



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:28 AM UTC

PDB ID : 6TTL / pdb_00006ttl
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)

This is a wwPDB X-ray Structure Validation Summary 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

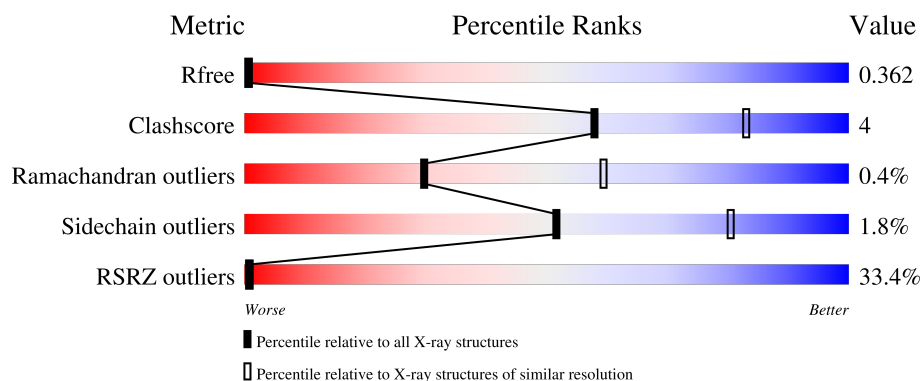
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	23% 64% 7% 29%
1	B	674	25% 62% 9% 29%

2 Entry composition

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	C	N	O	S	0	0	0
			3799	2407	643	725	24			
1	B	479	Total	C	N	O	S	0	0	0
			3799	2407	643	725	24			

There are 60 discrepancies between the modelled and reference sequences:

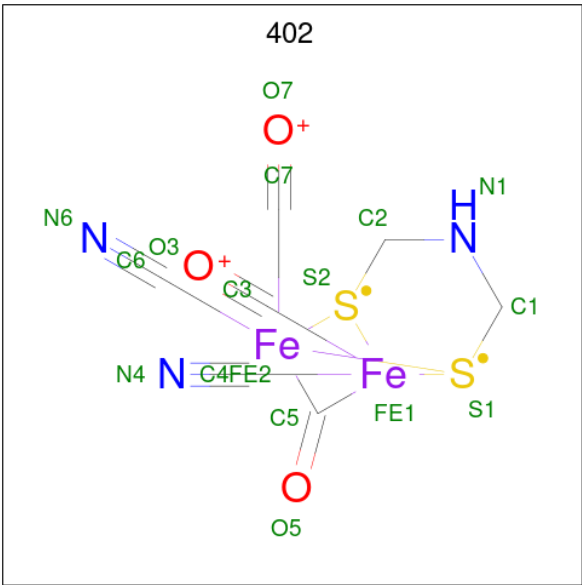
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ASP	-	expression tag	UNP A0A1I9RYV3
A	646	ILE	-	expression tag	UNP A0A1I9RYV3
A	647	TRP	-	expression tag	UNP A0A1I9RYV3
A	648	SER	-	expression tag	UNP A0A1I9RYV3
A	649	VAL	-	expression tag	UNP A0A1I9RYV3
A	650	GLY	-	expression tag	UNP A0A1I9RYV3
A	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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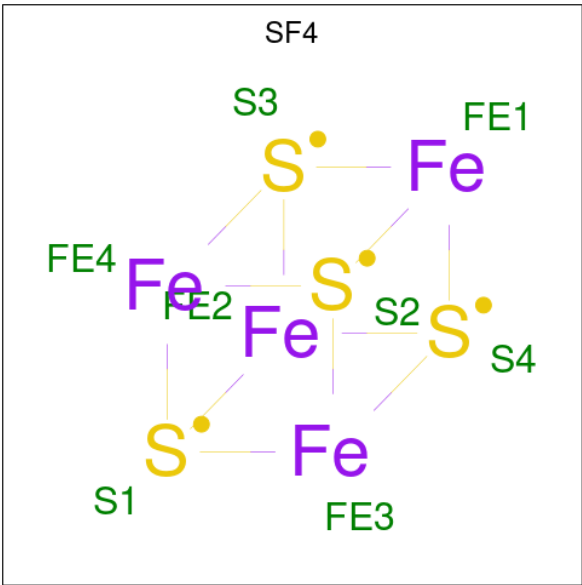
Chain	Residue	Modelled	Actual	Comment	Reference
A	670	PRO	-	expression tag	UNP A0A1I9RYV3
A	671	GLN	-	expression tag	UNP A0A1I9RYV3
A	672	PHE	-	expression tag	UNP A0A1I9RYV3
A	673	GLU	-	expression tag	UNP A0A1I9RYV3
A	674	LYS	-	expression tag	UNP A0A1I9RYV3
B	645	ASP	-	expression tag	UNP A0A1I9RYV3
B	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+) (CCD ID: 402) (formula: C₇H₅Fe₂N₃O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	S	0	0
			17	7	2	3	3	2		
2	B	1	Total	C	Fe	N	O	S	0	0
			17	7	2	3	3	2		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

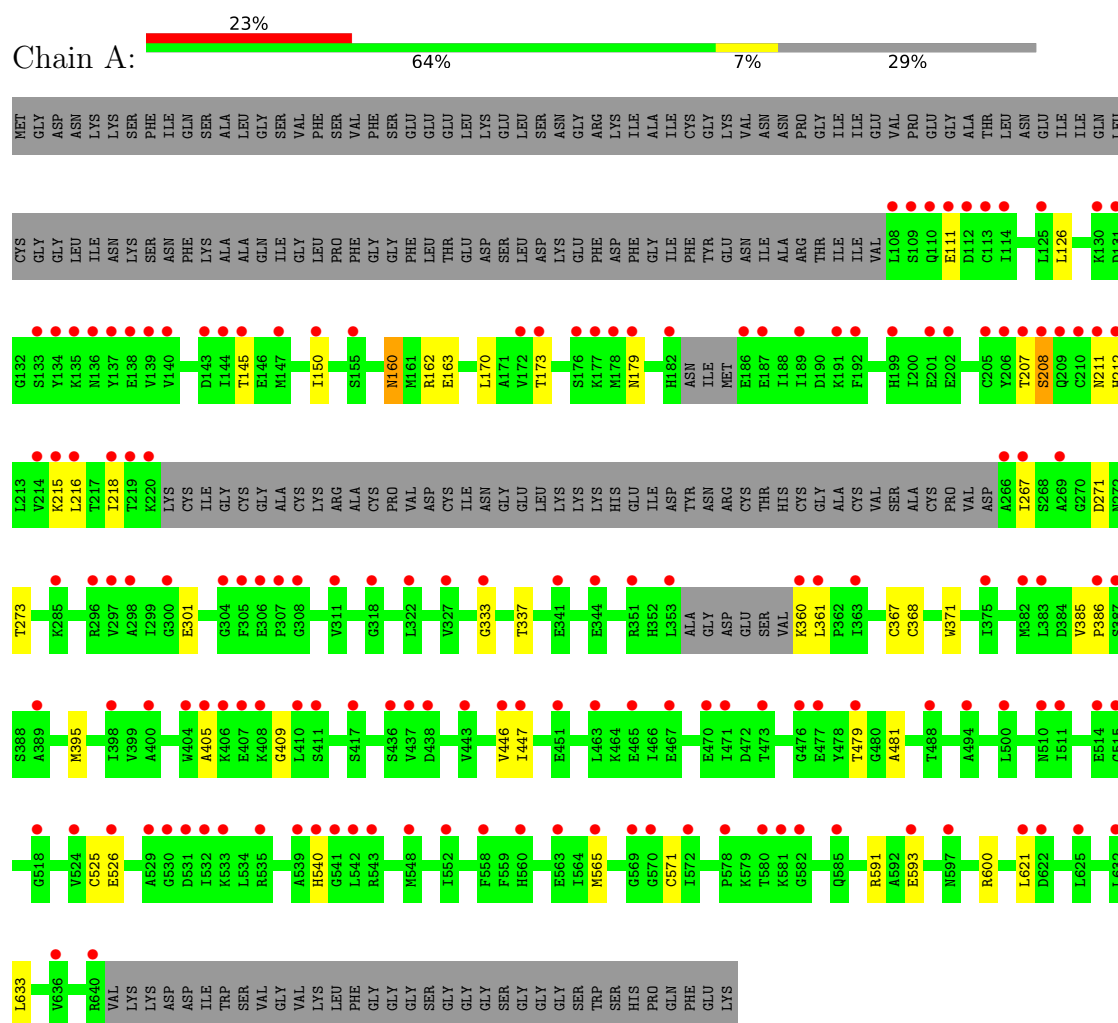


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

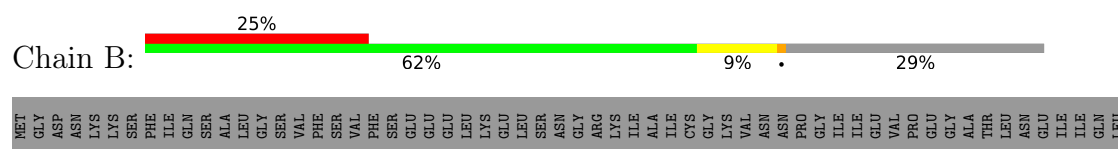
3 Residue-property plots

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



SER	K579	Y478	D384	A269	Q209	L195	CYS
HIS	T580	T479	V385	G270	C210	L126	GLY
PRO	K581	G490	P386	M274	H211	A127	GLY
GLN	G582	A481	S387	L275	H212	K128	LEU
PHE	N583	G490	P392	V295	L213	D131	ILE
GLU	K584	T498	M395	R296	V214	G132	ASN
LYS	Q585	A499	A400	V297	K215	S133	LYS
	A586	L500	W404	G304	L216	Y134	SER
	A587	R507	A405	E308	T217	K135	ASN
	L588	D509	K406	E309	L218	N136	PHE
	Q589	N510	K407	N310	T219	Y137	LYS
	K590	F511	K408	K313	K220	Y140	ALA
	E593	E512	G409	R320	L151	T145	ALA
	T598	F513	L410	K321	L150	M147	GLN
	D599	E514	S417	L322	L151	T145	ILE
	P599	G518	I420	D325	S155	T145	GLY
	R600	G521	M421	G333	M160	T145	LEU
	S601	F522	P422	A334	M161	M147	PRO
	K602	R523	K427	D335	E163	T145	PHE
	T603	V524	Y428	L336	E163	T145	GLY
	N608	E526	A430	T337	E163	T145	LEU
	L621	L527	S431	A342	K175	K175	THR
	P622	E528	R432	A343	K176	K176	GLU
	L633	A529	S436	E344	K177	K177	ASP
	V636	G530	D442	R348	M178	M178	PHE
	Y637	D531	V443	L349	Q180	Q180	ASP
	R640	F532	V446	L353	K181	K181	LYS
VAL	LYS	K533	I447	ALA	H182	H182	ILE
LYS	LYS	H540	E451	GLY	ASN	ASN	PHE
ASP	ASP	G541	L452	ASP	ILE	ILE	TYR
ILE	ILE	L542	GLU	GLY	MET	MET	GLU
TRP	TRP	R543	ASP	ASP	ASP	ASP	ASN
SER	SER	L549	GLU	TYR	ILE	ILE	ILE
VAL	VAL	I552	SER	ASN	E186	E186	ALA
GLY	GLY	L552	ARG	ASN	E187	E187	ALA
LYS	LYS	G555	VAL	ARG	T188	T188	ARG
LEU	LEU	E556	K360	CYS	D189	D189	THR
PHE	PHE	E556	L361	THR	K191	K191	ILE
GLY	GLY	A561	P362	HIS	F192	F192	ILE
GLY	GLY	I562	S366	CYS	L108	L108	VAL
SER	SER	I562	C367	ALA	S109	S109	
GLY	GLY	M565	C368	CYS	Q110	Q110	
GLY	GLY	V568	W371	VAL	E111	E111	
GLY	GLY	G569	I466	SER	D112	D112	
SER	SER	G570	D468	ALA	C113	C113	
GLY	GLY	C571	E470	ALA	I114	I114	
GLY	GLY	I572	K373	CYS	I115	I115	
GLY	GLY	G573	E471	PRO	Q116	Q116	
TRP	TRP		V474	VAL	F117	F117	
			E477	ASP	C205	C205	
				A266	T206	T206	
				L267	E123	E123	
				S268	Y124	Y124	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.339 , 0.353 0.345 , 0.362	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 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: 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	0.11	0/3859	0.27	0/5186
1	B	0.10	0/3859	0.29	0/5186
All	All	0.10	0/7718	0.28	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 [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	3799	0	3807	28	0
1	B	3799	0	3807	40	0
2	A	17	0	5	4	0
2	B	17	0	5	5	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
All	All	7648	0	7624	68	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.

The worst 5 of 68 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

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%)	30	59
1	B	471/674 (70%)	432 (92%)	37 (8%)	2 (0%)	30	59
All	All	942/1348 (70%)	864 (92%)	74 (8%)	4 (0%)	30	59

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%)	63	86
1	B	408/565 (72%)	398 (98%)	10 (2%)	42	74
All	All	816/1130 (72%)	801 (98%)	15 (2%)	51	80

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	180	GLN
1	B	215	LYS
1	B	181	LYS
1	B	621	LEU
1	B	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	179	ASN
1	A	378	ASN
1	B	152	ASN
1	B	378	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 ⓘ

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	A	701	1	0,12,12	-	-	-		
2	402	A	700	1	15,19,19	2.60	9 (60%)	1,36,36	2.07	1 (100%)
3	SF4	B	701	1	0,12,12	-	-	-		
2	402	B	700	1	15,19,19	2.57	8 (53%)	1,36,36	0.91	0

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

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	402	S1-FE2	4.40	2.32	2.26
2	A	700	402	S1-FE2	4.39	2.32	2.26
2	B	700	402	C4-N4	4.26	1.21	1.15
2	A	700	402	C4-N4	4.18	1.21	1.15
2	A	700	402	C2-N1	3.43	1.50	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	402	C1-N1-C2	2.07	119.93	114.31

There are no chirality outliers.

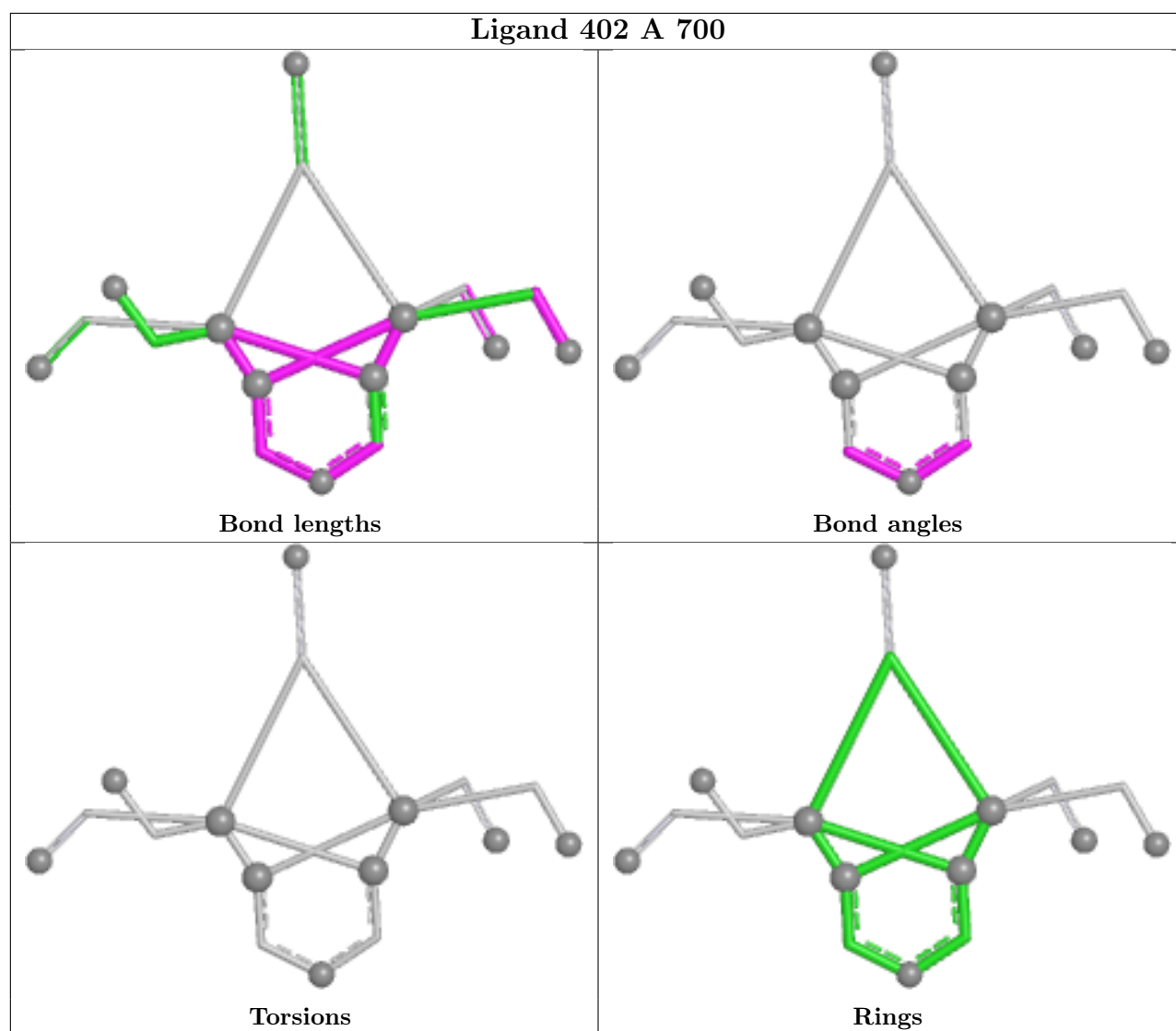
There are no torsion outliers.

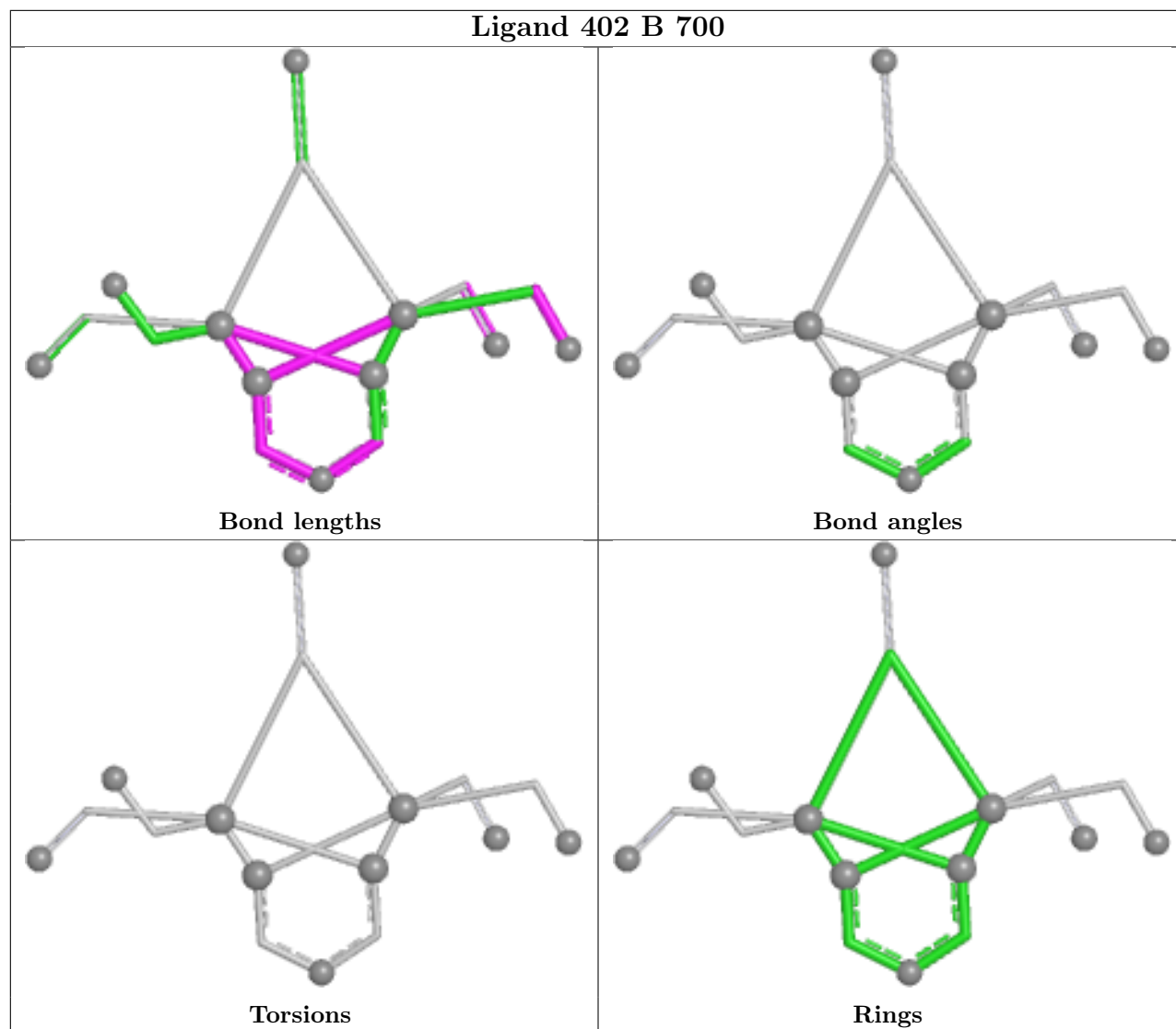
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	402	4	0
2	B	700	402	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	1.71	153 (31%)	1 1	54, 69, 90, 107	0
1	B	479/674 (71%)	1.71	167 (34%)	1 1	53, 70, 93, 109	0
All	All	958/1348 (71%)	1.71	320 (33%)	1 1	53, 69, 92, 109	0

The worst 5 of 320 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	7.7
1	A	543	ARG	6.8
1	A	210	CYS	6.8
1	A	266	ALA	6.7
1	B	266	ALA	6.6

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](#)

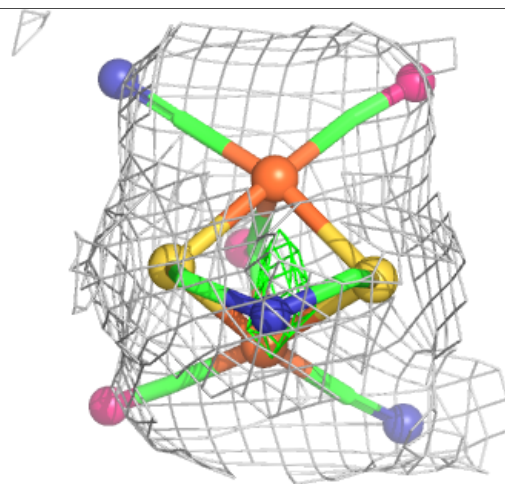
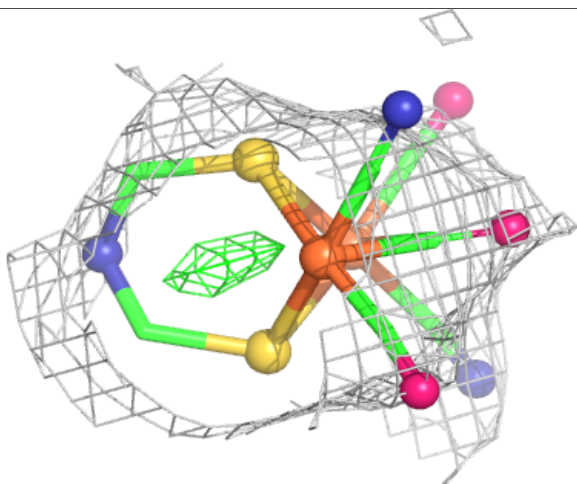
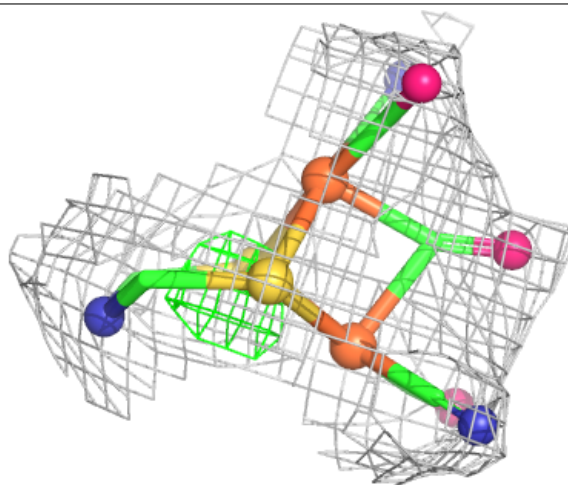
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	402	B	700	17/17	0.96	0.13	56,59,67,69	0
3	SF4	A	701	8/8	0.96	0.07	58,62,68,68	8
2	402	A	700	17/17	0.97	0.10	58,61,71,75	0
3	SF4	B	701	8/8	0.98	0.06	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.

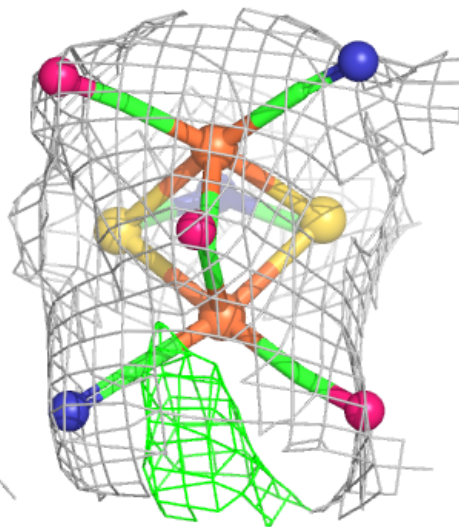
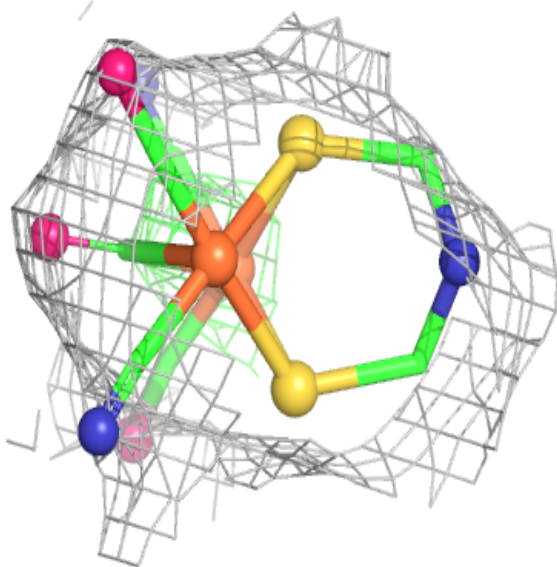
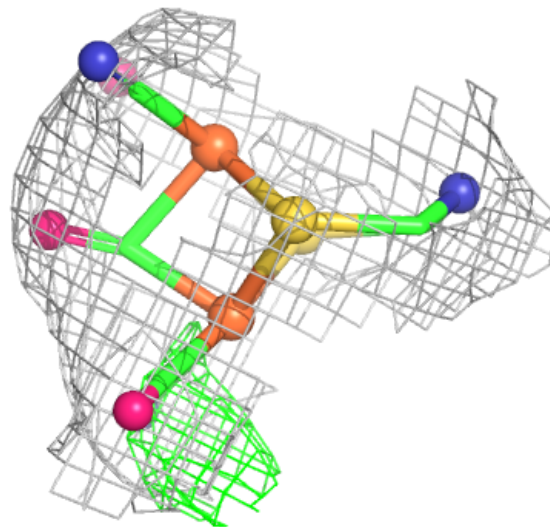
Electron density around 402 B 700:

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.