



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 04:08 pm BST

PDB ID : 9HB9 / pdb\_00009hb9  
Title : A. vinelandii nitrogenase MoFe protein Anc1a  
Authors : Detemple, F.; Kacar, B.; Einsle, O.  
Deposited on : 2024-11-05  
Resolution : 2.66 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

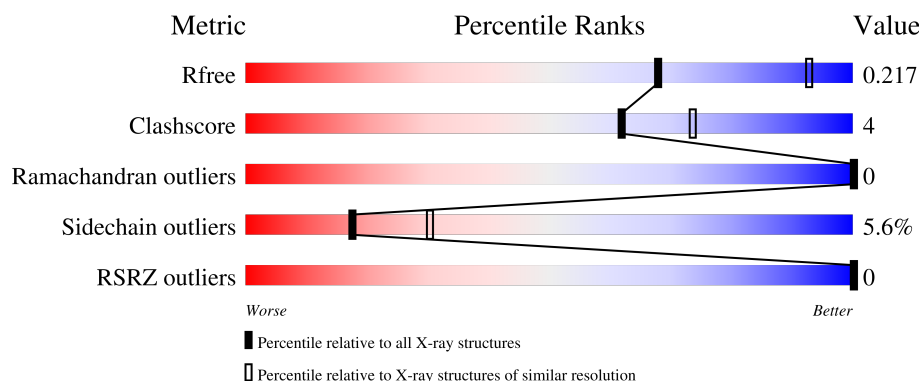
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.66 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))
$R_{free}$	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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  $\geq 3$ , 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	503	
1	C	503	
2	B	523	
2	D	523	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ICS	A	501	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16172 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.

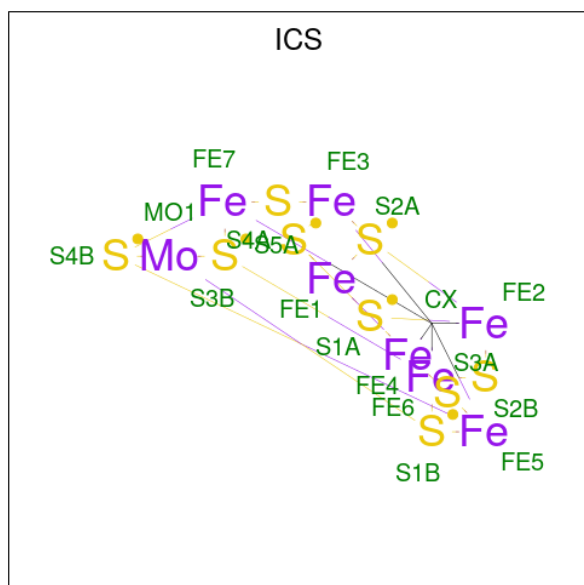
- Molecule 1 is a protein called MoFe nitrogenase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3805	2416	648	718	23			
1	C	477	Total	C	N	O	S	0	0	0
			3801	2414	648	716	23			

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

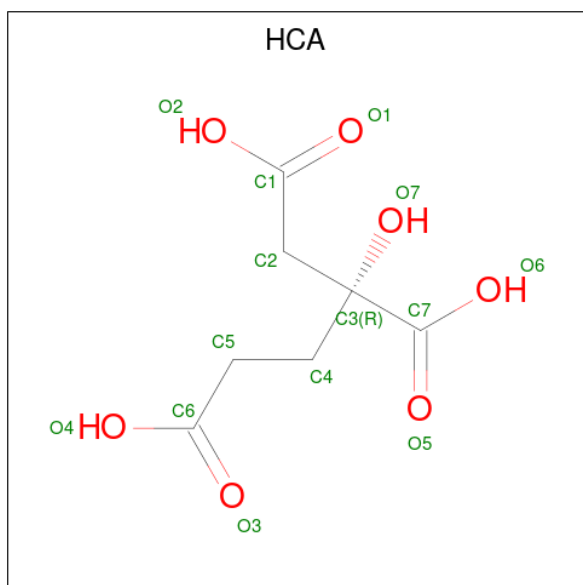
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4166	2660	703	775	28			

- Molecule 3 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula:  $\text{CFe}_7\text{MoS}_9$ ) (labeled as "Ligand of Interest" by depositor).



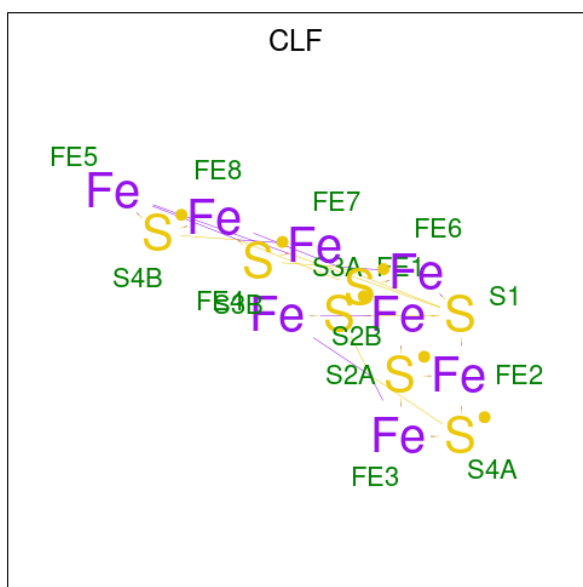
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	
3	C	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	

- Molecule 4 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
4	A	1	Total	C	O		
			14	7	7	0	0
4	C	1	Total	C	O		
			14	7	7	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
5	B	1	Total	Fe	S	0	0
			15	8	7		
5	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

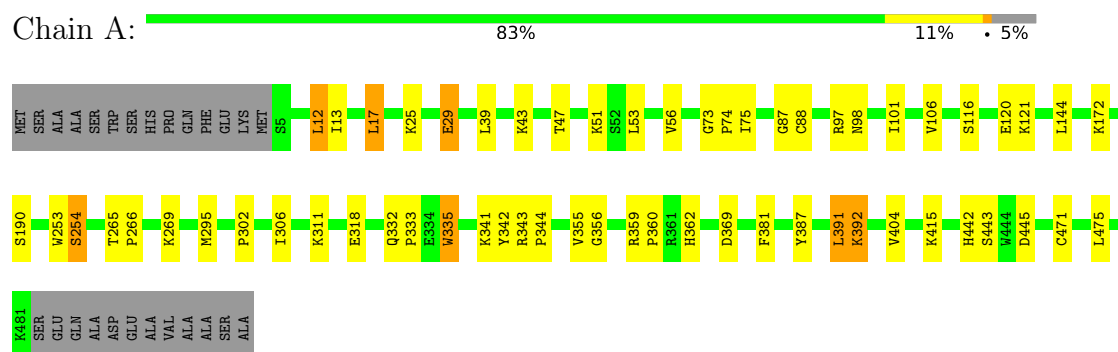
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	39	Total	O	0	0
			39	39		
7	C	24	Total	O	0	0
			24	24		
7	D	47	Total	O	0	0
			47	47		

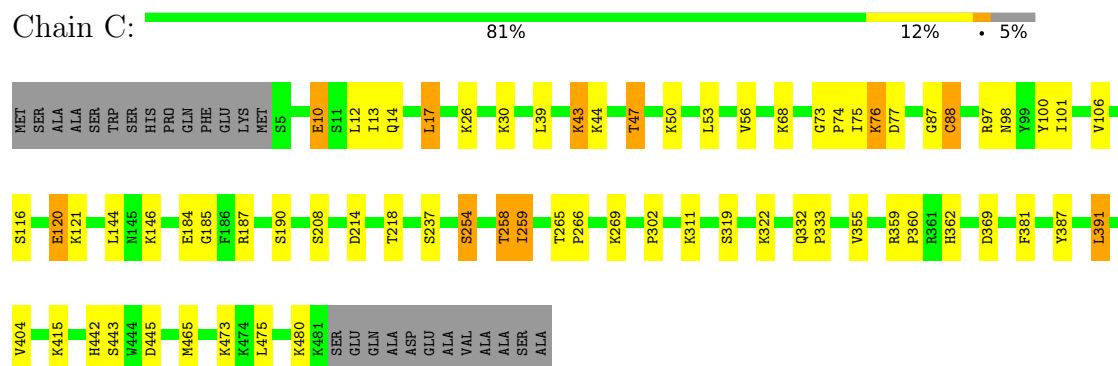
### 3 Residue-property plots [i](#)

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.

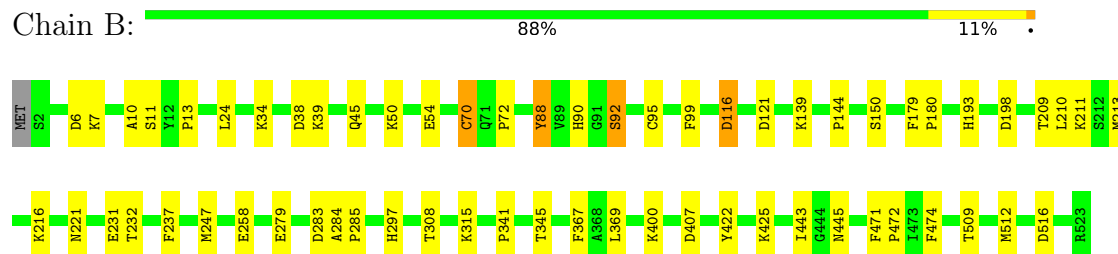
#### • Molecule 1: MoFe nitrogenase subunit D



#### • Molecule 1: MoFe nitrogenase subunit D



#### • Molecule 2: Nitrogenase molybdenum-iron protein beta chain

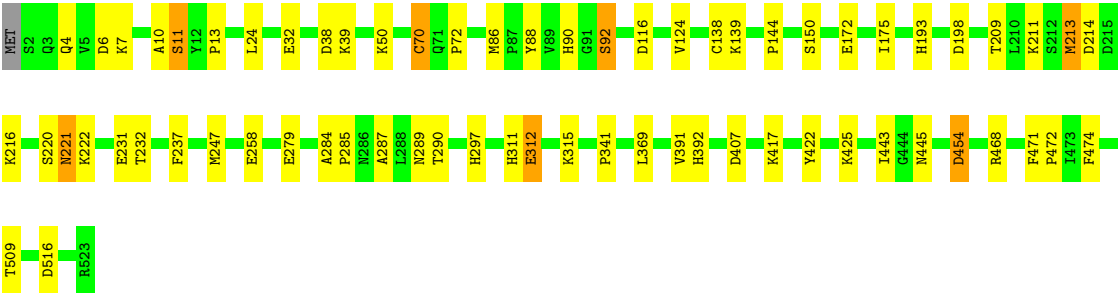


#### • Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D: 

87%

11%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.29Å 138.62Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.66 19.88 – 2.66	Depositor EDS
% Data completeness (in resolution range)	77.8 (19.88-2.66) 77.8 (19.88-2.66)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.169 , 0.220 0.172 , 0.217	Depositor DCC
$R_{free}$ test set	2377 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CLF, ICS, MG, 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	0.49	0/3894	0.98	0/5249
1	C	0.50	0/3890	1.00	2/5244 (0.0%)
2	B	0.50	0/4276	0.99	3/5782 (0.1%)
2	D	0.49	0/4272	0.97	3/5778 (0.1%)
All	All	0.50	0/16332	0.99	8/22053 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	CYS	CB-CA-C	-8.14	92.99	109.68
2	D	70	CYS	CB-CA-C	-7.18	94.97	109.68
1	C	76	LYS	CB-CA-C	-6.48	100.66	110.90
1	C	120	GLU	CB-CA-C	-6.07	101.35	110.88
2	B	116	ASP	CA-CB-CG	5.40	118.00	112.60
2	D	407	ASP	CA-CB-CG	5.39	117.99	112.60
2	B	407	ASP	CA-CB-CG	5.31	117.91	112.60
2	D	454	ASP	CA-CB-CG	5.07	117.67	112.60

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	3805	0	3727	31	0
1	C	3801	0	3723	33	0
2	B	4170	0	4077	30	0
2	D	4166	0	4066	39	0
3	A	18	0	0	4	0
3	C	18	0	0	3	0
4	A	14	0	6	0	0
4	C	14	0	6	1	0
5	B	15	0	0	1	0
5	D	15	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	24	0	0	1	0
7	B	39	0	0	1	0
7	C	24	0	0	0	0
7	D	47	0	0	1	0
All	All	16172	0	15605	125	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 (125) 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:90:HIS:HA	2:D:116:ASP:OD2	1.72	0.89
2:D:289:ASN:HD22	2:D:290:THR:H	1.35	0.73
1:C:146:LYS:HB2	1:C:259:ILE:HD11	1.72	0.69
2:D:221:ASN:HD21	2:D:287:ALA:HA	1.56	0.69
2:D:221:ASN:ND2	2:D:287:ALA:HA	2.11	0.66
2:B:70:CYS:HB3	2:B:72:PRO:HD2	1.80	0.64
1:C:184:GLU:HG3	1:C:187:ARG:NH1	2.14	0.62
2:D:209:THR:HB	2:D:213:MET:HE1	1.82	0.61
2:D:70:CYS:O	2:D:193:HIS:HA	2.02	0.60
2:B:70:CYS:O	2:B:193:HIS:HA	2.01	0.60
2:D:92:SER:HB2	5:D:601:CLF:S2A	2.43	0.58
1:A:442:HIS:HE1	3:A:501:ICS:S1B	2.28	0.57
1:A:306:ILE:HD11	1:A:335:TRP:CH2	2.40	0.56
2:D:221:ASN:C	2:D:221:ASN:HD22	2.13	0.56
1:C:74:PRO:HB2	1:C:254:SER:HB2	1.88	0.56
1:A:335:TRP:C	1:A:335:TRP:CD1	2.83	0.56
1:A:471:CYS:HB3	7:A:609:HOH:O	2.05	0.56
1:C:77:ASP:OD2	1:C:258:THR:OG1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:HIS:ND1	2:D:116:ASP:OD2	2.39	0.55
1:A:51:LYS:NZ	2:B:121:ASP:OD2	2.39	0.54
2:D:445:ASN:HB2	2:D:472:PRO:O	2.08	0.54
2:B:34:LYS:HE2	7:B:723:HOH:O	2.07	0.54
2:B:445:ASN:HB2	2:B:472:PRO:O	2.08	0.53
2:B:472:PRO:HB2	2:B:474:PHE:CE1	2.42	0.53
2:B:509:THR:O	2:B:516:ASP:HA	2.08	0.53
2:D:70:CYS:HB3	2:D:72:PRO:HD2	1.89	0.53
1:C:332:GLN:N	1:C:333:PRO:HD2	2.24	0.53
2:D:509:THR:O	2:D:516:ASP:HA	2.08	0.52
1:A:356:GLY:HA3	3:A:501:ICS:S1B	2.50	0.52
1:A:332:GLN:N	1:A:333:PRO:HD2	2.25	0.51
2:B:92:SER:HB2	5:B:601:CLF:S2A	2.49	0.51
1:C:302:PRO:HD2	1:C:369:ASP:OD2	2.11	0.51
1:C:190:SER:HB2	1:C:381:PHE:HB3	1.92	0.51
2:D:472:PRO:HB2	2:D:474:PHE:CE1	2.45	0.51
1:C:101:ILE:CD1	2:D:24:LEU:HD13	2.41	0.51
2:D:139:LYS:HD2	2:D:175:ILE:HD11	1.93	0.51
1:C:442:HIS:HE1	3:C:501:ICS:S1B	2.34	0.50
1:A:74:PRO:HB2	1:A:254:SER:HB2	1.94	0.50
2:B:345:THR:HG21	1:C:480:LYS:HE2	1.92	0.50
1:C:101:ILE:HD11	2:D:24:LEU:HD13	1.93	0.50
1:A:190:SER:HB2	1:A:381:PHE:HB3	1.91	0.50
2:B:10:ALA:O	2:B:11:SER:C	2.54	0.50
2:B:221:ASN:OD1	2:B:283:ASP:OD2	2.29	0.50
2:D:10:ALA:O	2:D:11:SER:C	2.54	0.50
2:D:88:TYR:OH	2:D:116:ASP:OD1	2.20	0.49
1:C:146:LYS:HB2	1:C:259:ILE:CD1	2.41	0.49
1:C:258:THR:HG21	2:D:32:GLU:HA	1.95	0.49
1:C:359:ARG:N	1:C:360:PRO:CD	2.75	0.49
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.47	0.49
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.46	0.49
1:A:359:ARG:N	1:A:360:PRO:CD	2.75	0.49
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.42	0.48
2:D:290:THR:OG1	2:D:311:HIS:CD2	2.66	0.48
1:A:302:PRO:HD2	1:A:369:ASP:OD2	2.13	0.48
1:C:30:LYS:HB3	1:C:47:THR:OG1	2.14	0.48
2:B:213:MET:HE3	2:B:308:THR:HG22	1.95	0.47
2:D:86:MET:HG2	2:D:138:CYS:SG	2.55	0.47
1:A:101:ILE:CD1	2:B:24:LEU:HD13	2.45	0.47
2:B:209:THR:HB	2:B:213:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:MET:HA	2:D:213:MET:HE2	1.96	0.47
1:C:10:GLU:O	1:C:14:GLN:HG2	2.15	0.47
1:A:97:ARG:NH1	1:A:443:SER:O	2.48	0.46
1:A:392:LYS:HD3	1:A:392:LYS:H	1.80	0.46
2:D:369:LEU:HA	2:D:443:ILE:O	2.15	0.46
1:A:253:TRP:HA	1:A:254:SER:HA	1.76	0.46
1:A:17:LEU:HD21	1:A:29:GLU:HB2	1.98	0.46
1:C:73:GLY:N	1:C:74:PRO:CD	2.79	0.45
1:C:442:HIS:HB3	4:C:502:HCA:O5	2.16	0.45
2:B:367:PHE:CD2	2:B:443:ILE:HD11	2.50	0.45
2:B:422:TYR:HB3	2:B:425:LYS:HG3	1.99	0.45
1:A:295:MET:HE1	1:A:311:LYS:HG3	1.99	0.45
1:C:265:THR:N	1:C:266:PRO:CD	2.80	0.45
2:D:290:THR:OG1	2:D:311:HIS:HD2	2.00	0.45
1:A:87:GLY:HA3	2:B:70:CYS:SG	2.56	0.45
1:C:76:LYS:HD3	1:C:100:TYR:HB2	1.99	0.45
2:D:422:TYR:HB3	2:D:425:LYS:HG3	1.98	0.45
1:A:381:PHE:CZ	3:A:501:ICS:S2B	3.10	0.44
2:D:198:ASP:HB2	2:D:297:HIS:O	2.17	0.44
1:A:73:GLY:N	1:A:74:PRO:CD	2.80	0.44
1:C:87:GLY:O	1:C:88:CYS:C	2.59	0.44
1:C:259:ILE:HD12	1:C:259:ILE:H	1.83	0.44
2:D:284:ALA:N	2:D:285:PRO:CD	2.80	0.44
2:D:312:GLU:O	2:D:312:GLU:CD	2.60	0.44
2:B:139:LYS:HA	2:B:144:PRO:HD2	2.00	0.44
2:B:284:ALA:N	2:B:285:PRO:CD	2.80	0.44
1:C:97:ARG:NH1	1:C:443:SER:O	2.50	0.44
2:B:88:TYR:OH	2:B:116:ASP:HB3	2.18	0.44
1:C:381:PHE:CZ	3:C:501:ICS:S2B	3.11	0.44
2:D:312:GLU:O	2:D:312:GLU:CG	2.66	0.44
1:C:43:LYS:HE3	1:C:47:THR:HG23	2.00	0.43
1:C:185:GLY:HA3	5:D:601:CLF:S2A	2.58	0.43
1:A:265:THR:N	1:A:266:PRO:CD	2.81	0.43
2:B:369:LEU:HA	2:B:443:ILE:O	2.18	0.43
2:D:289:ASN:ND2	2:D:290:THR:H	2.10	0.43
1:C:387:TYR:O	1:C:391:LEU:HD13	2.19	0.43
2:B:198:ASP:HB2	2:B:297:HIS:O	2.18	0.42
1:A:12:LEU:HD21	1:A:415:LYS:HG3	2.02	0.42
1:A:387:TYR:O	1:A:391:LEU:HD13	2.20	0.42
1:A:442:HIS:HA	3:A:501:ICS:S4B	2.59	0.42
1:A:106:VAL:O	1:A:144:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HD3	1:A:342:TYR:CZ	2.55	0.42
1:C:53:LEU:O	1:C:56:VAL:HG22	2.20	0.42
1:C:442:HIS:HA	3:C:501:ICS:S4B	2.60	0.42
1:C:106:VAL:O	1:C:144:LEU:HB2	2.19	0.41
1:A:87:GLY:O	1:A:88:CYS:C	2.61	0.41
2:B:179:PHE:HA	2:B:180:PRO:HD3	1.95	0.41
2:B:231:GLU:HB3	2:B:237:PHE:CZ	2.55	0.41
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.55	0.41
2:D:247:MET:HG2	2:D:341:PRO:HD3	2.01	0.41
1:A:120:GLU:O	1:A:121:LYS:C	2.64	0.41
1:A:13:ILE:O	1:A:17:LEU:HB2	2.21	0.41
2:B:247:MET:HG2	2:B:341:PRO:HD3	2.01	0.41
1:A:53:LEU:O	1:A:56:VAL:HG22	2.21	0.41
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.56	0.41
2:B:512:MET:HE1	2:D:454:ASP:HA	2.03	0.41
2:D:139:LYS:HA	2:D:144:PRO:HD2	2.02	0.41
2:D:211:LYS:HB2	7:D:742:HOH:O	2.21	0.41
2:B:209:THR:O	2:B:210:LEU:C	2.64	0.41
1:C:13:ILE:O	1:C:17:LEU:HB2	2.20	0.41
1:C:120:GLU:O	1:C:121:LYS:C	2.63	0.41
2:D:468:ARG:HG3	2:D:468:ARG:HH11	1.86	0.41
2:D:289:ASN:HD22	2:D:290:THR:N	2.10	0.40
1:A:343:ARG:N	1:A:344:PRO:CD	2.85	0.40
1:C:184:GLU:HG3	1:C:187:ARG:HH11	1.81	0.40
2:D:391:VAL:HG12	2:D:392:HIS:CE1	2.56	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	475/503 (94%)	450 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	475/503 (94%)	448 (94%)	27 (6%)	0	100	100
2	B	520/523 (99%)	501 (96%)	19 (4%)	0	100	100
2	D	520/523 (99%)	502 (96%)	18 (4%)	0	100	100
All	All	1990/2052 (97%)	1901 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	410/429 (96%)	388 (95%)	22 (5%)	18	32
1	C	409/429 (95%)	375 (92%)	34 (8%)	9	15
2	B	453/455 (100%)	436 (96%)	17 (4%)	28	47
2	D	452/455 (99%)	429 (95%)	23 (5%)	20	34
All	All	1724/1768 (98%)	1628 (94%)	96 (6%)	17	30

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LEU
1	A	25	LYS
1	A	29	GLU
1	A	39	LEU
1	A	43	LYS
1	A	47	THR
1	A	75	ILE
1	A	98	ASN
1	A	116	SER
1	A	172	LYS
1	A	254	SER
1	A	269	LYS

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Mol	Chain	Res	Type
1	A	318	GLU
1	A	335	TRP
1	A	355	VAL
1	A	362	HIS
1	A	391	LEU
1	A	392	LYS
1	A	404	VAL
1	A	445	ASP
1	A	475	LEU
2	B	6	ASP
2	B	7	LYS
2	B	13	PRO
2	B	38	ASP
2	B	39	LYS
2	B	45	GLN
2	B	50	LYS
2	B	54	GLU
2	B	88	TYR
2	B	92	SER
2	B	150	SER
2	B	211	LYS
2	B	216	LYS
2	B	258	GLU
2	B	279	GLU
2	B	315	LYS
2	B	400	LYS
1	C	10	GLU
1	C	12	LEU
1	C	17	LEU
1	C	26	LYS
1	C	39	LEU
1	C	43	LYS
1	C	44	LYS
1	C	47	THR
1	C	50	LYS
1	C	68	LYS
1	C	75	ILE
1	C	88	CYS
1	C	98	ASN
1	C	116	SER
1	C	208	SER
1	C	214	ASP

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Mol	Chain	Res	Type
1	C	218	THR
1	C	237	SER
1	C	254	SER
1	C	258	THR
1	C	259	ILE
1	C	269	LYS
1	C	311	LYS
1	C	319	SER
1	C	322	LYS
1	C	355	VAL
1	C	362	HIS
1	C	391	LEU
1	C	404	VAL
1	C	415	LYS
1	C	445	ASP
1	C	465	MET
1	C	473	LYS
1	C	475	LEU
2	D	4	GLN
2	D	6	ASP
2	D	7	LYS
2	D	11	SER
2	D	13	PRO
2	D	38	ASP
2	D	39	LYS
2	D	50	LYS
2	D	92	SER
2	D	124	VAL
2	D	150	SER
2	D	172	GLU
2	D	213	MET
2	D	214	ASP
2	D	216	LYS
2	D	220	SER
2	D	221	ASN
2	D	222	LYS
2	D	258	GLU
2	D	279	GLU
2	D	312	GLU
2	D	315	LYS
2	D	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	98	ASN
1	A	432	GLN
2	B	37	GLN
2	B	317	ASN
2	B	363	HIS
2	B	418	ASN
2	B	518	ASN
1	C	98	ASN
1	C	196	HIS
1	C	432	GLN
1	C	476	GLN
2	D	45	GLN
2	D	130	ASN
2	D	221	ASN
2	D	225	ASN
2	D	289	ASN
2	D	311	HIS
2	D	317	ASN
2	D	338	GLN
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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	ICS	A	501	1	18,30,30	2.46	9 (50%)	-		
5	CLF	B	601	2,1	0,24,24	-	-	-		
4	HCA	C	502	-	13,13,13	1.21	0	14,18,18	2.60	3 (21%)
5	CLF	D	601	2,1	0,24,24	-	-	-		
3	ICS	C	501	1	18,30,30	2.63	9 (50%)	-		
4	HCA	A	502	-	13,13,13	1.23	1 (7%)	14,18,18	2.51	4 (28%)

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
4	HCA	A	502	-	-	7/17/17/17	-
5	CLF	D	601	2,1	-	-	0/12/10/10
5	CLF	B	601	2,1	-	-	0/12/10/10
4	HCA	C	502	-	-	6/17/17/17	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	ICS	S3B-FE6	-5.19	2.19	2.32
3	C	501	ICS	S1B-FE6	-5.03	2.20	2.32
3	A	501	ICS	S3B-FE6	-4.28	2.21	2.32
3	C	501	ICS	S4B-FE7	-3.99	2.22	2.32
3	A	501	ICS	S1B-FE6	-3.73	2.23	2.32
3	A	501	ICS	S4A-FE3	-3.68	2.23	2.32
3	A	501	ICS	S4B-FE7	-3.64	2.23	2.32
3	C	501	ICS	S2B-FE6	-3.57	2.16	2.24
3	C	501	ICS	S2A-FE2	-3.37	2.24	2.32
3	A	501	ICS	S2B-FE6	-3.18	2.17	2.24
3	A	501	ICS	S2A-FE2	-2.93	2.25	2.32
3	C	501	ICS	S4A-FE3	-2.69	2.25	2.32
3	A	501	ICS	S3B-FE7	-2.59	2.26	2.32
3	A	501	ICS	S4B-FE5	-2.51	2.26	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	ICS	S1A-FE2	-2.41	2.26	2.32
3	C	501	ICS	S5A-FE7	-2.28	2.19	2.24
4	A	502	HCA	O5-C7	2.24	1.29	1.22
3	A	501	ICS	S1B-FE5	-2.19	2.26	2.32
3	C	501	ICS	S2A-FE3	-2.02	2.27	2.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	HCA	O6-C7-C3	5.33	122.31	113.05
4	C	502	HCA	O7-C3-C7	-5.26	101.48	108.86
4	C	502	HCA	O5-C7-C3	-4.97	115.22	122.25
4	A	502	HCA	O7-C3-C7	-4.67	102.31	108.86
4	A	502	HCA	O6-C7-C3	4.47	120.82	113.05
4	A	502	HCA	O5-C7-C3	-4.17	116.34	122.25
4	A	502	HCA	O2-C1-C2	2.71	123.05	114.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	HCA	C3-C4-C5-C6
4	C	502	HCA	C1-C2-C3-C7
4	C	502	HCA	O7-C3-C4-C5
4	C	502	HCA	C2-C3-C4-C5
4	A	502	HCA	O2-C1-C2-C3
4	C	502	HCA	C1-C2-C3-C4
4	C	502	HCA	C4-C5-C6-O3
4	C	502	HCA	C4-C5-C6-O4
4	A	502	HCA	C4-C5-C6-O4
4	A	502	HCA	O1-C1-C2-C3
4	A	502	HCA	C4-C5-C6-O3
4	A	502	HCA	O7-C3-C4-C5
4	A	502	HCA	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 11 short contacts:

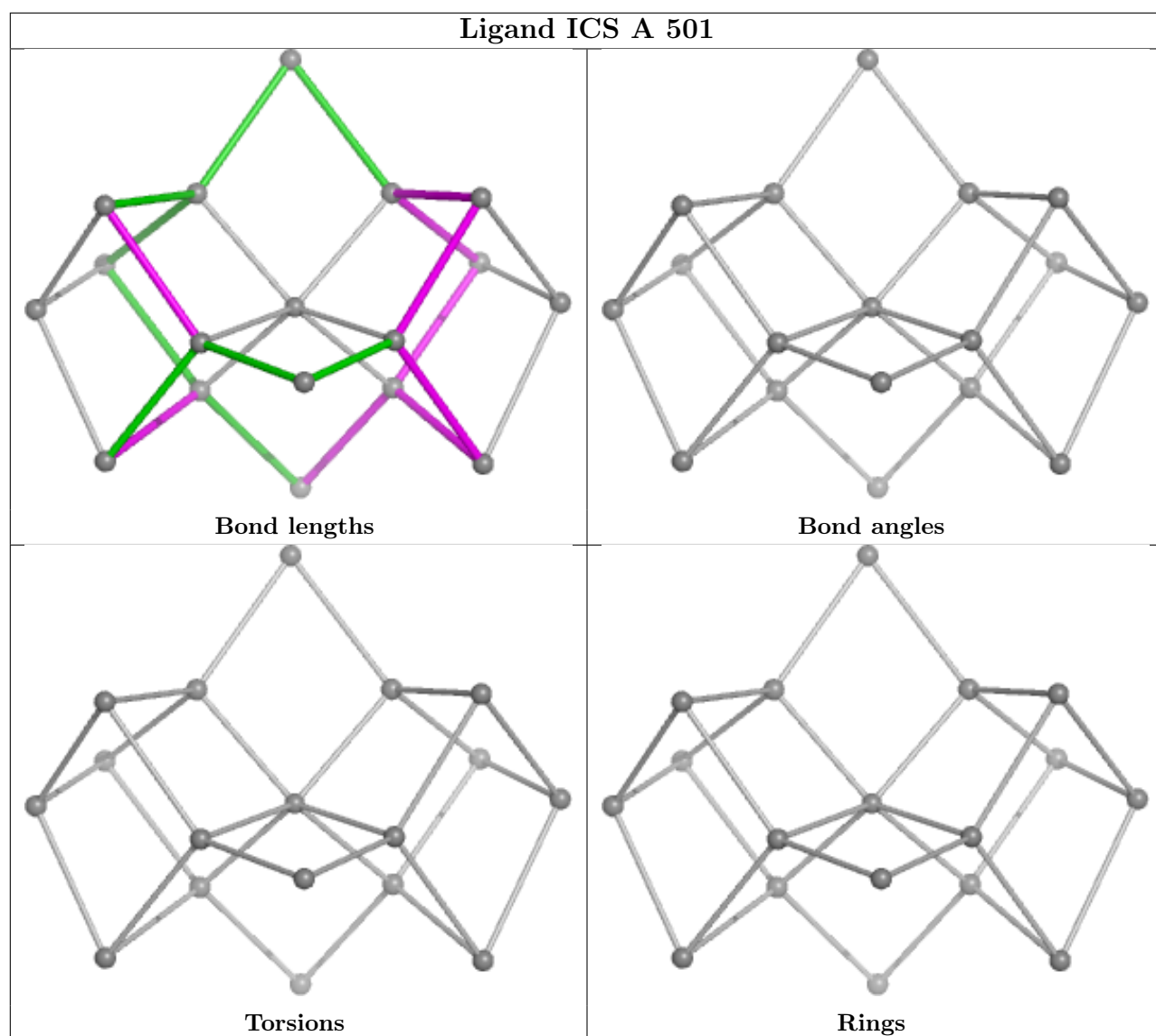
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ICS	4	0
5	B	601	CLF	1	0

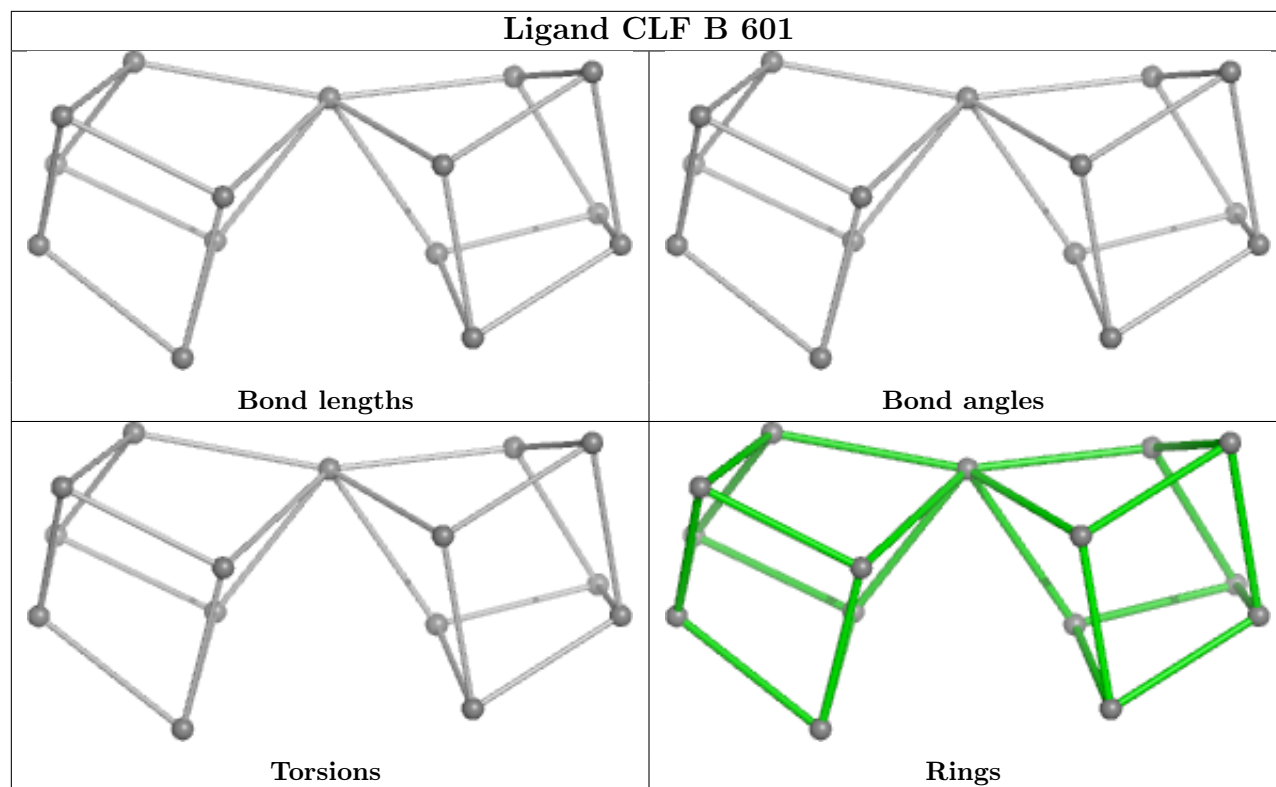
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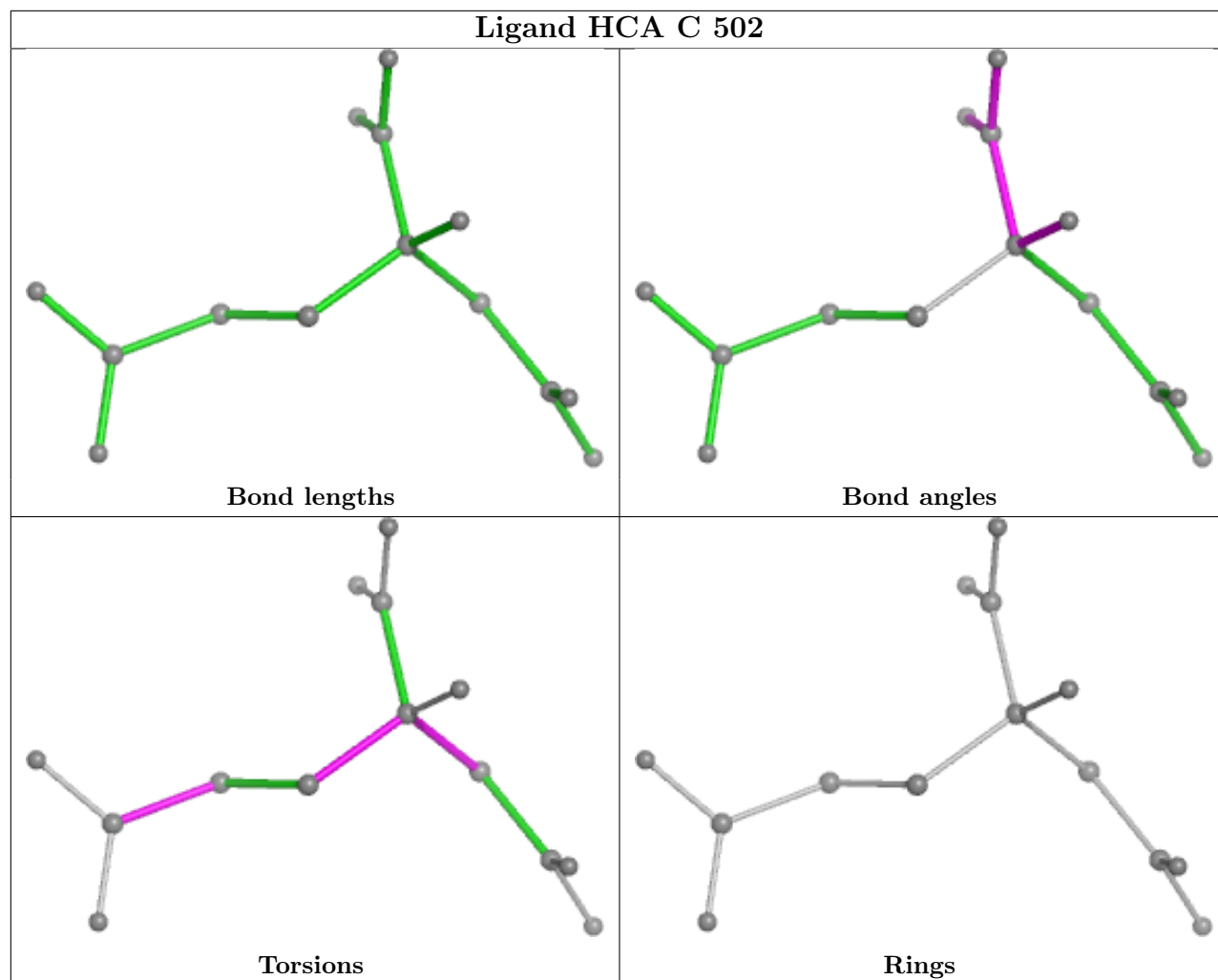
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	HCA	1	0
5	D	601	CLF	2	0
3	C	501	ICS	3	0

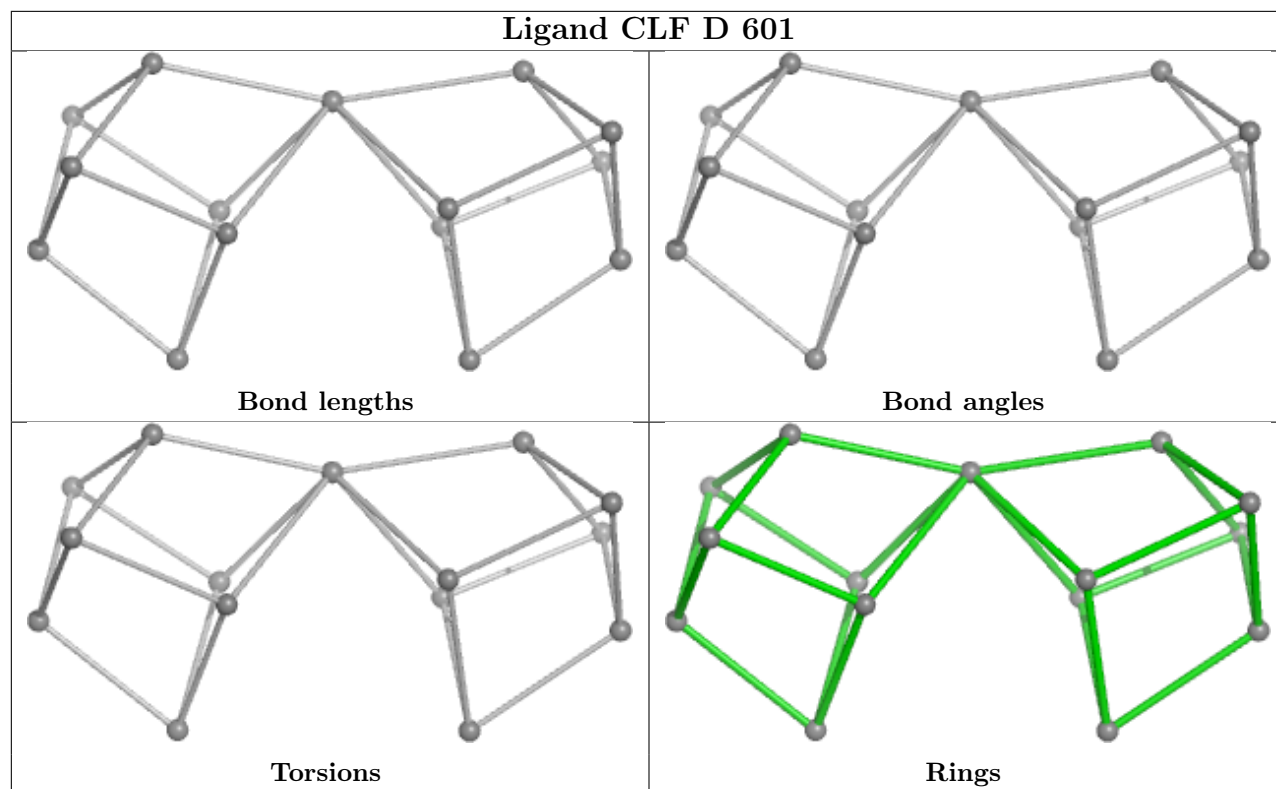
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



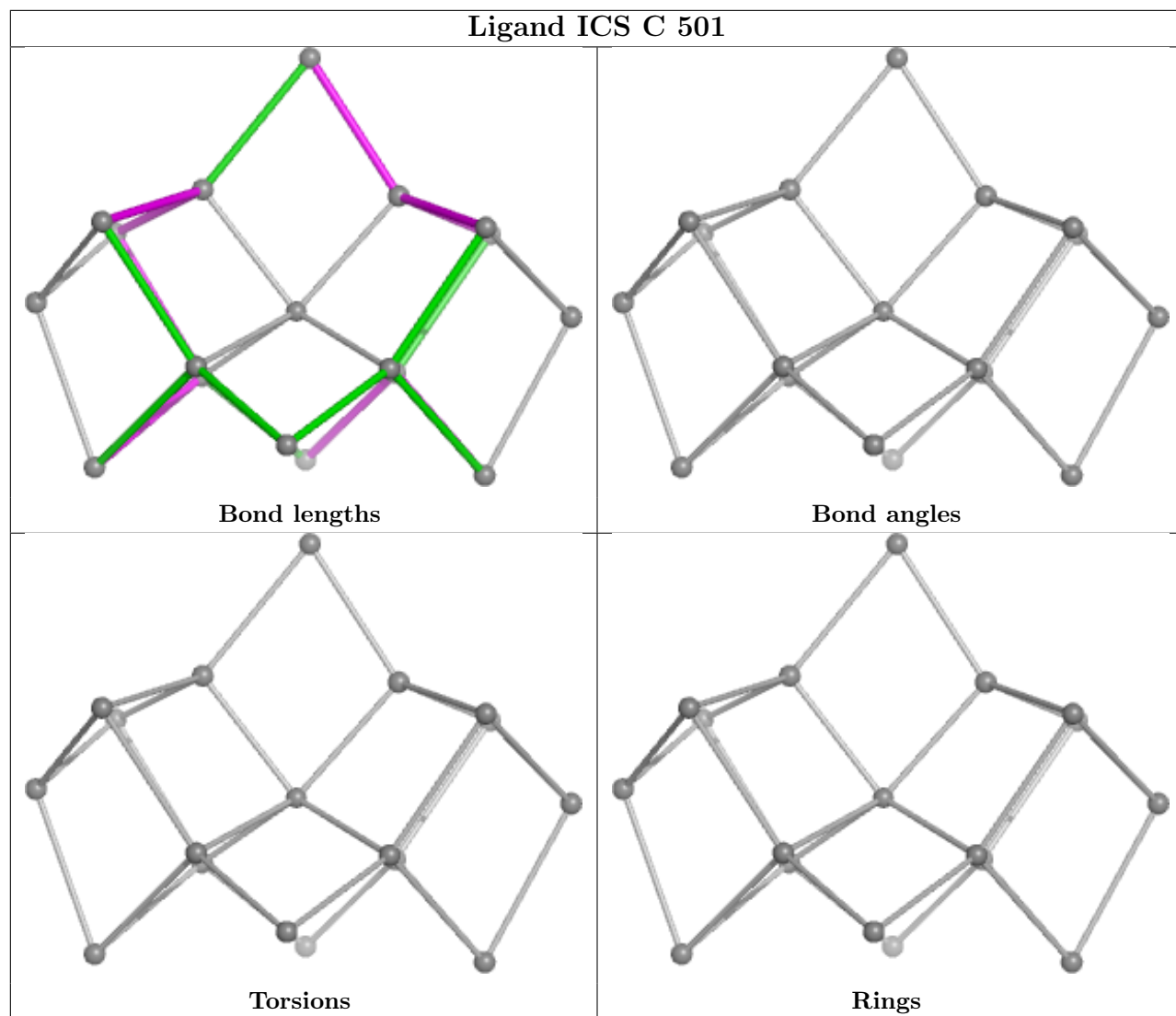


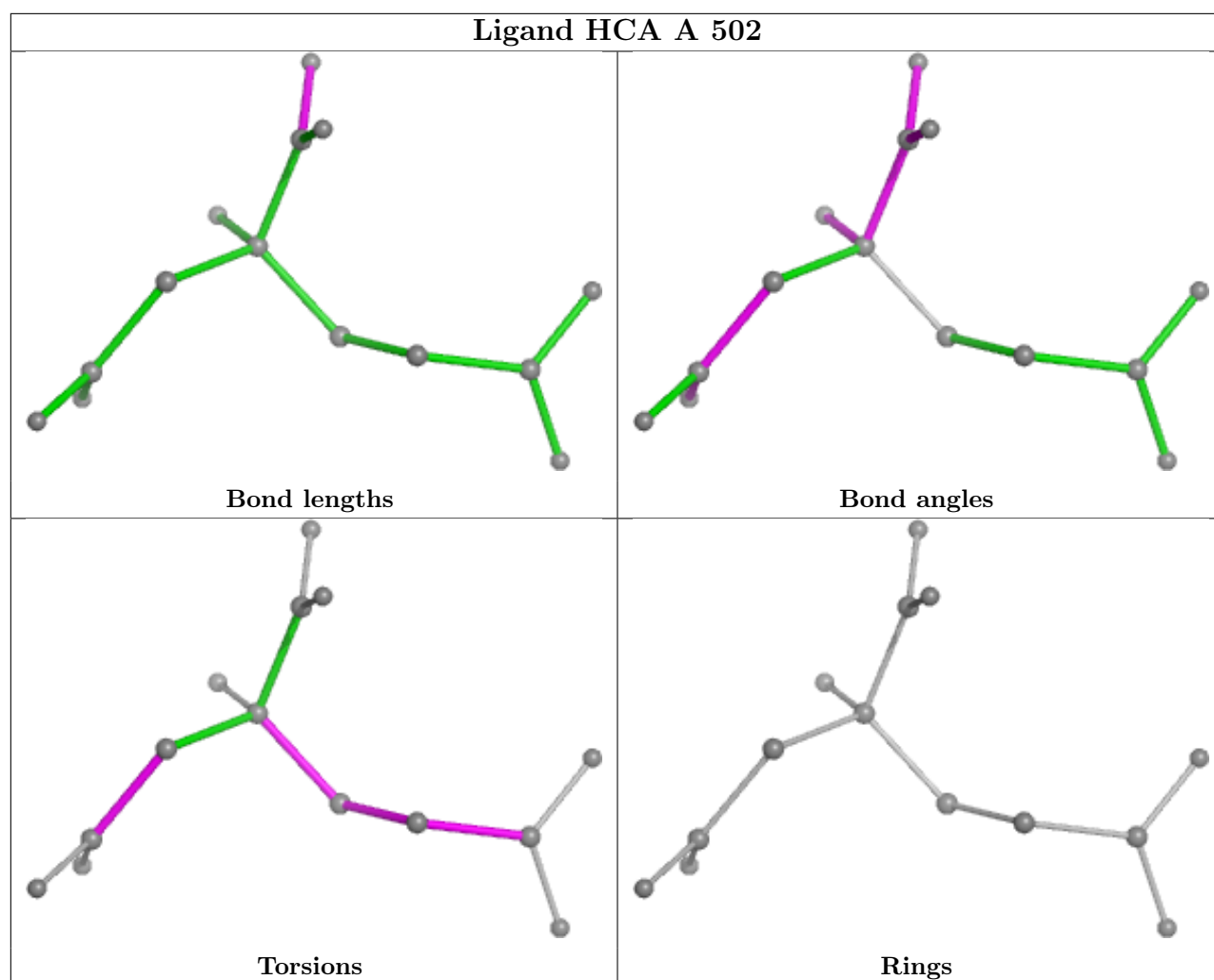






## Ligand ICS C 501





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	477/503 (94%)	-0.70	0 100 100	22, 43, 74, 108	5 (1%)
1	C	477/503 (94%)	-0.66	0 100 100	27, 45, 75, 100	6 (1%)
2	B	522/523 (99%)	-0.86	0 100 100	19, 37, 54, 83	4 (0%)
2	D	522/523 (99%)	-0.85	0 100 100	22, 37, 56, 79	4 (0%)
All	All	1998/2052 (97%)	-0.77	0 100 100	19, 40, 67, 108	19 (0%)

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	HCA	C	502	14/14	0.95	0.07	42,53,59,61	0
4	HCA	A	502	14/14	0.96	0.07	44,51,54,56	0
3	ICS	C	501	18/18	0.99	0.03	39,45,52,54	0
5	CLF	B	601	15/15	0.99	0.03	25,29,33,36	0

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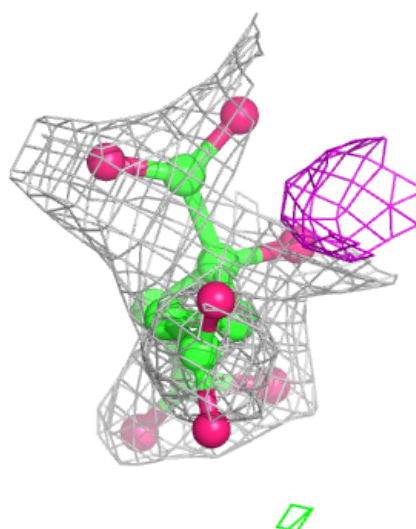
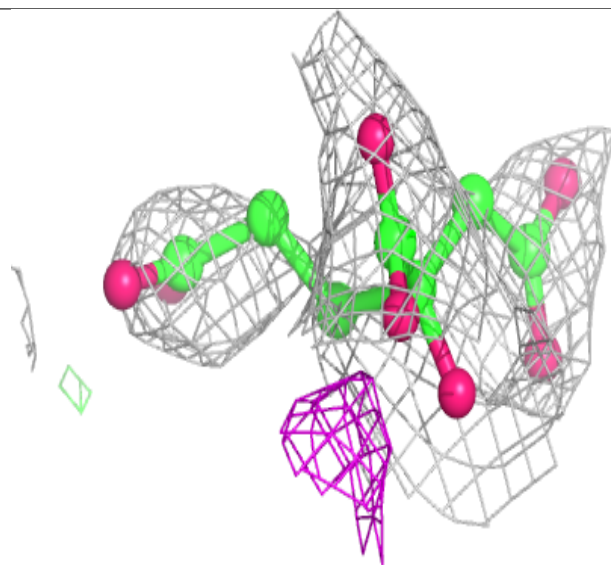
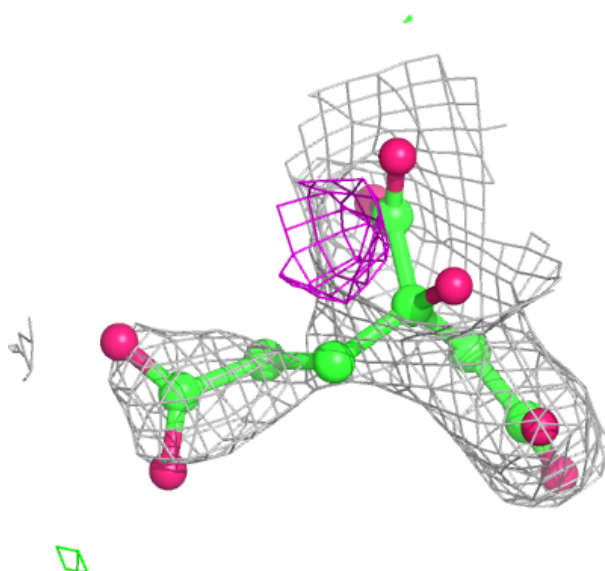
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CLF	D	601	15/15	0.99	0.03	23,27,30,30	0
6	MG	B	602	1/1	0.99	0.06	21,21,21,21	0
3	ICS	A	501	18/18	1.00	0.02	43,47,50,50	0
6	MG	D	602	1/1	1.00	0.03	19,19,19,19	0

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.

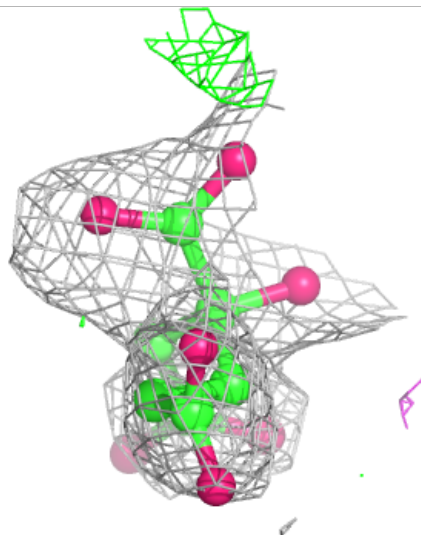
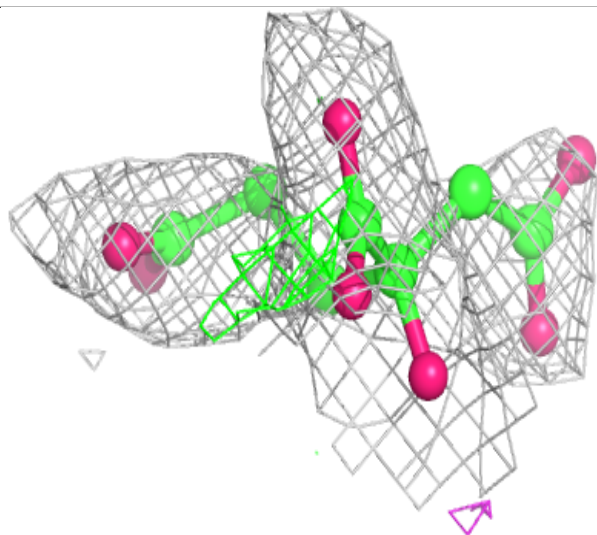
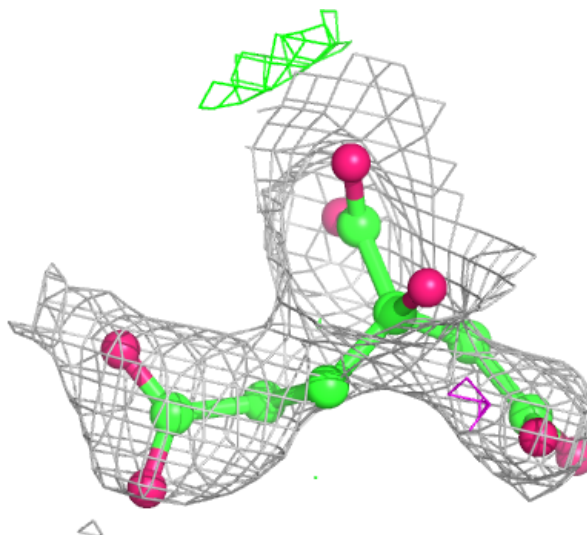
**Electron density around HCA C 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



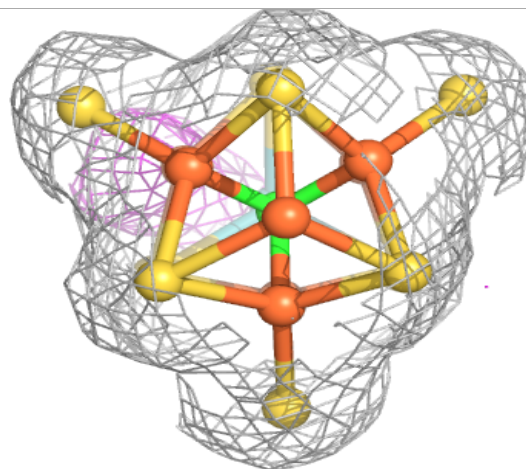
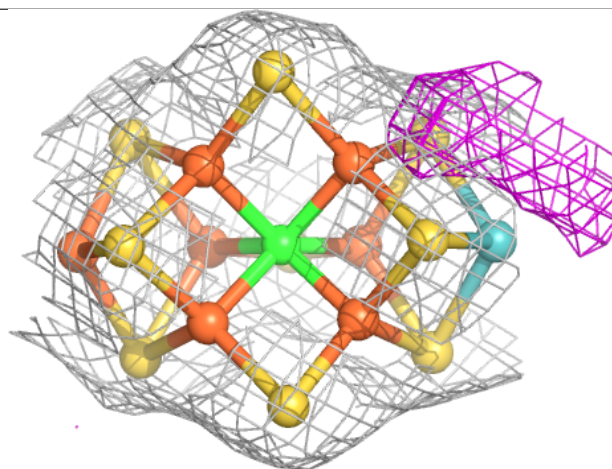
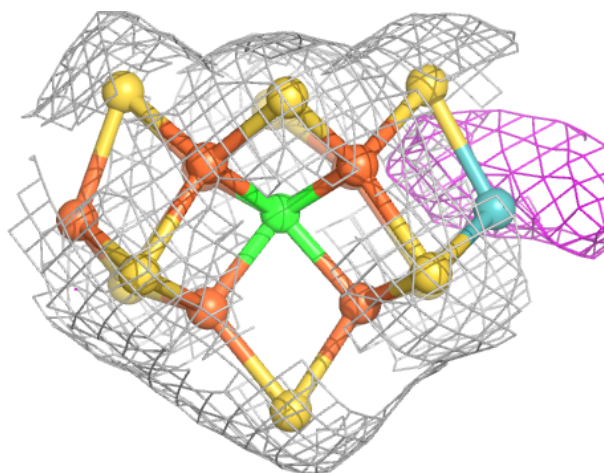
**Electron density around HCA A 502:**

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



**Electron density around ICS C 501:**

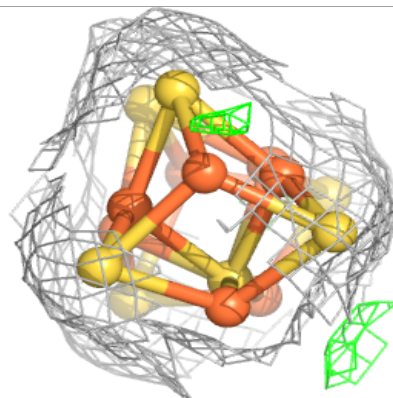
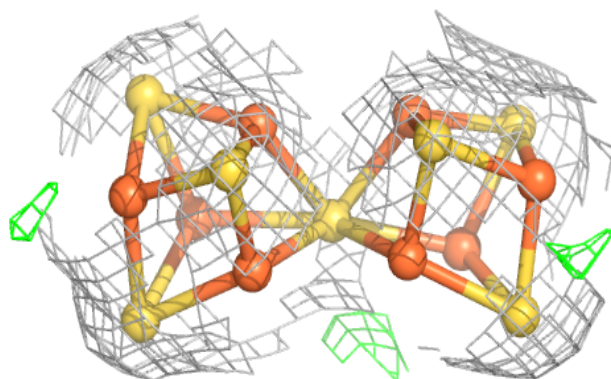
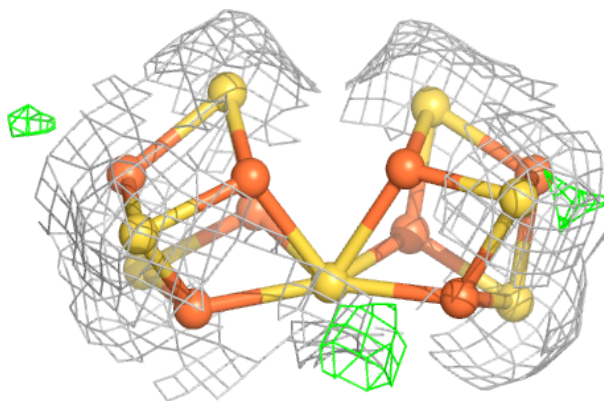
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



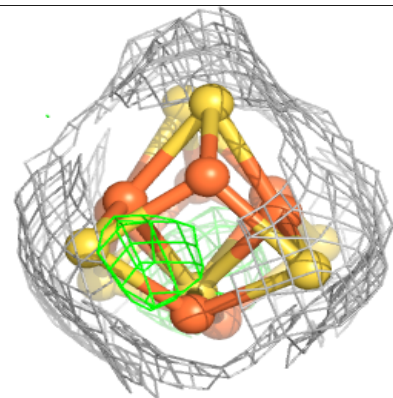
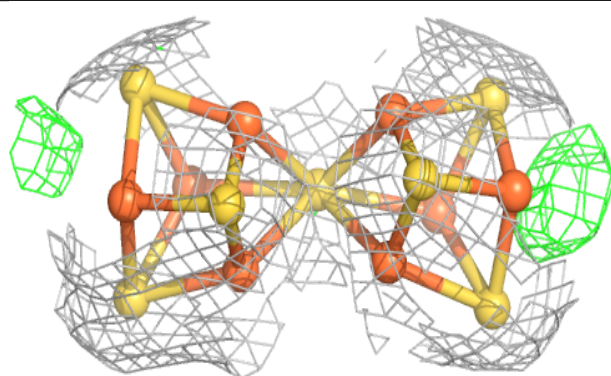
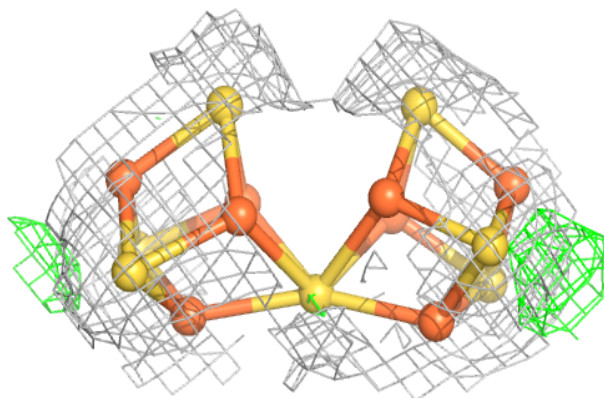


**Electron density around CLF B 601:**

$2mF_o-DF_c$  (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:**

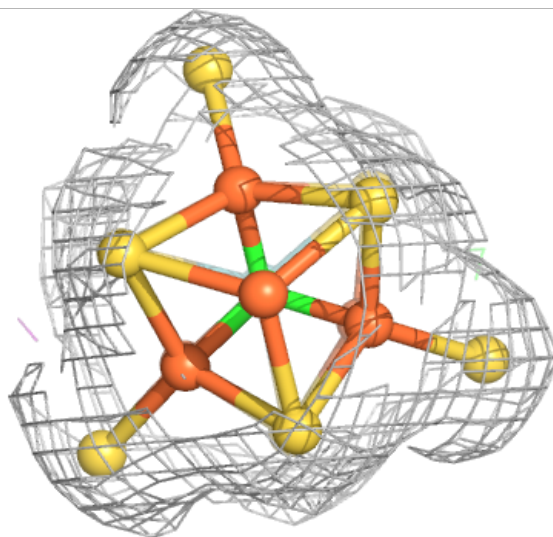
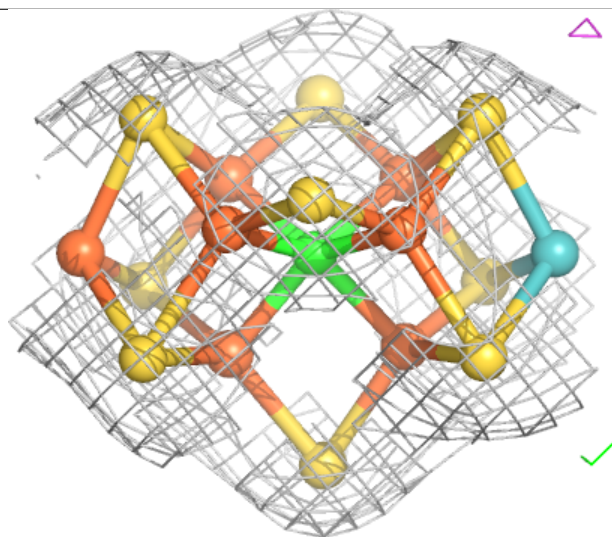
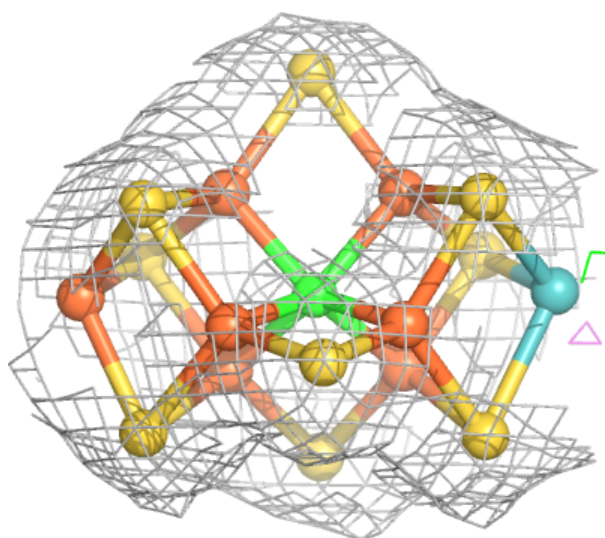
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ICS A 501:**

$2mF_o-DF_c$  (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.