



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 06:28 am BST

PDB ID : 3U7Q
Title : A. vinelandii nitrogenase MoFe protein at atomic resolution
Authors : Spatzal, T.; Einsle, O.
Deposited on : 2011-10-14
Resolution : 1.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

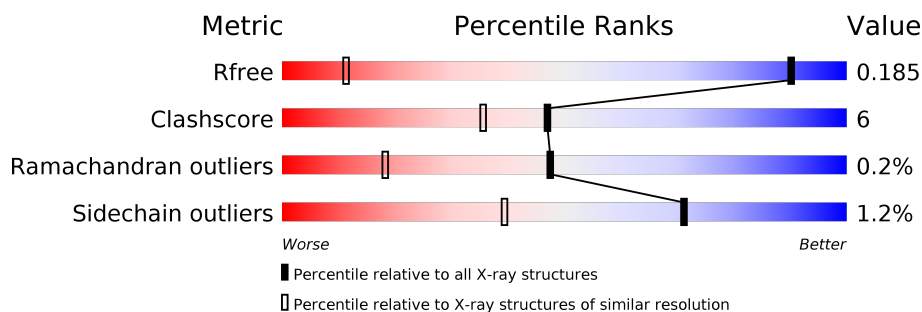
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)

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

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 18955 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.

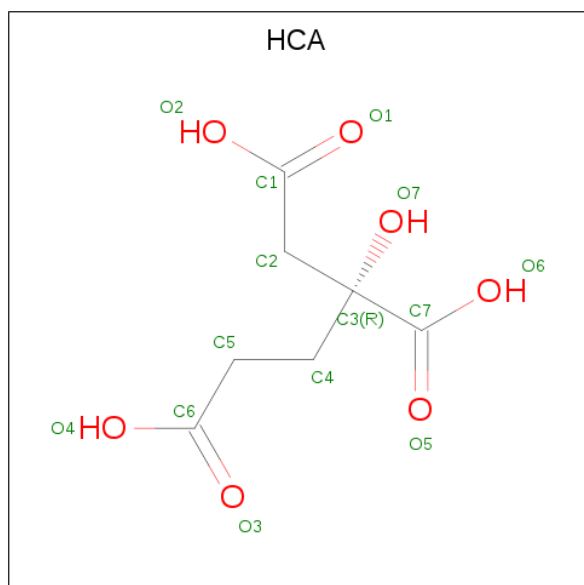
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	3	4	0
			3811	2426	648	710	27			
1	C	477	Total	C	N	O	S	33	8	0
			3826	2438	648	712	28			

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

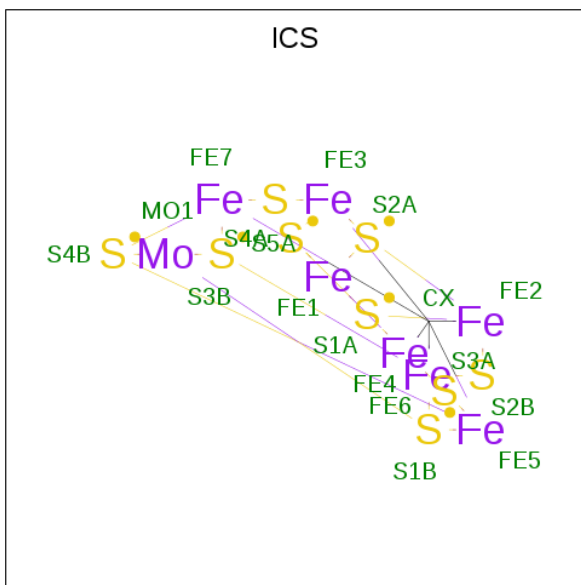
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	28	14	0
			4247	2722	707	783	35			
2	D	522	Total	C	N	O	S	20	16	0
			4301	2749	723	793	36			

- 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
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

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



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

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

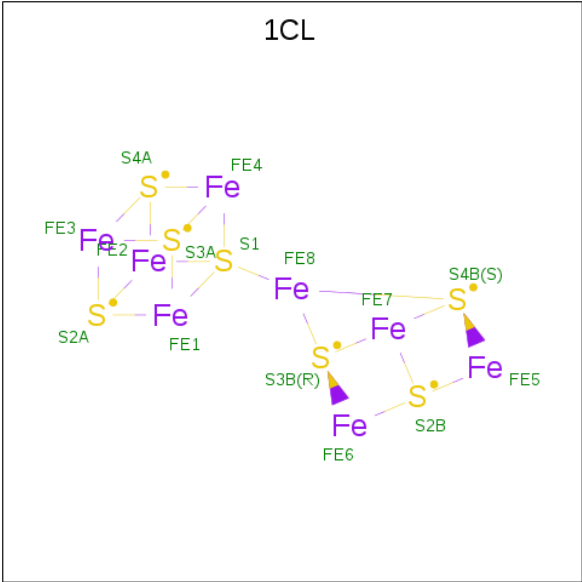


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	A	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		
5	C	1	Total	C	N	0	0
			5	3	2		
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

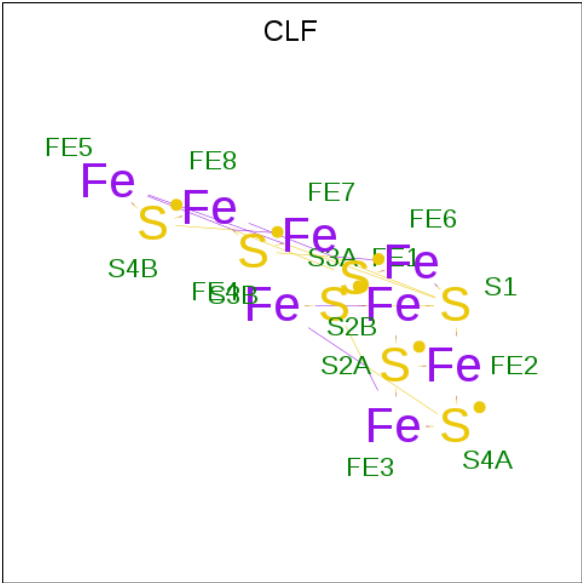
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is FE(8)-S(7) CLUSTER, OXIDIZED (three-letter code: 1CL) (formula: Fe₈S₇).



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

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



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

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

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

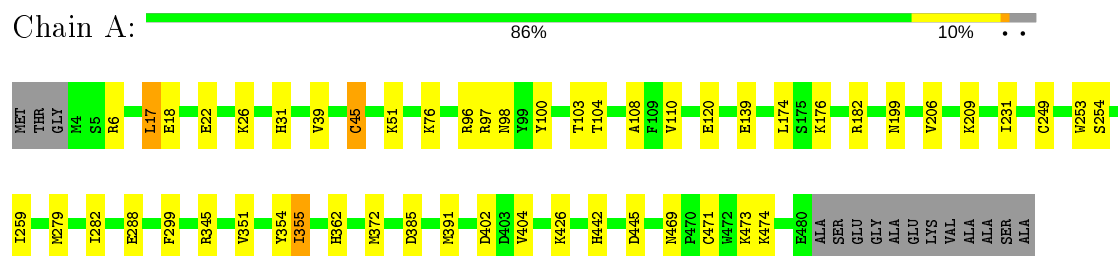
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	588	Total	O	0	0
			588	588		
10	B	726	Total	O	0	0
			726	726		
10	C	557	Total	O	0	0
			557	557		
10	D	731	Total	O	0	0
			731	731		

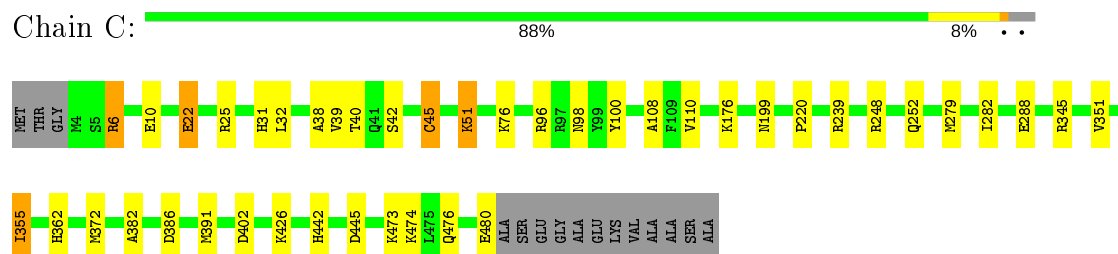
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

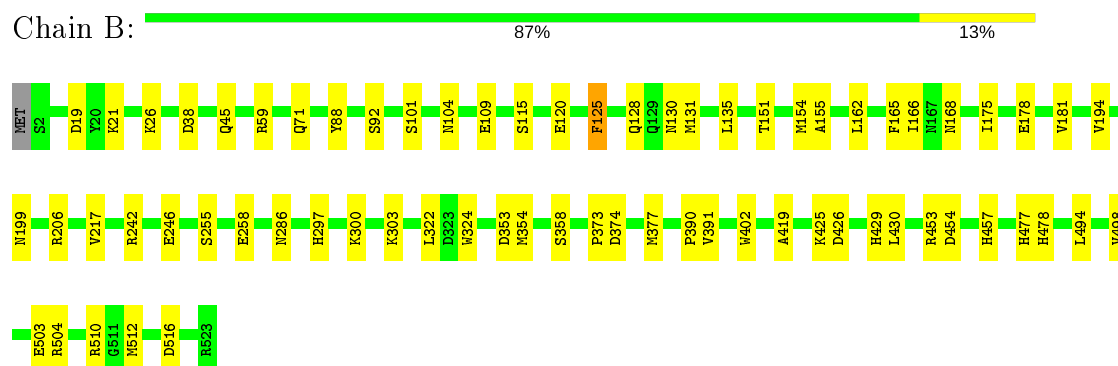
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

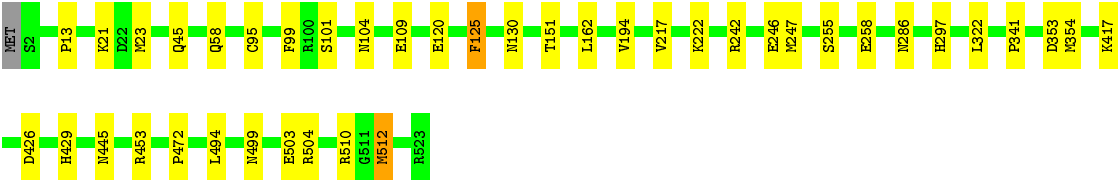


- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 130.70Å 107.22Å 90.00° 110.67° 90.00°	Depositor
Resolution (Å)	47.46 – 1.00 47.46 – 1.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.46-1.00) 99.1 (47.46-1.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.00Å)	Xtriage
Refinement program	REFMAC 5.6.0113	Depositor
R, R_{free}	0.128 , 0.146 0.172 , 0.185	Depositor DCC
R_{free} test set	55903 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18955	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IMD, CLF, HCA, ICS, CA, 1CL

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	2/3908 (0.1%)	0.84	6/5268 (0.1%)
1	C	0.73	5/3941 (0.1%)	0.86	8/5311 (0.2%)
2	B	0.62	2/4389 (0.0%)	0.79	5/5930 (0.1%)
2	D	0.61	1/4420 (0.0%)	0.79	3/5966 (0.1%)
All	All	0.65	10/16658 (0.1%)	0.82	22/22475 (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	A	0	1
1	C	0	1
2	B	0	1
2	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	GLU	CD-OE2	-14.01	1.10	1.25
1	C	22	GLU	CD-OE1	11.07	1.37	1.25
1	C	10	GLU	CD-OE1	7.80	1.34	1.25
1	C	45[A]	CYS	CB-SG	-7.60	1.69	1.82
1	C	45[B]	CYS	CB-SG	-7.60	1.69	1.82
2	B	125	PHE	CB-CG	-5.22	1.42	1.51
2	B	178	GLU	CD-OE2	-5.14	1.20	1.25
1	A	51[A]	LYS	CE-NZ	5.05	1.61	1.49
1	A	51[B]	LYS	CE-NZ	5.05	1.61	1.49
2	D	503	GLU	CD-OE2	5.04	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51[A]	LYS	CD-CE-NZ	10.21	135.18	111.70
1	A	51[B]	LYS	CD-CE-NZ	10.21	135.18	111.70
1	C	6	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	C	248	ARG	NE-CZ-NH1	8.69	124.65	120.30
2	B	125	PHE	N-CA-CB	8.44	125.79	110.60
2	D	510	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	B	125	PHE	CB-CA-C	-7.67	95.06	110.40
2	B	510	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	345	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	248	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	C	345	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	51[A]	LYS	CD-CE-NZ	-6.40	96.98	111.70
1	C	51[B]	LYS	CD-CE-NZ	-6.40	96.98	111.70
2	D	417	LYS	CA-CB-CG	6.14	126.91	113.40
1	A	385	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	39	VAL	CB-CA-C	-5.37	101.19	111.40
1	A	6	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	B	19	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	C	40	THR	N-CA-CB	5.12	120.02	110.30
2	B	59	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	299	PHE	CB-CG-CD1	5.05	124.34	120.80
2	D	222	LYS	CD-CE-NZ	-5.00	100.19	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ARG	Sidechain
2	B	125	PHE	Peptide
1	C	96	ARG	Sidechain
2	D	125[B]	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3811	0	3763	51	0
1	C	3826	0	3797	30	0
2	B	4247	0	4202	93	0
2	D	4301	0	4227	57	0
3	A	14	0	6	2	0
3	C	14	0	6	2	0
4	A	18	0	0	0	0
4	C	18	0	0	0	0
5	A	10	0	10	1	0
5	B	10	0	10	1	0
5	C	10	0	10	3	0
5	D	10	0	10	1	0
6	B	2	0	0	0	0
7	B	15	0	0	0	0
7	D	15	0	0	0	0
8	B	15	0	0	0	0
8	D	15	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	A	588	0	0	13	1
10	B	726	0	0	31	0
10	C	557	0	0	9	0
10	D	731	0	0	16	0
All	All	18955	0	16041	201	1

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 6.

All (201) 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:494:IMD:H5	10:D:878:HOH:O	1.29	1.29
1:A:249:CYS:HB3	10:A:1157:HOH:O	1.11	1.28
2:B:425:LYS:HE2	10:B:2302:HOH:O	1.28	1.28
1:A:182:ARG:HG3	10:A:2215:HOH:O	1.33	1.27
1:A:22:GLU:OE2	1:A:26:LYS:HE3	1.49	1.09
2:B:45:GLN:HB3	10:B:2214:HOH:O	0.90	1.07
2:B:512[B]:MET:HG2	2:D:453[B]:ARG:HD3	1.35	1.07
2:B:21:LYS:HD3	10:B:2340:HOH:O	1.52	1.06
2:D:45:GLN:HB3	10:D:2175:HOH:O	0.87	1.04
2:B:38:ASP:HB2	10:B:2233:HOH:O	1.60	0.98
1:C:473:LYS:HG2	10:C:2388:HOH:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:HD3	2:D:23[A]:MET:SD	2.07	0.94
2:D:453[B]:ARG:NH1	10:D:808:HOH:O	1.86	0.92
2:B:453:ARG:O	2:D:512[B]:MET:CE	2.19	0.90
2:B:454:ASP:HA	2:D:512[B]:MET:HE1	1.49	0.90
2:B:373:PRO:O	2:B:377[A]:MET:HE2	1.72	0.90
2:B:477:HIS:H	2:D:499:ASN:HD21	1.13	0.90
2:B:512[B]:MET:SD	2:D:453[B]:ARG:HD2	2.10	0.90
2:B:454:ASP:HA	2:D:512[B]:MET:CE	2.01	0.89
5:C:493:IMD:H4	10:C:1611:HOH:O	1.74	0.87
1:A:103:THR:HA	2:D:512[C]:MET:HE2	1.57	0.87
2:B:45:GLN:HG2	10:B:1167:HOH:O	1.73	0.86
2:B:246:GLU:CD	10:B:2210:HOH:O	2.15	0.85
2:B:512[B]:MET:CG	2:D:453[B]:ARG:HD3	2.04	0.85
2:B:426:ASP:H	2:B:429:HIS:HD2	1.25	0.84
2:D:45:GLN:HG2	10:D:1061:HOH:O	1.77	0.84
5:D:524:IMD:H4	10:D:527:HOH:O	1.78	0.83
1:A:17:LEU:HG	10:A:1697:HOH:O	1.78	0.83
2:D:426:ASP:H	2:D:429:HIS:HD2	1.27	0.83
2:D:58:GLN:HG2	10:D:2378:HOH:O	1.77	0.83
2:B:374:ASP:HA	2:B:377[A]:MET:CE	2.12	0.80
1:A:17:LEU:CG	10:A:1697:HOH:O	2.29	0.79
2:B:374:ASP:HA	2:B:377[A]:MET:HE3	1.64	0.79
2:B:503[B]:GLU:CG	10:B:2293:HOH:O	2.30	0.79
2:B:503[B]:GLU:OE2	10:B:2293:HOH:O	2.01	0.78
1:A:120:GLU:HG2	10:A:2381:HOH:O	1.84	0.77
2:B:390:PRO:C	10:B:1757:HOH:O	2.22	0.77
2:D:125[A]:PHE:HZ	10:D:2091:HOH:O	1.67	0.76
2:B:303:LYS:HE2	10:B:2111:HOH:O	1.87	0.75
2:B:453:ARG:O	2:D:512[B]:MET:HE3	1.85	0.75
2:B:377[A]:MET:HE1	2:B:402:TRP:CD1	2.22	0.75
2:B:21:LYS:HG2	10:B:1635:HOH:O	1.88	0.74
1:C:22:GLU:OE1	1:C:25:ARG:NH2	2.17	0.74
1:A:209:LYS:HZ1	1:A:259:ILE:HD11	1.53	0.74
1:A:209:LYS:NZ	1:A:259:ILE:HD11	2.03	0.73
2:B:377[A]:MET:CE	2:B:402:TRP:HE1	2.00	0.73
1:A:249:CYS:CB	10:A:1157:HOH:O	1.88	0.73
2:B:512[B]:MET:CG	2:D:453[B]:ARG:CD	2.65	0.73
2:B:453:ARG:C	2:D:512[B]:MET:CE	2.57	0.72
1:A:22:GLU:CD	1:A:26:LYS:HE3	2.11	0.71
1:C:45[A]:CYS:SG	1:C:391:MET:CE	2.79	0.71
2:B:453:ARG:C	2:D:512[B]:MET:HE2	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76[B]:LYS:NZ	10:C:549:HOH:O	2.21	0.70
2:B:71:GLN:HE22	2:B:199:ASN:HD22	1.38	0.70
2:B:512[B]:MET:SD	2:D:453[B]:ARG:CD	2.80	0.70
2:B:353:ASP:OD2	10:D:1263:HOH:O	2.11	0.68
2:D:109[B]:GLU:OE2	10:D:1263:HOH:O	2.11	0.68
2:D:242:ARG:HD3	2:D:246:GLU:OE2	1.92	0.68
1:A:199:ASN:HD22	1:A:282:ILE:H	1.42	0.67
2:D:21:LYS:HG2	10:D:1771:HOH:O	1.92	0.67
1:C:31:HIS:HE1	10:C:609:HOH:O	1.78	0.67
2:D:353:ASP:OD2	10:D:2575:HOH:O	2.13	0.66
2:B:21:LYS:HE2	10:B:2099:HOH:O	1.96	0.66
2:B:109[B]:GLU:OE2	10:D:2575:HOH:O	2.14	0.65
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.41	0.65
1:A:31:HIS:HE1	10:A:614:HOH:O	1.79	0.65
1:A:469:ASN:HD22	1:A:471:CYS:H	1.45	0.65
2:B:120:GLU:OE2	5:B:525:IMD:H2	1.97	0.64
2:B:21:LYS:CE	10:B:2099:HOH:O	2.45	0.64
2:B:246:GLU:OE1	10:B:2210:HOH:O	2.15	0.64
2:B:377[A]:MET:HE1	2:B:402:TRP:NE1	2.13	0.64
2:B:454:ASP:N	2:D:512[B]:MET:HE2	2.13	0.63
1:A:22:GLU:OE2	1:A:26:LYS:CE	2.36	0.63
1:A:120:GLU:CG	10:A:2381:HOH:O	2.45	0.63
2:B:454:ASP:CA	2:D:512[B]:MET:CE	2.76	0.63
2:B:503[B]:GLU:HG3	10:B:2293:HOH:O	1.95	0.63
1:C:199:ASN:HD22	1:C:282:ILE:H	1.46	0.62
1:A:17:LEU:CD1	10:A:1697:HOH:O	2.47	0.62
1:C:31:HIS:HD2	1:C:402:ASP:OD2	1.82	0.62
2:D:247[B]:MET:HG2	2:D:341:PRO:HD3	1.81	0.62
1:A:31:HIS:HD2	1:A:402:ASP:OD2	1.83	0.61
1:A:104:THR:H	2:D:512[C]:MET:CE	2.13	0.61
1:A:17:LEU:HD12	10:A:1697:HOH:O	1.99	0.61
1:A:45[A]:CYS:SG	1:A:391:MET:HE2	2.41	0.61
2:B:242:ARG:HD3	2:B:246:GLU:OE2	2.00	0.60
2:D:125[A]:PHE:CZ	10:D:2091:HOH:O	2.45	0.60
2:B:454:ASP:CA	2:D:512[B]:MET:HE1	2.29	0.60
1:A:206:VAL:HA	1:A:209:LYS:HE2	1.82	0.60
1:C:45[A]:CYS:SG	1:C:391:MET:HE1	2.41	0.59
1:A:249:CYS:SG	10:A:1157:HOH:O	2.49	0.58
2:B:300:LYS:CE	10:B:2307:HOH:O	2.49	0.58
2:B:391:VAL:N	10:B:1757:HOH:O	2.35	0.58
5:C:494:IMD:H4	2:D:120:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG11	1:A:45[B]:CYS:SG	2.44	0.57
2:B:453:ARG:HG2	2:D:512[B]:MET:CE	2.34	0.57
2:B:377[A]:MET:HE2	2:B:402:TRP:HE1	1.69	0.57
1:A:45[A]:CYS:SG	1:A:391:MET:CE	2.92	0.57
2:B:206:ARG:HD3	10:B:1970:HOH:O	2.05	0.57
5:C:493:IMD:H2	10:C:607:HOH:O	2.04	0.57
2:B:454:ASP:HA	2:D:512[B]:MET:HE2	1.84	0.56
1:C:45[A]:CYS:SG	1:C:391:MET:HE2	2.45	0.56
1:C:199:ASN:HD21	1:C:279[A]:MET:HA	1.71	0.55
2:D:247[B]:MET:HG2	2:D:341:PRO:CD	2.37	0.55
1:A:104:THR:H	2:D:512[C]:MET:HE2	1.70	0.55
2:B:92:SER:N	2:B:154[B]:MET:HE1	2.21	0.55
2:B:21:LYS:CD	10:B:2340:HOH:O	2.30	0.55
2:B:377[A]:MET:HE1	2:B:402:TRP:HE1	1.72	0.55
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.89	0.54
1:A:199:ASN:HD21	1:A:279[B]:MET:HA	1.71	0.54
1:C:199:ASN:HD21	1:C:279[B]:MET:HA	1.73	0.54
1:A:474:LYS:HB3	2:D:322:LEU:HD21	1.90	0.53
2:B:373:PRO:C	2:B:377[A]:MET:HE2	2.28	0.53
2:B:391:VAL:HA	10:B:1757:HOH:O	2.07	0.53
2:D:217:VAL:H	2:D:286:ASN:ND2	2.06	0.53
1:A:139:GLU:OE2	1:A:176:LYS:HE3	2.07	0.53
2:B:115[B]:SER:HB2	10:B:624:HOH:O	2.07	0.53
1:A:199:ASN:HD21	1:A:279[A]:MET:HA	1.73	0.53
2:B:303:LYS:CE	10:B:2111:HOH:O	2.53	0.53
2:B:454:ASP:CA	2:D:512[B]:MET:HE2	2.38	0.52
2:B:457:HIS:HB2	2:D:512[B]:MET:CE	2.40	0.52
2:B:374:ASP:HA	2:B:377[A]:MET:HE2	1.92	0.51
2:B:494:LEU:O	2:B:498[B]:VAL:HG23	2.10	0.51
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.93	0.51
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.26	0.51
1:C:25:ARG:HD3	10:C:1229:HOH:O	2.09	0.51
1:C:32:LEU:O	10:C:1421:HOH:O	2.19	0.51
1:C:42:SER:HB2	1:C:391:MET:HE1	1.92	0.51
2:B:358:SER:HB3	2:B:498[B]:VAL:HG21	1.92	0.51
2:B:130:ASN:ND2	10:B:1738:HOH:O	2.44	0.51
2:B:300:LYS:NZ	10:B:2307:HOH:O	2.03	0.51
2:B:426:ASP:H	2:B:429:HIS:CD2	2.16	0.50
2:D:101[B]:SER:HA	2:D:104:ASN:HD22	1.76	0.50
2:B:217:VAL:H	2:B:286:ASN:ND2	2.09	0.49
2:B:175[A]:ILE:CD1	2:B:181:VAL:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LYS:NZ	10:B:2362:HOH:O	2.40	0.49
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.95	0.49
1:C:476:GLN:NE2	1:C:480:GLU:HB2	2.28	0.49
2:D:130:ASN:ND2	10:D:2082:HOH:O	2.44	0.48
2:B:21:LYS:HB3	10:B:2340:HOH:O	2.13	0.48
2:B:377[A]:MET:CE	2:B:402:TRP:NE1	2.68	0.47
1:A:442:HIS:HB3	3:A:6494:HCA:O5	2.15	0.47
1:C:100:TYR:CE2	1:C:110:VAL:HB	2.50	0.47
1:C:442:HIS:HB3	3:C:7494:HCA:O5	2.15	0.47
2:D:512[A]:MET:HG2	10:D:584:HOH:O	2.15	0.47
2:B:504:ARG:NH2	10:B:2296:HOH:O	2.47	0.46
1:A:199:ASN:HD22	1:A:282:ILE:N	2.12	0.46
2:B:503[B]:GLU:CD	10:B:2293:HOH:O	2.44	0.46
2:B:478:HIS:NE2	2:D:354[B]:MET:HG3	2.30	0.46
1:A:17:LEU:N	1:A:17:LEU:HD23	2.31	0.46
2:B:131[B]:MET:SD	2:B:166:ILE:HG13	2.56	0.46
2:D:504:ARG:NH2	10:D:2174:HOH:O	2.48	0.46
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.98	0.45
2:B:516:ASP:OD2	2:D:453[B]:ARG:NH1	2.49	0.45
1:A:351[A]:VAL:CG2	1:A:372:MET:CE	2.94	0.45
1:A:206:VAL:HA	1:A:209:LYS:CE	2.46	0.45
1:A:100:TYR:CE2	1:A:110:VAL:HB	2.51	0.45
2:B:425:LYS:CE	10:B:2302:HOH:O	2.11	0.45
1:A:442:HIS:CG	3:A:6494:HCA:H52	2.52	0.44
2:B:101[B]:SER:HA	2:B:104:ASN:HD22	1.82	0.44
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.83	0.44
1:C:426:LYS:HA	2:D:104:ASN:ND2	2.32	0.44
2:D:194:VAL:HB	2:D:297:HIS:CG	2.52	0.44
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.32	0.44
1:A:76:LYS:O	1:A:108:ALA:HA	2.18	0.44
1:A:45[B]:CYS:HB2	1:A:391:MET:HE1	1.99	0.44
2:B:194:VAL:HB	2:B:297:HIS:CG	2.53	0.44
2:B:128:GLN:NE2	2:B:168:ASN:HD22	2.15	0.44
1:A:22:GLU:CG	1:A:26:LYS:HE3	2.48	0.43
1:C:442:HIS:CG	3:C:7494:HCA:H52	2.52	0.43
2:D:426:ASP:H	2:D:429:HIS:CD2	2.19	0.43
1:A:426:LYS:HA	2:B:104:ASN:HD21	1.83	0.43
1:A:199:ASN:ND2	1:A:282:ILE:H	2.13	0.43
1:C:351[A]:VAL:CG2	1:C:372:MET:CE	2.97	0.43
1:A:18:GLU:HG3	10:A:2373:HOH:O	2.19	0.43
2:B:453:ARG:HG2	2:D:512[B]:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASN:HD22	1:C:282:ILE:N	2.14	0.43
1:A:253:TRP:HA	1:A:254:SER:HA	1.84	0.43
2:B:419:ALA:HB2	10:B:1757:HOH:O	2.18	0.43
1:C:288:GLU:HG3	10:C:1540:HOH:O	2.18	0.43
2:B:71:GLN:HE21	2:B:71:GLN:HB3	1.72	0.42
2:B:324:TRP:CH2	2:B:377[B]:MET:HG2	2.54	0.42
2:B:453:ARG:HG2	2:D:512[B]:MET:HE3	2.01	0.42
1:C:382:ALA:HB1	1:C:386:ASP:HB2	2.01	0.42
2:B:354[B]:MET:SD	2:B:494:LEU:HD22	2.59	0.42
2:D:101[B]:SER:HA	2:D:104:ASN:ND2	2.34	0.42
2:B:391:VAL:CA	10:B:1757:HOH:O	2.63	0.42
2:D:494:LEU:HD23	2:D:494:LEU:C	2.40	0.42
1:C:426:LYS:HA	2:D:104:ASN:HD21	1.85	0.41
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.55	0.41
2:B:154[B]:MET:HE3	2:B:155:ALA:H	1.85	0.41
1:A:103:THR:CA	2:D:512[C]:MET:HE2	2.37	0.41
2:D:445:ASN:HB2	2:D:472:PRO:O	2.21	0.41
2:B:135:LEU:HB3	2:B:175[A]:ILE:HG21	2.03	0.41
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.56	0.40
1:C:38:ALA:CB	10:C:2334:HOH:O	2.69	0.40
1:A:288:GLU:HG3	10:A:1600:HOH:O	2.21	0.40
1:A:351[A]:VAL:CG2	1:A:372:MET:HE2	2.52	0.40
1:A:97:ARG:O	1:A:231:ILE:HA	2.22	0.40

All (1) 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:A:1986:HOH:O	10:A:2381:HOH:O[2_646]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	479/492 (97%)	462 (96%)	16 (3%)	1 (0%)	47	18
1	C	484/492 (98%)	464 (96%)	19 (4%)	1 (0%)	47	18
2	B	534/523 (102%)	526 (98%)	7 (1%)	1 (0%)	47	18
2	D	537/523 (103%)	528 (98%)	8 (2%)	1 (0%)	47	18
All	All	2034/2030 (100%)	1980 (97%)	50 (2%)	4 (0%)	47	18

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 ⓘ

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	411/415 (99%)	403 (98%)	8 (2%)	57	23
1	C	416/415 (100%)	407 (98%)	9 (2%)	52	18
2	B	468/455 (103%)	466 (100%)	2 (0%)	91	70
2	D	471/455 (104%)	466 (99%)	5 (1%)	73	43
All	All	1766/1740 (102%)	1742 (99%)	24 (1%)	71	34

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	45[A]	CYS
1	A	45[B]	CYS
1	A	98	ASN
1	A	355	ILE
1	A	362	HIS
1	A	445	ASP

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Mol	Chain	Res	Type
1	A	473	LYS
2	B	88	TYR
2	B	258	GLU
1	C	6	ARG
1	C	51[A]	LYS
1	C	51[B]	LYS
1	C	98	ASN
1	C	176	LYS
1	C	220	PRO
1	C	355	ILE
1	C	362	HIS
1	C	445	ASP
2	D	13	PRO
2	D	258	GLU
2	D	512[A]	MET
2	D	512[B]	MET
2	D	512[C]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	199	ASN
1	A	271	ASN
1	A	384	ASN
1	A	468	ASN
1	A	469	ASN
2	B	71	GLN
2	B	104	ASN
2	B	128	GLN
2	B	130	ASN
2	B	225	ASN
2	B	286	ASN
2	B	294	GLN
2	B	363	HIS
2	B	418	ASN
2	B	429	HIS
2	B	518	ASN
1	C	31	HIS
1	C	199	ASN
1	C	252	GLN
1	C	271	ASN

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Mol	Chain	Res	Type
1	C	384	ASN
1	C	468	ASN
1	C	476	GLN
2	D	104	ASN
2	D	130	ASN
2	D	225	ASN
2	D	286	ASN
2	D	294	GLN
2	D	363	HIS
2	D	418	ASN
2	D	429	HIS
2	D	499	ASN
2	D	518	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	A	494	-	3,5,5	0.28	0	4,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IMD	C	494	-	3,5,5	0.34	0	4,5,5	0.46	0
3	HCA	A	6494	-	4,13,13	1.14	0	4,18,18	2.64	1 (25%)
5	IMD	D	525	-	3,5,5	0.46	0	4,5,5	0.83	0
8	CLF	D	7499[B]	1,2	0,24,24	0.00	-	-	-	-
5	IMD	C	493	-	3,5,5	0.54	0	4,5,5	0.40	0
5	IMD	B	525	-	3,5,5	0.36	0	4,5,5	0.42	0
5	IMD	A	493	-	3,5,5	0.40	0	4,5,5	0.82	0
7	1CL	B	6498[A]	1,2	0,22,22	0.00	-	-	-	-
4	ICS	C	7496	1	18,30,30	2.44	11 (61%)	-	-	-
8	CLF	B	6499[B]	1,2	0,24,24	0.00	-	-	-	-
4	ICS	A	6496	1	18,30,30	2.44	10 (55%)	-	-	-
7	1CL	D	7498[A]	1,2	0,22,22	0.00	-	-	-	-
5	IMD	B	524	-	3,5,5	0.15	0	4,5,5	0.77	0
5	IMD	D	524	-	3,5,5	0.44	0	4,5,5	0.46	0
3	HCA	C	7494	-	4,13,13	0.92	0	4,18,18	2.55	1 (25%)

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	A	494	-	-	-	0/1/1/1
5	IMD	C	494	-	-	-	0/1/1/1
3	HCA	A	6494	-	-	0/7/17/17	-
5	IMD	D	525	-	-	-	0/1/1/1
8	CLF	D	7499[B]	1,2	-	-	0/12/10/10
5	IMD	C	493	-	-	-	0/1/1/1
5	IMD	B	525	-	-	-	0/1/1/1
5	IMD	A	493	-	-	-	0/1/1/1
7	1CL	B	6498[A]	1,2	-	-	0/9/8/8
8	CLF	B	6499[B]	1,2	-	-	0/12/10/10
7	1CL	D	7498[A]	1,2	-	-	0/9/8/8
5	IMD	B	524	-	-	-	0/1/1/1
5	IMD	D	524	-	-	-	0/1/1/1
3	HCA	C	7494	-	-	0/7/17/17	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6496	ICS	S3B-FE6	-4.08	2.22	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6496	ICS	S4B-FE7	-4.04	2.22	2.32
4	C	7496	ICS	S3B-FE6	-4.03	2.22	2.32
4	C	7496	ICS	S4B-FE7	-4.01	2.22	2.32
4	A	6496	ICS	S1B-FE6	-3.44	2.23	2.32
4	C	7496	ICS	S1B-FE6	-3.34	2.24	2.32
4	A	6496	ICS	S2B-FE6	-3.03	2.17	2.24
4	C	7496	ICS	S2A-FE2	-2.97	2.25	2.32
4	A	6496	ICS	S3B-FE7	-2.96	2.25	2.32
4	C	7496	ICS	S2B-FE6	-2.84	2.18	2.24
4	A	6496	ICS	S4B-FE5	-2.81	2.25	2.32
4	C	7496	ICS	S4A-FE3	-2.78	2.25	2.32
4	C	7496	ICS	S3B-FE7	-2.69	2.25	2.32
4	A	6496	ICS	S2A-FE2	-2.64	2.25	2.32
4	A	6496	ICS	S4A-FE3	-2.62	2.25	2.32
4	C	7496	ICS	S4B-FE5	-2.54	2.26	2.32
4	C	7496	ICS	S1B-FE5	-2.36	2.26	2.32
4	A	6496	ICS	S1A-FE2	-2.34	2.26	2.32
4	C	7496	ICS	S1A-FE2	-2.26	2.26	2.32
4	C	7496	ICS	S2A-FE3	-2.10	2.27	2.32
4	A	6496	ICS	S1B-FE5	-2.07	2.27	2.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	6494	HCA	C4-C5-C6	5.06	119.06	111.39
3	C	7494	HCA	C4-C5-C6	5.00	118.97	111.39

There are no chirality outliers.

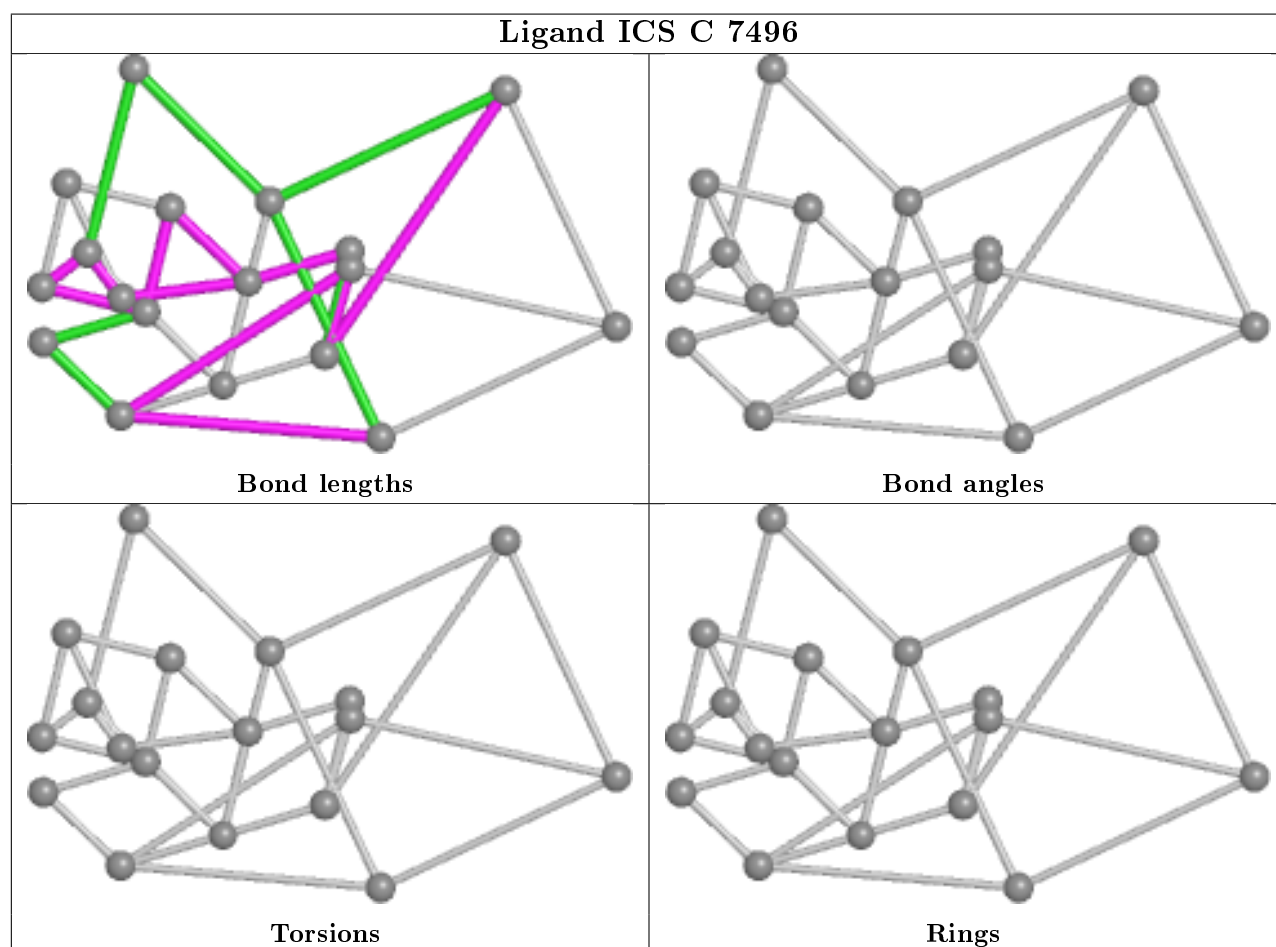
There are no torsion outliers.

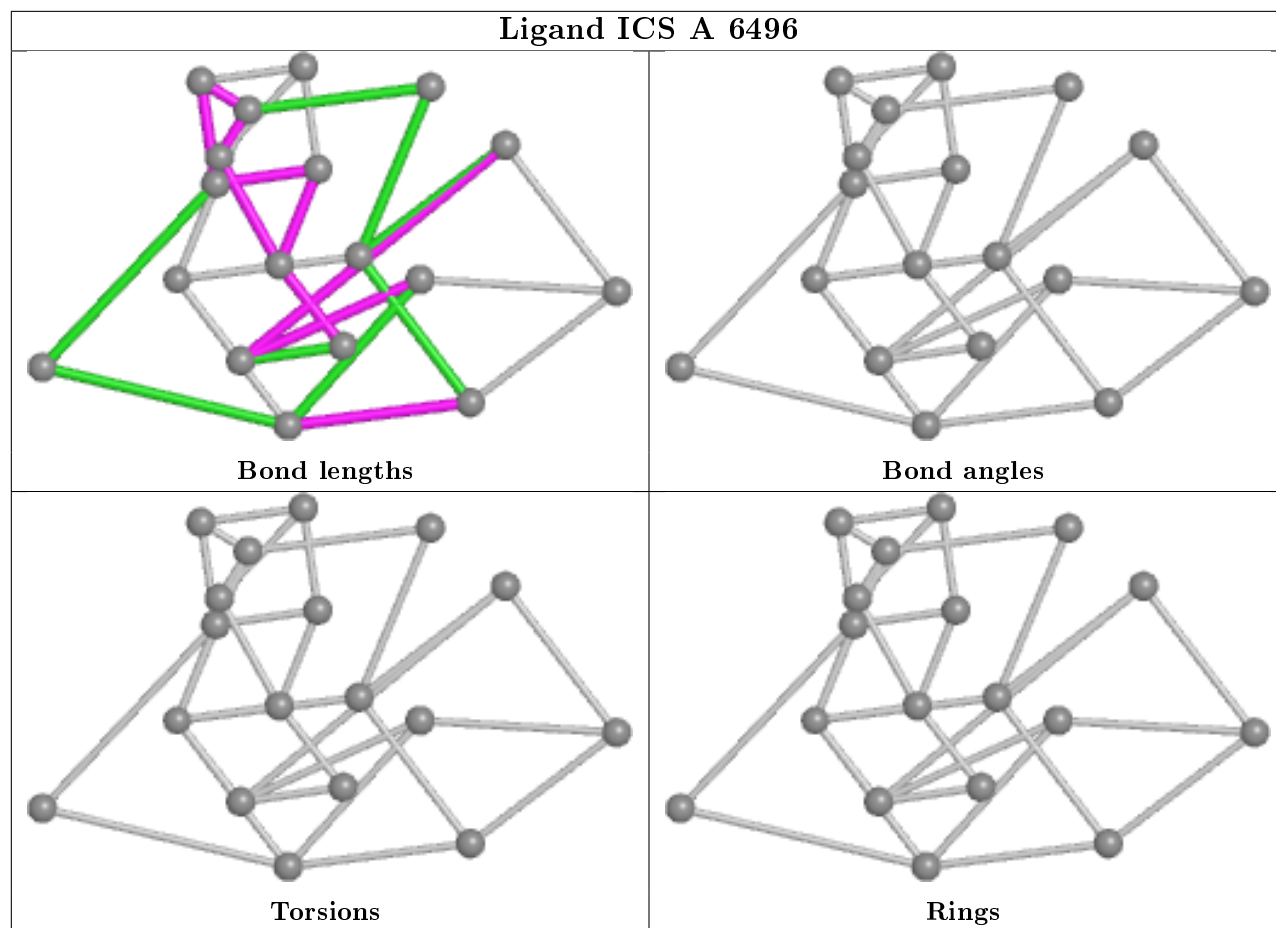
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	494	IMD	1	0
5	C	494	IMD	1	0
3	A	6494	HCA	2	0
5	C	493	IMD	2	0
5	B	525	IMD	1	0
5	D	524	IMD	1	0
3	C	7494	HCA	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

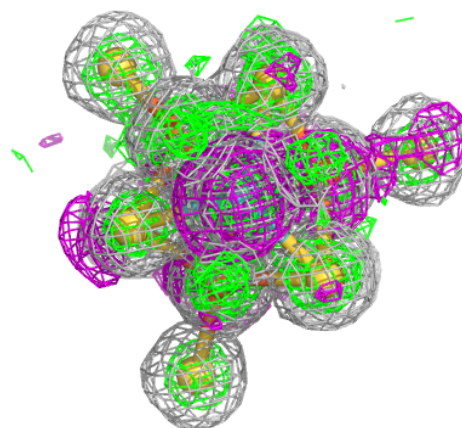
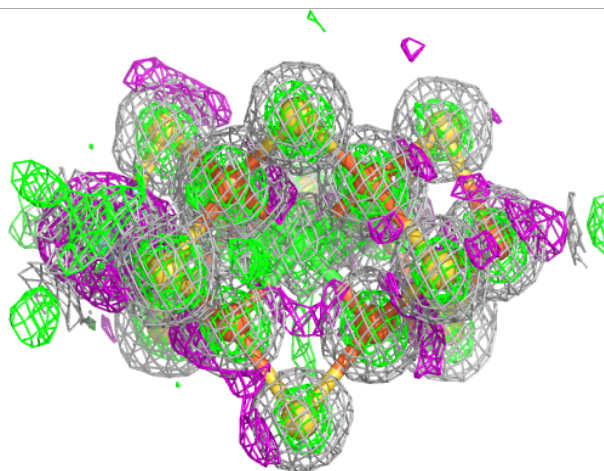
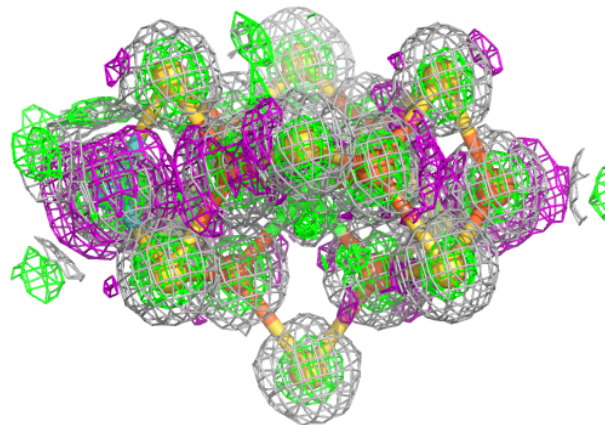
6.4 Ligands

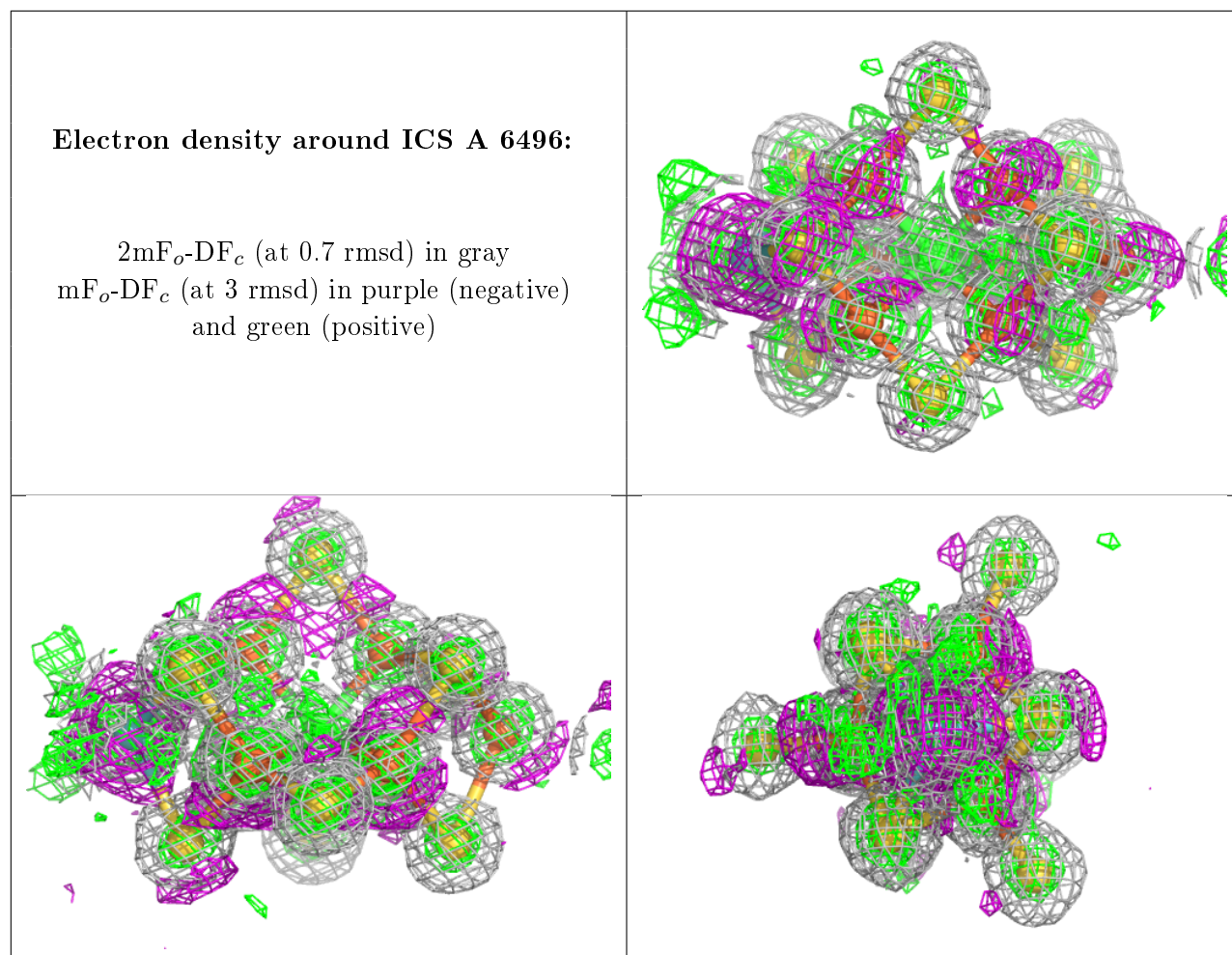
Unable to reproduce the depositors R factor - this section is therefore empty.

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 7496:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.