Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 05:32 PM EDT

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 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:

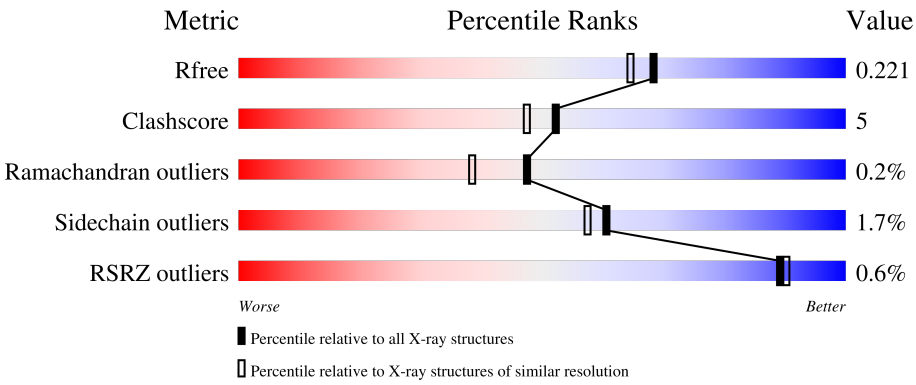
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 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 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	477	% 88% 11% •
1	C	477	% 91% 9% •
2	B	522	92% 8%
2	D	522	90% 10%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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.

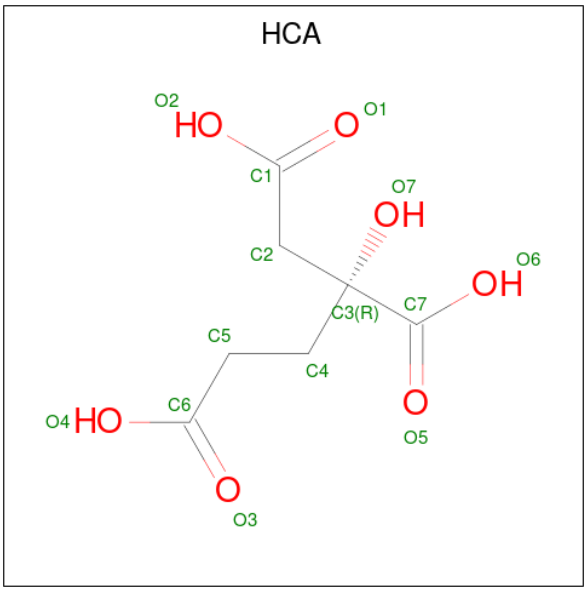
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

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

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

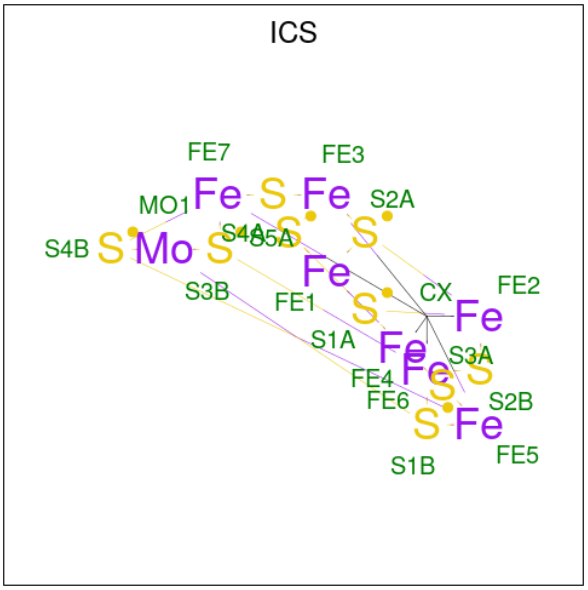
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4149	2651	699	771	28	0	0	0
2	D	522	4154	2654	699	773	28	0	0	0

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



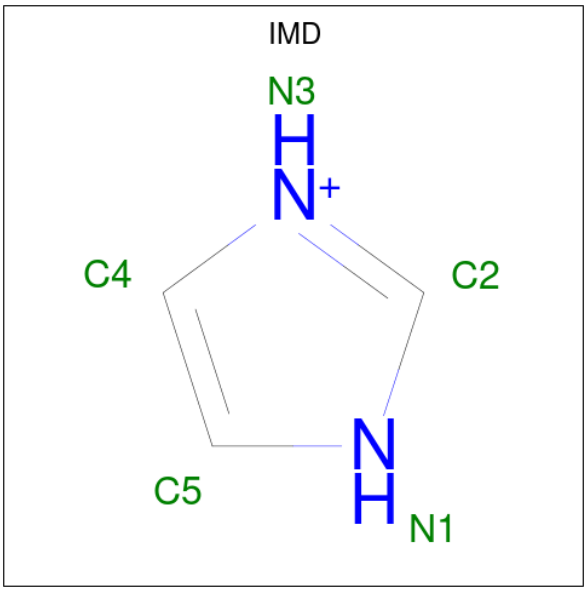
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	14	7	7	0	0
			Total	C	O		
3	C	1	14	7	7	0	0

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



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

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

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

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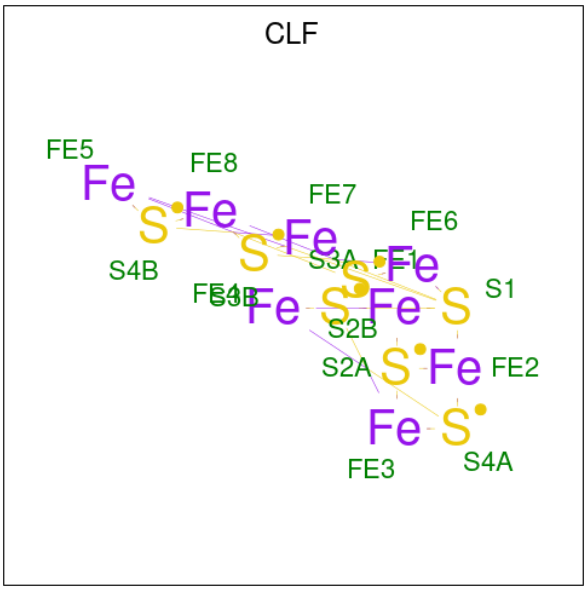
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Se 1 1	0	0

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

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

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



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

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

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

- Molecule 10 is water.

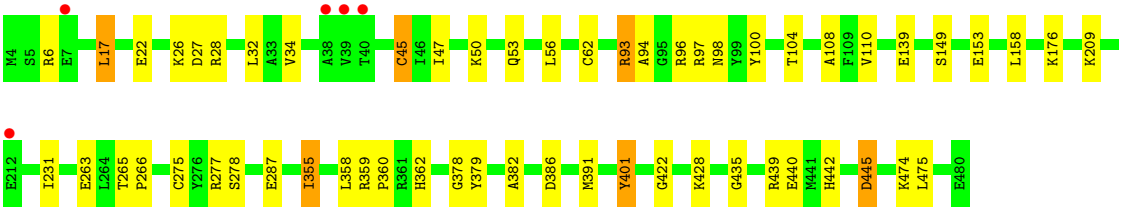
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	248	248	248	0	0
			Total	O		
10	B	337	337	337	0	0
			Total	O		
10	C	240	240	240	0	0
			Total	O		
10	D	321	321	321	0	0

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.

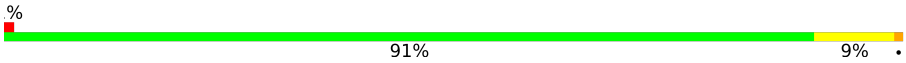
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

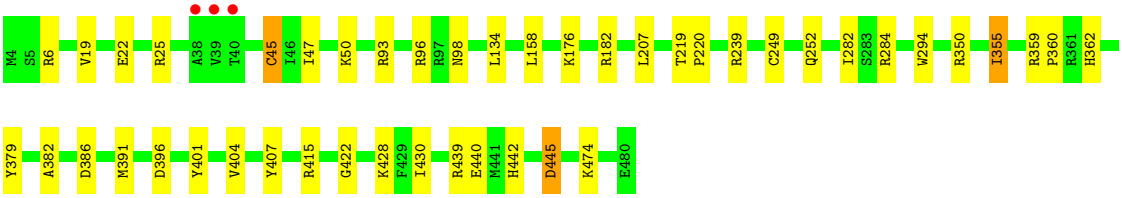
Chain A:



• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

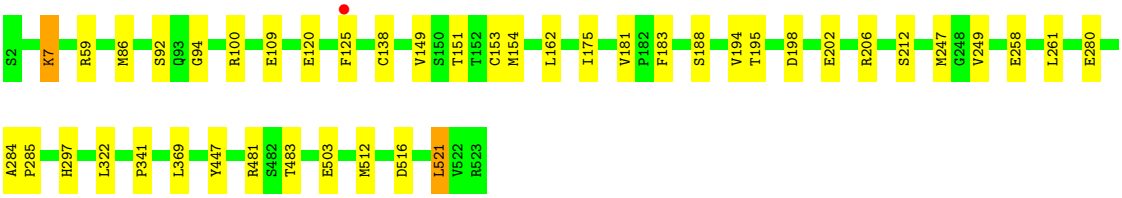
Chain C:





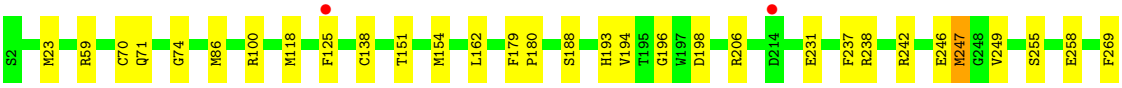
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

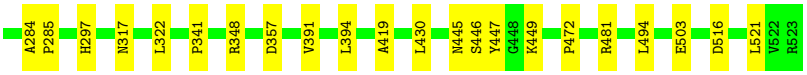
Chain B:



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:




A284
P285
H297
N317
L322
P341
R348
D357
V391
L394
A419
L430
N445
S446
Y447
G448
K449
P472
R481
L494
E503
D516
L521
V522
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	80.76Å 130.38Å 106.90Å 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
$< I/\sigma(I) >$ [1]	3.20 (at 1.89Å)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: MG, IMD, ICS, HCA, CA, SE, 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	0.65	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.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	A	277	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	277	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (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	182	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	96	ARG	Sidechain
2	D	206	ARG	Sidechain
2	D	238	ARG	Sidechain
2	D	59	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
4:C:502:ICS:S1B	10:C:811:HOH:O	2.03	1.16
1:A:445:ASP:OD1	10:A:601:HOH:O	1.69	1.10
1:C:379:TYR:CE2	10:C:629:HOH:O	2.05	1.09
1:C:360:PRO:HD2	10:C:629:HOH:O	1.54	1.04
1:C:284:ARG:HG2	10:C:683:HOH:O	1.60	1.02
1:C:428:LYS:HD2	10:C:636:HOH:O	1.60	1.01
2:D:447:TYR:CE1	10:D:990:HOH:O	2.13	1.00
10:B:1007:HOH:O	2:D:521:LEU:CD1	2.09	0.98
10:C:815:HOH:O	2:D:23:MET:HG2	1.63	0.98
1:C:93:ARG:HG3	10:C:611:HOH:O	1.65	0.97
2:B:447:TYR:CE1	10:B:1007:HOH:O	2.21	0.94
1:C:440:GLU:CG	10:C:636:HOH:O	2.18	0.92
2:D:446:SER:O	10:D:701:HOH:O	1.88	0.91
10:C:815:HOH:O	2:D:23:MET:CE	2.19	0.89
1:A:93:ARG:C	10:A:602:HOH:O	2.09	0.89
1:C:360:PRO:CD	10:C:629:HOH:O	2.14	0.88
1:C:445:ASP:OD1	10:C:601:HOH:O	1.92	0.86
2:D:449:LYS:HG2	10:D:701:HOH:O	1.73	0.86
1:C:428:LYS:CD	10:C:636:HOH:O	2.18	0.85
1:A:442:HIS:CG	10:A:605:HOH:O	2.30	0.84
1:A:442:HIS:CB	10:A:605:HOH:O	2.23	0.84
4:C:502:ICS:S5A	10:C:614:HOH:O	2.34	0.83
10:B:1007:HOH:O	2:D:521:LEU:HD11	1.74	0.81
1:C:45:CYS:SG	1:C:391:MET:CE	2.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ARG:CG	10:C:683:HOH:O	2.20	0.77
5:B:607:IMD:H4	10:B:891:HOH:O	1.84	0.76
1:C:6:ARG:NH2	1:C:396:ASP:OD1	2.20	0.75
1:C:440:GLU:HG2	10:C:636:HOH:O	1.85	0.75
1:A:445:ASP:CG	10:A:601:HOH:O	2.18	0.74
2:B:521:LEU:CG	10:D:990:HOH:O	2.28	0.74
1:C:45:CYS:SG	1:C:391:MET:HE1	2.30	0.72
2:D:447:TYR:CD1	10:D:990:HOH:O	2.36	0.71
1:C:249:CYS:CB	10:C:818:HOH:O	2.03	0.70
1:C:415:ARG:NE	1:C:415:ARG:NH1	2.39	0.69
2:B:521:LEU:CD1	10:D:990:HOH:O	2.04	0.69
4:C:502:ICS:S4B	10:C:730:HOH:O	2.50	0.68
2:B:280:GLU:OE1	5:B:606:IMD:H5	1.94	0.68
10:A:614:HOH:O	8:B:602:CLF:S1	2.52	0.68
1:C:45:CYS:SG	1:C:391:MET:HE2	2.34	0.67
1:C:440:GLU:CD	10:C:636:HOH:O	2.33	0.67
1:A:94:ALA:HB3	10:A:602:HOH:O	1.94	0.67
2:B:521:LEU:HD21	10:D:990:HOH:O	1.95	0.67
2:B:447:TYR:CD1	10:B:1007:HOH:O	2.47	0.65
2:D:503:GLU:OE1	2:D:503:GLU:OE2	2.13	0.65
1:A:93:ARG:O	10:A:602:HOH:O	2.12	0.65
1:A:47:ILE:HD12	1:A:50:LYS:HG3	1.78	0.64
10:C:815:HOH:O	2:D:23:MET:CG	2.31	0.63
1:A:93:ARG:CZ	10:A:607:HOH:O	2.47	0.62
8:B:602:CLF:FE1	8:B:602:CLF:S2A	1.92	0.61
4:A:502:ICS:S1A	10:A:801:HOH:O	2.56	0.61
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.84	0.60
1:A:474:LYS:HB3	2:D:322:LEU:HD21	1.82	0.60
1:A:94:ALA:CB	10:A:602:HOH:O	2.49	0.59
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.84	0.59
5:C:504:IMD:H4	10:C:679:HOH:O	2.03	0.58
1:A:93:ARG:NE	10:A:607:HOH:O	2.36	0.57
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.86	0.56
1:A:45:CYS:SG	1:A:391:MET:CE	2.93	0.56
2:B:198:ASP:HB2	2:B:297:HIS:O	2.05	0.56
1:C:22:GLU:OE1	1:C:25:ARG:NH2	2.28	0.56
1:A:27:ASP:OD1	10:A:603:HOH:O	2.17	0.56
5:C:504:IMD:C4	10:C:679:HOH:O	2.54	0.56
2:B:503:GLU:OE1	2:B:503:GLU:CG	2.54	0.55
2:D:503:GLU:OE1	2:D:503:GLU:CG	2.54	0.55
1:A:445:ASP:OD2	10:A:601:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:MET:HG3	2:D:341:PRO:HD3	1.89	0.55
2:D:494:LEU:HD23	2:D:494:LEU:C	2.27	0.53
2:D:242:ARG:HD3	2:D:246:GLU:OE2	2.08	0.53
1:A:278:SER:HB3	10:A:801:HOH:O	2.08	0.53
2:D:198:ASP:HB2	2:D:297:HIS:O	2.09	0.53
2:D:317:ASN:ND2	10:D:704:HOH:O	2.39	0.53
10:C:815:HOH:O	2:D:23:MET:HE3	1.94	0.53
1:A:442:HIS:HB2	10:A:641:HOH:O	2.08	0.53
1:C:360:PRO:CB	10:C:629:HOH:O	2.56	0.53
1:A:209:LYS:NZ	1:A:263:GLU:OE2	2.41	0.53
1:A:45:CYS:SG	1:A:391:MET:HE2	2.48	0.52
1:C:239:ARG:HD3	10:C:815:HOH:O	2.08	0.52
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.09	0.52
1:C:442:HIS:HE1	10:C:744:HOH:O	1.91	0.52
10:C:815:HOH:O	2:D:23:MET:SD	2.59	0.52
1:C:428:LYS:HD3	10:C:636:HOH:O	1.98	0.52
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.91	0.52
1:A:97:ARG:O	1:A:231:ILE:HA	2.09	0.52
1:C:442:HIS:CD2	3:C:501:HCA:H52	2.45	0.52
1:C:442:HIS:CE1	10:C:744:HOH:O	2.62	0.52
2:D:118:MET:HB2	2:D:154:MET:HE1	1.93	0.51
2:D:194:VAL:HB	2:D:297:HIS:CG	2.46	0.51
1:C:19:VAL:HG11	1:C:407:TYR:CE2	2.46	0.51
2:D:242:ARG:CD	2:D:246:GLU:OE2	2.59	0.51
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.93	0.51
2:B:120:GLU:OE2	5:B:604:IMD:H2	2.11	0.51
5:B:606:IMD:H2	10:B:1003:HOH:O	2.11	0.50
1:A:265:THR:N	1:A:266:PRO:CD	2.74	0.50
1:C:294:TRP:O	5:C:503:IMD:H2	2.12	0.49
1:C:359:ARG:NH2	10:C:614:HOH:O	2.44	0.49
1:C:428:LYS:NZ	10:C:602:HOH:O	2.18	0.49
1:C:422:GLY:HA2	1:C:439:ARG:O	2.13	0.49
3:C:501:HCA:O7	3:C:501:HCA:O1	2.31	0.49
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.47	0.49
1:C:219:THR:HB	1:C:220:PRO:HD2	1.94	0.49
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.94	0.48
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.95	0.48
1:C:442:HIS:CG	3:C:501:HCA:H52	2.48	0.48
1:A:209:LYS:HE3	1:A:263:GLU:OE2	2.13	0.48
1:A:209:LYS:CE	1:A:263:GLU:OE2	2.62	0.47
1:C:360:PRO:CG	10:C:629:HOH:O	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:MET:CB	2:D:154:MET:HE1	2.45	0.47
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.96	0.47
1:C:360:PRO:HB2	10:C:629:HOH:O	2.12	0.47
1:C:239:ARG:HD2	1:C:252:GLN:OE1	2.15	0.47
1:A:153:GLU:HB3	10:A:614:HOH:O	2.13	0.46
1:A:428:LYS:HE3	10:A:667:HOH:O	2.14	0.46
2:D:70:CYS:HB2	2:D:188:SER:HB2	1.98	0.46
2:B:194:VAL:HB	2:B:297:HIS:CG	2.50	0.46
1:C:445:ASP:CG	10:C:601:HOH:O	2.47	0.46
2:D:86:MET:HG2	2:D:138:CYS:SG	2.55	0.46
1:A:442:HIS:HB2	10:A:605:HOH:O	2.06	0.46
1:C:158:LEU:HD11	2:D:154:MET:HG3	1.98	0.45
1:C:359:ARG:N	1:C:360:PRO:CD	2.79	0.45
2:B:153:CYS:HB3	2:B:188:SER:OG	2.17	0.45
2:B:202:GLU:OE2	2:B:206:ARG:NH2	2.44	0.45
1:C:379:TYR:CD2	1:C:382:ALA:HB2	2.51	0.45
2:B:284:ALA:N	2:B:285:PRO:CD	2.80	0.45
2:B:92:SER:HB3	10:B:867:HOH:O	2.16	0.44
1:A:378:GLY:HA3	1:A:401:TYR:O	2.16	0.44
1:C:47:ILE:HG23	1:C:50:LYS:HE2	1.98	0.44
1:A:158:LEU:HD11	2:B:154:MET:HG3	1.98	0.44
1:C:440:GLU:HG3	10:C:601:HOH:O	2.16	0.44
2:D:357:ASP:HA	10:D:806:HOH:O	2.17	0.44
1:A:422:GLY:HA2	1:A:439:ARG:O	2.18	0.44
1:A:435:GLY:CA	1:A:475:LEU:HD22	2.47	0.44
1:A:440:GLU:HG3	10:A:601:HOH:O	2.18	0.44
2:B:86:MET:HG2	2:B:138:CYS:SG	2.58	0.43
2:B:109:GLU:OE1	10:B:701:HOH:O	2.21	0.43
2:B:247:MET:HB3	2:B:249:VAL:HG23	2.00	0.43
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.99	0.43
1:A:93:ARG:CD	10:A:607:HOH:O	2.66	0.43
1:C:207:LEU:HD22	1:C:282:ILE:HD11	2.00	0.43
1:A:442:HIS:HB3	10:A:605:HOH:O	2.06	0.43
2:B:7:LYS:HE3	10:B:996:HOH:O	2.17	0.43
1:A:22:GLU:HG3	1:A:26:LYS:HE3	2.01	0.42
1:C:134:LEU:C	1:C:134:LEU:HD23	2.40	0.42
2:B:149:VAL:O	2:B:183:PHE:HA	2.19	0.42
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.54	0.42
1:A:139:GLU:OE2	1:A:176:LYS:HE3	2.20	0.42
1:A:6:ARG:HG3	1:A:34:VAL:HG11	2.01	0.42
1:A:62:CYS:HB3	2:B:94:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:HA	1:A:108:ALA:O	2.20	0.42
1:A:17:LEU:HD21	1:A:32:LEU:CD1	2.50	0.42
1:A:17:LEU:HD23	1:A:17:LEU:N	2.36	0.41
1:A:47:ILE:HD11	10:A:603:HOH:O	2.19	0.41
2:D:284:ALA:N	2:D:285:PRO:CD	2.84	0.41
2:B:175:ILE:HD13	2:B:181:VAL:HG21	2.03	0.41
2:B:483:THR:O	5:B:603:IMD:H5	2.19	0.41
1:A:379:TYR:CD2	1:A:382:ALA:HB2	2.56	0.41
2:B:109:GLU:HG3	2:B:261:LEU:O	2.21	0.41
1:A:275:CYS:HA	1:A:358:LEU:HD22	2.03	0.41
1:C:294:TRP:HZ2	10:C:683:HOH:O	2.02	0.41
2:D:445:ASN:HB2	2:D:472:PRO:O	2.21	0.41
2:B:512:MET:HE2	2:B:512:MET:HB2	1.93	0.41
2:D:391:VAL:HA	2:D:419:ALA:HA	2.02	0.41
2:D:179:PHE:HA	2:D:180:PRO:HD3	1.92	0.40
2:D:71:GLN:O	2:D:196:GLY:HA3	2.21	0.40
1:A:287:GLU:OE1	10:A:604:HOH:O	2.22	0.40
1:A:359:ARG:N	1:A:360:PRO:CD	2.85	0.40
1:C:430:ILE:HG23	2:D:269:PHE:CG	2.57	0.40
2:D:74:GLY:HA3	2:D:193:HIS:O	2.22	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	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

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	45	CYS
1	A	98	ASN
1	A	149	SER
1	A	355	ILE
1	A	362	HIS
1	A	401	TYR
1	A	445	ASP
2	B	7	LYS
2	B	125	PHE
2	B	195	THR
2	B	212	SER
2	B	258	GLU
2	B	369	LEU
2	B	516	ASP
2	B	521	LEU
1	C	45	CYS

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	176	LYS
1	C	355	ILE
1	C	362	HIS
1	C	401	TYR
1	C	404	VAL
1	C	445	ASP
2	D	125	PHE
2	D	247	MET
2	D	258	GLU
2	D	516	ASP

Sometimes 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 (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 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	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
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	C	501	-	13,13,13	1.37	1 (7%)	14,18,18	1.36	2 (14%)
5	IMD	A	503	-	3,5,5	0.23	0	4,5,5	0.74	0
5	IMD	D	602	-	3,5,5	0.29	0	4,5,5	0.83	0
8	CLF	B	602	1,10,2	0,24,24	-	-	-		
4	ICS	C	502	1,10,6	12,28,30	2.69	6 (50%)	-		
5	IMD	B	604	-	3,5,5	0.28	0	4,5,5	0.57	0
5	IMD	C	503	-	3,5,5	0.35	0	4,5,5	0.63	0
5	IMD	D	605	-	3,5,5	0.35	0	4,5,5	0.63	0
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%)	-		
3	HCA	A	501	-	13,13,13	0.96	0	14,18,18	2.76	5 (35%)
5	IMD	C	504	-	3,5,5	0.32	0	4,5,5	0.72	0
8	CLF	D	603	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
5	IMD	B	603	-	-	-	0/1/1/1
5	IMD	A	504	-	-	-	0/1/1/1
5	IMD	B	607	-	-	-	0/1/1/1
5	IMD	D	604	-	-	-	0/1/1/1
3	HCA	C	501	-	-	5/17/17/17	-
5	IMD	A	503	-	-	-	0/1/1/1
5	IMD	D	602	-	-	-	0/1/1/1
8	CLF	B	602	1,10,2	-	-	0/12/10/10
5	IMD	C	503	-	-	-	0/1/1/1
5	IMD	D	605	-	-	-	0/1/1/1
5	IMD	B	606	-	-	-	0/1/1/1
5	IMD	B	604	-	-	-	0/1/1/1
3	HCA	A	501	-	-	6/17/17/17	-
5	IMD	C	504	-	-	-	0/1/1/1
8	CLF	D	603	1,2	-	-	0/12/10/10

All (13) 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
4	C	502	ICS	S4B-FE5	-4.06	2.22	2.32
4	C	502	ICS	S3B-FE7	-3.94	2.22	2.32
4	C	502	ICS	S1A-FE4	-3.77	2.23	2.32
4	A	502	ICS	S2A-FE3	-3.30	2.24	2.32
4	C	502	ICS	S5A-FE3	-3.16	2.17	2.24
4	A	502	ICS	S4B-FE7	-3.04	2.24	2.32
3	C	501	HCA	C2-C3	2.76	1.57	1.53
4	C	502	ICS	S3A-FE4	2.27	2.30	2.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	HCA	O5-C7-C3	-5.18	114.92	122.25
3	A	501	HCA	O7-C3-C7	-5.06	101.76	108.86
3	A	501	HCA	O6-C7-C3	4.56	120.98	113.05
3	A	501	HCA	C4-C5-C6	3.48	120.64	112.75
3	A	501	HCA	O3-C6-C5	-2.83	113.99	123.08
3	C	501	HCA	O6-C7-C3	2.48	117.36	113.05
3	C	501	HCA	O5-C7-C3	-2.30	119.00	122.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	C	501	HCA	C2-C3-C4-C5
3	A	501	HCA	C7-C3-C4-C5
3	C	501	HCA	C7-C3-C4-C5
3	C	501	HCA	C1-C2-C3-C4
3	C	501	HCA	O7-C3-C4-C5
3	A	501	HCA	O1-C1-C2-C3
3	A	501	HCA	O2-C1-C2-C3
3	C	501	HCA	C1-C2-C3-C7
3	A	501	HCA	C4-C5-C6-O4
3	A	501	HCA	C4-C5-C6-O3

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	603	IMD	1	0
5	B	607	IMD	1	0
3	C	501	HCA	4	0
8	B	602	CLF	2	0
4	C	502	ICS	3	0
5	B	604	IMD	1	0
5	C	503	IMD	1	0
5	B	606	IMD	2	0
4	A	502	ICS	1	0
5	C	504	IMD	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.

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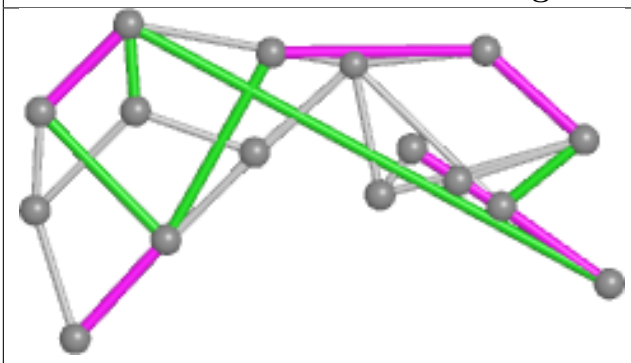
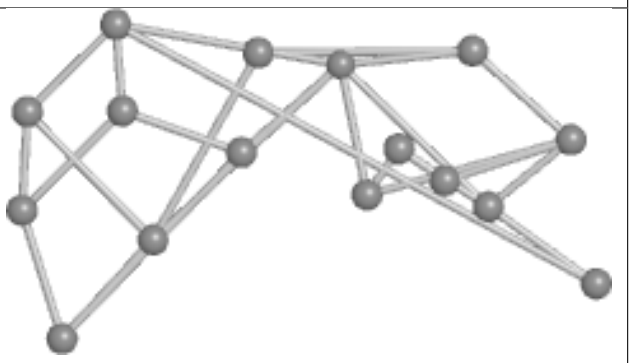
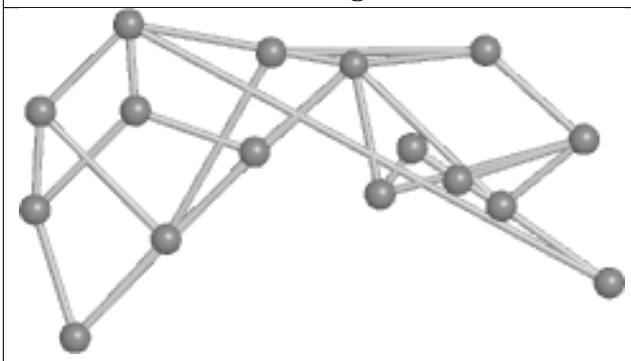


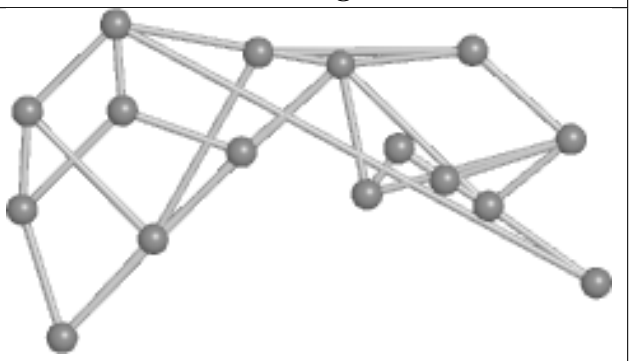
Bond lengths



Bond angles

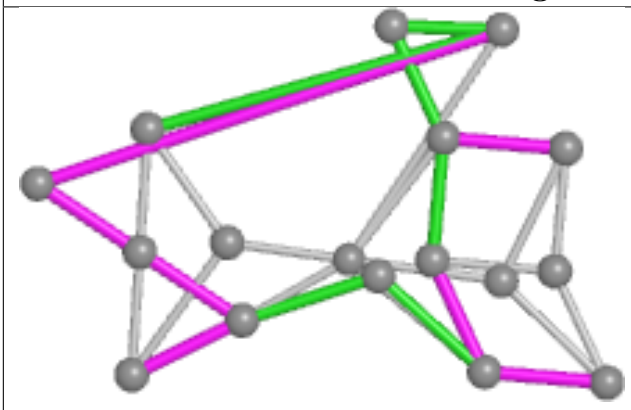


Torsions

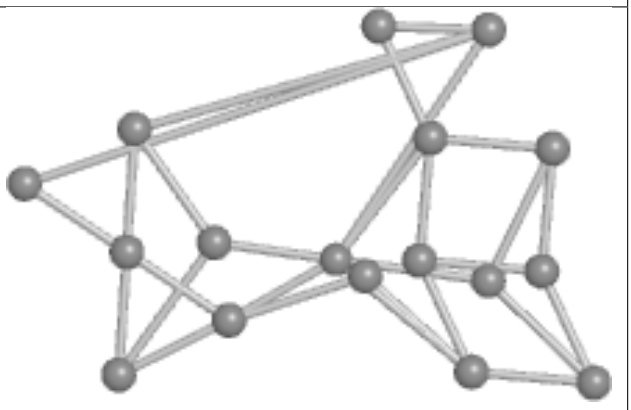


Rings

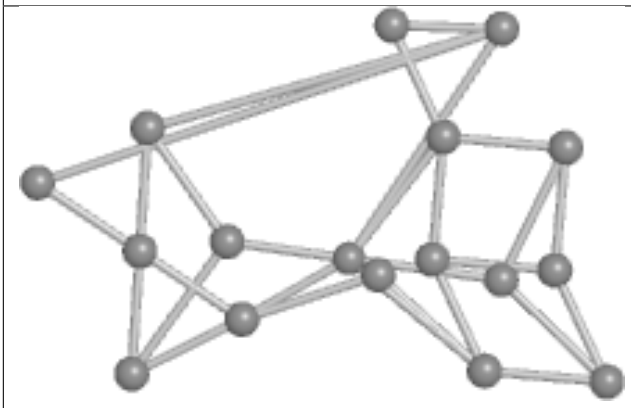
Ligand ICS A 502



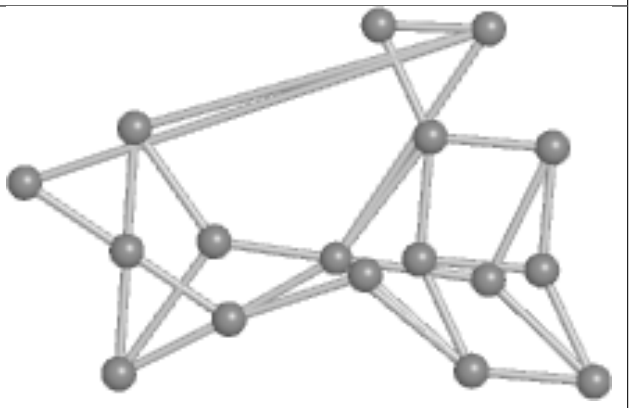
Bond lengths



Bond angles



Torsions



Rings

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

All (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
1	C	40	THR	2.5
1	A	39	VAL	2.4
1	A	38	ALA	2.3
1	A	7	GLU	2.3
1	A	212	GLU	2.2
1	A	40	THR	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)

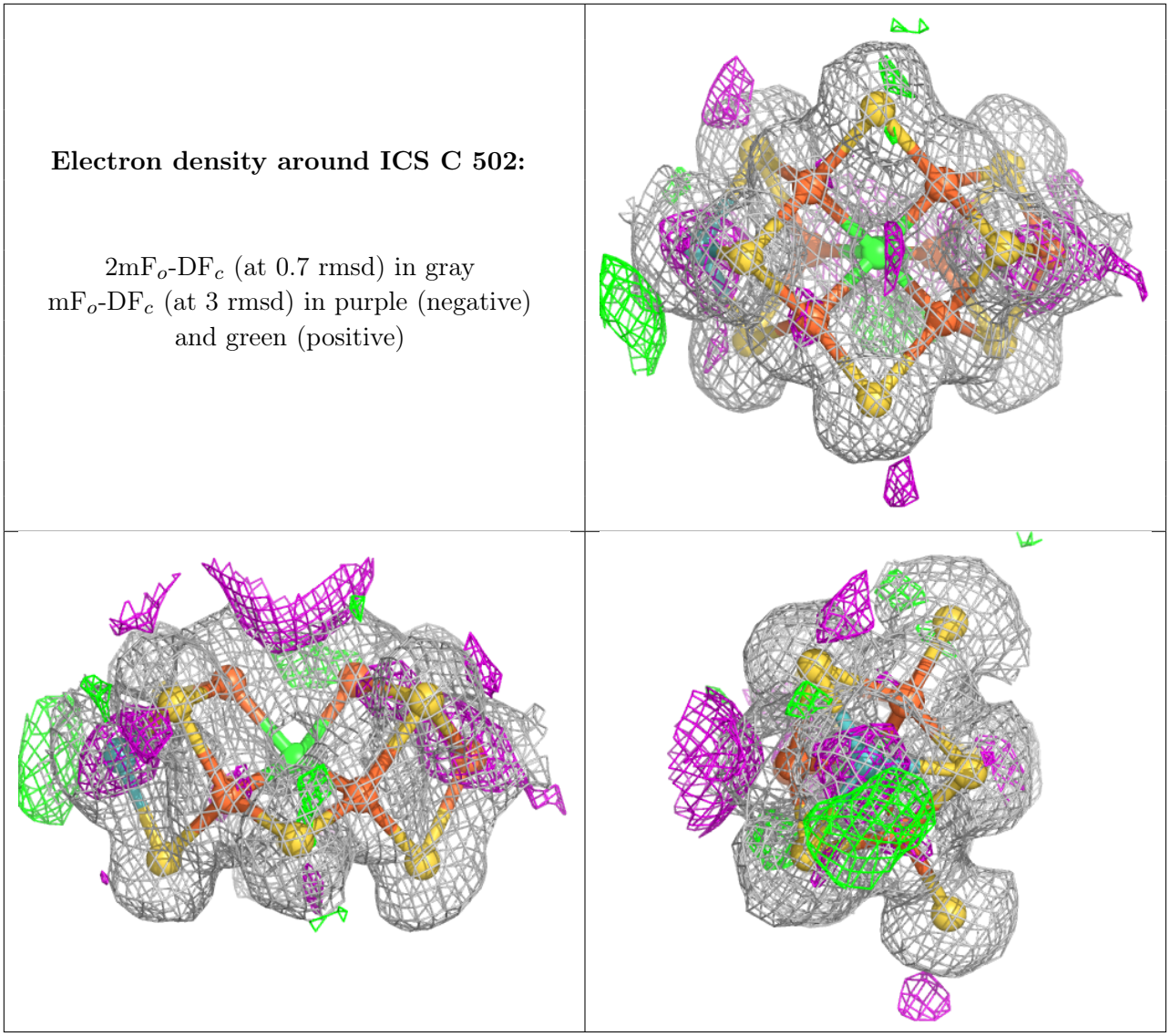
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
7	CA	B	601	1/1	0.95	0.06	36,36,36,36	0
3	HCA	C	501	14/14	0.95	0.10	9,11,13,13	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	B	602	15/15	0.97	0.07	7,8,10,12	0
8	CLF	D	603	15/15	0.97	0.06	8,9,10,13	0
6	SE	A	505	1/1	0.99	0.16	11,11,11,11	0
6	SE	C	505	1/1	0.99	0.18	14,14,14,14	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

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.

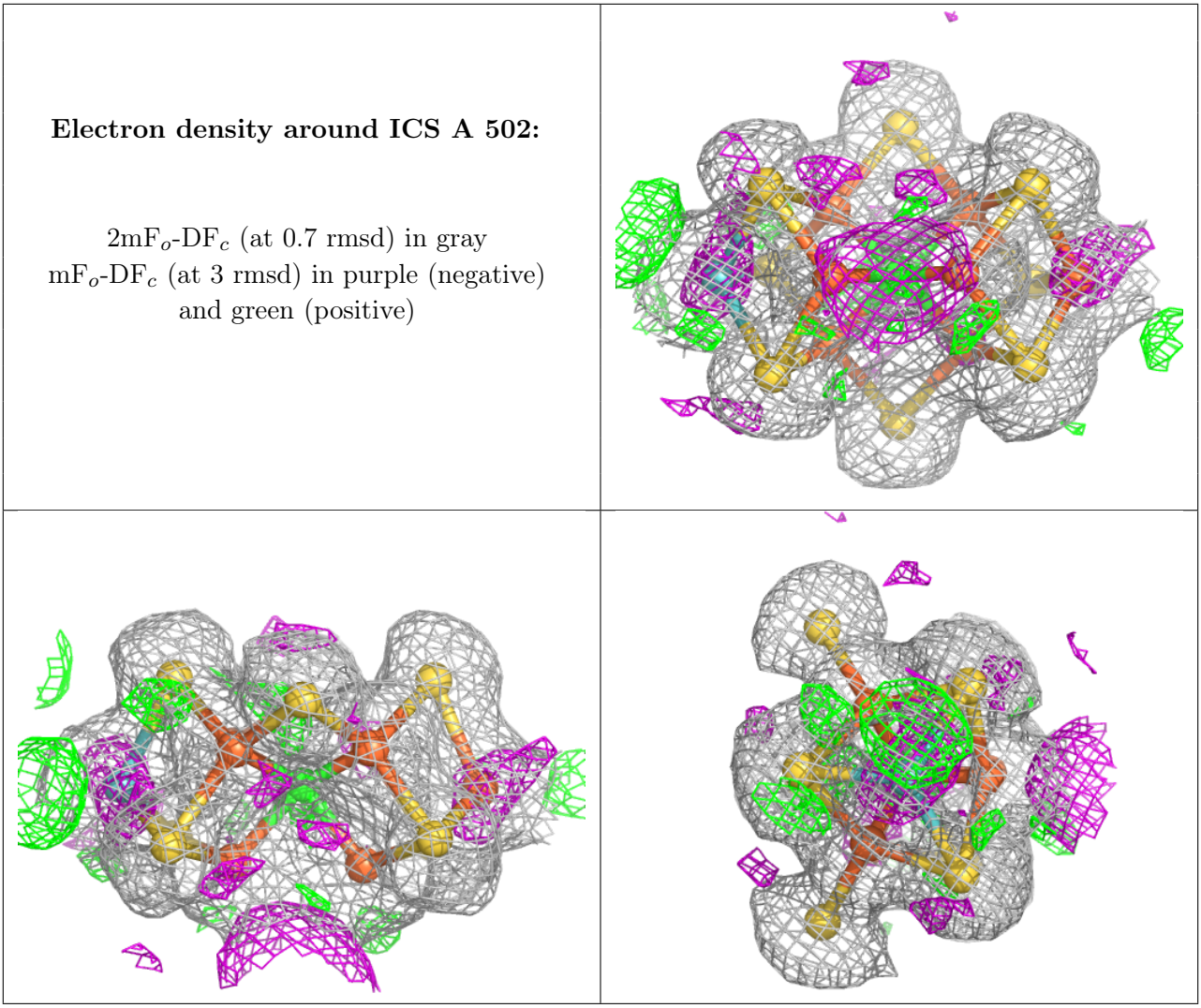
Electron density around ICS C 502:

$2mF_o$-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.