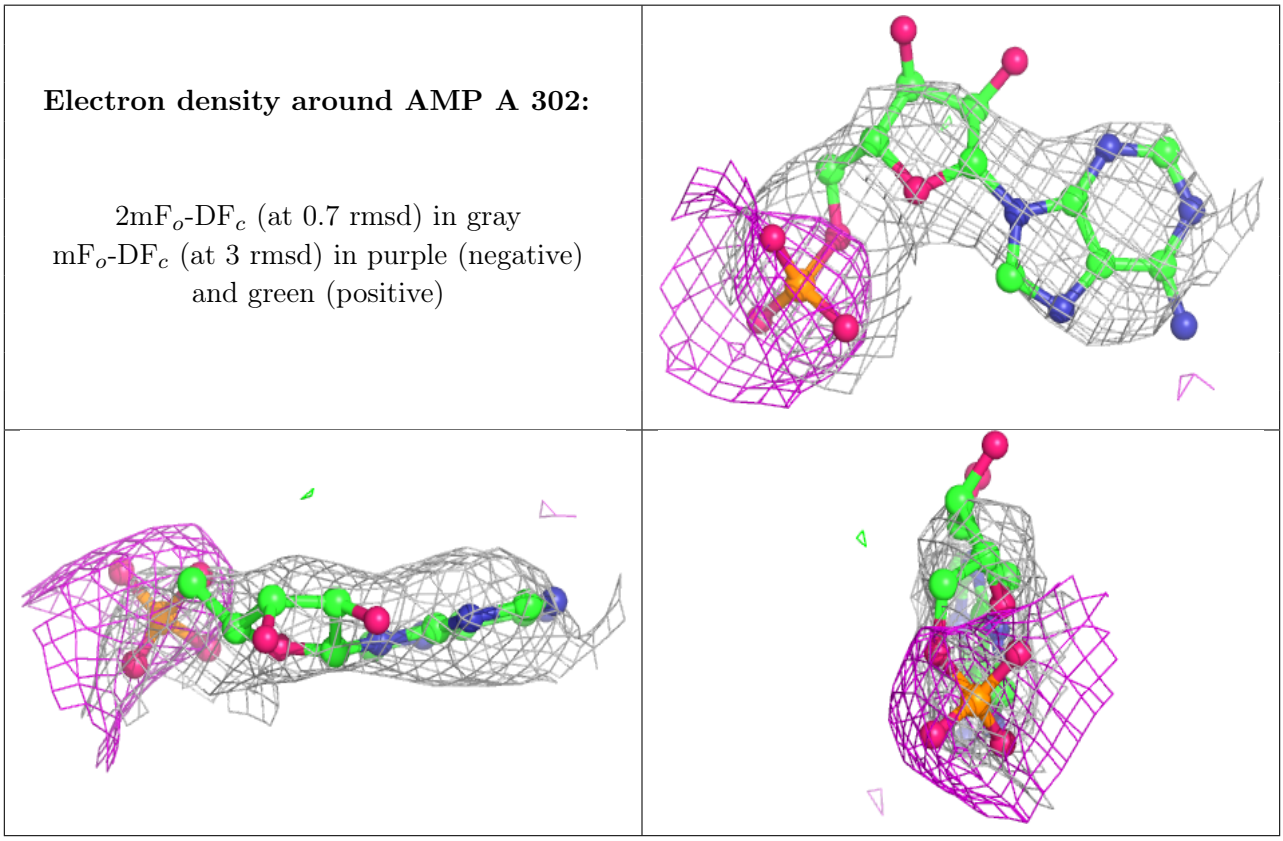
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	D	302	1/1	0.97	0.32	125,125,125,125	0
2	SF4	G	301	8/8	0.97	0.25	101,104,117,120	0
4	CL	G	302	1/1	0.97	0.29	154,154,154,154	0
2	SF4	F	301	8/8	0.98	0.24	100,102,115,139	0
4	CL	C	302	1/1	0.98	0.49	116,116,116,116	0
4	CL	B	302	1/1	0.99	0.46	113,113,113,113	0
2	SF4	E	301	8/8	0.99	0.26	100,100,100,119	0
4	CL	E	302	1/1	0.99	0.28	130,130,130,130	0
2	SF4	A	301	8/8	0.99	0.25	100,100,112,116	0
2	SF4	C	301	8/8	0.99	0.25	100,100,101,117	0
2	SF4	D	301	8/8	1.00	0.24	100,100,100,113	0
2	SF4	B	301	8/8	1.00	0.27	100,100,100,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

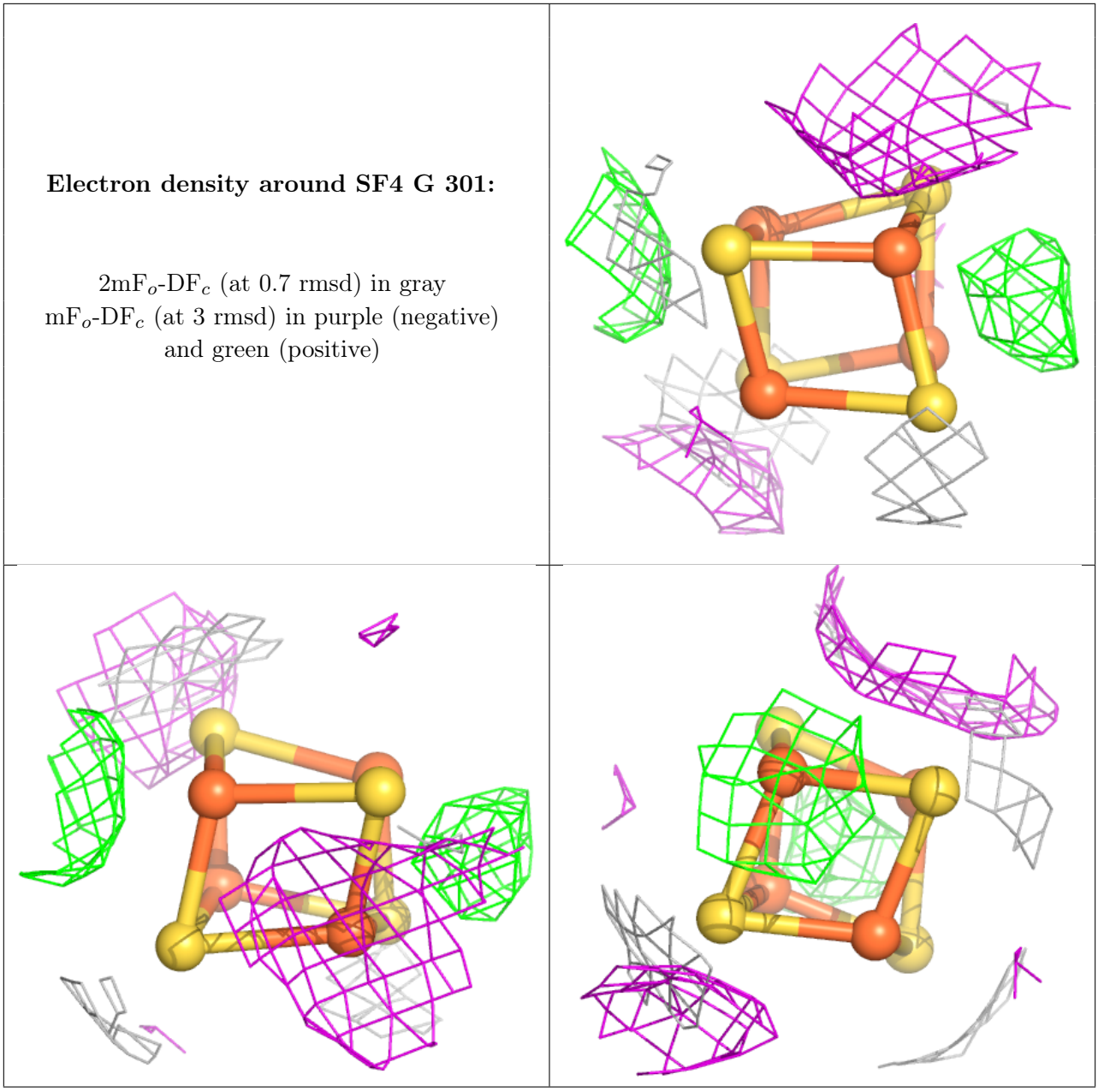
Electron density around AMP A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



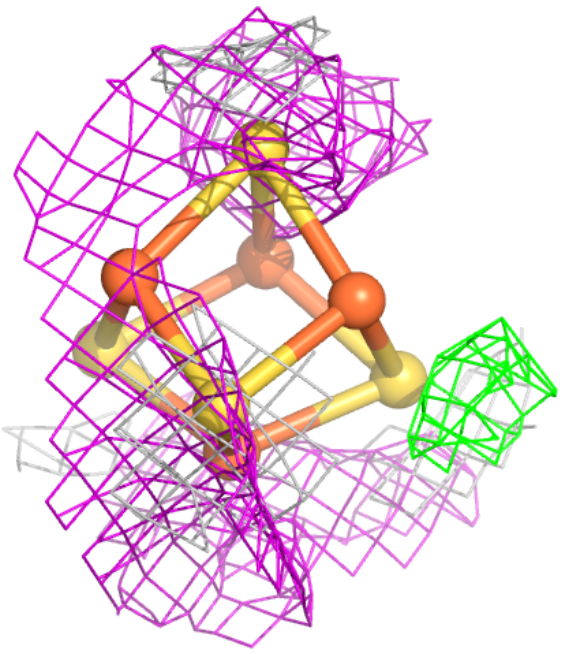
Electron density around SF4 G 301:

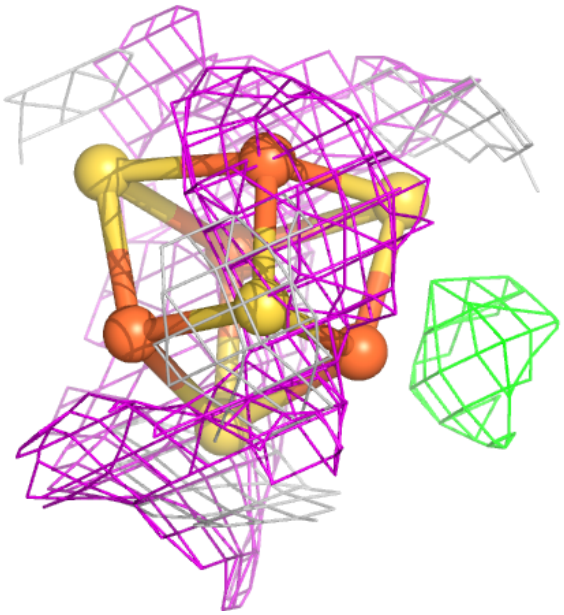
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

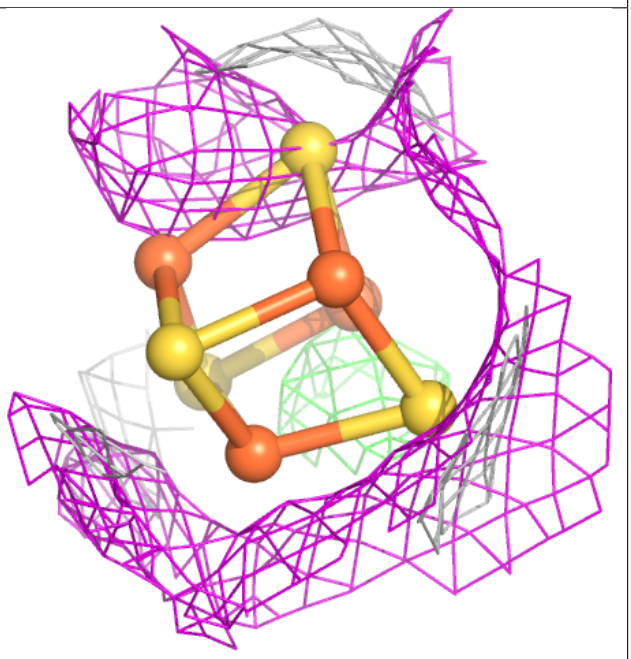


Electron density around SF4 F 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

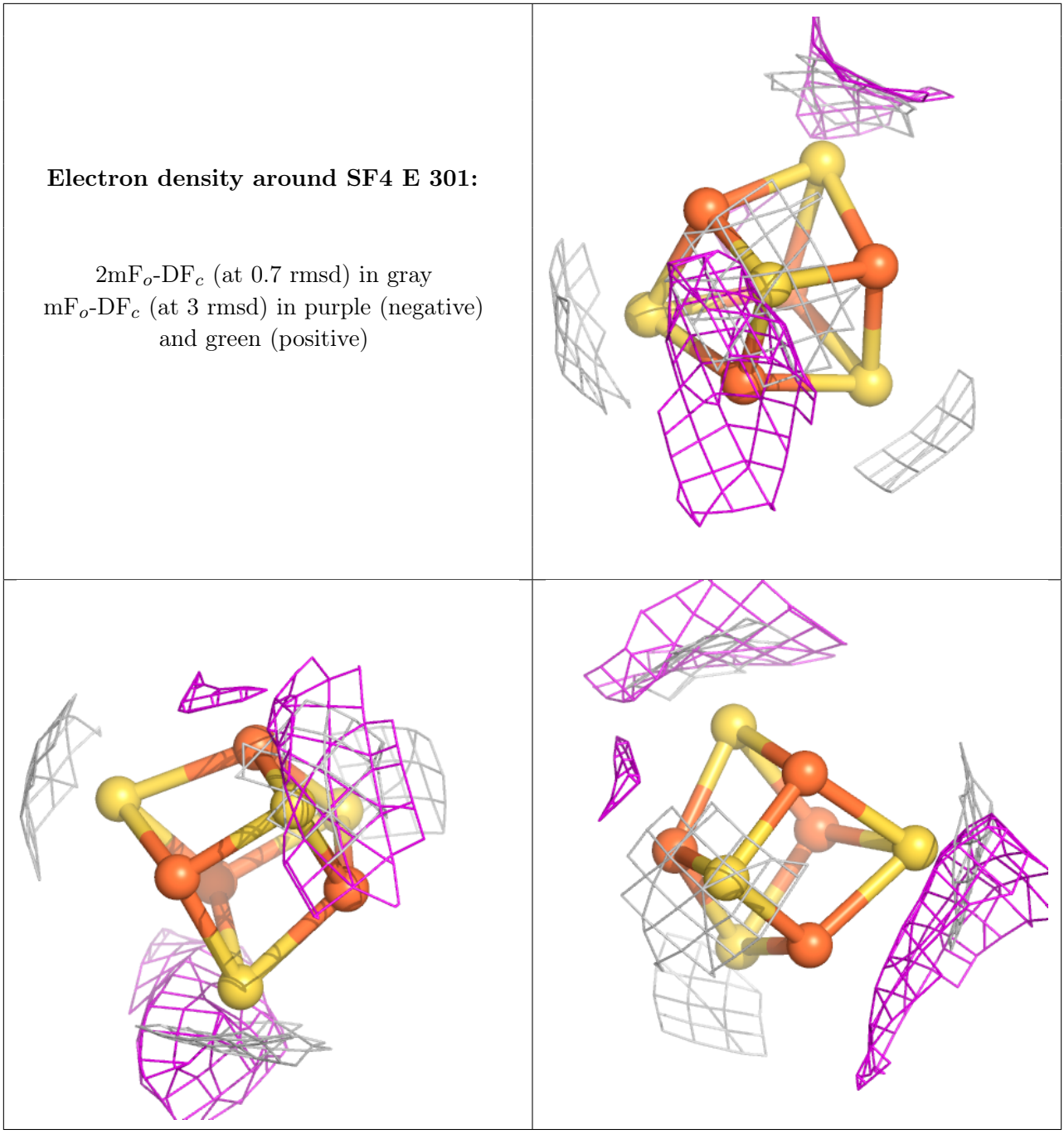






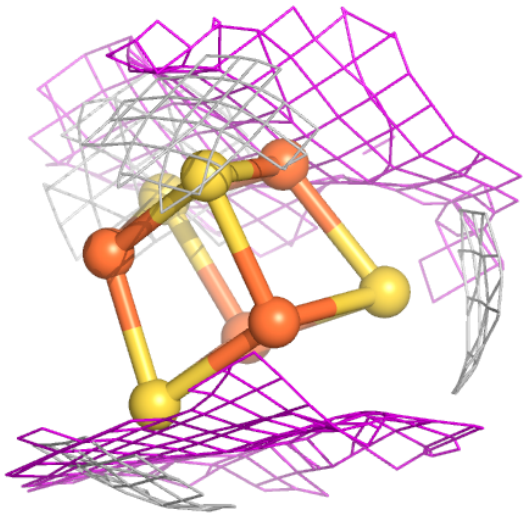
Electron density around SF4 E 301:

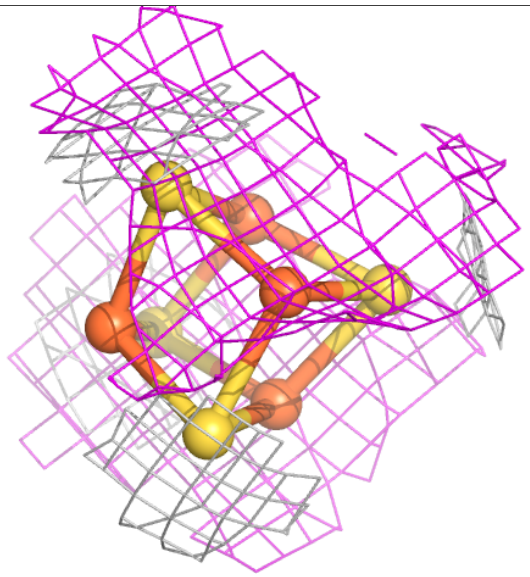
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

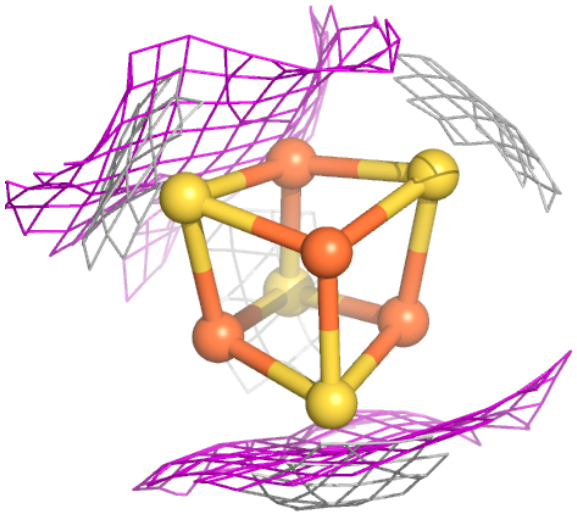


Electron density around SF4 A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

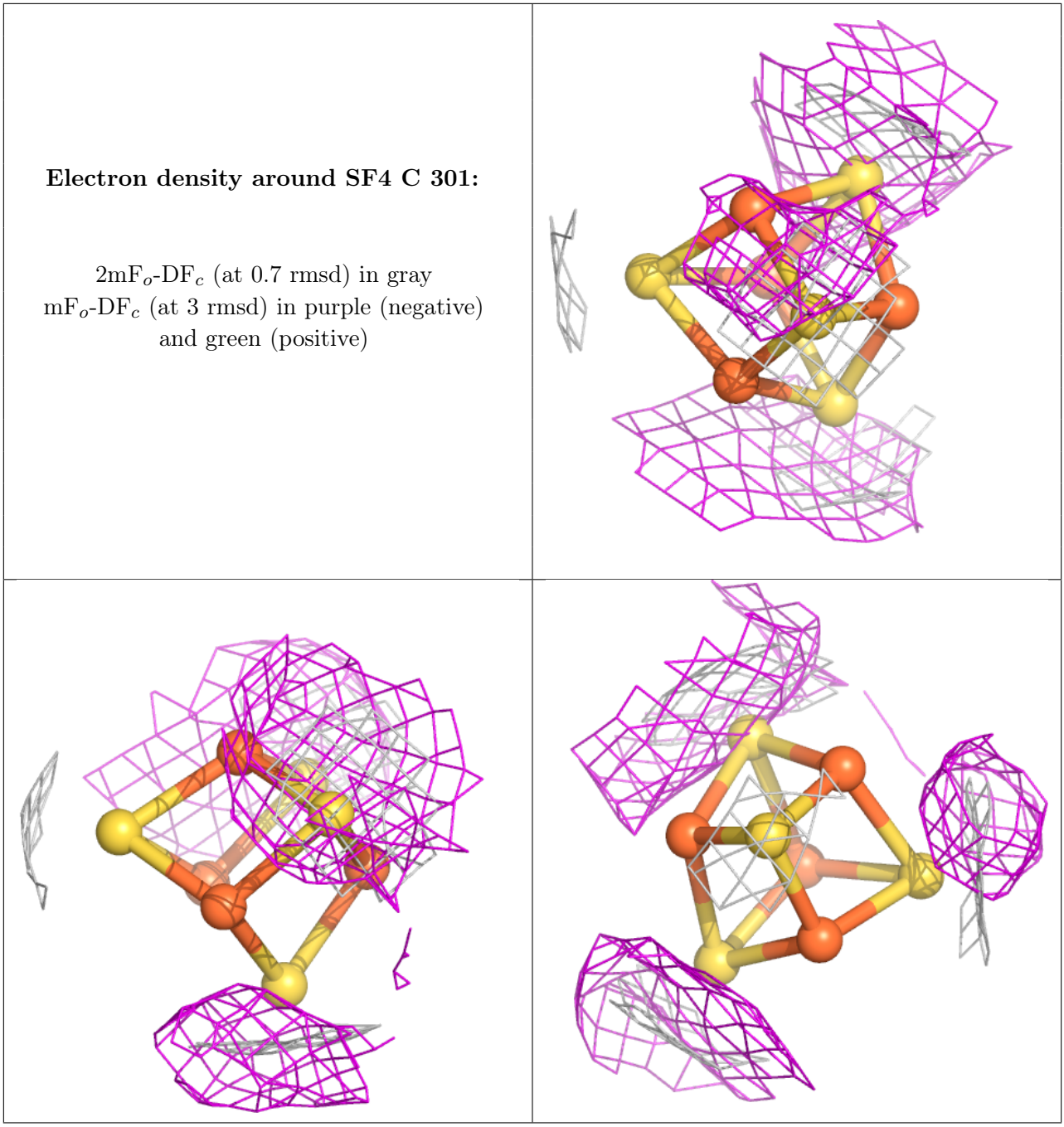






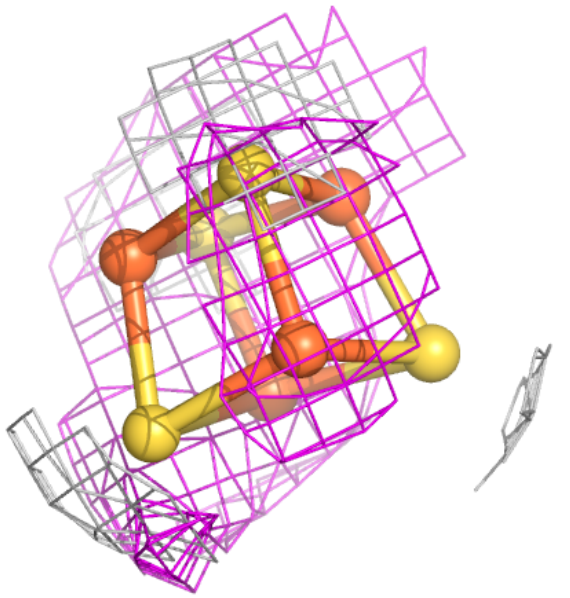
Electron density around SF4 C 301:

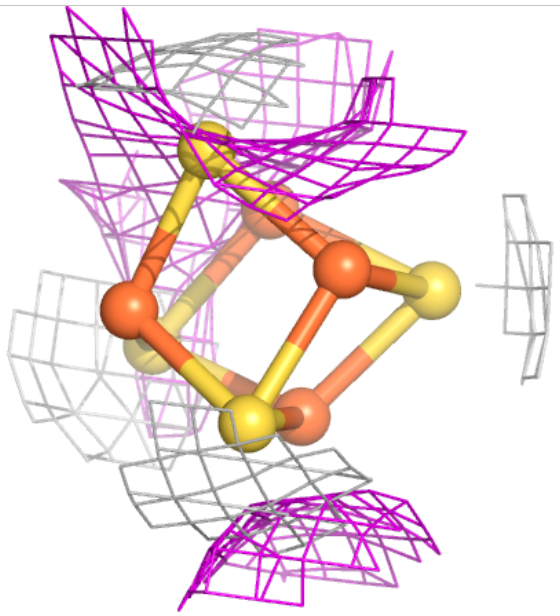
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

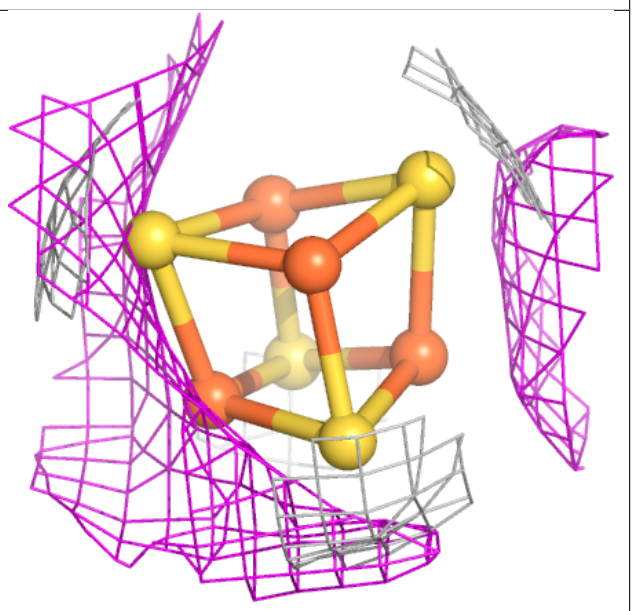


Electron density around SF4 D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

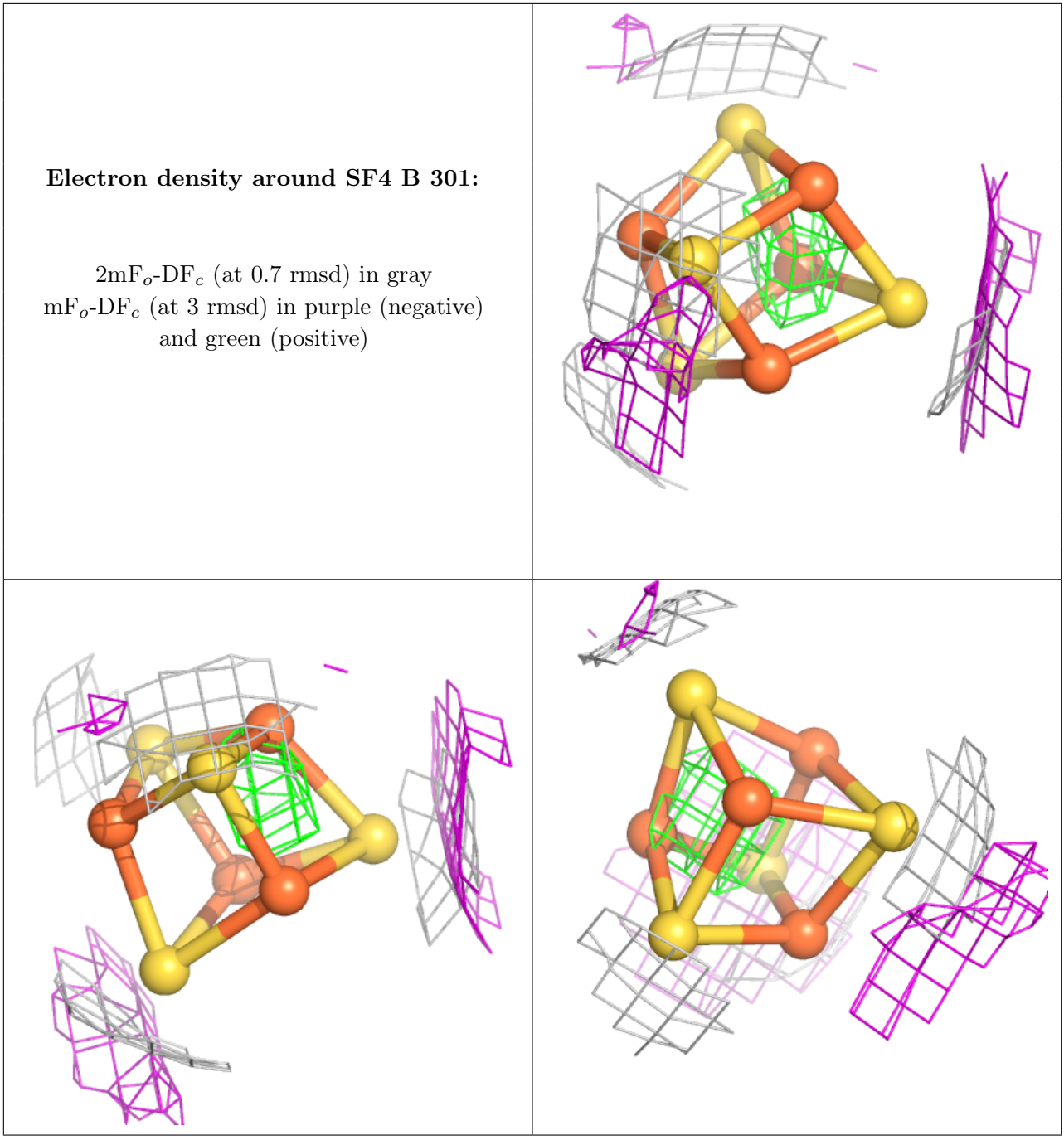






Electron density around SF4 B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.