



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 10:52 AM BST

PDB ID : 6OP2
Title : Selenium incorporated FeMo-cofactor of nitrogenase from azotobacter vinelandii at high concentration of selenium
Authors : Arias, R.J.; Rees, D.C.
Deposited on : 2019-04-24
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

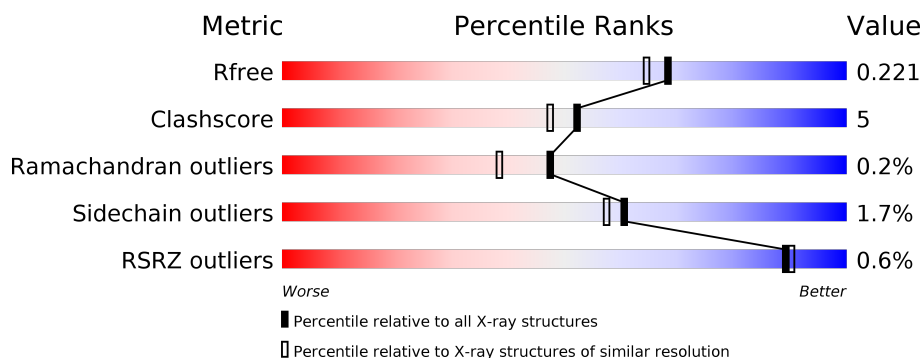
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	477	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 11% . </div> </div>
1	C	477	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 91% 9% . </div> </div>
2	B	522	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 92%, yellow 8%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 92% 8% </div> </div>
2	D	522	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 90%, yellow 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 90% 10% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IMD	B	607	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

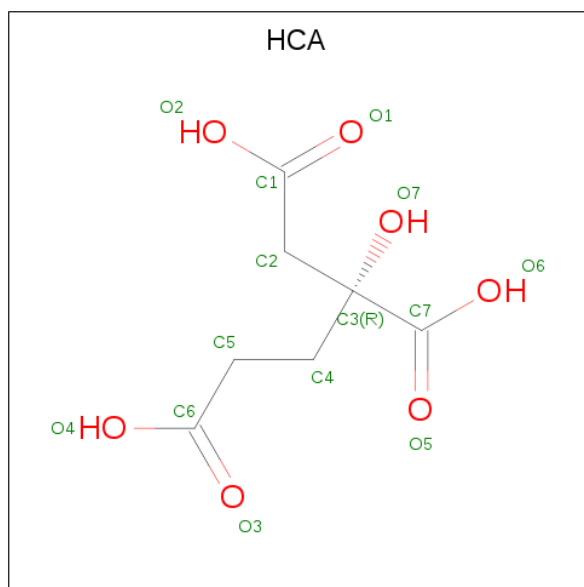
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3787	2408	645	709	25			
1	C	477	Total	C	N	O	S	0	0	0
			3757	2392	641	699	25			

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

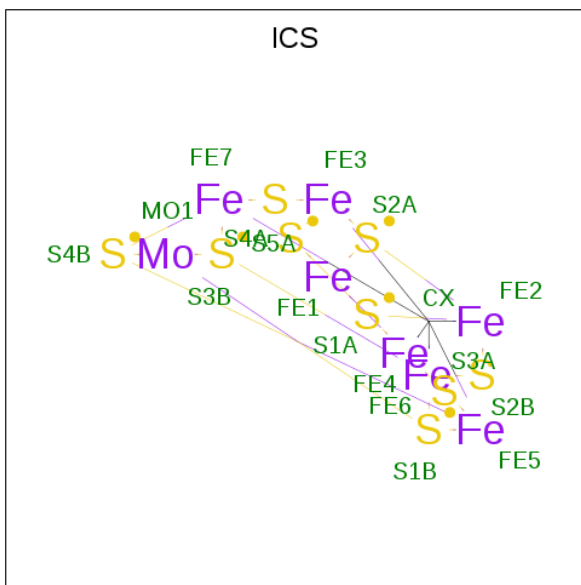
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4149	2651	699	771	28			
2	D	522	Total	C	N	O	S	0	0	0
			4154	2654	699	773	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



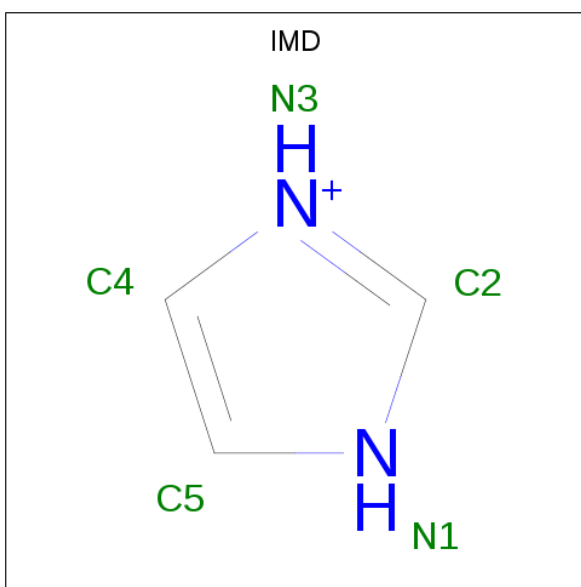
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			17	1	7	1	8		
4	C	1	Total	C	Fe	Mo	S	0	0
			17	1	7	1	8		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $\text{C}_3\text{H}_5\text{N}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	A	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	C	1	Total	C	N	0	0
			5	3	2		
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Se	0	0
			1	1		

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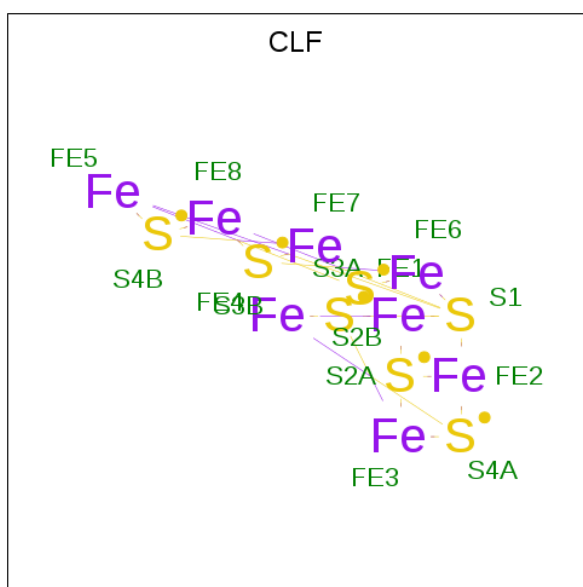
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Se	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).



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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	248	Total 248	O 248	0	0
10	B	337	Total 337	O 337	0	0
10	C	240	Total 240	O 240	0	0
10	D	321	Total 321	O 321	0	0

A284	P285	E297	N317	L322	P341	R348	D357	V391	L394	A419	L430	N445	S446	Y447	G448	K449	P472	R481	L494	E503	D516	L521	V522	R523
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.76 Å 130.38 Å 106.90 Å 90.00° 110.54° 90.00°	Depositor
Resolution (Å)	37.81 – 1.90 38.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.81-1.90) 98.6 (38.56-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.177 , 0.214 0.185 , 0.221	Depositor DCC
R_{free} test set	8048 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17146	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/3875	0.75	3/5226 (0.1%)
1	C	0.65	0/3839	0.75	0/5179
2	B	0.64	0/4253	0.74	1/5755 (0.0%)
2	D	0.61	0/4256	0.74	3/5758 (0.1%)
All	All	0.63	0/16223	0.75	7/21918 (0.0%)

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	2
1	C	0	3
2	B	0	2
2	D	0	3
All	All	0	10

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	100	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	D	348	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	28	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	D	481	ARG	NE-CZ-NH2	-5.44	117.58	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	93	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	481	ARG	Sidechain
2	B	59	ARG	Sidechain
1	C	96	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	3787	0	3720	49	0
1	C	3757	0	3662	49	0
2	B	4149	0	4028	29	0
2	D	4154	0	4027	40	0
3	A	14	0	6	0	0
3	C	14	0	6	4	0
4	A	17	0	0	1	0
4	C	17	0	0	3	0
5	A	10	0	10	0	0
5	B	20	0	20	5	0
5	C	10	0	10	3	0
5	D	15	0	15	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	15	0	0	2	0
8	D	15	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	248	0	0	25	0
10	B	337	0	0	11	0
10	C	240	0	0	36	0
10	D	321	0	0	10	0
All	All	17146	0	15504	172	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 5.

The worst 5 of 172 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:93:ARG:HG2	10:A:602:HOH:O	1.27	1.32
2:B:521:LEU:HD11	10:D:990:HOH:O	1.35	1.22
1:C:249:CYS:HB3	10:C:818:HOH:O	1.28	1.22
10:B:1007:HOH:O	2:D:521:LEU:HD21	1.38	1.21
10:B:1007:HOH:O	2:D:521:LEU:CD2	1.84	1.20

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/477 (100%)	455 (96%)	19 (4%)	1 (0%)	47	38
1	C	475/477 (100%)	456 (96%)	18 (4%)	1 (0%)	47	38
2	B	520/522 (100%)	510 (98%)	10 (2%)	0	100	100
2	D	520/522 (100%)	511 (98%)	8 (2%)	1 (0%)	47	38
All	All	1990/1998 (100%)	1932 (97%)	55 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/407 (100%)	398 (98%)	8 (2%)	55	51
1	C	394/407 (97%)	386 (98%)	8 (2%)	55	51
2	B	446/454 (98%)	438 (98%)	8 (2%)	59	55
2	D	445/454 (98%)	441 (99%)	4 (1%)	78	79
All	All	1691/1722 (98%)	1663 (98%)	28 (2%)	60	57

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	258	GLU
2	B	521	LEU
2	D	247	MET
2	B	369	LEU
2	B	516	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	442	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	IMD	C	504	-	3,5,5	0.32	0	4,5,5	0.72	0
5	IMD	B	607	-	3,5,5	0.42	0	4,5,5	0.54	0
5	IMD	D	604	-	3,5,5	0.37	0	4,5,5	0.50	0
3	HCA	A	501	-	4,13,13	0.82	0	4,18,18	3.24	1 (25%)
8	CLF	D	603	1,2	0,24,24	0.00	-	-	-	-
5	IMD	D	605	-	3,5,5	0.35	0	4,5,5	0.63	0
3	HCA	C	501	-	4,13,13	1.14	0	4,18,18	2.85	3 (75%)
5	IMD	D	602	-	3,5,5	0.29	0	4,5,5	0.83	0
4	ICS	C	502	1,10,6	12,28,30	2.69	6 (50%)	-	-	-
5	IMD	B	606	-	3,5,5	0.40	0	4,5,5	0.45	0
4	ICS	A	502	1,6	12,28,30	3.21	6 (50%)	-	-	-
5	IMD	B	604	-	3,5,5	0.28	0	4,5,5	0.57	0
5	IMD	A	503	-	3,5,5	0.23	0	4,5,5	0.74	0
5	IMD	C	503	-	3,5,5	0.35	0	4,5,5	0.63	0
8	CLF	B	602	1,10,2	0,24,24	0.00	-	-	-	-
5	IMD	B	603	-	3,5,5	0.28	0	4,5,5	0.66	0
5	IMD	A	504	-	3,5,5	0.34	0	4,5,5	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	C	504	-	-	-	0/1/1/1
5	IMD	B	607	-	-	-	0/1/1/1
5	IMD	D	604	-	-	-	0/1/1/1
5	IMD	D	605	-	-	-	0/1/1/1
8	CLF	D	603	1,2	-	-	0/12/10/10
3	HCA	A	501	-	-	2/7/17/17	-
3	HCA	C	501	-	-	4/7/17/17	-
5	IMD	D	602	-	-	-	0/1/1/1
8	CLF	B	602	1,10,2	-	-	0/12/10/10
5	IMD	B	606	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	C	503	-	-	-	0/1/1/1
5	IMD	B	604	-	-	-	0/1/1/1
5	IMD	A	503	-	-	-	0/1/1/1
5	IMD	B	603	-	-	-	0/1/1/1
5	IMD	A	504	-	-	-	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S4B-FE5	-5.41	2.19	2.32
4	A	502	ICS	S1A-FE4	-5.02	2.20	2.32
4	A	502	ICS	S4A-FE3	-4.61	2.21	2.32
4	A	502	ICS	S3B-FE7	-4.57	2.21	2.32
4	C	502	ICS	S4A-FE3	-4.55	2.21	2.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	C4-C5-C6	6.11	120.64	111.39
3	C	501	HCA	C4-C5-C6	3.53	116.74	111.39
3	C	501	HCA	C3-C2-C1	-3.44	109.48	114.98
3	C	501	HCA	C4-C3-C7	-2.87	106.47	111.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 18 short contacts:

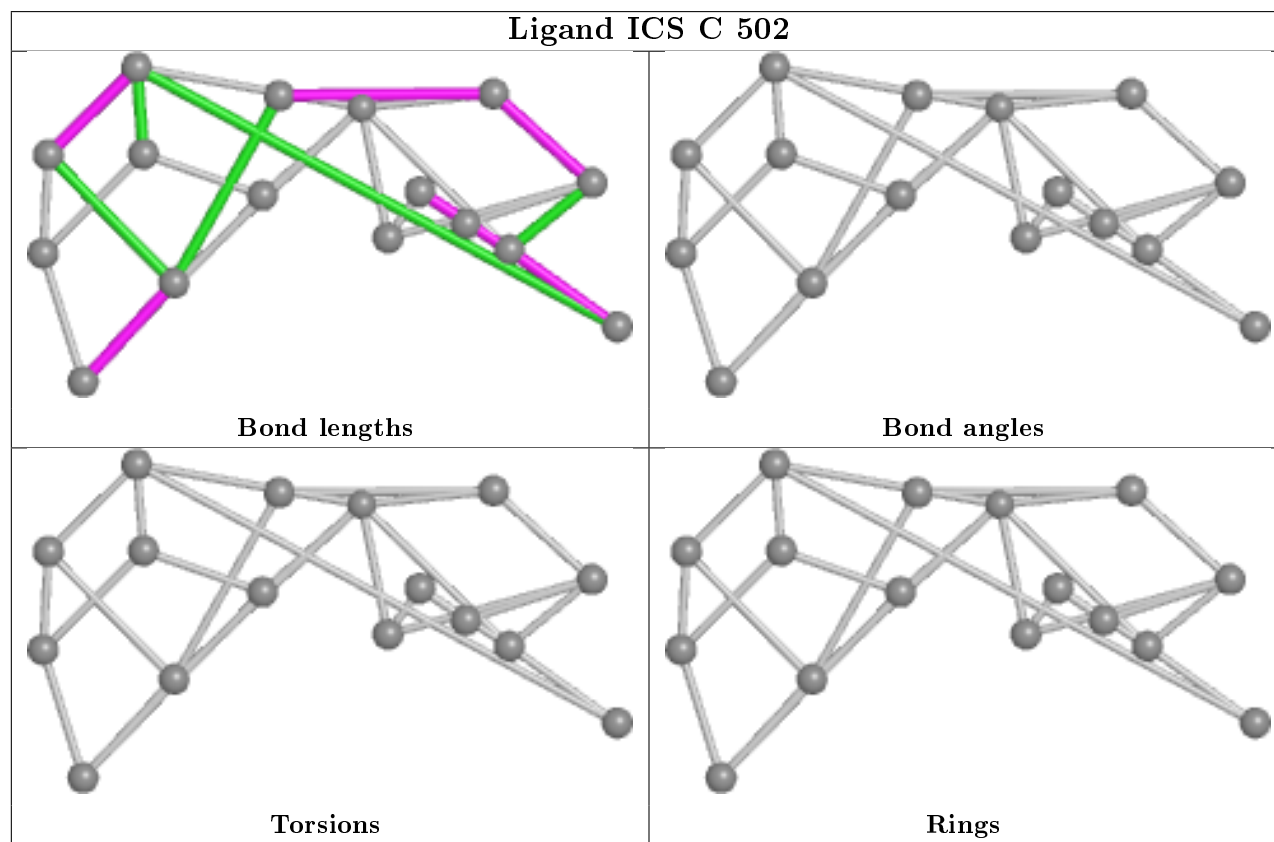
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	IMD	2	0
5	B	607	IMD	1	0
3	C	501	HCA	4	0
4	C	502	ICS	3	0

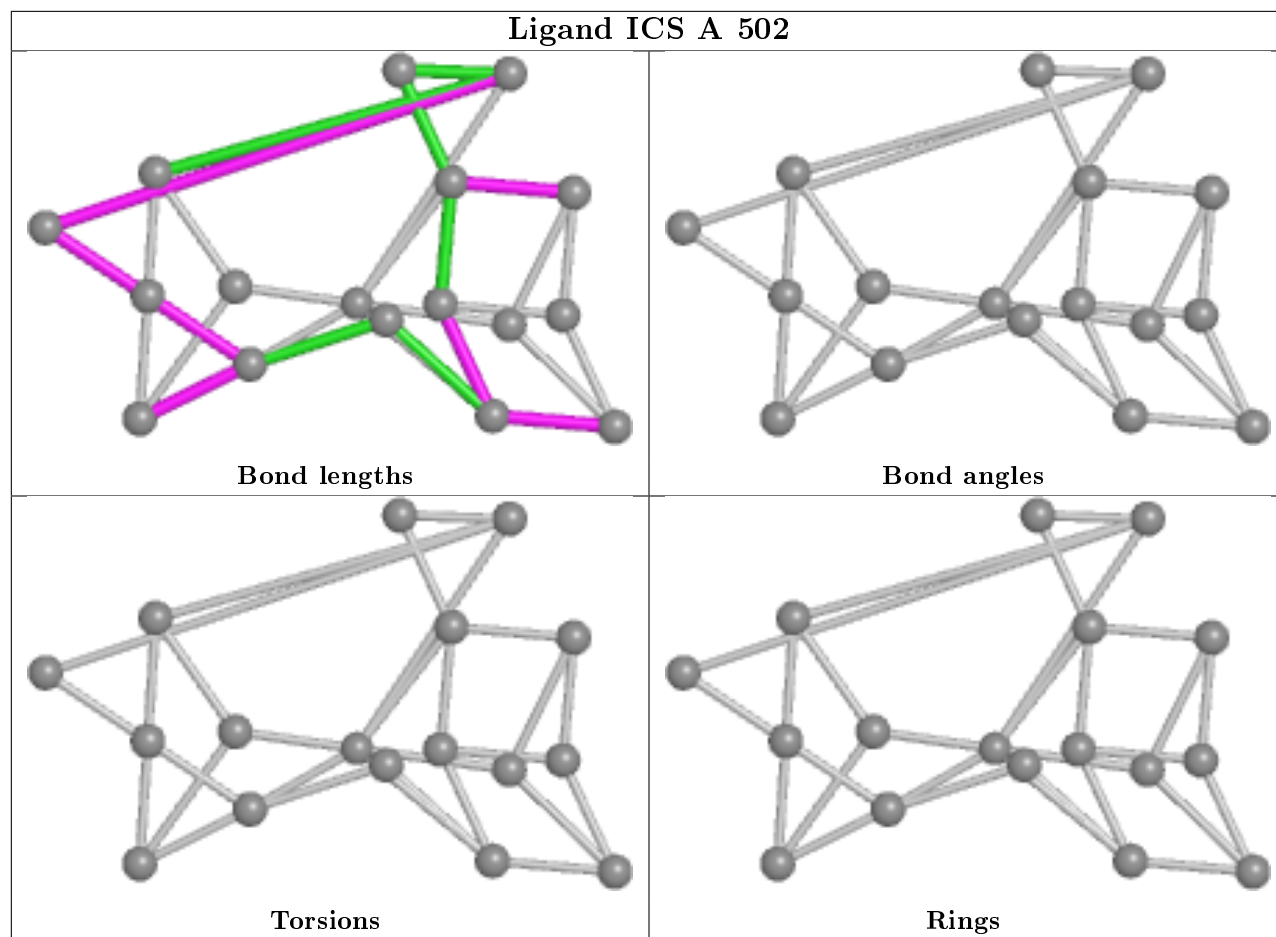
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	IMD	2	0
4	A	502	ICS	1	0
5	B	604	IMD	1	0
5	C	503	IMD	1	0
8	B	602	CLF	2	0
5	B	603	IMD	1	0

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 [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	477/477 (100%)	-0.13	5 (1%) 82 84	7, 14, 30, 45	0
1	C	477/477 (100%)	-0.14	3 (0%) 89 90	8, 14, 28, 55	0
2	B	522/522 (100%)	-0.30	1 (0%) 95 95	7, 14, 23, 55	0
2	D	522/522 (100%)	-0.27	2 (0%) 92 93	8, 14, 24, 49	0
All	All	1998/1998 (100%)	-0.21	11 (0%) 89 90	7, 14, 27, 55	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	125	PHE	5.4
1	C	39	VAL	4.2
1	C	38	ALA	4.0
2	D	125	PHE	3.7
2	D	214	ASP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

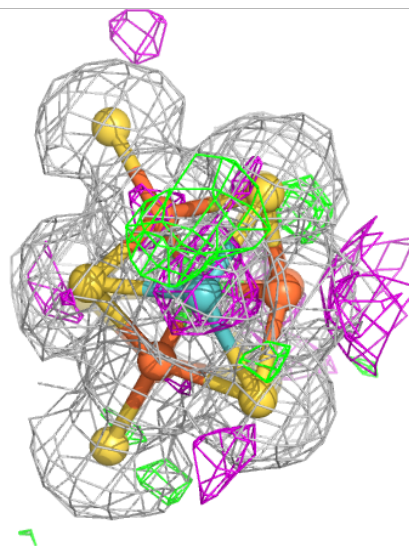
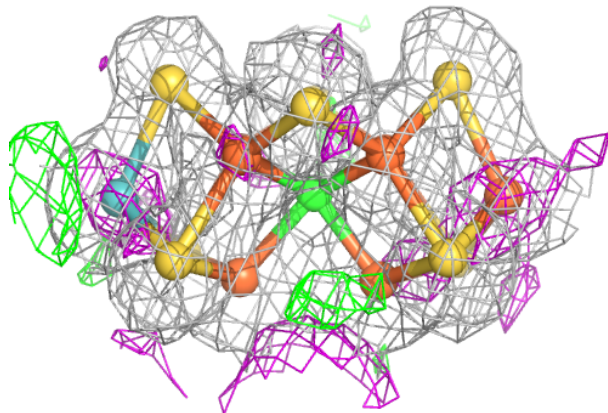
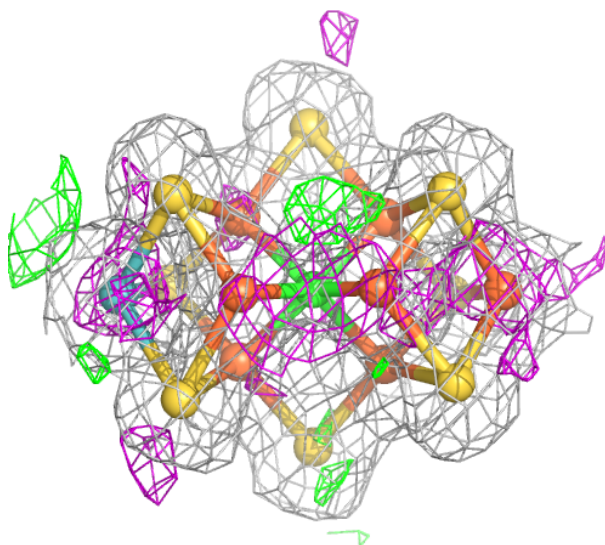
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IMD	B	607	5/5	0.14	0.99	98,100,101,101	0
5	IMD	D	605	5/5	0.76	0.17	40,40,40,42	0
5	IMD	B	606	5/5	0.78	0.15	34,35,36,36	0
9	MG	D	606	1/1	0.80	0.33	54,54,54,54	0
5	IMD	D	602	5/5	0.83	0.10	28,28,30,30	0
5	IMD	A	503	5/5	0.85	0.21	31,32,34,35	0
5	IMD	A	504	5/5	0.87	0.17	28,29,30,31	0
9	MG	B	605	1/1	0.89	0.08	36,36,36,36	0
5	IMD	B	604	5/5	0.90	0.12	27,27,28,28	0
5	IMD	C	503	5/5	0.91	0.15	30,31,32,33	0
5	IMD	C	504	5/5	0.91	0.14	24,26,26,27	0
5	IMD	D	604	5/5	0.94	0.10	16,16,17,18	0
3	HCA	C	501	14/14	0.95	0.10	9,11,13,13	0
7	CA	B	601	1/1	0.95	0.06	36,36,36,36	0
5	IMD	B	603	5/5	0.95	0.10	16,16,16,17	0
3	HCA	A	501	14/14	0.96	0.12	10,12,15,15	0
7	CA	D	601	1/1	0.96	0.06	32,32,32,32	0
8	CLF	D	603	15/15	0.97	0.06	8,9,10,13	0
8	CLF	B	602	15/15	0.97	0.07	7,8,10,12	0
4	ICS	C	502	17/18	0.99	0.05	7,8,9,9	0
4	ICS	A	502	17/18	0.99	0.05	6,8,9,10	0
6	SE	C	505	1/1	0.99	0.18	14,14,14,14	0
6	SE	A	505	1/1	0.99	0.16	11,11,11,11	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.

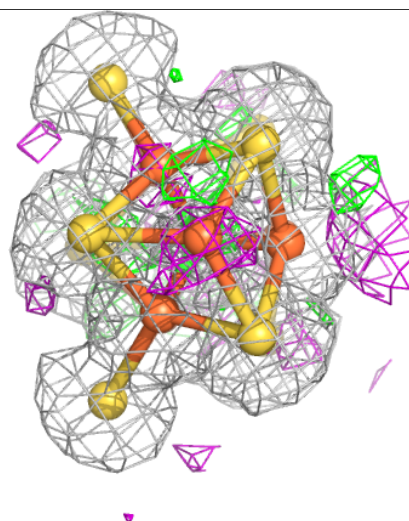
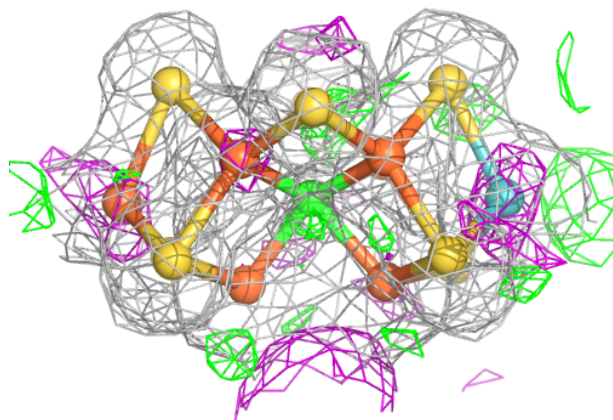
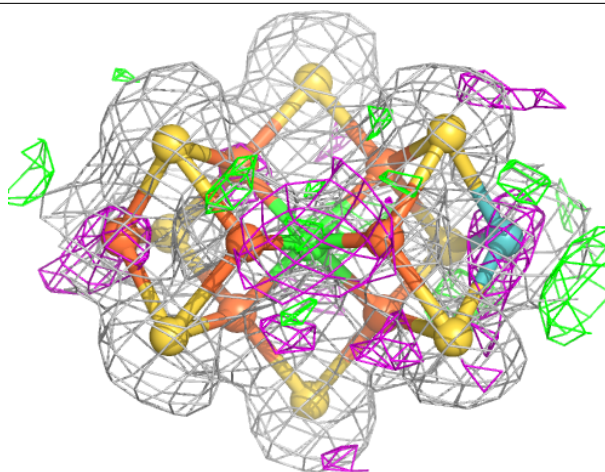
Electron density around ICS C 502:

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.