



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:28 PM EDT

PDB ID : 6VXT / pdb_00006vxt
Title : Activated Nitrogenase MoFe-protein from Azotobacter vinelandii
Authors : Kang, W.; Hu, Y.; Ribbe, M.W.
Deposited on : 2020-02-24
Resolution : 1.74 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

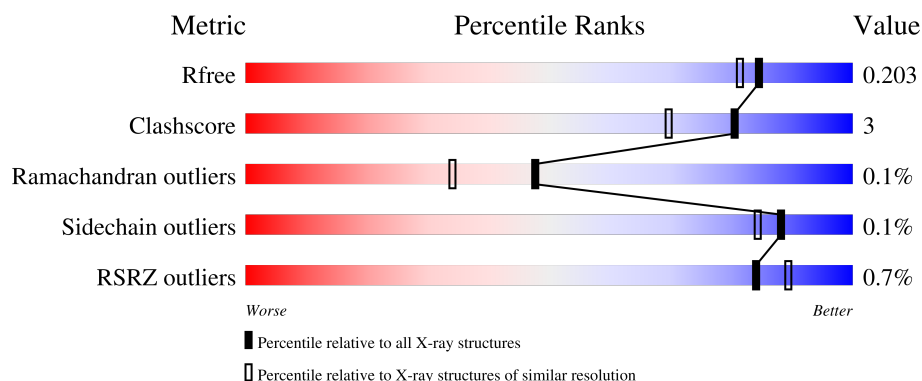
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	492	% 92% 5% .
1	C	492	% 90% 7% .
2	B	523	95% 5%
2	D	523	% 94% 6%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17021 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.

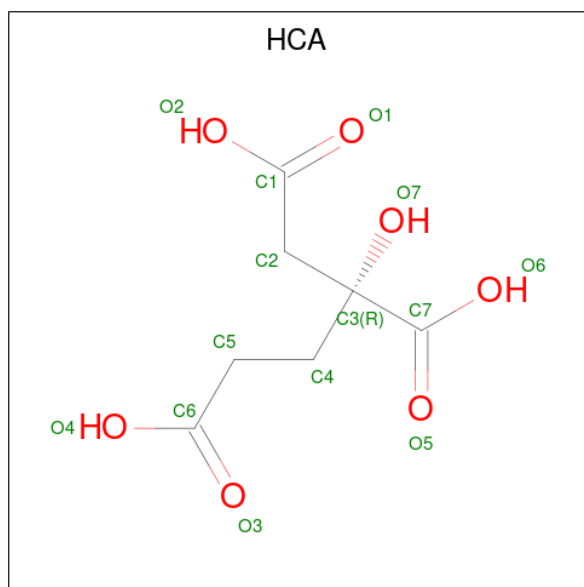
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	1	0
			3710	2365	630	690	25			
1	C	477	Total	C	N	O	S	0	2	0
			3712	2368	638	680	26			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

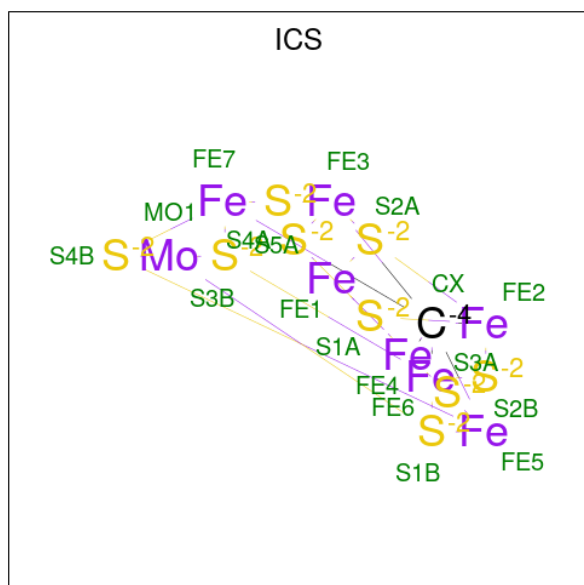
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	2	0
			4123	2632	696	766	29			
2	D	522	Total	C	N	O	S	0	0	0
			4094	2616	692	758	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).

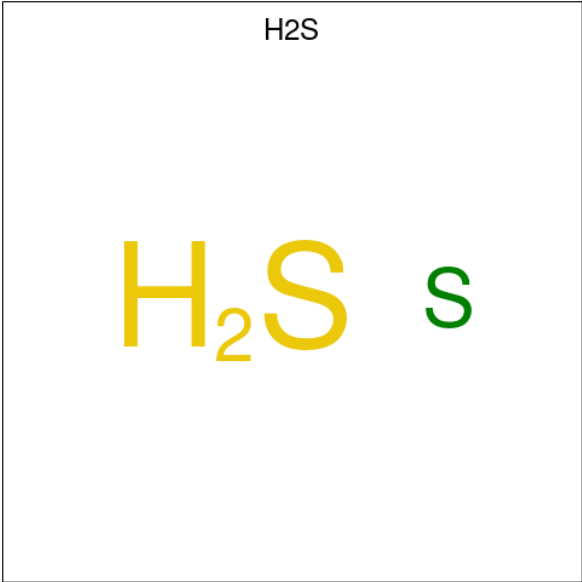


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

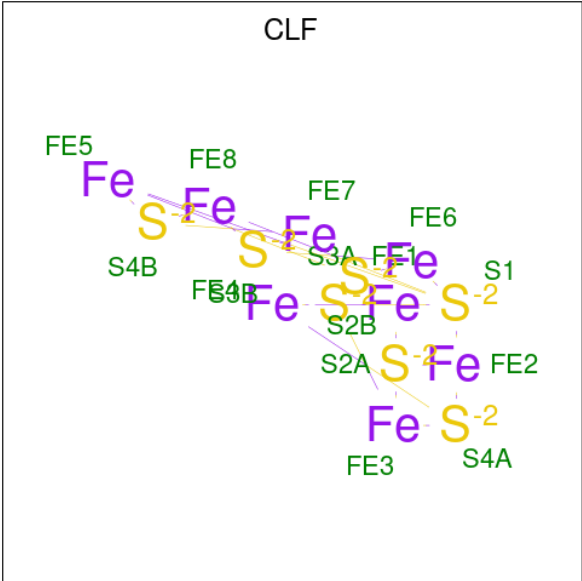
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mo	0	0
			4	4		
5	C	4	Total	Mo	0	0
			4	4		

- Molecule 6 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	S	0	0
			1	1		
6	D	1	Total	S	0	0
			1	1		

- Molecule 7 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			15	8	7		

Continued on next page...

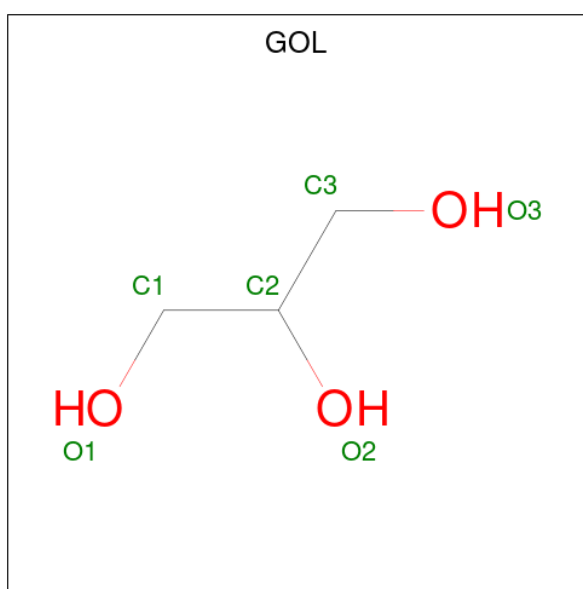
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Fe	0	0
			2	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

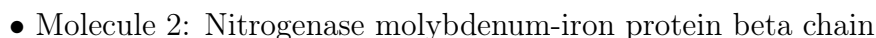
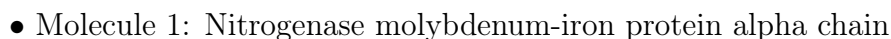


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	272	Total 272	O 272	0	0
10	B	358	Total 358	O 358	0	0
10	C	256	Total 256	O 256	0	0
10	D	348	Total 348	O 348	0	0

- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.53Å 203.44Å 83.86Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	41.71 – 1.74 41.71 – 1.74	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.71-1.74) 96.7 (41.71-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.172 , 0.203 0.173 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17021	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HCA, GOL, H2S, MO, ICS, FE, CLF

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	0.31	0/3801	0.52	0/5140
1	C	0.31	0/3806	0.51	0/5147
2	B	0.30	0/4231	0.51	0/5733
2	D	0.30	0/4199	0.48	0/5694
All	All	0.30	0/16037	0.50	0/21714

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	3710	0	3592	16	0
1	C	3712	0	3601	22	0
2	B	4123	0	3977	20	0
2	D	4094	0	3928	20	0
3	A	14	0	6	2	0
3	C	14	0	6	3	0
4	A	18	0	0	1	0
4	C	18	0	0	0	0
5	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	15	0	0	0	0
7	C	15	0	0	0	0
8	B	2	0	0	0	0
9	B	24	0	32	3	0
9	D	18	0	24	1	0
10	A	272	0	0	1	0
10	B	358	0	0	1	0
10	C	256	0	0	0	0
10	D	348	0	0	2	0
All	All	17021	0	15166	79	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 3.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:MET:HE2	2:D:154:MET:HE3	1.57	0.87
2:D:296:TRP:CD1	2:D:377:MET:HE1	2.26	0.70
2:D:213:MET:HA	2:D:213:MET:HE2	1.74	0.69
1:A:176:LYS:HD3	1:A:177:THR:H	1.58	0.67
2:B:118:MET:HB2	2:B:154:MET:HE1	1.76	0.67
2:B:247:MET:O	2:B:338:GLN:HG2	1.96	0.64
2:D:217:VAL:HG13	2:D:220:SER:HB3	1.82	0.60
2:B:213:MET:HA	2:B:213:MET:HE2	1.82	0.60
2:D:118:MET:HB2	2:D:154:MET:HE1	1.83	0.59
2:D:213:MET:HE1	2:D:285:PRO:HG2	1.85	0.59
2:B:232:THR:HG1	9:B:602:GOL:HO1	1.50	0.58
1:C:6:ARG:NH2	1:C:35:ASN:O	2.36	0.58
1:C:158:LEU:HD11	2:D:154:MET:HG3	1.87	0.56
2:B:232:THR:OG1	9:B:602:GOL:O1	2.18	0.56
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.05	0.56
2:D:226:ILE:HD13	2:D:291:VAL:HB	1.90	0.54
1:A:341:LYS:NZ	10:A:702:HOH:O	2.35	0.53
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.90	0.53
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.90	0.53
2:B:333:SER:OG	2:B:338:GLN:O	2.21	0.52
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:NZ	1:A:263:GLU:OE2	2.41	0.51
2:B:237:PHE:O	2:B:241:LYS:HG3	2.11	0.51
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.46	0.51
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.91	0.51
2:D:170:LYS:HD3	2:D:177:ASP:HA	1.93	0.51
2:D:213:MET:HE1	2:D:285:PRO:CG	2.41	0.50
1:C:429:PHE:O	1:C:433:LYS:HG2	2.11	0.50
3:C:601:HCA:O7	3:C:601:HCA:O1	2.29	0.50
2:B:299:GLU:CD	2:B:401:ARG:HH22	2.21	0.49
2:D:118:MET:CB	2:D:154:MET:HE1	2.41	0.49
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.13	0.49
2:D:194:VAL:HB	2:D:297:HIS:CG	2.48	0.48
1:C:225:ILE:HG13	1:C:249[A]:CYS:SG	2.54	0.48
1:A:442:HIS:HB3	3:A:601:HCA:O6	2.15	0.46
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.96	0.46
9:D:603:GOL:H11	10:D:729:HOH:O	2.15	0.46
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.50	0.46
2:B:512:MET:HB3	2:B:512:MET:HE2	1.62	0.46
2:B:154:MET:HE2	2:B:154:MET:HB3	1.70	0.46
2:B:213:MET:SD	2:B:308:THR:HG22	2.56	0.45
2:B:509:THR:O	2:B:516:ASP:HA	2.16	0.45
2:D:9:LYS:HE3	10:D:808:HOH:O	2.17	0.44
2:D:341:PRO:HD2	2:D:344:LEU:HD12	1.98	0.44
1:C:467:LEU:HD23	1:C:467:LEU:O	2.17	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.44
2:B:494:LEU:C	2:B:494:LEU:HD23	2.42	0.44
1:A:253:TRP:HA	1:A:254:SER:HA	1.81	0.44
1:C:98:ASN:O	1:C:98:ASN:ND2	2.50	0.44
2:D:43:VAL:O	2:D:47:THR:HG23	2.17	0.43
9:B:602:GOL:H12	10:B:766:HOH:O	2.17	0.43
1:A:176:LYS:HD3	1:A:177:THR:N	2.30	0.43
1:C:298:ASN:HA	1:C:362:HIS:NE2	2.34	0.43
1:C:253:TRP:HA	1:C:254:SER:HA	1.77	0.43
2:D:445:ASN:HB2	2:D:472:PRO:O	2.19	0.43
2:B:213:MET:HE1	2:B:285:PRO:CG	2.49	0.42
1:C:177:THR:OG1	1:C:209:LYS:NZ	2.51	0.42
2:D:509:THR:O	2:D:516:ASP:HA	2.19	0.42
1:C:5:SER:O	1:C:9:VAL:HG23	2.20	0.42
1:C:382:ALA:HB1	1:C:386:ASP:CB	2.50	0.42
3:A:601:HCA:O2	3:A:601:HCA:O7	2.37	0.42
2:B:390:PRO:O	2:B:419:ALA:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:HB3	2:D:322:LEU:HD21	2.01	0.41
1:A:5:SER:O	1:A:9:VAL:HG23	2.20	0.41
1:A:36:ASP:H	1:A:391:MET:HE2	1.84	0.41
2:B:258:GLU:HG3	2:B:259:GLU:N	2.35	0.41
1:C:165:SER:O	1:C:169:VAL:HG22	2.21	0.41
1:A:97:ARG:O	1:A:231:ILE:HA	2.20	0.41
1:C:97:ARG:O	1:C:231:ILE:HA	2.21	0.41
1:A:394:MET:HE3	1:A:394:MET:HB3	1.95	0.41
1:C:410:GLU:HG2	1:C:414:LYS:HD2	2.03	0.41
2:B:458:LYS:HG2	2:B:462:PHE:CD2	2.56	0.41
1:C:442:HIS:HB3	3:C:601:HCA:O5	2.21	0.41
1:A:66:GLY:O	1:A:70:VAL:HB	2.21	0.40
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.91	0.40
1:A:158:LEU:HD11	2:B:154:MET:HG3	2.03	0.40
1:A:356:GLY:HA3	4:A:602:ICS:S1B	2.61	0.40
1:C:442:HIS:CG	3:C:601:HCA:H52	2.57	0.40
2:D:153:CYS:HB3	2:D:188:SER:OG	2.22	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	475/492 (96%)	453 (95%)	21 (4%)	1 (0%)	43	29
1	C	477/492 (97%)	460 (96%)	16 (3%)	1 (0%)	43	29
2	B	522/523 (100%)	512 (98%)	10 (2%)	0	100	100
2	D	520/523 (99%)	508 (98%)	12 (2%)	0	100	100
All	All	1994/2030 (98%)	1933 (97%)	59 (3%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ILE
1	C	355	ILE

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	388/415 (94%)	388 (100%)	0	100	100
1	C	385/415 (93%)	385 (100%)	0	100	100
2	B	440/455 (97%)	440 (100%)	0	100	100
2	D	432/455 (95%)	431 (100%)	1 (0%)	87	84
All	All	1645/1740 (94%)	1644 (100%)	1 (0%)	88	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
2	B	18	GLN
2	B	163	ASN
2	B	317	ASN
2	B	363	HIS
2	B	457	HIS
2	B	518	ASN
1	C	14	GLN
1	C	98	ASN
1	C	384	ASN
2	D	163	ASN
2	D	317	ASN
2	D	338	GLN
2	D	363	HIS

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 25 ligands modelled in this entry, 10 are monoatomic and 2 are modelled with single atom - leaving 13 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
9	GOL	B	602	-	5,5,5	0.97	0	5,5,5	1.11	0
9	GOL	B	604	-	5,5,5	1.06	0	5,5,5	0.80	0
9	GOL	B	603	-	5,5,5	0.82	0	5,5,5	1.03	0
3	HCA	C	601	4	13,13,13	1.29	2 (15%)	15,18,18	1.78	3 (20%)
7	CLF	C	607	2,1	0,24,24	-	-	-		
4	ICS	C	602	3,1	6,30,30	1.77	2 (33%)	-		
9	GOL	D	602	-	5,5,5	0.83	0	5,5,5	1.12	0
9	GOL	D	604	-	5,5,5	1.03	0	5,5,5	0.85	0
4	ICS	A	602	3,1	6,30,30	1.24	1 (16%)	-		
3	HCA	A	601	4	13,13,13	0.95	0	15,18,18	1.72	2 (13%)
7	CLF	A	608	2,1	0,24,24	-	-	-		
9	GOL	D	603	-	5,5,5	0.86	0	5,5,5	0.96	1 (20%)
9	GOL	B	605	-	5,5,5	0.91	0	5,5,5	1.07	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
9	GOL	B	602	-	-	1/4/4/4	-
9	GOL	B	604	-	-	1/4/4/4	-
9	GOL	B	603	-	-	2/4/4/4	-
3	HCA	C	601	4	-	2/17/17/17	-
7	CLF	C	607	2,1	-	-	0/12/10/10
9	GOL	D	602	-	-	2/4/4/4	-
9	GOL	D	604	-	-	2/4/4/4	-
3	HCA	A	601	4	-	2/17/17/17	-
7	CLF	A	608	2,1	-	-	0/12/10/10
9	GOL	D	603	-	-	1/4/4/4	-
9	GOL	B	605	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ICS	S5A-FE7	-2.64	2.18	2.24
4	C	602	ICS	S2B-FE2	-2.48	2.19	2.24
3	C	601	HCA	C3-C7	-2.43	1.50	1.53
3	C	601	HCA	O7-C3	2.27	1.47	1.43
4	A	602	ICS	S5A-FE7	-2.02	2.20	2.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HCA	O6-C7-C3	4.30	121.39	113.14
3	C	601	HCA	O6-C7-C3	4.08	120.96	113.14
3	C	601	HCA	O2-C1-C2	2.37	121.87	114.35
3	C	601	HCA	O4-C6-C5	2.26	121.14	114.00
3	A	601	HCA	O6-C7-O5	-2.07	117.24	123.86
9	D	603	GOL	C3-C2-C1	-2.02	104.39	111.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	HCA	C2-C3-C4-C5
9	D	602	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	602	GOL	C1-C2-C3-O3
9	B	603	GOL	O1-C1-C2-C3
9	D	604	GOL	O1-C1-C2-C3
9	B	603	GOL	O1-C1-C2-O2
9	D	602	GOL	O1-C1-C2-O2
9	D	604	GOL	O1-C1-C2-O2
3	A	601	HCA	C2-C3-C4-C5
9	D	603	GOL	O1-C1-C2-C3
9	B	604	GOL	O2-C2-C3-O3
3	C	601	HCA	C1-C2-C3-C4
3	A	601	HCA	O1-C1-C2-C3

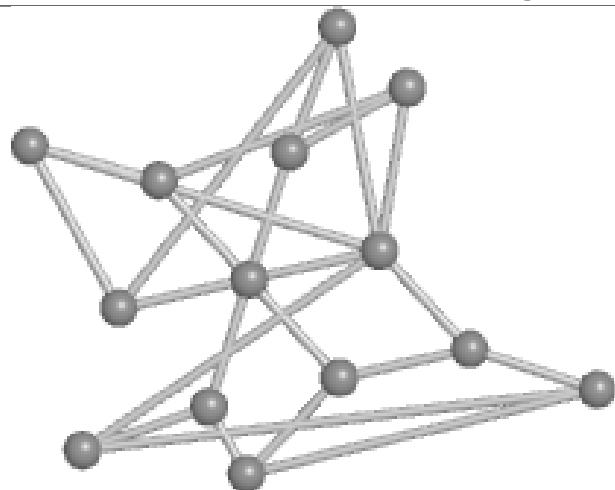
There are no ring outliers.

5 monomers are involved in 10 short contacts:

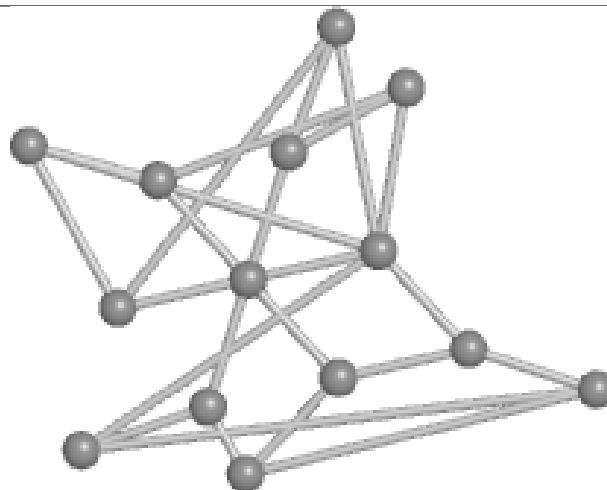
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	602	GOL	3	0
3	C	601	HCA	3	0
4	A	602	ICS	1	0
3	A	601	HCA	2	0
9	D	603	GOL	1	0

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.

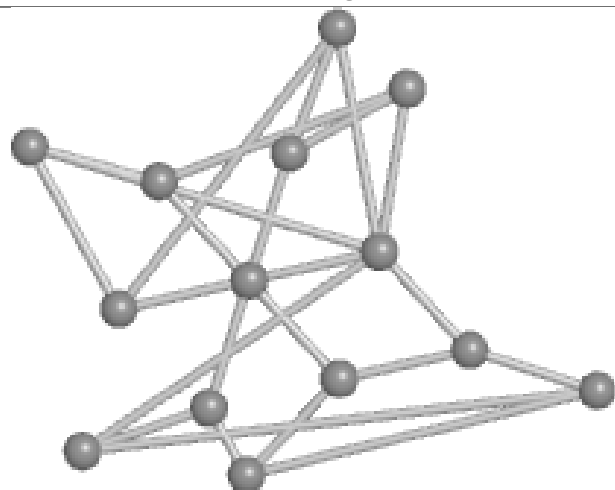
Ligand CLF C 607



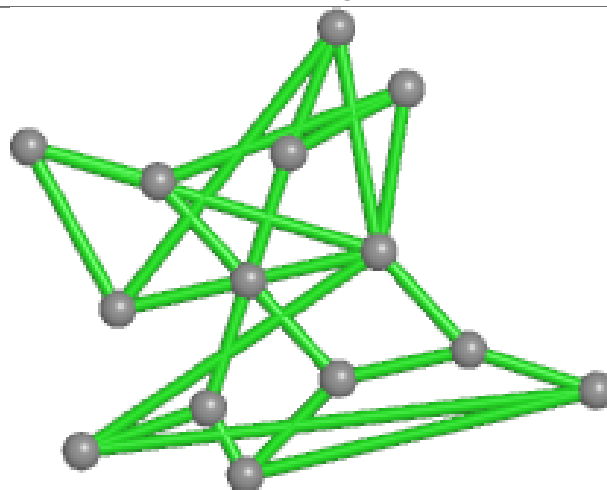
Bond lengths



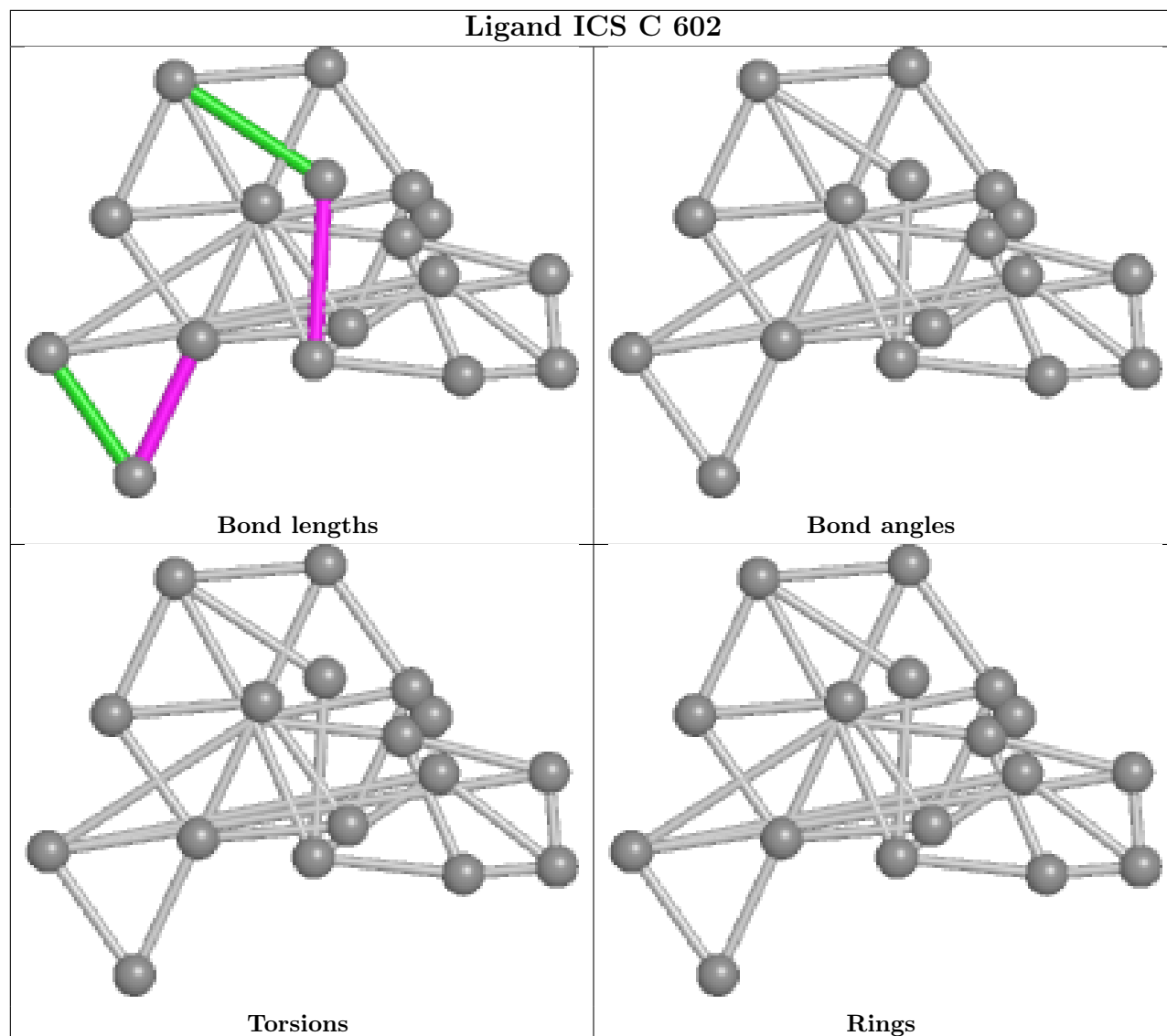
Bond angles

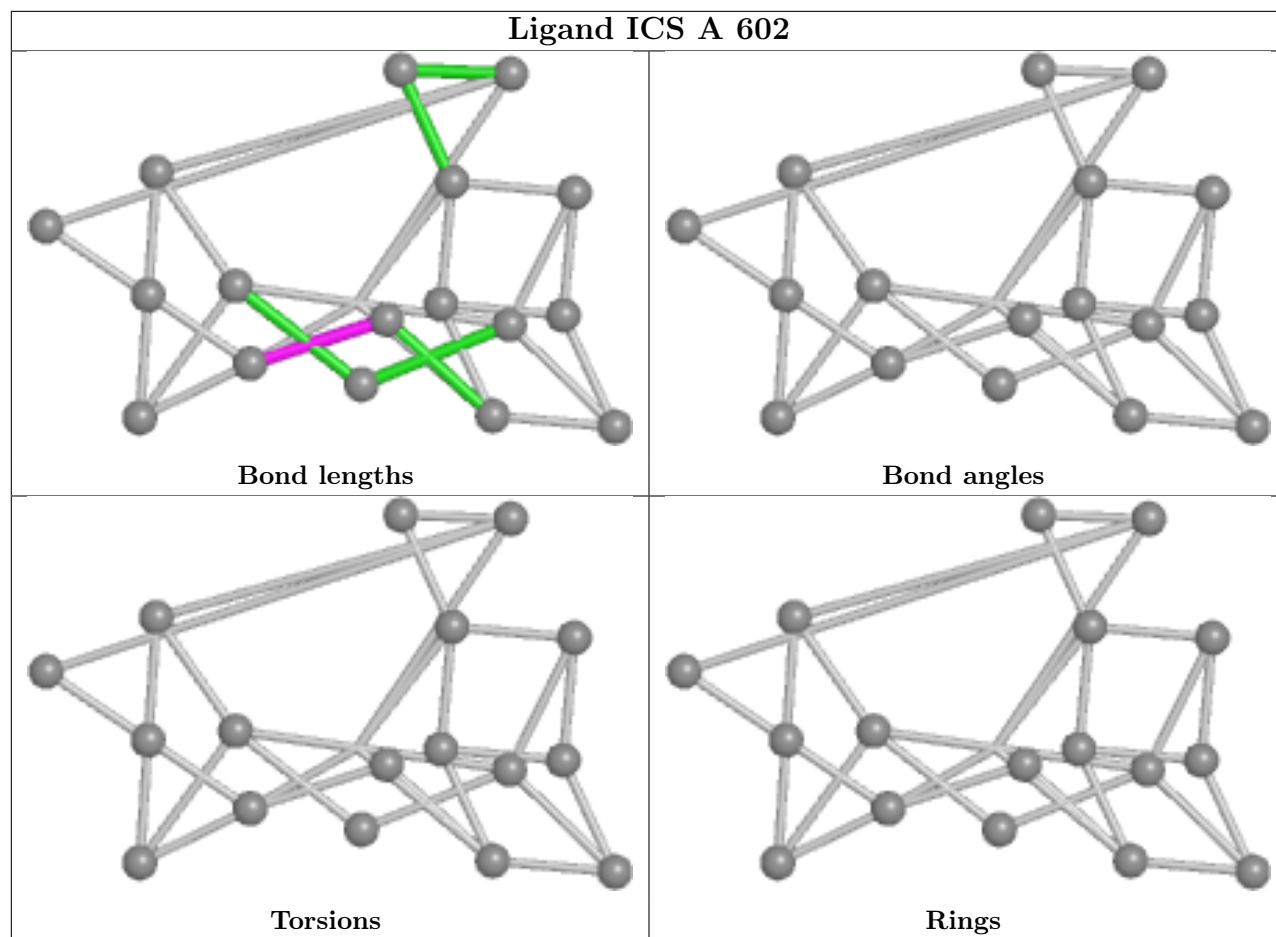


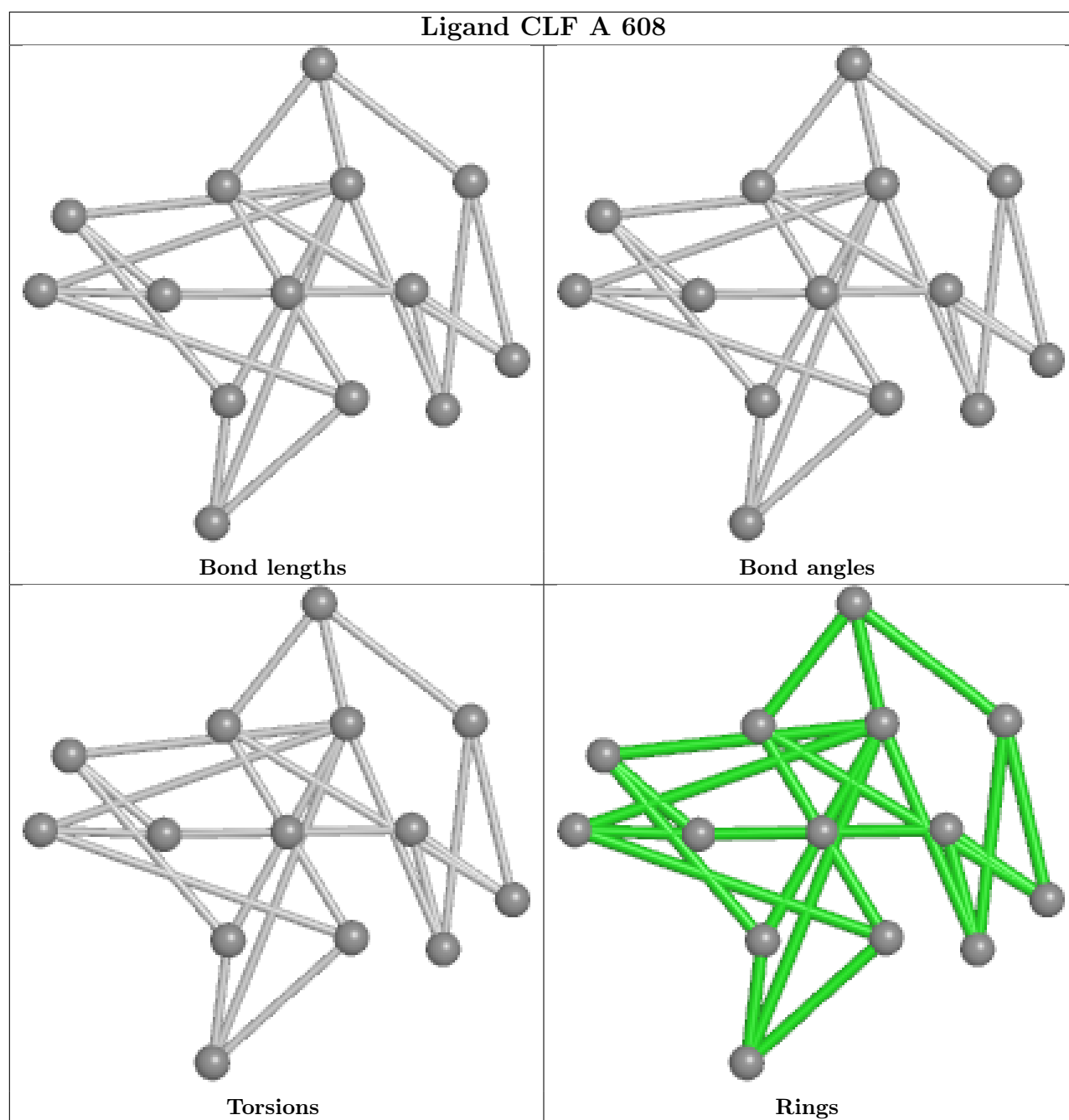
Torsions



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	476/492 (96%)	0.12	3 (0%) 85 90	30, 42, 61, 76	2 (0%)
1	C	477/492 (96%)	0.22	6 (1%) 75 82	24, 43, 61, 82	2 (0%)
2	B	522/523 (99%)	0.04	2 (0%) 88 92	15, 41, 60, 74	2 (0%)
2	D	522/523 (99%)	0.12	3 (0%) 85 90	29, 43, 62, 77	0
All	All	1997/2030 (98%)	0.13	14 (0%) 84 89	15, 42, 61, 82	6 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	CYS	3.4
1	C	480	GLU	3.4
1	A	362	HIS	3.3
2	B	215	ASP	3.2
2	D	214	ASP	3.1
2	D	125	PHE	2.9
1	C	362	HIS	2.5
1	A	5	SER	2.5
2	D	215	ASP	2.4
2	B	125	PHE	2.2
1	C	159	ILE	2.2
1	A	176	LYS	2.1
1	C	176	LYS	2.1
1	C	397	SER	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

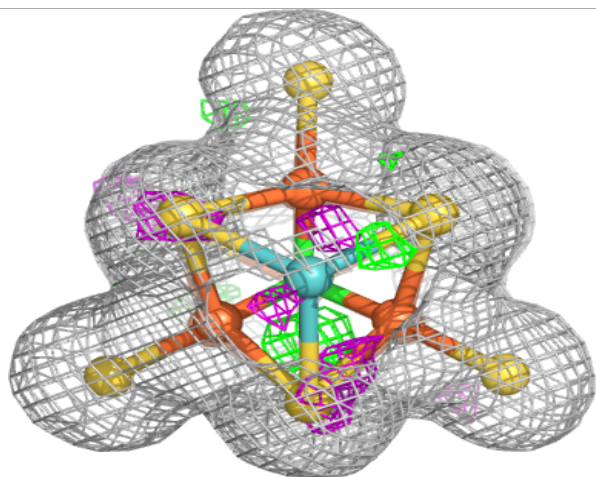
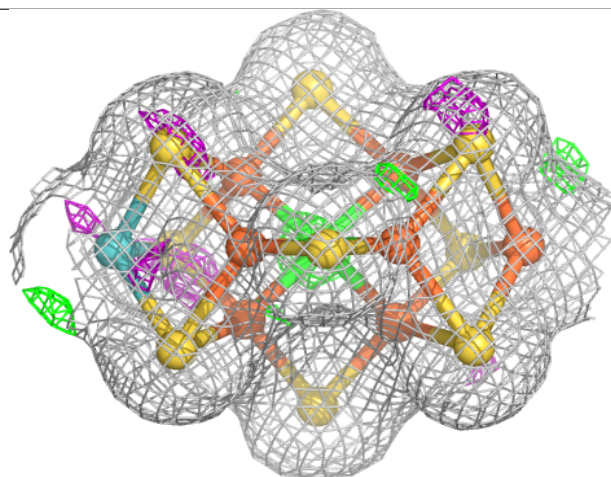
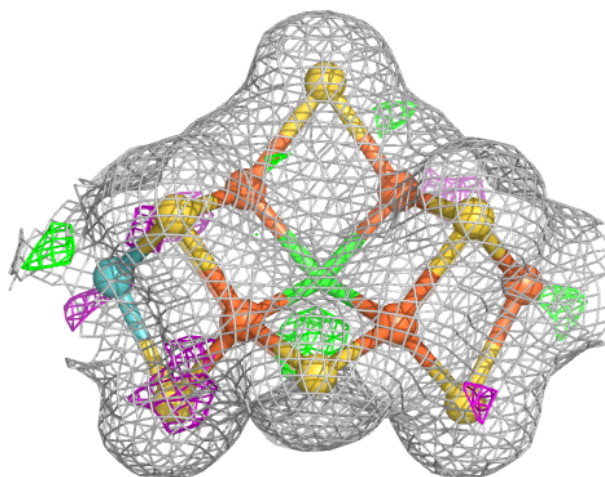
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	B	603	6/6	0.85	0.18	45,54,61,73	0
9	GOL	D	603	6/6	0.90	0.17	46,63,63,63	0
9	GOL	B	604	6/6	0.93	0.10	52,54,61,68	0
9	GOL	B	602	6/6	0.93	0.11	40,48,49,50	0
9	GOL	D	602	6/6	0.94	0.09	52,62,63,70	0
9	GOL	D	604	6/6	0.94	0.11	40,47,52,54	0
5	MO	C	606	1/1	0.95	0.09	76,76,76,76	1
9	GOL	B	605	6/6	0.95	0.09	54,61,66,69	0
8	FE	B	606	1/1	0.95	0.07	51,51,51,51	1
3	HCA	C	601	14/14	0.95	0.08	27,33,36,39	0
5	MO	A	607	1/1	0.95	0.07	71,71,71,71	1
3	HCA	A	601	14/14	0.96	0.07	24,32,36,36	0
8	FE	B	601	1/1	0.96	0.08	59,59,59,59	1
5	MO	A	606	1/1	0.97	0.06	53,53,53,53	1
5	MO	C	604	1/1	0.98	0.05	58,58,58,58	1
5	MO	A	603	1/1	0.98	0.05	45,45,45,45	1
6	H2S	D	601	1/1	0.98	0.06	40,40,40,40	0
5	MO	A	604	1/1	0.98	0.04	53,53,53,53	1
4	ICS	C	602	18/18	0.99	0.03	24,31,33,34	0
7	CLF	A	608	15/15	0.99	0.03	29,32,34,35	0
7	CLF	C	607	15/15	0.99	0.03	29,33,36,37	0
5	MO	C	605	1/1	0.99	0.05	44,44,44,44	1
5	MO	C	603	1/1	0.99	0.04	44,44,44,44	1
6	H2S	A	605	1/1	0.99	0.04	37,37,37,37	0
4	ICS	A	602	18/18	1.00	0.03	27,30,32,33	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.

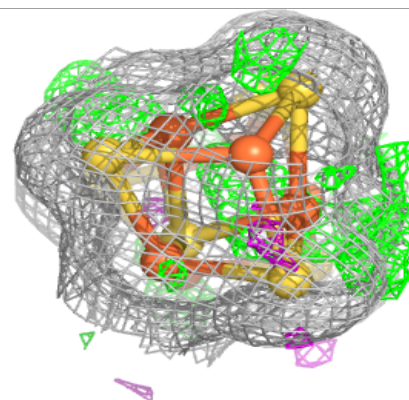
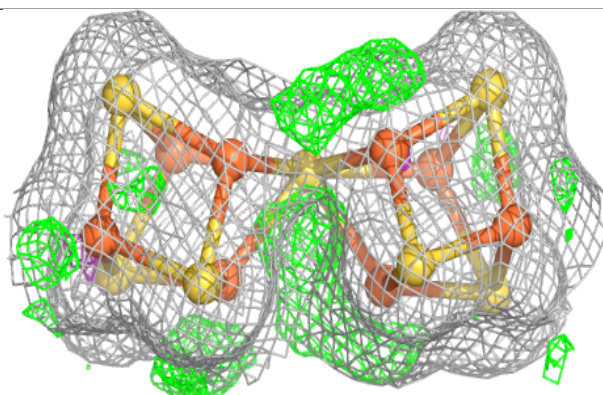
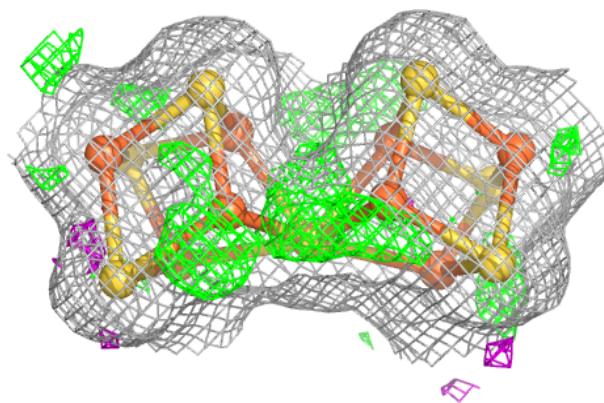
Electron density around ICS C 602:

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

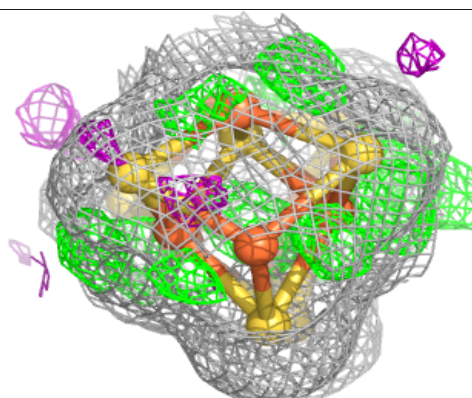
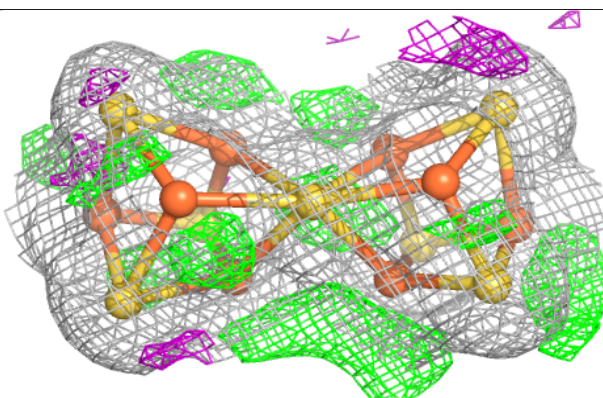
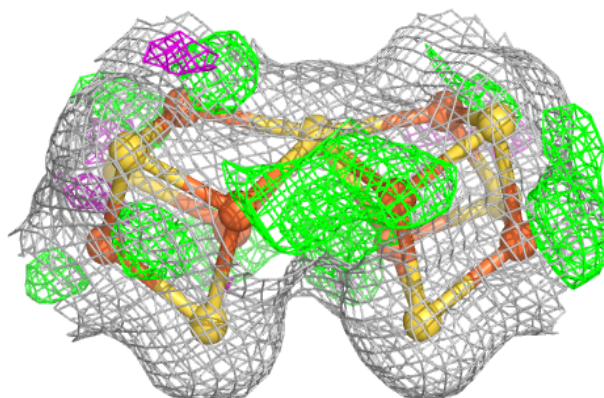


Electron density around CLF A 608:

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

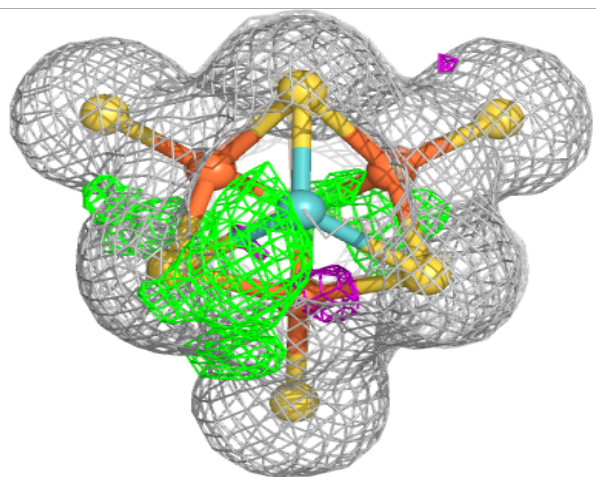
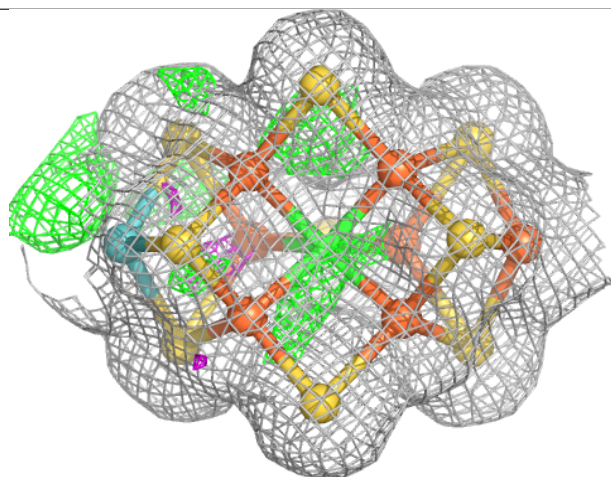
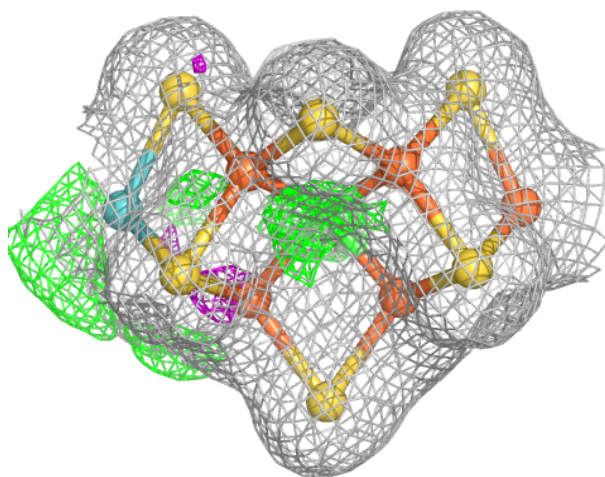
**Electron density around CLF C 607:**

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



Electron density around ICS A 602:

$2mF_o-DF_c$ (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.