



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:07 PM BST

PDB ID : 6VXT
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

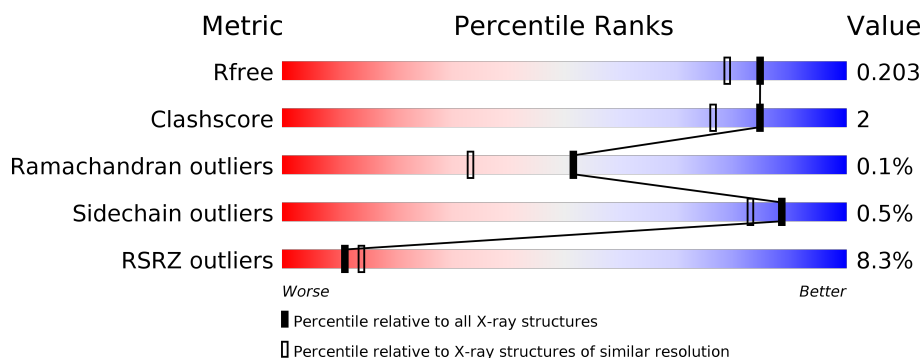
1 Overall quality at a glance

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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 $\leq 5\%$. 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	<div> <div>9%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	C	492	<div> <div>10%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
2	B	523	<div> <div>7%</div> <div> <div></div> <div>95%</div> <div>5%</div> <div></div> </div> </div>
2	D	523	<div> <div>8%</div> <div> <div></div> <div>94%</div> <div>6%</div> <div></div> </div> </div>

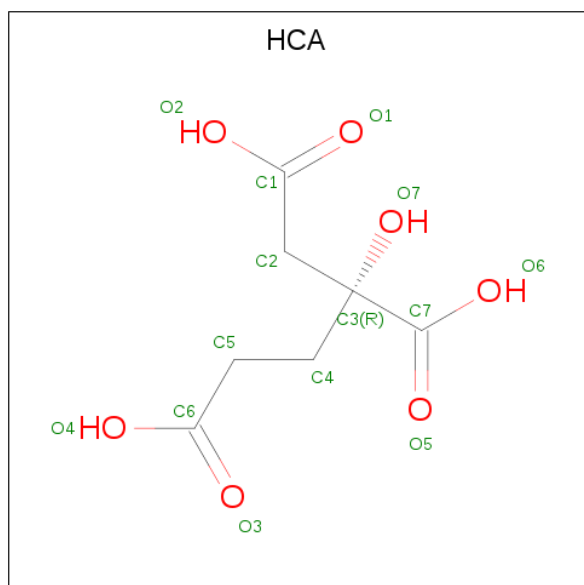
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

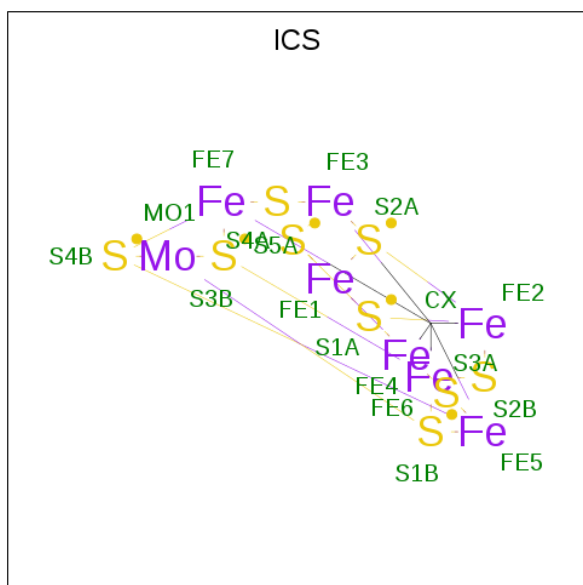
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total 4123	C 2632	N 696	O 766	S 29	0	2	0
2	D	522	Total 4094	C 2616	N 692	O 758	S 28	0	0	0

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIIC ACID (three-letter code: 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 (three-letter code: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by author).

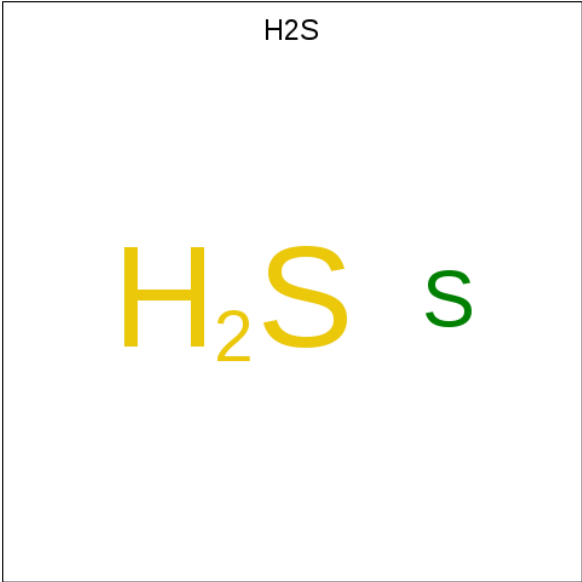


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

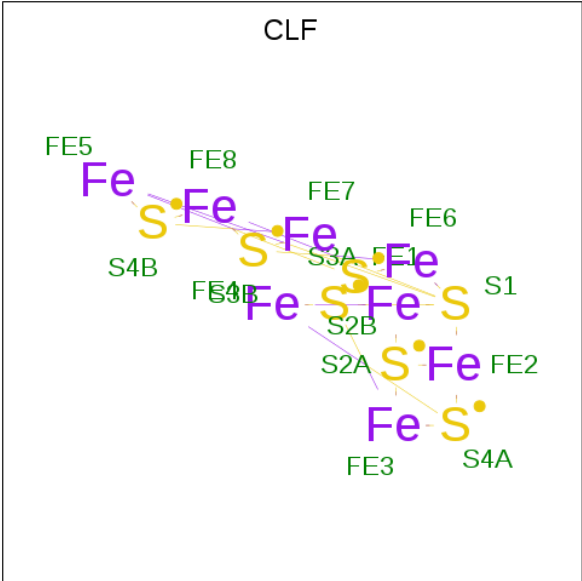
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mo	0	0
			4	4		
5	C	4	Total	Mo	0	0
			4	4		

- Molecule 6 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



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

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by author).



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

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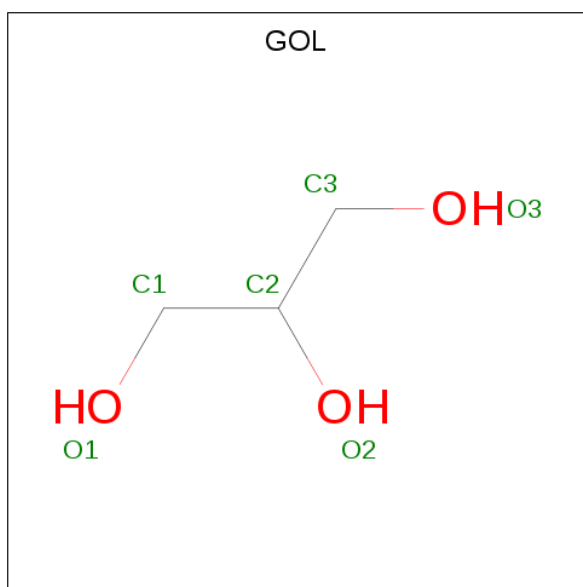
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is GLYCEROL (three-letter code: 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		

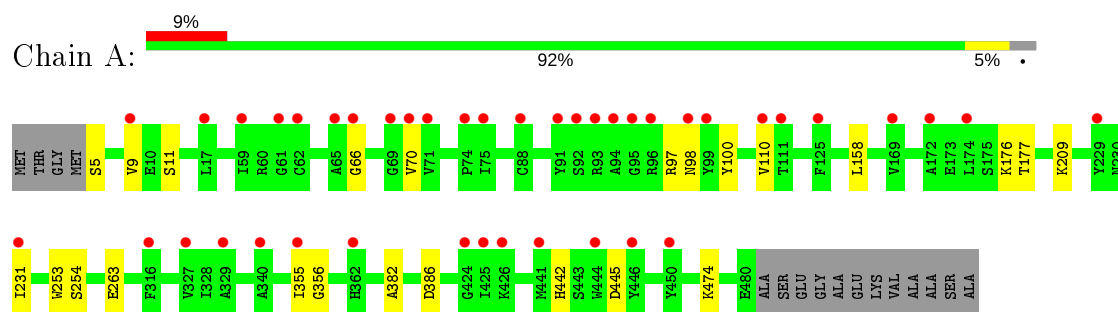
- Molecule 10 is water.

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

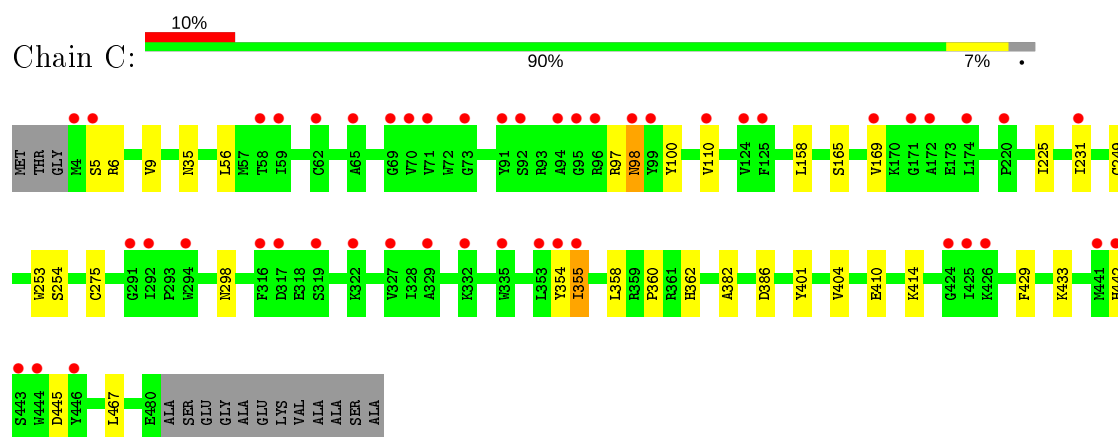
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

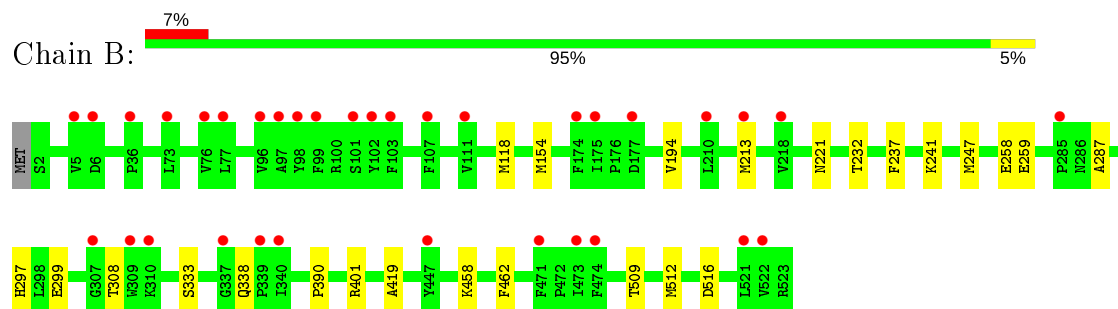
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



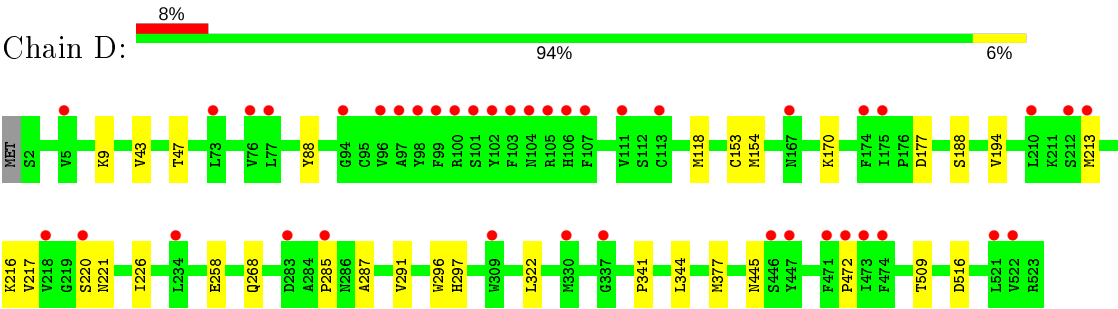
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta 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) 96.1 (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 0.172 , 0.203	Depositor DCC
R_{free} test set	1983 reflections (0.76%)	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)	0.36 , 59.5	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: GOL, CLF, H2S, HCA, FE, ICS, MO

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	0.39	0/3801	0.54	0/5140
1	C	0.38	0/3806	0.55	0/5147
2	B	0.37	0/4231	0.54	0/5733
2	D	0.36	0/4199	0.53	0/5694
All	All	0.38	0/16037	0.54	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	13	0
1	C	3712	0	3601	21	0
2	B	4123	0	3977	17	0
2	D	4094	0	3928	19	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

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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	0	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	71	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 2.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD3	1:A:177:THR:H	1.58	0.67
2:B:247:MET:O	2:B:338:GLN:HG2	1.96	0.64
2:B:118:MET:HB2	2:B:154:MET:HE1	1.81	0.62
2:B:232:THR:OG1	9:B:602:GOL:O1	2.18	0.61
2:D:217:VAL:HG13	2:D:220:SER:HB3	1.82	0.60
2:B:232:THR:HG1	9:B:602:GOL:HO1	1.48	0.60
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: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: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:D:213:MET:HE3	2:D:285:PRO:HG2	1.91	0.52
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
2:D:296:TRP:CD1	2:D:377:MET:HE1	2.46	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
1:C:429:PHE:O	1:C:433:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:MET:HB3	2:D:154:MET:HE3	1.93	0.50
3:C:601:HCA:O1	3:C:601:HCA:O7	2.29	0.50
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
2:D:213:MET:HE1	2:D:216:LYS:HG3	1.96	0.47
2:B:118:MET:CB	2:B:154:MET:HE1	2.44	0.46
2:D:118:MET:CB	2:D:154:MET:HE3	2.46	0.46
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: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:341:PRO:HD2	2:D:344:LEU:HD12	1.98	0.44
2:D:9:LYS:HE3	10:D:808:HOH:O	2.17	0.44
2:B:299:GLU:CD	2:B:401:ARG:HH22	2.21	0.44
1:C:467:LEU:O	1:C:467:LEU:HD23	2.17	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	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:512:MET:HE2	2:B:512:MET:HB3	1.95	0.42
2:D:509:THR:O	2:D:516:ASP:HA	2.19	0.42
1:C:382:ALA:HB1	1:C:386:ASP:CB	2.50	0.42
1:C:5:SER:O	1:C:9:VAL:HG23	2.20	0.42
3:A:601:HCA:O7	3:A:601:HCA:O2	2.37	0.42
2:B:390:PRO:O	2:B:419:ALA:HB2	2.20	0.42
2:D:377:MET:HB3	2:D:377:MET:HE3	1.65	0.42
1:A:474:LYS:HB3	2:D:322:LEU:HD21	2.01	0.41
1:A:209:LYS:NZ	1:A:263:GLU:OE2	2.41	0.41
1:A:5:SER:O	1:A:9:VAL:HG23	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	475/492 (96%)	453 (95%)	21 (4%)	1 (0%)	47	29
1	C	477/492 (97%)	460 (96%)	16 (3%)	1 (0%)	47	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%)	51	33

All (2) Ramachandran outliers are listed below:

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

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	388/415 (94%)	385 (99%)	3 (1%)	81	72
1	C	385/415 (93%)	382 (99%)	3 (1%)	81	72
2	B	440/455 (97%)	440 (100%)	0	100	100
2	D	432/455 (95%)	429 (99%)	3 (1%)	84	75
All	All	1645/1740 (94%)	1636 (100%)	9 (0%)	88	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	98	ASN
1	A	445	ASP
1	C	98	ASN
1	C	401	TYR
1	C	445	ASP
2	D	88	TYR
2	D	258	GLU
2	D	268	GLN

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](#)

Of 25 ligands modelled in this entry, 2 are modelled with single atom and 10 are monoatomic - 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	D	604	-	5,5,5	0.99	0	5,5,5	0.79	0
9	GOL	B	603	-	5,5,5	0.78	0	5,5,5	0.96	0
9	GOL	B	604	-	5,5,5	1.03	0	5,5,5	0.74	0
7	CLF	A	608	1,2	0,24,24	0.00	-	-		
3	HCA	A	601	-	4,13,13	0.71	0	4,18,18	2.82	3 (75%)
9	GOL	D	603	-	5,5,5	0.84	0	5,5,5	0.89	0
9	GOL	B	602	-	5,5,5	0.94	0	5,5,5	1.05	0
9	GOL	D	602	-	5,5,5	0.82	0	5,5,5	1.04	0
7	CLF	C	607	1,2	0,24,24	0.00	-	-		
4	ICS	C	602	1	18,30,30	2.90	12 (66%)	-		
9	GOL	B	605	-	5,5,5	0.88	0	5,5,5	1.00	0
3	HCA	C	601	-	4,13,13	1.49	1 (25%)	4,18,18	2.75	2 (50%)
4	ICS	A	602	1	18,30,30	2.83	11 (61%)	-		

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	D	604	-	-	2/4/4/4	-
9	GOL	B	603	-	-	2/4/4/4	-
9	GOL	B	604	-	-	1/4/4/4	-
7	CLF	A	608	1,2	-	-	0/12/10/10

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCA	A	601	-	-	3/7/17/17	-
9	GOL	D	603	-	-	1/4/4/4	-
9	GOL	B	602	-	-	1/4/4/4	-
9	GOL	D	602	-	-	2/4/4/4	-
7	CLF	C	607	1,2	-	-	0/12/10/10
9	GOL	B	605	-	-	0/4/4/4	-
3	HCA	C	601	-	-	3/7/17/17	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ICS	S1B-FE6	-5.82	2.18	2.32
4	C	602	ICS	S1B-FE6	-4.88	2.20	2.32
4	C	602	ICS	S2A-FE2	-4.58	2.21	2.32
4	C	602	ICS	S3B-FE7	-4.50	2.21	2.32
4	A	602	ICS	S2A-FE2	-4.21	2.22	2.32
4	A	602	ICS	S4B-FE7	-3.99	2.22	2.32
4	A	602	ICS	S3B-FE7	-3.89	2.22	2.32
4	C	602	ICS	S1B-FE5	-3.71	2.23	2.32
4	C	602	ICS	S4B-FE7	-3.69	2.23	2.32
4	C	602	ICS	S3B-FE6	-3.53	2.23	2.32
4	A	602	ICS	S1B-FE5	-3.31	2.24	2.32
4	A	602	ICS	S3B-FE6	-2.98	2.25	2.32
4	A	602	ICS	S4A-FE3	-2.95	2.25	2.32
4	A	602	ICS	S4B-FE5	-2.86	2.25	2.32
3	C	601	HCA	O7-C3	2.83	1.47	1.43
4	C	602	ICS	S5A-FE7	-2.64	2.18	2.24
4	A	602	ICS	S2A-FE3	-2.54	2.26	2.32
4	C	602	ICS	S4B-FE5	-2.51	2.26	2.32
4	C	602	ICS	S2B-FE2	-2.48	2.19	2.24
4	C	602	ICS	S4A-FE3	-2.47	2.26	2.32
4	C	602	ICS	S4A-FE4	-2.23	2.26	2.32
4	C	602	ICS	S2A-FE3	-2.18	2.27	2.32
4	A	602	ICS	S1A-FE2	-2.15	2.27	2.32
4	A	602	ICS	S5A-FE7	-2.02	2.20	2.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	HCA	C3-C2-C1	-3.99	108.60	114.98
3	A	601	HCA	C3-C2-C1	-3.57	109.27	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HCA	C4-C5-C6	3.42	116.58	111.39
3	C	601	HCA	C4-C3-C7	-3.20	105.89	111.52
3	A	601	HCA	C4-C3-C7	-2.70	106.77	111.52

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	HCA	C2-C3-C4-C5
9	D	602	GOL	O1-C1-C2-C3
3	C	601	HCA	C2-C3-C4-C5
9	B	603	GOL	O1-C1-C2-C3
9	D	604	GOL	O1-C1-C2-C3
9	B	602	GOL	C1-C2-C3-O3
9	B	603	GOL	O1-C1-C2-O2
9	D	604	GOL	O1-C1-C2-O2
9	D	602	GOL	O1-C1-C2-O2
3	C	601	HCA	C1-C2-C3-C4
3	A	601	HCA	O7-C3-C4-C5
3	C	601	HCA	O7-C3-C4-C5
9	D	603	GOL	O1-C1-C2-C3
9	B	604	GOL	O2-C2-C3-O3
3	A	601	HCA	C7-C3-C4-C5

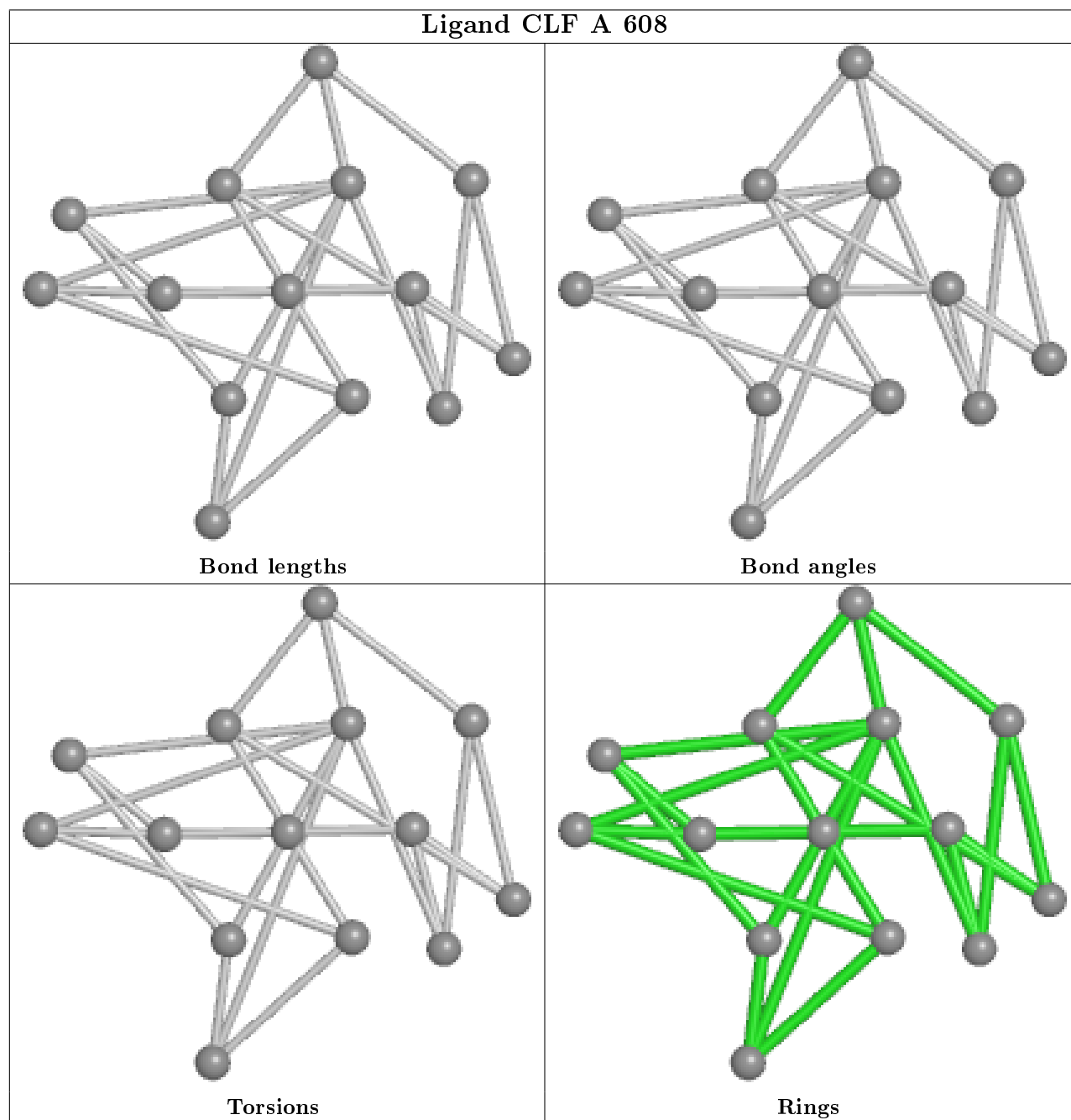
There are no ring outliers.

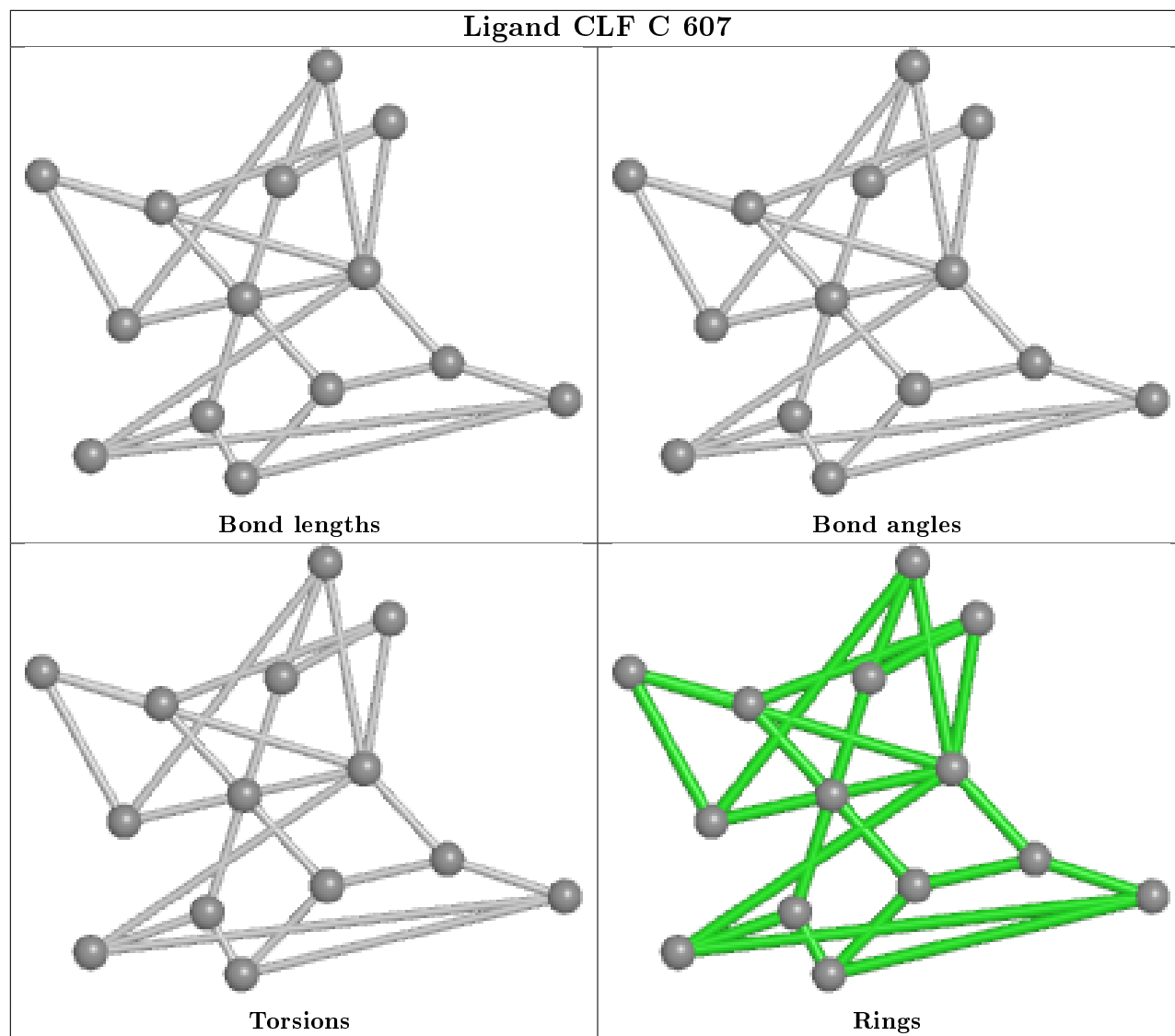
5 monomers are involved in 10 short contacts:

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

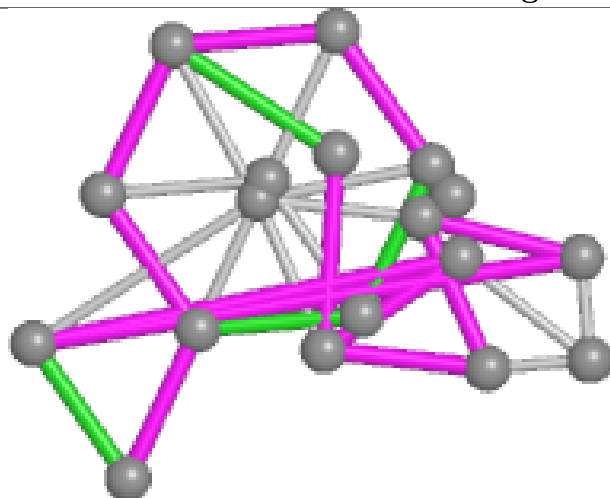
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

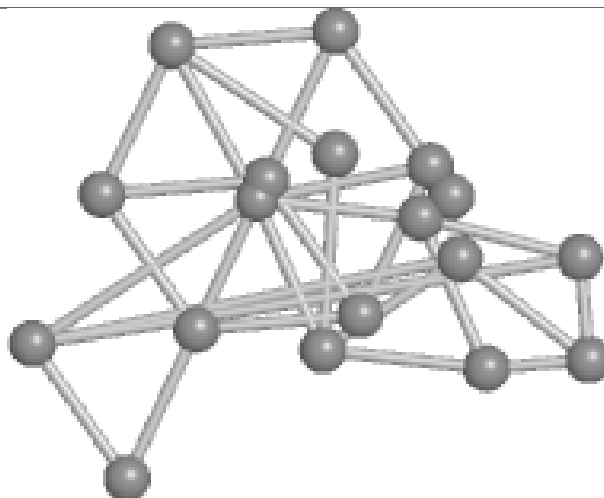




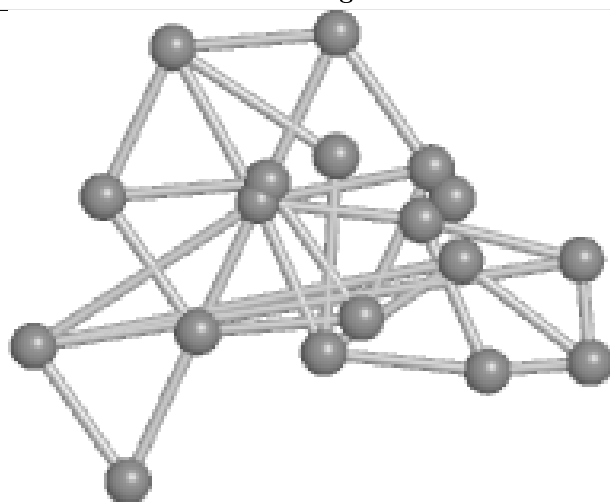
Ligand ICS C 602



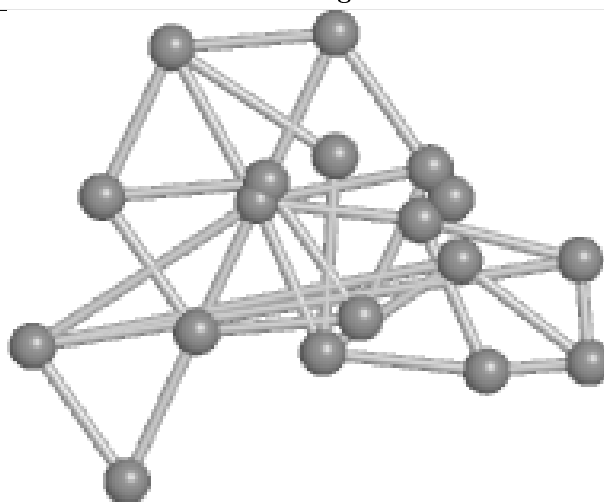
Bond lengths



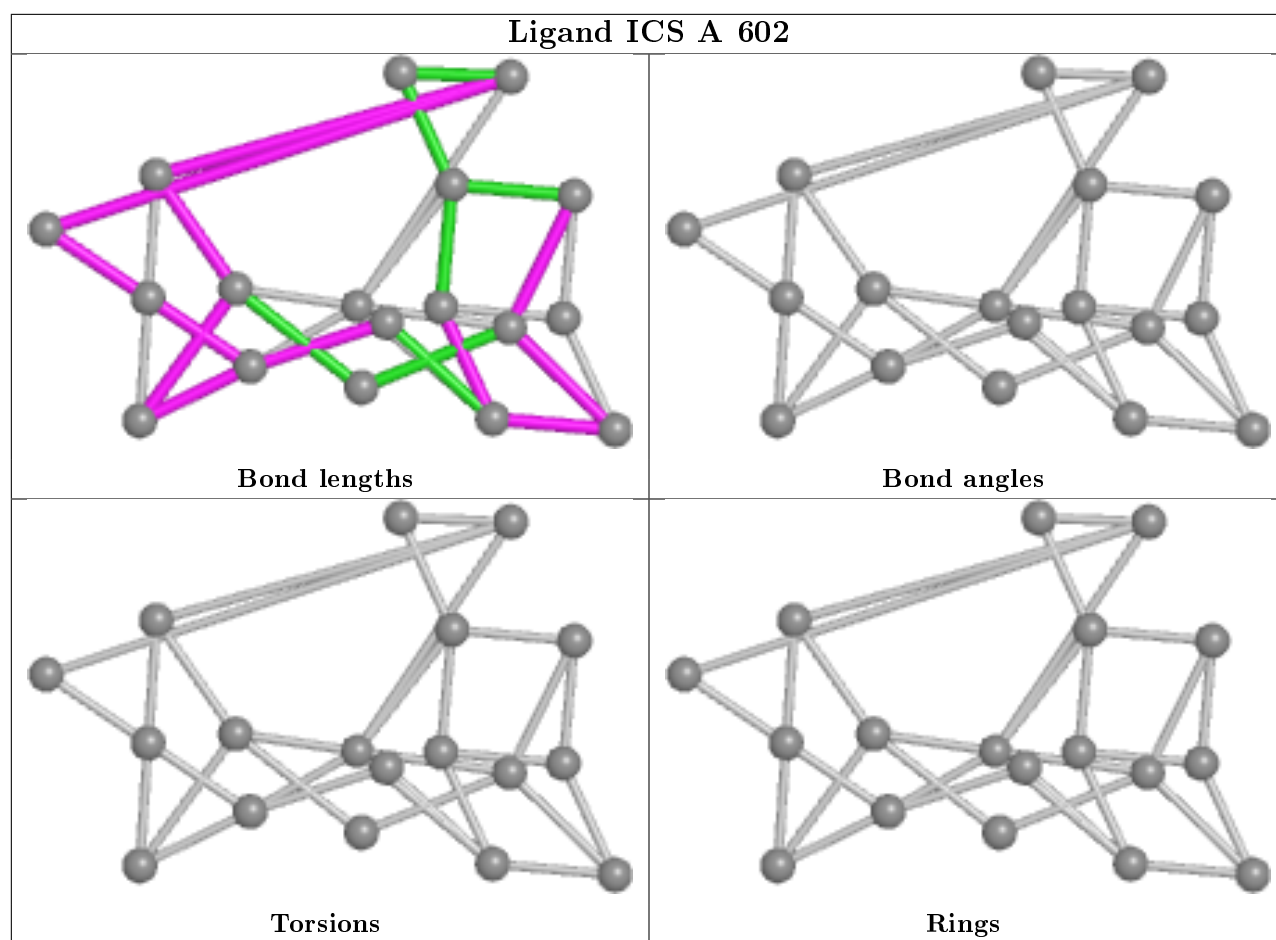
Bond angles



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

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	476/492 (96%)	0.36	42 (8%) 10 12	30, 42, 61, 76	1 (0%)
1	C	477/492 (96%)	0.42	48 (10%) 7 8	31, 43, 61, 82	0
2	B	522/523 (99%)	0.19	34 (6%) 18 23	28, 41, 60, 74	0
2	D	522/523 (99%)	0.32	41 (7%) 12 16	29, 43, 62, 77	0
All	All	1997/2030 (98%)	0.32	165 (8%) 11 14	28, 43, 61, 82	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	ILE	5.9
2	D	103	PHE	5.3
2	B	98	TYR	5.0
2	D	98	TYR	4.8
2	D	102	TYR	4.7
1	A	95	GLY	4.6
1	A	70	VAL	4.6
2	B	102	TYR	4.5
2	B	522	VAL	4.5
2	D	97	ALA	4.4
1	C	91	TYR	4.3
1	A	94	ALA	4.2
2	D	521	LEU	4.1
1	C	172	ALA	4.1
1	C	95	GLY	4.1
1	C	70	VAL	4.1
2	D	218	VAL	4.0
2	D	522	VAL	4.0
1	A	425	ILE	3.9
2	B	97	ALA	3.8
2	D	101	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	521	LEU	3.8
1	C	125	PHE	3.8
2	D	474	PHE	3.7
1	C	59	ILE	3.6
2	B	307	GLY	3.5
1	A	65	ALA	3.5
2	D	99	PHE	3.5
2	D	107	PHE	3.5
1	A	169	VAL	3.4
2	D	76	VAL	3.4
2	D	111	VAL	3.4
2	B	103	PHE	3.4
2	D	73	LEU	3.4
1	A	231	ILE	3.4
1	A	91	TYR	3.3
1	A	444	TRP	3.3
1	C	94	ALA	3.2
1	C	292	ILE	3.2
2	D	309	TRP	3.2
1	A	446	TYR	3.2
1	C	424	GLY	3.2
1	C	65	ALA	3.2
2	B	5	VAL	3.2
1	C	316	PHE	3.1
1	A	172	ALA	3.1
2	B	101[A]	SER	3.0
2	D	473	ILE	3.0
2	D	471	PHE	3.0
2	D	337	GLY	3.0
2	D	175	ILE	3.0
1	A	110	VAL	3.0
2	D	96	VAL	3.0
1	A	125	PHE	2.9
1	A	98	ASN	2.9
2	D	104	ASN	2.9
1	A	69	GLY	2.8
1	C	319	SER	2.8
1	C	124	VAL	2.8
2	D	77	LEU	2.8
2	D	94	GLY	2.8
1	A	99	TYR	2.8
1	A	174	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	329	ALA	2.8
1	A	59	ILE	2.8
1	C	4	MET	2.8
1	C	92	SER	2.8
1	C	444	TRP	2.8
1	C	71	VAL	2.7
2	B	474	PHE	2.7
2	D	174	PHE	2.7
1	A	62	CYS	2.7
1	C	62	CYS	2.7
1	C	355	ILE	2.7
2	B	309	TRP	2.7
1	C	327	VAL	2.7
2	D	105	ARG	2.7
2	D	285	PRO	2.7
1	C	291	GLY	2.7
2	B	107	PHE	2.6
1	C	322	LYS	2.6
2	D	472	PRO	2.6
1	A	9	VAL	2.6
1	A	327	VAL	2.6
2	B	111	VAL	2.6
1	C	446	TYR	2.6
1	C	335	TRP	2.6
1	C	99	TYR	2.5
1	C	174	LEU	2.5
1	C	441	MET	2.5
2	D	330	MET	2.5
1	C	169	VAL	2.5
1	A	92	SER	2.5
1	C	353	LEU	2.5
1	C	96	ARG	2.4
2	B	340	ILE	2.4
2	B	473	ILE	2.4
2	D	100	ARG	2.4
1	A	93	ARG	2.4
1	A	71	VAL	2.4
1	C	110	VAL	2.4
2	D	234	LEU	2.4
1	A	229	TYR	2.4
2	D	447	TYR	2.4
2	B	96	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	231	ILE	2.3
1	A	329	ALA	2.3
1	C	69	GLY	2.3
2	B	175	ILE	2.3
1	C	426	LYS	2.3
2	B	310	LYS	2.3
2	B	177	ASP	2.3
1	A	355	ILE	2.3
2	B	99	PHE	2.3
2	B	339	PRO	2.3
2	B	210	LEU	2.3
1	A	96	ARG	2.2
2	B	76	VAL	2.2
2	D	5	VAL	2.2
1	A	17	LEU	2.2
1	C	294	TRP	2.2
1	A	66	GLY	2.2
1	A	424	GLY	2.2
1	C	171	GLY	2.2
1	A	111	THR	2.2
2	D	220	SER	2.2
1	C	442	HIS	2.2
1	C	98	ASN	2.2
2	B	174	PHE	2.2
1	A	426	LYS	2.2
2	D	167	ASN	2.2
1	A	61	GLY	2.2
1	A	450	TYR	2.1
2	B	213	MET	2.1
2	B	77	LEU	2.1
2	D	212	SER	2.1
2	B	218	VAL	2.1
2	D	210	LEU	2.1
1	C	5	SER	2.1
1	A	441	MET	2.1
2	D	283	ASP	2.1
1	A	74	PRO	2.1
1	C	220	PRO	2.1
2	D	106	HIS	2.1
1	A	340	ALA	2.1
2	B	73	LEU	2.1
2	B	36	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	285	PRO	2.1
1	C	354	TYR	2.1
2	B	447	TYR	2.1
1	A	316	PHE	2.1
2	B	6	ASP	2.1
2	D	113	CYS	2.1
1	A	75	ILE	2.1
1	C	443	SER	2.1
1	C	332	LYS	2.0
2	B	337	GLY	2.0
2	D	446	SER	2.0
1	A	88	CYS	2.0
1	C	58	THR	2.0
2	D	213	MET	2.0
1	A	362	HIS	2.0
2	B	471	PHE	2.0
1	C	317	ASP	2.0
1	C	73	GLY	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
9	GOL	B	603	6/6	0.78	0.22	45,54,61,73	0
5	MO	C	606	1/1	0.90	0.04	76,76,76,76	1
9	GOL	B	604	6/6	0.90	0.15	52,54,61,68	0
9	GOL	D	603	6/6	0.91	0.23	46,63,63,63	0
9	GOL	B	602	6/6	0.92	0.12	40,48,49,50	0

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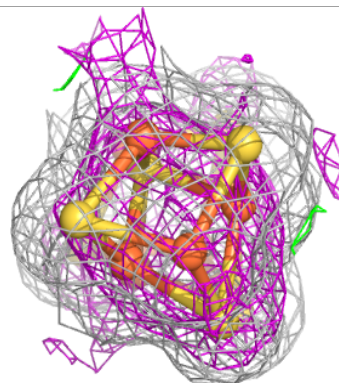
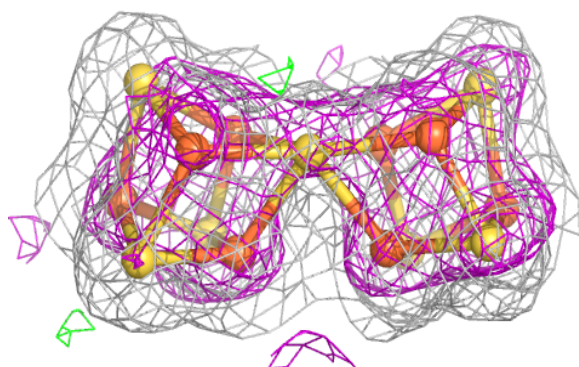
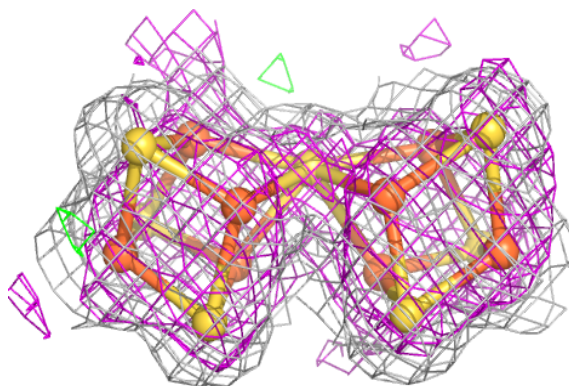
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HCA	C	601	14/14	0.93	0.19	27,33,36,39	0
9	GOL	D	604	6/6	0.94	0.12	40,47,52,54	0
3	HCA	A	601	14/14	0.94	0.19	24,32,36,36	0
5	MO	A	607	1/1	0.95	0.06	71,71,71,71	1
9	GOL	D	602	6/6	0.96	0.17	52,62,63,70	0
8	FE	B	606	1/1	0.97	0.14	51,51,51,51	1
9	GOL	B	605	6/6	0.97	0.10	54,61,66,69	0
6	H2S	D	601	1/1	0.97	0.17	40,40,40,40	0
5	MO	A	606	1/1	0.98	0.04	53,53,53,53	1
7	CLF	A	608	15/15	0.98	0.07	29,32,34,35	0
8	FE	B	601	1/1	0.98	0.17	59,59,59,59	1
5	MO	A	603	1/1	0.98	0.06	45,45,45,45	1
7	CLF	C	607	15/15	0.98	0.06	29,33,36,37	0
4	ICS	C	602	18/18	0.98	0.07	24,31,33,34	0
5	MO	C	603	1/1	0.99	0.06	44,44,44,44	1
5	MO	A	604	1/1	0.99	0.03	53,53,53,53	1
5	MO	C	605	1/1	0.99	0.06	44,44,44,44	1
5	MO	C	604	1/1	0.99	0.03	58,58,58,58	1
4	ICS	A	602	18/18	0.99	0.09	27,30,32,33	0
6	H2S	A	605	1/1	1.00	0.18	37,37,37,37	0

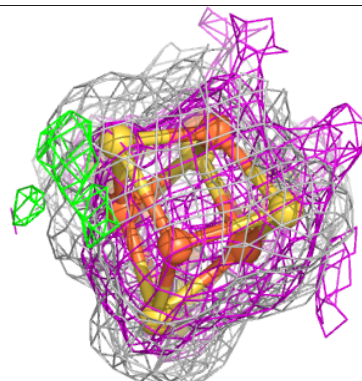
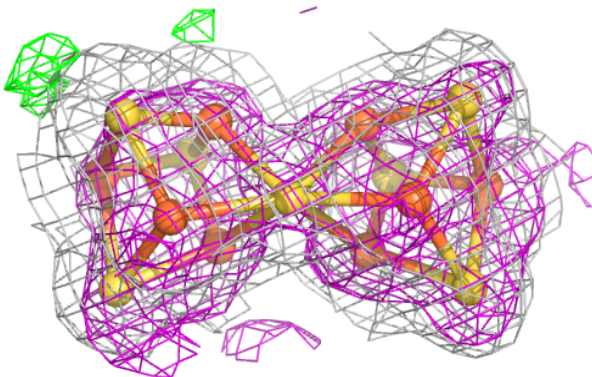
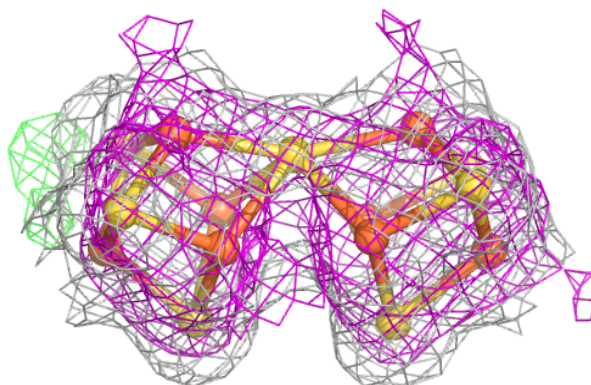
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

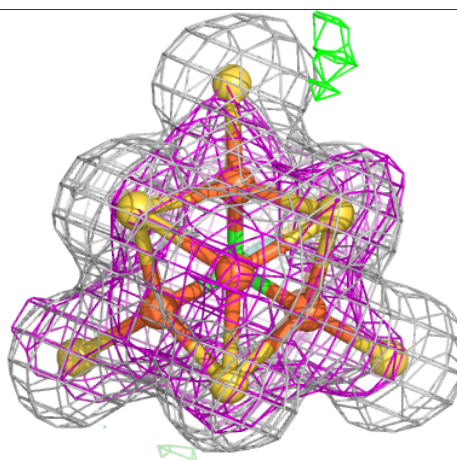
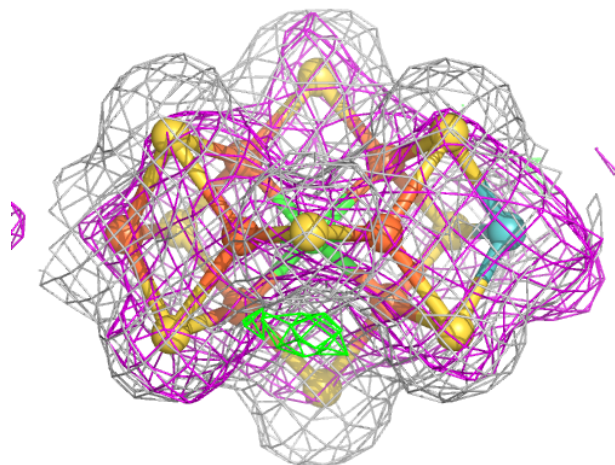
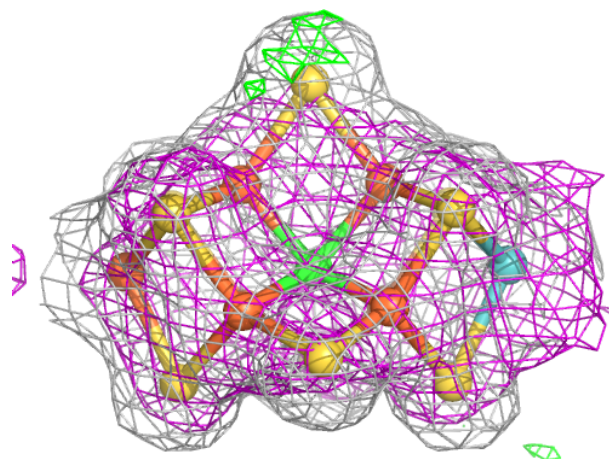
**Electron density around CLF C 607:**

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



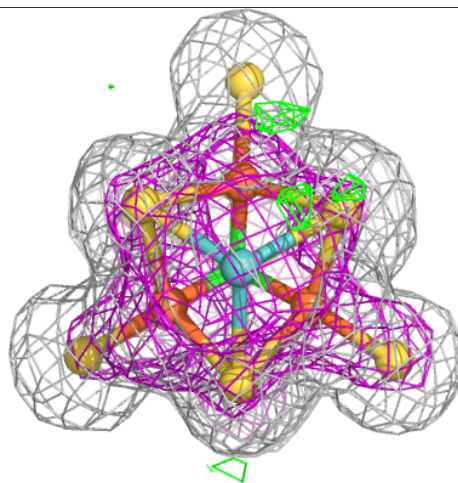
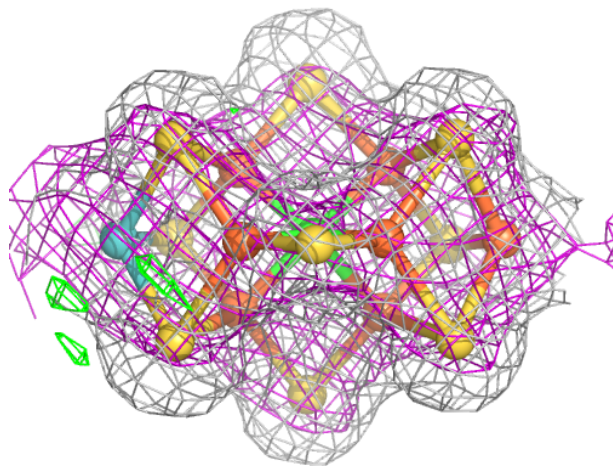
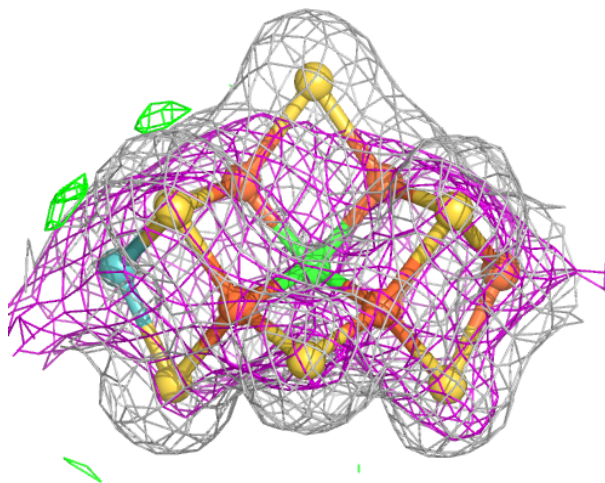
Electron density around ICS C 602:

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



Electron density around 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.