wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 08:15 AM EDT

PDB ID	:	5BVH / pdb_00005bvh
Title	:	CO-bound form of Selenium incorporated nitrogenase MoFe-protein (Av1-Se-CO) from A. vinelandii
Authors	:	Spatzal, T.; Perez, K.A.; Howard, J.B.; Rees, D.C.
Deposited on	:	2015-06-05
Resolution	:	1.53 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 (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:

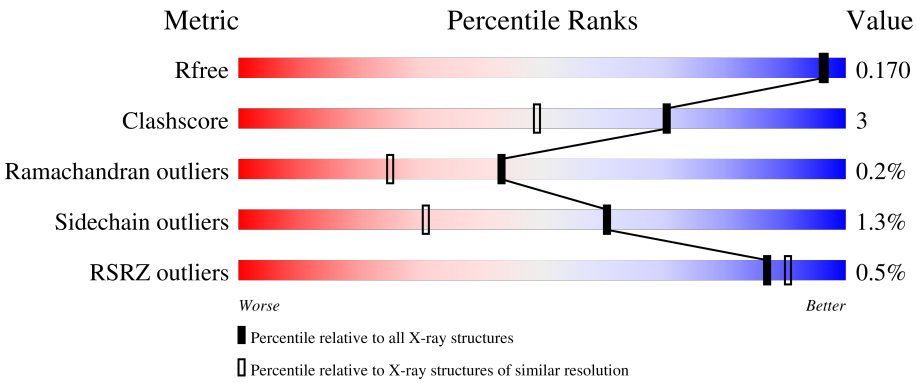
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.53 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	492	% 88% 9% •
1	C	492	% 90% 7% •
2	B	523	93% 7%
2	D	523	93% 7%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18236 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
			Total	C	N	O	S			
1	A	477	3859	2452	662	717	28	0	10	0
1	C	477	3868	2455	663	722	28	0	11	0

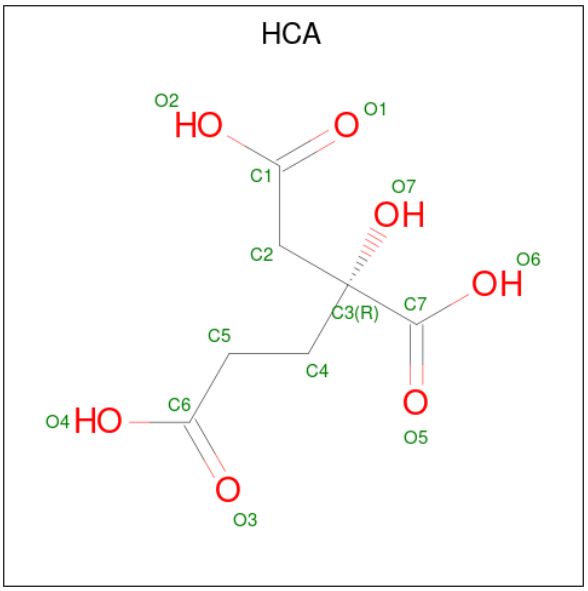
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLN	GLU	conflict	UNP P07328
C	440	GLN	GLU	conflict	UNP P07328

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

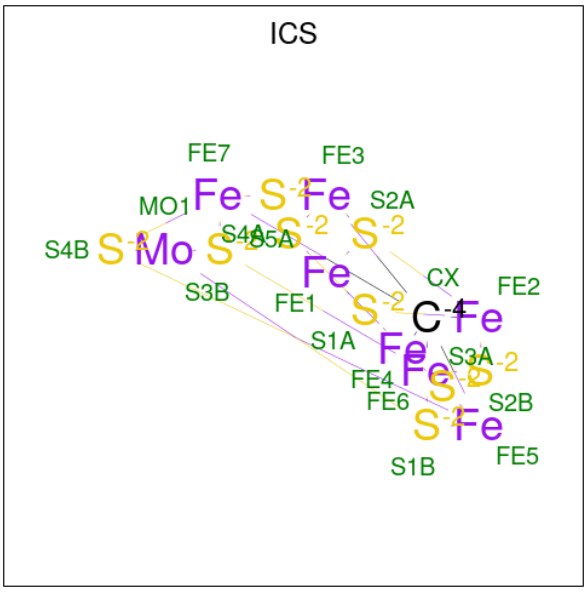
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4243	2704	718	791	30	0	11	0
2	D	522	4277	2727	722	795	33	0	13	0

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



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).



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

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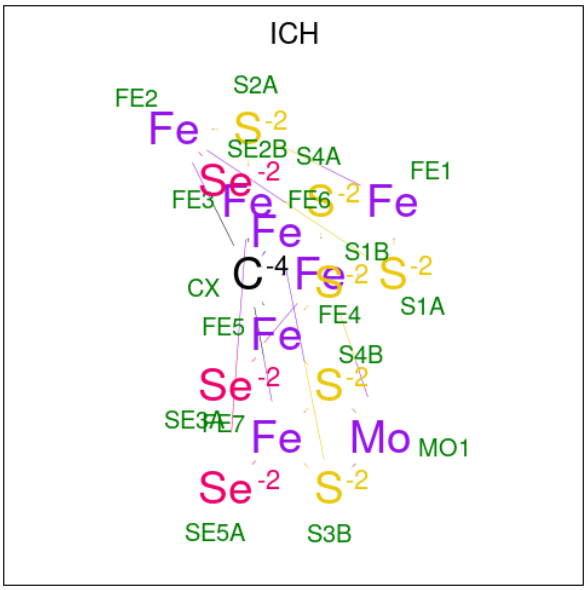
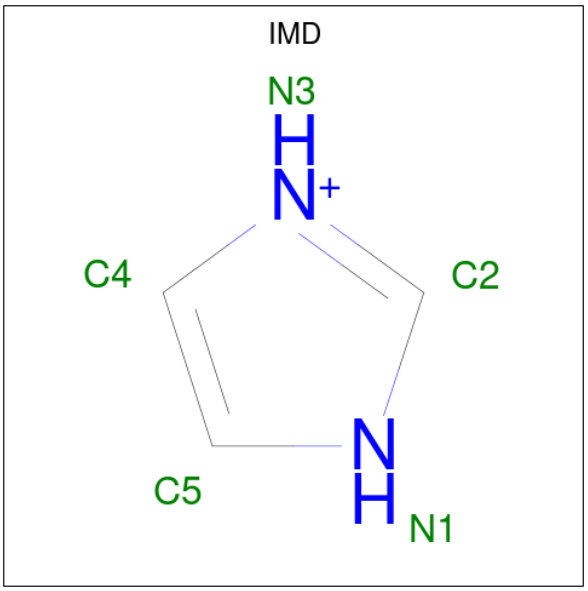
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	Mo	S		
4	C	1	17	1	7	1	8	0	1

- Molecule 5 is iron-sulfur-molybdenum cluster with interstitial carbon with selenium incorporated (CCD ID: ICH) (formula: $CFe_7MoS_6Se_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	Mo	S	Se		
5	A	1	18	1	7	1	6	3	0	1
5	C	1	18	1	7	1	6	3	0	1

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).

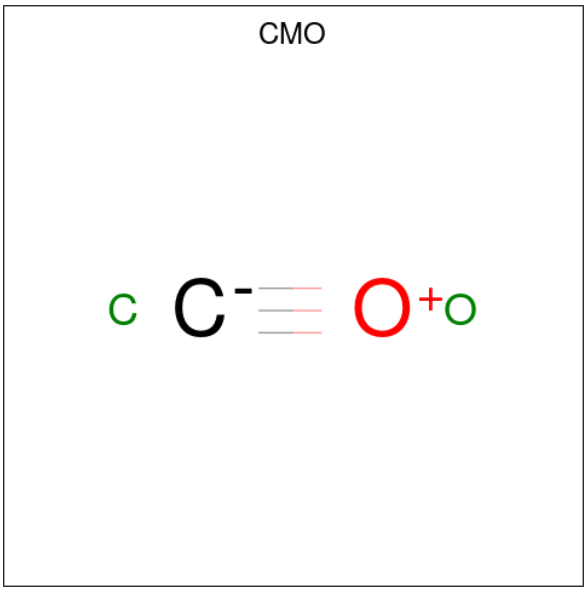


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	C	1	Total C N 5 3 2	0	0
6	D	1	Total C N 5 3 2	0	0
6	D	1	Total C N 5 3 2	0	0
6	D	1	Total C N 5 3 2	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

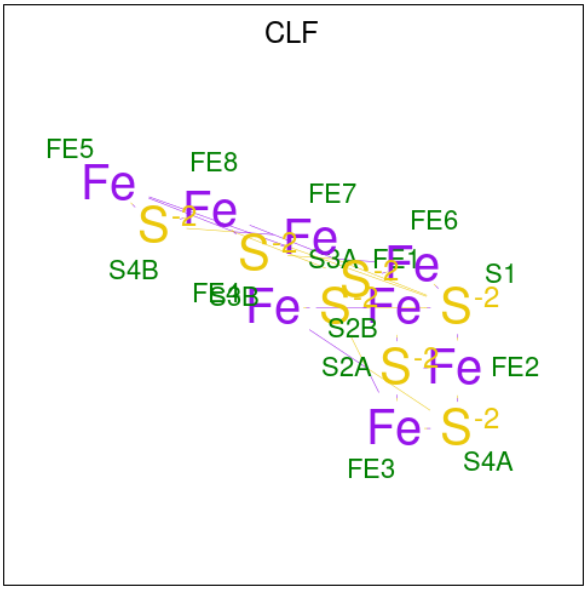
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	2	1	1	0	1
			Total	C	O		
8	C	1	2	1	1	0	1

- Molecule 9 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).



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

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 11 is water.

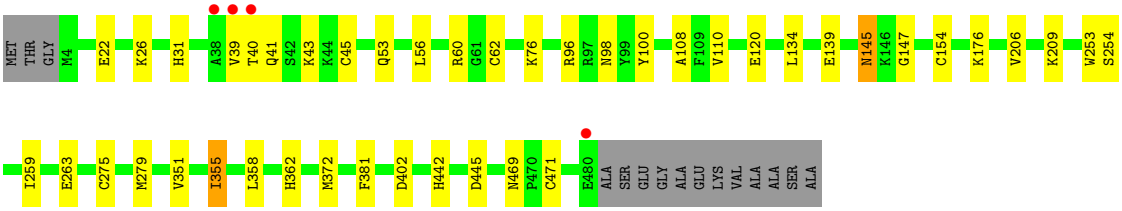
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	383	383	383	0	0
			Total	O		
11	B	509	509	509	0	0
			Total	O		
11	C	389	389	389	0	0
			Total	O		
11	D	532	532	532	0	0

3 Residue-property plots (i)

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

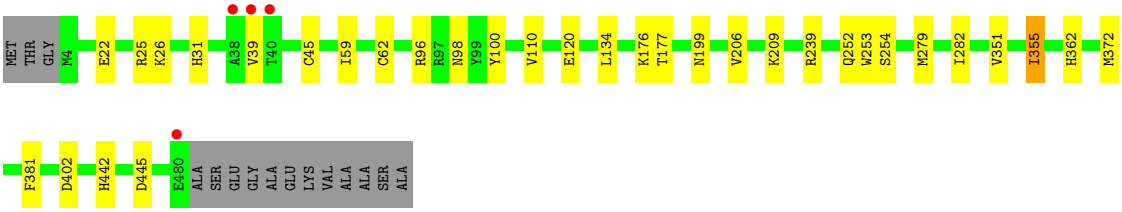
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain A:



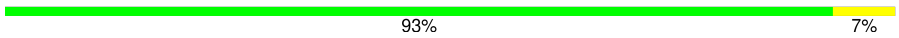
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

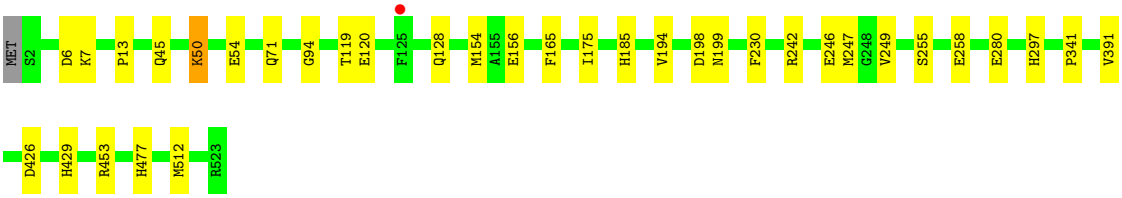
Chain C:



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

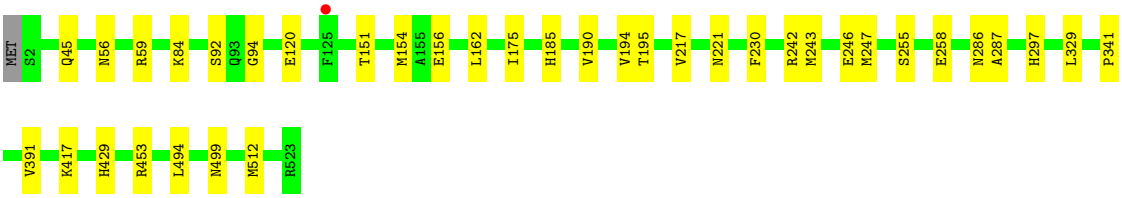
Chain B:





• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:


MET
S2
Q45
N56
R59
K84
S92
Q93
G94
E120
F125
T151
M154
A155
E156
L162
I175
H185
V190
V194
T195
V217
N221
F230
R242
M243
E246
M247
S255
E258
N286
A287
H297
L329
P341
V391
K417
H429
R453
L494
N499
M512
R523

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.07Å 130.83Å 107.32Å 90.00° 110.64° 90.00°	Depositor
Resolution (Å)	100.43 – 1.53 100.43 – 1.53	Depositor EDS
% Data completeness (in resolution range)	96.1 (100.43-1.53) 96.1 (100.43-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.144 , 0.160 0.157 , 0.170	Depositor DCC
R_{free} test set	14889 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18236	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: IMD, ICH, FE2, CMO, CL, HCA, ICS, CLF

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	0.87	0/3946	0.95	3/5315 (0.1%)
1	C	0.88	0/3956	0.95	2/5332 (0.0%)
2	B	0.90	0/4350	0.92	1/5878 (0.0%)
2	D	0.87	0/4381	0.90	1/5916 (0.0%)
All	All	0.88	0/16633	0.93	7/22441 (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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	39	VAL	N-CA-C	5.81	117.22	109.37
1	A	60	ARG	N-CA-C	5.42	117.73	110.35
2	B	391	VAL	N-CA-C	5.32	116.10	110.72
1	A	154	CYS	CA-C-N	-5.14	114.37	119.56
1	A	154	CYS	C-N-CA	-5.14	114.37	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ARG	Sidechain
1	C	96	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	3859	0	3800	26	0
1	C	3868	0	3785	23	0
2	B	4243	0	4125	36	0
2	D	4277	0	4164	37	0
3	A	14	0	6	2	0
3	C	14	0	6	1	0
4	A	17	0	0	0	0
4	C	17	0	0	0	0
5	A	18	0	0	2	0
5	C	18	0	0	1	0
6	A	5	0	5	0	0
6	B	15	0	15	2	0
6	C	5	0	5	1	0
6	D	15	0	15	2	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
9	A	15	0	0	0	0
9	C	15	0	0	0	0
10	B	2	0	0	0	0
11	A	383	0	0	1	0
11	B	509	0	0	5	0
11	C	389	0	0	3	0
11	D	532	0	0	5	0
All	All	18236	0	15926	111	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 3.

The worst 5 of 111 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:453[B]:ARG:HD3	2:D:512[B]:MET:HG2	1.09	1.05
2:B:453[B]:ARG:CD	2:D:512[B]:MET:HG2	1.87	1.05
2:B:453[B]:ARG:CD	2:D:512[B]:MET:CG	2.35	1.04
2:B:453[B]:ARG:HD3	2:D:512[B]:MET:CG	1.87	1.03
2:B:453[B]:ARG:HD2	2:D:512[B]:MET:SD	2.01	0.99

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	484/492 (98%)	463 (96%)	20 (4%)	1 (0%)	43	25
1	C	486/492 (99%)	468 (96%)	17 (4%)	1 (0%)	43	25
2	B	531/523 (102%)	523 (98%)	7 (1%)	1 (0%)	43	25
2	D	533/523 (102%)	523 (98%)	9 (2%)	1 (0%)	43	25
All	All	2034/2030 (100%)	1977 (97%)	53 (3%)	4 (0%)	43	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	255	SER
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	415/415 (100%)	408 (98%)	7 (2%)	53	23
1	C	414/415 (100%)	407 (98%)	7 (2%)	53	23
2	B	460/455 (101%)	453 (98%)	7 (2%)	57	27
2	D	463/455 (102%)	459 (99%)	4 (1%)	70	46
All	All	1752/1740 (101%)	1727 (99%)	25 (1%)	61	29

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	45[A]	CYS
1	C	176	LYS
2	D	417	LYS
1	C	98	ASN
1	C	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	429	HIS
2	D	297	HIS
1	C	199	ASN
2	D	429	HIS
2	D	185	HIS

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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
8	CMO	A	506[C]	-	0,1,1	-	-	-		
6	IMD	B	601	-	5,5,5	0.70	0	5,5,5	0.73	0
6	IMD	B	602	-	5,5,5	0.27	0	5,5,5	0.74	0
6	IMD	B	603	-	5,5,5	0.45	0	5,5,5	0.37	0
9	CLF	A	507	2,1	0,24,24	-	-	-		
5	ICH	C	503[B]	3,1	0,30,30	-	-	-		
4	ICS	C	502[A]	3,1	4,28,30	1.84	1 (25%)	-		
8	CMO	C	506[C]	-	0,1,1	-	-	-		
3	HCA	C	501	5,4	13,13,13	1.08	0	15,18,18	1.32	2 (13%)
6	IMD	A	504	-	5,5,5	0.49	0	5,5,5	0.46	0
6	IMD	D	602	-	5,5,5	0.57	0	5,5,5	0.51	0
6	IMD	D	603	-	5,5,5	0.48	0	5,5,5	0.29	0
6	IMD	C	504	-	5,5,5	0.55	0	5,5,5	0.45	0
5	ICH	A	503[B]	3,1	0,30,30	-	-	-		
9	CLF	C	507	2,1	0,24,24	-	-	-		
4	ICS	A	502[A]	3,1	4,28,30	1.66	1 (25%)	-		
6	IMD	D	601	-	5,5,5	0.56	0	5,5,5	0.38	0
3	HCA	A	501	5,4	13,13,13	1.05	0	15,18,18	1.61	5 (33%)

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
6	IMD	B	601	-	-	-	0/1/1/1
6	IMD	B	602	-	-	-	0/1/1/1
6	IMD	B	603	-	-	-	0/1/1/1
3	HCA	C	501	5,4	-	0/17/17/17	-
6	IMD	A	504	-	-	-	0/1/1/1
6	IMD	D	602	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IMD	D	603	-	-	-	0/1/1/1
6	IMD	C	504	-	-	-	0/1/1/1
9	CLF	C	507	2,1	-	-	0/12/10/10
9	CLF	A	507	2,1	-	-	0/12/10/10
6	IMD	D	601	-	-	-	0/1/1/1
3	HCA	A	501	5,4	-	3/17/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502[A]	ICS	S3A-FE5	2.85	2.31	2.24
4	A	502[A]	ICS	S3A-FE5	2.79	2.31	2.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	HCA	C4-C5-C6	3.01	119.75	112.77
3	A	501	HCA	C4-C5-C6	2.78	119.21	112.77
3	A	501	HCA	O6-C7-C3	2.74	118.40	113.14
3	C	501	HCA	O6-C7-C3	2.44	117.82	113.14
3	A	501	HCA	O4-C6-C5	2.37	121.47	114.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C4-C3-C7-O6
3	A	501	HCA	O1-C1-C2-C3
3	A	501	HCA	O2-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	IMD	1	0
6	B	603	IMD	1	0
5	C	503[B]	ICH	1	0
3	C	501	HCA	1	0
6	D	603	IMD	1	0
6	C	504	IMD	1	0

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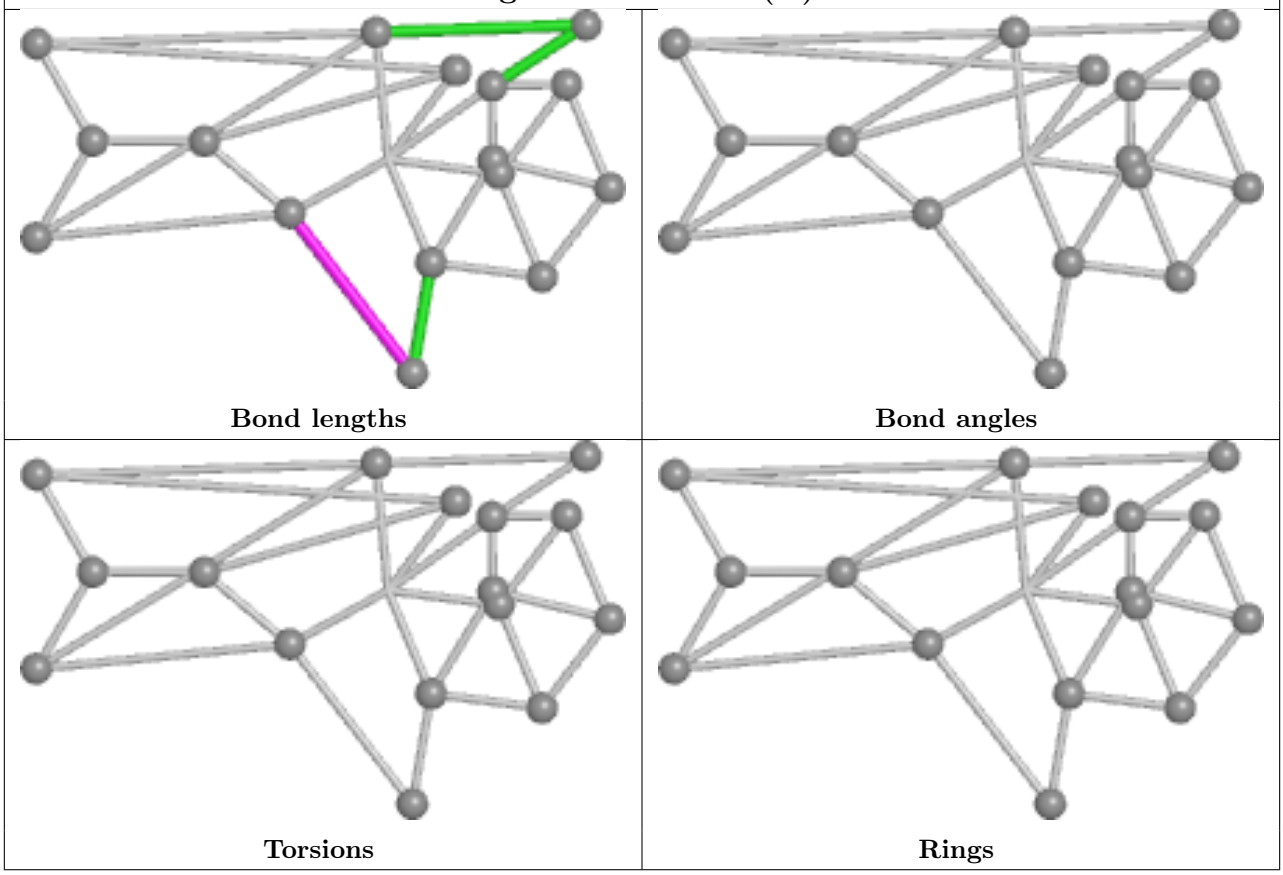
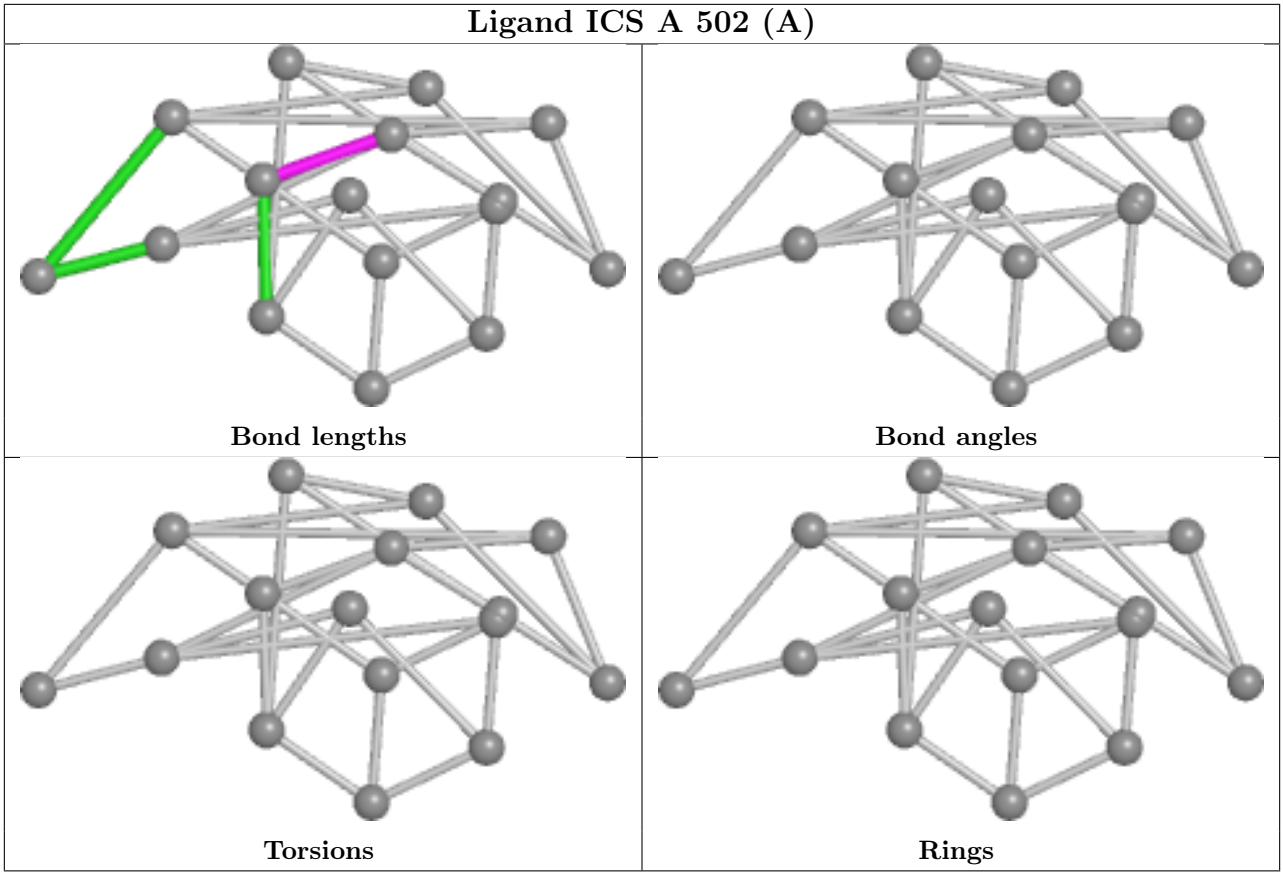
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503[B]	ICH	2	0
6	D	601	IMD	1	0
3	A	501	HCA	2	0

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 ICS C 502 (A)





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	477/492 (96%)	-0.37	4 (0%)	82	87	5, 12, 24, 39	22 (4%)
1	C	477/492 (96%)	-0.40	4 (0%)	82	87	5, 12, 23, 37	24 (5%)
2	B	522/523 (99%)	-0.48	1 (0%)	91	93	4, 11, 20, 27	21 (4%)
2	D	522/523 (99%)	-0.48	1 (0%)	91	93	4, 11, 21, 33	20 (3%)
All	All	1998/2030 (98%)	-0.44	10 (0%)	87	90	4, 11, 21, 39	87 (4%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480[A]	GLU	8.8
1	C	38	ALA	5.4
2	D	125	PHE	5.4
2	B	125	PHE	4.4
1	A	38	ALA	4.3

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)

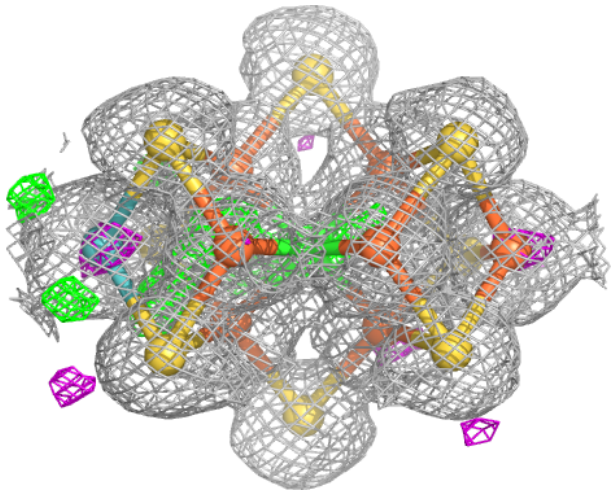
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

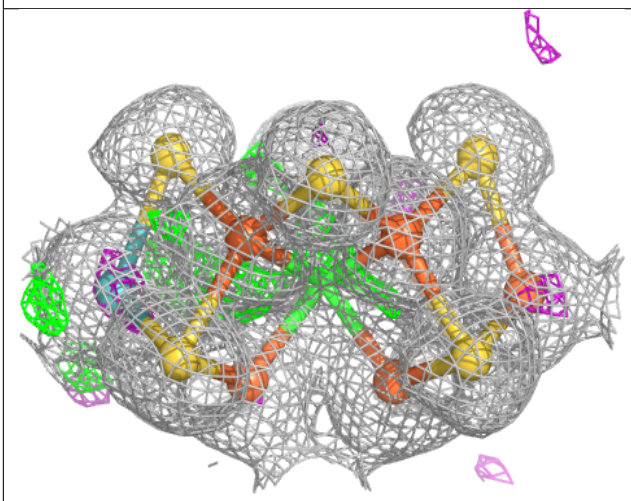
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IMD	B	601	5/5	0.87	0.12	24,25,25,25	0
6	IMD	B	603	5/5	0.87	0.11	24,25,26,26	0
6	IMD	D	603	5/5	0.90	0.11	27,27,27,28	0
6	IMD	C	504	5/5	0.91	0.09	22,22,23,24	0
6	IMD	A	504	5/5	0.94	0.08	24,24,25,25	0
6	IMD	D	601	5/5	0.95	0.06	11,12,12,13	0
6	IMD	B	602	5/5	0.95	0.06	11,11,11,12	0
6	IMD	D	602	5/5	0.96	0.07	19,20,20,20	0
3	HCA	A	501	14/14	0.98	0.04	8,8,10,10	0
3	HCA	C	501	14/14	0.99	0.03	8,8,11,11	0
7	CL	A	505	1/1	0.99	0.03	11,11,11,11	1
8	CMO	A	506[C]	2/2	0.99	0.05	7,7,7,8	0
8	CMO	C	506[C]	2/2	0.99	0.05	7,7,7,7	0
5	ICH	C	503[B]	18/18	1.00	0.01	4,8,9,10	18
4	ICS	A	502[A]	17/18	1.00	0.01	7,8,9,9	17
7	CL	C	505	1/1	1.00	0.02	10,10,10,10	1
4	ICS	C	502[A]	17/18	1.00	0.01	7,8,8,9	17
5	ICH	A	503[B]	18/18	1.00	0.01	4,8,9,10	18
9	CLF	A	507	15/15	1.00	0.01	8,8,8,8	0
9	CLF	C	507	15/15	1.00	0.01	8,8,9,9	0
10	FE2	B	604	1/1	1.00	0.03	9,9,9,9	1
10	FE2	B	605	1/1	1.00	0.02	10,10,10,10	1

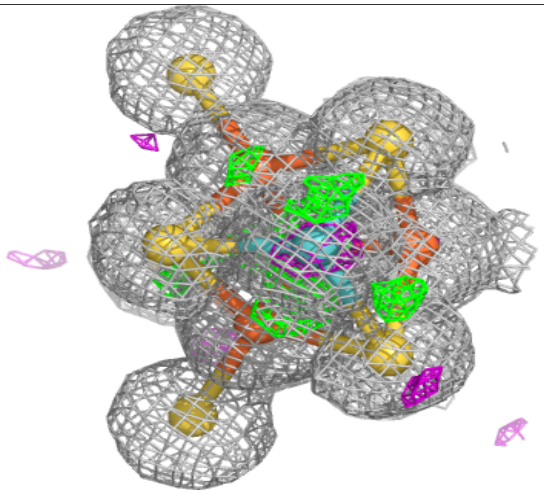
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

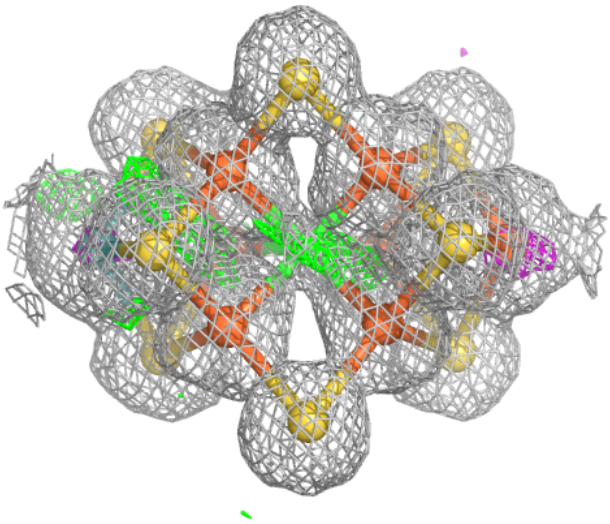
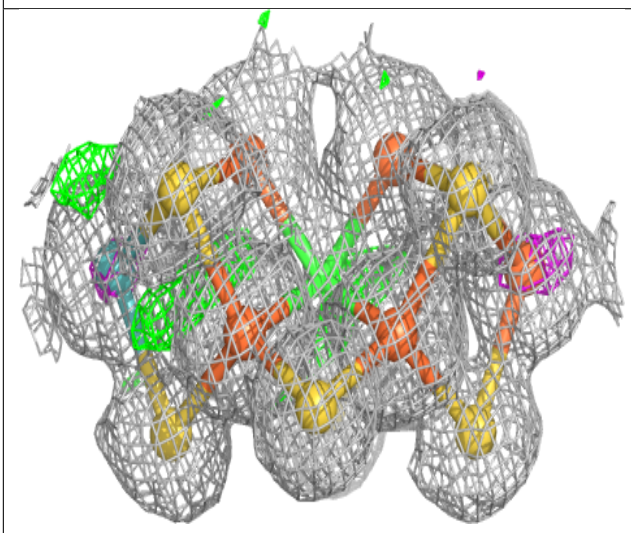
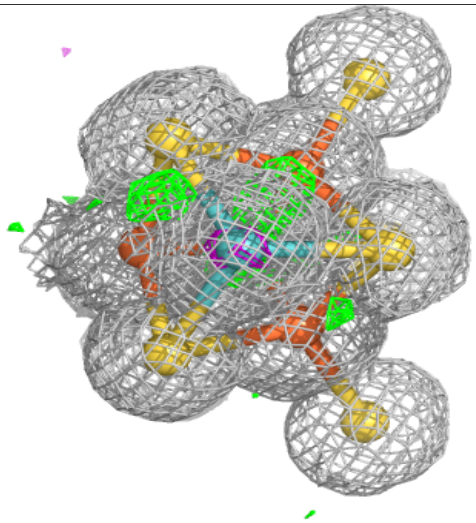
Electron density around ICS A 502 (A):

$2mF_o$-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 (A): 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.