Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:10 PM EDT

PDB ID	:	6OP3 / pdb_00006op3
Title	:	Selenium incorporated FeMo-cofactor of nitrogenase from Azotobacter vinelandii with low concentration of selenium
Authors	:	Arias, R.J.; Rees, D.C.
Deposited on	:	2019-04-24
Resolution	:	1.60 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 ⓘ 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 ⓘ) were used in the production of this report:

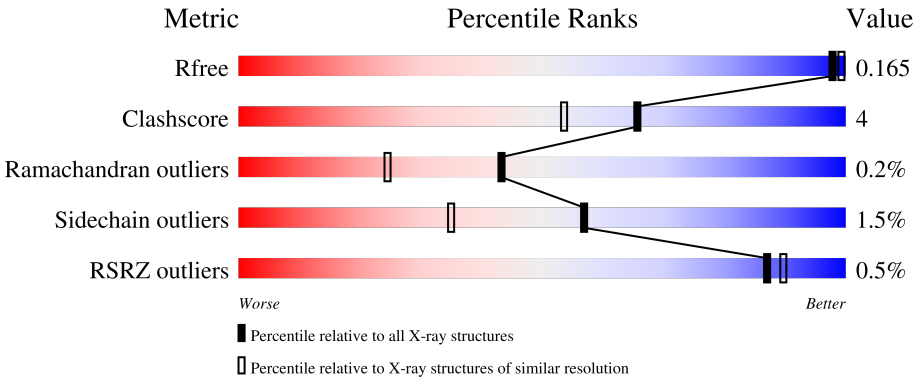
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	477	90% 10%
1	C	477	92% 8%
2	B	522	91% 7%
2	D	522	91% 9%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18377 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.

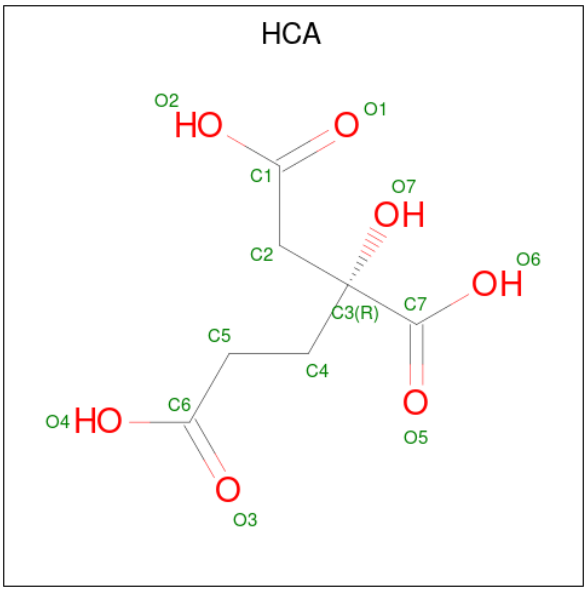
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	6	0
			3842	2442	656	718	26			
1	C	477	Total	C	N	O	S	0	6	0
			3819	2429	654	710	26			

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

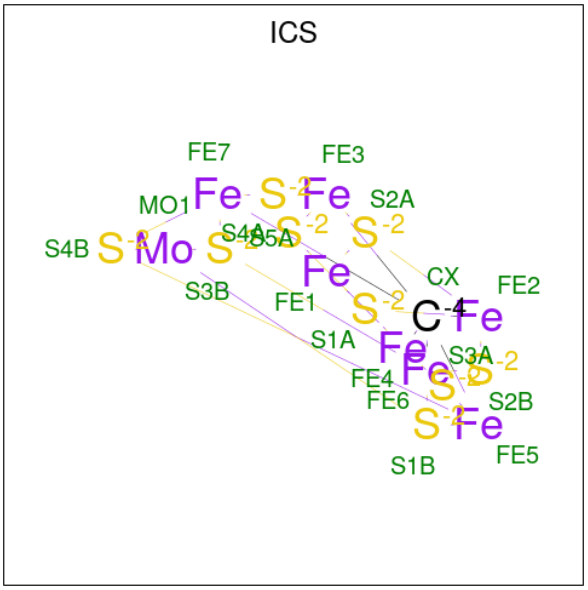
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	7	0
			4213	2690	712	783	28			
2	D	522	Total	C	N	O	S	0	4	0
			4193	2678	704	781	30			

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



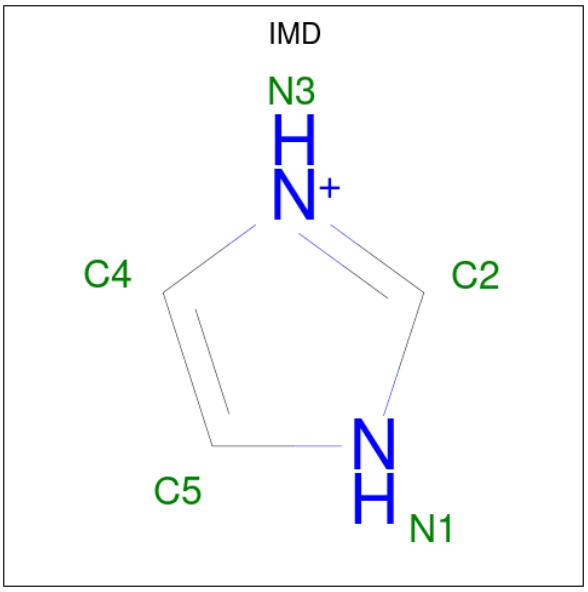
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 14 7 7	0	0
3	C	1	Total C O 14 7 7	0	0

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



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

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).

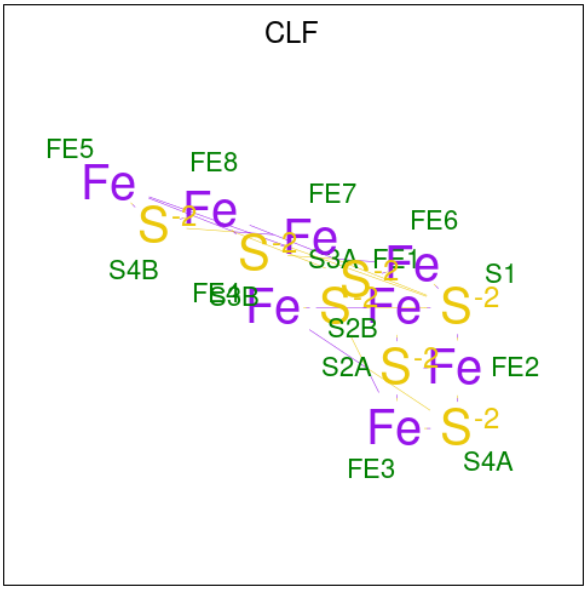


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	A	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0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

- Molecule 6 is SELENIUM ATOM (CCD ID: SE) (formula: Se).

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

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



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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Ca 1 1	0	0
9	D	2	Total Ca 2 2	0	0

- Molecule 10 is water.

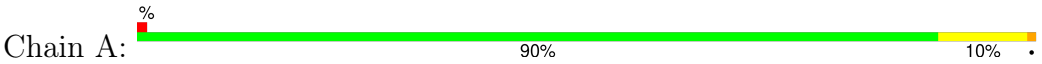
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	466	Total O 466 466	0	0
10	B	604	Total O 604 604	0	0
10	C	477	Total O 477 477	0	0
10	D	603	Total O 603 603	0	0

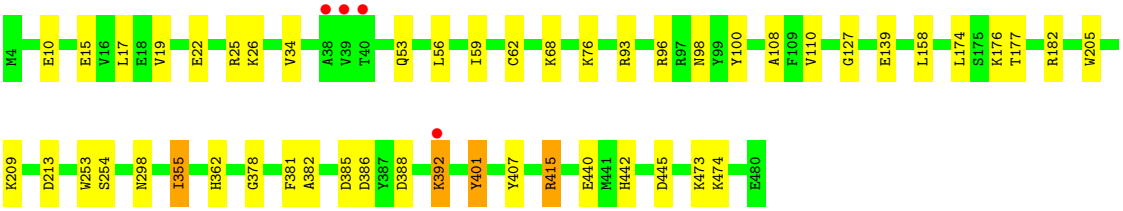
3 Residue-property plots (i)

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

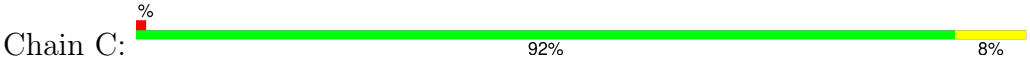
Chain A:

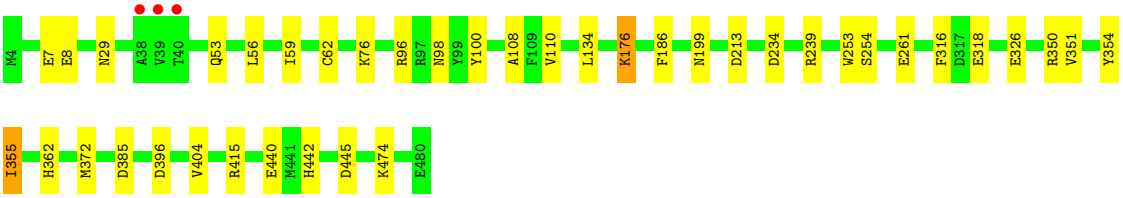




• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

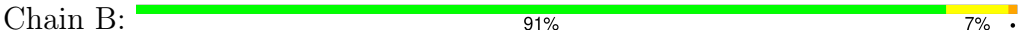
Chain C:

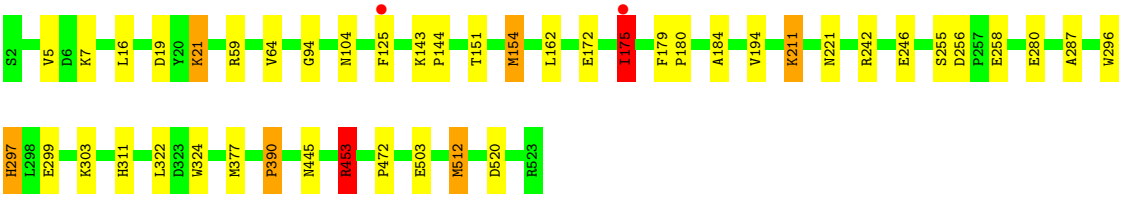




• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

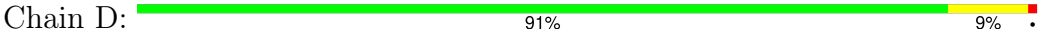
Chain B:





• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D:






E258
A287
H297
E306
L322
D323
P341
V391
R401
R453
H457
K458
H477
L494
E503
M512
Q513
A514
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	80.87Å 131.02Å 106.96Å 90.00° 110.62° 90.00°	Depositor
Resolution (Å)	37.85 – 1.60 37.85 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.85-1.60) 98.6 (37.85-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.127 , 0.152 0.142 , 0.165	Depositor DCC
R_{free} test set	13417 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	10.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18377	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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

5.1 Standard geometry

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

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	1.01	5/3931 (0.1%)	1.09	3/5298 (0.1%)
1	C	1.00	2/3903 (0.1%)	1.09	6/5261 (0.1%)
2	B	1.02	6/4315 (0.1%)	1.11	15/5831 (0.3%)
2	D	1.02	4/4299 (0.1%)	1.12	10/5814 (0.2%)
All	All	1.01	17/16448 (0.1%)	1.10	34/22204 (0.2%)

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	2
2	B	0	3
2	D	0	3
All	All	0	10

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	184	ALA	N-CA	-7.70	1.36	1.46
2	B	311	HIS	CE1-NE2	6.72	1.39	1.32
2	B	184	ALA	N-CA	-6.66	1.38	1.46
2	B	390	PRO	C-O	6.66	1.31	1.23
1	A	127	GLY	C-O	-6.15	1.20	1.24
1	C	440	GLU	CD-OE2	5.99	1.36	1.25
1	A	440	GLU	CD-OE2	5.80	1.36	1.25
1	A	93	ARG	N-CA	5.75	1.53	1.46
2	D	166	ILE	C-O	-5.66	1.17	1.24
2	D	171	LYS	N-CA	5.48	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	PHE	N-CA	5.25	1.51	1.46
2	B	5	VAL	N-CA	-5.12	1.40	1.46
2	D	477	HIS	CE1-NE2	5.09	1.37	1.32
2	B	64	VAL	C-O	-5.09	1.18	1.24
1	A	298	ASN	C-O	5.06	1.29	1.23
1	C	316	PHE	C-O	-5.05	1.17	1.24
2	B	453	ARG	CD-NE	-5.05	1.39	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	453	ARG	NE-CZ-NH2	9.73	127.96	119.20
2	B	390	PRO	CB-CA-C	9.58	122.00	111.56
2	B	390	PRO	N-CA-C	-8.88	96.56	110.50
2	D	453	ARG	NE-CZ-NH1	-8.46	113.03	121.50
2	B	154	MET	CG-SD-CE	-8.13	83.01	100.90
2	B	453	ARG	NE-CZ-NH2	8.07	126.47	119.20
2	D	453	ARG	CD-NE-CZ	7.94	135.52	124.40
2	D	175	ILE	N-CA-CB	-7.75	100.36	111.21
2	B	390	PRO	CA-C-N	-7.58	115.31	122.66
2	B	390	PRO	C-N-CA	-7.58	115.31	122.66
2	B	453	ARG	NE-CZ-NH1	-7.29	114.21	121.50
2	B	19	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	385	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	385	ASP	CA-CB-CG	6.09	118.69	112.60
2	B	390	PRO	O-C-N	-6.05	116.62	123.03
2	B	104	ASN	CA-CB-CG	5.91	118.50	112.60
1	C	59	ILE	N-CA-CB	-5.89	103.12	112.07
1	A	59	ILE	N-CA-CB	-5.83	103.21	112.07
2	D	104	ASN	CA-CB-CG	5.81	118.41	112.60
2	D	19	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	213	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	199	ASN	CA-CB-CG	5.67	118.27	112.60
1	C	213	ASP	CA-CB-CG	5.56	118.16	112.60
2	D	178	GLU	CB-CG-CD	5.55	122.03	112.60
2	B	175	ILE	N-CA-CB	-5.34	103.73	111.21
2	D	512	MET	CG-SD-CE	-5.34	89.14	100.90
1	C	261	GLU	CB-CG-CD	-5.27	103.64	112.60
1	C	234	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	520	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	297	HIS	CA-CB-CG	5.18	118.98	113.80
2	B	453	ARG	CD-NE-CZ	5.16	131.62	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	160	ASP	CA-CB-CG	5.16	117.75	112.60
2	D	323	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	180	PRO	N-CA-CB	5.08	107.37	103.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	415[A]	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	390	PRO	Mainchain
2	B	453	ARG	Sidechain
2	B	59	ARG	Sidechain
1	C	350[A]	ARG	Sidechain
1	C	96	ARG	Sidechain
2	D	206	ARG	Sidechain
2	D	453	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	3842	0	3777	30	0
1	C	3819	0	3743	24	0
2	B	4213	0	4105	38	0
2	D	4193	0	4073	33	0
3	A	14	0	6	3	0
3	C	14	0	6	2	0
4	A	17	0	0	0	0
4	C	17	0	0	0	0
5	A	10	0	10	1	0
5	B	20	0	20	2	0
5	C	10	0	10	1	0
5	D	20	0	20	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	15	0	0	0	0
7	D	15	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
10	A	466	0	0	7	0
10	B	604	0	0	7	2
10	C	477	0	0	5	2
10	D	603	0	0	19	0
All	All	18377	0	15770	120	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (120) 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)
5:A:504:IMD:H5	10:D:830:HOH:O	1.34	1.27
2:B:503[B]:GLU:OE2	2:B:503[B]:GLU:OE1	1.65	1.14
2:B:21[B]:LYS:HE2	10:B:861:HOH:O	1.53	1.07
2:B:503[B]:GLU:OE1	2:B:503[B]:GLU:CG	2.04	1.05
2:D:172[B]:GLU:OE1	10:D:701:HOH:O	1.80	0.98
2:D:391:VAL:HB	10:D:1129:HOH:O	1.65	0.96
2:D:391:VAL:CG2	10:D:1129:HOH:O	2.13	0.95
2:B:256:ASP:OD2	5:B:605:IMD:H2	1.72	0.90
1:C:8:GLU:CG	10:C:971:HOH:O	2.21	0.88
1:A:473:LYS:HG2	10:A:763:HOH:O	1.76	0.86
2:B:453:ARG:HD3	2:D:512:MET:SD	2.15	0.86
1:C:239:ARG:HD3	2:D:23[B]:MET:SD	2.17	0.85
2:B:512:MET:SD	2:D:453:ARG:HD3	2.19	0.82
1:C:396:ASP:CG	10:C:611:HOH:O	2.22	0.81
1:C:415:ARG:NH2	1:C:415:ARG:NH1	2.29	0.81
1:A:17:LEU:CD2	10:A:952:HOH:O	2.32	0.78
5:D:606:IMD:N1	10:D:702:HOH:O	2.12	0.76
1:A:17:LEU:HD23	10:A:952:HOH:O	1.86	0.75
5:D:603:IMD:H4	10:D:754:HOH:O	1.86	0.75
2:B:503[B]:GLU:CG	10:D:1050:HOH:O	2.36	0.74
2:D:21:LYS:HD3	10:D:1167:HOH:O	1.89	0.73
1:C:415:ARG:NH1	1:C:415:ARG:NE	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21[B]:LYS:CE	10:B:861:HOH:O	2.23	0.72
2:B:21[B]:LYS:HG2	10:D:702:HOH:O	1.91	0.71
2:B:280:GLU:OE1	5:B:605:IMD:H4	1.91	0.70
1:A:177:THR:OG1	1:A:209[B]:LYS:HE3	1.92	0.69
1:C:318:GLU:H	1:C:318:GLU:CD	2.01	0.69
1:A:17:LEU:HG	10:A:952:HOH:O	1.92	0.68
1:A:15:GLU:CD	1:A:415[B]:ARG:HH22	2.01	0.68
1:C:7:GLU:OE2	1:C:7:GLU:OE1	2.11	0.68
2:D:458[B]:LYS:NZ	10:D:704:HOH:O	2.27	0.66
2:B:242:ARG:HD3	2:B:246:GLU:OE1	1.96	0.66
1:A:15:GLU:OE1	1:A:415[B]:ARG:NH2	2.30	0.65
1:A:17:LEU:CG	10:A:952:HOH:O	2.46	0.64
2:D:503:GLU:CD	10:D:707:HOH:O	2.42	0.62
2:B:303:LYS:HE2	10:B:1221:HOH:O	1.97	0.62
2:D:242:ARG:HD3	2:D:246:GLU:OE2	1.99	0.62
1:A:22:GLU:HG3	1:A:26:LYS:HE3	1.83	0.61
1:A:388:ASP:O	1:A:392:LYS:NZ	2.33	0.61
1:A:182:ARG:HD3	10:A:605:HOH:O	2.02	0.59
2:B:125:PHE:HB3	10:B:1097:HOH:O	2.01	0.59
2:D:247[B]:MET:HG3	2:D:341:PRO:HD3	1.87	0.57
2:D:503:GLU:CG	10:D:709:HOH:O	2.54	0.56
10:B:989:HOH:O	5:C:505:IMD:H2	2.05	0.56
2:B:296:TRP:CD1	2:B:377:MET:HE1	2.41	0.55
2:D:391:VAL:HG21	10:D:1129:HOH:O	1.96	0.55
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.88	0.54
2:D:247[B]:MET:HB3	2:D:249:VAL:HG23	1.91	0.53
2:B:503[B]:GLU:OE2	2:B:503[B]:GLU:CB	2.57	0.53
1:A:22:GLU:OE2	1:A:25:ARG:NE	2.39	0.53
1:A:158:LEU:HD11	2:B:154:MET:HG3	1.90	0.52
1:C:29:ASN:ND2	10:C:605:HOH:O	2.43	0.52
2:B:503[B]:GLU:OE2	2:B:503[B]:GLU:HB3	2.10	0.51
2:D:503:GLU:HG3	10:D:709:HOH:O	2.09	0.51
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.11	0.51
2:B:299:GLU:HG2	10:B:842:HOH:O	2.11	0.50
1:C:351[A]:VAL:CG2	1:C:372[A]:MET:HE2	2.43	0.49
2:D:513:GLN:O	5:D:606:IMD:H4	2.12	0.49
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.94	0.49
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.95	0.48
1:A:474:LYS:HB3	2:D:322:LEU:HD21	1.96	0.48
1:A:25:ARG:HD3	10:A:764:HOH:O	2.14	0.47
1:A:442:HIS:HB3	3:A:501:HCA:O6	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:MET:HG3	2:D:457:HIS:HB2	1.96	0.47
2:D:391:VAL:CB	10:D:1129:HOH:O	2.25	0.47
2:D:514:ALA:O	5:D:606:IMD:H5	2.14	0.47
2:D:391:VAL:HG23	10:D:1129:HOH:O	2.00	0.46
2:B:16:LEU:HA	2:B:21[B]:LYS:HE3	1.97	0.46
2:D:401:ARG:HD2	10:D:847:HOH:O	2.15	0.46
1:C:134:LEU:C	1:C:134:LEU:HD23	2.41	0.46
1:A:205:TRP:O	1:A:209[B]:LYS:HE2	2.16	0.45
2:B:175:ILE:CD1	2:B:179:PHE:CD2	3.00	0.45
2:D:194:VAL:HB	2:D:297:HIS:CG	2.51	0.45
1:C:415:ARG:NH2	1:C:415:ARG:NE	2.64	0.45
2:D:120:GLU:OE2	5:D:601:IMD:H4	2.16	0.45
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.52	0.45
1:A:76:LYS:O	1:A:108:ALA:HA	2.16	0.45
2:B:322:LEU:HD21	1:C:474[A]:LYS:HB3	1.98	0.45
2:D:512:MET:HB3	2:D:512:MET:HE2	1.35	0.45
1:C:326:GLU:OE1	10:C:602:HOH:O	2.21	0.45
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.98	0.44
1:C:253:TRP:HA	1:C:254:SER:HA	1.80	0.44
2:D:494:LEU:HD23	2:D:494:LEU:C	2.43	0.44
1:C:62:CYS:HB3	2:D:94:GLY:HA3	2.00	0.44
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.17	0.44
2:B:322:LEU:HD21	1:C:474[B]:LYS:HB3	2.00	0.43
1:A:10:GLU:HG3	1:A:34:VAL:HG21	2.01	0.43
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.43
2:B:503[A]:GLU:OE2	2:B:503[A]:GLU:CG	2.67	0.43
2:B:151:THR:HG23	2:B:162:LEU:HD11	2.01	0.43
1:A:253:TRP:HA	1:A:254:SER:HA	1.83	0.43
1:C:76:LYS:O	1:C:108:ALA:HA	2.18	0.43
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.01	0.43
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.53	0.42
2:B:143:LYS:N	2:B:144:PRO:CD	2.82	0.42
1:A:442:HIS:CG	3:A:501:HCA:H52	2.55	0.42
3:A:501:HCA:O7	3:A:501:HCA:O2	2.37	0.42
2:B:512:MET:HE2	2:B:512:MET:HB3	1.38	0.42
2:B:377:MET:HB2	2:B:377:MET:HE2	1.78	0.42
2:B:445:ASN:HB2	2:B:472:PRO:O	2.20	0.42
1:C:176:LYS:HE3	10:C:914:HOH:O	2.19	0.42
2:B:7:LYS:HA	2:B:7:LYS:HD2	1.86	0.42
2:B:154:MET:HB3	2:B:154:MET:HE2	1.22	0.42
2:D:10:ALA:O	2:D:11:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PHE:CG	10:B:1097:HOH:O	2.71	0.42
2:B:324:TRP:HH2	2:B:377:MET:HG2	1.85	0.42
1:C:442:HIS:CG	3:C:501:HCA:H52	2.54	0.42
1:A:15:GLU:CD	1:A:415[B]:ARG:NH2	2.73	0.41
1:A:19:VAL:HG11	1:A:407[A]:TYR:CE2	2.55	0.41
2:D:175:ILE:HA	2:D:176:PRO:HD3	1.97	0.41
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.55	0.41
1:C:53:GLN:HB2	1:C:56:LEU:HD12	2.02	0.41
1:C:186:PHE:HA	10:D:845:HOH:O	2.19	0.41
2:D:306:GLU:OE1	10:D:703:HOH:O	2.22	0.41
1:A:378:GLY:HA3	1:A:401:TYR:O	2.20	0.41
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.21	0.41
2:B:211:LYS:HA	2:B:211:LYS:HD2	1.87	0.41
2:B:503[B]:GLU:OE2	2:B:503[B]:GLU:CG	2.69	0.40
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.57	0.40
1:A:68:LYS:C	1:A:68:LYS:HD3	2.47	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1229:HOH:O	10:C:1047:HOH:O[1_556]	1.87	0.33
10:B:998:HOH:O	10:C:698:HOH:O[1_556]	2.01	0.19

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	481/477 (101%)	463 (96%)	17 (4%)	1 (0%)	43	24
1	C	481/477 (101%)	464 (96%)	16 (3%)	1 (0%)	43	24
2	B	527/522 (101%)	517 (98%)	9 (2%)	1 (0%)	43	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	524/522 (100%)	513 (98%)	10 (2%)	1 (0%)	43 24
All	All	2013/1998 (101%)	1957 (97%)	52 (3%)	4 (0%)	43 24

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	413/407 (102%)	406 (98%)	7 (2%)	53 30
1	C	405/407 (100%)	400 (99%)	5 (1%)	63 43
2	B	454/454 (100%)	446 (98%)	8 (2%)	51 28
2	D	452/454 (100%)	446 (99%)	6 (1%)	61 40
All	All	1724/1722 (100%)	1698 (98%)	26 (2%)	57 35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	176	LYS
1	A	355	ILE
1	A	362	HIS
1	A	392	LYS
1	A	401	TYR
1	A	445	ASP
2	B	21[A]	LYS
2	B	21[B]	LYS
2	B	172	GLU

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Mol	Chain	Res	Type
2	B	175	ILE
2	B	211	LYS
2	B	258	GLU
2	B	453	ARG
2	B	512	MET
1	C	98	ASN
1	C	176	LYS
1	C	355	ILE
1	C	362	HIS
1	C	445	ASP
2	D	7	LYS
2	D	13	PRO
2	D	175	ILE
2	D	258	GLU
2	D	453	ARG
2	D	512	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
2	B	4	GLN
2	B	58	GLN
1	C	119	GLN
1	C	432	GLN
2	D	418	ASN

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 26 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
3	HCA	C	501	4	13,13,13	1.48	2 (15%)	15,18,18	1.44	2 (13%)
5	IMD	D	604	-	5,5,5	0.75	0	5,5,5	0.62	0
7	CLF	D	602	1,2	0,24,24	-	-	-		
5	IMD	D	606	-	5,5,5	0.74	0	5,5,5	0.48	0
5	IMD	B	602	-	5,5,5	0.59	0	5,5,5	1.33	1 (20%)
5	IMD	C	503	-	5,5,5	0.50	0	5,5,5	0.69	0
5	IMD	A	503	-	5,5,5	0.40	0	5,5,5	0.71	0
5	IMD	B	605	-	5,5,5	0.94	0	5,5,5	0.63	0
5	IMD	C	505	-	5,5,5	1.04	0	5,5,5	1.09	0
5	IMD	A	504	-	5,5,5	0.99	0	5,5,5	0.97	0
5	IMD	D	603	-	5,5,5	0.79	0	5,5,5	0.30	0
7	CLF	B	601	1,2	0,24,24	-	-	-		
5	IMD	B	603	-	5,5,5	0.66	0	5,5,5	0.93	0
4	ICS	C	502	1,6,3	4,28,30	1.49	1 (25%)	-		
3	HCA	A	501	4	13,13,13	1.09	0	15,18,18	1.51	1 (6%)
4	ICS	A	502	1,6,3	4,28,30	1.12	0	-		
5	IMD	D	601	-	5,5,5	0.19	0	5,5,5	0.87	0
5	IMD	B	606	-	5,5,5	0.77	0	5,5,5	0.78	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
3	HCA	C	501	4	-	0/17/17/17	-
5	IMD	D	604	-	-	-	0/1/1/1
7	CLF	D	602	1,2	-	-	0/12/10/10
5	IMD	D	606	-	-	-	0/1/1/1
5	IMD	B	602	-	-	-	0/1/1/1
5	IMD	C	503	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	503	-	-	-	0/1/1/1
5	IMD	B	605	-	-	-	0/1/1/1
5	IMD	C	505	-	-	-	0/1/1/1
5	IMD	D	603	-	-	-	0/1/1/1
7	CLF	B	601	1,2	-	-	0/12/10/10
5	IMD	B	603	-	-	-	0/1/1/1
3	HCA	A	501	4	-	3/17/17/17	-
5	IMD	A	504	-	-	-	0/1/1/1
5	IMD	D	601	-	-	-	0/1/1/1
5	IMD	B	606	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	HCA	C3-C7	-3.11	1.50	1.53
4	C	502	ICS	S3A-FE5	2.64	2.31	2.24
3	C	501	HCA	C5-C6	2.02	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	HCA	O6-C7-C3	3.46	119.78	113.14
3	A	501	HCA	C4-C5-C6	3.39	120.63	112.77
3	C	501	HCA	C4-C5-C6	2.61	118.83	112.77
5	B	602	IMD	C5-N1-C2	2.11	111.73	107.19

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	O2-C1-C2-C3
3	A	501	HCA	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	HCA	2	0
5	D	606	IMD	3	0

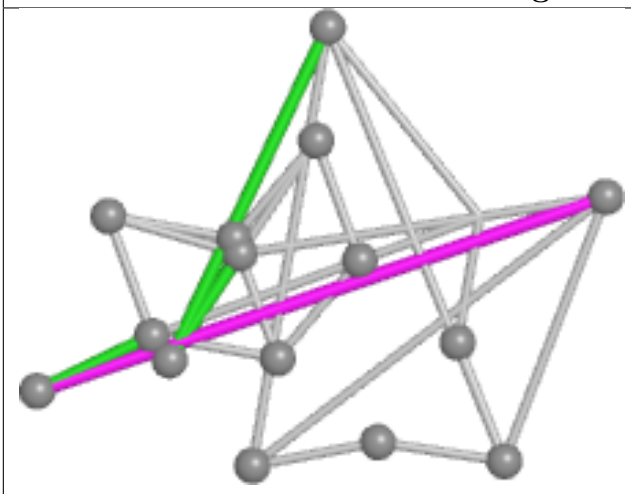
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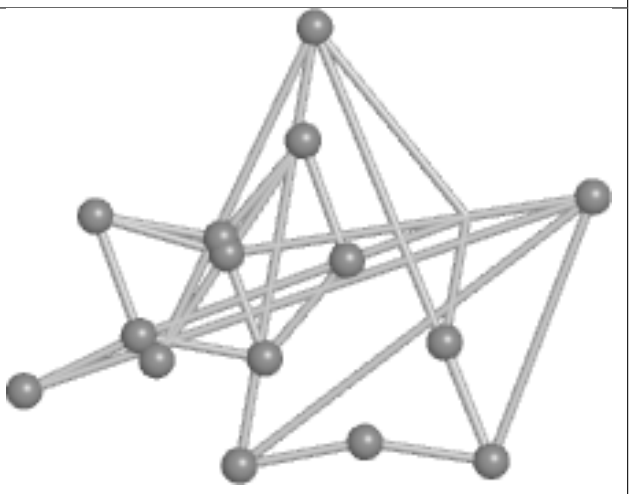
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	605	IMD	2	0
5	C	505	IMD	1	0
5	A	504	IMD	1	0
5	D	603	IMD	1	0
3	A	501	HCA	3	0
5	D	601	IMD	1	0

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 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.

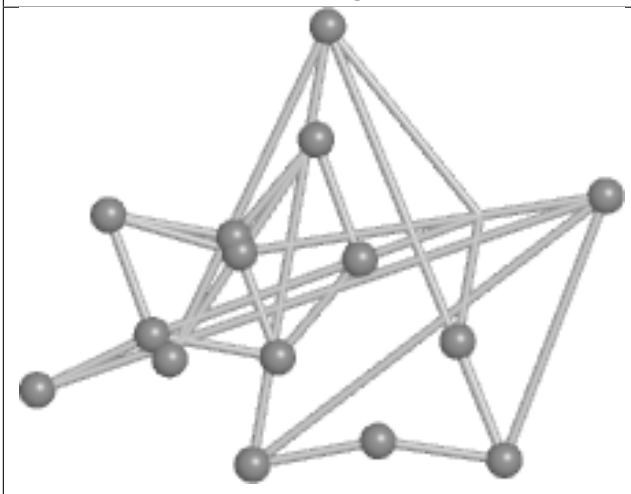
Ligand ICS C 502



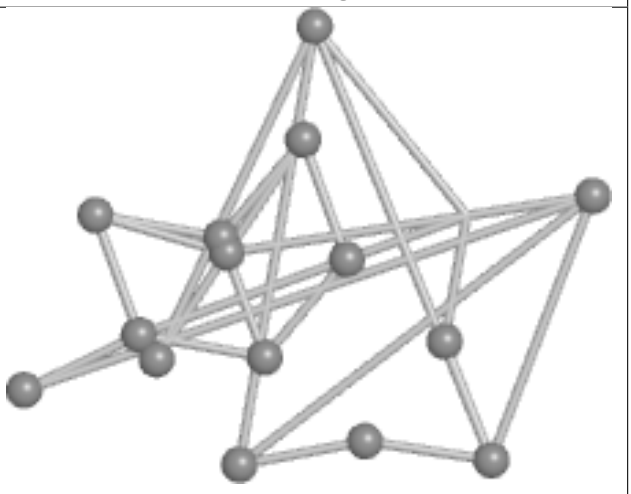
Bond lengths



Bond angles

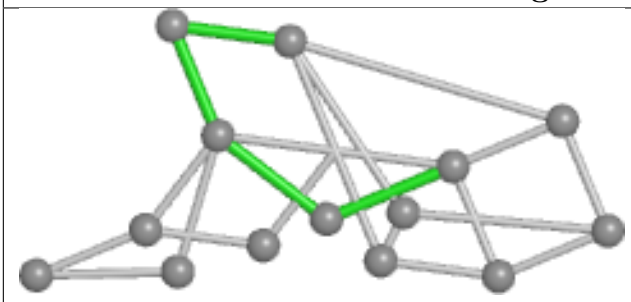


Torsions

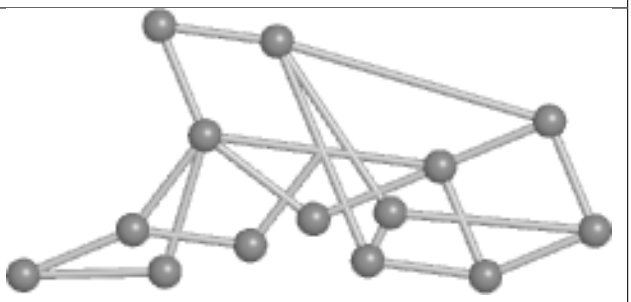


Rings

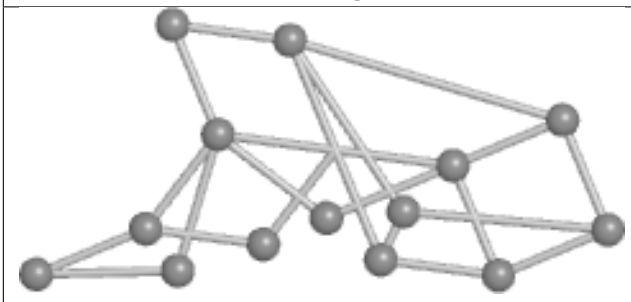
Ligand ICS A 502



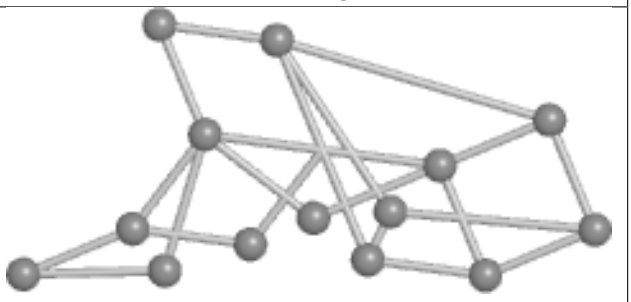
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.52	4 (0%)	82	86	5, 12, 26, 41	6 (1%)
1	C	477/477 (100%)	-0.54	3 (0%)	85	88	5, 11, 25, 42	6 (1%)
2	B	522/522 (100%)	-0.57	2 (0%)	88	91	4, 11, 22, 46	7 (1%)
2	D	522/522 (100%)	-0.58	1 (0%)	91	92	6, 11, 22, 42	4 (0%)
All	All	1998/1998 (100%)	-0.55	10 (0%)	87	90	4, 11, 24, 46	23 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	125	PHE	5.7
2	D	125	PHE	5.4
1	A	38	ALA	4.3
1	C	39	VAL	3.7
1	C	38	ALA	3.3
1	A	39	VAL	3.3
2	B	175	ILE	2.4
1	C	40	THR	2.4
1	A	392	LYS	2.2
1	A	40	THR	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

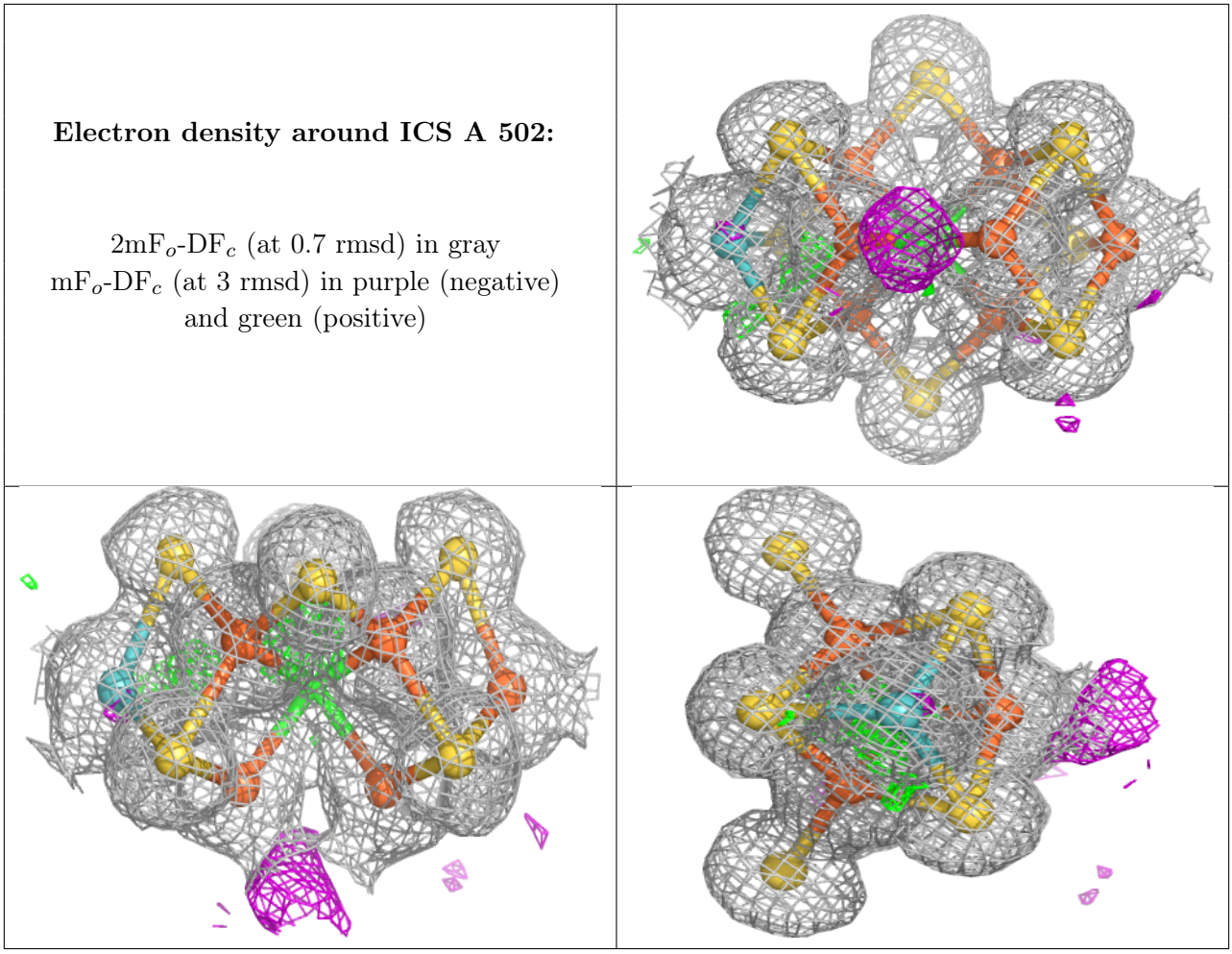
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C	505	5/5	0.80	0.18	21,22,30,32	0
5	IMD	B	606	5/5	0.81	0.14	32,35,38,41	0
5	IMD	A	504	5/5	0.84	0.20	24,25,29,30	0
5	IMD	B	605	5/5	0.84	0.13	25,27,30,30	0
5	IMD	D	601	5/5	0.87	0.11	22,23,25,27	0
5	IMD	D	606	5/5	0.88	0.13	31,32,35,40	0
8	MG	D	605	1/1	0.89	0.14	40,40,40,40	0
8	MG	B	604	1/1	0.90	0.11	45,45,45,45	0
5	IMD	B	603	5/5	0.91	0.09	21,24,24,24	0
5	IMD	D	604	5/5	0.94	0.09	21,22,22,23	0
5	IMD	A	503	5/5	0.95	0.08	22,26,28,31	0
9	CA	D	607	1/1	0.95	0.21	35,35,35,35	0
5	IMD	D	603	5/5	0.96	0.06	10,12,14,17	0
5	IMD	B	602	5/5	0.96	0.06	11,12,13,16	0
5	IMD	C	503	5/5	0.96	0.07	21,23,24,25	0
3	HCA	C	501	14/14	0.98	0.04	7,8,12,12	0
3	HCA	A	501	14/14	0.98	0.04	6,8,12,12	0
9	CA	C	506	1/1	0.99	0.17	36,36,36,36	0
9	CA	B	607	1/1	0.99	0.15	19,19,19,19	0
9	CA	D	608	1/1	0.99	0.16	19,19,19,19	0
4	ICS	A	502	17/18	1.00	0.01	6,7,8,8	0
4	ICS	C	502	17/18	1.00	0.01	6,7,8,8	0
6	SE	A	505	1/1	1.00	0.04	9,9,9,9	0
6	SE	C	504	1/1	1.00	0.04	9,9,9,9	0
7	CLF	B	601	15/15	1.00	0.02	7,7,8,9	0
7	CLF	D	602	15/15	1.00	0.02	7,8,8,9	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.

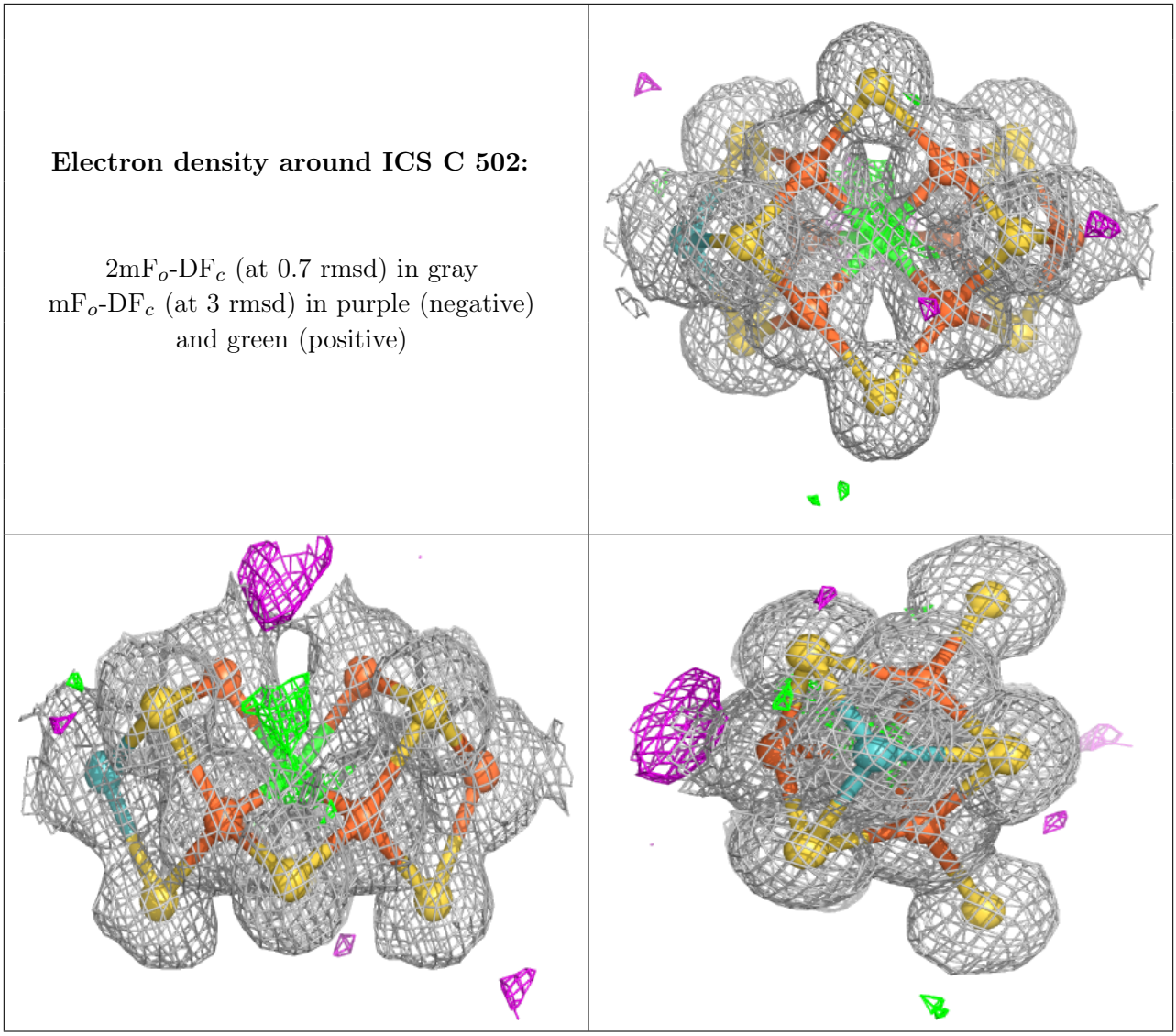
Electron density around ICS A 502:

$2mF_o$-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

There are no such residues in this entry.