Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 10:59 pm BST

PDB ID	:	9HBC / pdb_00009hbc
Title	:	A. vinelandii nitrogenase MoFe protein Anc2
Authors	:	Detemple, F.; Kacar, B.; Einsle, O.
Deposited on	:	2024-11-06
Resolution	:	1.82 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 (i) 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 (i)) were used in the production of this report:

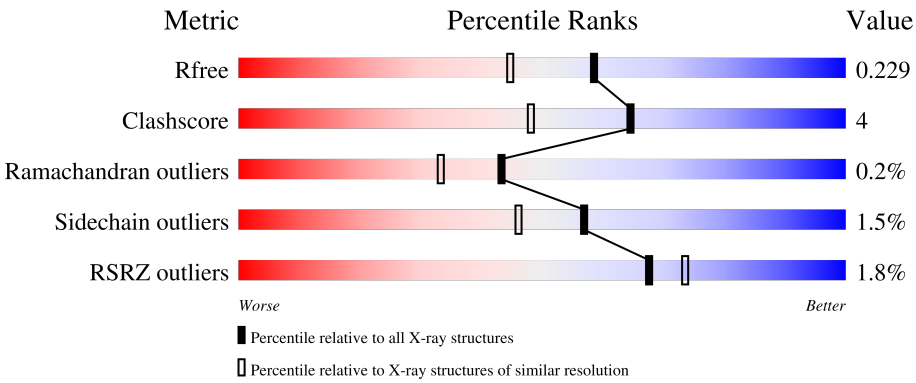
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 <=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	491	3% 84% 12% • •
1	C	491	2% 85% 12% •
2	B	523	.% 92% 8%
2	D	523	.% 91% 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17460 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.

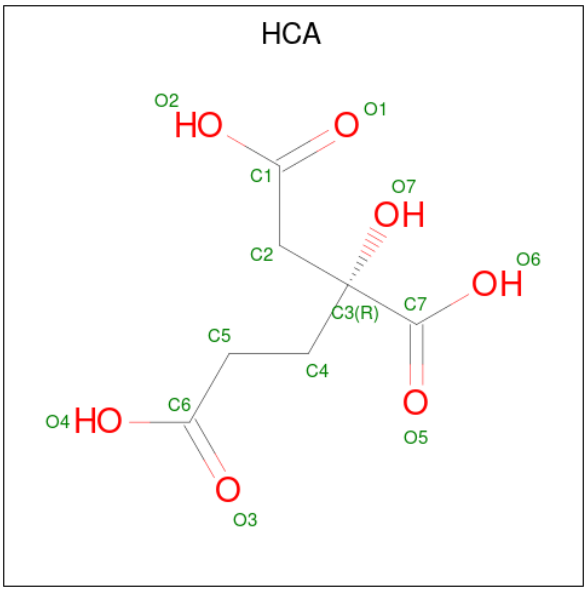
- Molecule 1 is a protein called MoFe nitrogenase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	3799	2411	655	708	25	0	1	0
1	C	478	3843	2437	665	716	25	0	6	0

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

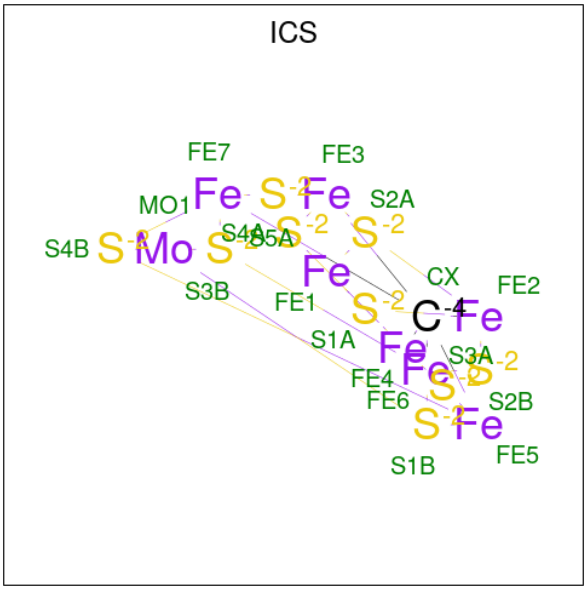
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4211	2689	714	779	29	0	5	0
2	D	522	4196	2678	710	780	28	0	3	0

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$) (labeled as "Ligand of Interest" by depositor).



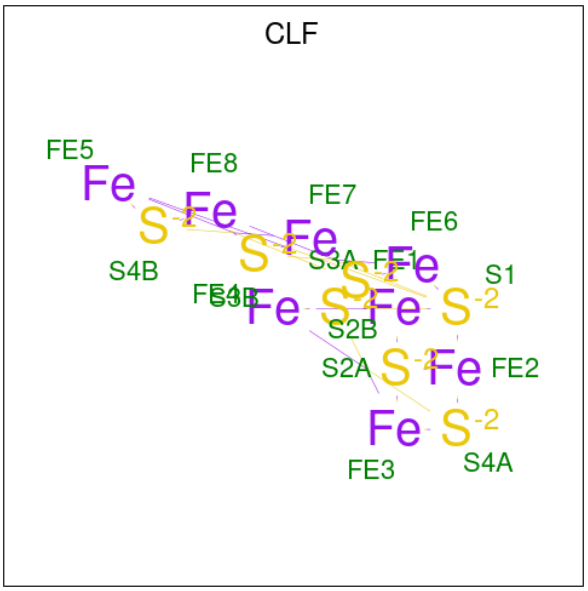
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	14	7	7	0	0
			Total	C	O		
3	C	1	14	7	7	0	0

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



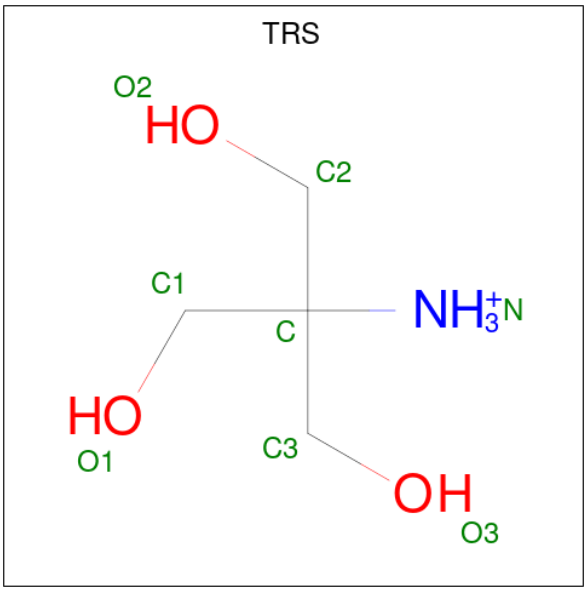
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	Mo	S		
4	A	1	18	1	7	1	9	0	0
			Total	C	Fe	Mo	S		
4	C	1	18	1	7	1	9	0	0

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).



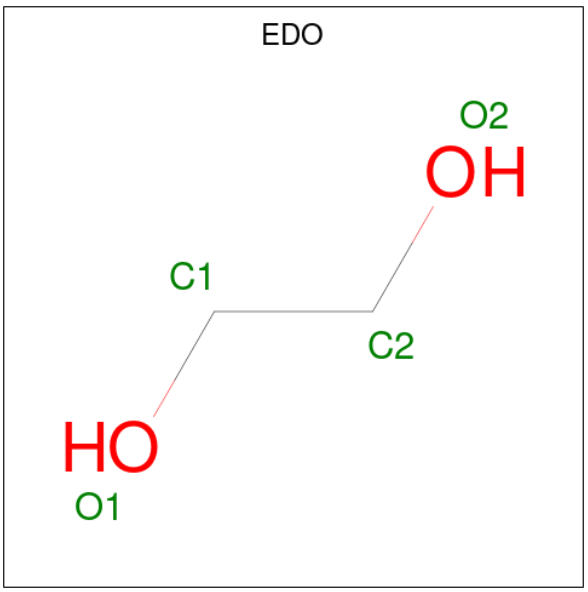
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	B	1	15	8	7	0	1
			Total	Fe	S		
5	D	1	15	8	7	0	1

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	8	4	1	3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	4	2	2	0	0
7	D	1	4	2	2	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	B	1	1	1	0	0
8	D	1	1	1	0	0

- Molecule 9 is water.

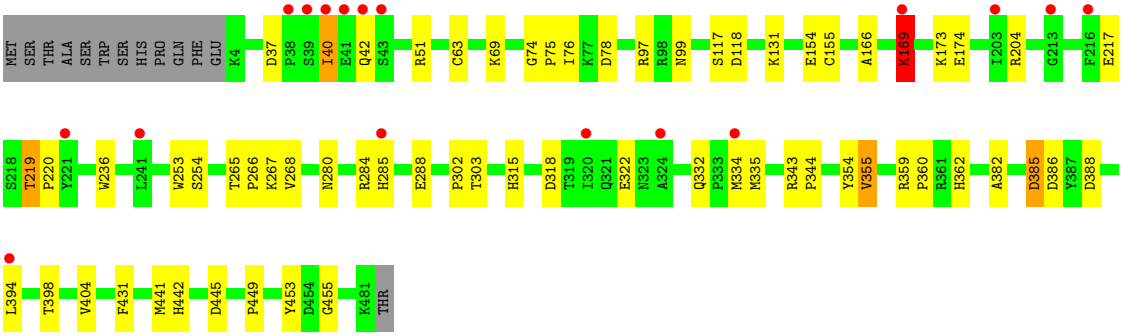
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	228	228	228	0	0
9	B	350	351	351	0	1
9	C	301	301	301	0	0
9	D	419	419	419	0	0

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.

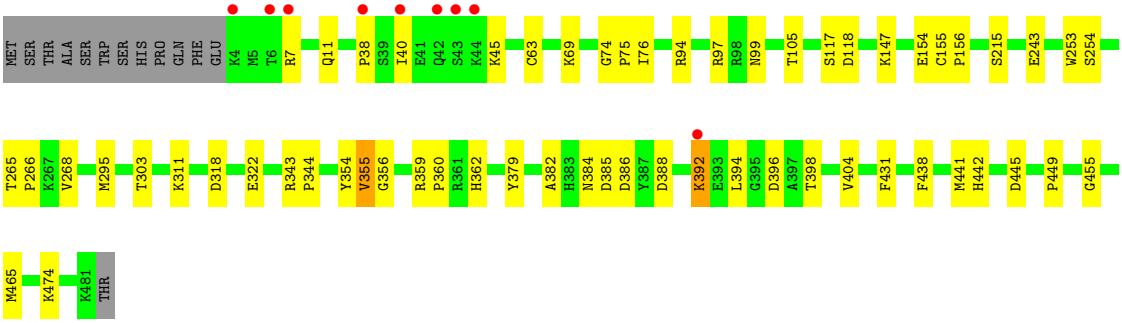
• Molecule 1: MoFe nitrogenase subunit D

Chain A:



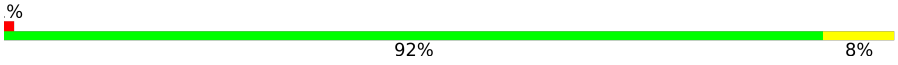
• Molecule 1: MoFe nitrogenase subunit D

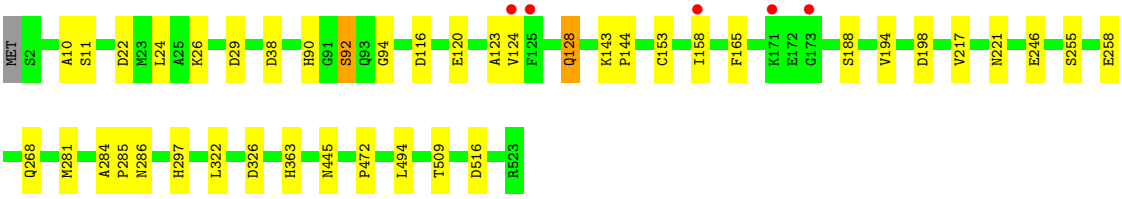
Chain C:



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

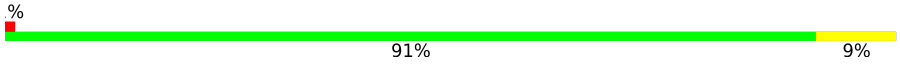
Chain B:

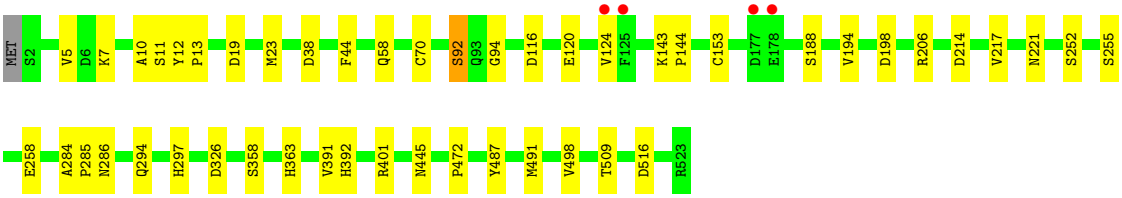




• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.94Å 130.13Å 209.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.49 – 1.82 110.49 – 1.82	Depositor EDS
% Data completeness (in resolution range)	66.1 (110.49-1.82) 66.1 (110.49-1.82)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.176 , 0.225 0.185 , 0.229	Depositor DCC
R_{free} test set	6145 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17460	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 38.71 % 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 3.5375e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, ICS, CLF, TRS, HCA

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	0.60	0/3887	1.07	8/5245 (0.2%)
1	C	0.62	0/3931	1.08	6/5301 (0.1%)
2	B	0.62	0/4323	1.05	5/5842 (0.1%)
2	D	0.62	0/4302	1.05	7/5817 (0.1%)
All	All	0.61	0/16443	1.06	26/22205 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	385	ASP	CA-CB-CG	8.10	120.70	112.60
1	C	385	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	431	PHE	CA-CB-CG	-6.75	107.05	113.80
1	A	441	MET	CG-SD-CE	-6.69	86.18	100.90
2	B	38	ASP	CA-CB-CG	6.17	118.77	112.60
2	D	198	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	441	MET	CG-SD-CE	-6.11	87.46	100.90
2	B	246	GLU	CB-CA-C	-6.05	100.75	110.79
2	D	116	ASP	CA-CB-CG	5.62	118.22	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	HIS	CA-CB-CG	5.56	119.36	113.80
2	D	19	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	105	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	303	THR	CA-CB-OG1	-5.50	101.34	109.60
2	B	198	ASP	CA-CB-CG	5.47	118.07	112.60
2	B	268	GLN	N-CA-CB	-5.44	101.16	111.00
1	C	388	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	303	THR	CA-CB-OG1	-5.40	101.50	109.60
2	D	326	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	431	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	388	ASP	CA-CB-CG	5.14	117.74	112.60
2	D	38	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	169	LYS	CB-CA-C	5.07	119.47	110.85
1	A	78	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	326	ASP	CA-CB-CG	5.03	117.63	112.60
2	D	44	PHE	CA-CB-CG	-5.03	108.77	113.80
2	D	214	ASP	CB-CA-C	-5.02	102.14	110.68

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ARG	Sidechain
1	C	97	ARG	Sidechain
2	D	206	ARG	Sidechain

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	3741	38	0
1	C	3843	0	3786	38	0
2	B	4211	0	4134	27	0
2	D	4196	0	4100	25	0
3	A	14	0	6	0	0
3	C	14	0	6	3	0
4	A	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	18	0	0	2	0
5	B	15	0	0	1	0
5	D	15	0	0	1	0
6	B	8	0	12	1	0
7	B	4	0	6	0	0
7	D	4	0	6	2	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	228	0	0	7	0
9	B	351	0	0	4	0
9	C	301	0	0	7	0
9	D	419	0	0	10	0
All	All	17460	0	15797	126	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 (126) 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:B:24:LEU:HD13	6:B:602:TRS:O1	1.48	1.12
1:A:335:MET:HE2	1:A:453:TYR:HD1	1.36	0.89
1:A:51:ARG:HD3	9:A:731:HOH:O	1.75	0.87
1:A:335:MET:HE2	1:A:453:TYR:CD1	2.14	0.83
2:D:120:GLU:OE1	9:D:701:HOH:O	2.06	0.73
2:D:363:HIS:HD2	9:D:1054:HOH:O	1.72	0.72
1:A:288:GLU:OE1	9:A:601:HOH:O	2.07	0.72
1:A:385:ASP:OD2	9:A:602:HOH:O	2.11	0.69
1:A:267:LYS:O	9:A:603:HOH:O	2.11	0.68
1:C:7[B]:ARG:NH1	1:C:11:GLN:HG3	2.09	0.68
2:B:128:GLN:HG3	9:B:831:HOH:O	1.95	0.67
1:C:243:GLU:OE1	9:C:601:HOH:O	2.13	0.67
1:C:7[B]:ARG:HH12	1:C:11:GLN:HG3	1.60	0.66
1:C:394:LEU:HD22	1:C:398:THR:HG21	1.78	0.66
7:D:602:EDO:C2	9:D:741:HOH:O	2.47	0.63
1:A:394:LEU:HD22	1:A:398:THR:HG21	1.81	0.62
2:B:128:GLN:HG2	2:B:165:PHE:CD1	2.35	0.62
2:D:401[A]:ARG:NE	9:D:702:HOH:O	2.30	0.60
2:D:401[A]:ARG:NH2	9:D:702:HOH:O	2.16	0.59
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.39	0.58
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:OD2	9:B:701:HOH:O	2.17	0.57
1:C:384:ASN:ND2	9:C:607:HOH:O	2.31	0.55
2:D:58:GLN:NE2	9:D:706:HOH:O	2.38	0.55
1:A:280:ASN:OD1	1:A:284:ARG:NH2	2.41	0.54
2:D:5:VAL:HG12	9:D:961:HOH:O	2.07	0.53
1:A:37:ASP:O	1:A:40:ILE:HB	2.08	0.53
1:A:335:MET:CE	1:A:453:TYR:HD1	2.16	0.53
1:A:76:ILE:CD1	1:A:254:SER:HB2	2.39	0.53
1:A:51:ARG:CD	9:A:731:HOH:O	2.44	0.52
2:B:22:ASP:O	2:B:26:LYS:HG2	2.10	0.52
2:D:358:SER:HB3	2:D:498:VAL:HG21	1.92	0.51
1:A:76:ILE:HD13	1:A:254:SER:HB2	1.91	0.51
1:A:166:ALA:O	1:A:169:LYS:HD3	2.10	0.51
2:B:153:CYS:HB3	2:B:188:SER:OG	2.11	0.51
1:A:63:CYS:HB3	2:B:94:GLY:HA3	1.93	0.50
2:B:445:ASN:HB2	2:B:472:PRO:O	2.11	0.50
2:B:10:ALA:O	2:B:11:SER:C	2.55	0.50
1:A:204:ARG:HG3	1:A:285:HIS:CE1	2.47	0.49
1:C:442:HIS:CG	3:C:501:HCA:H52	2.47	0.49
2:B:194:VAL:HB	2:B:297:HIS:CG	2.46	0.49
1:A:265:THR:O	1:A:268:VAL:HG22	2.13	0.49
1:C:63:CYS:HB3	2:D:94:GLY:HA3	1.95	0.49
1:A:42:GLN:H	1:A:42:GLN:CD	2.21	0.49
1:C:265:THR:O	1:C:268:VAL:HG22	2.13	0.49
1:A:265:THR:N	1:A:266:PRO:CD	2.75	0.48
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.95	0.48
1:A:302:PRO:HB3	1:A:335:MET:HE3	1.94	0.48
1:C:76:ILE:CD1	1:C:254:SER:HB2	2.44	0.48
1:A:449:PRO:O	1:A:455:GLY:HA2	2.14	0.48
2:D:10:ALA:O	2:D:11:SER:C	2.56	0.48
2:D:509:THR:O	2:D:516:ASP:HA	2.14	0.48
2:D:194:VAL:HB	2:D:297:HIS:CG	2.48	0.48
1:A:359:ARG:N	1:A:360:PRO:CD	2.77	0.47
1:C:392[A]:LYS:NZ	9:C:618:HOH:O	2.46	0.47
1:A:69:LYS:C	1:A:69:LYS:HD3	2.39	0.47
1:A:173:LYS:HG2	1:A:174:GLU:N	2.28	0.47
7:D:602:EDO:H11	9:D:905:HOH:O	2.15	0.47
2:B:92:SER:HB2	5:B:601[B]:CLF:S2A	2.55	0.47
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.96	0.47
1:C:392[A]:LYS:HE3	9:C:618:HOH:O	2.15	0.47
1:C:155:CYS:HB2	1:C:156:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HD2	9:A:658:HOH:O	2.15	0.47
2:B:120:GLU:HB3	9:B:707:HOH:O	2.14	0.47
1:C:74:GLY:N	1:C:75:PRO:CD	2.78	0.46
1:C:359:ARG:N	1:C:360:PRO:CD	2.77	0.46
2:D:153:CYS:HB3	2:D:188:SER:OG	2.15	0.46
1:C:94:ARG:O	9:C:602:HOH:O	2.21	0.46
1:C:392[A]:LYS:H	1:C:392[A]:LYS:HZ3	1.64	0.46
1:A:315:HIS:O	1:A:315:HIS:ND1	2.49	0.46
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.97	0.46
2:D:221:ASN:C	2:D:221:ASN:OD1	2.59	0.46
2:D:445:ASN:HB2	2:D:472:PRO:O	2.15	0.46
1:C:76:ILE:HD13	1:C:254:SER:HB2	1.97	0.45
1:C:295:MET:HE1	1:C:311:LYS:HG2	1.97	0.45
2:B:128:GLN:HG2	2:B:165:PHE:CE1	2.51	0.45
2:B:128:GLN:HG2	2:B:165:PHE:CG	2.51	0.45
2:B:221:ASN:OD1	2:B:221:ASN:C	2.59	0.45
1:C:69:LYS:HD3	1:C:69:LYS:C	2.41	0.45
2:B:509:THR:O	2:B:516:ASP:HA	2.17	0.45
1:C:147:LYS:NZ	9:C:622:HOH:O	2.49	0.45
3:C:501:HCA:O7	3:C:501:HCA:O1	2.32	0.45
1:C:356:GLY:HA3	4:C:502:ICS:S1B	2.57	0.45
2:D:294:GLN:NE2	9:D:735:HOH:O	2.50	0.45
1:C:449:PRO:O	1:C:455:GLY:HA2	2.17	0.45
2:D:143:LYS:N	2:D:144:PRO:CD	2.80	0.45
1:C:253:TRP:HA	1:C:254:SER:HA	1.78	0.44
2:B:143:LYS:N	2:B:144:PRO:CD	2.81	0.44
9:C:601:HOH:O	2:D:23:MET:HG3	2.17	0.44
2:D:284:ALA:N	2:D:285:PRO:CD	2.81	0.44
1:C:343:ARG:N	1:C:344:PRO:CD	2.80	0.43
2:B:281[A]:MET:CA	2:B:281[A]:MET:HE2	2.48	0.43
1:C:265:THR:N	1:C:266:PRO:CD	2.80	0.43
2:D:217:VAL:H	2:D:286:ASN:ND2	2.17	0.43
2:D:92:SER:HB2	5:D:601[B]:CLF:S2A	2.58	0.43
1:A:334[B]:MET:HB2	9:A:699:HOH:O	2.18	0.43
1:A:74:GLY:N	1:A:75:PRO:CD	2.81	0.42
1:A:253:TRP:HA	1:A:254:SER:HA	1.80	0.42
1:C:38:PRO:HD2	1:C:396:ASP:OD1	2.19	0.42
1:C:379:TYR:CD2	1:C:382:ALA:HB2	2.54	0.42
1:A:284:ARG:CB	1:A:284:ARG:HH11	2.32	0.42
1:A:318:ASP:O	1:A:322:GLU:HG3	2.20	0.42
2:B:123:ALA:HA	2:B:158:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:HIS:CG	1:C:465:MET:HG3	2.55	0.42
1:A:117:SER:O	1:A:118:ASP:C	2.62	0.42
1:A:219:THR:HB	1:A:220:PRO:HD2	2.01	0.42
2:D:7:LYS:HG3	9:D:708:HOH:O	2.19	0.42
2:D:391[B]:VAL:HG22	2:D:392:HIS:CE1	2.55	0.42
1:A:343:ARG:N	1:A:344:PRO:CD	2.82	0.42
2:B:217:VAL:H	2:B:286:ASN:ND2	2.18	0.41
1:C:392[A]:LYS:NZ	1:C:392[A]:LYS:HB3	2.35	0.41
1:C:438:PHE:CD1	1:C:438:PHE:C	2.98	0.41
2:B:284:ALA:N	2:B:285:PRO:CD	2.84	0.41
1:A:154:GLU:O	1:A:155:CYS:C	2.64	0.41
2:D:12:TYR:HA	2:D:13:PRO:HA	1.84	0.41
1:A:236:TRP:CD1	2:B:24:LEU:HD21	2.56	0.41
1:C:117:SER:O	1:C:118:ASP:C	2.63	0.41
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.54	0.40
2:B:26:LYS:HE2	9:B:859:HOH:O	2.20	0.40
1:C:154:GLU:O	1:C:155:CYS:C	2.64	0.40
2:D:487:TYR:O	2:D:491:MET:HG3	2.21	0.40
1:C:318:ASP:O	1:C:322:GLU:HG3	2.21	0.40
1:C:442:HIS:CE1	4:C:502:ICS:S1B	3.14	0.40
2:B:494:LEU:HD23	2:B:494:LEU:C	2.46	0.40
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.21	0.40
2:D:70:CYS:HB2	2:D:188:SER:HB2	2.03	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	477/491 (97%)	456 (96%)	20 (4%)	1 (0%)	43	33
1	C	482/491 (98%)	460 (95%)	21 (4%)	1 (0%)	43	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	525/523 (100%)	511 (97%)	13 (2%)	1 (0%)	43	33
2	D	523/523 (100%)	509 (97%)	13 (2%)	1 (0%)	43	33
All	All	2007/2028 (99%)	1936 (96%)	67 (3%)	4 (0%)	43	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	255	SER
2	D	255	SER
1	A	355	VAL
1	C	355	VAL

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	404/416 (97%)	395 (98%)	9 (2%)	45	30
1	C	409/416 (98%)	400 (98%)	9 (2%)	45	30
2	B	459/455 (101%)	455 (99%)	4 (1%)	70	62
2	D	456/455 (100%)	452 (99%)	4 (1%)	70	62
All	All	1728/1742 (99%)	1702 (98%)	26 (2%)	57	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	99	ASN
1	A	169	LYS
1	A	217	GLU
1	A	219	THR
1	A	332	GLN
1	A	355	VAL
1	A	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	445	ASP
2	B	92	SER
2	B	124	VAL
2	B	128	GLN
2	B	258	GLU
1	C	40	ILE
1	C	45	LYS
1	C	99	ASN
1	C	215	SER
1	C	355	VAL
1	C	362	HIS
1	C	392[A]	LYS
1	C	392[B]	LYS
1	C	445	ASP
2	D	92	SER
2	D	124	VAL
2	D	252	SER
2	D	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	271	ASN
1	A	432	GLN
1	A	468	ASN
2	B	45	GLN
2	B	104	ASN
2	B	130	ASN
2	B	163	ASN
2	B	225	ASN
2	B	286	ASN
2	B	294	GLN
2	B	317	ASN
2	B	418	ASN
1	C	11	GLN
1	C	214	GLN
1	C	271	ASN
1	C	468	ASN
2	D	104	ASN
2	D	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	130	ASN
2	D	163	ASN
2	D	168	ASN
2	D	225	ASN
2	D	278	GLN
2	D	286	ASN
2	D	294	GLN
2	D	317	ASN
2	D	363	HIS
2	D	418	ASN
2	D	513	GLN

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)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	CLF	B	601[B]	1,2	0,24,24	-	-	-		
3	HCA	C	501	4	13,13,13	1.62	4 (30%)	14,18,18	2.29	6 (42%)
7	EDO	D	602	-	3,3,3	0.52	0	2,2,2	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HCA	A	501	4	13,13,13	1.38	2 (15%)	14,18,18	3.12	8 (57%)
7	EDO	B	603	-	3,3,3	0.10	0	2,2,2	0.28	0
4	ICS	C	502	1,3	18,30,30	3.16	12 (66%)	-		
5	CLF	D	601[B]	1,2	0,24,24	-	-	-		
6	TRS	B	602	-	7,7,7	0.21	0	9,9,9	0.58	0
4	ICS	A	502	1,3	18,30,30	3.54	13 (72%)	-		

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
5	CLF	B	601[B]	1,2	-	-	0/12/10/10
3	HCA	C	501	4	-	4/17/17/17	-
7	EDO	D	602	-	-	0/1/1/1	-
3	HCA	A	501	4	-	3/17/17/17	-
7	EDO	B	603	-	-	1/1/1/1	-
6	TRS	B	602	-	-	3/9/9/9	-
5	CLF	D	601[B]	1,2	-	-	0/12/10/10

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S2B-FE2	-7.25	2.07	2.24
4	A	502	ICS	S3B-FE7	-5.91	2.17	2.32
4	A	502	ICS	S1B-FE5	-4.86	2.20	2.32
4	C	502	ICS	S3B-FE7	-4.80	2.20	2.32
4	A	502	ICS	S1B-FE6	-4.65	2.20	2.32
4	A	502	ICS	S1A-FE2	-4.64	2.21	2.32
4	C	502	ICS	S2A-FE2	-4.64	2.21	2.32
4	C	502	ICS	S4B-FE5	-4.54	2.21	2.32
4	C	502	ICS	S2B-FE6	-4.50	2.14	2.24
4	C	502	ICS	S1B-FE5	-3.97	2.22	2.32
4	C	502	ICS	S4B-FE7	-3.94	2.22	2.32
4	C	502	ICS	S1A-FE2	-3.89	2.22	2.32
4	A	502	ICS	S4B-FE7	-3.74	2.23	2.32
4	A	502	ICS	S3B-FE6	-3.51	2.23	2.32
3	C	501	HCA	C4-C3	3.30	1.59	1.54
4	A	502	ICS	S2B-FE6	-3.25	2.17	2.24
4	C	502	ICS	S1A-FE4	-3.23	2.24	2.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S1B-FE6	-3.04	2.24	2.32
4	C	502	ICS	S3B-FE6	-2.71	2.25	2.32
4	C	502	ICS	S2A-FE3	-2.66	2.25	2.32
4	C	502	ICS	S3A-FE5	2.66	2.31	2.24
3	A	501	HCA	O7-C3	2.52	1.48	1.43
4	A	502	ICS	S4A-FE4	-2.50	2.26	2.32
3	C	501	HCA	O3-C6	2.49	1.30	1.22
3	C	501	HCA	C2-C3	2.43	1.56	1.53
3	A	501	HCA	O3-C6	2.31	1.29	1.22
4	A	502	ICS	S4A-FE3	-2.24	2.26	2.32
4	A	502	ICS	S2A-FE2	-2.23	2.26	2.32
4	A	502	ICS	S3A-FE5	2.20	2.30	2.24
4	A	502	ICS	S5A-FE3	2.20	2.30	2.24
3	C	501	HCA	C3-C7	2.06	1.55	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	HCA	O6-C7-C3	7.89	126.76	113.05
3	C	501	HCA	O6-C7-C3	4.35	120.61	113.05
3	A	501	HCA	C4-C5-C6	4.26	122.40	112.75
3	C	501	HCA	C2-C3-C7	-3.77	102.01	110.11
3	A	501	HCA	O5-C7-C3	-3.20	117.72	122.25
3	A	501	HCA	C2-C3-C7	-3.18	103.27	110.11
3	A	501	HCA	O2-C1-C2	3.00	123.99	114.35
3	C	501	HCA	O3-C6-C5	-2.86	113.90	123.08
3	A	501	HCA	O6-C7-O5	-2.61	115.52	123.82
3	A	501	HCA	O4-C6-C5	2.32	121.47	114.03
3	C	501	HCA	O2-C1-C2	2.27	121.64	114.35
3	C	501	HCA	C3-C2-C1	-2.25	108.38	113.81
3	C	501	HCA	O7-C3-C7	2.20	111.96	108.86
3	A	501	HCA	O1-C1-C2	-2.15	116.66	122.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	C	501	HCA	C2-C3-C4-C5
6	B	602	TRS	C2-C-C1-O1
6	B	602	TRS	C3-C-C1-O1
6	B	602	TRS	N-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	603	EDO	O1-C1-C2-O2
3	A	501	HCA	O7-C3-C4-C5
3	C	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C1-C2-C3-C4
3	C	501	HCA	C4-C5-C6-O4
3	A	501	HCA	C3-C4-C5-C6

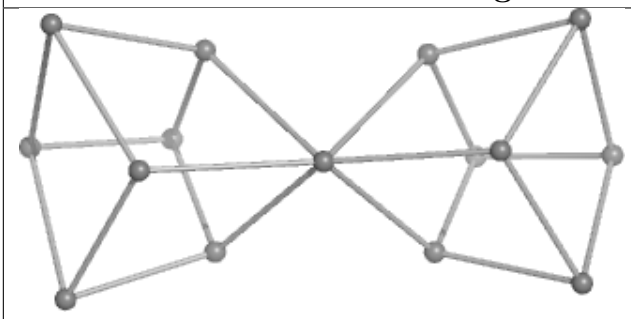
There are no ring outliers.

6 monomers are involved in 10 short contacts:

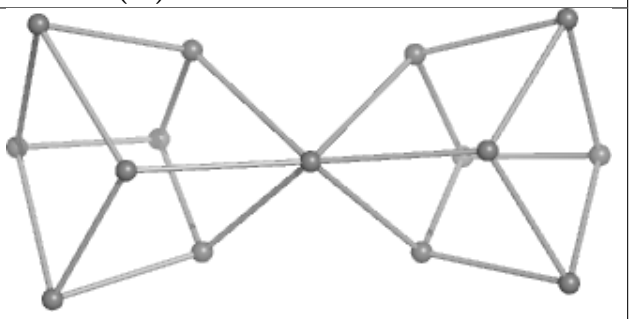
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601[B]	CLF	1	0
3	C	501	HCA	3	0
7	D	602	EDO	2	0
4	C	502	ICS	2	0
5	D	601[B]	CLF	1	0
6	B	602	TRS	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

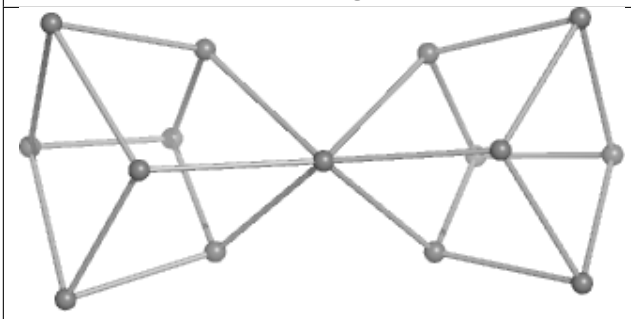
Ligand CLF B 601 (B)



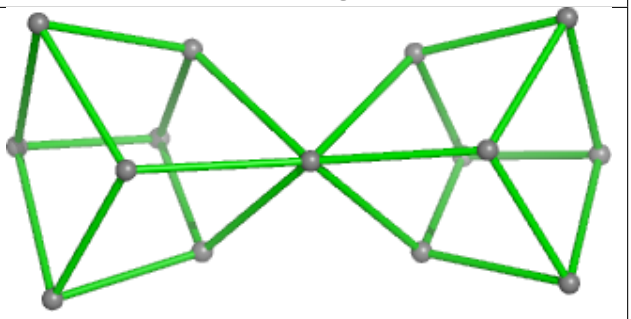
Bond lengths



Bond angles

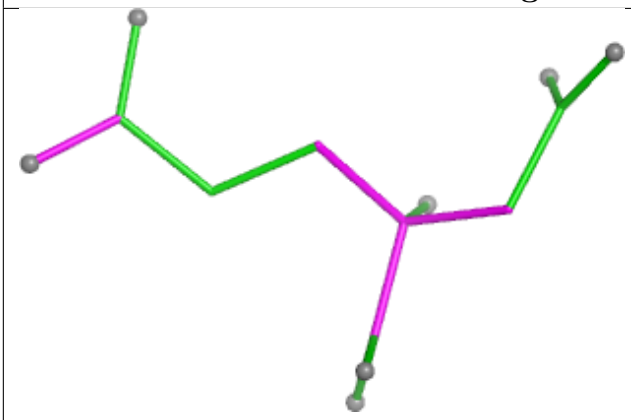


Torsions

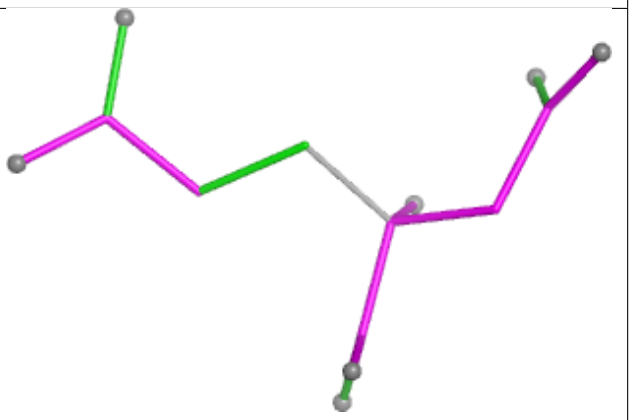


Rings

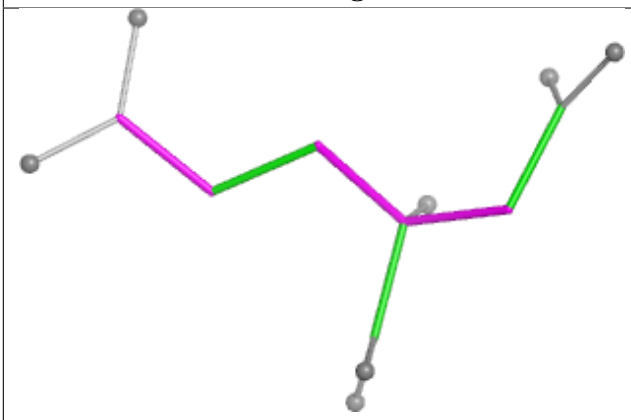
Ligand HCA C 501



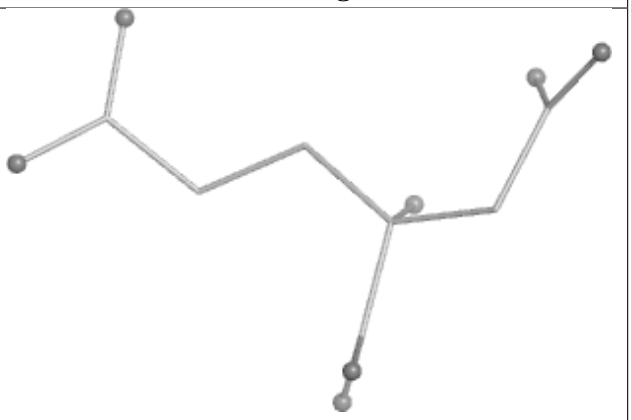
Bond lengths



Bond angles

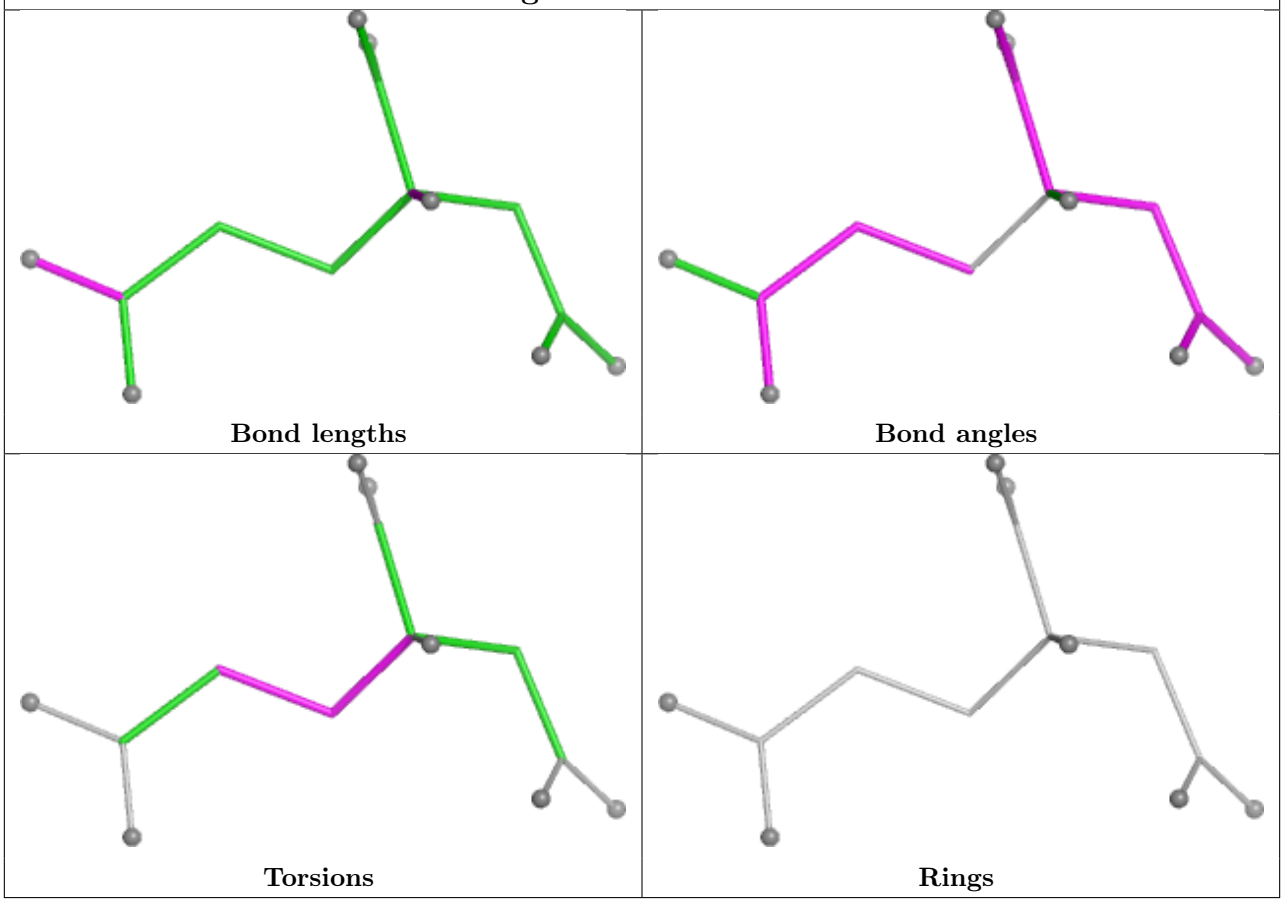


Torsions

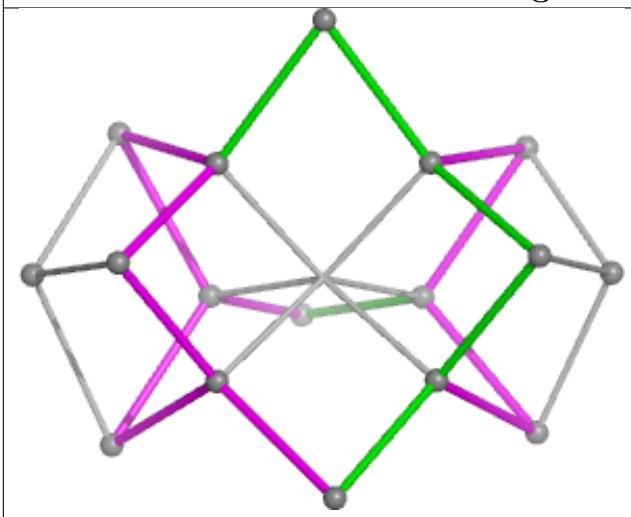


Rings

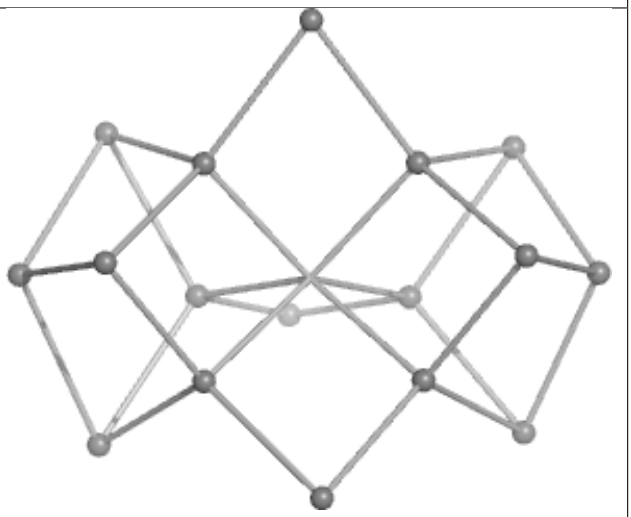
Ligand HCA A 501



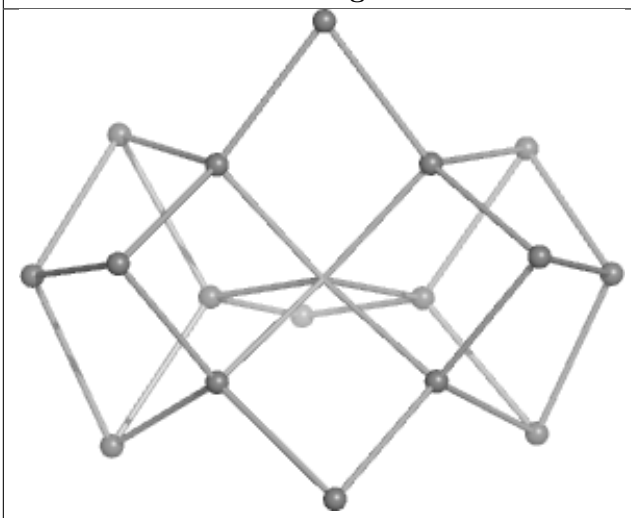
Ligand ICS C 502



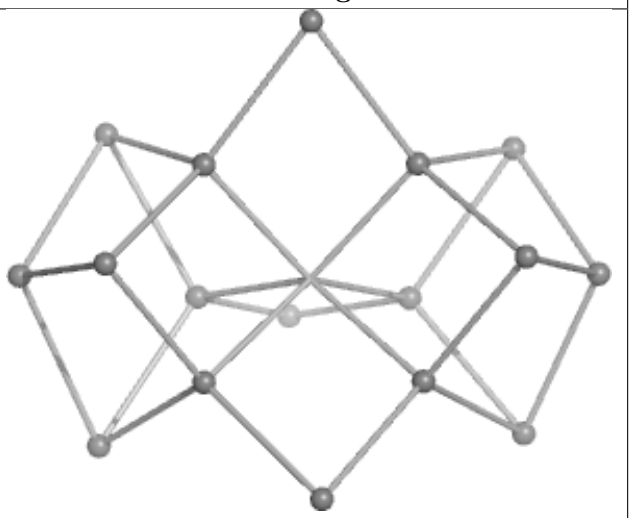
Bond lengths



Bond angles

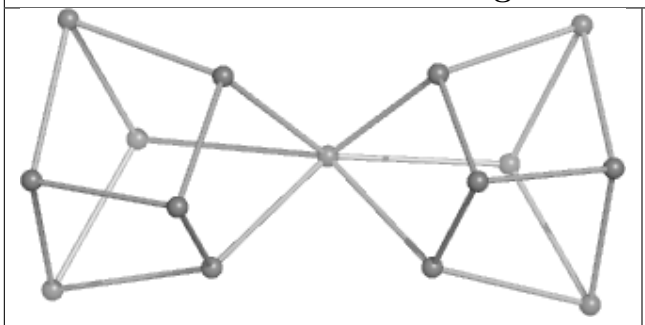


Torsions

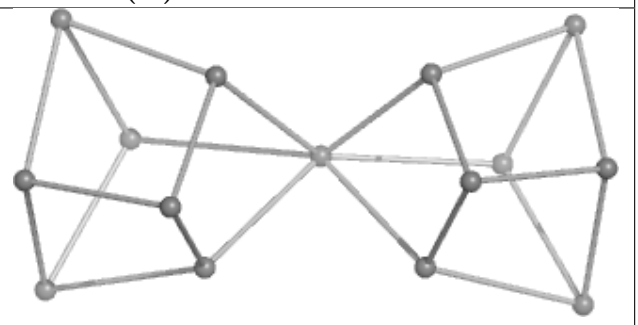


Rings

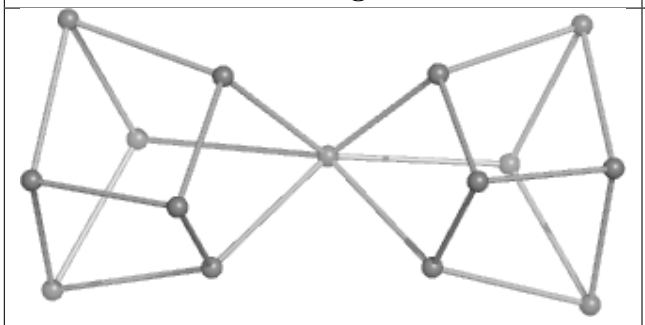
Ligand CLF D 601 (B)



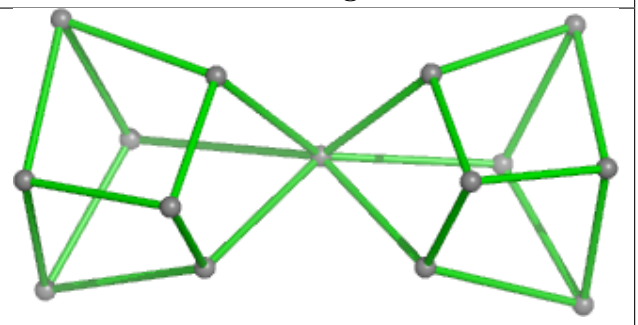
Bond lengths



Bond angles

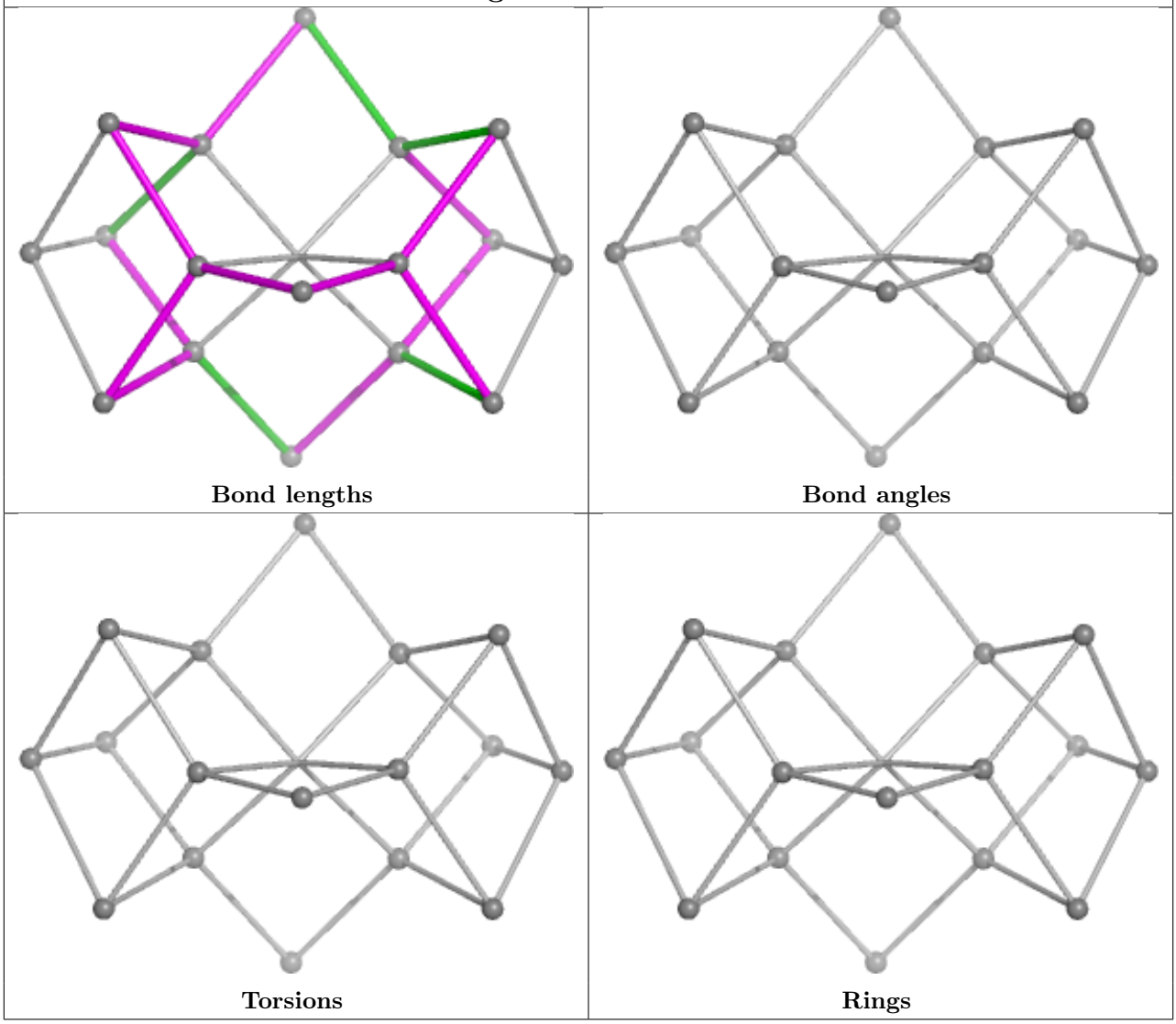


Torsions



Rings

Ligand ICS A 502



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	478/491 (97%)	0.33	17 (3%)	46	53	17, 31, 54, 109	5 (1%)
1	C	478/491 (97%)	-0.18	9 (1%)	66	72	9, 23, 45, 110	8 (1%)
2	B	522/523 (99%)	-0.18	5 (0%)	79	84	9, 24, 43, 68	6 (1%)
2	D	522/523 (99%)	-0.37	4 (0%)	82	87	12, 22, 36, 71	5 (0%)
All	All	2000/2028 (98%)	-0.11	35 (1%)	67	73	9, 25, 46, 110	24 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	ILE	5.3
1	A	40	ILE	5.1
2	D	125	PHE	5.0
2	B	125	PHE	4.3
1	C	38	PRO	3.4
2	D	124	VAL	3.3
1	A	42	GLN	3.2
1	C	7[A]	ARG	3.2
1	A	38	PRO	3.1
2	B	124	VAL	2.8
1	A	324	ALA	2.8
1	C	42	GLN	2.7
1	A	169	LYS	2.7
1	C	392[A]	LYS	2.7
1	A	43	SER	2.7
1	A	213	GLY	2.6
1	A	285	HIS	2.6
1	A	334[A]	MET	2.6
1	A	39	SER	2.5
1	A	203	ILE	2.4
1	A	320	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	6	THR	2.4
2	B	158	ILE	2.4
1	C	43	SER	2.3
2	B	173	GLY	2.3
1	C	4	LYS	2.3
1	A	41	GLU	2.2
2	D	178	GLU	2.2
1	A	394	LEU	2.2
1	A	221	TYR	2.1
2	D	177	ASP	2.1
1	C	44	LYS	2.1
2	B	171	LYS	2.1
1	A	241	LEU	2.1
1	A	216	PHE	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
6	TRS	B	602	8/8	0.82	0.17	48,56,60,63	0
7	EDO	B	603	4/4	0.89	0.12	37,44,44,45	0
7	EDO	D	602	4/4	0.89	0.11	28,34,34,37	0
3	HCA	A	501	14/14	0.95	0.06	12,17,23,24	0
3	HCA	C	501	14/14	0.96	0.06	12,17,21,22	0
4	ICS	A	502	18/18	0.99	0.03	17,20,23,24	0
5	CLF	B	601[B]	15/15	0.99	0.03	21,23,27,28	0
5	CLF	D	601[B]	15/15	0.99	0.02	16,18,20,21	0
8	MG	B	604	1/1	0.99	0.02	18,18,18,18	0

Continued on next page...

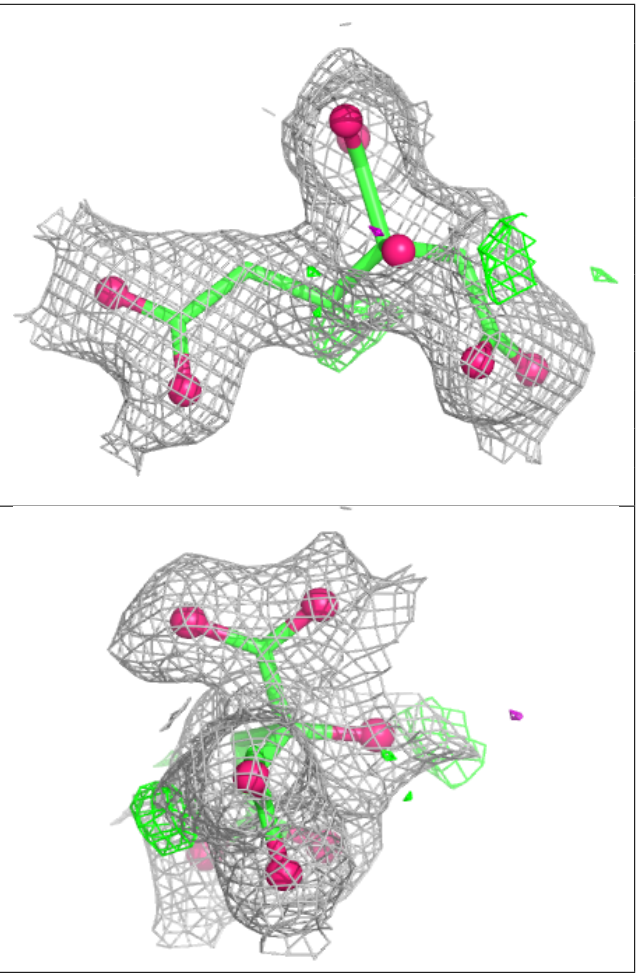
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ICS	C	502	18/18	1.00	0.02	15,16,18,20	0
8	MG	D	603	1/1	1.00	0.02	17,17,17,17	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.

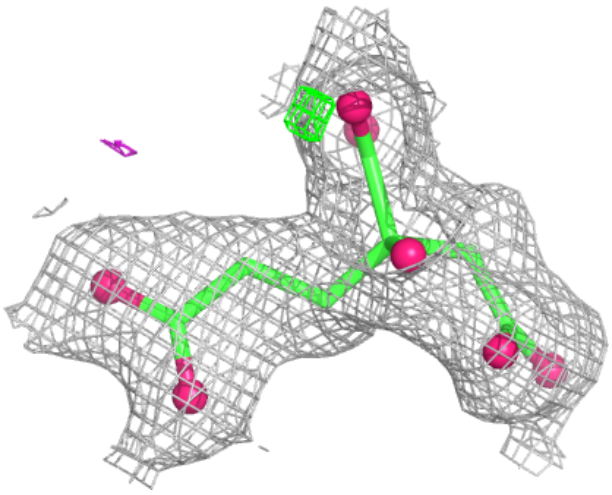
Electron density around HCA A 501:

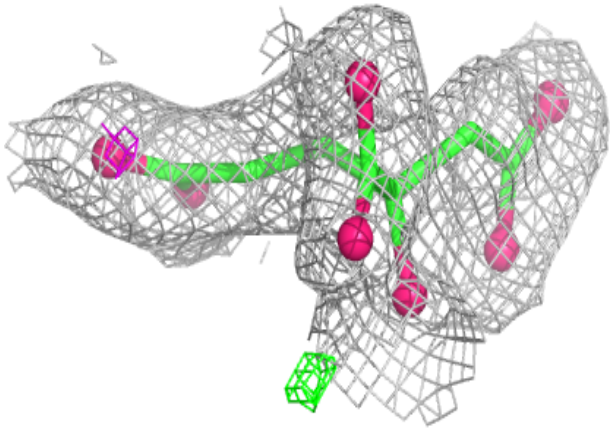
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

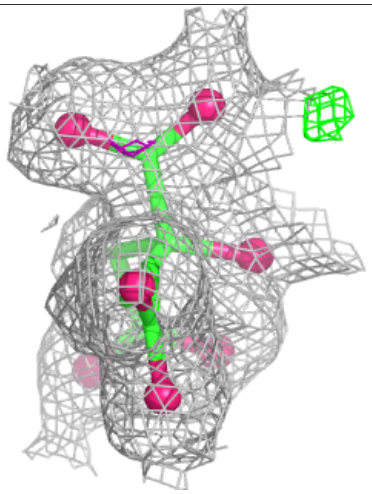


Electron density around HCA C 501:

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

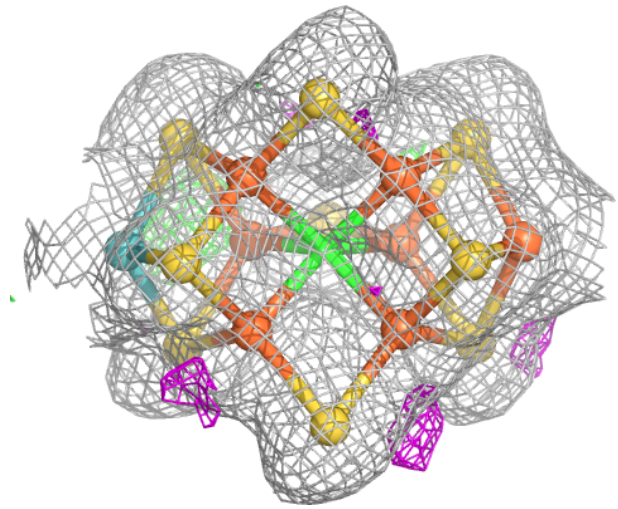


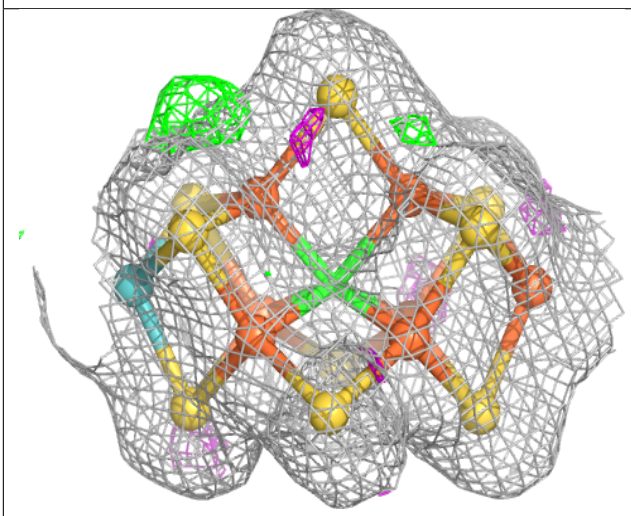


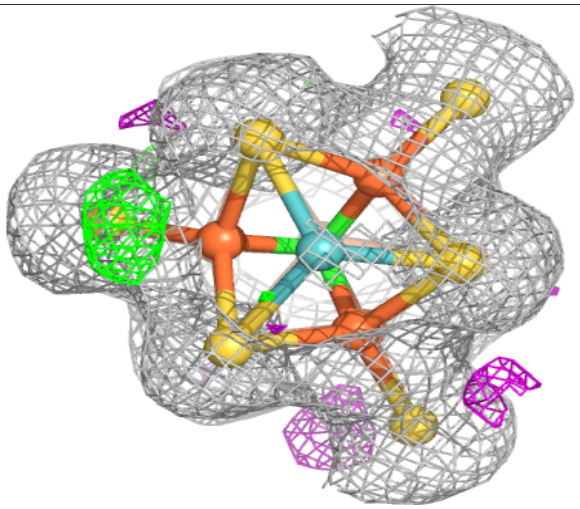


Electron density around ICS A 502:

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

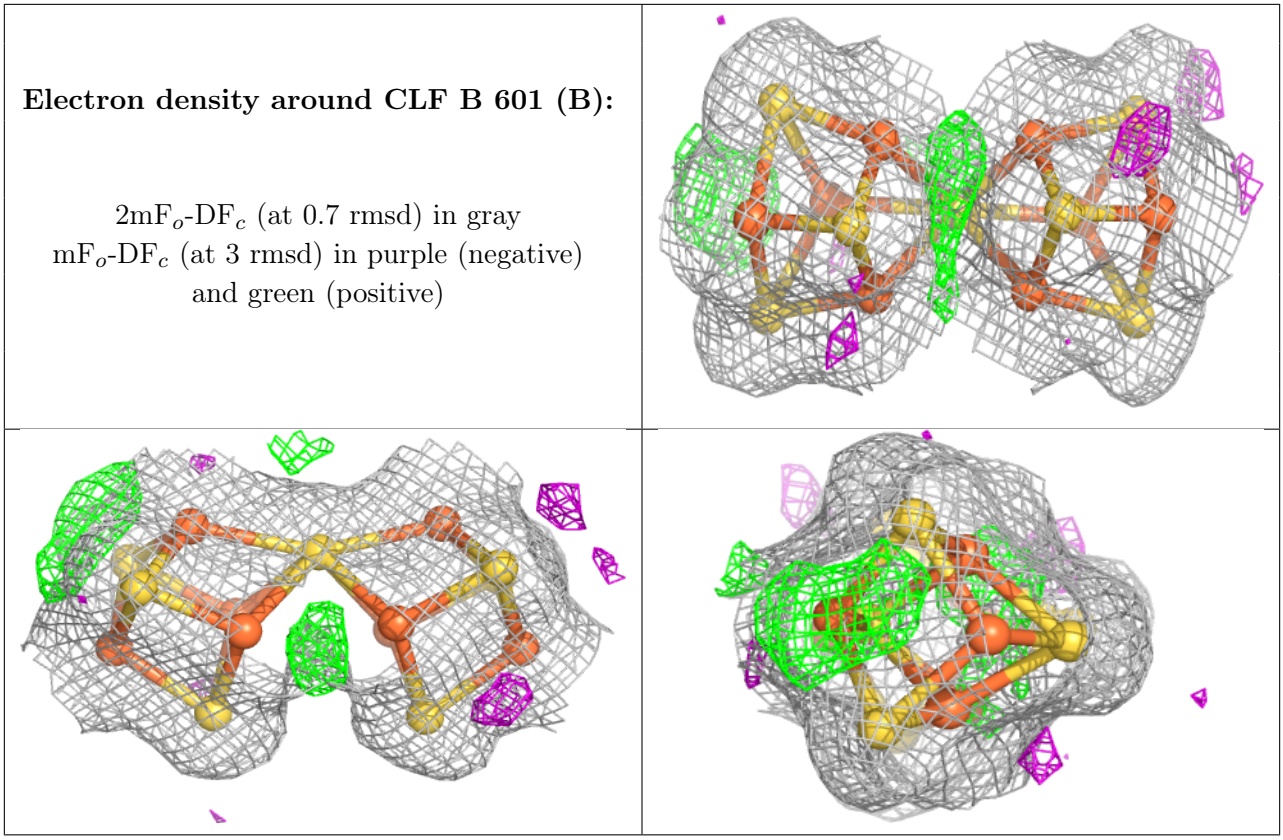






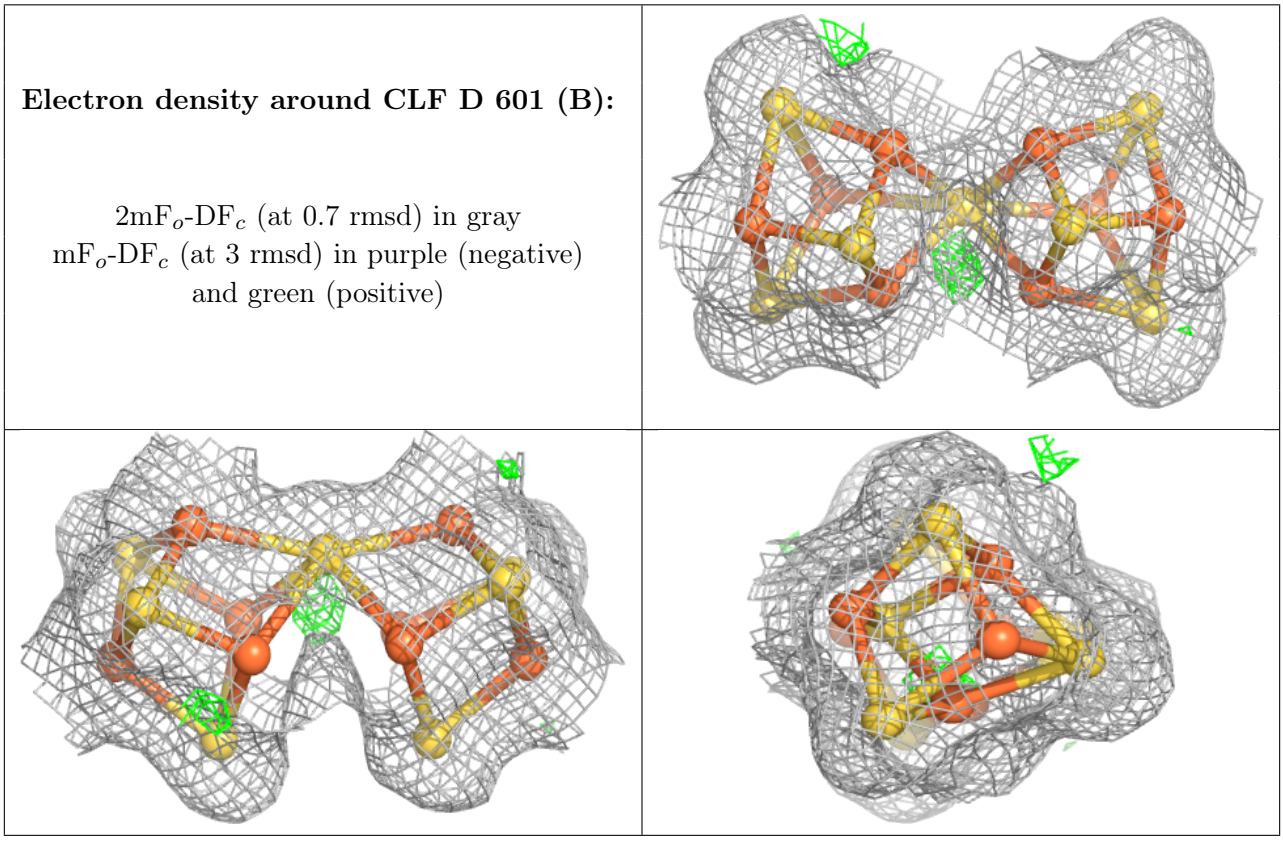
Electron density around CLF B 601 (B):

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



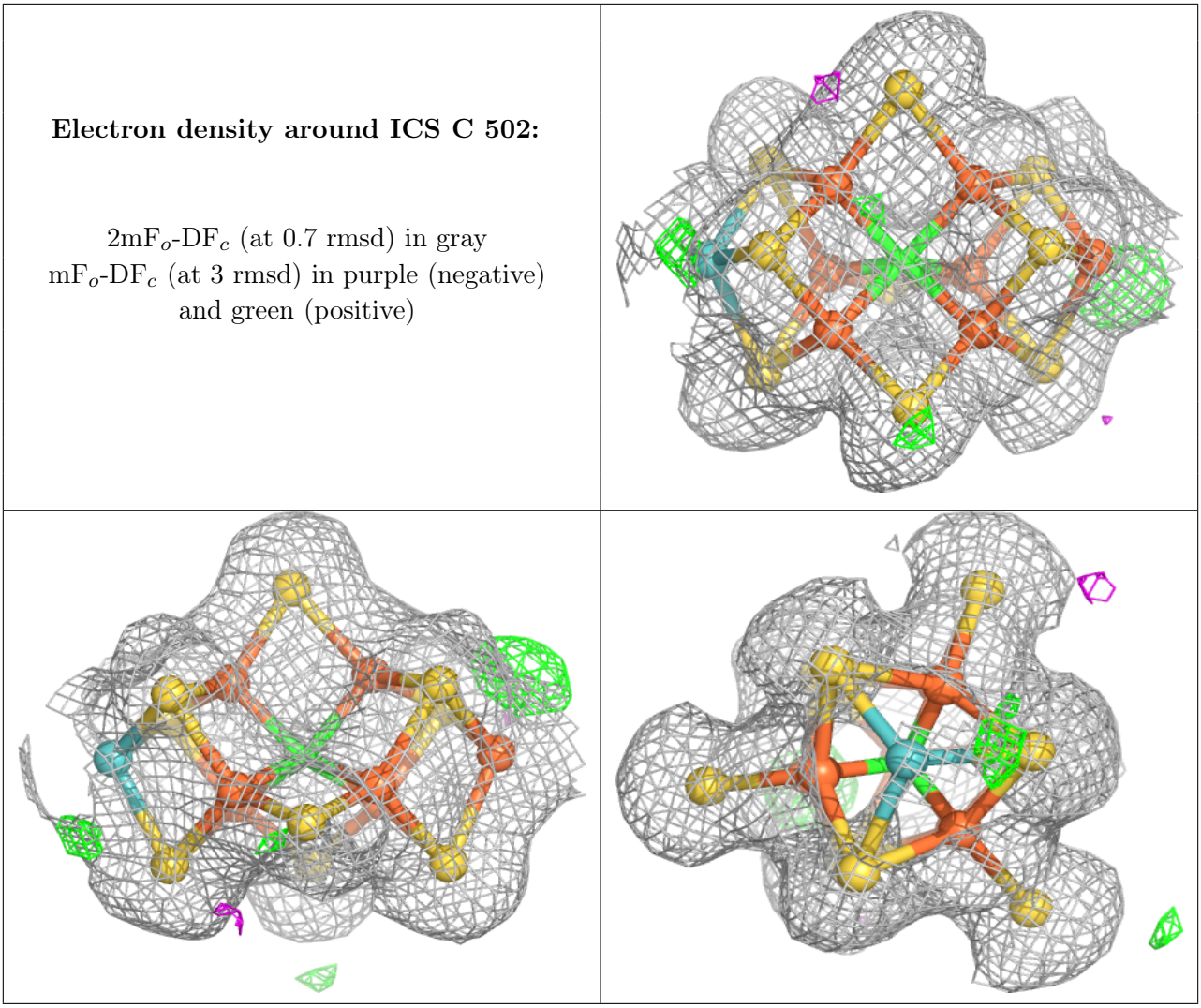
Electron density around CLF D 601 (B):

$2mF_o$-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 502:

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.