



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:12 am BST

PDB ID : 6O7S  
Title : Nitrogenase MoFeP mutant S188A from *Azotobacter vinelandii* in the indigo carmine oxidized state  
Authors : Rutledge, H.L.; Tezcan, F.A.  
Deposited on : 2019-03-08  
Resolution : 2.27 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.

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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 : 2.11  
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) : 2.11

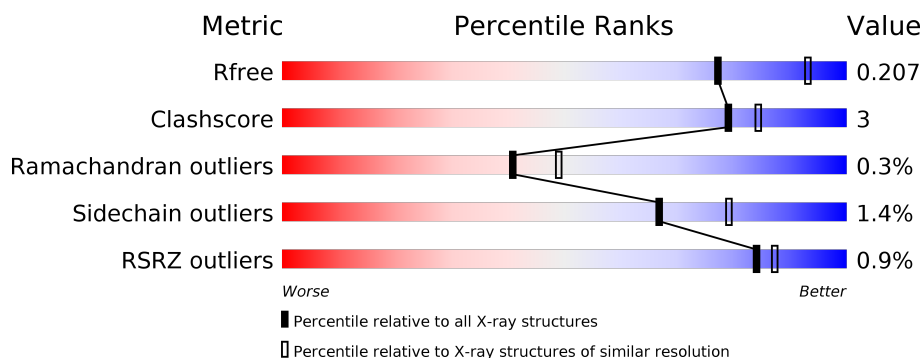
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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  $\geq 3$ , 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	492	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 88%, green 88%, grey 88%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>88%</span> <span>8%</span> </div> </div>
1	C	492	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 88%, green 88%, grey 88%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>88%</span> <span>9%</span> </div> </div>
2	B	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 94%, green 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>94%</span> <span>6%</span> </div> </div>
2	D	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 92%, green 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>92%</span> <span>7%</span> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32420 atoms, of which 15273 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	476	Total	C	H	N	O	S	0	0	0
			7314	2367	3591	637	695	24			
1	C	476	Total	C	H	N	O	S	0	0	0
			7275	2364	3566	629	692	24			

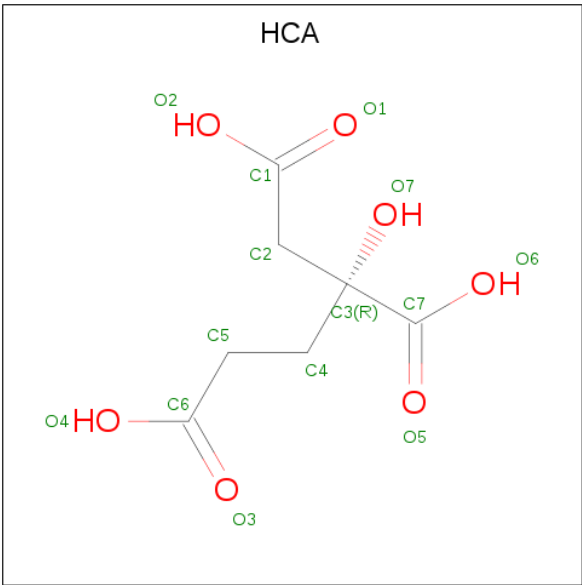
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	522	Total	C	H	N	O	S	0	0	0
			8169	2649	4026	699	767	28			
2	D	522	Total	C	H	N	O	S	0	0	0
			8245	2663	4078	704	772	28			

There are 2 discrepancies between the modelled and reference sequences:

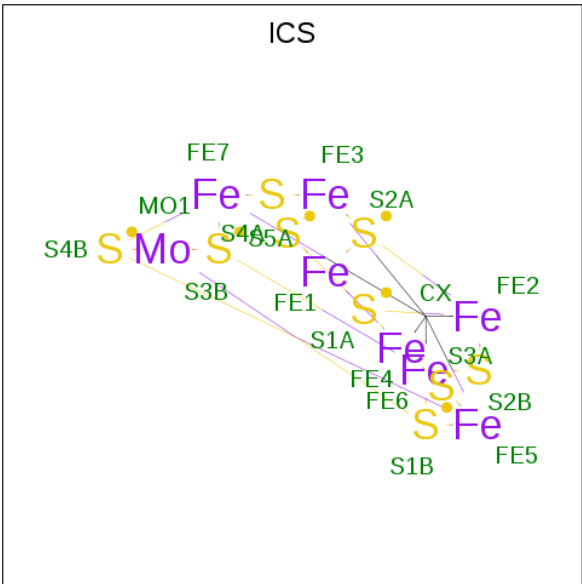
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	ALA	SER	engineered mutation	UNP P07329
D	188	ALA	SER	engineered mutation	UNP P07329

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	7	6	7		
3	C	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe<sub>7</sub>MoS<sub>9</sub>).



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

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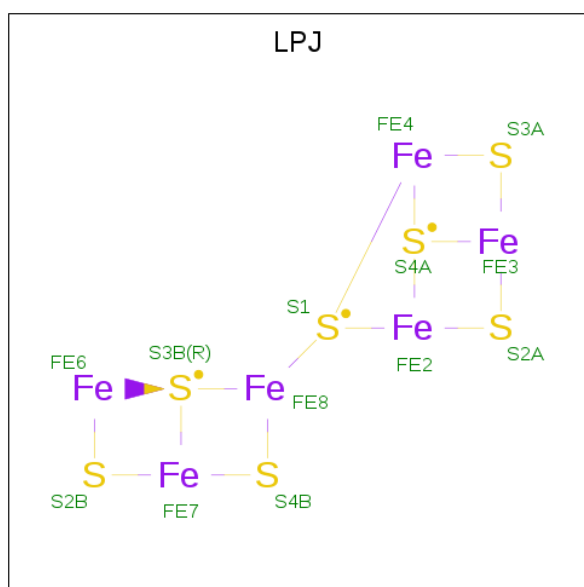
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is FE(6)-S(7) CLUSTER (three-letter code: LPJ) (formula: Fe<sub>6</sub>S<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			13	6	7		
6	D	1	Total	Fe	S	0	0
			13	6	7		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Fe	0	0
			1	1		
7	D	1	Total	Fe	0	0
			1	1		

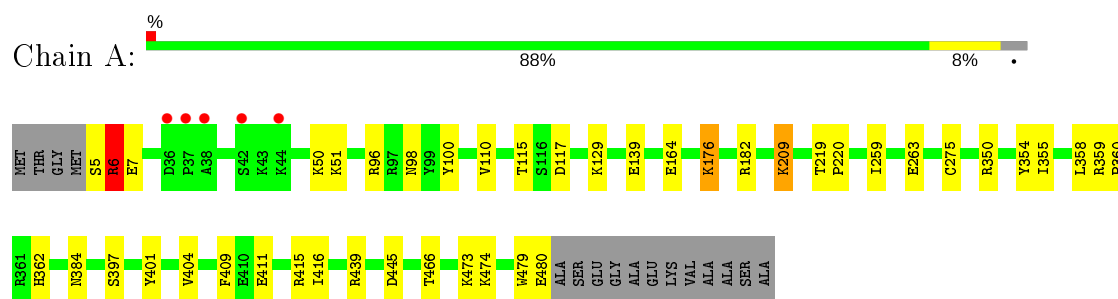
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	247	Total 247	O 247	0	0
8	B	417	Total 417	O 417	0	0
8	C	247	Total 247	O 247	0	0
8	D	400	Total 400	O 400	0	0

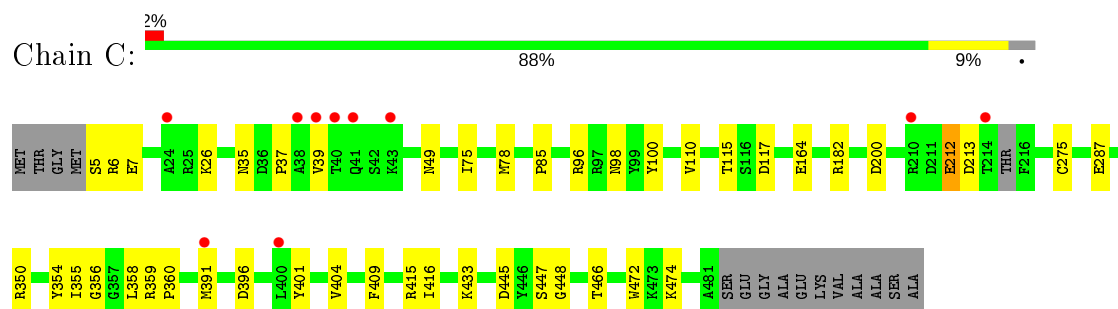
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

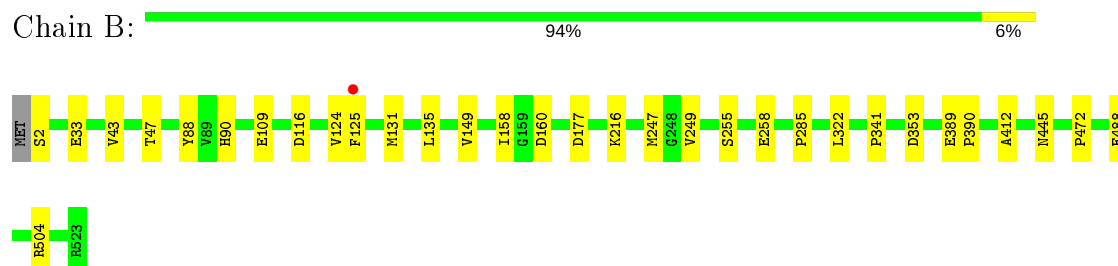
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



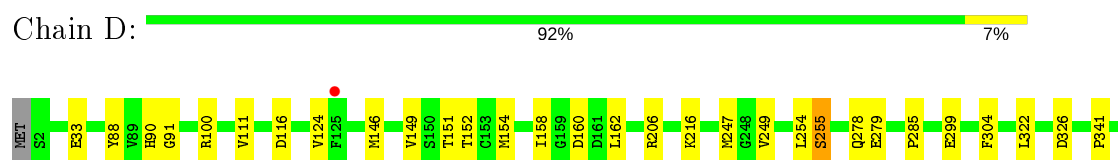
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- 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	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.78Å 128.05Å 107.54Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	35.45 – 2.27 79.64 – 2.27	Depositor EDS
% Data completeness (in resolution range)	91.5 (35.45-2.27) 91.6 (79.64-2.27)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.170 , 0.208 0.170 , 0.207	Depositor DCC
$R_{free}$ test set	8453 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: ICS, NA, HCA, FE, LPJ

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	0.26	0/3811	0.46	0/5149
1	C	0.31	0/3796	0.49	1/5132 (0.0%)
2	B	0.31	1/4249 (0.0%)	0.45	0/5751
2	D	0.32	0/4273	0.46	0/5778
All	All	0.30	1/16129 (0.0%)	0.46	1/21810 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	109	GLU	CD-OE1	-7.55	1.17	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	ASN	O-C-N	-5.18	114.42	122.70

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	3723	3591	3598	20	0
1	C	3709	3566	3568	27	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4143	4026	4027	21	0
2	D	4167	4078	4077	21	2
3	A	14	6	6	1	0
3	C	14	6	6	1	0
4	A	18	0	0	1	0
4	C	18	0	0	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	13	0	0	0	0
6	D	13	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	A	247	0	0	3	0
8	B	417	0	0	8	0
8	C	247	0	0	5	0
8	D	400	0	0	2	0
All	All	17147	15273	15282	88	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (88) 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:6:ARG:NH1	1:A:397:SER:OG	2.03	0.92
1:C:49:ASN:O	8:C:601:HOH:O	2.01	0.78
1:C:75:ILE:HG21	1:C:78:MET:HE2	1.67	0.75
1:A:350:ARG:NH1	8:A:603:HOH:O	2.22	0.73
1:C:350:ARG:NH1	8:C:604:HOH:O	2.23	0.71
2:D:389:GLU:OE1	8:D:701:HOH:O	2.08	0.71
1:A:411:GLU:OE1	8:A:601:HOH:O	2.10	0.69
1:C:200:ASP:OD2	8:C:602:HOH:O	2.09	0.68
2:D:33:GLU:OE1	8:D:702:HOH:O	2.12	0.67
2:B:33:GLU:OE1	8:B:701:HOH:O	2.11	0.67
1:C:287:GLU:OE1	8:C:603:HOH:O	2.13	0.66
1:C:39:VAL:HG12	1:C:391:MET:SD	2.37	0.65
2:B:389:GLU:OE1	8:B:702:HOH:O	2.14	0.65
2:B:488:GLU:OE2	8:B:703:HOH:O	2.15	0.63
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.30	0.61
1:A:96:ARG:NH2	4:A:502:ICS:S5A	2.72	0.61
1:A:50:LYS:NZ	8:A:610:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HG21	1:C:78:MET:CE	2.32	0.60
2:B:177:ASP:OD2	8:B:704:HOH:O	2.17	0.58
2:D:100:ARG:HD2	2:D:111:VAL:O	2.04	0.58
1:C:350:ARG:NH2	1:C:416:ILE:O	2.35	0.57
1:C:115:THR:HG22	1:C:117:ASP:H	1.69	0.57
1:A:115:THR:HG22	1:A:117:ASP:H	1.70	0.56
1:A:350:ARG:NH2	1:A:416:ILE:O	2.36	0.56
2:D:152:THR:HG22	2:D:154:MET:H	1.72	0.55
1:C:39:VAL:O	1:C:39:VAL:HG12	2.07	0.55
2:D:90:HIS:ND1	2:D:116:ASP:OD2	2.37	0.55
2:B:504:ARG:NH1	8:B:716:HOH:O	2.33	0.54
1:C:96:ARG:NH2	4:C:502:ICS:S5A	2.80	0.54
2:B:353:ASP:OD1	1:C:433:LYS:NZ	2.37	0.54
1:C:26:LYS:NZ	8:C:611:HOH:O	2.30	0.54
2:B:124:VAL:HG13	2:B:125:PHE:CD2	2.44	0.53
1:C:39:VAL:O	1:C:391:MET:CE	2.57	0.52
1:C:5:SER:O	1:C:7:GLU:N	2.43	0.52
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.93	0.51
2:B:258:GLU:OE2	8:B:705:HOH:O	2.19	0.50
1:A:259:ILE:O	1:A:263:GLU:HG3	2.12	0.50
2:B:2:SER:N	8:B:726:HOH:O	2.45	0.50
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.47	0.49
1:C:37:PRO:HD3	1:C:396:ASP:OD1	2.12	0.49
1:A:479:TRP:O	1:A:480:GLU:HB2	2.13	0.49
3:A:501:HCA:O1	3:A:501:HCA:O7	2.31	0.49
2:D:247:MET:HG2	2:D:341:PRO:HD3	1.94	0.48
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.95	0.48
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.95	0.48
2:B:412:ALA:O	8:B:706:HOH:O	2.20	0.48
2:D:146:MET:CE	2:D:278:GLN:HG2	2.44	0.48
2:D:299:GLU:OE1	2:D:401:ARG:NH1	2.42	0.47
2:B:247:MET:HB3	2:B:249:VAL:HG23	1.96	0.47
2:B:216:LYS:HG2	2:B:285:PRO:HB2	1.96	0.47
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.49	0.47
2:D:216:LYS:HG2	2:D:285:PRO:HB2	1.97	0.46
2:B:90:HIS:NE2	2:B:160:ASP:OD2	2.49	0.46
2:B:158:ILE:HD11	2:B:160:ASP:CG	2.36	0.46
2:D:206:ARG:HG2	2:D:304:PHE:CE1	2.51	0.46
2:D:158:ILE:HD11	2:D:160:ASP:CG	2.37	0.45
2:D:91:GLY:HA3	2:D:152:THR:HB	1.99	0.45
3:C:501:HCA:O2	3:C:501:HCA:O7	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:OE2	1:A:176:LYS:HE2	2.17	0.45
1:C:447:SER:OG	1:C:448:GLY:N	2.48	0.45
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.99	0.44
2:B:131:MET:HE2	2:B:135:LEU:HD11	1.99	0.44
1:A:5:SER:O	1:A:7:GLU:N	2.51	0.44
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.51	0.44
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.52	0.44
2:D:88:TYR:O	2:D:149:VAL:HA	2.17	0.44
1:A:164:GLU:OE2	1:A:182:ARG:HD2	2.18	0.44
2:B:445:ASN:HB2	2:B:472:PRO:O	2.19	0.43
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.99	0.43
1:C:39:VAL:O	1:C:391:MET:HE3	2.19	0.42
1:C:356:GLY:HA3	4:C:502:ICS:S1B	2.59	0.42
2:B:43:VAL:O	2:B:47:THR:HG23	2.20	0.41
1:C:466:THR:O	1:C:472:TRP:NE1	2.49	0.41
2:B:322:LEU:HD21	1:C:474:LYS:HB3	2.03	0.41
2:D:254:LEU:O	2:D:255:SER:HB3	2.21	0.41
1:A:439:ARG:HD3	1:A:466:THR:OG1	2.20	0.41
1:C:85:PRO:HB2	6:D:601:LPJ:S2B	2.60	0.41
1:A:474:LYS:HB3	2:D:322:LEU:HD21	2.02	0.41
1:C:164:GLU:OE2	1:C:182:ARG:HD2	2.20	0.41
1:A:219:THR:HB	1:A:220:PRO:HD2	2.03	0.41
2:B:88:TYR:O	2:B:149:VAL:HA	2.20	0.41
1:C:359:ARG:N	1:C:360:PRO:CD	2.84	0.41
1:A:359:ARG:N	1:A:360:PRO:CD	2.83	0.40
2:D:326:ASP:OD1	2:D:487:TYR:OH	2.31	0.40
2:D:445:ASN:HB2	2:D:472:PRO:O	2.21	0.40
2:D:379:LEU:HD21	2:D:443:ILE:HG21	2.02	0.40
1:A:209:LYS:HE3	1:A:263:GLU:OE1	2.22	0.40
2:D:509:THR:O	2:D:516:ASP:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLU:HG3	2:D:279:GLU:HB3[1_455]	1.05	0.55
1:C:212:GLU:HB2	2:D:279:GLU:HG2[1_455]	1.33	0.27

## 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	474/492 (96%)	453 (96%)	19 (4%)	2 (0%)	34	40
1	C	472/492 (96%)	450 (95%)	20 (4%)	2 (0%)	34	40
2	B	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	47	57
2	D	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	47	57
All	All	1986/2030 (98%)	1917 (96%)	63 (3%)	6 (0%)	41	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	ARG
1	A	6	ARG
2	D	255	SER
2	B	255	SER
1	A	355	ILE
1	C	355	ILE

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/415 (94%)	376 (97%)	13 (3%)	38	51
1	C	384/415 (92%)	377 (98%)	7 (2%)	59	72
2	B	444/454 (98%)	443 (100%)	1 (0%)	93	97
2	D	451/454 (99%)	449 (100%)	2 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1668/1738 (96%)	1645 (99%)	23 (1%)	67 79

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	51	LYS
1	A	98	ASN
1	A	129	LYS
1	A	176	LYS
1	A	209	LYS
1	A	362	HIS
1	A	384	ASN
1	A	401	TYR
1	A	409	PHE
1	A	415	ARG
1	A	445	ASP
1	A	473	LYS
2	B	390	PRO
1	C	98	ASN
1	C	212	GLU
1	C	213	ASP
1	C	401	TYR
1	C	409	PHE
1	C	415	ARG
1	C	445	ASP
2	D	124	VAL
2	D	404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 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	$\# Z  > 2$
6	LPJ	B	601	1,2	0,17,17	0.00	-	-		
3	HCA	A	501	-	4,13,13	0.72	0	4,18,18	1.68	1 (25%)
3	HCA	C	501	-	4,13,13	0.68	0	4,18,18	1.55	1 (25%)
4	ICS	C	502	1	18,30,30	2.63	11 (61%)	-		
4	ICS	A	502	1	18,30,30	2.63	11 (61%)	-		
6	LPJ	D	601	1,2	0,17,17	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCA	C	501	-	-	3/7/17/17	-
3	HCA	A	501	-	-	1/7/17/17	-
6	LPJ	D	601	1,2	-	-	0/5/5/5
6	LPJ	B	601	1,2	-	-	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S4B-FE7	-4.38	2.21	2.32
4	A	502	ICS	S4B-FE7	-4.37	2.21	2.32
4	A	502	ICS	S3B-FE6	-4.19	2.22	2.32
4	C	502	ICS	S3B-FE6	-4.01	2.22	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S1B-FE6	-3.83	2.22	2.32
4	C	502	ICS	S1B-FE6	-3.82	2.23	2.32
4	C	502	ICS	S2A-FE2	-3.25	2.24	2.32
4	C	502	ICS	S3B-FE7	-3.22	2.24	2.32
4	A	502	ICS	S2A-FE2	-3.19	2.24	2.32
4	A	502	ICS	S4B-FE5	-3.18	2.24	2.32
4	A	502	ICS	S3B-FE7	-3.14	2.24	2.32
4	C	502	ICS	S4B-FE5	-3.03	2.24	2.32
4	C	502	ICS	S4A-FE3	-2.91	2.25	2.32
4	A	502	ICS	S2B-FE6	-2.82	2.18	2.24
4	A	502	ICS	S4A-FE3	-2.79	2.25	2.32
4	C	502	ICS	S2B-FE6	-2.76	2.18	2.24
4	C	502	ICS	S1A-FE2	-2.58	2.26	2.32
4	A	502	ICS	S1A-FE2	-2.55	2.26	2.32
4	C	502	ICS	S1B-FE5	-2.30	2.26	2.32
4	A	502	ICS	S1B-FE5	-2.22	2.26	2.32
4	C	502	ICS	S2A-FE3	-2.14	2.27	2.32
4	A	502	ICS	S2A-FE3	-2.05	2.27	2.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	C3-C2-C1	-2.80	110.50	114.98
3	C	501	HCA	C3-C2-C1	-2.43	111.10	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	HCA	C2-C3-C4-C5
3	C	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C7-C3-C4-C5
3	A	501	HCA	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

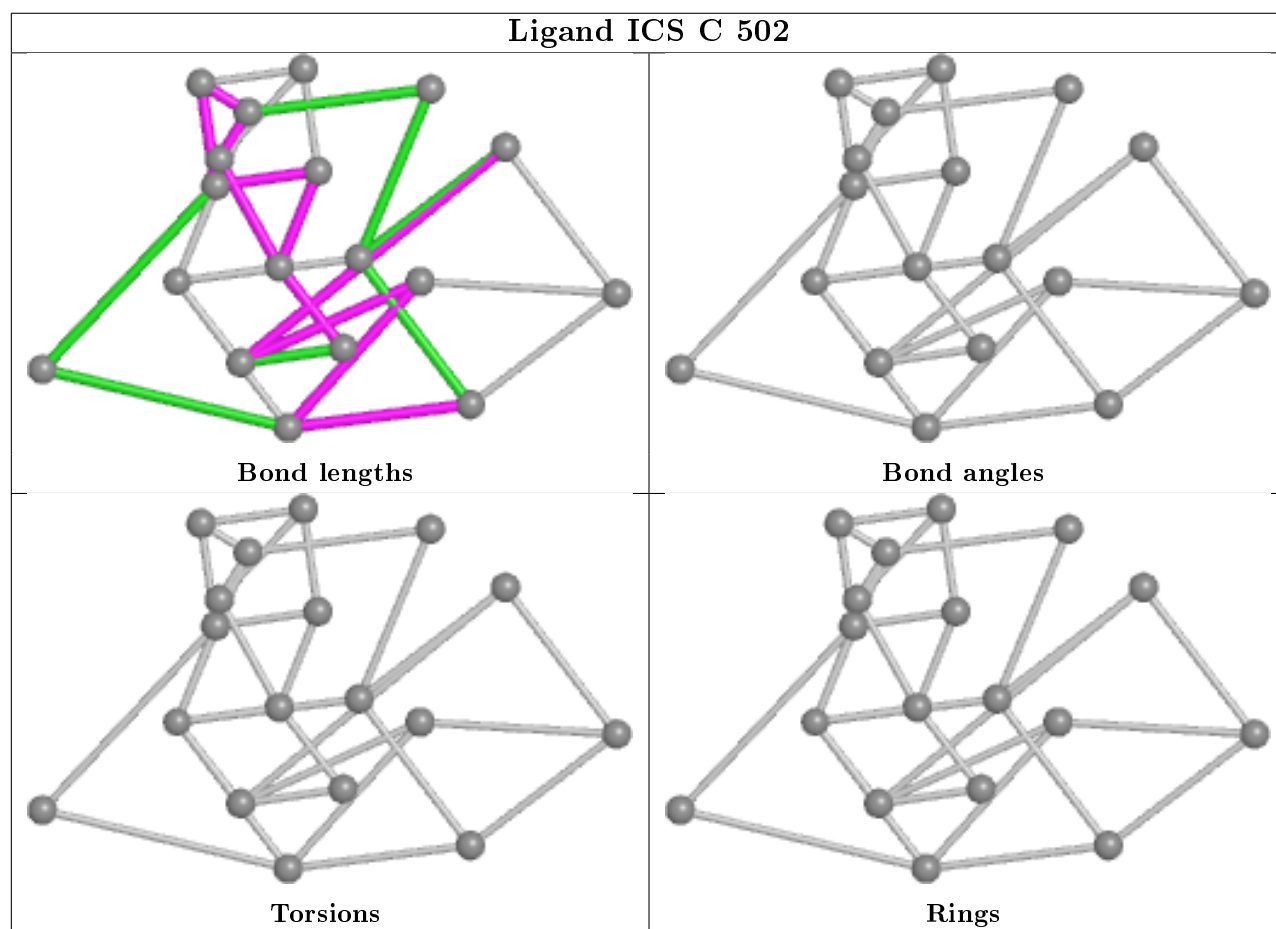
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	1	0
3	C	501	HCA	1	0
4	C	502	ICS	2	0

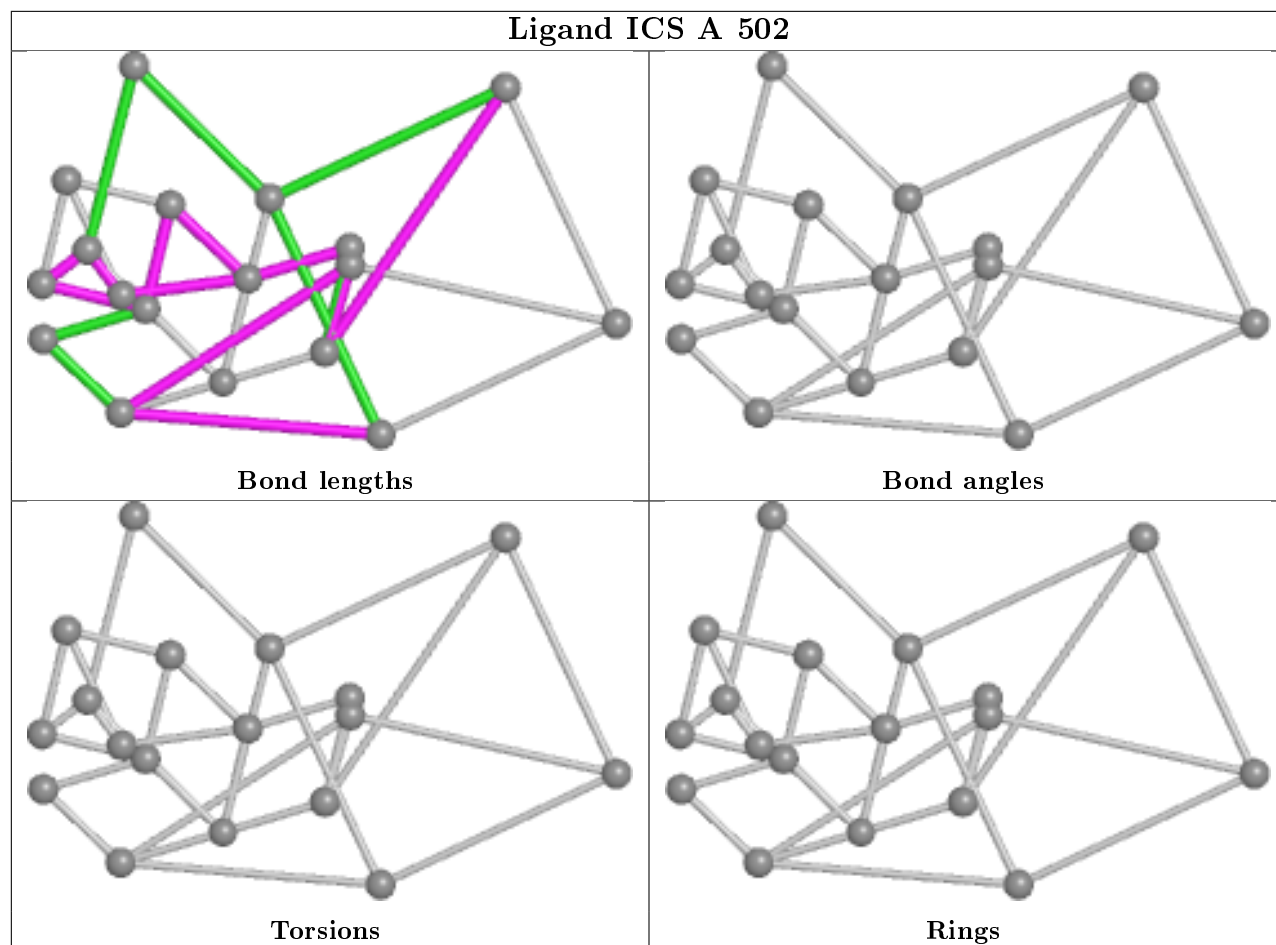
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	ICS	1	0
6	D	601	LPJ	1	0

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.





## 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, 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	476/492 (96%)	-0.04	5 (1%) 80 84	18, 27, 50, 144	0
1	C	476/492 (96%)	-0.02	10 (2%) 63 69	17, 26, 50, 123	0
2	B	522/523 (99%)	-0.30	1 (0%) 95 96	15, 22, 34, 50	0
2	D	522/523 (99%)	-0.29	1 (0%) 95 96	14, 21, 33, 57	0
All	All	1996/2030 (98%)	-0.17	17 (0%) 84 87	14, 24, 41, 144	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	125	PHE	5.2
1	C	40	THR	5.1
1	C	41	GLN	4.5
1	C	43	LYS	3.8
1	A	38	ALA	3.1
1	A	37	PRO	3.0
1	C	391	MET	2.6
1	C	24	ALA	2.6
1	C	38	ALA	2.6
1	C	39	VAL	2.5
1	C	214	THR	2.5
1	C	210	ARG	2.4
1	A	44	LYS	2.2
2	B	125	PHE	2.2
1	A	42	SER	2.1
1	A	36	ASP	2.1
1	C	400	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

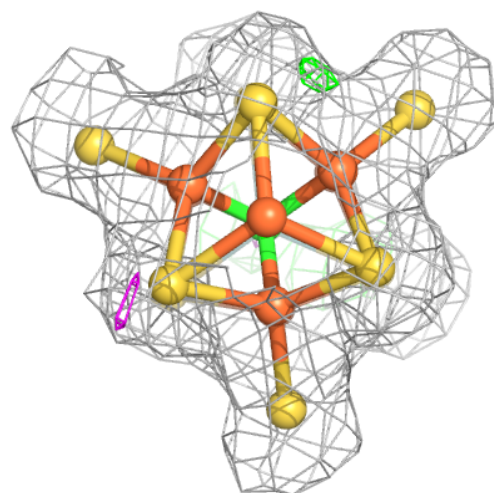
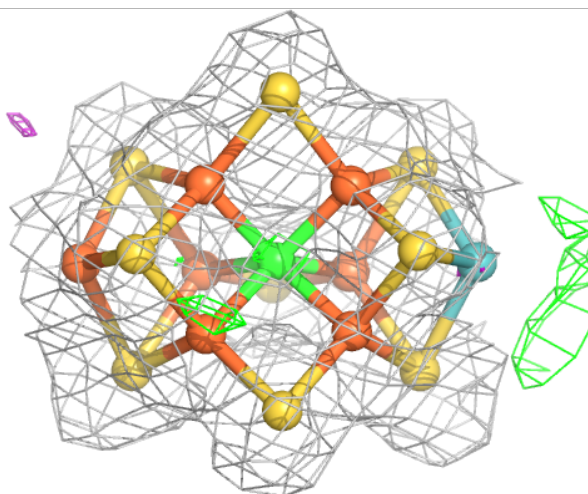
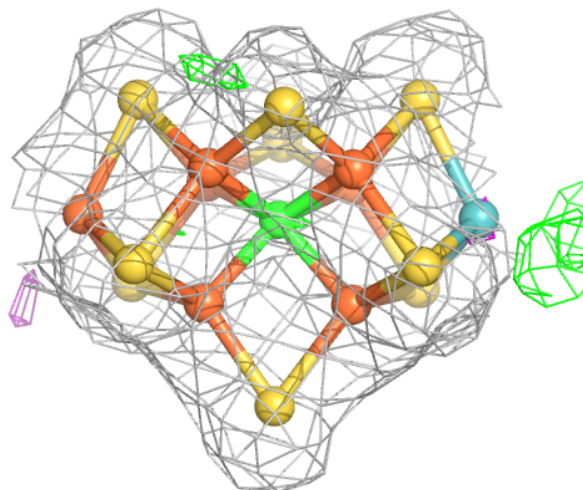
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	503	1/1	0.81	0.12	28,28,28,28	0
5	NA	C	503	1/1	0.86	0.10	24,24,24,24	0
3	HCA	C	501	14/14	0.90	0.21	22,26,31,31	0
3	HCA	A	501	14/14	0.93	0.19	25,29,35,35	0
6	LPJ	D	601	13/13	0.97	0.09	17,20,25,25	0
6	LPJ	B	601	13/13	0.97	0.08	17,24,26,27	0
4	ICS	C	502	18/18	0.99	0.08	17,21,25,26	0
4	ICS	A	502	18/18	0.99	0.07	20,23,26,27	0
7	FE	D	602	1/1	0.99	0.12	14,14,14,14	1
7	FE	B	602	1/1	1.00	0.12	18,18,18,18	0

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

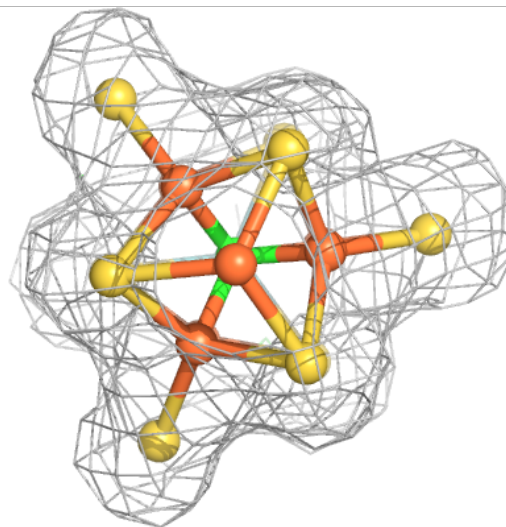
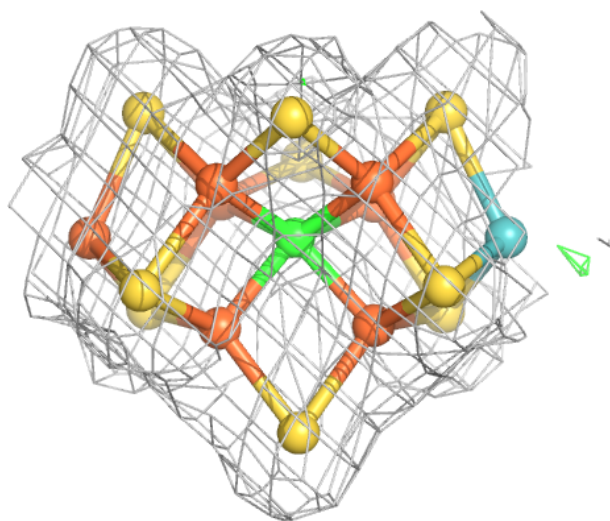
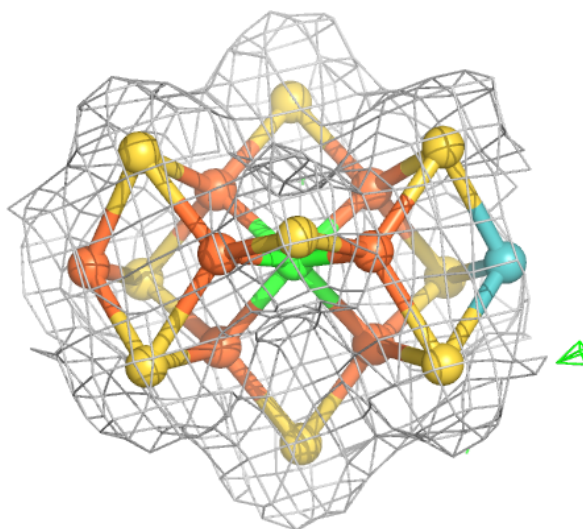
**Electron density around ICS C 502:**

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



**Electron density around ICS 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.