



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:59 PM UTC

PDB ID : 9F46 / pdb_00009f46
Title : crystal structure of apo-[FeFe]-hydrogenase CbA5H from *Clostridium beijerinckii*
Authors : Duan, J.; Rutz, A.; Hofmann, E.; Happe, T.; Kurisu, G.
Deposited on : 2024-04-26
Resolution : 2.45 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

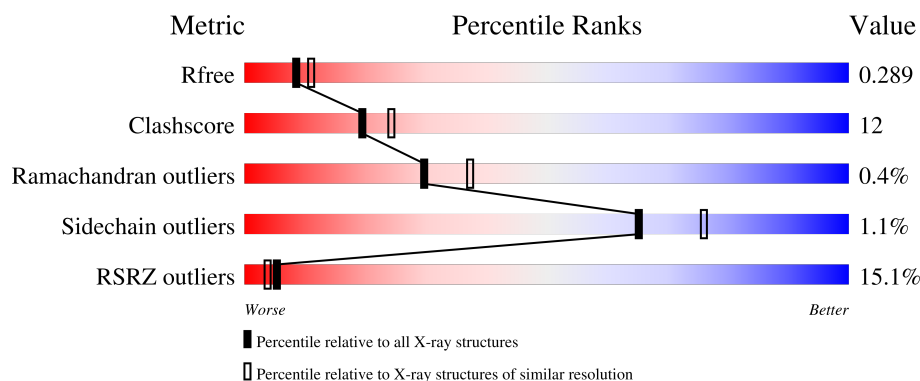
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	674	11% 72% 20% 8%
1	B	674	17% 72% 19% 8%

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	B	702	-	-	X	-
4	CL	A	711	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19448 atoms, of which 9666 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 [FeFe]-hydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	621	Total	C	H	N	O	S	0	0	0
			9696	3070	4844	819	927	36			
1	B	618	Total	C	H	N	O	S	0	0	0
			9654	3057	4822	816	923	36			

There are 60 discrepancies between the modelled and reference sequences:

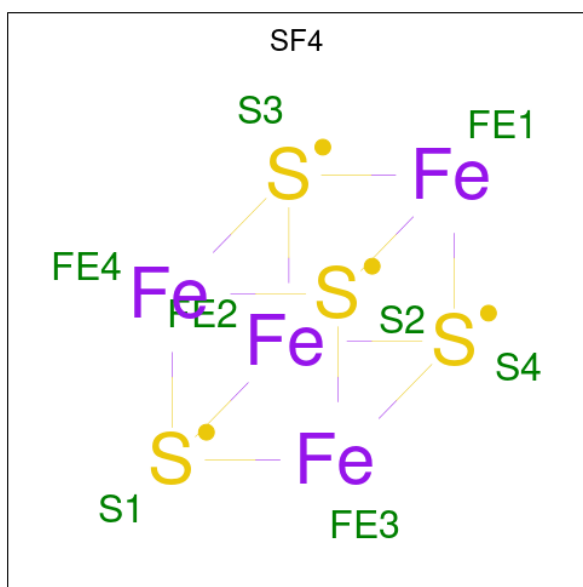
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ASP	-	expression tag	UNP A0A1I9RYV3
A	646	ILE	-	expression tag	UNP A0A1I9RYV3
A	647	TRP	-	expression tag	UNP A0A1I9RYV3
A	648	SER	-	expression tag	UNP A0A1I9RYV3
A	649	VAL	-	expression tag	UNP A0A1I9RYV3
A	650	GLY	-	expression tag	UNP A0A1I9RYV3
A	651	VAL	-	expression tag	UNP A0A1I9RYV3
A	652	LYS	-	expression tag	UNP A0A1I9RYV3
A	653	LEU	-	expression tag	UNP A0A1I9RYV3
A	654	PHE	-	expression tag	UNP A0A1I9RYV3
A	655	GLY	-	expression tag	UNP A0A1I9RYV3
A	656	GLY	-	expression tag	UNP A0A1I9RYV3
A	657	GLY	-	expression tag	UNP A0A1I9RYV3
A	658	SER	-	expression tag	UNP A0A1I9RYV3
A	659	GLY	-	expression tag	UNP A0A1I9RYV3
A	660	GLY	-	expression tag	UNP A0A1I9RYV3
A	661	GLY	-	expression tag	UNP A0A1I9RYV3
A	662	SER	-	expression tag	UNP A0A1I9RYV3
A	663	GLY	-	expression tag	UNP A0A1I9RYV3
A	664	GLY	-	expression tag	UNP A0A1I9RYV3
A	665	GLY	-	expression tag	UNP A0A1I9RYV3
A	666	SER	-	expression tag	UNP A0A1I9RYV3
A	667	TRP	-	expression tag	UNP A0A1I9RYV3
A	668	SER	-	expression tag	UNP A0A1I9RYV3
A	669	HIS	-	expression tag	UNP A0A1I9RYV3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	670	PRO	-	expression tag	UNP A0A1I9RYV3
A	671	GLN	-	expression tag	UNP A0A1I9RYV3
A	672	PHE	-	expression tag	UNP A0A1I9RYV3
A	673	GLU	-	expression tag	UNP A0A1I9RYV3
A	674	LYS	-	expression tag	UNP A0A1I9RYV3
B	645	ASP	-	expression tag	UNP A0A1I9RYV3
B	646	ILE	-	expression tag	UNP A0A1I9RYV3
B	647	TRP	-	expression tag	UNP A0A1I9RYV3
B	648	SER	-	expression tag	UNP A0A1I9RYV3
B	649	VAL	-	expression tag	UNP A0A1I9RYV3
B	650	GLY	-	expression tag	UNP A0A1I9RYV3
B	651	VAL	-	expression tag	UNP A0A1I9RYV3
B	652	LYS	-	expression tag	UNP A0A1I9RYV3
B	653	LEU	-	expression tag	UNP A0A1I9RYV3
B	654	PHE	-	expression tag	UNP A0A1I9RYV3
B	655	GLY	-	expression tag	UNP A0A1I9RYV3
B	656	GLY	-	expression tag	UNP A0A1I9RYV3
B	657	GLY	-	expression tag	UNP A0A1I9RYV3
B	658	SER	-	expression tag	UNP A0A1I9RYV3
B	659	GLY	-	expression tag	UNP A0A1I9RYV3
B	660	GLY	-	expression tag	UNP A0A1I9RYV3
B	661	GLY	-	expression tag	UNP A0A1I9RYV3
B	662	SER	-	expression tag	UNP A0A1I9RYV3
B	663	GLY	-	expression tag	UNP A0A1I9RYV3
B	664	GLY	-	expression tag	UNP A0A1I9RYV3
B	665	GLY	-	expression tag	UNP A0A1I9RYV3
B	666	SER	-	expression tag	UNP A0A1I9RYV3
B	667	TRP	-	expression tag	UNP A0A1I9RYV3
B	668	SER	-	expression tag	UNP A0A1I9RYV3
B	669	HIS	-	expression tag	UNP A0A1I9RYV3
B	670	PRO	-	expression tag	UNP A0A1I9RYV3
B	671	GLN	-	expression tag	UNP A0A1I9RYV3
B	672	PHE	-	expression tag	UNP A0A1I9RYV3
B	673	GLU	-	expression tag	UNP A0A1I9RYV3
B	674	LYS	-	expression tag	UNP A0A1I9RYV3

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Cl	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	Cl	0	0
			5	5		

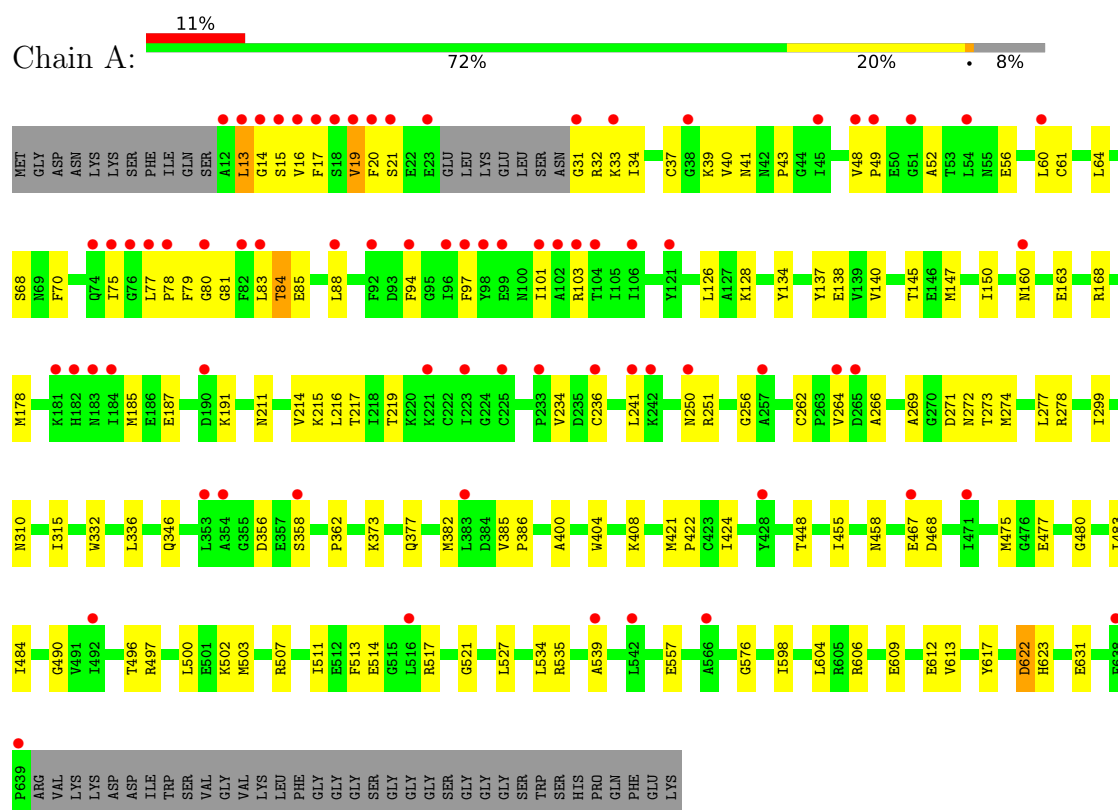
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	20	Total	O	0	0
			20	20		

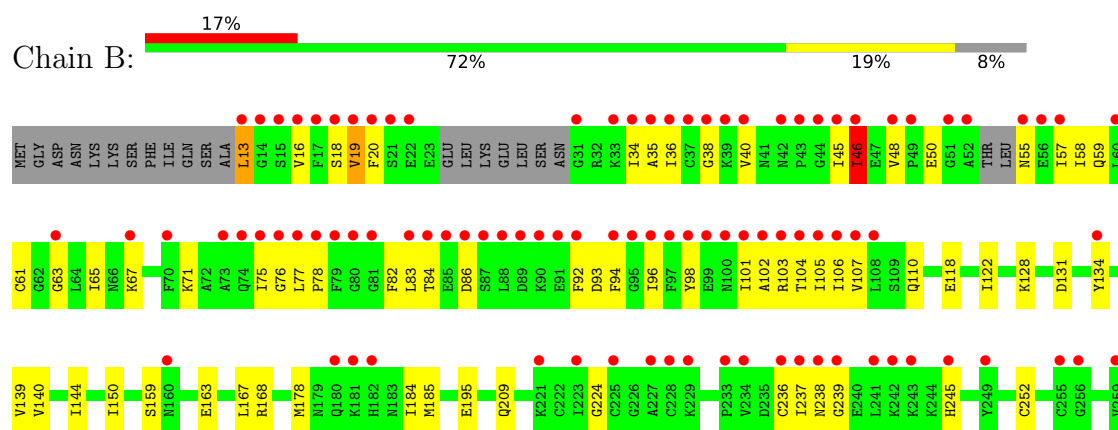
3 Residue-property plots [i](#)

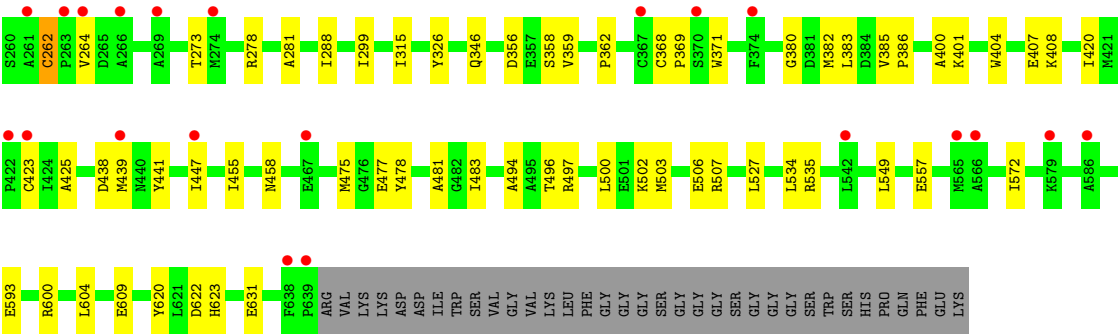
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: [FeFe]-hydrogenase



- Molecule 1: [FeFe]-hydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.90Å 167.90Å 125.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.45 48.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.89-2.45) 100.0 (48.89-2.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.239 , 0.289 0.239 , 0.289	Depositor DCC
R_{free} test set	3308 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19448	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0114e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SF4, ZN

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	0.20	0/4931	0.42	1/6635 (0.0%)
1	B	0.18	0/4910	0.44	3/6604 (0.0%)
All	All	0.19	0/9841	0.43	4/13239 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	THR	CA-CB-CG2	-6.50	99.46	110.50
1	B	239	GLY	N-CA-C	-6.07	98.80	113.18
1	B	262	CYS	CA-C-N	-5.44	114.07	119.56
1	B	262	CYS	C-N-CA	-5.44	114.07	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4852	4844	4845	115	0
1	B	4832	4822	4821	114	0
2	A	24	0	0	0	0
2	B	24	0	0	3	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	7	0	0	1	0
4	B	5	0	0	1	0
5	A	16	0	0	1	0
5	B	20	0	0	1	0
All	All	9782	9666	9666	225	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 12.

All (225) 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:19:VAL:HG13	1:A:277:LEU:HD11	1.32	1.06
1:A:84:THR:HG21	1:A:191:LYS:HE3	1.42	1.02
1:B:34:ILE:HD12	1:B:48:VAL:HG11	1.48	0.95
1:A:19:VAL:HG21	1:A:273:THR:CG2	2.02	0.90
1:A:19:VAL:HG13	1:A:277:LEU:CD1	2.06	0.85
1:A:19:VAL:HG21	1:A:273:THR:HG22	1.59	0.81
1:B:19:VAL:HG11	1:B:455:ILE:HA	1.63	0.81
1:B:58:ILE:HD12	1:B:59:GLN:N	1.97	0.80
1:B:140:VAL:HG23	1:B:144:ILE:HD12	1.62	0.80
1:A:84:THR:HG21	1:A:191:LYS:CE	2.13	0.79
1:B:58:ILE:HD13	1:B:63:GLY:HA2	1.66	0.76
1:A:19:VAL:HG11	1:A:455:ILE:HG12	1.67	0.75
1:B:76:GLY:HA2	1:B:102:ALA:HB3	1.69	0.74
1:B:245:HIS:ND1	2:B:702:SF4:S3	2.61	0.72
1:A:273:THR:HG23	1:A:455:ILE:HD11	1.72	0.72
1:B:101:ILE:HG23	1:B:103:ARG:H	1.55	0.70
1:B:369:PRO:HG2	1:B:425:ALA:HB1	1.74	0.69
1:B:593:GLU:OE2	1:B:600:ARG:NH2	2.26	0.68
1:A:77:LEU:HB3	1:A:78:PRO:HD3	1.76	0.67
1:A:19:VAL:HG21	1:A:273:THR:HG21	1.76	0.66
1:B:400:ALA:HA	1:B:475:MET:HE1	1.77	0.65
1:A:16:VAL:HG13	1:A:19:VAL:H	1.61	0.65
1:B:362:PRO:O	1:B:385:VAL:HG13	1.97	0.65
1:B:140:VAL:HG23	1:B:144:ILE:CD1	2.26	0.64
1:A:168:ARG:NH2	1:B:631:GLU:OE2	2.30	0.64
1:A:187:GLU:O	1:A:191:LYS:HD3	2.00	0.62
1:A:14:GLY:O	1:A:15:SER:OG	2.14	0.62
1:B:185:MET:HE2	1:B:185:MET:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD1	1:A:273:THR:OG1	2.13	0.61
1:A:467:GLU:OE2	1:A:468:ASP:O	2.19	0.61
1:B:13:LEU:HD12	1:B:281:ALA:HB1	1.81	0.61
1:B:423:CYS:SG	1:B:425:ALA:HB3	2.41	0.60
1:A:64:LEU:HD12	1:A:68:SER:O	2.02	0.60
1:A:400:ALA:HA	1:A:475:MET:HE1	1.83	0.59
1:B:57:ILE:HD11	1:B:92:PHE:CG	2.37	0.59
1:A:216:LEU:HD13	1:A:269:ALA:HB2	1.85	0.59
1:B:16:VAL:CG1	1:B:20:PHE:HB2	2.33	0.59
1:B:75:ILE:HD13	1:B:105:ILE:HD12	1.85	0.59
1:B:604:LEU:HD22	1:B:609:GLU:HB3	1.83	0.59
1:B:45:ILE:C	1:B:46:ILE:HG13	2.28	0.58
1:B:36:ILE:CG2	1:B:40:VAL:HG21	2.33	0.58
1:A:16:VAL:HG13	1:A:19:VAL:N	2.18	0.57
1:B:139:VAL:HG13	1:B:140:VAL:HG13	1.86	0.57
1:B:237:ILE:HD12	1:B:237:ILE:N	2.20	0.57
1:A:17:PHE:O	1:A:19:VAL:HG23	2.05	0.57
1:A:97:PHE:HA	1:A:101:ILE:HG21	1.88	0.56
1:A:33:LYS:O	1:A:34:ILE:HD13	2.06	0.56
1:B:36:ILE:HG22	1:B:40:VAL:HG21	1.87	0.56
1:A:19:VAL:O	1:A:458:ASN:HB2	2.06	0.55
1:B:82:PHE:HB2	1:B:184:ILE:HG12	1.87	0.55
1:B:262:CYS:SG	1:B:264:VAL:O	2.64	0.55
1:B:34:ILE:HG22	1:B:35:ALA:N	2.21	0.55
1:B:16:VAL:HG12	1:B:20:PHE:HB2	1.89	0.55
1:B:75:ILE:CD1	1:B:105:ILE:HD12	2.38	0.54
1:B:356:ASP:OD1	1:B:358:SER:OG	2.26	0.54
1:A:215:LYS:O	1:A:217:THR:HG23	2.08	0.53
1:B:118:GLU:HG2	1:B:185:MET:HE1	1.90	0.53
1:B:84:THR:OG1	1:B:86:ASP:OD1	2.23	0.53
1:A:75:ILE:O	1:A:80:GLY:HA3	2.09	0.53
1:A:79:PHE:HE2	1:A:134:TYR:CZ	2.26	0.52
1:A:211:ASN:HB3	1:A:272:ASN:OD1	2.09	0.52
1:A:211:ASN:O	1:A:214:VAL:HG22	2.10	0.52
1:A:85:GLU:OE1	1:A:85:GLU:C	2.53	0.52
1:A:21:SER:OG	1:A:277:LEU:HD22	2.09	0.52
1:A:70:PHE:HB3	1:A:88:LEU:HD11	1.91	0.52
1:A:13:LEU:HD12	1:A:77:LEU:HD22	1.91	0.52
1:A:83:LEU:HD12	1:A:83:LEU:N	2.24	0.52
1:A:496:THR:HG21	1:A:527:LEU:CD1	2.38	0.52
1:B:36:ILE:HD12	1:B:105:ILE:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:HD11	1:B:92:PHE:CD1	2.45	0.51
1:B:77:LEU:HB3	1:B:78:PRO:HD3	1.92	0.51
1:B:496:THR:HG21	1:B:527:LEU:HD13	1.92	0.51
1:A:41:ASN:O	1:A:61:CYS:O	2.28	0.51
1:A:79:PHE:HE2	1:A:134:TYR:CE2	2.28	0.51
1:B:86:ASP:OD1	1:B:86:ASP:N	2.44	0.51
1:B:58:ILE:HD12	1:B:59:GLN:HG2	1.93	0.51
1:A:219:THR:OG1	1:A:266:ALA:O	2.26	0.50
1:B:38:GLY:HA3	1:B:107:VAL:H	1.75	0.50
1:B:98:TYR:O	1:B:101:ILE:N	2.44	0.50
1:B:407:GLU:OE2	1:B:620:TYR:OH	2.23	0.50
1:B:34:ILE:O	1:B:45:ILE:O	2.29	0.50
1:B:481:ALA:HB1	1:B:494:ALA:HB1	1.93	0.50
1:A:15:SER:HB2	1:A:37:CYS:O	2.11	0.50
1:A:33:LYS:O	1:A:33:LYS:HD2	2.11	0.50
1:A:604:LEU:HD22	1:A:609:GLU:HB3	1.92	0.50
1:B:224:GLY:HA2	1:B:245:HIS:CE1	2.46	0.50
1:B:122:ILE:HG23	1:B:144:ILE:CG2	2.42	0.49
1:A:16:VAL:O	1:A:19:VAL:HA	2.13	0.49
1:A:19:VAL:HG13	1:A:277:LEU:CG	2.42	0.49
1:A:496:THR:HG21	1:A:527:LEU:HD13	1.95	0.49
1:B:209:GLN:HE22	1:B:278:ARG:HH12	1.59	0.49
1:B:19:VAL:HG21	1:B:455:ILE:HG13	1.93	0.49
1:B:128:LYS:HB3	1:B:134:TYR:CE2	2.48	0.49
1:A:400:ALA:CA	1:A:475:MET:HE1	2.43	0.48
1:A:147:MET:HE2	1:A:185:MET:HG2	1.95	0.48
1:A:511:ILE:HD13	1:A:606:ARG:CZ	2.43	0.48
1:A:16:VAL:CG1	1:A:19:VAL:N	2.77	0.48
1:A:49:PRO:HG2	1:A:52:ALA:HB2	1.95	0.48
1:B:45:ILE:O	1:B:46:ILE:HD12	2.13	0.48
1:B:380:GLY:HA2	1:B:383:LEU:HD21	1.96	0.48
1:A:362:PRO:O	1:A:385:VAL:HG13	2.14	0.48
1:A:346:GLN:OE1	1:A:502:LYS:HE3	2.13	0.48
1:B:299:ILE:HG21	1:B:315:ILE:HD11	1.95	0.48
1:B:500:LEU:HD21	1:B:534:LEU:CD1	2.44	0.48
1:B:438:ASP:O	1:B:439:MET:HG2	2.13	0.48
1:A:617:TYR:O	1:A:622:ASP:N	2.46	0.47
1:B:45:ILE:O	1:B:46:ILE:O	2.32	0.47
1:A:140:VAL:HG13	1:A:178:MET:HE3	1.96	0.47
1:A:404:TRP:CE2	1:A:408:LYS:HD2	2.49	0.47
1:B:58:ILE:CD1	1:B:59:GLN:HG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:HIS:CE1	2:B:702:SF4:S3	3.07	0.47
1:A:400:ALA:CB	1:A:475:MET:HE1	2.44	0.47
1:A:17:PHE:HB2	1:A:39:LYS:HE3	1.96	0.47
1:A:40:VAL:HG12	1:A:64:LEU:HD23	1.96	0.47
1:B:159:SER:HB3	1:B:163:GLU:HG3	1.97	0.47
1:B:346:GLN:HG3	1:B:503:MET:HG3	1.97	0.47
1:B:622:ASP:O	1:B:623:HIS:HB3	2.15	0.47
1:B:236:CYS:SG	1:B:252:CYS:HA	2.54	0.47
1:A:78:PRO:HB2	1:A:79:PHE:CD2	2.50	0.47
1:A:511:ILE:O	1:A:511:ILE:HG13	2.14	0.47
1:A:310:ASN:HB2	1:A:598:ILE:HD11	1.95	0.46
1:A:622:ASP:O	1:A:623:HIS:HB3	2.15	0.46
1:B:101:ILE:HG23	1:B:103:ARG:N	2.27	0.46
1:A:138:GLU:C	1:A:138:GLU:OE1	2.58	0.46
1:B:19:VAL:HG21	1:B:455:ILE:CG1	2.45	0.46
1:A:251:ARG:HG2	1:A:377:GLN:HG3	1.97	0.46
1:A:31:GLY:C	1:A:103:ARG:HH22	2.24	0.46
1:A:137:TYR:O	1:A:140:VAL:HG22	2.15	0.46
1:B:71:LYS:HG3	1:B:110:GLN:OE1	2.16	0.46
1:B:507:ARG:NH1	5:B:801:HOH:O	2.48	0.46
1:A:32:ARG:NE	1:A:48:VAL:HG23	2.31	0.46
1:A:299:ILE:HG21	1:A:315:ILE:HD11	1.98	0.46
1:B:262:CYS:SG	1:B:264:VAL:HG23	2.56	0.45
1:B:506:GLU:HA	1:B:506:GLU:OE1	2.16	0.45
1:B:535:ARG:HH21	1:B:557:GLU:HB3	1.81	0.45
1:A:150:ILE:HG23	1:A:163:GLU:HB3	1.99	0.45
1:A:514:GLU:HA	1:A:517:ARG:HD2	1.98	0.45
1:B:401:LYS:NZ	1:B:441:TYR:O	2.50	0.45
1:A:19:VAL:O	1:A:458:ASN:CB	2.64	0.45
1:A:40:VAL:HA	1:A:64:LEU:HA	1.98	0.45
1:A:97:PHE:CA	1:A:101:ILE:HG21	2.46	0.45
1:A:507:ARG:NH1	5:A:801:HOH:O	2.50	0.45
1:A:631:GLU:OE2	1:B:168:ARG:NH2	2.50	0.45
1:B:150:ILE:HG23	1:B:163:GLU:HB3	1.99	0.45
1:B:34:ILE:HG22	1:B:36:ILE:HD13	1.99	0.45
1:B:209:GLN:HE22	1:B:278:ARG:NH1	2.15	0.45
1:B:288:ILE:HG22	1:B:326:TYR:HB2	1.99	0.44
1:B:36:ILE:HG22	1:B:40:VAL:CG2	2.47	0.44
1:A:13:LEU:HG	1:A:14:GLY:N	2.33	0.44
1:B:50:GLU:N	1:B:50:GLU:OE1	2.51	0.44
1:B:385:VAL:N	1:B:386:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HD12	1:B:58:ILE:C	2.41	0.44
1:A:250:ASN:O	1:A:373:LYS:NZ	2.50	0.44
1:B:382:MET:SD	1:B:549:LEU:HD22	2.58	0.44
1:B:478:TYR:CE1	1:B:483:ILE:HD13	2.52	0.44
1:B:104:THR:O	1:B:105:ILE:HD13	2.18	0.44
1:B:420:ILE:HA	1:B:447:ILE:O	2.18	0.44
1:A:138:GLU:OE1	1:A:138:GLU:O	2.36	0.43
1:B:19:VAL:HG22	1:B:273:THR:CG2	2.48	0.43
1:B:46:ILE:HD13	1:B:48:VAL:HG12	1.99	0.43
1:B:477:GLU:OE2	4:B:707:CL:CL	2.73	0.43
1:A:262:CYS:SG	1:A:264:VAL:HG23	2.58	0.43
1:B:16:VAL:HG11	1:B:20:PHE:HB2	2.01	0.43
1:A:234:VAL:HG23	1:A:236:CYS:HB2	1.99	0.43
1:B:19:VAL:O	1:B:458:ASN:HB3	2.18	0.43
1:B:34:ILE:CG2	1:B:105:ILE:HG12	2.48	0.43
1:B:77:LEU:HB3	1:B:78:PRO:CD	2.48	0.43
1:A:128:LYS:HD2	1:A:128:LYS:HA	1.80	0.43
1:A:631:GLU:OE1	1:B:168:ARG:NH2	2.52	0.43
1:B:77:LEU:HD13	1:B:106:ILE:CD1	2.49	0.43
1:A:382:MET:HB3	1:A:385:VAL:HG21	2.00	0.43
1:A:617:TYR:O	1:A:622:ASP:HA	2.18	0.43
1:B:368:CYS:O	1:B:371:TRP:CD1	2.72	0.43
1:A:19:VAL:CG1	1:A:455:ILE:HG12	2.43	0.43
1:A:168:ARG:HH21	1:B:631:GLU:CD	2.27	0.43
1:A:356:ASP:OD1	1:A:358:SER:HB3	2.19	0.43
1:A:496:THR:HG22	1:A:513:PHE:CE2	2.54	0.43
1:A:480:GLY:O	1:A:483:ILE:HG22	2.18	0.43
1:A:521:GLY:O	1:A:539:ALA:HA	2.19	0.43
1:B:19:VAL:HG22	1:B:273:THR:HG21	2.00	0.42
1:B:237:ILE:HD11	2:B:703:SF4:S1	2.59	0.42
1:B:404:TRP:CE2	1:B:408:LYS:HD2	2.54	0.42
1:A:274:MET:O	1:A:278:ARG:HG3	2.19	0.42
1:A:48:VAL:HG21	1:A:94:PHE:CZ	2.54	0.42
1:A:500:LEU:HD21	1:A:534:LEU:CD1	2.49	0.42
1:A:75:ILE:HB	1:A:81:GLY:H	1.85	0.42
1:A:56:GLU:O	1:A:60:LEU:HG	2.20	0.42
1:A:101:ILE:HG23	1:A:103:ARG:H	1.84	0.42
1:A:37:CYS:O	1:A:37:CYS:SG	2.77	0.41
1:A:535:ARG:HH12	1:A:557:GLU:HB3	1.84	0.41
1:B:16:VAL:CG2	1:B:65:ILE:HD11	2.50	0.41
1:A:421:MET:O	1:A:448:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:HE1	1:A:612:GLU:HB2	1.86	0.41
1:A:422:PRO:O	1:A:576:GLY:N	2.50	0.41
1:B:131:ASP:OD1	1:B:131:ASP:C	2.63	0.41
1:B:140:VAL:CG1	1:B:178:MET:HE3	2.50	0.41
1:A:126:LEU:HD11	1:A:145:THR:HA	2.02	0.41
1:A:385:VAL:N	1:A:386:PRO:HD2	2.34	0.41
1:B:34:ILE:CG2	1:B:35:ALA:N	2.83	0.41
1:A:496:THR:HG22	1:A:513:PHE:HE2	1.85	0.41
1:B:75:ILE:HD11	1:B:83:LEU:HD13	2.02	0.41
1:A:16:VAL:HB	1:A:43:PRO:HG3	2.01	0.41
1:A:32:ARG:HE	1:A:48:VAL:HG23	1.85	0.41
1:B:36:ILE:CD1	1:B:105:ILE:HB	2.51	0.41
1:B:71:LYS:HG3	1:B:110:GLN:CD	2.46	0.41
1:B:423:CYS:SG	1:B:425:ALA:N	2.91	0.41
1:A:33:LYS:O	1:A:33:LYS:CD	2.68	0.41
1:A:346:GLN:HG3	1:A:503:MET:CG	2.51	0.41
1:A:477:GLU:OE2	4:A:706:CL:CL	2.75	0.41
1:A:507:ARG:HH11	1:A:507:ARG:HG2	1.86	0.41
1:B:93:ASP:HB3	1:B:96:ILE:HG12	2.02	0.41
1:A:336:LEU:HD13	1:A:613:VAL:HG13	2.03	0.41
1:B:55:ASN:OD1	1:B:55:ASN:C	2.64	0.41
1:A:216:LEU:CD1	1:A:269:ALA:HB2	2.49	0.40
1:A:484:ILE:O	1:A:490:GLY:HA3	2.21	0.40
1:B:34:ILE:HD12	1:B:48:VAL:CG1	2.34	0.40
1:B:77:LEU:HD13	1:B:106:ILE:HD11	2.03	0.40
1:B:92:PHE:CE2	1:B:94:PHE:CE1	3.09	0.40
1:B:496:THR:HG21	1:B:527:LEU:CD1	2.51	0.40
1:A:20:PHE:HB2	1:A:458:ASN:HB3	2.03	0.40
1:B:71:LYS:NZ	1:B:195:GLU:OE1	2.53	0.40
1:B:167:LEU:HD22	1:B:185:MET:SD	2.62	0.40
1:B:496:THR:O	1:B:497:ARG:C	2.64	0.40
1:A:256:GLY:HA2	1:A:424:ILE:HD11	2.02	0.40
1:A:496:THR:O	1:A:497:ARG:C	2.62	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 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	617/674 (92%)	584 (95%)	30 (5%)	3 (0%)	24	32
1	B	612/674 (91%)	578 (94%)	32 (5%)	2 (0%)	36	45
All	All	1229/1348 (91%)	1162 (94%)	62 (5%)	5 (0%)	30	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	B	46	ILE
1	B	19	VAL
1	A	19	VAL
1	A	13	LEU

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 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	523/565 (93%)	521 (100%)	2 (0%)	84	89
1	B	521/565 (92%)	512 (98%)	9 (2%)	53	67
All	All	1044/1130 (92%)	1033 (99%)	11 (1%)	65	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN

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Mol	Chain	Res	Type
1	A	622	ASP
1	B	13	LEU
1	B	18	SER
1	B	46	ILE
1	B	61	CYS
1	B	67	LYS
1	B	238	ASN
1	B	359	VAL
1	B	502	LYS
1	B	572	ILE

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

Mol	Chain	Res	Type
1	A	250	ASN
1	A	458	ASN
1	B	160	ASN
1	B	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 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	B	703	1	0,12,12	-	-	-		
2	SF4	A	702	1	0,12,12	-	-	-		
2	SF4	A	701	1	0,12,12	-	-	-		
2	SF4	B	701	1	0,12,12	-	-	-		
2	SF4	B	702	1	0,12,12	-	-	-		
2	SF4	A	703	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	B	703	1	-	-	0/6/5/5
2	SF4	A	702	1	-	-	0/6/5/5
2	SF4	A	701	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
2	SF4	B	702	1	-	-	0/6/5/5
2	SF4	A	703	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.

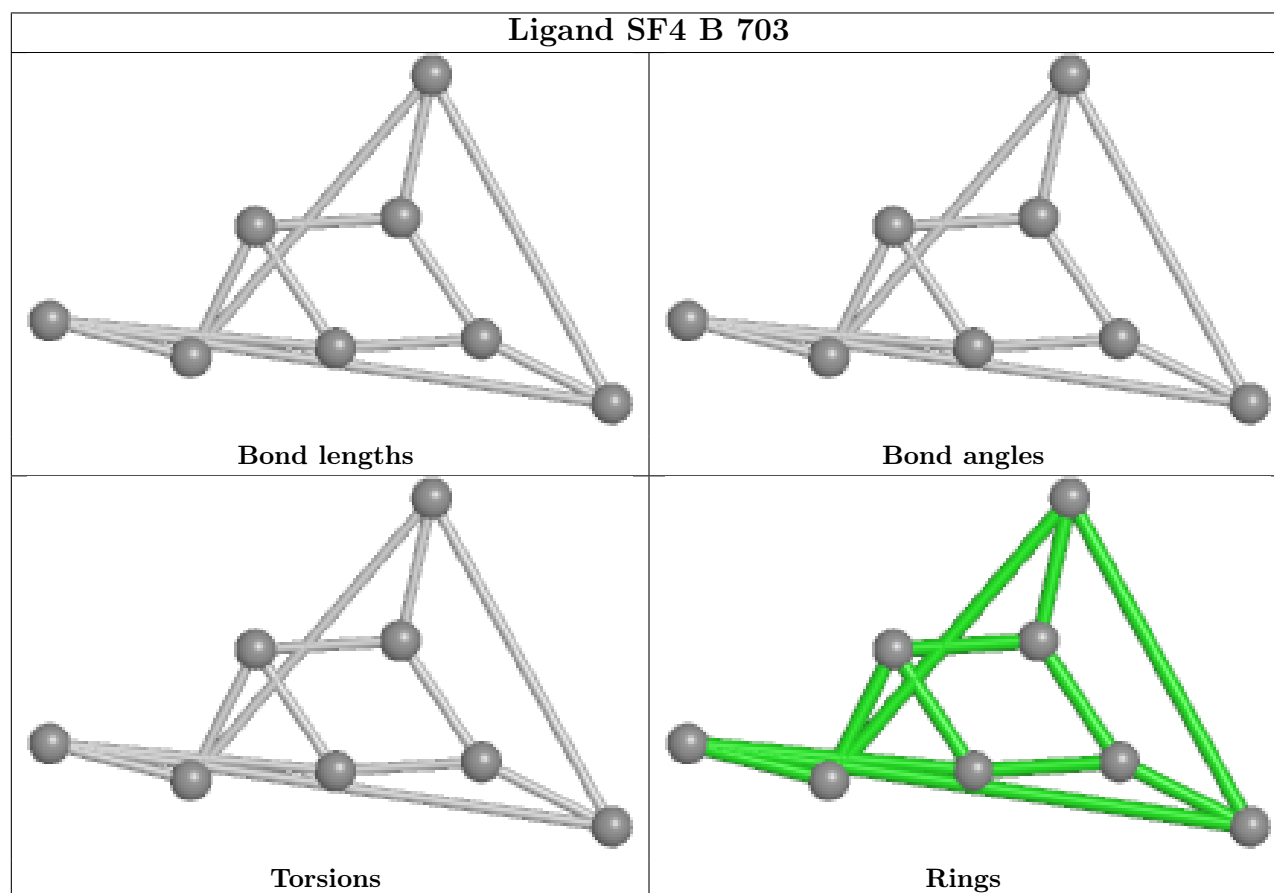
There are no ring outliers.

2 monomers are involved in 3 short contacts:

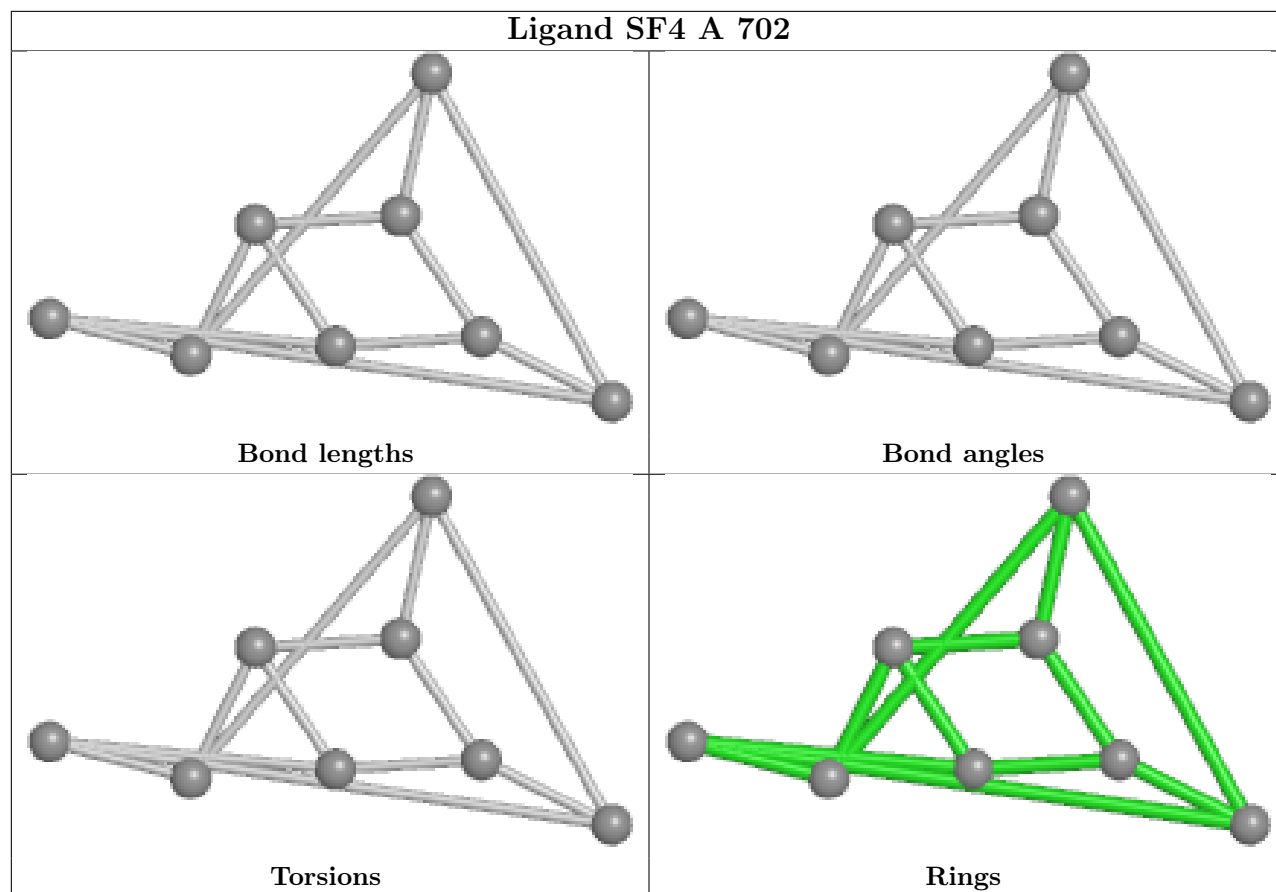
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	703	SF4	1	0
2	B	702	SF4	2	0

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

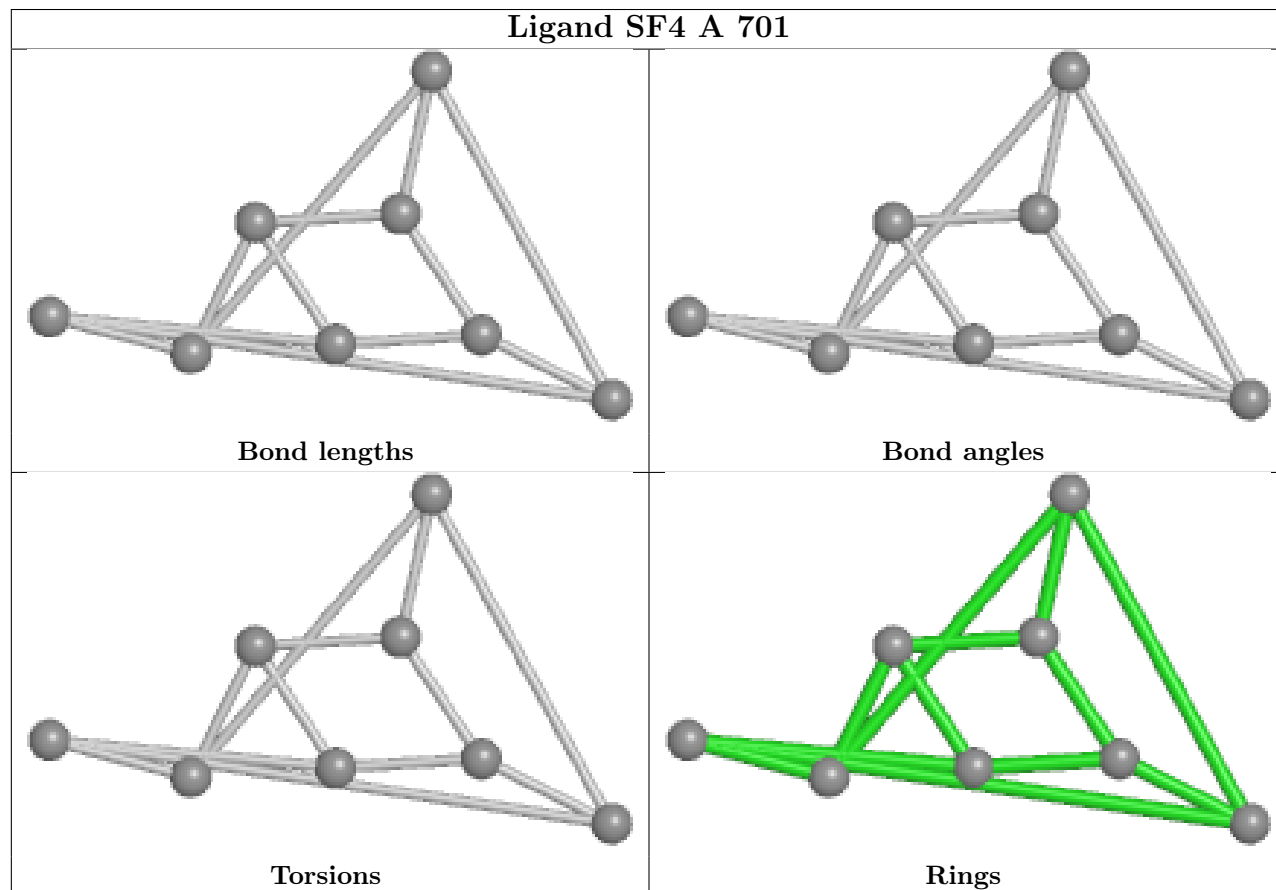
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



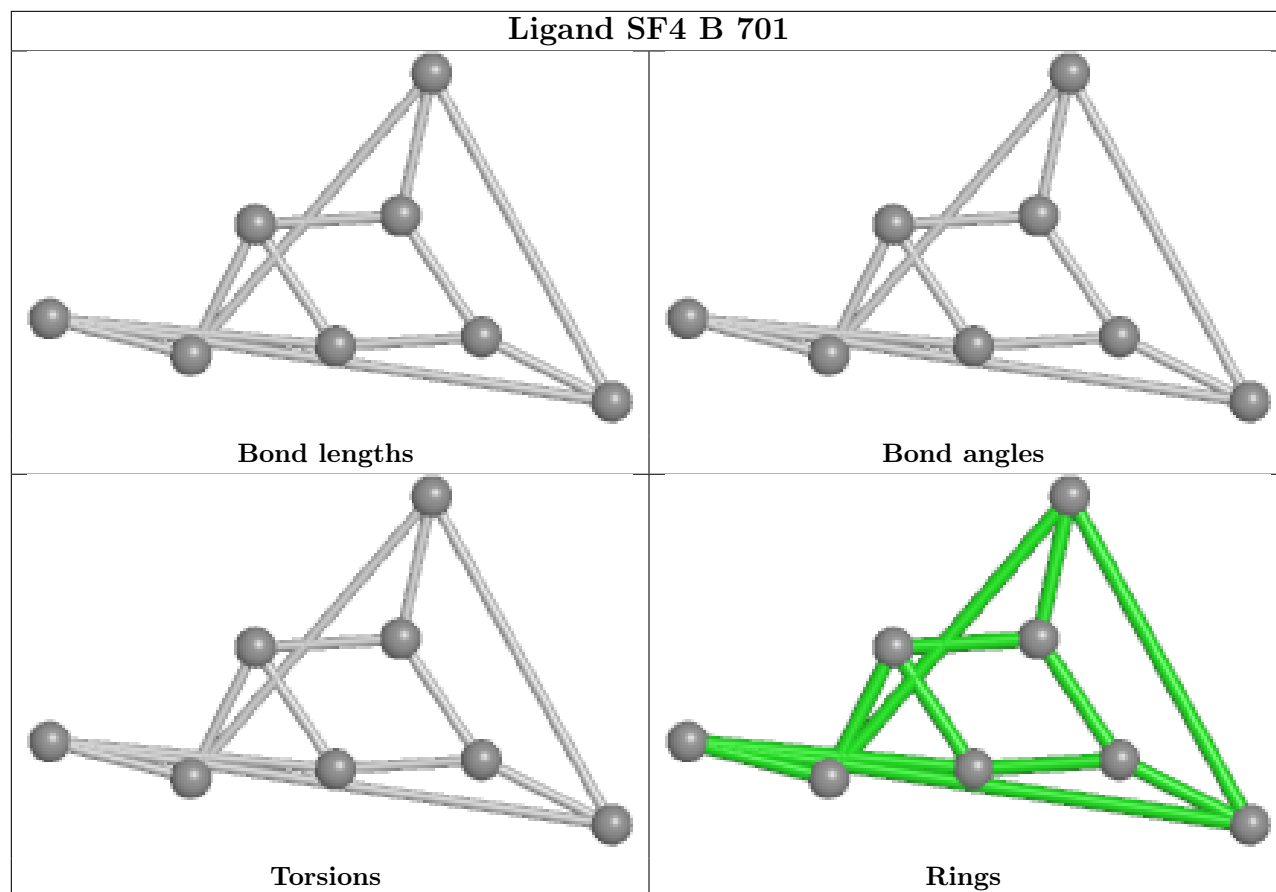
Ligand SF4 A 702



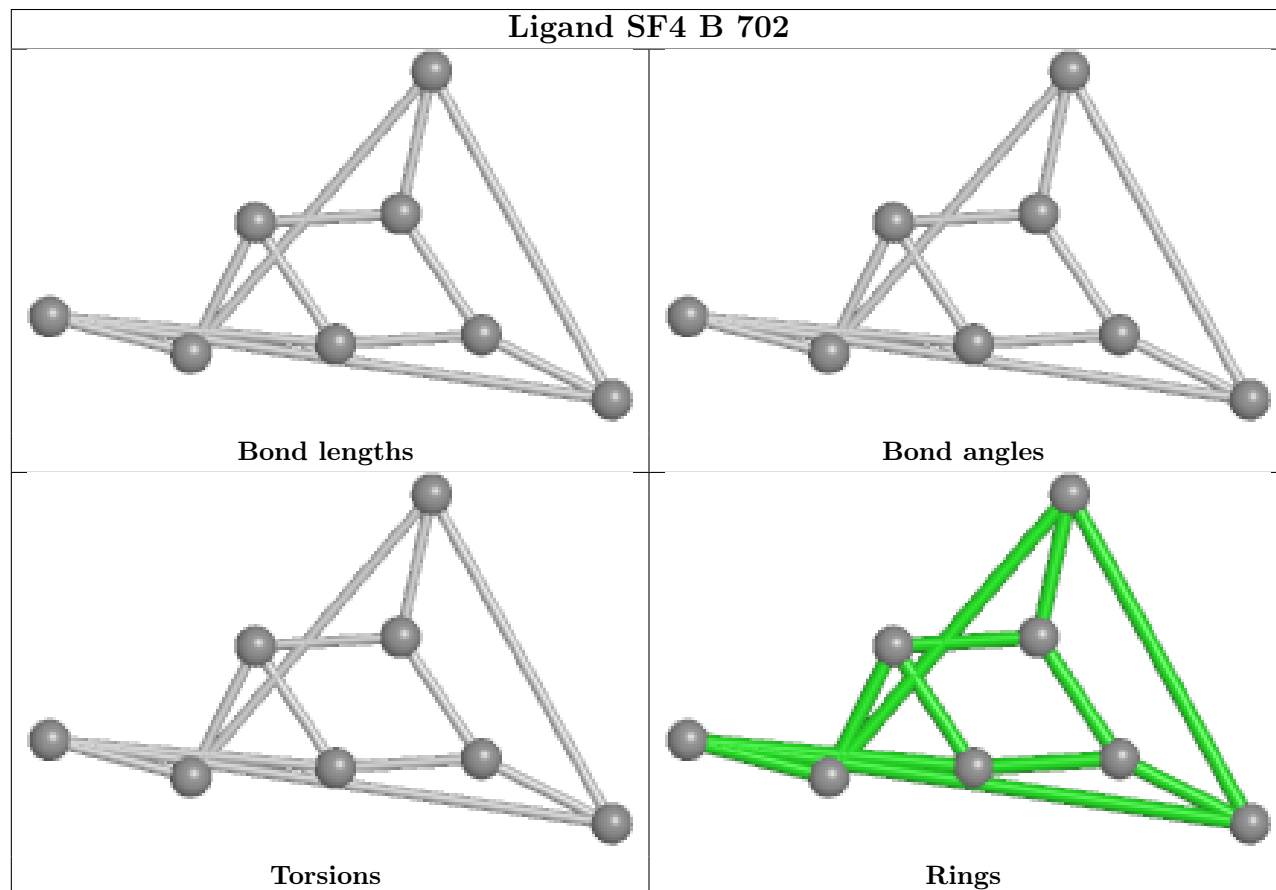
Ligand SF4 A 701

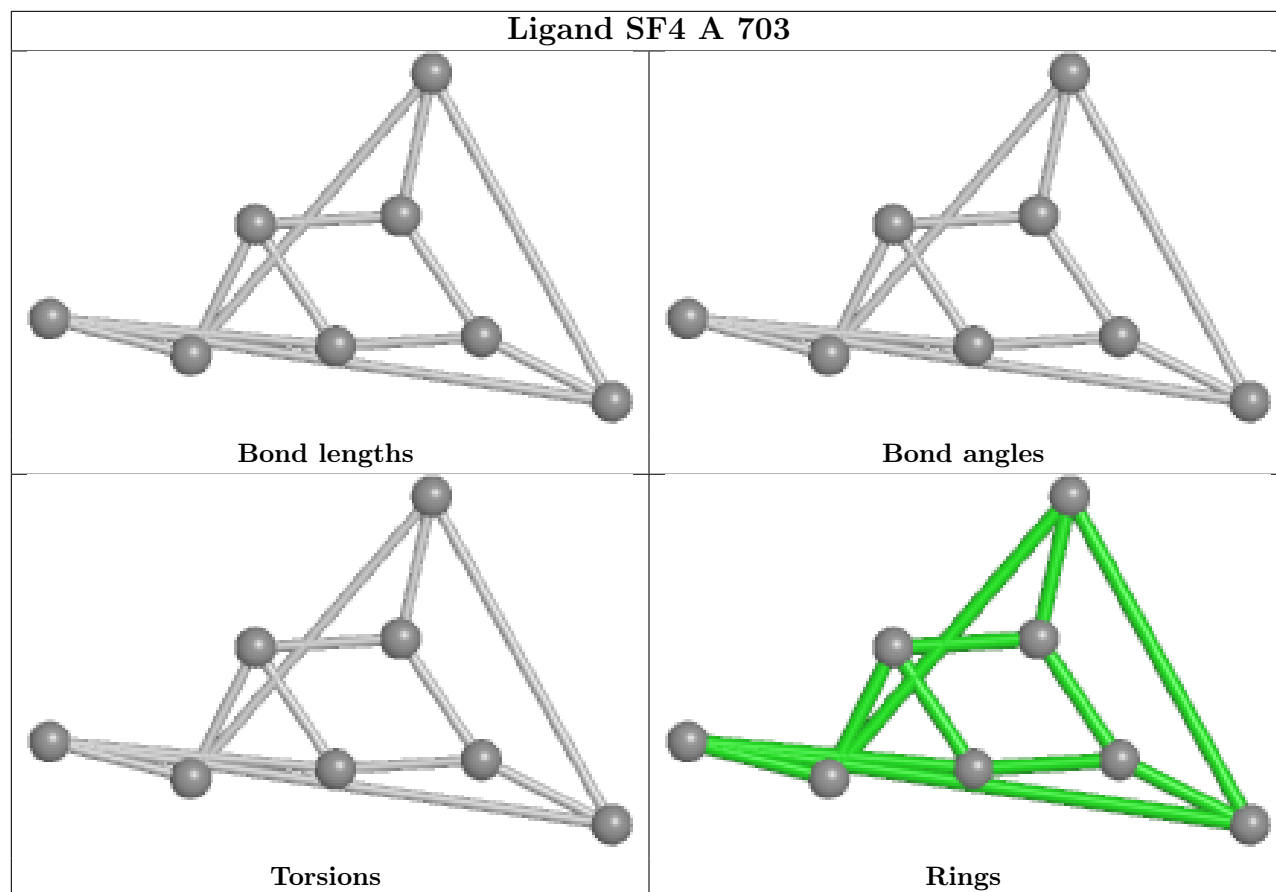


Ligand SF4 B 701



Ligand SF4 B 702





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

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, 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	621/674 (92%)	0.84	72 (11%) 9 8	53, 76, 124, 171	0
1	B	618/674 (91%)	1.07	115 (18%) 3 2	52, 77, 147, 185	0
All	All	1239/1348 (91%)	0.95	187 (15%) 5 4	52, 76, 137, 185	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	PHE	6.9
1	A	17	PHE	6.6
1	B	101	ILE	6.5
1	A	77	LEU	6.5
1	B	239	GLY	5.8
1	A	96	ILE	5.5
1	A	19	VAL	5.3
1	B	96	ILE	5.3
1	B	19	VAL	5.2
1	B	20	PHE	5.2
1	B	52	ALA	5.2
1	B	104	THR	5.1
1	A	16	VAL	5.1
1	B	256	GLY	5.0
1	B	97	PHE	4.9
1	B	98	TYR	4.8
1	A	102	ALA	4.7
1	A	20	PHE	4.7
1	B	57	ILE	4.7
1	B	241	LEU	4.6
1	B	13	LEU	4.6
1	B	102	ALA	4.6
1	B	40	VAL	4.6
1	B	60	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	92	PHE	4.5
1	B	45	ILE	4.5
1	B	106	ILE	4.5
1	A	12	ALA	4.4
1	B	80	GLY	4.4
1	B	44	GLY	4.4
1	B	70	PHE	4.3
1	B	87	SER	4.2
1	B	21	SER	4.2
1	B	79	PHE	4.2
1	B	42	ASN	4.2
1	A	18	SER	4.2
1	B	37	CYS	4.1
1	A	76	GLY	4.0
1	B	88	LEU	4.0
1	B	105	ILE	3.8
1	B	223	ILE	3.8
1	B	18	SER	3.8
1	B	35	ALA	3.8
1	B	76	GLY	3.8
1	B	43	PRO	3.7
1	A	13	LEU	3.7
1	B	83	LEU	3.7
1	B	15	SER	3.7
1	A	74	GLN	3.7
1	B	94	PHE	3.6
1	B	77	LEU	3.6
1	B	259	VAL	3.5
1	B	586	ALA	3.5
1	B	229	LYS	3.5
1	B	46	ILE	3.5
1	A	638	PHE	3.5
1	A	15	SER	3.4
1	A	97	PHE	3.3
1	A	54	LEU	3.3
1	B	245	HIS	3.3
1	B	34	ILE	3.3
1	A	241	LEU	3.3
1	A	80	GLY	3.3
1	B	238	ASN	3.2
1	A	264	VAL	3.2
1	A	31	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	31	GLY	3.1
1	A	45	ILE	3.1
1	A	492	ILE	3.1
1	B	439	MET	3.1
1	B	36	ILE	3.1
1	B	249	TYR	3.1
1	B	55	ASN	3.1
1	A	51	GLY	3.1
1	A	101	ILE	3.1
1	B	367	CYS	3.1
1	B	16	VAL	3.1
1	A	98	TYR	3.0
1	B	84	THR	3.0
1	B	233	PRO	3.0
1	A	184	ILE	3.0
1	A	78	PRO	3.0
1	B	86	ASP	3.0
1	A	236	CYS	3.0
1	B	74	GLN	3.0
1	B	90	LYS	3.0
1	A	38	GLY	3.0
1	B	237	ILE	2.9
1	A	49	PRO	2.9
1	B	33	LYS	2.9
1	B	266	ALA	2.9
1	A	182	HIS	2.9
1	B	236	CYS	2.9
1	B	263	PRO	2.9
1	A	103	ARG	2.8
1	B	14	GLY	2.8
1	B	51	GLY	2.8
1	B	100	ASN	2.8
1	A	639	PRO	2.8
1	A	104	THR	2.8
1	A	99	GLU	2.8
1	B	447	ILE	2.7
1	B	182	HIS	2.7
1	B	49	PRO	2.7
1	A	566	ALA	2.7
1	B	423	CYS	2.7
1	B	242	LYS	2.7
1	B	274	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	56	GLU	2.7
1	B	73	ALA	2.7
1	B	181	LYS	2.6
1	B	103	ARG	2.6
1	B	225	CYS	2.6
1	B	221	LYS	2.6
1	B	91	GLU	2.5
1	B	374	PHE	2.5
1	B	48	VAL	2.5
1	A	14	GLY	2.5
1	A	358	SER	2.5
1	A	160	ASN	2.5
1	B	81	GLY	2.5
1	B	134	TYR	2.5
1	B	75	ILE	2.5
1	B	269	ALA	2.5
1	A	92	PHE	2.4
1	A	21	SER	2.4
1	A	88	LEU	2.4
1	A	82	PHE	2.4
1	A	428	TYR	2.4
1	B	264	VAL	2.4
1	A	181	LYS	2.4
1	B	22	GLU	2.4
1	A	60	LEU	2.4
1	B	108	LEU	2.4
1	B	99	GLU	2.4
1	A	242	LYS	2.3
1	B	67	LYS	2.3
1	A	183	ASN	2.3
1	B	370	SER	2.3
1	B	38	GLY	2.3
1	B	95	GLY	2.3
1	B	255	CYS	2.3
1	B	160	ASN	2.3
1	A	354	ALA	2.3
1	A	190	ASP	2.3
1	A	33	LYS	2.3
1	B	39	LYS	2.3
1	B	638	PHE	2.3
1	B	467	GLU	2.3
1	A	467	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	639	PRO	2.3
1	A	539	ALA	2.2
1	A	223	ILE	2.2
1	A	265	ASP	2.2
1	B	85	GLU	2.2
1	A	121	TYR	2.2
1	A	542	LEU	2.2
1	A	23	GLU	2.2
1	B	107	VAL	2.2
1	B	180	GLN	2.2
1	A	75	ILE	2.2
1	A	94	PHE	2.2
1	B	78	PRO	2.2
1	A	221	LYS	2.2
1	A	250	ASN	2.2
1	B	261	ALA	2.2
1	A	383	LEU	2.2
1	A	83	LEU	2.1
1	A	353	LEU	2.1
1	A	516	LEU	2.1
1	B	63	GLY	2.1
1	B	542	LEU	2.1
1	A	48	VAL	2.1
1	B	227	ALA	2.1
1	A	471	ILE	2.1
1	B	422	PRO	2.1
1	B	566	ALA	2.1
1	B	579	LYS	2.1
1	A	225	CYS	2.1
1	A	233	PRO	2.1
1	B	228	CYS	2.1
1	B	565	MET	2.1
1	A	257	ALA	2.0
1	B	89	ASP	2.0
1	B	234	VAL	2.0
1	B	243	LYS	2.0
1	A	106	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

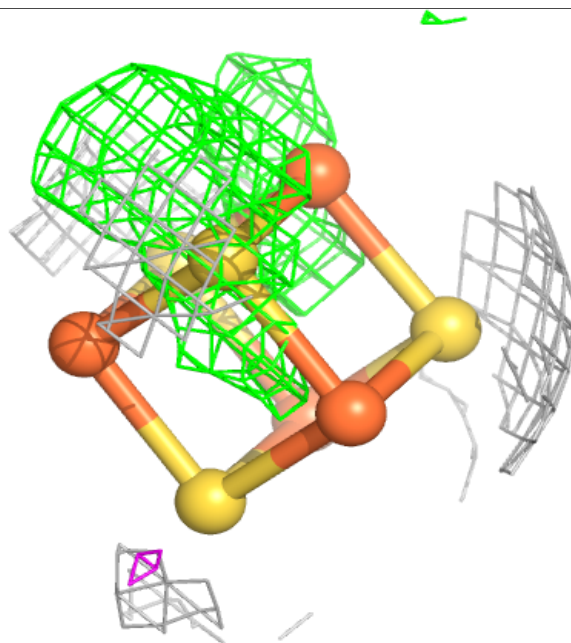
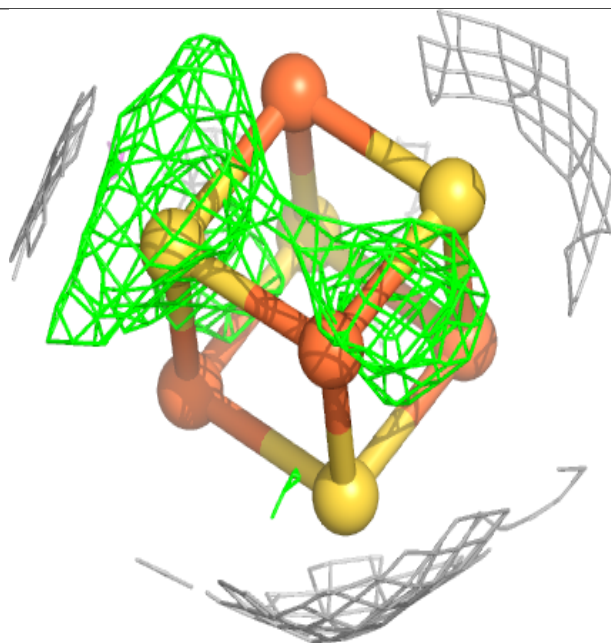
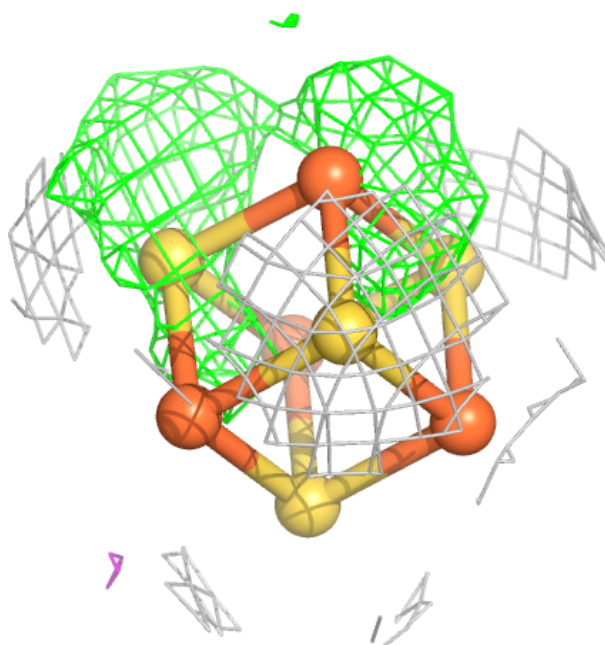
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	707	1/1	0.72	0.39	88,88,88,88	0
4	CL	A	711	1/1	0.78	0.58	106,106,106,106	0
4	CL	A	708	1/1	0.81	0.40	98,98,98,98	0
4	CL	A	706	1/1	0.83	0.36	83,83,83,83	0
4	CL	A	707	1/1	0.86	0.35	90,90,90,90	0
4	CL	A	709	1/1	0.86	0.38	95,95,95,95	0
4	CL	B	708	1/1	0.86	0.44	101,101,101,101	0
4	CL	B	706	1/1	0.90	0.20	94,94,94,94	0
4	CL	B	709	1/1	0.92	0.27	88,88,88,88	0
4	CL	A	710	1/1	0.93	0.24	84,84,84,84	0
2	SF4	A	702	8/8	0.96	0.07	77,90,97,102	0
2	SF4	B	702	8/8	0.96	0.07	89,101,126,130	0
4	CL	B	705	1/1	0.97	0.06	56,56,56,56	0
4	CL	A	705	1/1	0.98	0.05	54,54,54,54	0
2	SF4	A	703	8/8	0.98	0.05	63,66,73,74	0
2	SF4	B	701	8/8	0.98	0.04	48,58,66,66	0
2	SF4	A	701	8/8	0.98	0.04	51,55,63,63	0
2	SF4	B	703	8/8	0.98	0.04	67,75,79,80	0
3	ZN	A	704	1/1	0.98	0.05	70,70,70,70	0
3	ZN	B	704	1/1	0.99	0.04	69,69,69,69	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.

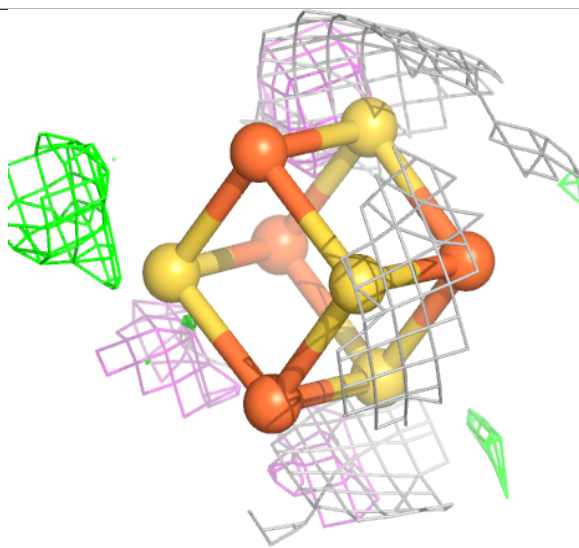
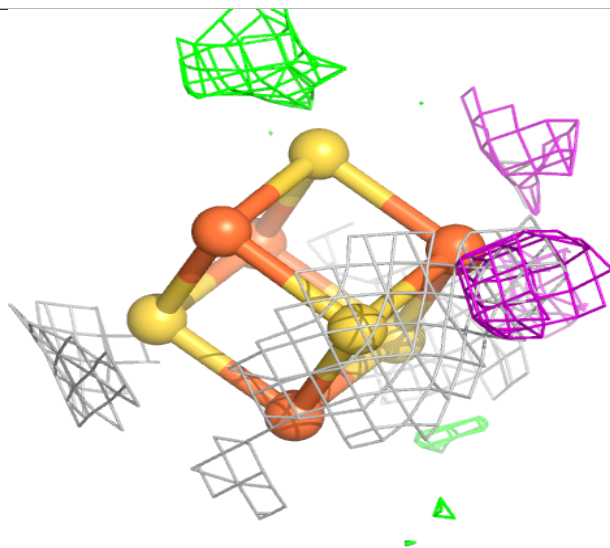
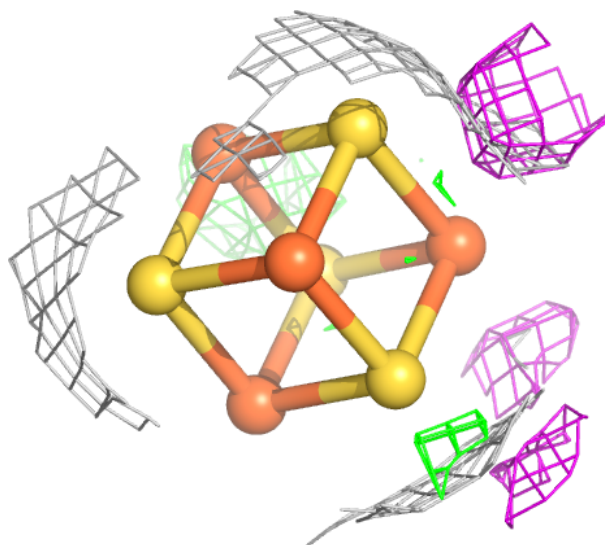
Electron density around SF4 A 702:

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



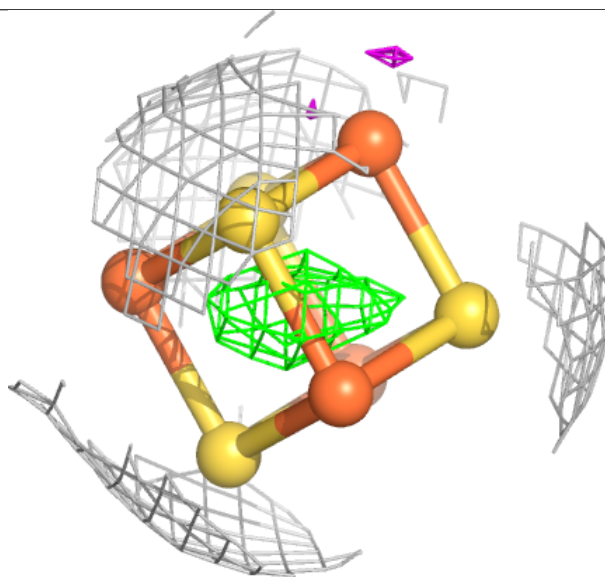
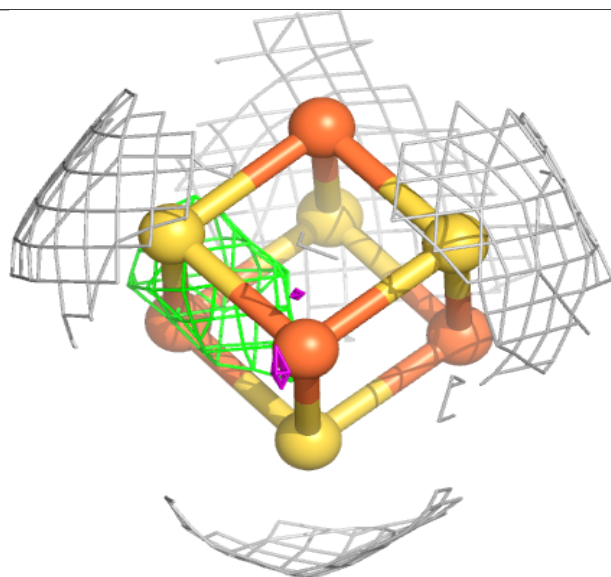
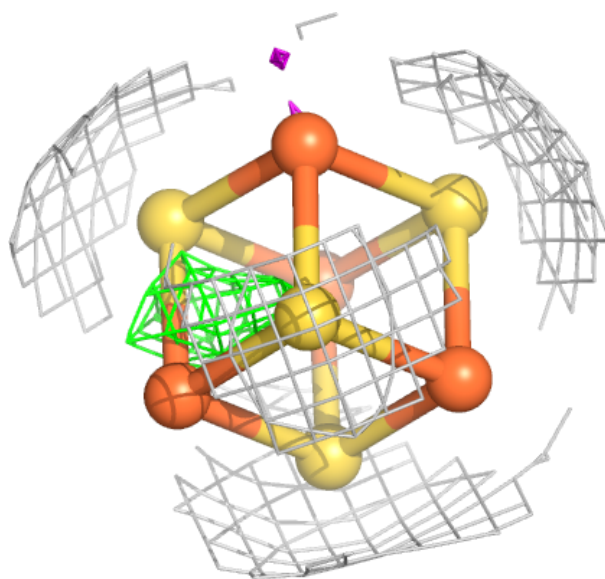
Electron density around SF4 B 702:

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



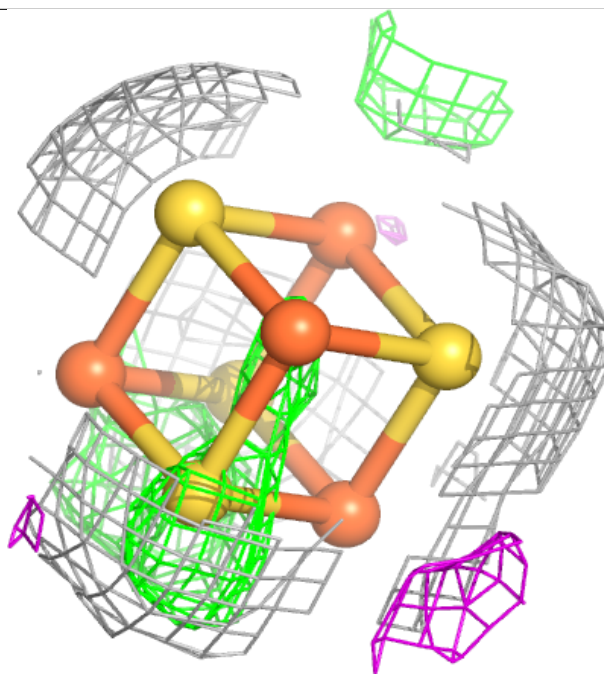
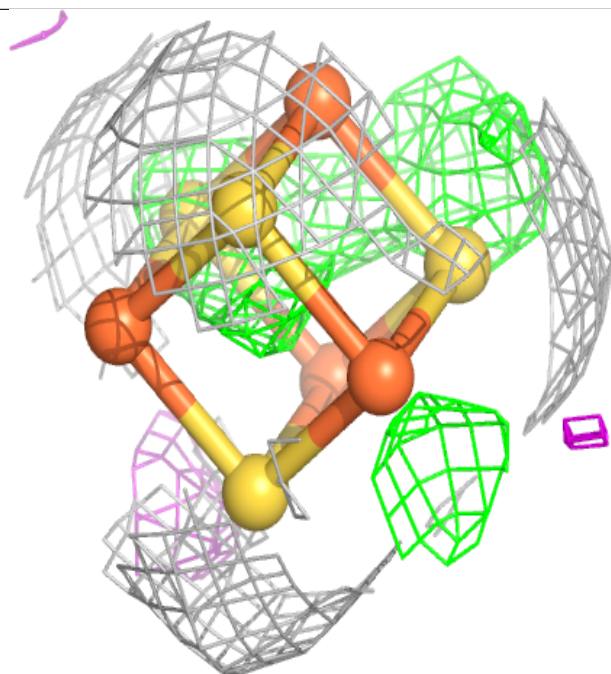
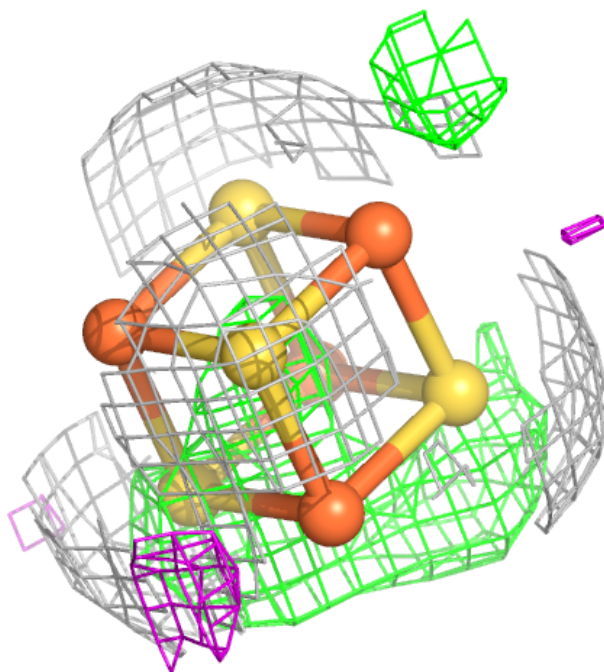
Electron density around SF4 A 703:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



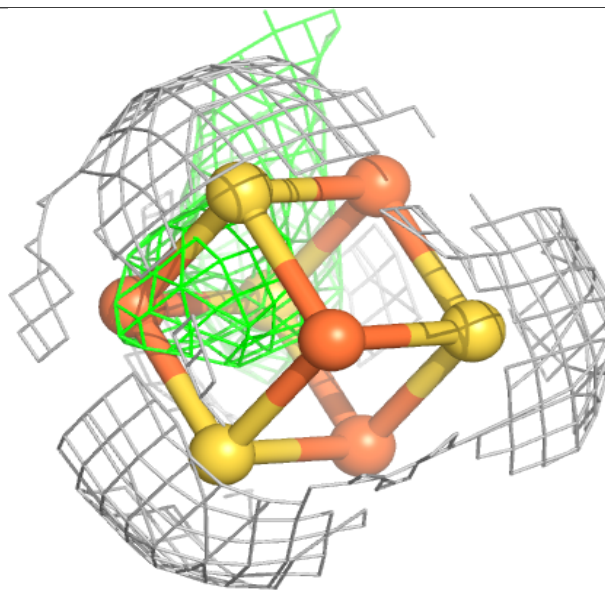
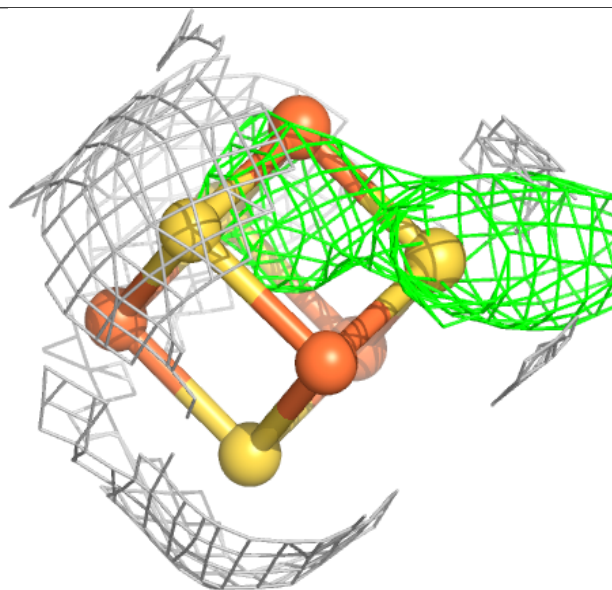
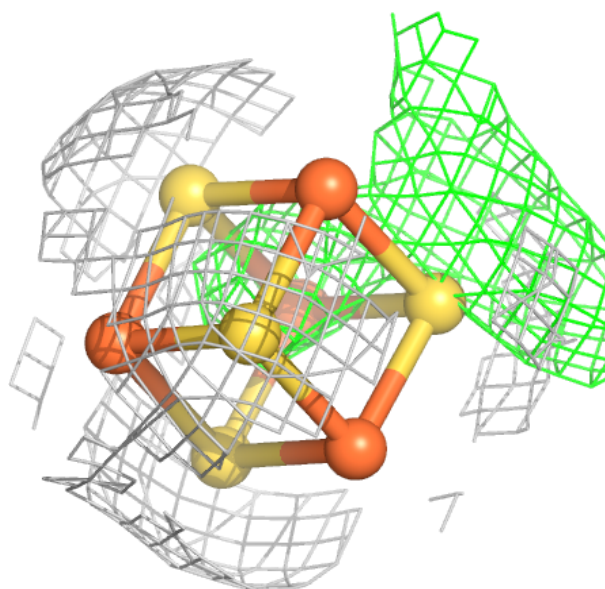
Electron density around SF4 B 701:

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



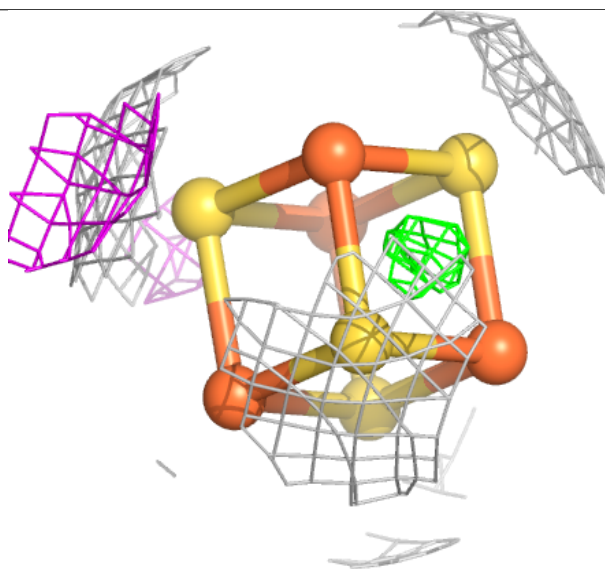
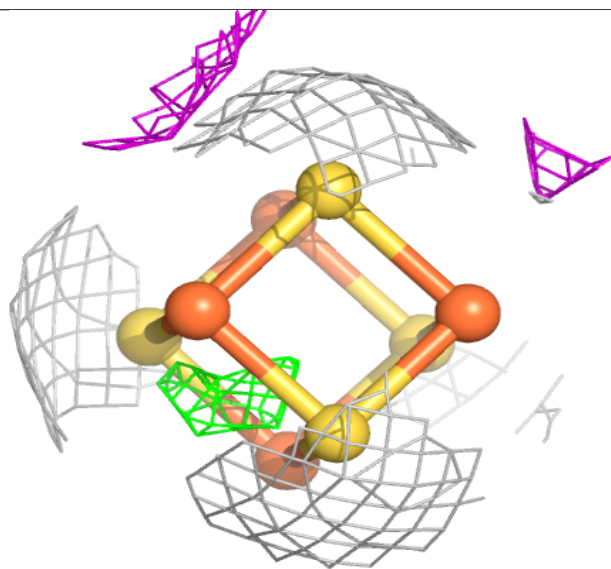
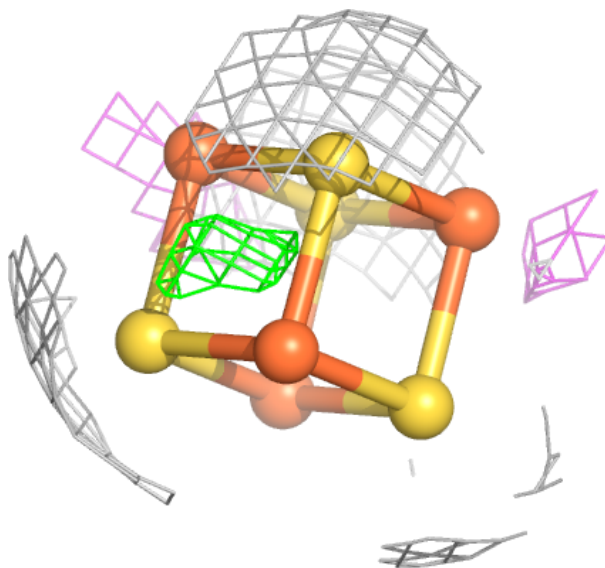
Electron density around SF4 A 701:

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



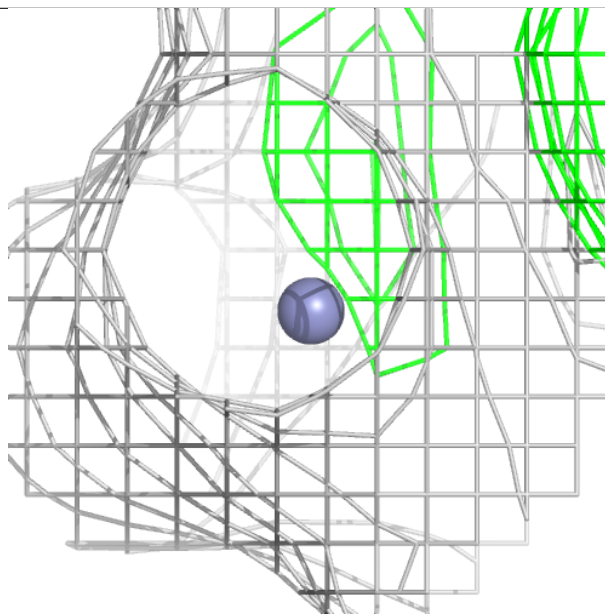
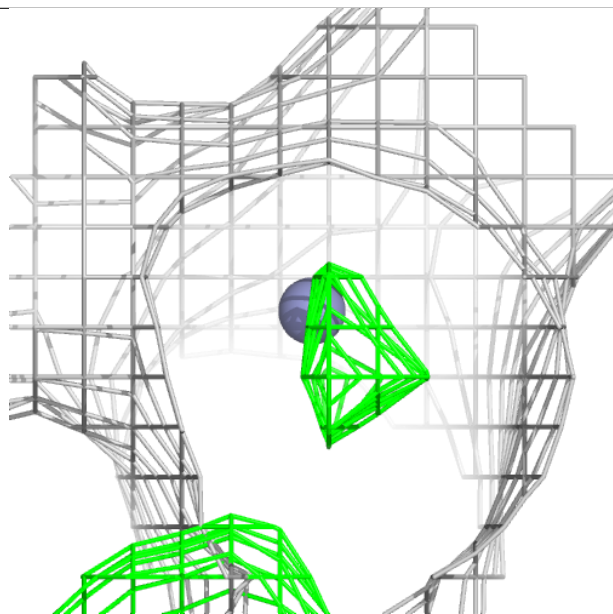
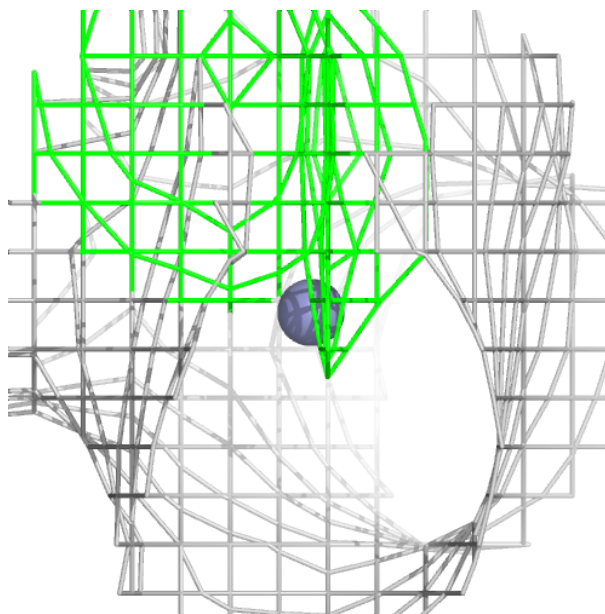
Electron density around SF4 B 703:

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



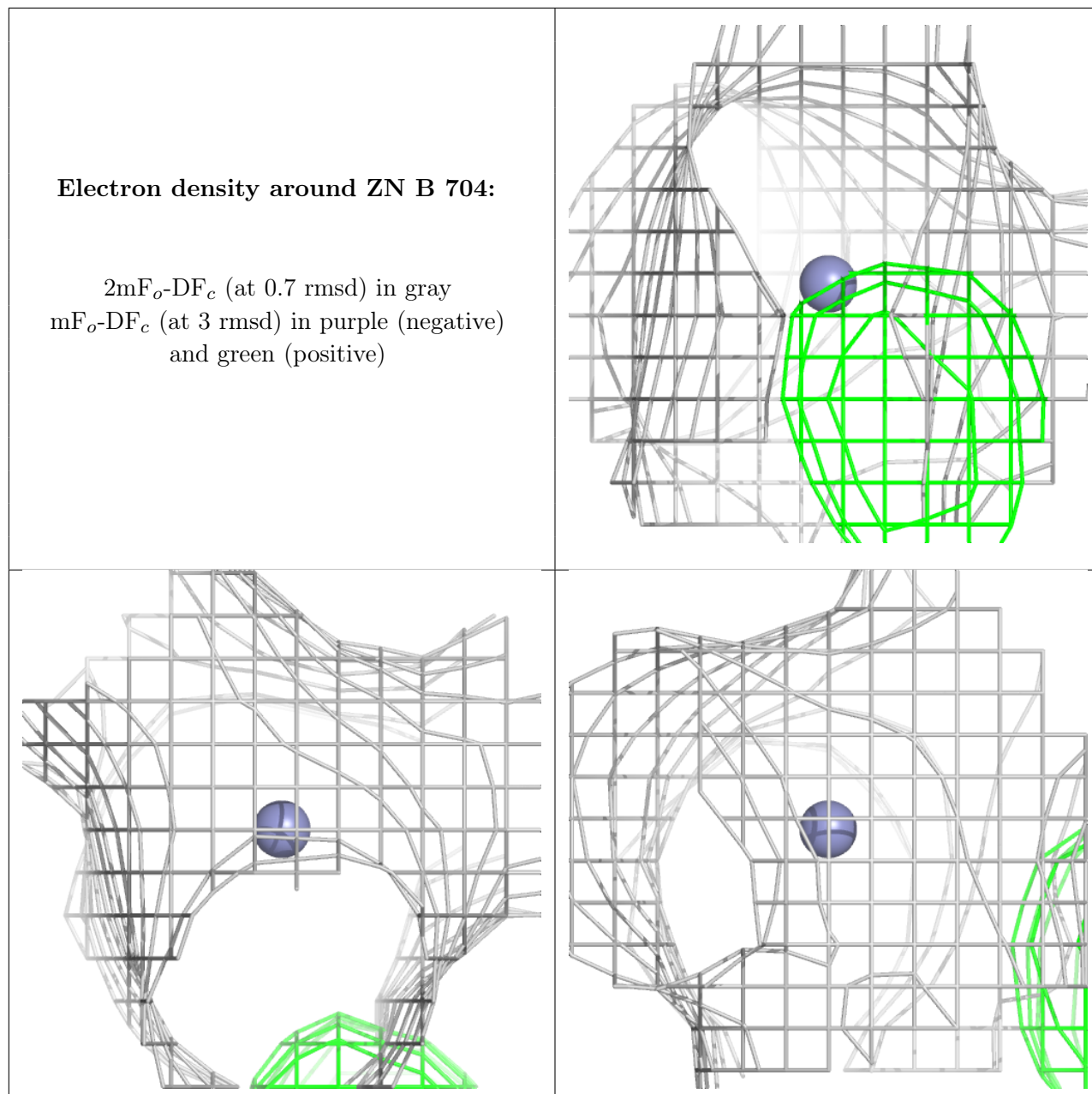
Electron density around ZN A 704:

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



Electron density around ZN B 704:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.