Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 04:12 PM EST

PDB ID	:	5KOJ
Title	:	Nitrogenase MoFeP protein in the IDS oxidized state
Authors	:	Owens, C.P.; Tezcan, F.A.
Deposited on	:	2016-06-30
Resolution	:	2.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

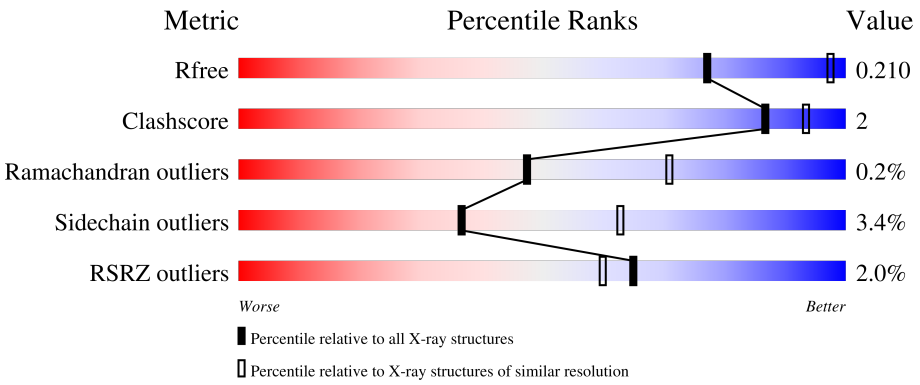
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	499	.% 88% 8% • •
1	C	499	4% 86% 9% • •
2	B	511	2% 95% 5% •
2	D	511	.% 93% 6% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16070 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.

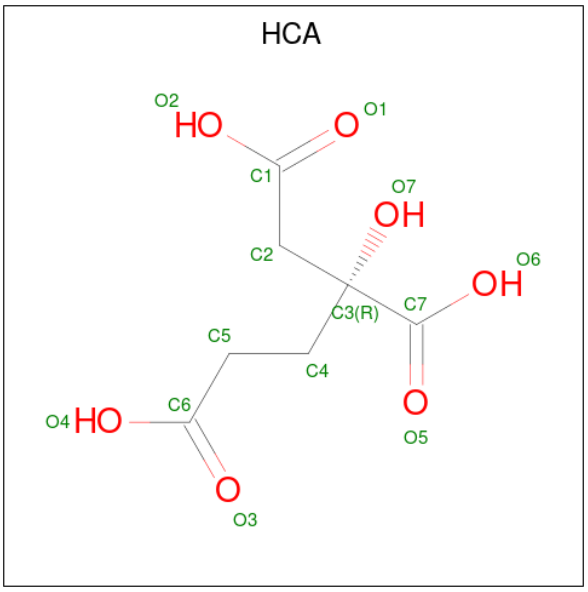
- Molecule 1 is a protein called Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3804	2420	663	701	20	0	0	0
1	C	480	3800	2418	662	700	20	0	0	0

- Molecule 2 is a protein called Nitrogenase FeMo beta subunit protein NifK.

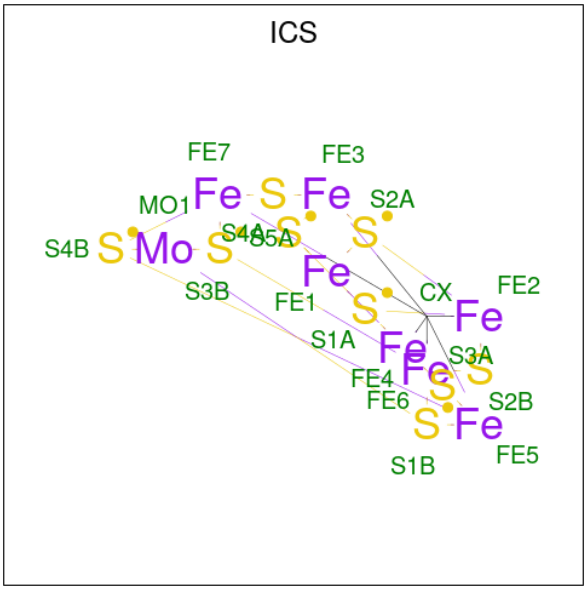
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	510	4006	2547	676	760	23	0	0	0
2	D	510	4006	2547	676	760	23	0	0	0

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



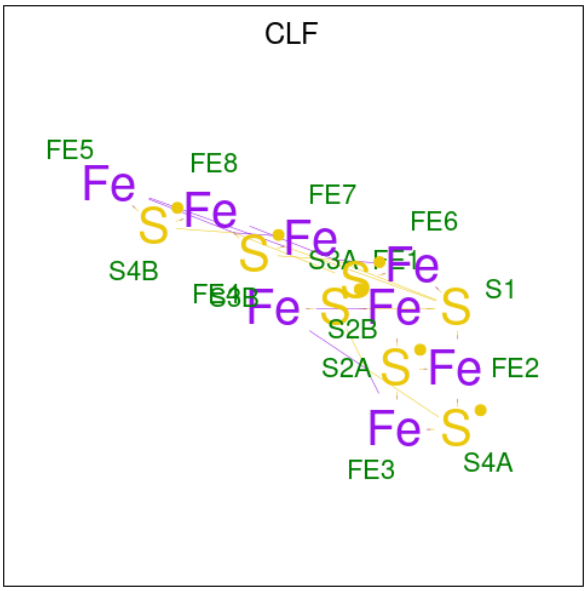
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	14	7	7	0	0
			Total	C	O		
3	C	1	14	7	7	0	0

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9).



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

- Molecule 5 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 7 is water.

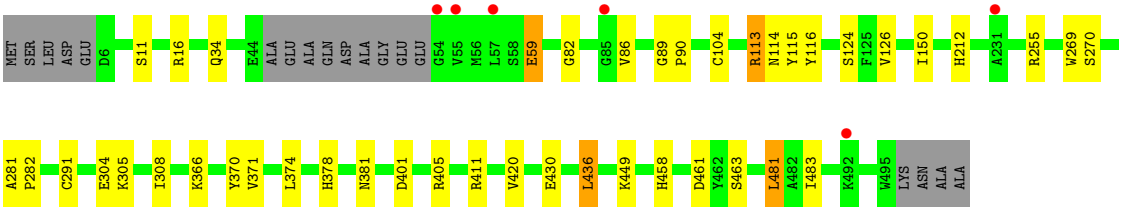
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	87	Total O 87 87	0	0
7	B	93	Total O 93 93	0	0
7	C	76	Total O 76 76	0	0
7	D	102	Total O 102 102	0	0

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.

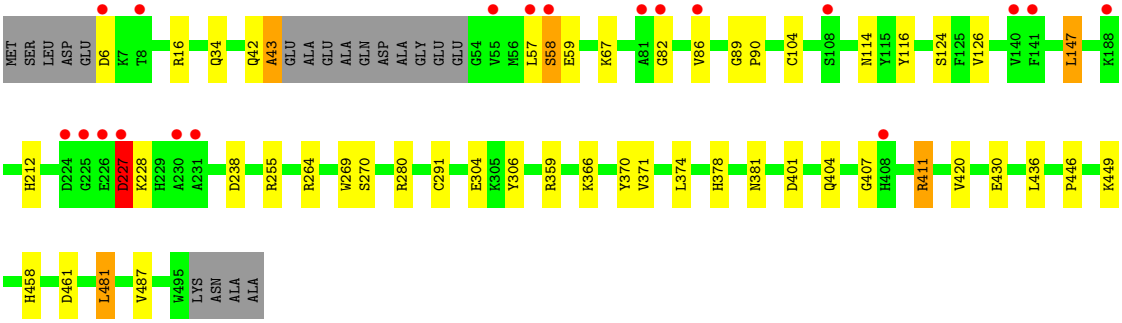
• Molecule 1: Nitrogenase protein alpha chain

Chain A:



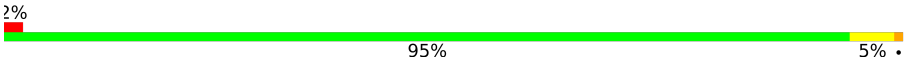
• Molecule 1: Nitrogenase protein alpha chain

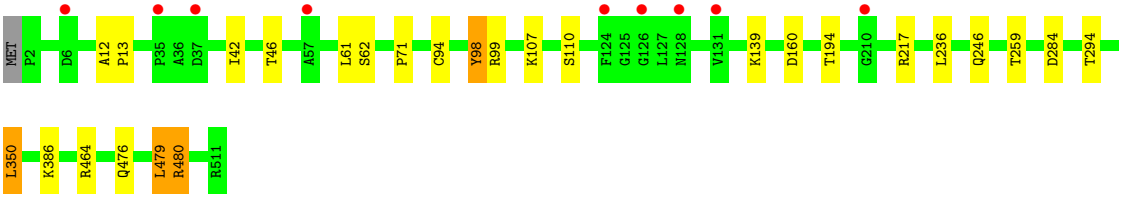
Chain C:



• Molecule 2: Nitrogenase FeMo beta subunit protein NifK

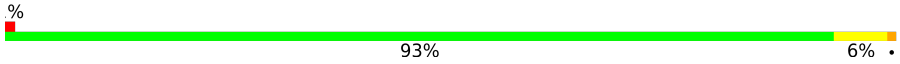
Chain B:

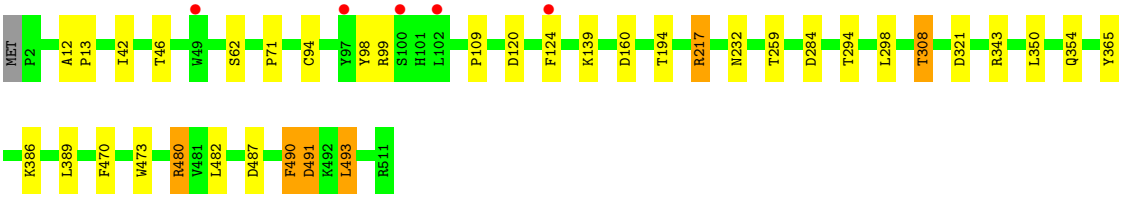




• Molecule 2: Nitrogenase FeMo beta subunit protein NifK

Chain D:




MET
P2
A12
P13
I42
T46
W49
S62
P71
C94
Y97
Y98
R99
S100
H101
L102
P109
D120
F124
K139
D160
T194
R217
N232
T259
D284
T294
L298
T308
D321
R343
L350
Q354
Y365
K386
L389
F470
W473
R480
V481
L482
D487
F490
D491
K492
L493
R511

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	201.57Å 201.57Å 132.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.59 39.59 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.59-2.59) 99.6 (39.59-2.59)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	0.42	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.168 , 0.208 0.174 , 0.210	Depositor DCC
R_{free} test set	4244 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16070	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: ICS, HCA, FE, 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	0.70	0/3896	0.86	5/5263 (0.1%)
1	C	0.70	1/3892 (0.0%)	0.88	8/5257 (0.2%)
2	B	0.72	1/4109 (0.0%)	0.81	2/5566 (0.0%)
2	D	0.71	0/4109	0.83	9/5566 (0.2%)
All	All	0.71	2/16006 (0.0%)	0.84	24/21652 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	TYR	CZ-OH	5.35	1.47	1.37
1	C	43	ALA	N-CA	5.08	1.56	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	99	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	255	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	411	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	280	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	147	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	16	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	D	490	PHE	N-CA-C	-5.99	94.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	401	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	16	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	99	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	405	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	306	TYR	N-CA-C	-5.52	96.08	111.00
2	D	493	LEU	CA-CB-CG	5.51	127.97	115.30
2	B	160	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	464	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	C	401	ASP	CB-CG-OD1	5.34	123.10	118.30
2	D	160	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	411	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	D	343	ARG	NE-CZ-NH2	-5.15	117.73	120.30
2	D	124	PHE	CB-CG-CD1	5.12	124.38	120.80
1	C	359	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	D	321	ASP	CB-CG-OD1	5.05	122.85	118.30
2	D	217	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	58	SER	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	227	ASP	Peptide

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	3804	0	3710	19	0
1	C	3800	0	3710	19	0
2	B	4006	0	3869	15	0
2	D	4006	0	3869	20	0
3	A	14	0	6	1	0
3	C	14	0	6	1	0
4	A	18	0	0	0	0
4	C	18	0	0	0	0
5	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	87	0	0	2	0
7	B	93	0	0	1	0
7	C	76	0	0	2	0
7	D	102	0	0	2	0
All	All	16070	0	15170	64	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 2.

All (64) 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:490:PHE:O	2:D:491:ASP:CB	2.11	0.98
2:D:490:PHE:O	2:D:491:ASP:HB3	1.79	0.81
1:C:212:HIS:NE2	7:C:601:HOH:O	1.93	0.76
2:D:490:PHE:O	2:D:491:ASP:HB2	1.90	0.72
2:B:99:ARG:HD2	2:B:110:SER:O	1.92	0.69
1:A:212:HIS:NE2	7:A:601:HOH:O	1.93	0.66
2:D:94:CYS:HB3	2:D:98:TYR:CE2	2.34	0.63
2:B:94:CYS:HB3	2:B:98:TYR:CE2	2.35	0.61
1:A:113:ARG:NH2	1:A:463:SER:O	2.35	0.59
1:C:42:GLN:O	1:C:43:ALA:CB	2.52	0.57
1:A:449:LYS:HE3	2:B:259:THR:OG1	2.07	0.55
1:C:227:ASP:CB	1:C:228:LYS:HA	2.36	0.55
1:C:458:HIS:HB3	3:C:501:HCA:O5	2.06	0.55
1:C:449:LYS:HE3	2:D:259:THR:OG1	2.07	0.53
2:D:298:LEU:HD13	2:D:308:THR:HG23	1.90	0.53
2:D:480:ARG:HB3	7:D:788:HOH:O	2.09	0.53
1:C:449:LYS:CE	2:D:259:THR:OG1	2.58	0.52
1:A:113:ARG:NH1	1:A:115:TYR:OH	2.44	0.51
1:A:449:LYS:CE	2:B:259:THR:OG1	2.59	0.51
2:D:487:ASP:O	2:D:490:PHE:O	2.29	0.51
2:B:480:ARG:HH22	2:D:480:ARG:HH22	1.58	0.50
1:C:116:TYR:CE1	1:C:126:VAL:HB	2.46	0.50
2:D:42:ILE:O	2:D:46:THR:HG23	2.12	0.50
2:B:42:ILE:O	2:B:46:THR:HG23	2.12	0.49
2:B:107:LYS:HG2	7:B:747:HOH:O	2.11	0.49
1:A:82:GLY:O	1:A:86:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:O	1:C:407:GLY:O	2.31	0.48
1:A:458:HIS:HB3	3:A:501:HCA:O5	2.14	0.48
1:A:59:GLU:HA	1:A:59:GLU:OE2	2.13	0.48
1:C:238:ASP:OD1	1:C:264:ARG:HD3	2.13	0.48
1:C:82:GLY:O	1:C:86:VAL:HB	2.14	0.47
2:B:350:LEU:HD13	1:C:487:VAL:HG23	1.96	0.47
1:A:116:TYR:CE1	1:A:126:VAL:HB	2.49	0.47
1:C:481:LEU:C	1:C:481:LEU:HD12	2.35	0.47
1:A:291:CYS:HA	1:A:374:LEU:HD22	1.97	0.46
1:C:291:CYS:HA	1:C:374:LEU:HD22	1.96	0.46
2:D:354:GLN:HB2	7:D:757:HOH:O	2.15	0.45
1:A:481:LEU:C	1:A:481:LEU:HD12	2.38	0.44
2:B:217:ARG:NH1	2:B:284:ASP:OD2	2.49	0.44
1:C:255:ARG:NH2	7:C:606:HOH:O	2.51	0.44
1:C:446:PRO:HG3	2:D:109:PRO:HB3	1.99	0.44
2:B:94:CYS:HB3	2:B:98:TYR:CZ	2.53	0.44
1:A:269:TRP:HA	1:A:270:SER:HA	1.78	0.44
2:D:71:PRO:HB2	2:D:98:TYR:CZ	2.53	0.44
1:A:150:ILE:HG23	2:B:61:LEU:HD13	2.00	0.43
1:C:89:GLY:N	1:C:90:PRO:CD	2.82	0.43
1:A:89:GLY:N	1:A:90:PRO:CD	2.82	0.43
2:B:12:ALA:HB3	2:B:13:PRO:CD	2.49	0.43
2:D:94:CYS:HB3	2:D:98:TYR:CZ	2.53	0.43
2:B:479:LEU:HD13	2:D:470:PHE:CZ	2.54	0.43
2:D:12:ALA:HB3	2:D:13:PRO:CD	2.49	0.43
1:A:212:HIS:CE1	7:A:601:HOH:O	2.60	0.42
1:A:370:TYR:CZ	1:A:420:VAL:HG12	2.55	0.42
2:B:71:PRO:HB2	2:B:98:TYR:CZ	2.55	0.42
1:C:370:TYR:CZ	1:C:420:VAL:HG12	2.55	0.42
1:A:436:LEU:HG	1:A:483:ILE:HD11	2.01	0.42
2:D:217:ARG:NH1	2:D:284:ASP:OD2	2.50	0.41
1:A:281:ALA:N	1:A:282:PRO:CD	2.82	0.41
1:C:269:TRP:HA	1:C:270:SER:HA	1.77	0.41
2:D:365:TYR:HA	2:D:389:LEU:O	2.21	0.41
1:C:42:GLN:O	1:C:43:ALA:HB2	2.21	0.40
1:A:282:PRO:O	1:A:308:ILE:HD11	2.22	0.40
2:B:476:GLN:CD	2:B:480:ARG:HH21	2.23	0.40
2:D:232:ASN:HB3	2:D:473:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/499 (96%)	455 (95%)	22 (5%)	0	100	100
1	C	476/499 (95%)	453 (95%)	22 (5%)	1 (0%)	47	71
2	B	508/511 (99%)	496 (98%)	11 (2%)	1 (0%)	47	71
2	D	508/511 (99%)	497 (98%)	9 (2%)	2 (0%)	34	57
All	All	1969/2020 (98%)	1901 (96%)	64 (3%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	ASP
2	D	491	ASP
2	B	294	THR
2	D	294	THR

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	398/413 (96%)	381 (96%)	17 (4%)	29	54
1	C	398/413 (96%)	378 (95%)	20 (5%)	24	47
2	B	427/428 (100%)	418 (98%)	9 (2%)	53	77
2	D	427/428 (100%)	417 (98%)	10 (2%)	50	75
All	All	1650/1682 (98%)	1594 (97%)	56 (3%)	37	63

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	34	GLN
1	A	59	GLU
1	A	104	CYS
1	A	113	ARG
1	A	114	ASN
1	A	124	SER
1	A	304	GLU
1	A	305	LYS
1	A	366	LYS
1	A	371	VAL
1	A	378	HIS
1	A	381	ASN
1	A	430	GLU
1	A	436	LEU
1	A	461	ASP
1	A	481	LEU
2	B	62	SER
2	B	139	LYS
2	B	194	THR
2	B	236	LEU
2	B	246	GLN
2	B	350	LEU
2	B	386	LYS
2	B	479	LEU
2	B	480	ARG
1	C	6	ASP
1	C	34	GLN
1	C	58	SER
1	C	59	GLU
1	C	67	LYS
1	C	104	CYS
1	C	114	ASN
1	C	124	SER
1	C	147	LEU
1	C	304	GLU
1	C	366	LYS
1	C	371	VAL
1	C	378	HIS
1	C	381	ASN
1	C	404	GLN
1	C	411	ARG

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Mol	Chain	Res	Type
1	C	430	GLU
1	C	436	LEU
1	C	461	ASP
1	C	481	LEU
2	D	62	SER
2	D	120	ASP
2	D	139	LYS
2	D	194	THR
2	D	308	THR
2	D	350	LEU
2	D	386	LYS
2	D	480	ARG
2	D	482	LEU
2	D	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	GLN
1	C	448	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 monosaccharides 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	$\#\|Z\| > 2$
4	ICS	C	502	1	18,30,30	3.45	13 (72%)	-		
3	HCA	A	501	-	13,13,13	0.83	0	14,18,18	2.10	4 (28%)
5	CLF	C	503	1,2	0,24,24	-	-	-		
4	ICS	A	502	1	18,30,30	3.06	10 (55%)	-		
3	HCA	C	501	-	13,13,13	0.94	0	14,18,18	1.52	5 (35%)
5	CLF	A	503	1,2	0,24,24	-	-	-		

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	A	501	-	-	3/17/17/17	-
3	HCA	C	501	-	-	7/17/17/17	-
5	CLF	C	503	1,2	-	-	0/12/10/10
5	CLF	A	503	1,2	-	-	0/12/10/10

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S2A-FE2	-6.09	2.17	2.32
4	A	502	ICS	S3B-FE7	-5.49	2.18	2.32
4	A	502	ICS	S2A-FE2	-4.90	2.20	2.32
4	C	502	ICS	S1A-FE2	-4.87	2.20	2.32
4	C	502	ICS	S3B-FE6	-4.59	2.21	2.32
4	C	502	ICS	S4B-FE7	-4.44	2.21	2.32
4	A	502	ICS	S1B-FE6	-4.33	2.21	2.32
4	C	502	ICS	S3B-FE7	-4.26	2.21	2.32
4	A	502	ICS	S2A-FE3	-4.20	2.22	2.32
4	A	502	ICS	S3B-FE6	-4.11	2.22	2.32
4	A	502	ICS	S4B-FE7	-3.95	2.22	2.32
4	C	502	ICS	S1B-FE5	-3.91	2.22	2.32
4	C	502	ICS	S4A-FE3	-3.90	2.22	2.32
4	C	502	ICS	S4B-FE5	-3.89	2.22	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S1B-FE6	-3.49	2.23	2.32
4	A	502	ICS	S1A-FE2	-3.41	2.24	2.32
4	C	502	ICS	S2A-FE3	-3.33	2.24	2.32
4	C	502	ICS	S3A-FE5	3.07	2.32	2.24
4	A	502	ICS	S1B-FE5	-2.83	2.25	2.32
4	A	502	ICS	S4A-FE3	-2.76	2.25	2.32
4	A	502	ICS	S4B-FE5	-2.44	2.26	2.32
4	C	502	ICS	S5A-FE3	-2.14	2.19	2.24
4	C	502	ICS	S2B-FE6	-2.11	2.19	2.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	HCA	O6-C7-C3	5.60	122.78	113.05
3	A	501	HCA	O5-C7-C3	-3.17	117.77	122.25
3	A	501	HCA	O3-C6-C5	-3.08	113.19	123.08
3	C	501	HCA	O7-C3-C7	-2.66	105.13	108.86
3	A	501	HCA	O4-C6-C5	2.29	121.38	114.03
3	C	501	HCA	O1-C1-C2	-2.25	116.36	122.94
3	C	501	HCA	O6-C7-C3	2.16	116.79	113.05
3	C	501	HCA	O2-C1-C2	2.03	120.86	114.35
3	C	501	HCA	O4-C6-C5	2.02	120.52	114.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	A	501	HCA	C7-C3-C4-C5
3	A	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C2-C3-C4-C5
3	C	501	HCA	C7-C3-C4-C5
3	C	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C3-C4-C5-C6
3	C	501	HCA	C4-C5-C6-O4
3	C	501	HCA	C4-C5-C6-O3
3	C	501	HCA	C1-C2-C3-C7

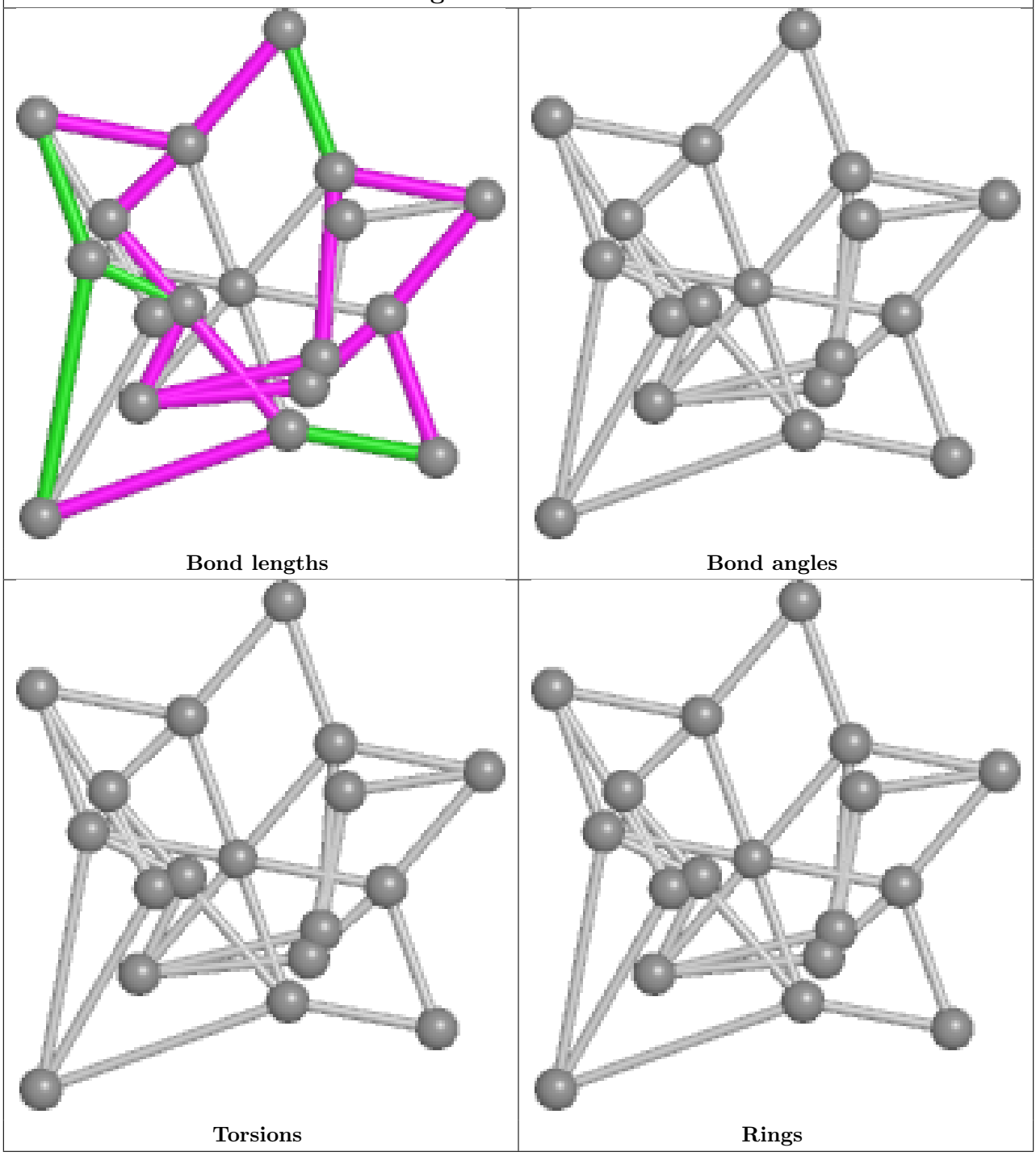
There are no ring outliers.

2 monomers are involved in 2 short contacts:

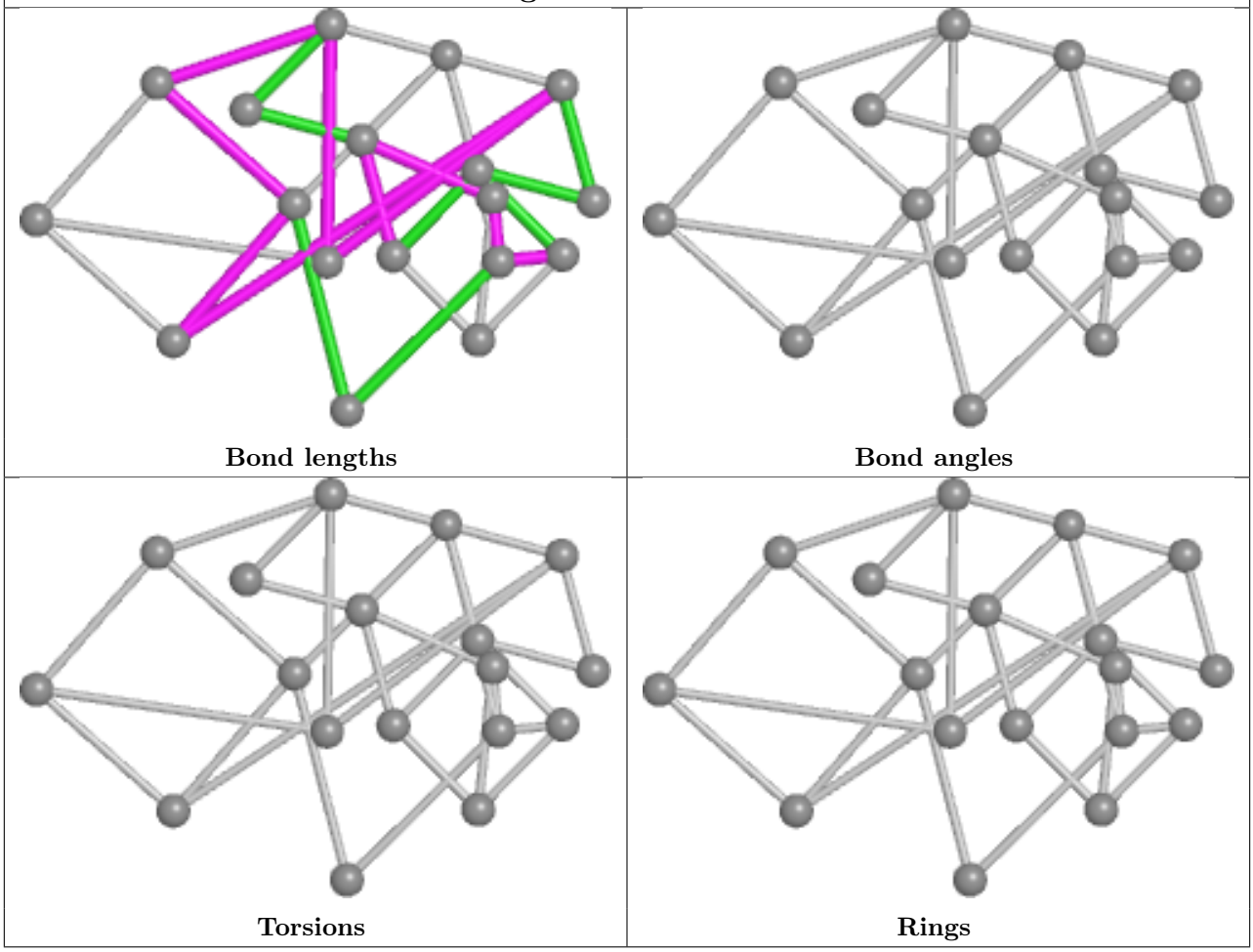
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	1	0
3	C	501	HCA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ICS C 502



Ligand ICS A 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	481/499 (96%)	0.30	6 (1%)	79	76	28, 38, 61, 79	0
1	C	480/499 (96%)	0.44	19 (3%)	38	31	28, 39, 64, 100	0
2	B	510/511 (99%)	0.22	9 (1%)	68	64	25, 36, 56, 76	0
2	D	510/511 (99%)	0.23	5 (0%)	82	80	25, 37, 57, 86	0
All	All	1981/2020 (98%)	0.30	39 (1%)	65	60	25, 38, 59, 100	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	ASP	4.2
2	B	124	PHE	3.8
1	C	224	ASP	3.4
2	D	124	PHE	3.3
1	C	6	ASP	3.3
1	C	226	GLU	3.3
2	B	57	ALA	3.0
1	C	81	ALA	2.9
1	C	57	LEU	2.8
1	C	86	VAL	2.8
2	B	131	VAL	2.8
1	A	57	LEU	2.8
1	C	231	ALA	2.7
1	A	54	GLY	2.7
2	B	6	ASP	2.6
1	C	140	VAL	2.5
1	C	55	VAL	2.5
2	D	97	TYR	2.5
1	C	108	SER	2.4
1	C	141	PHE	2.4
1	A	231	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	55	VAL	2.4
2	D	102	LEU	2.4
2	D	49	TRP	2.3
1	C	8	THR	2.3
1	C	82	GLY	2.3
2	B	37	ASP	2.3
2	D	100	SER	2.2
1	C	188	LYS	2.2
1	C	408	HIS	2.2
1	A	492	LYS	2.2
1	C	230	ALA	2.1
1	C	225	GLY	2.1
2	B	126	GLY	2.1
2	B	128	ASN	2.1
2	B	210	GLY	2.0
1	A	85	GLY	2.0
1	C	58	SER	2.0
2	B	35	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no 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(Å^2)	Q<0.9
6	FE	B	601	1/1	0.91	0.06	81,81,81,81	0
6	FE	D	601	1/1	0.92	0.09	62,62,62,62	0
5	CLF	C	503	15/15	0.94	0.10	34,38,49,54	0
5	CLF	A	503	15/15	0.95	0.10	28,34,38,44	2
3	HCA	A	501	14/14	0.97	0.19	28,33,38,43	0

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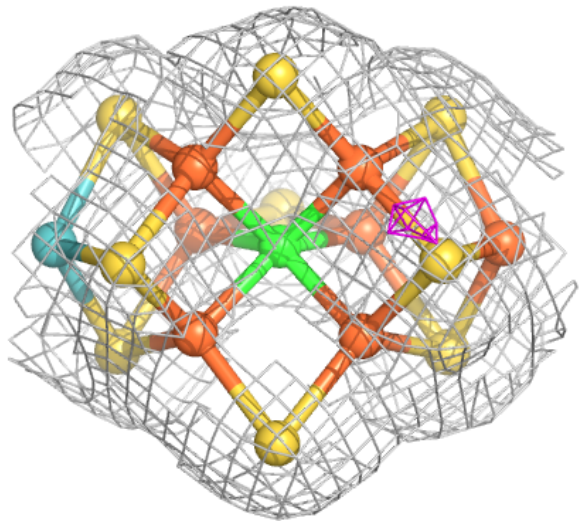
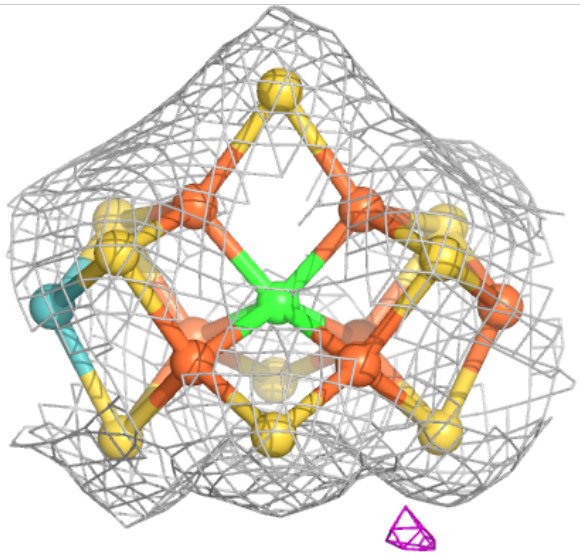
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HCA	C	501	14/14	0.97	0.22	31,37,39,43	0
4	ICS	A	502	18/18	0.99	0.11	27,32,34,37	0
4	ICS	C	502	18/18	0.99	0.11	31,34,38,40	0

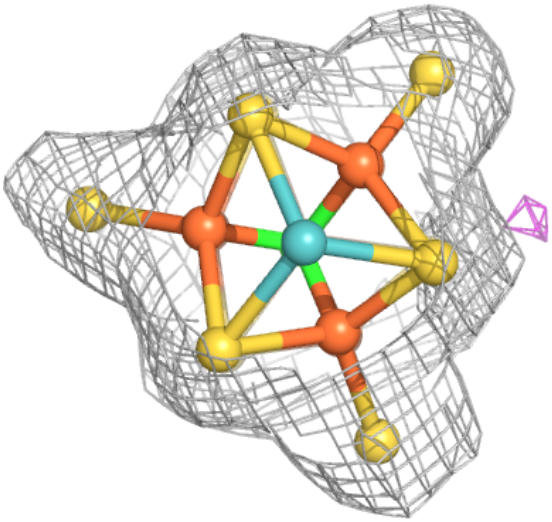
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ICS 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)

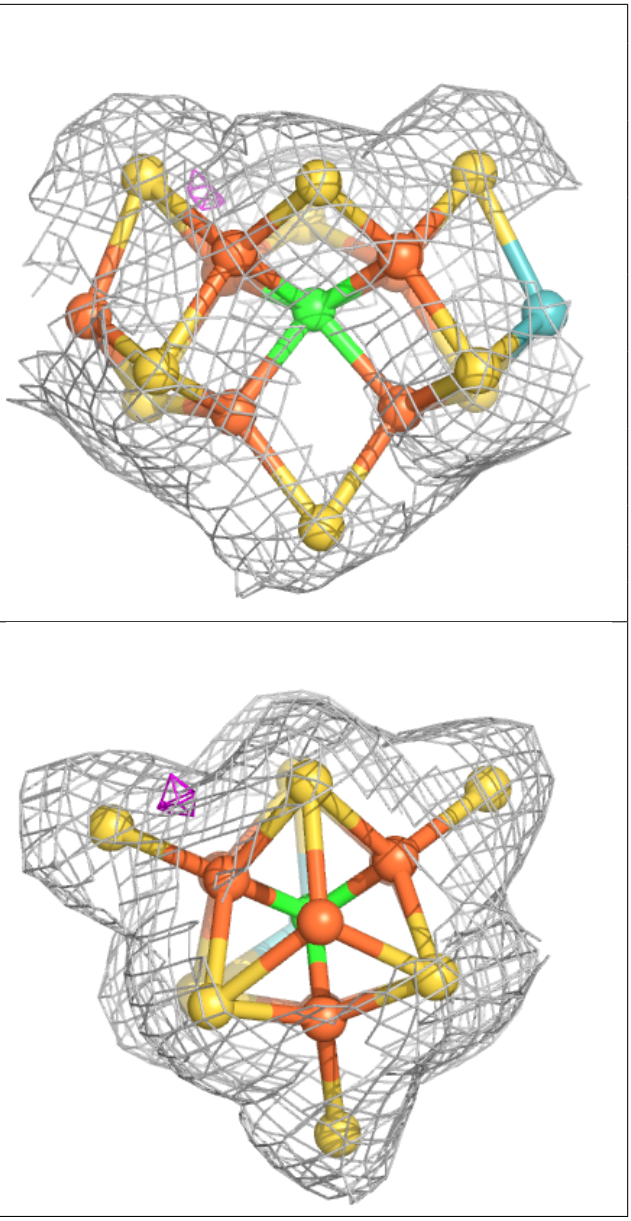






Electron density around ICS C 502:

$2mF_o$-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.