



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 04:06 pm BST

PDB ID : 9HAZ / pdb_00009haz
Title : A. vinelandii nitrogenase Fe protein Anc1b
Authors : Detemple, F.; Kacar, B.; Einsle, O.
Deposited on : 2024-11-05
Resolution : 2.43 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

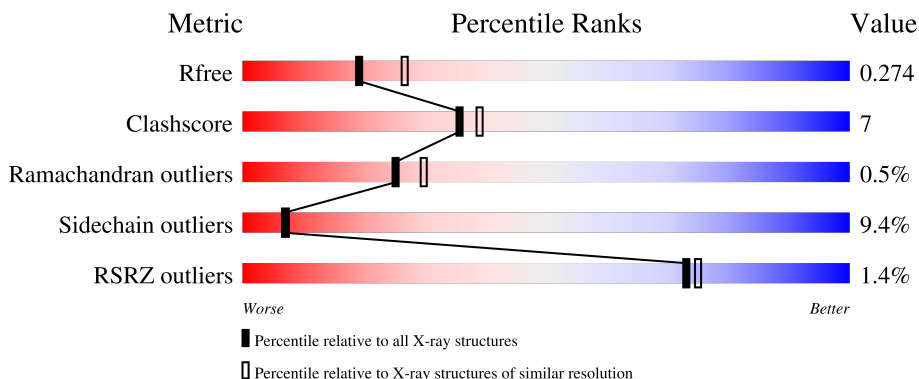
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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 $\leq 5\%$. 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	290	
1	B	290	
1	C	290	
2	D	290	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8854 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.

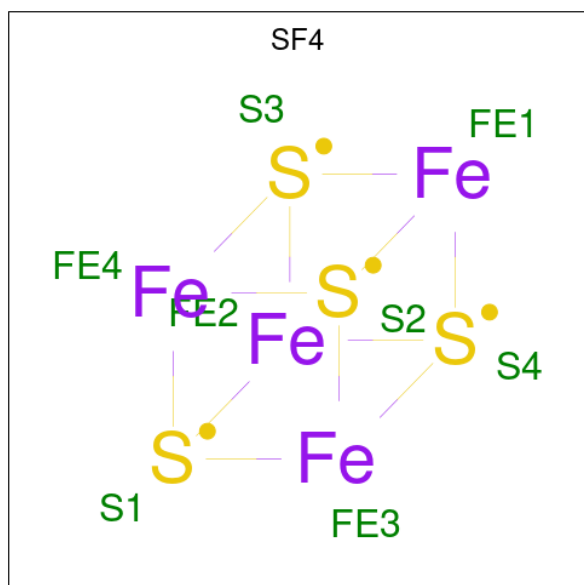
- Molecule 1 is a protein called Fe protein NifH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2169	1352	364	431	22			
1	B	289	Total	C	N	O	S	0	3	0
			2199	1373	368	435	23			
1	C	289	Total	C	N	O	S	0	2	0
			2201	1372	367	439	23			

- Molecule 2 is a protein called Fe protein NifH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	289	Total	C	N	O	S	0	2	0
			2194	1368	367	436	23			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Mg	0	0
			3	3		

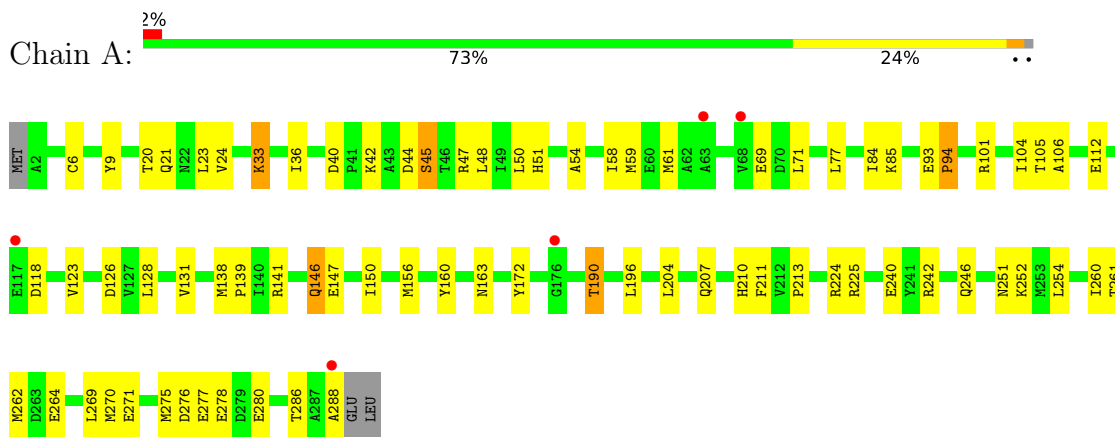
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	13	Total	O	0	0
			13	13		
5	C	26	Total	O	0	0
			26	26		
5	D	14	Total	O	0	0
			14	14		

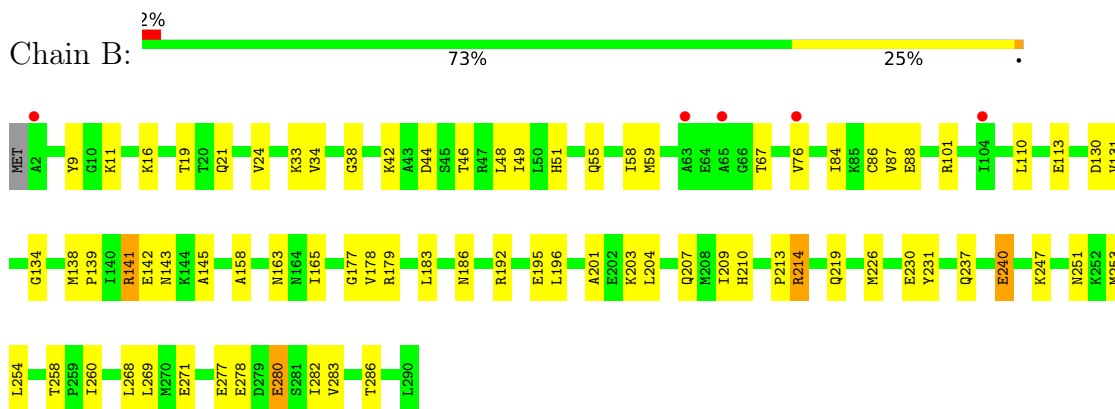
3 Residue-property plots [i](#)

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.

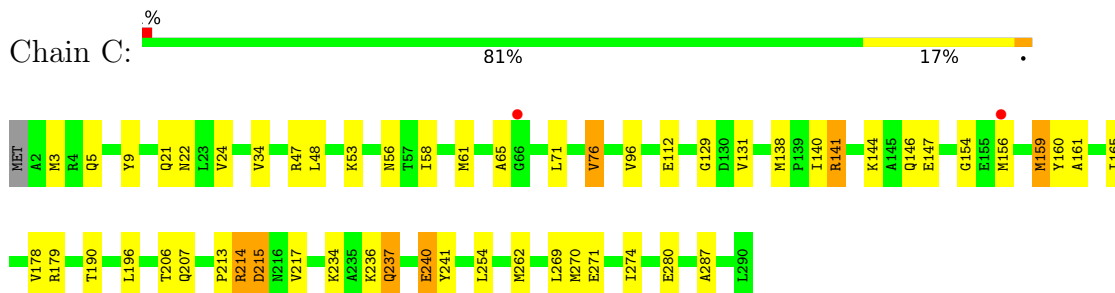
• Molecule 1: Fe protein NifH



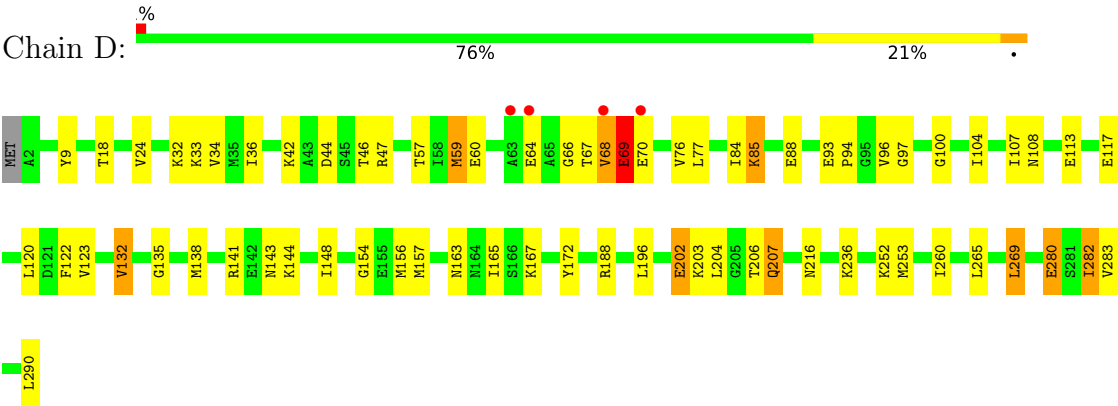
• Molecule 1: Fe protein NifH



• Molecule 1: Fe protein NifH



● Molecule 2: Fe protein NifH



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.35Å 109.78Å 95.21Å 90.00° 118.61° 90.00°	Depositor
Resolution (Å)	69.84 – 2.43 69.84 – 2.43	Depositor EDS
% Data completeness (in resolution range)	64.2 (69.84-2.43) 64.2 (69.84-2.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.195 , 0.272 0.199 , 0.274	Depositor DCC
R_{free} test set	1313 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SF4, MG

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	0.48	0/2192	1.04	3/2949 (0.1%)
1	B	0.48	0/2223	1.01	4/2993 (0.1%)
1	C	0.48	0/2225	1.04	1/2994 (0.0%)
2	D	0.49	0/2218	1.00	2/2988 (0.1%)
All	All	0.48	0/8858	1.03	10/11924 (0.1%)

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	C	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	THR	CA-CB-OG1	-5.71	101.03	109.60
1	B	258	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	190	THR	CA-CB-OG1	-5.62	101.17	109.60
1	C	215	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	44	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	18	THR	CA-CB-OG1	-5.21	101.79	109.60
2	D	46	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	146	GLN	N-CA-CB	5.12	117.88	110.26
1	B	19	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	33	LYS	CB-CA-C	5.07	118.12	109.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	141	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	214	ARG	Sidechain

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	2169	0	2159	37	0
1	B	2199	0	2197	31	1
1	C	2201	0	2196	28	0
2	D	2194	0	2185	34	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	C	3	0	0	0	0
5	A	19	0	0	1	0
5	B	13	0	0	0	0
5	C	26	0	0	0	0
5	D	14	0	0	1	0
All	All	8854	0	8737	126	1

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 7.

All (126) 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)
2:D:143:ASN:HB2	5:D:311:HOH:O	1.79	0.82
1:A:213:PRO:HD2	1:A:240:GLU:HG2	1.60	0.81
1:C:61:MET:HB3	1:C:71:LEU:HD11	1.66	0.77
1:A:240:GLU:OE1	5:A:401:HOH:O	2.01	0.77
1:C:21:GLN:HE22	1:C:48:LEU:H	1.32	0.76
1:A:207:GLN:HE22	1:A:251:ASN:HD21	1.40	0.70
1:B:210:HIS:HE2	1:B:240:GLU:HG3	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:MET:HG3	2:D:157:MET:HE2	1.74	0.69
1:A:261:THR:OG1	1:A:264:GLU:HB2	1.99	0.62
1:B:21:GLN:HE22	1:B:48:LEU:H	1.47	0.62
1:B:192:ARG:NH1	1:B:195:GLU:OE1	2.34	0.60
1:C:213:PRO:HD2	1:C:237:GLN:HE22	1.65	0.60
1:A:286:THR:HG22	1:A:288:ALA:H	1.67	0.60
1:A:213:PRO:CD	1:A:240:GLU:HG2	2.32	0.59
2:D:68:VAL:O	2:D:70:GLU:N	2.35	0.59
1:A:163:ASN:HD21	1:A:260:ILE:H	1.49	0.59
1:B:163:ASN:HD21	1:B:260:ILE:H	1.49	0.59
1:B:58:ILE:HG12	1:B:76:VAL:HG21	1.85	0.59
1:B:51:HIS:HE2	1:B:230:GLU:CD	2.10	0.58
1:A:61:MET:O	1:A:71:LEU:HD11	2.05	0.57
1:C:213:PRO:CD	1:C:240:GLU:HG2	2.36	0.56
2:D:156:MET:CG	2:D:157:MET:HE2	2.37	0.55
1:C:24:VAL:HG13	1:C:34:VAL:HG11	1.89	0.54
1:B:213:PRO:CD	1:B:240:GLU:HG2	2.38	0.54
2:D:24:VAL:HG12	2:D:84:ILE:HD13	1.90	0.54
1:A:210:HIS:NE2	1:A:240:GLU:HG3	2.22	0.54
2:D:24:VAL:HG11	2:D:36:ILE:HD11	1.89	0.53
1:B:179:ARG:HB2	1:B:254[A]:LEU:HD12	1.90	0.53
1:C:21:GLN:NE2	1:C:48:LEU:H	2.06	0.52
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.74	0.52
2:D:154:GLY:O	2:D:188:ARG:NH2	2.42	0.52
2:D:132:VAL:CG2	2:D:132:VAL:O	2.58	0.51
1:A:45:SER:HB2	1:A:126:ASP:OD2	2.10	0.51
1:A:44[B]:ASP:O	1:A:47:ARG:NH1	2.43	0.51
1:C:147:GLU:HG2	1:C:254:LEU:HD11	1.93	0.51
1:A:21:GLN:HE22	1:A:48:LEU:H	1.60	0.50
1:A:51:HIS:O	1:A:225:ARG:NH1	2.39	0.50
1:C:140:ILE:HG23	1:C:178:VAL:HG11	1.92	0.50
1:A:224:ARG:HG2	2:D:282:ILE:HG23	1.93	0.50
2:D:207:GLN:HG2	2:D:253:MET:SD	2.51	0.50
1:C:56:ASN:HB2	1:C:61:MET:HE1	1.93	0.50
2:D:100:GLY:HA3	2:D:138:MET:HE2	1.93	0.50
1:A:77:LEU:HD21	1:A:85:LYS:HD2	1.93	0.50
1:A:242:ARG:O	1:A:246:GLN:HB2	2.11	0.49
2:D:107:ILE:HG21	2:D:144:LYS:HD2	1.94	0.49
1:A:24:VAL:HG12	1:A:84:ILE:HD13	1.95	0.49
1:A:44[A]:ASP:O	1:A:47:ARG:NH1	2.44	0.49
1:A:270:MET:HA	1:A:275:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:MET:HE1	1:C:141:ARG:NH1	2.28	0.49
1:B:209:ILE:O	1:B:247:LYS:HD3	2.13	0.49
1:B:9:TYR:HB3	1:B:165:ILE:HD13	1.95	0.49
2:D:77:LEU:HD21	2:D:85:LYS:HG2	1.95	0.49
2:D:135:GLY:O	2:D:138:MET:HB2	2.13	0.49
1:B:87:VAL:HG11	1:B:110:LEU:HD11	1.95	0.48
2:D:141:ARG:HG3	2:D:172:TYR:CE1	2.49	0.48
1:B:143:ASN:HD21	1:B:177:GLY:H	1.62	0.48
1:C:206:THR:OG1	1:C:207:GLN:N	2.46	0.48
2:D:282:ILE:HD12	2:D:290:LEU:CD2	2.44	0.47
1:B:21:GLN:HE21	1:B:49:ILE:HG12	1.80	0.47
1:C:160:TYR:CE1	1:C:262:MET:HE1	2.49	0.47
1:A:211:PHE:O	1:A:213:PRO:HD3	2.14	0.47
1:B:280:GLU:O	1:B:283:VAL:HG12	2.14	0.47
2:D:163:ASN:HD21	2:D:260:ILE:H	1.60	0.47
1:A:50:LEU:O	1:A:51:HIS:HB2	2.14	0.47
1:B:251:ASN:ND2	1:B:253:MET:H	2.13	0.47
2:D:9:TYR:HB3	2:D:165:ILE:HD13	1.97	0.47
2:D:216[A]:ASN:O	2:D:216[A]:ASN:OD1	2.31	0.47
1:A:141:ARG:HG3	1:A:172:TYR:CE1	2.50	0.47
2:D:59[A]:MET:HG3	2:D:60:GLU:N	2.28	0.46
1:A:94:PRO:HG3	2:D:167:LYS:HD3	1.97	0.46
1:C:159:MET:HE3	1:C:159:MET:HB3	1.84	0.46
1:A:207:GLN:HE22	1:A:251:ASN:ND2	2.09	0.46
2:D:34:VAL:HA	2:D:122:PHE:O	2.16	0.46
2:D:44:ASP:HB2	2:D:47:ARG:HD2	1.97	0.46
1:A:160:TYR:HE2	2:D:42:LYS:HA	1.81	0.46
2:D:265:LEU:O	2:D:269:LEU:HD22	2.15	0.46
1:B:46:THR:HB	1:B:86:CYS:HB3	1.98	0.46
1:C:9:TYR:HB3	1:C:165:ILE:HD13	1.98	0.45
1:B:38:GLY:HA3	1:B:88:GLU:OE1	2.16	0.45
1:A:147:GLU:HG2	1:A:254:LEU:HD11	1.98	0.45
1:B:11:LYS:HD2	1:B:158:ALA:HA	1.98	0.45
1:B:24:VAL:HG13	1:B:34:VAL:HG11	1.99	0.45
1:C:21:GLN:HE22	1:C:48:LEU:N	2.09	0.45
1:A:9:TYR:O	1:A:150:ILE:HA	2.16	0.45
1:B:231:TYR:CE1	1:C:287:ALA:HB2	2.52	0.44
1:C:5:GLN:HB3	1:C:144:LYS:O	2.18	0.44
1:A:58:ILE:HD12	1:A:106:ALA:HB1	1.99	0.44
1:C:61:MET:HE2	1:C:61:MET:HB2	1.90	0.44
1:A:40:ASP:OD1	1:A:128:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:HG21	1:B:55:GLN:HE22	1.83	0.43
1:C:154:GLY:O	1:C:274:ILE:HG12	2.16	0.43
1:C:71:LEU:HD21	1:C:76:VAL:HG21	2.00	0.43
2:D:280:GLU:HA	2:D:283:VAL:HG23	1.99	0.43
1:B:138:MET:HB3	1:B:139:PRO:HD3	2.00	0.43
1:A:104:ILE:O	1:A:105:THR:C	2.62	0.43
1:A:44[B]:ASP:OD2	1:A:54:ALA:HA	2.18	0.43
1:B:214:ARG:NH2	1:B:219:GLN:OE1	2.52	0.43
1:B:48:LEU:O	1:B:226:MET:HA	2.19	0.43
1:B:213:PRO:HD2	1:B:237:GLN:HE22	1.83	0.43
2:D:57:THR:HA	2:D:88:GLU:O	2.19	0.43
2:D:96:VAL:HG23	2:D:97:GLY:N	2.34	0.42
1:A:138:MET:HB3	1:A:139:PRO:HD3	2.00	0.42
1:C:237:GLN:HE21	1:C:237:GLN:HA	1.85	0.42
1:A:59:MET:HE1	1:A:93:GLU:HG2	2.01	0.42
1:B:207:GLN:HE22	1:B:251:ASN:ND2	2.18	0.42
1:C:215:ASP:OD1	1:C:217:VAL:HG12	2.19	0.42
1:B:134:GLY:O	1:B:141:ARG:NH1	2.52	0.42
1:B:145:ALA:O	1:B:178:VAL:HG22	2.19	0.42
1:A:20:THR:O	1:A:24:VAL:HG23	2.20	0.42
1:C:22:ASN:HB3	1:C:241:TYR:CD2	2.55	0.42
1:C:129:GLY:O	1:C:161:ALA:HB1	2.20	0.42
1:C:179:ARG:HB2	1:C:254:LEU:HD12	2.02	0.41
2:D:68:VAL:C	2:D:69:GLU:HG3	2.45	0.41
2:D:132:VAL:O	2:D:132:VAL:HG23	2.19	0.41
1:A:6:CYS:HA	1:A:147:GLU:O	2.21	0.41
2:D:202:GLU:HG2	2:D:203:LYS:N	2.35	0.41
1:A:24:VAL:HG11	1:A:36:ILE:HD11	2.01	0.41
1:B:24:VAL:HG12	1:B:84:ILE:HD13	2.02	0.41
1:C:47:ARG:NH1	1:C:53:LYS:O	2.53	0.41
1:C:58:ILE:HG12	1:C:76:VAL:HG22	2.02	0.41
1:C:237:GLN:HA	1:C:237:GLN:NE2	2.36	0.41
1:A:156:MET:HE1	1:A:262:MET:SD	2.60	0.41
2:D:93:GLU:O	2:D:94:PRO:C	2.64	0.41
1:B:183:LEU:HD12	1:B:201:ALA:HB2	2.03	0.40
2:D:108:ASN:HD22	2:D:108:ASN:HA	1.72	0.40
2:D:282:ILE:CD1	2:D:290:LEU:HD23	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:OE2	1:B:271:GLU:OE2[2_656]	2.02	0.18

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	286/290 (99%)	272 (95%)	13 (4%)	1 (0%)	37	44
1	B	290/290 (100%)	281 (97%)	9 (3%)	0	100	100
1	C	289/290 (100%)	277 (96%)	10 (4%)	2 (1%)	19	22
2	D	289/290 (100%)	273 (94%)	13 (4%)	3 (1%)	13	13
All	All	1154/1160 (100%)	1103 (96%)	45 (4%)	6 (0%)	25	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	69	GLU
1	C	65	ALA
2	D	64	GLU
1	C	3	MET
1	A	94	PRO
2	D	66	GLY

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	228/232 (98%)	207 (91%)	21 (9%)	7	7
1	B	232/232 (100%)	209 (90%)	23 (10%)	6	6
1	C	233/232 (100%)	215 (92%)	18 (8%)	10	12
2	D	231/232 (100%)	205 (89%)	26 (11%)	4	4
All	All	924/928 (100%)	836 (90%)	88 (10%)	7	7

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	33	LYS
1	A	42	LYS
1	A	45	SER
1	A	69	GLU
1	A	101	ARG
1	A	112	GLU
1	A	118	ASP
1	A	123	VAL
1	A	131	VAL
1	A	146	GLN
1	A	190	THR
1	A	196	LEU
1	A	204	LEU
1	A	252	LYS
1	A	269	LEU
1	A	271	GLU
1	A	276	ASP
1	A	277	GLU
1	A	278	GLU
1	A	280	GLU
1	B	16	LYS
1	B	33	LYS
1	B	42	LYS
1	B	59[A]	MET
1	B	59[B]	MET
1	B	67	THR
1	B	101	ARG
1	B	113	GLU
1	B	130	ASP
1	B	131	VAL
1	B	142	GLU
1	B	186	ASN

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Mol	Chain	Res	Type
1	B	196	LEU
1	B	203	LYS
1	B	204	LEU
1	B	214	ARG
1	B	240	GLU
1	B	268	LEU
1	B	269	LEU
1	B	277	GLU
1	B	278	GLU
1	B	280	GLU
1	B	282	ILE
1	C	76	VAL
1	C	96	VAL
1	C	112	GLU
1	C	131	VAL
1	C	146	GLN
1	C	156	MET
1	C	159	MET
1	C	190	THR
1	C	196	LEU
1	C	214	ARG
1	C	234	LYS
1	C	236	LYS
1	C	237	GLN
1	C	240	GLU
1	C	269	LEU
1	C	270	MET
1	C	271	GLU
1	C	280	GLU
2	D	32	LYS
2	D	33	LYS
2	D	59[A]	MET
2	D	59[B]	MET
2	D	67	THR
2	D	68	VAL
2	D	69	GLU
2	D	76	VAL
2	D	85	LYS
2	D	104	ILE
2	D	113	GLU
2	D	117	GLU
2	D	120	LEU

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Mol	Chain	Res	Type
2	D	123	VAL
2	D	132	VAL
2	D	148	ILE
2	D	196	LEU
2	D	202	GLU
2	D	204	LEU
2	D	206	THR
2	D	207	GLN
2	D	236	LYS
2	D	252	LYS
2	D	269	LEU
2	D	280	GLU
2	D	282	ILE

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	55	GLN
1	A	163	ASN
1	A	164	ASN
1	A	251	ASN
1	B	21	GLN
1	B	55	GLN
1	B	108	ASN
1	B	143	ASN
1	B	146	GLN
1	B	163	ASN
1	B	164	ASN
1	B	186	ASN
1	B	237	GLN
1	B	251	ASN
1	C	21	GLN
1	C	108	ASN
1	C	146	GLN
1	C	163	ASN
1	C	164	ASN
1	C	186	ASN
1	C	237	GLN
1	C	251	ASN
2	D	108	ASN
2	D	146	GLN

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Mol	Chain	Res	Type
2	D	163	ASN
2	D	164	ASN
2	D	186	ASN
2	D	219	GLN
2	D	237	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
3	SF4	A	301	2,1	0,12,12	-	-	-		
3	SF4	B	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
3	SF4	A	301	2,1	-	-	0/6/5/5
3	SF4	B	301	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

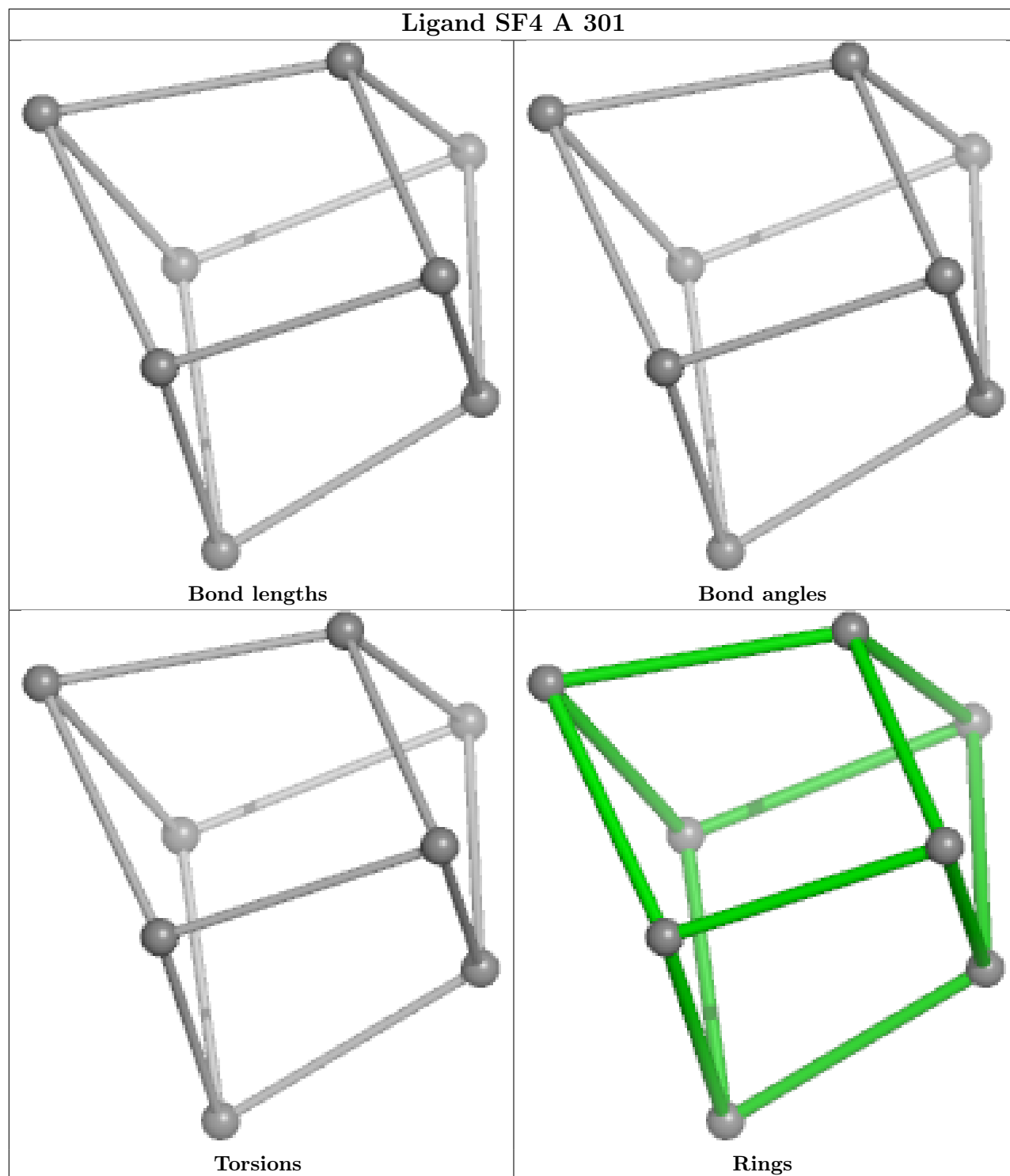
There are no torsion outliers.

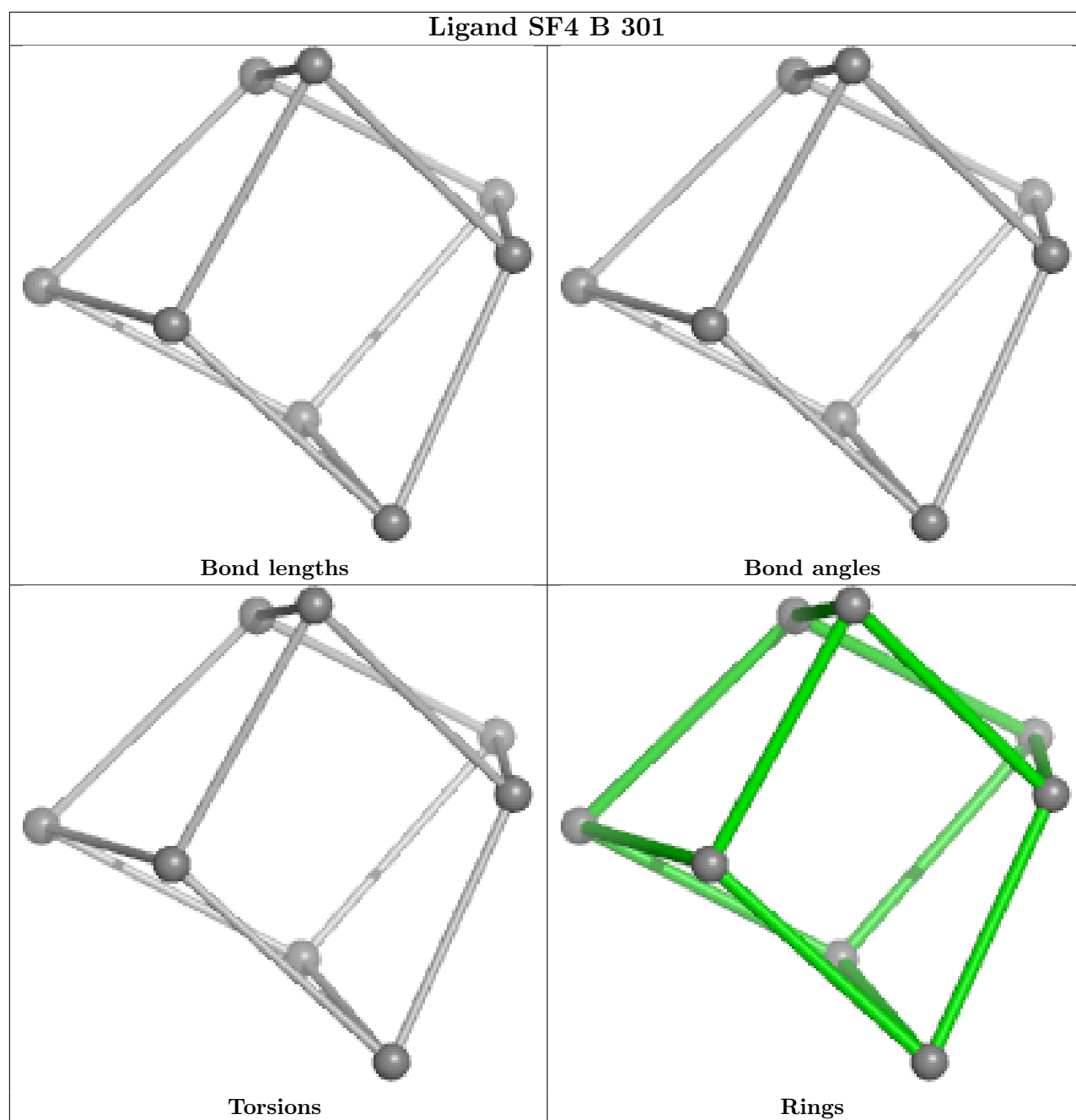
There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand SF4 A 301





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	287/290 (98%)	-0.24	5 (1%) 69 70	11, 24, 56, 69	1 (0%)
1	B	289/290 (99%)	-0.14	5 (1%) 69 70	10, 26, 49, 75	3 (1%)
1	C	289/290 (99%)	-0.21	2 (0%) 84 85	12, 27, 46, 63	2 (0%)
2	D	289/290 (99%)	-0.14	4 (1%) 73 75	9, 28, 52, 82	2 (0%)
All	All	1154/1160 (99%)	-0.18	16 (1%) 73 75	9, 27, 52, 82	8 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	64	GLU	3.9
1	B	65	ALA	3.5
1	B	2	ALA	2.9
1	C	156	MET	2.6
2	D	63	ALA	2.6
1	B	104	ILE	2.6
1	A	117	GLU	2.5
1	A	68	VAL	2.5
1	A	288	ALA	2.5
1	B	63	ALA	2.3
1	B	76	VAL	2.2
1	C	66	GLY	2.1
1	A	176	GLY	2.1
1	A	63	ALA	2.1
2	D	70	GLU	2.0
2	D	68	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

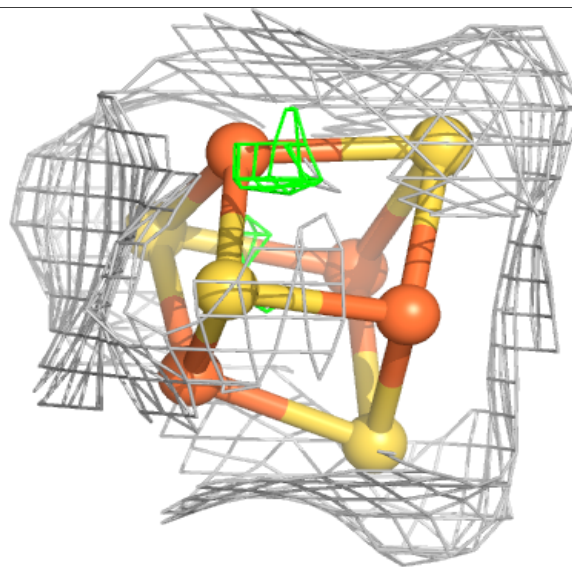
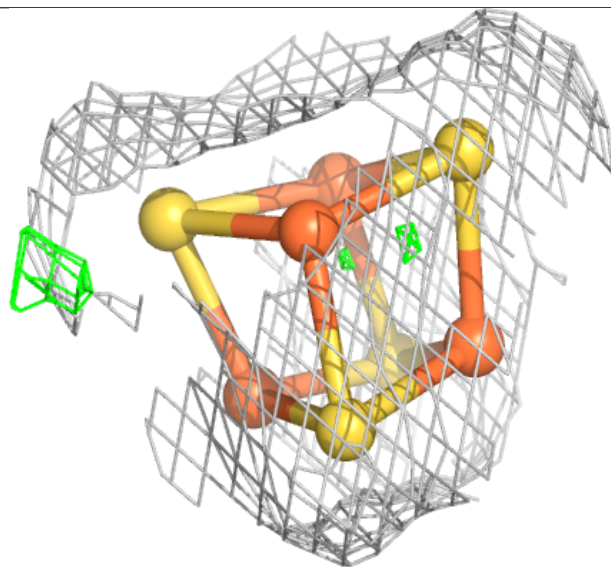
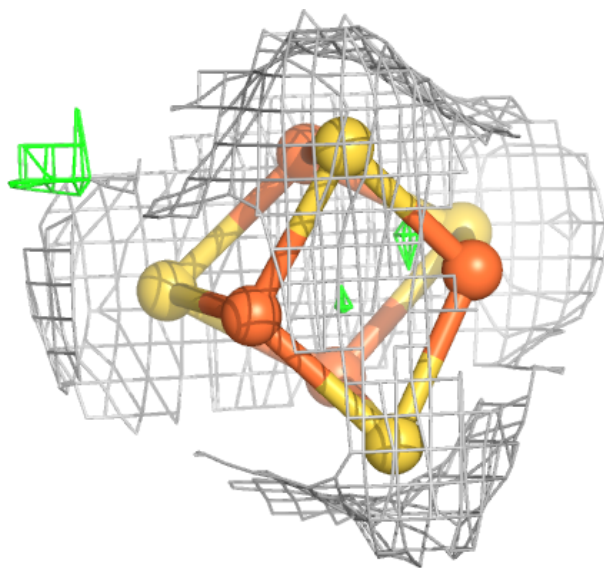
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	301	1/1	0.95	0.03	22,22,22,22	1
4	MG	C	302	1/1	0.96	0.04	24,24,24,24	0
4	MG	C	303	1/1	0.97	0.13	13,13,13,13	0
3	SF4	B	301	8/8	0.98	0.04	18,19,22,22	0
3	SF4	A	301	8/8	0.99	0.03	17,19,20,20	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.

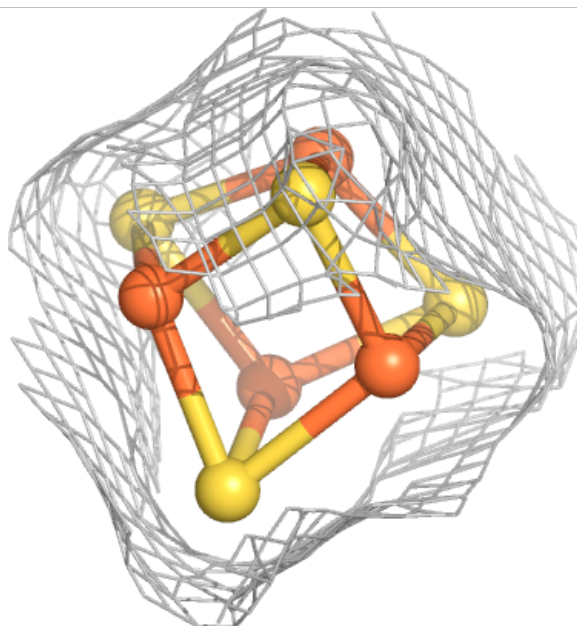
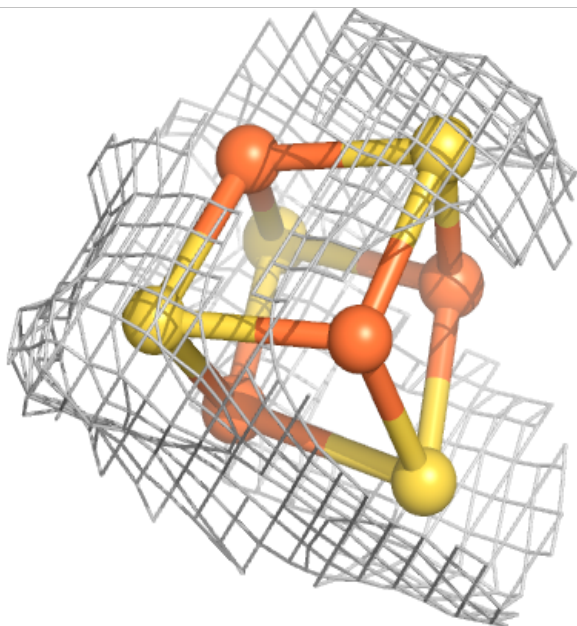
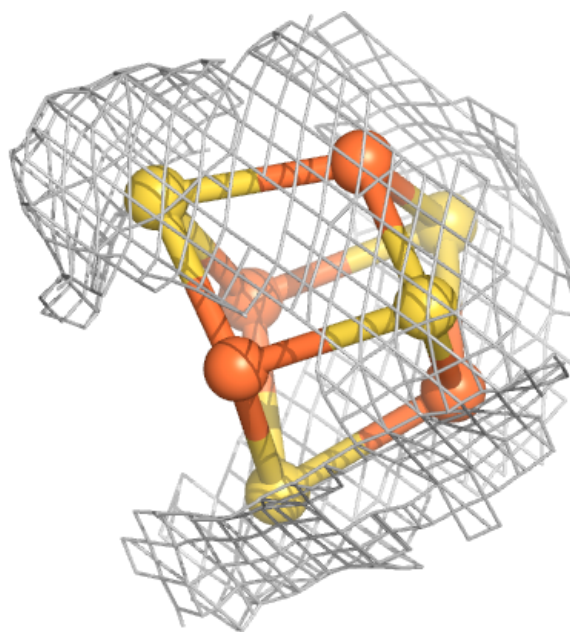
Electron density around SF4 B 301:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.