Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2020 – 01:10 pm GMT

PDB ID	:	6TTL
Title	:	crystal structure of [FeFe]-hydrogenase CbA5H (partial) from Clostridium beijerinckii in Hinact state
Authors	:	Duan, J.; Rutz, A.; Hofmann, E.; Happe, T.
Deposited on	:	2019-12-28
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

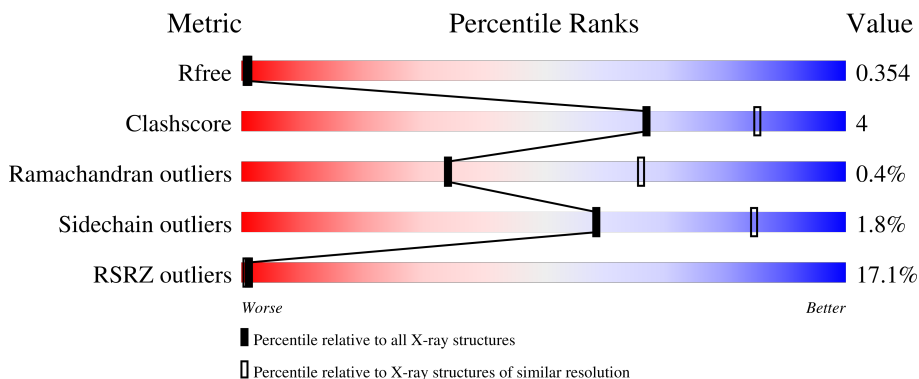|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.90 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	Percentile Ranks	Value
Rfree		0.354
Clashscore		4
Ramachandran outliers		0.4%
Sidechain outliers		1.8%
RSRZ outliers		17.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	674	11% / 65% / 6% / 29%
1	B	674	14% / 62% / 8% · / 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7648 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 [FeFe]-hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total 3799	C 2407	N 643	O 725	S 24	0	0	0
1	B	479	Total 3799	C 2407	N 643	O 725	S 24	0	0	0

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 dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolatato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (three-letter code: 402) (formula: $C_7H_5Fe_2N_3O_3S_2$) (labeled as "Ligand of Interest" by author).
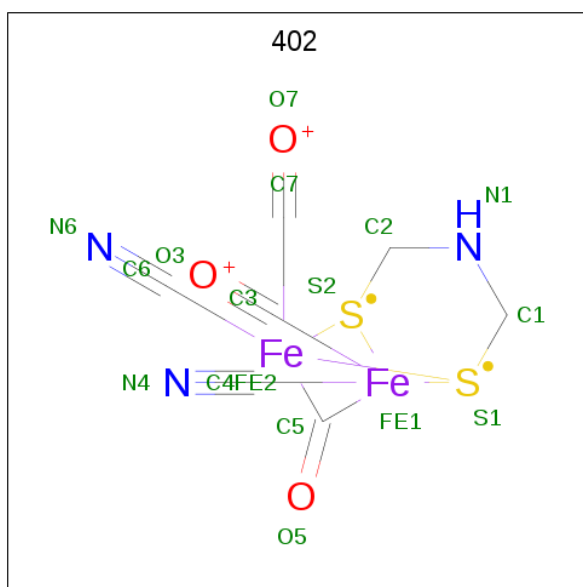
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 17	C 7	Fe 2	N 2	O 3	S 3	2	0	0
2	B	1	Total 17	C 7	Fe 2	N 2	O 3	S 3	2	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
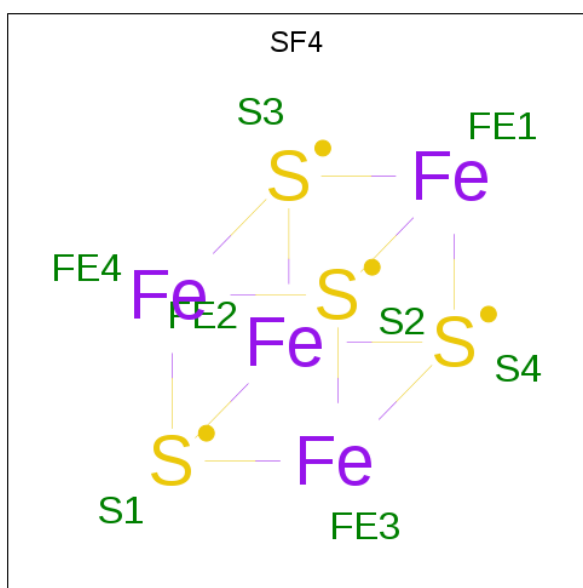
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	Fe 4	S 4	0	0
3	B	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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
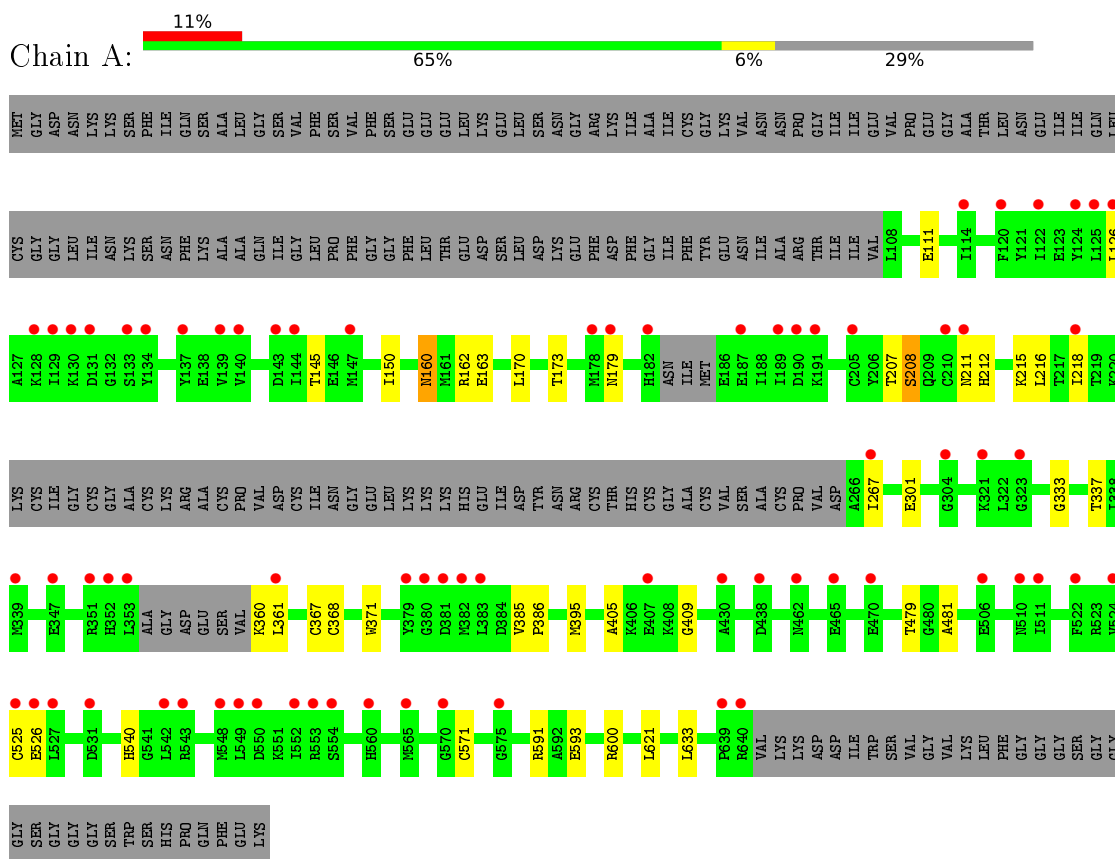
- Molecule 1: [FeFe]-hydrogenase
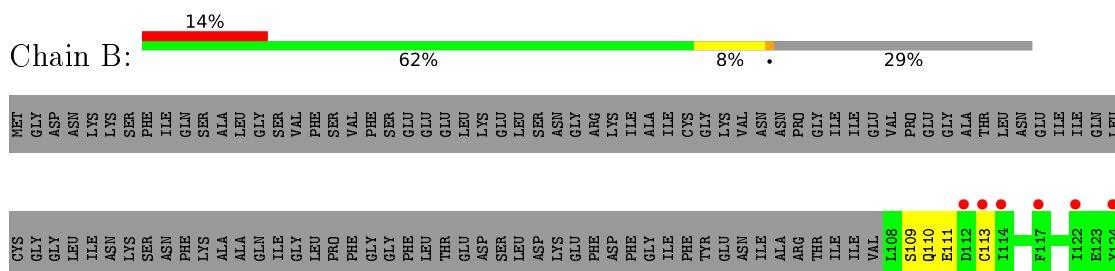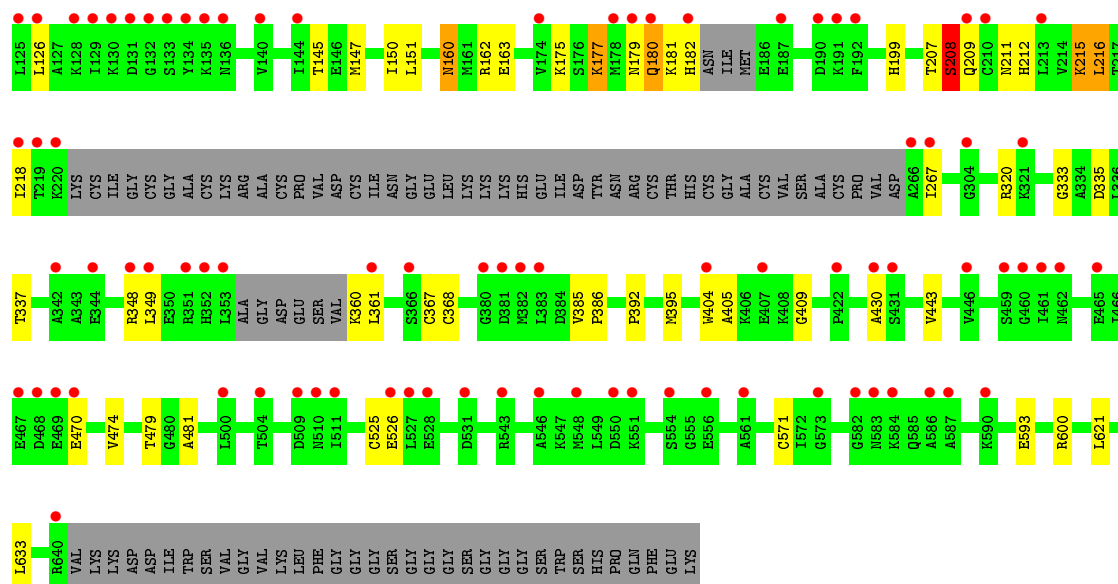
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.00Å 169.00Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.90 49.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.26-2.90) 100.0 (49.26-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.339 , 0.353 0.341 , 0.354	Depositor DCC
R_{free} test set	2065 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	87.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7648	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.04 % 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 1.1968e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: SF4, 402

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	0.24	0/3859	0.41	0/5186
1	B	0.24	0/3859	0.41	0/5186
All	All	0.24	0/7718	0.41	0/10372

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3799	0	3807	25	0
1	B	3799	0	3807	35	0
2	A	17	0	5	3	0
2	B	17	0	5	3	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
All	All	7648	0	7624	60	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 4.

All (60) 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:B:207:THR:O	1:B:208:SER:HB2	1.84	0.77
1:B:405:ALA:O	1:B:409:GLY:N	2.24	0.70
1:A:405:ALA:O	1:A:409:GLY:N	2.25	0.69
1:B:160:ASN:OD1	1:B:162:ARG:NH1	2.27	0.68
1:A:160:ASN:OD1	1:A:162:ARG:NH1	2.27	0.67
1:A:368:CYS:N	2:A:700:402:H8	2.13	0.63
1:B:368:CYS:N	2:B:700:402:H8	2.17	0.59
1:A:218:ILE:HG22	1:A:267:ILE:HG12	1.86	0.57
1:B:218:ILE:HG22	1:B:267:ILE:HG12	1.86	0.57
1:B:179:ASN:ND2	1:B:179:ASN:O	2.41	0.54
1:A:111:GLU:O	1:A:207:THR:HG23	2.09	0.53
1:A:207:THR:O	1:A:208:SER:CB	2.58	0.52
1:B:175:LYS:HG2	1:B:180:GLN:HA	1.91	0.51
1:B:126:LEU:HD21	1:B:145:THR:HG22	1.93	0.51
1:A:179:ASN:O	1:A:179:ASN:ND2	2.44	0.50
1:B:571:CYS:CB	2:B:700:402:C4	2.89	0.50
1:A:479:THR:HG22	1:A:481:ALA:H	1.77	0.50
1:B:360:LYS:C	1:B:361:LEU:HD12	2.33	0.49
1:A:571:CYS:CB	2:A:700:402:C4	2.89	0.49
1:A:301:GLU:OE2	1:A:591:ARG:NE	2.44	0.49
1:B:571:CYS:SG	2:B:700:402:H7	2.52	0.49
1:B:177:LYS:N	1:B:177:LYS:HD2	2.27	0.49
1:A:593:GLU:OE2	1:A:600:ARG:NH2	2.46	0.48
1:A:395:MET:SD	1:A:633:LEU:HD22	2.54	0.48
1:B:111:GLU:O	1:B:207:THR:HG23	2.14	0.48
1:A:525:CYS:SG	1:A:526:GLU:N	2.86	0.48
1:B:479:THR:HG22	1:B:481:ALA:H	1.79	0.48
1:A:526:GLU:OE1	1:A:526:GLU:N	2.47	0.47
1:B:526:GLU:OE1	1:B:526:GLU:N	2.48	0.47
1:A:211:ASN:O	1:A:212:HIS:HB2	2.15	0.46
1:A:333:GLY:O	1:A:337:THR:HG23	2.15	0.46
1:B:333:GLY:O	1:B:337:THR:HG23	2.16	0.45
1:B:337:THR:HG21	1:B:392:PRO:HG3	1.99	0.45
1:B:404:TRP:HZ3	1:B:474:VAL:HG11	1.82	0.45
1:B:113:CYS:SG	1:B:199:HIS:NE2	2.89	0.44
1:B:348:ARG:NH1	1:B:360:LYS:O	2.50	0.44
1:B:593:GLU:OE2	1:B:600:ARG:NH2	2.50	0.44
1:B:385:VAL:N	1:B:386:PRO:CD	2.81	0.44
1:B:385:VAL:N	1:B:386:PRO:HD3	2.33	0.44
1:A:126:LEU:HD21	1:A:145:THR:HG22	1.99	0.43
1:B:211:ASN:O	1:B:212:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HD12	1:B:361:LEU:HD21	2.00	0.43
1:B:430:ALA:HB1	1:B:443:VAL:HG23	2.00	0.43
1:A:571:CYS:SG	2:A:700:402:H7	2.59	0.43
1:A:150:ILE:HG23	1:A:163:GLU:HB3	2.00	0.42
1:A:385:VAL:N	1:A:386:PRO:HD3	2.34	0.42
1:B:525:CYS:SG	1:B:526:GLU:N	2.93	0.42
1:B:147:MET:O	1:B:151:LEU:HD23	2.20	0.42
1:B:150:ILE:HG23	1:B:163:GLU:HB3	2.00	0.42
1:B:395:MET:SD	1:B:633:LEU:HD22	2.59	0.42
1:A:360:LYS:C	1:A:361:LEU:HD12	2.41	0.42
1:B:335:ASP:OD2	1:B:479:THR:HB	2.20	0.41
1:B:320:ARG:NH2	1:B:470:GLU:O	2.52	0.41
1:B:215:LYS:O	1:B:216:LEU:HB2	2.19	0.41
1:A:170:LEU:HA	1:A:173:THR:HG22	2.01	0.41
1:A:385:VAL:N	1:A:386:PRO:CD	2.84	0.41
1:B:109:SER:O	1:B:110:GLN:HB3	2.21	0.41
1:B:348:ARG:HB3	1:B:361:LEU:HD11	2.02	0.41
1:A:368:CYS:O	1:A:371:TRP:NE1	2.55	0.40
1:A:395:MET:SD	1:A:633:LEU:HB3	2.61	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	471/674 (70%)	432 (92%)	37 (8%)	2 (0%)	34	66
1	B	471/674 (70%)	432 (92%)	37 (8%)	2 (0%)	34	66
All	All	942/1348 (70%)	864 (92%)	74 (8%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	B	208	SER
1	A	216	LEU
1	B	216	LEU

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	408/565 (72%)	403 (99%)	5 (1%)	71	91
1	B	408/565 (72%)	398 (98%)	10 (2%)	47	78
All	All	816/1130 (72%)	801 (98%)	15 (2%)	59	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	215	LYS
1	A	367	CYS
1	A	540	HIS
1	A	621	LEU
1	B	160	ASN
1	B	177	LYS
1	B	180	GLN
1	B	181	LYS
1	B	182	HIS
1	B	208	SER
1	B	209	GLN
1	B	215	LYS
1	B	367	CYS
1	B	621	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SF4	B	701	1	0,12,12	0.00	-	-		
2	402	A	700	1	13,19,19	2.36	7 (53%)	2,36,36	1.23	0
3	SF4	A	701	1	0,12,12	0.00	-	-		
2	402	B	700	1	13,19,19	2.33	6 (46%)	2,36,36	1.55	1 (50%)

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	B	701	1	-	-	0/6/5/5
2	402	A	700	1	-	-	0/5/3/3
3	SF4	A	701	1	-	-	0/6/5/5
2	402	B	700	1	-	-	0/5/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	402	S1-FE2	4.13	2.32	2.26
2	A	700	402	S1-FE2	4.12	2.32	2.26
2	B	700	402	C4-N4	3.81	1.21	1.15
2	A	700	402	C4-N4	3.73	1.21	1.15
2	A	700	402	O3-C3	3.04	1.23	1.15
2	B	700	402	O3-C3	3.02	1.23	1.15
2	A	700	402	S2-FE1	2.83	2.30	2.26
2	B	700	402	S2-FE1	2.70	2.30	2.26
2	A	700	402	S2-FE2	2.60	2.30	2.26
2	B	700	402	S2-FE2	2.54	2.29	2.26
2	A	700	402	C2-S2	2.45	1.89	1.85
2	B	700	402	C2-S2	2.41	1.89	1.85
2	A	700	402	S1-FE1	2.08	2.29	2.26

All (1) bond angle outliers are listed below:

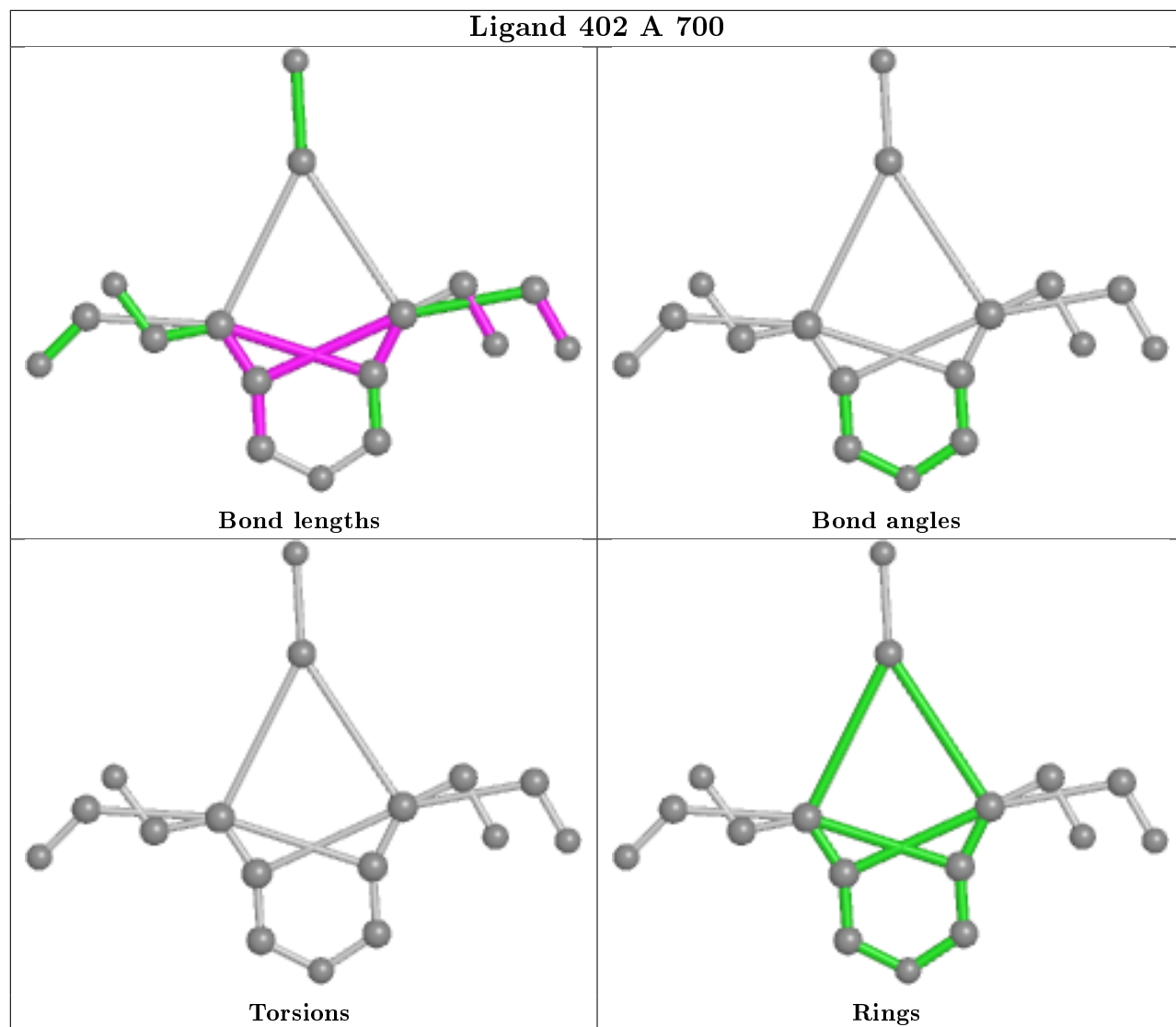| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	700	402	S2-C2-N1	2.18	123.17	117.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	402	3	0
2	B	700	402	3	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 402 A 700

Bond lengths

Bond angles

Torsions

Rings

Ligand 402 B 700

Bond lengths

Bond angles

Torsions

Rings
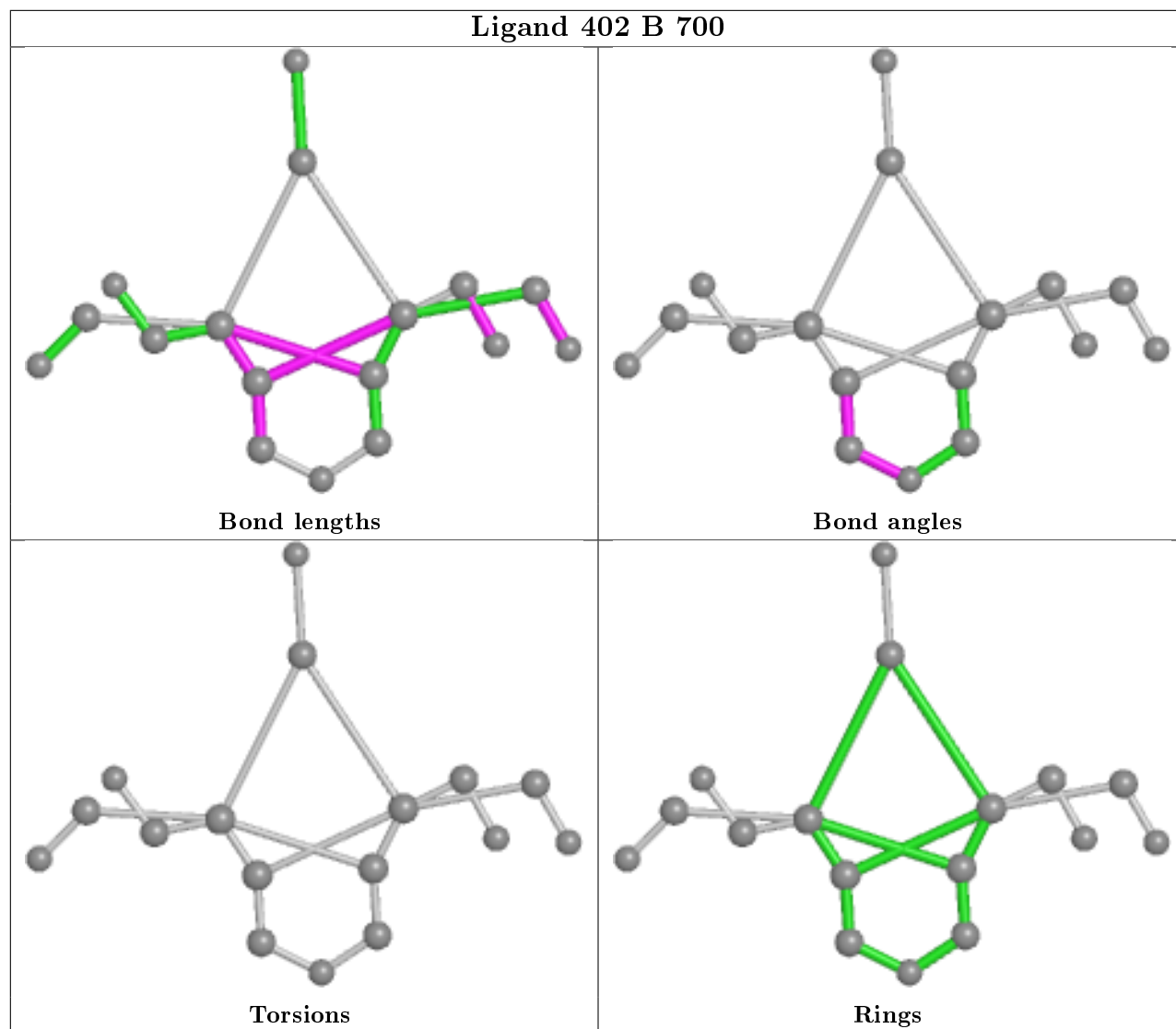
5.7 Other polymers (i)

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	479/674 (71%)	1.07	73 (15%)	2 1	54, 69, 90, 107	0
1	B	479/674 (71%)	1.11	91 (18%)	1 0	53, 70, 93, 109	0
All	All	958/1348 (71%)	1.09	164 (17%)	1 1	53, 69, 92, 109	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	ILE	7.9
1	A	134	TYR	7.2
1	A	353	LEU	6.9
1	A	140	VAL	6.7
1	A	133	SER	6.4
1	A	267	ILE	6.0
1	B	267	ILE	5.7
1	B	131	ASP	5.7
1	B	191	LYS	5.6
1	A	543	ARG	5.4
1	B	190	ASP	5.3
1	A	190	ASP	5.3
1	A	351	ARG	5.2
1	A	182	HIS	5.2
1	B	465	GLU	5.2
1	A	380	GLY	5.1
1	B	353	LEU	5.0
1	B	509	ASP	5.0
1	B	133	SER	4.8
1	B	219	THR	4.8
1	B	135	LYS	4.7
1	B	122	ILE	4.6
1	A	575	GLY	4.6
1	A	531	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	4.4
1	A	383	LEU	4.4
1	B	526	GLU	4.4
1	A	640	ARG	4.4
1	A	131	ASP	4.4
1	B	132	GLY	4.2
1	B	361	LEU	4.2
1	B	383	LEU	4.2
1	B	640	ARG	4.1
1	B	349	LEU	4.1
1	A	548	MET	4.0
1	A	143	ASP	3.9
1	B	467	GLU	3.9
1	B	510	ASN	3.9
1	B	174	VAL	3.9
1	A	465	GLU	3.9
1	B	461	ILE	3.8
1	B	543	ARG	3.8
1	B	140	VAL	3.8
1	B	422	PRO	3.7
1	B	321	LYS	3.7
1	B	586	ALA	3.6
1	B	554	SER	3.6
1	B	125	LEU	3.6
1	B	511	ILE	3.6
1	A	137	TYR	3.6
1	B	209	GLN	3.5
1	A	510	ASN	3.5
1	B	342	ALA	3.5
1	A	122	ILE	3.5
1	A	553	ARG	3.4
1	B	266	ALA	3.4
1	B	130	LYS	3.4
1	B	304	GLY	3.4
1	A	361	LEU	3.4
1	B	136	ASN	3.3
1	B	134	TYR	3.3
1	A	542	LEU	3.3
1	A	139	VAL	3.3
1	B	583	ASN	3.3
1	A	639	PRO	3.3
1	A	218	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	178	MET	3.2
1	B	528	GLU	3.2
1	A	129	ILE	3.1
1	B	129	ILE	3.1
1	B	551	LYS	3.1
1	B	382	MET	3.1
1	A	187	GLU	3.1
1	B	218	ILE	3.1
1	B	187	GLU	3.1
1	A	524	VAL	3.0
1	A	527	LEU	3.0
1	B	126	LEU	3.0
1	A	304	GLY	3.0
1	A	552	ILE	2.9
1	A	522	PHE	2.9
1	A	526	GLU	2.9
1	B	459	SER	2.9
1	A	205	CYS	2.9
1	A	430	ALA	2.9
1	A	554	SER	2.8
1	B	407	GLU	2.8
1	B	180	GLN	2.8
1	B	112	ASP	2.8
1	B	527	LEU	2.8
1	B	179	ASN	2.8
1	B	550	ASP	2.8
1	B	213	LEU	2.8
1	B	220	LYS	2.8
1	B	582	GLY	2.8
1	B	470	GLU	2.8
1	B	210	CYS	2.8
1	B	124	TYR	2.7
1	B	117	PHE	2.7
1	A	128	LYS	2.7
1	A	130	LYS	2.7
1	B	584	LYS	2.7
1	B	531	ASP	2.7
1	A	550	ASP	2.6
1	A	462	ASN	2.6
1	A	549	LEU	2.6
1	A	178	MET	2.6
1	B	182	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	500	LEU	2.6
1	B	504	THR	2.6
1	A	210	CYS	2.5
1	A	125	LEU	2.5
1	A	147	MET	2.5
1	B	462	ASN	2.5
1	B	556	GLU	2.5
1	A	189	ILE	2.5
1	A	179	ASN	2.5
1	A	381	ASP	2.5
1	A	323	GLY	2.5
1	B	114	ILE	2.5
1	B	344	GLU	2.4
1	A	511	ILE	2.4
1	B	352	HIS	2.4
1	B	430	ALA	2.4
1	A	407	GLU	2.3
1	A	570	GLY	2.3
1	B	351	ARG	2.3
1	A	191	LYS	2.3
1	A	379	TYR	2.3
1	A	382	MET	2.3
1	A	124	TYR	2.3
1	A	321	LYS	2.3
1	A	211	ASN	2.2
1	B	548	MET	2.2
1	A	560	HIS	2.2
1	A	347	GLU	2.2
1	B	380	GLY	2.2
1	B	446	VAL	2.2
1	B	468	ASP	2.2
1	B	113	CYS	2.2
1	B	587	ALA	2.2
1	A	352	HIS	2.2
1	B	128	LYS	2.2
1	A	339	MET	2.2
1	A	525	CYS	2.2
1	A	565	MET	2.2
1	A	114	ILE	2.1
1	B	460	GLY	2.1
1	B	573	GLY	2.1
1	B	192	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	506	GLU	2.1
1	B	366	SER	2.1
1	A	470	GLU	2.1
1	B	404	TRP	2.1
1	A	120	PHE	2.1
1	B	431	SER	2.1
1	B	144	ILE	2.1
1	B	561	ALA	2.1
1	B	469	GLU	2.1
1	A	438	ASP	2.1
1	B	546	ALA	2.1
1	B	381	ASP	2.0
1	B	348	ARG	2.0
1	B	590	LYS	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, 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
2	402	A	700	17/17	0.96	0.23	58,61,71,75	0
3	SF4	A	701	8/8	0.96	0.17	58,62,68,68	8
2	402	B	700	17/17	0.96	0.28	56,59,67,69	0
3	SF4	B	701	8/8	0.98	0.19	60,62,66,74	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.
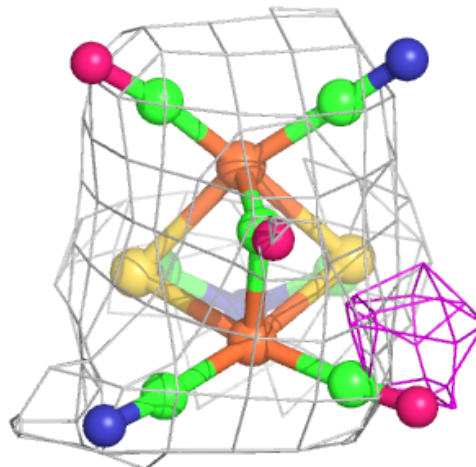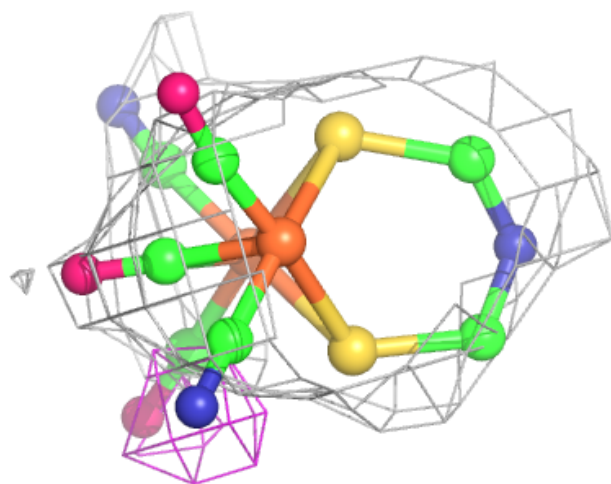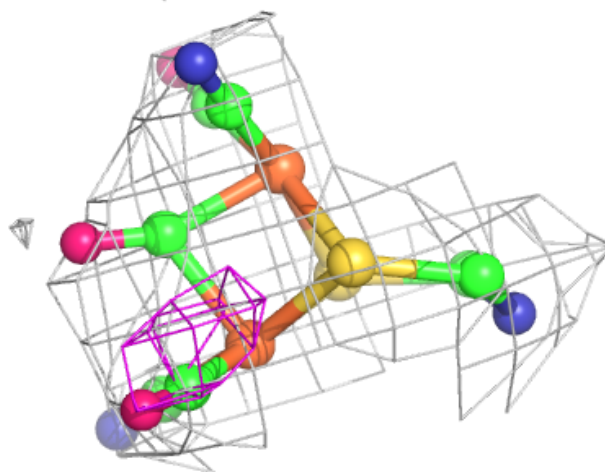
Electron density around 402 A 700:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
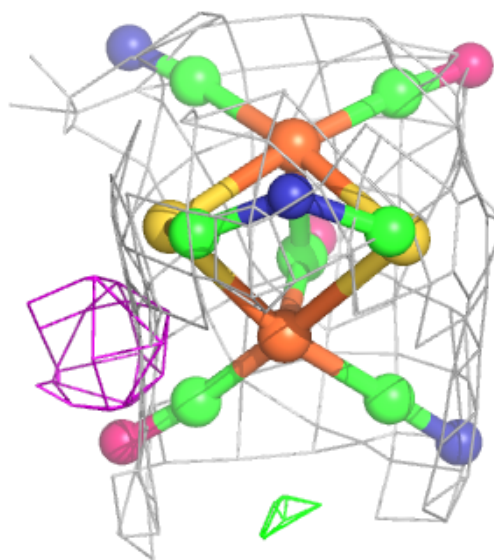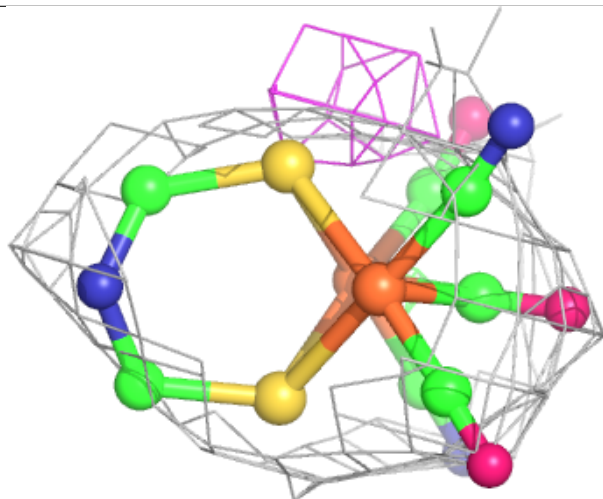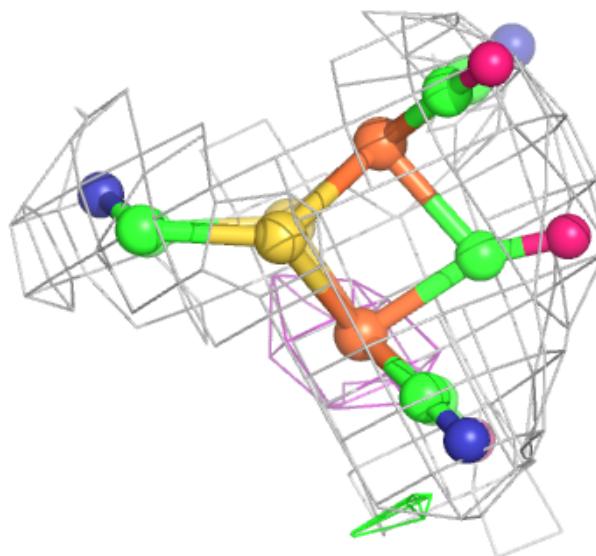
Electron density around 402 B 700:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.