



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:29 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 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

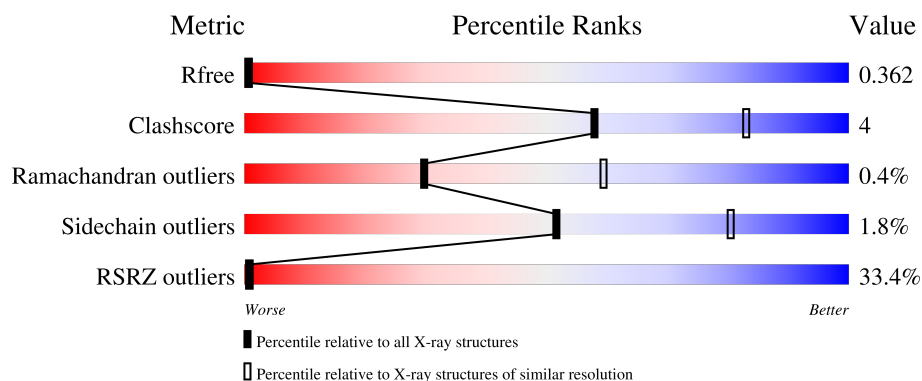
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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:

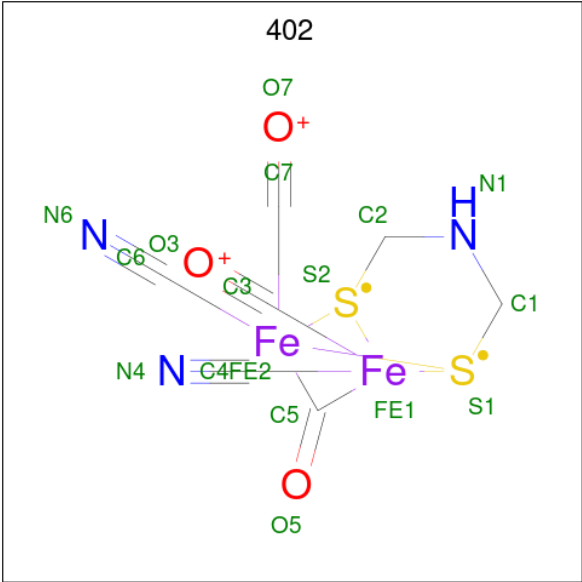
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ASP	-	expression tag	UNP A0A1I9RYV3
A	646	ILE	-	expression tag	UNP A0A1I9RYV3
A	647	TRP	-	expression tag	UNP A0A1I9RYV3
A	648	SER	-	expression tag	UNP A0A1I9RYV3
A	649	VAL	-	expression tag	UNP A0A1I9RYV3
A	650	GLY	-	expression tag	UNP A0A1I9RYV3
A	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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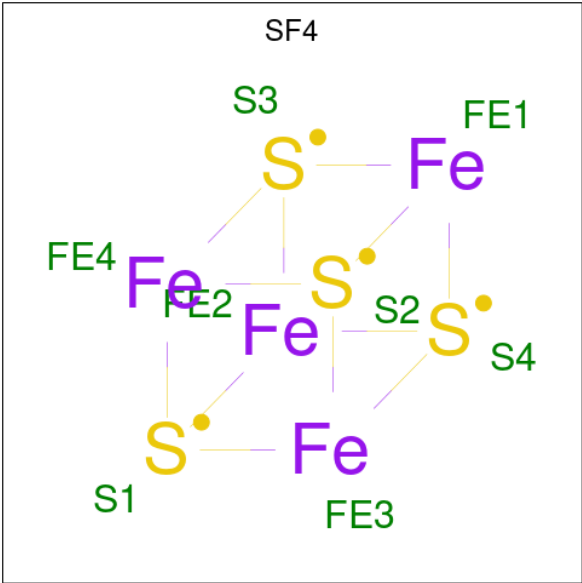
Chain	Residue	Modelled	Actual	Comment	Reference
A	670	PRO	-	expression tag	UNP A0A1I9RYV3
A	671	GLN	-	expression tag	UNP A0A1I9RYV3
A	672	PHE	-	expression tag	UNP A0A1I9RYV3
A	673	GLU	-	expression tag	UNP A0A1I9RYV3
A	674	LYS	-	expression tag	UNP A0A1I9RYV3
B	645	ASP	-	expression tag	UNP A0A1I9RYV3
B	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).

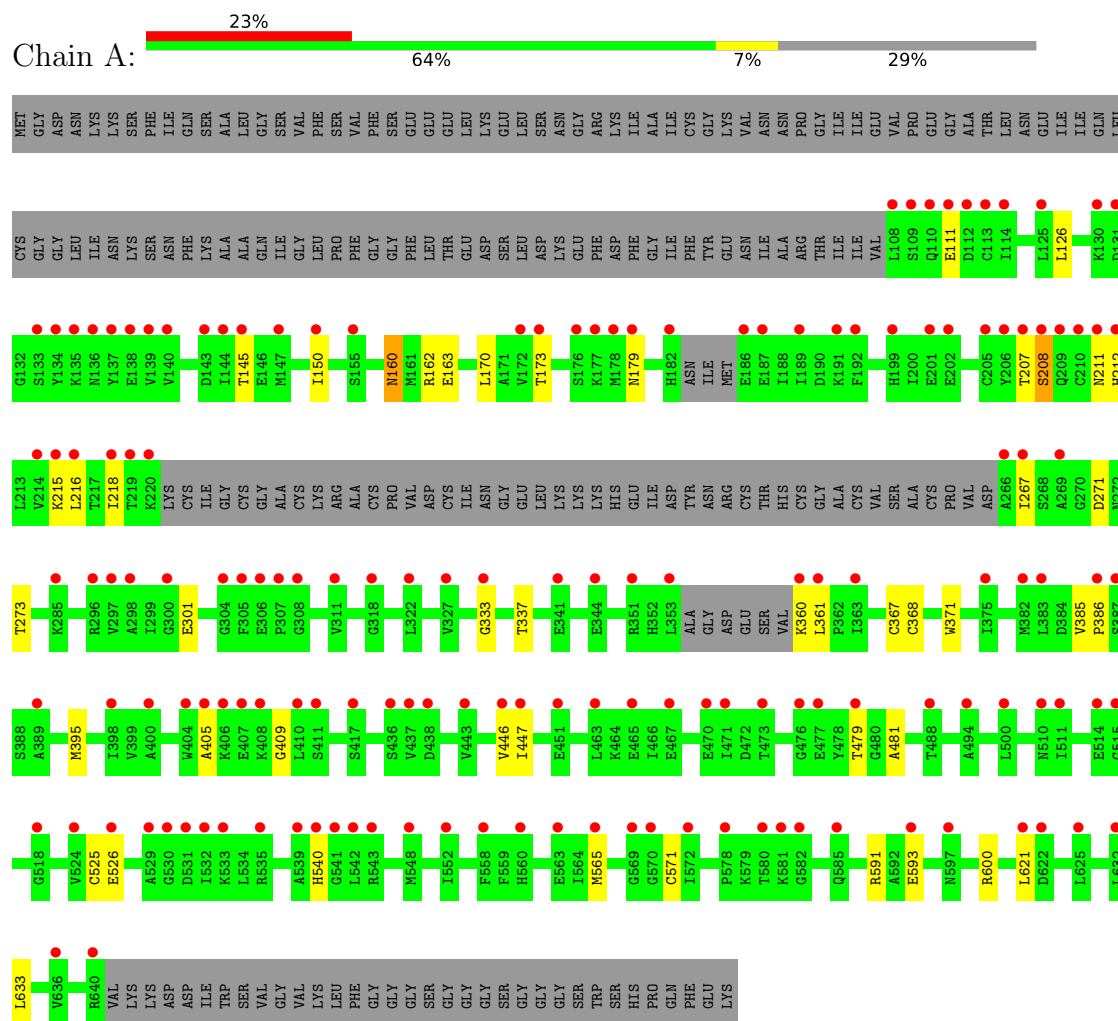


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

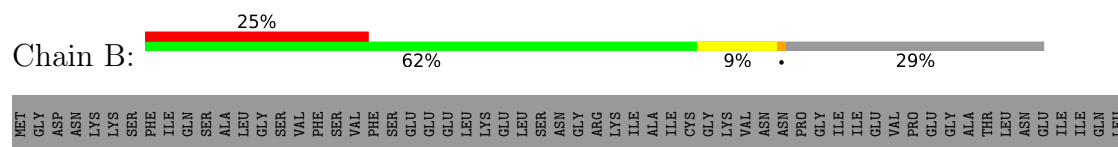
3 Residue-property plots

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	M147	LEU
	S601	F522	P422	A334	M161	M147	PRO
	K602	R523	K427	D335	E163	T150	PHE
	T603	V524	Y428	L336	E163	T150	GLY
	N608	E526	A430	T337	K175	T150	LEU
	L621	L527	R432	A342	K176	K175	THR
	P622	A529	S436	E343	K177	K176	GLU
	L633	G530	D442	E344	K178	K177	ASP
	V636	D531	V443	R348	Q180	K181	SER
	Y637	F532	V446	L349	Q180	K181	LEU
	R640	K533	I447	L353	H182	H182	ASP
VAL	LYS	H540	E451	ALA	ASN	ASN	LYS
LYS	LYS	G541	L452	GLY	ILE	ILE	GLY
ASP	ASP	L542	ASP	ASP	MET	MET	PHE
ILE	ILE	R543	GLU	TYR	E186	E186	ASP
TRP	TRP	L549	VAL	VAL	E187	E187	PHE
SER	SER	I552	K453	SER	I188	I188	GLY
GLY	VAL	L552	K454	VAL	D190	D190	ILE
VAL	VAL	G555	I455	K360	K191	K191	THR
LYS	LYS	E556	F456	L361	F192	F192	ILE
LEU	PHE	G556	E457	P362	F192	F192	ILE
PHE	GLY	E556	E457	P362	F192	F192	VAL
GLY	GLY	A561	K464	S366	E196	E196	L108
GLY	GLY	I562	E465	C367	I196	I196	S109
SER	SER	M565	I466	C368	E197	E197	Q110
GLY	GLY	V568	E467	W371	E198	E198	E111
GLY	GLY	G569	D468	I372	H199	H199	D112
SER	SER	G570	E469	K373	L200	L200	C113
GLY	GLY	C571	E470	E376	E201	E201	I114
GLY	GLY	I572	I471	E376	E201	E201	I115
GLY	GLY	G573	V474	M382	C205	C205	Q116
TRP	TRP	E477	E477	L383	T206	T206	F117
					T207	T207	E123
					S208	S208	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.

All (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
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:271:ASP:OD1	1:A:273:THR:OG1	2.15	0.57
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:360:LYS:C	1:B:361:LEU:HD12	2.33	0.54
1:B:179:ASN:O	1:B:179:ASN:ND2	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: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:N	1:A:526:GLU:OE1	2.47	0.47
1:B:526:GLU:N	1:B:526:GLU:OE1	2.48	0.47
1:A:360:LYS:C	1:A:361:LEU:HD12	2.41	0.46
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:A:565:MET:HE1	2:A:700:402:N1	2.31	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:446:VAL:C	1:B:447:ILE:HD12	2.44	0.43
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:A:446:VAL:C	1:A:447:ILE:HD12	2.45	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:B:565:MET:HE1	2:B:700:402:N1	2.35	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:565:MET:HE1	2:B:700:402:H7	2.03	0.41
1:B:211:ASN:C	1:B:213:LEU:H	2.27	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:382:MET:HE1	1:B:549:LEU:HB3	2.02	0.41
1:B:215:LYS:O	1:B:216:LEU:HB2	2.19	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

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	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 ⓘ

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

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	198	GLU
1	B	208	SER

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Mol	Chain	Res	Type
1	B	209	GLN
1	B	215	LYS
1	B	621	LEU

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 [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](#)

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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
2	B	700	402	C2-N1	3.42	1.50	1.40
2	A	700	402	O3-C3	3.18	1.23	1.15
2	B	700	402	O3-C3	3.16	1.23	1.15
2	A	700	402	S2-FE1	2.99	2.30	2.26
2	A	700	402	C1-N1	2.88	1.48	1.40
2	B	700	402	C1-N1	2.85	1.48	1.40
2	B	700	402	S2-FE1	2.84	2.30	2.26
2	A	700	402	S2-FE2	2.74	2.30	2.26
2	B	700	402	S2-FE2	2.67	2.29	2.26
2	A	700	402	C2-S2	2.43	1.89	1.85
2	B	700	402	C2-S2	2.39	1.89	1.85
2	A	700	402	S1-FE1	2.18	2.29	2.26

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.

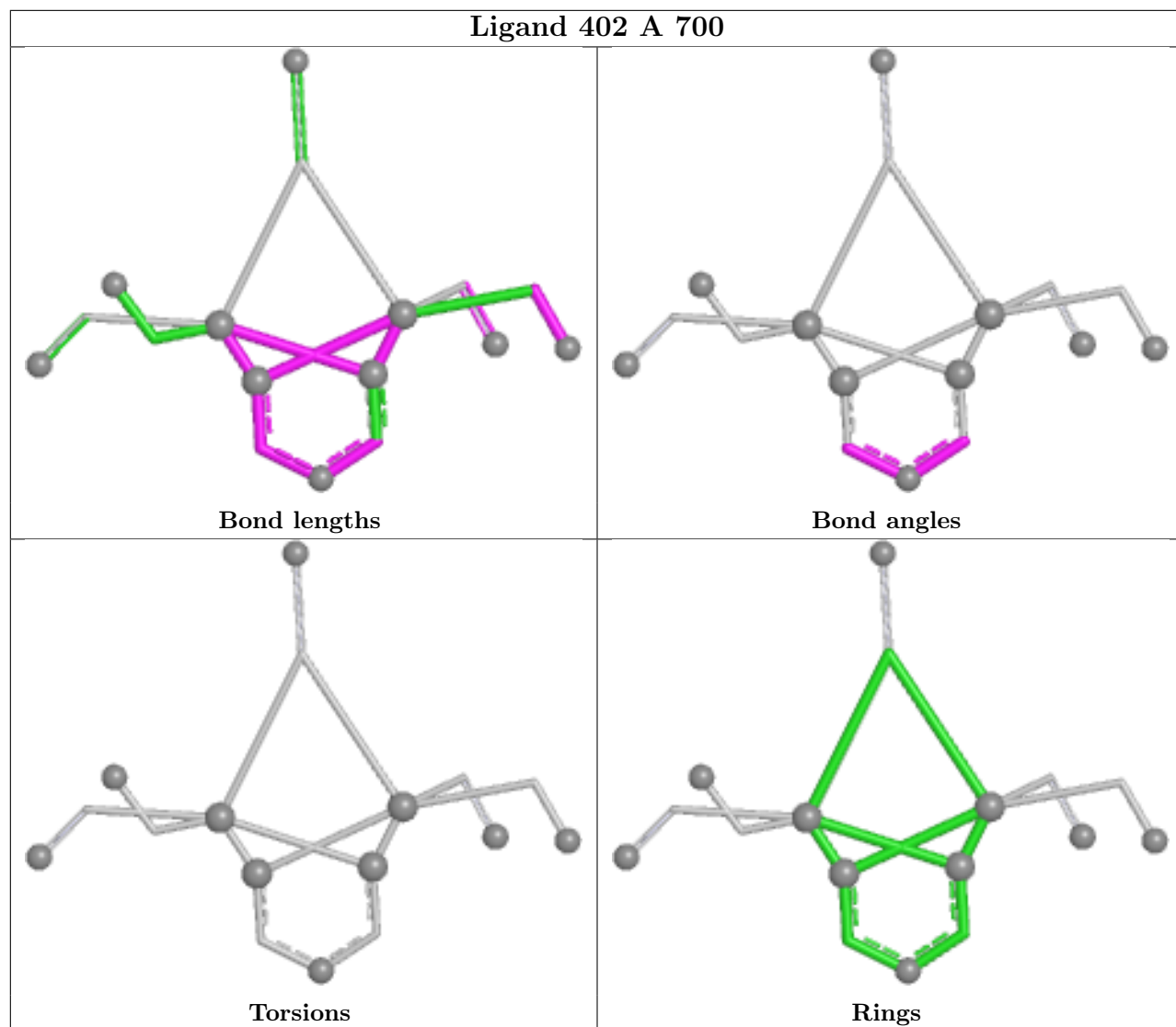
There are no ring outliers.

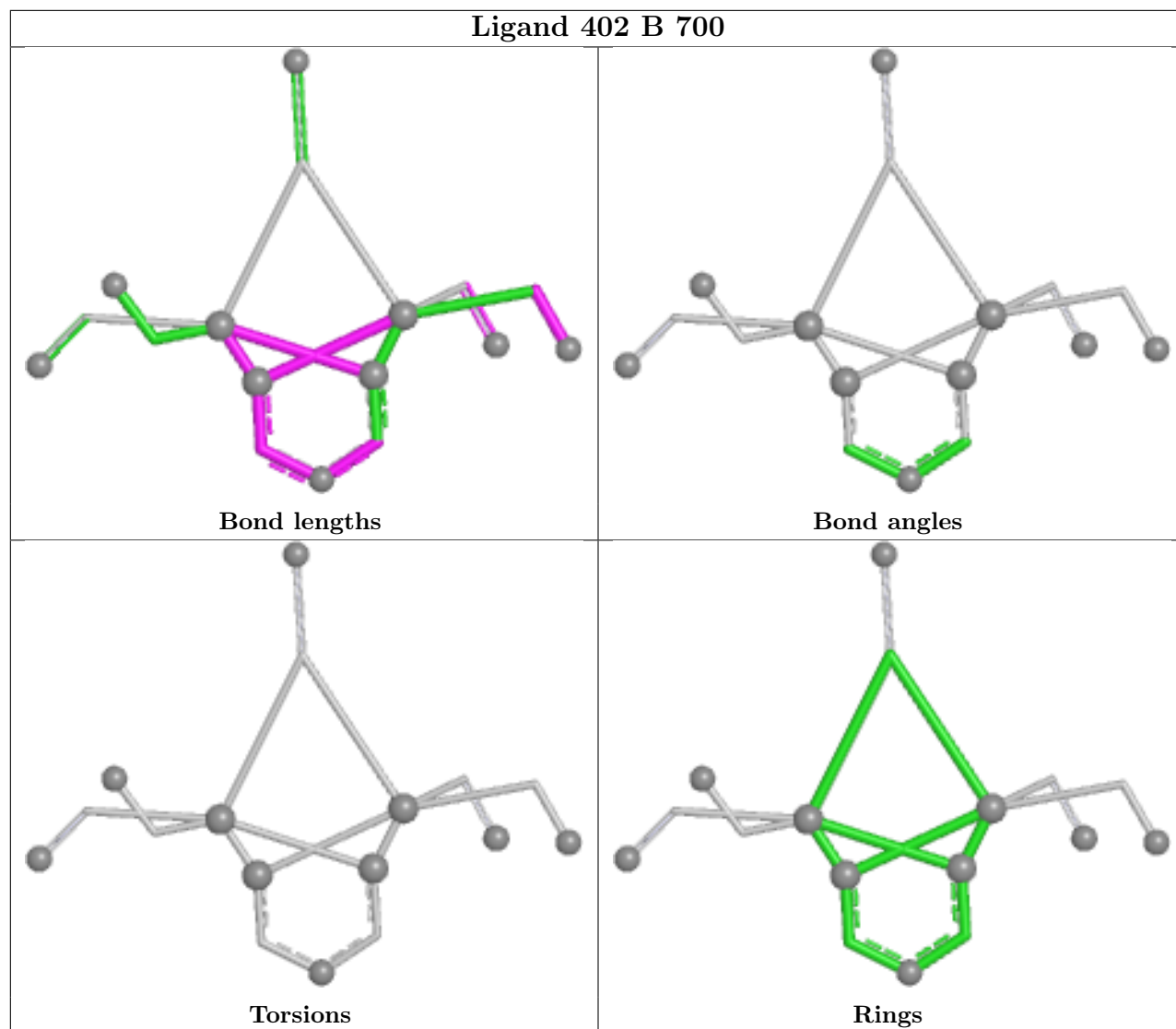
2 monomers are involved in 9 short contacts:

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.

Ligand 402 A 700





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	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

All (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
1	A	186	GLU	6.2
1	A	205	CYS	6.1
1	A	134	TYR	6.0
1	B	113	CYS	6.0
1	B	210	CYS	5.9
1	B	543	ARG	5.9
1	A	211	ASN	5.2
1	A	353	LEU	5.0
1	A	297	VAL	5.0
1	A	515	GLY	4.9
1	B	407	GLU	4.9
1	B	186	GLU	4.9
1	B	404	TRP	4.9
1	A	531	ASP	4.9
1	A	267	ILE	4.8
1	A	407	GLU	4.7
1	A	177	LYS	4.7
1	B	360	LYS	4.7
1	B	353	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	140	VAL	4.7
1	B	112	ASP	4.6
1	B	465	GLU	4.5
1	A	220	LYS	4.5
1	B	471	ILE	4.5
1	A	216	LEU	4.5
1	A	218	ILE	4.4
1	B	209	GLN	4.3
1	B	108	LEU	4.3
1	B	361	LEU	4.3
1	A	541	GLY	4.2
1	A	137	TYR	4.2
1	A	360	LYS	4.2
1	A	108	LEU	4.2
1	A	470	GLU	4.2
1	B	220	LYS	4.1
1	A	578	PRO	4.1
1	A	144	ILE	4.1
1	B	509	ASP	4.1
1	B	342	ALA	4.0
1	B	134	TYR	3.9
1	B	427	LYS	3.9
1	B	400	ALA	3.9
1	A	636	VAL	3.8
1	A	514	GLU	3.8
1	B	114	ILE	3.8
1	B	529	ALA	3.8
1	B	603	THR	3.8
1	A	306	GLU	3.8
1	B	201	GLU	3.8
1	A	110	GLN	3.8
1	B	199	HIS	3.7
1	A	542	LEU	3.7
1	B	526	GLU	3.7
1	A	404	TRP	3.7
1	B	211	ASN	3.7
1	B	205	CYS	3.7
1	A	565	MET	3.6
1	B	215	LYS	3.6
1	A	187	GLU	3.6
1	A	382	MET	3.6
1	A	113	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	135	LYS	3.6
1	B	470	GLU	3.5
1	B	216	LEU	3.5
1	B	131	ASP	3.5
1	A	518	GLY	3.5
1	A	307	PRO	3.5
1	B	586	ALA	3.5
1	B	214	VAL	3.5
1	A	465	GLU	3.5
1	A	133	SER	3.5
1	B	349	LEU	3.4
1	B	362	PRO	3.4
1	A	540	HIS	3.4
1	B	217	THR	3.4
1	B	219	THR	3.4
1	B	510	ASN	3.4
1	A	138	GLU	3.4
1	A	199	HIS	3.4
1	A	212	HIS	3.4
1	B	200	ILE	3.4
1	B	598	ILE	3.4
1	B	213	LEU	3.3
1	B	308	GLY	3.3
1	A	207	THR	3.3
1	A	471	ILE	3.3
1	B	182	HIS	3.2
1	B	206	TYR	3.2
1	B	115	ILE	3.2
1	A	563	GLU	3.2
1	A	109	SER	3.2
1	B	498	THR	3.2
1	A	178	MET	3.2
1	A	208	SER	3.2
1	B	335	ASP	3.2
1	A	219	THR	3.2
1	B	218	ILE	3.1
1	B	366	SER	3.1
1	A	182	HIS	3.1
1	B	468	ASP	3.1
1	B	518	GLY	3.1
1	B	562	ILE	3.1
1	B	572	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	467	GLU	3.1
1	A	400	ALA	3.0
1	B	405	ALA	3.0
1	A	510	ASN	3.0
1	B	116	GLN	3.0
1	B	521	GLY	3.0
1	B	507	ARG	3.0
1	B	268	SER	3.0
1	A	201	GLU	3.0
1	B	530	GLY	3.0
1	B	446	VAL	3.0
1	A	581	LYS	3.0
1	A	322	LEU	3.0
1	A	214	VAL	3.0
1	B	533	LYS	2.9
1	A	209	GLN	2.9
1	B	208	SER	2.9
1	A	463	LEU	2.9
1	B	383	LEU	2.9
1	A	570	GLY	2.9
1	B	304	GLY	2.9
1	B	110	GLN	2.9
1	A	179	ASN	2.9
1	A	269	ALA	2.9
1	B	561	ALA	2.9
1	B	447	ILE	2.9
1	A	112	ASP	2.9
1	A	131	ASP	2.9
1	B	531	ASP	2.9
1	B	636	VAL	2.9
1	B	155	SER	2.9
1	A	398	ILE	2.9
1	B	187	GLU	2.8
1	A	524	VAL	2.8
1	B	310	ASN	2.8
1	B	178	MET	2.8
1	B	454	LYS	2.8
1	B	136	ASN	2.8
1	B	464	LYS	2.8
1	B	422	PRO	2.8
1	B	428	TYR	2.8
1	A	189	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	420	ILE	2.8
1	B	590	LYS	2.8
1	B	490	GLY	2.8
1	A	383	LEU	2.7
1	B	140	VAL	2.7
1	A	150	ILE	2.7
1	B	192	PHE	2.7
1	B	584	LYS	2.7
1	A	569	GLY	2.7
1	B	270	GLY	2.7
1	A	145	THR	2.7
1	B	109	SER	2.7
1	A	539	ALA	2.7
1	A	530	GLY	2.7
1	B	207	THR	2.7
1	B	188	ILE	2.6
1	B	410	LEU	2.7
1	B	269	ALA	2.6
1	A	477	GLU	2.6
1	B	511	ILE	2.6
1	A	476	GLY	2.6
1	A	582	GLY	2.6
1	B	579	LYS	2.6
1	A	494	ALA	2.6
1	B	581	LYS	2.6
1	A	361	LEU	2.6
1	A	410	LEU	2.6
1	B	190	ASP	2.6
1	A	206	TYR	2.6
1	B	175	LYS	2.6
1	B	479	THR	2.6
1	A	511	ILE	2.5
1	A	572	ILE	2.5
1	A	451	GLU	2.5
1	A	351	ARG	2.5
1	A	176	SER	2.5
1	B	325	ASP	2.5
1	A	436	SER	2.5
1	B	133	SER	2.5
1	B	387	SER	2.5
1	B	376	GLU	2.5
1	A	389	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	THR	2.5
1	A	296	ARG	2.5
1	B	274	MET	2.5
1	A	363	ILE	2.5
1	B	295	VAL	2.5
1	A	305	PHE	2.5
1	A	526	GLU	2.5
1	A	500	LEU	2.4
1	B	542	LEU	2.4
1	B	569	GLY	2.4
1	A	406	LYS	2.4
1	B	466	ILE	2.4
1	A	533	LYS	2.4
1	B	117	PHE	2.4
1	A	529	ALA	2.4
1	A	446	VAL	2.4
1	A	387	SER	2.4
1	B	513	PHE	2.4
1	B	125	LEU	2.4
1	A	375	ILE	2.4
1	B	532	ILE	2.4
1	A	308	GLY	2.4
1	B	432	ARG	2.4
1	B	195	GLU	2.4
1	A	405	ALA	2.4
1	A	580	THR	2.4
1	A	135	LYS	2.3
1	A	640	ARG	2.3
1	A	558	PHE	2.3
1	A	298	ALA	2.3
1	B	451	GLU	2.3
1	A	632	LEU	2.3
1	A	130	LYS	2.3
1	B	177	LYS	2.3
1	B	313	LYS	2.3
1	B	297	VAL	2.3
1	A	341	GLU	2.3
1	A	593	GLU	2.3
1	A	147	MET	2.3
1	B	431	SER	2.3
1	A	114	ILE	2.3
1	B	637	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	128	LYS	2.3
1	A	386	PRO	2.3
1	A	467	GLU	2.3
1	B	477	GLU	2.3
1	A	417	SER	2.3
1	B	601	SER	2.3
1	B	582	GLY	2.3
1	B	588	LEU	2.3
1	B	181	LYS	2.3
1	A	333	GLY	2.3
1	A	532	ILE	2.2
1	A	535	ARG	2.2
1	A	139	VAL	2.2
1	A	548	MET	2.2
1	A	136	ASN	2.2
1	B	608	ASN	2.2
1	A	443	VAL	2.2
1	B	514	GLU	2.2
1	A	597	ASN	2.2
1	B	442	ASP	2.2
1	A	437	VAL	2.2
1	B	137	TYR	2.2
1	A	192	PHE	2.2
1	B	191	LYS	2.2
1	B	540	HIS	2.2
1	A	327	VAL	2.2
1	A	622	ASP	2.2
1	A	479	THR	2.2
1	A	304	GLY	2.2
1	B	373	LYS	2.2
1	B	452	LEU	2.2
1	B	500	LEU	2.2
1	A	111	GLU	2.2
1	A	447	ILE	2.1
1	B	523	ARG	2.1
1	A	143	ASP	2.1
1	B	622	ASP	2.1
1	A	300	GLY	2.1
1	A	488	THR	2.1
1	A	621	LEU	2.1
1	A	625	LEU	2.1
1	A	411	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLU	2.1
1	B	348	ARG	2.1
1	A	318	GLY	2.1
1	B	541	GLY	2.1
1	B	322	LEU	2.1
1	A	155	SER	2.1
1	A	552	ILE	2.1
1	B	123	GLU	2.1
1	B	552	ILE	2.1
1	B	556	GLU	2.1
1	B	395	MET	2.1
1	A	125	LEU	2.1
1	B	371	TRP	2.1
1	B	640	ARG	2.1
1	B	528	GLU	2.1
1	A	585	GLN	2.1
1	A	172	VAL	2.1
1	A	408	LYS	2.1
1	A	560	HIS	2.1
1	B	275	LEU	2.1
1	A	173	THR	2.1
1	B	196	ILE	2.1
1	B	455	ILE	2.1
1	B	309	GLU	2.1
1	B	344	GLU	2.1
1	B	568	VAL	2.0
1	B	573	GLY	2.0
1	A	438	ASP	2.0
1	B	430	ALA	2.0
1	A	344	GLU	2.0
1	B	111	GLU	2.0
1	A	285	LYS	2.0
1	B	417	SER	2.0
1	B	436	SER	2.0
1	B	443	VAL	2.0
1	B	474	VAL	2.0
1	B	336	LEU	2.0
1	B	555	GLY	2.0
1	A	191	LYS	2.0
1	A	215	LYS	2.0
1	B	457	GLU	2.0
1	B	124	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	311	VAL	2.0
1	B	524	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](#)

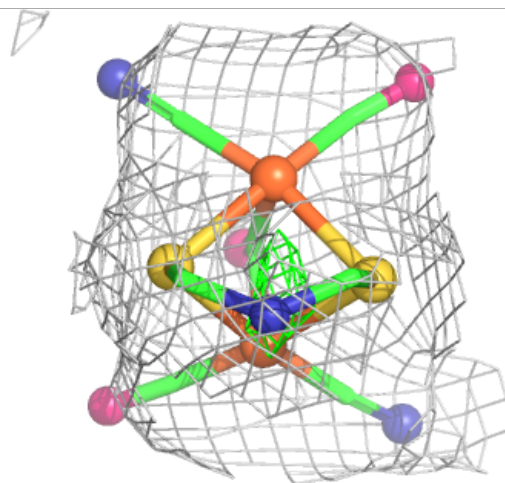
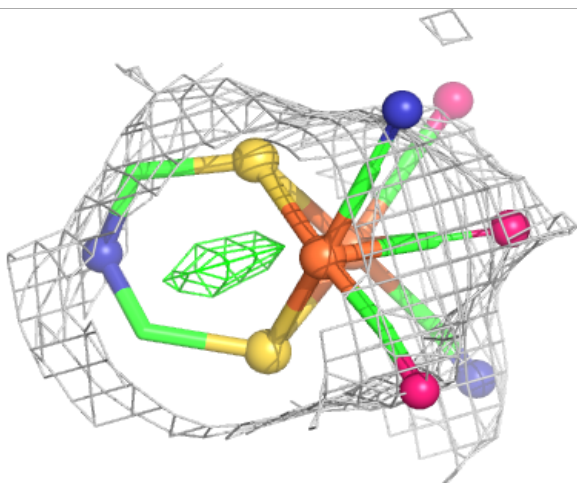
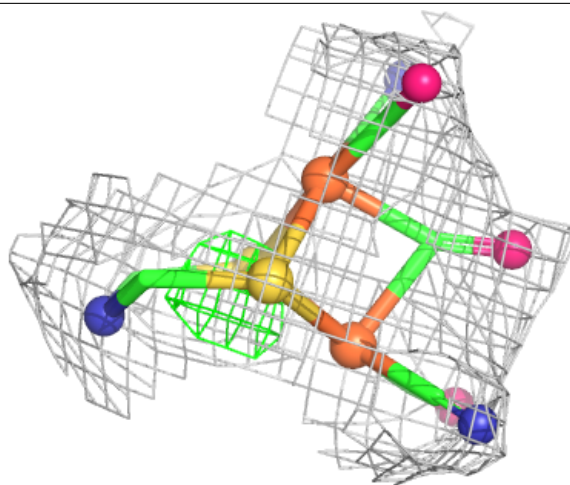
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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.

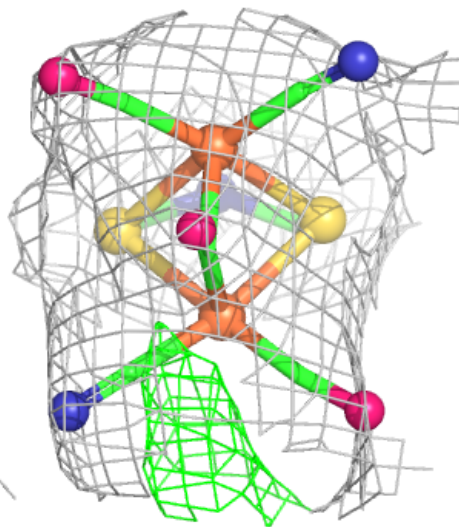
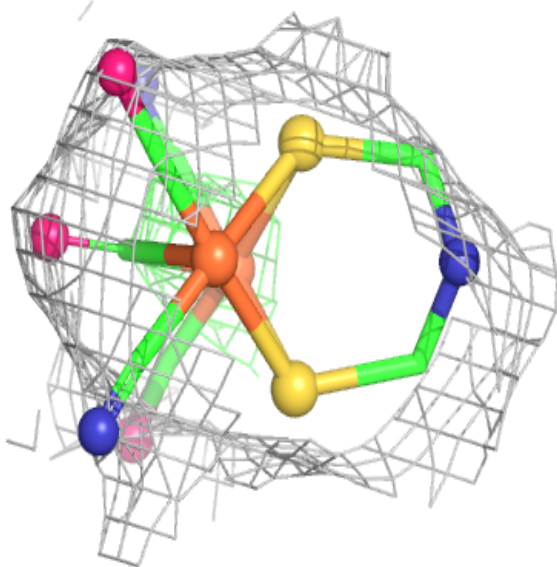
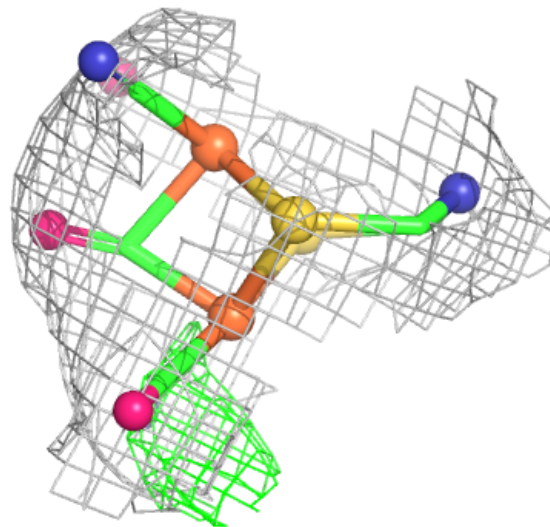
Electron density around 402 B 700:

$2mF_o-DF_c$ (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.