



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 07:17 am BST

PDB ID : 4TKV
Title : CO-bound Nitrogenase MoFe-protein from *A. vinelandii*
Authors : Spatzal, T.; Perez, K.; Einsle, O.; Howard, J.B.; Rees, D.C.
Deposited on : 2014-05-28
Resolution : 1.50 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

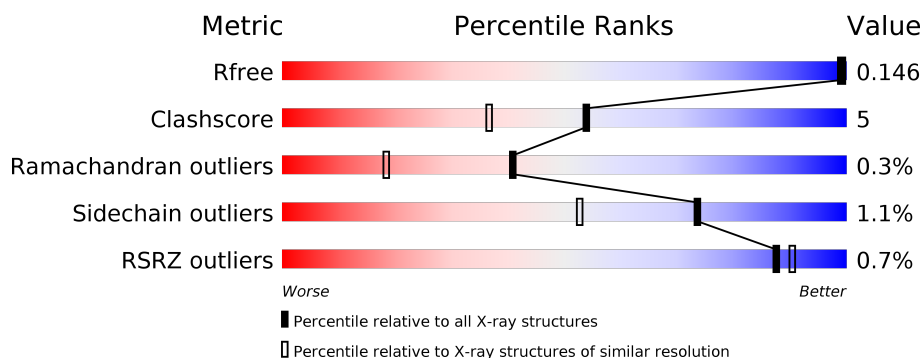
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	492	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 9% ... </div> </div>
1	C	492	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 9% ... </div> </div>
2	B	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 91% 8% </div> </div>
2	D	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 90% 10% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CMO	A	505	-	-	X	-
6	CMO	B	604	-	-	X	-
6	CMO	C	505	-	-	X	-
6	CMO	D	604	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18221 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	15	0
			3914	2482	678	726	28			
1	C	477	Total	C	N	O	S	0	12	0
			3878	2461	664	725	28			

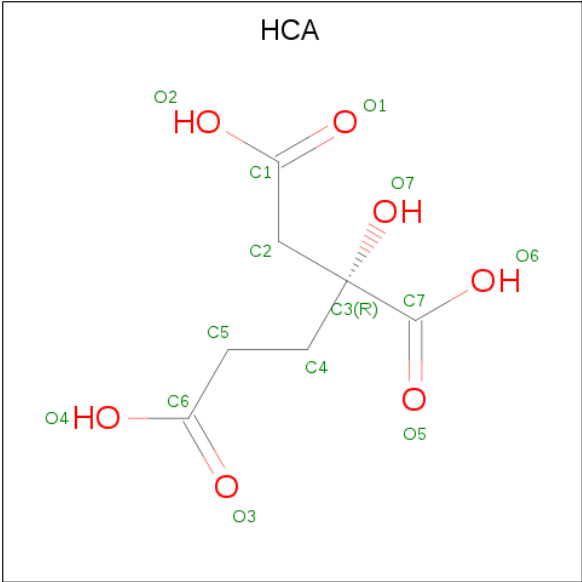
There are 2 discrepancies between the modelled and reference sequences:

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

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

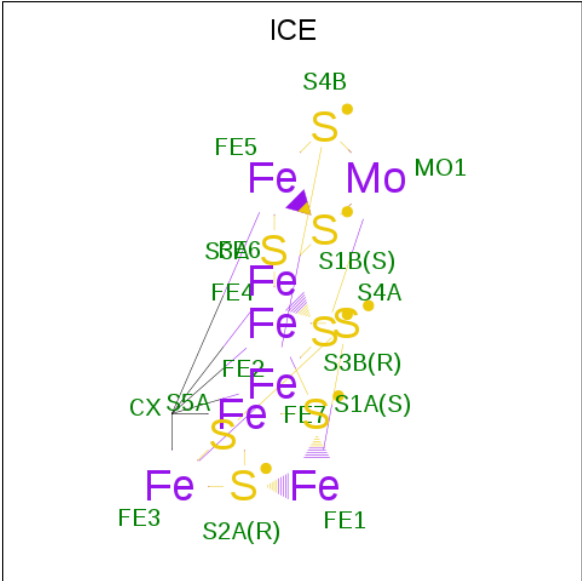
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	17	0
			4301	2739	728	803	31			
2	D	522	Total	C	N	O	S	0	19	0
			4344	2767	732	812	33			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



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: ICE) (formula: CFe₇MoS₈).



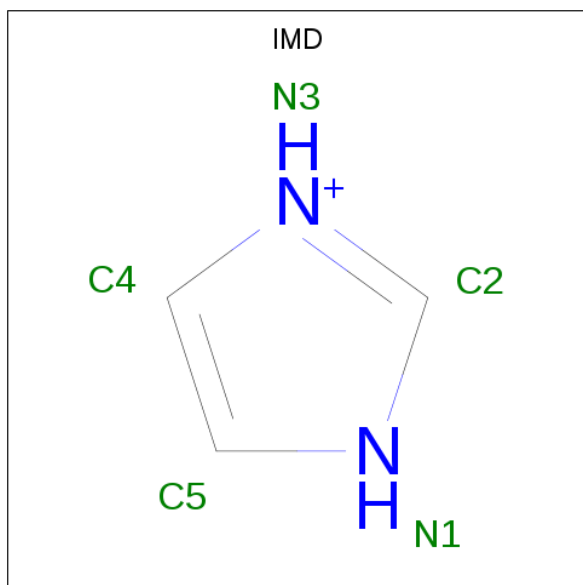
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			17	1	7	1	8		

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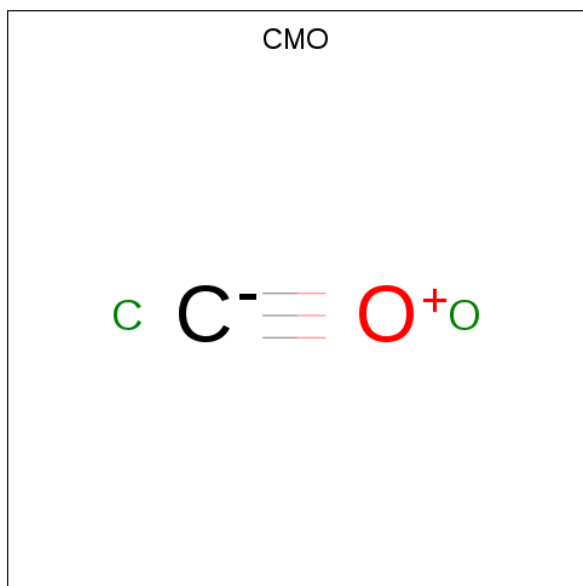
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total S 1 1	0	0
4	C	1	Total C Fe Mo S 17 1 7 1 8	0	0
4	C	1	Total S 1 1	0	0

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



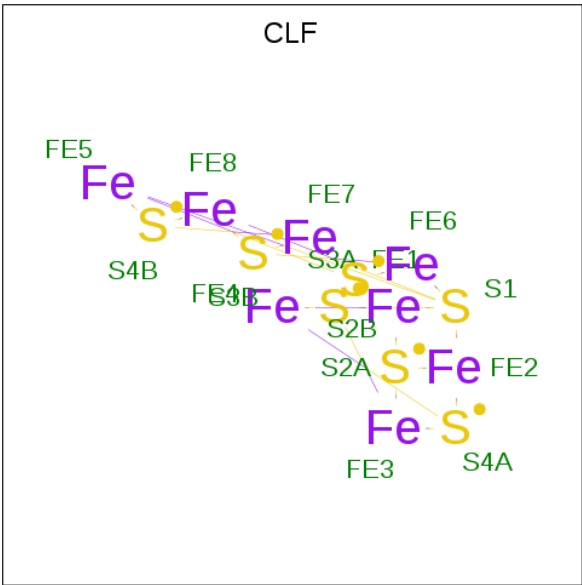
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	B	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0
5	D	1	Total C N 5 3 2	0	0

- Molecule 6 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			2	1	1		
6	A	1	Total	C	O	0	0
			2	1	1		
6	B	1	Total	C	O	0	0
			2	1	1		
6	C	1	Total	C	O	0	0
			2	1	1		
6	C	1	Total	C	O	0	0
			2	1	1		
6	D	1	Total	C	O	0	0
			2	1	1		

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



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

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

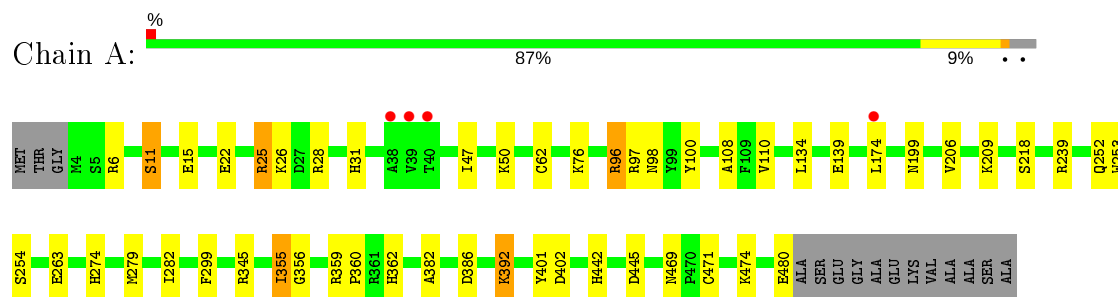
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	351	Total	O	0	0
			351	351		
9	B	466	Total	O	0	0
			466	466		
9	C	362	Total	O	0	0
			362	362		
9	D	457	Total	O	0	0
			457	457		

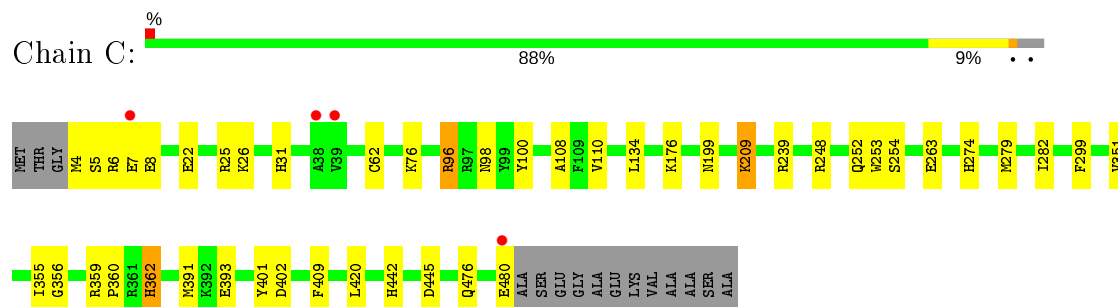
3 Residue-property plots [i](#)

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 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.

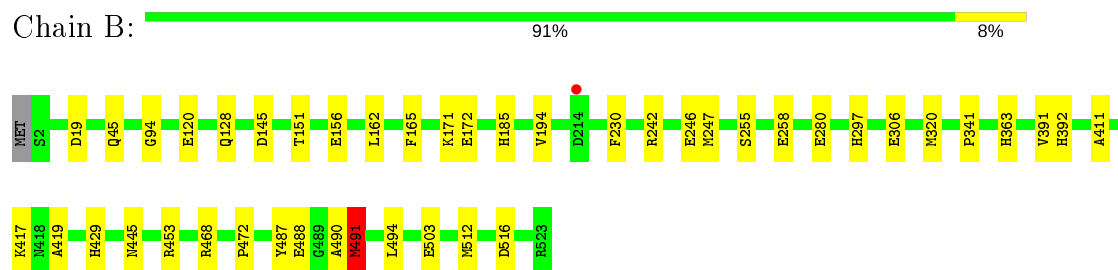
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



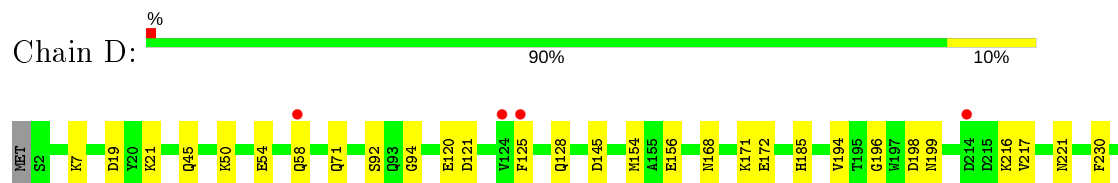
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- 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	81.17Å 130.62Å 107.00Å 90.00° 110.65° 90.00°	Depositor
Resolution (Å)	38.74 – 1.50 38.74 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.74-1.50) 98.1 (38.74-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.138 , 0.154 0.146 , 0.146	Depositor DCC
R_{free} test set	16172 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18221	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CMO, IMD, CLF, ICE, HCA, FE2

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	0.53	0/4001	0.85	15/5385 (0.3%)
1	C	0.54	0/3966	0.80	7/5346 (0.1%)
2	B	0.54	0/4406	0.77	3/5949 (0.1%)
2	D	0.54	0/4450	0.77	3/6006 (0.0%)
All	All	0.54	0/16823	0.80	28/22686 (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
2	B	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25[A]	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	A	25[B]	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	C	96	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	25[A]	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	25[B]	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	25[A]	ARG	CG-CD-NE	-6.95	97.20	111.80
1	A	25[B]	ARG	CG-CD-NE	-6.95	97.20	111.80
2	D	320	MET	CG-SD-CE	6.52	110.64	100.20
2	B	320	MET	CG-SD-CE	6.16	110.05	100.20
1	A	345[A]	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	345[B]	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	209[A]	LYS	CD-CE-NZ	6.00	125.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209[B]	LYS	CD-CE-NZ	6.00	125.51	111.70
1	A	345[A]	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	345[B]	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	D	198	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	6	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	6	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	D	19	ASP	CB-CG-OD1	5.35	123.12	118.30
2	B	145	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	96	ARG	CG-CD-NE	5.32	122.96	111.80
1	C	248	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	6	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	96	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	19	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	28	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	409	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	97	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	491[B]	MET	Mainchain

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	3914	0	3854	38	0
1	C	3878	0	3794	39	0
2	B	4301	0	4185	51	0
2	D	4344	0	4230	52	0
3	A	14	0	6	2	0
3	C	14	0	6	2	0
4	A	18	0	0	1	0
4	C	18	0	0	1	0
5	A	5	0	5	0	0
5	B	15	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	5	0	5	2	0
5	D	15	0	15	2	0
6	A	4	0	0	2	0
6	B	2	0	0	3	0
6	C	4	0	0	2	0
6	D	2	0	0	2	0
7	A	15	0	0	0	0
7	C	15	0	0	0	0
8	B	2	0	0	0	0
9	A	351	0	0	4	0
9	B	466	0	0	13	0
9	C	362	0	0	11	0
9	D	457	0	0	13	0
All	All	18221	0	16115	173	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 (173) 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:C:22:GLU:OE1	1:C:26:LYS:CE	1.69	1.41
2:D:125:PHE:HZ	9:D:1107:HOH:O	1.03	1.35
2:B:453[B]:ARG:HD3	2:D:512[B]:MET:CG	1.62	1.29
2:B:45[A]:GLN:NE2	9:B:702:HOH:O	1.86	1.07
2:B:453[B]:ARG:HD3	2:D:512[B]:MET:HG2	1.31	1.05
1:C:22:GLU:CD	1:C:26:LYS:HE3	1.77	1.05
2:B:512[B]:MET:HB2	2:D:453[B]:ARG:HD3	1.37	1.04
1:C:22:GLU:OE1	1:C:26:LYS:HE3	0.83	1.00
2:D:303:LYS:HE2	9:D:1078:HOH:O	1.62	0.97
2:B:453[B]:ARG:HD3	2:D:512[B]:MET:HG3	1.43	0.97
2:D:125:PHE:CZ	9:D:1107:HOH:O	1.88	0.96
2:B:453[B]:ARG:CD	2:D:512[B]:MET:CG	2.42	0.96
2:B:280:GLU:OE1	5:B:601:IMD:H5	1.67	0.95
2:B:453[B]:ARG:CD	2:D:512[B]:MET:HG3	1.97	0.94
2:B:171:LYS:NZ	2:B:172:GLU:OE2	2.09	0.84
1:A:11:SER:O	1:A:15[A]:GLU:HG3	1.79	0.83
2:D:499:ASN:O	2:D:503[A]:GLU:HG3	1.80	0.80
2:B:512[B]:MET:HB2	2:D:453[B]:ARG:CD	2.11	0.79
5:C:503:IMD:H4	9:C:605:HOH:O	1.82	0.79
6:D:604:CMO:O	9:D:701:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:ASP:H	2:D:429:HIS:HD2	1.30	0.77
1:C:274:HIS:HE1	1:C:299:PHE:H	1.32	0.77
5:D:601:IMD:H4	9:D:748:HOH:O	1.85	0.77
6:B:604:CMO:O	9:B:703:HOH:O	2.04	0.76
2:B:490:ALA:O	2:B:491[B]:MET:O	2.04	0.75
2:D:45[B]:GLN:HG2	9:D:944:HOH:O	1.86	0.75
1:A:274:HIS:HE1	1:A:299:PHE:H	1.35	0.75
2:B:45[B]:GLN:NE2	9:B:706:HOH:O	2.21	0.73
1:C:209[A]:LYS:HE3	9:C:859:HOH:O	1.88	0.72
1:A:480[B]:GLU:O	9:A:602:HOH:O	2.09	0.71
2:D:230:PHE:H	2:D:297:HIS:HE1	1.40	0.69
2:D:92:SER:OG	2:D:154[B]:MET:HG2	1.93	0.69
2:B:453[B]:ARG:NH2	9:B:707:HOH:O	2.22	0.68
2:D:230:PHE:H	2:D:297:HIS:CE1	2.11	0.68
2:B:306:GLU:OE1	9:B:704:HOH:O	2.10	0.68
1:C:391:MET:CE	9:C:609:HOH:O	2.41	0.68
2:D:468:ARG:HH11	6:D:604:CMO:C	2.05	0.68
2:B:230:PHE:H	2:B:297:HIS:HE1	1.39	0.68
2:D:120:GLU:OE2	5:D:603:IMD:H4	1.94	0.68
2:D:21[A]:LYS:HG2	9:D:710:HOH:O	1.91	0.67
2:D:279[A]:GLU:OE2	9:D:702:HOH:O	2.12	0.67
2:B:230:PHE:H	2:B:297:HIS:CE1	2.13	0.66
2:B:453[B]:ARG:HD2	2:D:512[B]:MET:HG3	1.76	0.66
2:D:71:GLN:HE22	2:D:199:ASN:HD22	1.44	0.66
2:B:503[B]:GLU:CD	9:B:709:HOH:O	2.34	0.65
2:D:453[B]:ARG:NH2	9:D:704:HOH:O	2.29	0.65
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.44	0.64
1:C:31:HIS:HE1	9:C:603:HOH:O	1.79	0.64
6:C:505:CMO:C	9:D:704:HOH:O	2.45	0.64
2:B:468:ARG:HH11	6:B:604:CMO:C	2.11	0.64
1:A:15[B]:GLU:O	1:A:15[B]:GLU:HG2	1.97	0.64
1:C:351[B]:VAL:HG12	1:C:420:LEU:HB3	1.78	0.64
2:B:242:ARG:HD3	2:B:246[B]:GLU:OE1	1.98	0.63
1:A:31:HIS:HD2	1:A:402:ASP:OD2	1.81	0.63
6:A:505:CMO:C	9:B:707:HOH:O	2.47	0.63
1:A:25[B]:ARG:NH1	1:A:26:LYS:HG2	2.15	0.62
5:C:503:IMD:H2	9:C:831:HOH:O	1.99	0.62
1:C:22:GLU:OE1	1:C:26:LYS:HE2	1.93	0.61
1:A:31:HIS:HE1	9:A:608:HOH:O	1.82	0.61
1:A:239:ARG:HH11	1:A:252:GLN:HE21	1.48	0.60
2:D:297:HIS:HD2	9:D:719:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:HIS:HD2	1:C:402:ASP:OD2	1.84	0.59
1:A:206:VAL:O	1:A:209[B]:LYS:HG2	2.03	0.59
2:B:297:HIS:HD2	9:B:759:HOH:O	1.85	0.59
2:D:145:ASP:OD2	9:D:703:HOH:O	2.17	0.58
2:D:50:LYS:CE	2:D:54[B]:GLU:OE1	2.52	0.58
2:B:45[B]:GLN:NE2	9:B:705:HOH:O	2.12	0.57
1:C:199:ASN:HD22	1:C:282:ILE:H	1.52	0.56
2:D:171:LYS:NZ	2:D:172:GLU:OE2	2.38	0.56
2:D:185:HIS:HE1	9:D:899:HOH:O	1.87	0.56
1:A:469:ASN:HD22	1:A:471:CYS:H	1.54	0.56
1:C:199:ASN:HD21	1:C:279[A]:MET:HA	1.70	0.56
1:C:391:MET:HE1	9:C:609:HOH:O	2.03	0.56
2:B:453[B]:ARG:C	2:B:453[B]:ARG:HD2	2.26	0.56
2:D:426:ASP:H	2:D:429:HIS:CD2	2.19	0.56
2:D:247[A]:MET:HG3	2:D:341:PRO:HD3	1.86	0.55
1:A:22:GLU:HG3	1:A:26:LYS:HE3	1.89	0.54
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.24	0.53
1:A:22:GLU:OE2	1:A:25[B]:ARG:NE	2.41	0.53
2:B:512[B]:MET:SD	2:D:453[B]:ARG:NE	2.82	0.52
1:C:25:ARG:HD3	9:C:723:HOH:O	2.10	0.52
2:B:156:GLU:OE2	2:B:185:HIS:HD2	1.92	0.52
1:A:199:ASN:HD21	1:A:279[A]:MET:HA	1.75	0.51
1:A:209[A]:LYS:NZ	1:A:263:GLU:OE2	2.39	0.51
1:A:199:ASN:HD22	1:A:282:ILE:H	1.59	0.51
2:B:120:GLU:OE2	5:B:603:IMD:H2	2.10	0.51
2:B:185:HIS:HE1	9:B:933:HOH:O	1.92	0.50
2:B:512[B]:MET:CB	2:D:453[B]:ARG:HD3	2.26	0.50
1:C:22:GLU:CG	1:C:26:LYS:HE3	2.42	0.50
2:D:194:VAL:HB	2:D:297:HIS:CG	2.46	0.50
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.27	0.49
2:B:487:TYR:O	2:B:491[B]:MET:HG3	2.13	0.49
2:B:453[B]:ARG:CD	2:D:512[B]:MET:SD	3.00	0.49
1:C:4:MET:HA	1:C:8:GLU:OE1	2.12	0.49
1:C:96:ARG:HH11	1:C:98:ASN:HD22	1.58	0.48
1:A:218:SER:HB2	9:A:611:HOH:O	2.12	0.48
1:C:476:GLN:OE1	1:C:480:GLU:HB2	2.13	0.48
1:A:442:HIS:HB3	3:A:501:HCA:O6	2.13	0.48
6:B:604:CMO:C	9:B:703:HOH:O	2.56	0.48
1:C:442:HIS:HB3	3:C:501:HCA:O5	2.14	0.48
1:A:392:LYS:HB3	1:A:392:LYS:NZ	2.29	0.48
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453[B]:ARG:O	2:B:453[B]:ARG:HD2	2.14	0.48
2:D:156:GLU:OE2	2:D:185:HIS:HD2	1.97	0.48
2:D:45[B]:GLN:HE22	2:D:458[B]:LYS:HE3	1.79	0.48
1:C:362:HIS:HD2	9:C:890:HOH:O	1.96	0.47
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.96	0.47
1:C:76:LYS:O	1:C:108:ALA:HA	2.14	0.47
1:A:96:ARG:HH11	1:A:98:ASN:HD22	1.62	0.47
2:D:50:LYS:HD2	2:D:54[B]:GLU:OE1	2.15	0.47
2:D:50:LYS:CD	2:D:54[B]:GLU:OE1	2.63	0.47
2:B:363:HIS:HD2	9:B:1099:HOH:O	1.98	0.46
1:A:442:HIS:CG	3:A:501:HCA:H52	2.51	0.46
1:A:274:HIS:CE1	1:A:299:PHE:H	2.23	0.46
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.82	0.45
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.97	0.45
2:D:128:GLN:NE2	2:D:168:ASN:HD22	2.14	0.45
2:D:247[A]:MET:HG3	2:D:341:PRO:CD	2.45	0.45
1:A:253:TRP:HA	1:A:254:SER:HA	1.81	0.45
1:C:253:TRP:HA	1:C:254:SER:HA	1.77	0.45
1:A:134:LEU:HD23	1:A:134:LEU:C	2.37	0.45
2:B:194:VAL:HB	2:B:297:HIS:CG	2.51	0.45
2:B:247[B]:MET:HG3	2:B:341:PRO:HD3	1.99	0.45
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.99	0.45
2:B:488:GLU:O	2:B:491[B]:MET:HB2	2.16	0.45
1:A:25[B]:ARG:NH1	1:A:26:LYS:CG	2.80	0.44
2:B:445:ASN:HB2	2:B:472:PRO:O	2.17	0.44
2:B:391[B]:VAL:HG12	2:B:392:HIS:CE1	2.52	0.44
2:B:490:ALA:O	2:B:491[B]:MET:C	2.54	0.44
1:C:393:GLU:OE1	9:C:601:HOH:O	2.20	0.44
6:C:505:CMO:C	2:D:453[A]:ARG:NH1	2.80	0.44
2:B:411:ALA:HB3	9:B:1081:HOH:O	2.18	0.44
1:A:22:GLU:OE1	1:A:25[A]:ARG:NH1	2.45	0.44
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.53	0.43
1:A:274:HIS:HD2	9:A:846:HOH:O	2.01	0.43
1:C:199:ASN:HD22	1:C:282:ILE:N	2.16	0.43
1:A:474:LYS:HB3	2:D:322:LEU:HD21	1.99	0.43
1:A:47:ILE:HG23	1:A:50:LYS:HE2	2.00	0.43
1:C:5:SER:OG	1:C:8:GLU:HG3	2.19	0.43
2:B:516:ASP:OD2	2:D:453[B]:ARG:NH2	2.51	0.43
1:C:239:ARG:HH11	1:C:252:GLN:NE2	2.13	0.43
2:B:391[A]:VAL:HA	2:B:419:ALA:HA	2.01	0.43
1:C:274:HIS:HD2	9:C:845:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:O	1:A:108:ALA:HA	2.18	0.42
2:D:217:VAL:H	2:D:286:ASN:ND2	2.17	0.42
1:C:134:LEU:HD23	1:C:134:LEU:C	2.40	0.42
2:D:71:GLN:HE22	2:D:199:ASN:ND2	2.15	0.42
1:C:274:HIS:CE1	1:C:299:PHE:H	2.22	0.42
1:A:22:GLU:OE2	1:A:25[B]:ARG:NH1	2.48	0.41
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.03	0.41
1:C:209[A]:LYS:NZ	1:C:263:GLU:OE2	2.45	0.41
6:A:505:CMO:C	2:B:453[A]:ARG:NH2	2.84	0.41
2:D:445:ASN:HB2	2:D:472:PRO:O	2.20	0.41
1:C:391:MET:HE3	9:C:609:HOH:O	2.16	0.41
2:D:509:THR:O	2:D:516:ASP:HA	2.21	0.41
2:B:512[A]:MET:HE2	2:B:512[A]:MET:HB2	1.81	0.41
1:C:359:ARG:N	1:C:360:PRO:CD	2.83	0.41
1:C:62:CYS:HB3	2:D:94:GLY:HA3	2.03	0.41
1:A:209[B]:LYS:H	1:A:209[B]:LYS:HG2	1.75	0.41
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.21	0.41
2:B:491[B]:MET:O	2:B:494:LEU:N	2.54	0.41
1:C:442:HIS:CG	3:C:501:HCA:H52	2.55	0.41
1:C:356:GLY:HA3	4:C:502:ICE:S1B	2.61	0.41
2:D:216:LYS:HA	2:D:286:ASN:HD21	1.85	0.41
1:C:199:ASN:HD21	1:C:279[B]:MET:HA	1.85	0.41
2:D:71:GLN:O	2:D:196:GLY:HA3	2.21	0.40
2:D:121:ASP:O	2:D:125:PHE:CE2	2.74	0.40
1:A:359:ARG:N	1:A:360:PRO:CD	2.84	0.40
1:A:356:GLY:HA3	4:A:502:ICE:S1B	2.62	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	489/492 (99%)	470 (96%)	18 (4%)	1 (0%)	47	23
1	C	487/492 (99%)	468 (96%)	18 (4%)	1 (0%)	47	23
2	B	537/523 (103%)	522 (97%)	12 (2%)	3 (1%)	25	7
2	D	540/523 (103%)	526 (97%)	13 (2%)	1 (0%)	47	23
All	All	2053/2030 (101%)	1986 (97%)	61 (3%)	6 (0%)	41	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491[A]	MET
2	B	491[B]	MET
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	420/415 (101%)	414 (99%)	6 (1%)	67	42
1	C	415/415 (100%)	410 (99%)	5 (1%)	71	48
2	B	468/455 (103%)	466 (100%)	2 (0%)	91	82
2	D	472/455 (104%)	465 (98%)	7 (2%)	65	39
All	All	1775/1740 (102%)	1755 (99%)	20 (1%)	73	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	355	ILE
1	A	362	HIS
1	A	392	LYS
1	A	401	TYR

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Mol	Chain	Res	Type
1	A	445	ASP
2	B	258	GLU
2	B	417	LYS
1	C	7	GLU
1	C	176	LYS
1	C	362	HIS
1	C	401	TYR
1	C	445	ASP
2	D	7	LYS
2	D	58	GLN
2	D	247[A]	MET
2	D	247[B]	MET
2	D	258	GLU
2	D	279[A]	GLU
2	D	279[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	98	ASN
1	A	199	ASN
1	A	252	GLN
1	A	271	ASN
1	A	274	HIS
1	A	384	ASN
1	A	432	GLN
1	A	468	ASN
1	A	469	ASN
2	B	128	GLN
2	B	130	ASN
2	B	185	HIS
2	B	199	ASN
2	B	225	ASN
2	B	286	ASN
2	B	297	HIS
2	B	363	HIS
2	B	418	ASN
2	B	429	HIS
2	B	518	ASN
1	C	31	HIS
1	C	98	ASN

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Mol	Chain	Res	Type
1	C	199	ASN
1	C	252	GLN
1	C	271	ASN
1	C	274	HIS
1	C	321	GLN
1	C	362	HIS
1	C	384	ASN
1	C	468	ASN
2	D	58	GLN
2	D	71	GLN
2	D	93	GLN
2	D	128	GLN
2	D	130	ASN
2	D	185	HIS
2	D	225	ASN
2	D	286	ASN
2	D	294	GLN
2	D	297	HIS
2	D	418	ASN
2	D	429	HIS
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 24 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 20 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	A	501	4	4,13,13	0.67	0	4,18,18	3.00	1 (25%)
5	IMD	D	603	-	3,5,5	0.37	0	4,5,5	0.55	0
6	CMO	A	504	4	0,1,1	0.00	-	-	-	-
3	HCA	C	501	4	4,13,13	0.65	0	4,18,18	2.97	1 (25%)
7	CLF	A	507	1,2	0,24,24	0.00	-	-	-	-
6	CMO	A	505	-	0,1,1	0.00	-	-	-	-
5	IMD	D	601	-	3,5,5	0.48	0	4,5,5	0.59	0
5	IMD	A	503	-	3,5,5	0.35	0	4,5,5	0.52	0
6	CMO	D	604	-	0,1,1	0.00	-	-	-	-
7	CLF	C	507	1,2	0,24,24	0.00	-	-	-	-
6	CMO	B	604	-	0,1,1	0.00	-	-	-	-
5	IMD	B	601	-	3,5,5	0.49	0	4,5,5	0.47	0
5	IMD	D	602	-	3,5,5	0.41	0	4,5,5	0.58	0
4	ICE	A	502	1,3,6	12,28,28	2.48	5 (41%)	-	-	-
5	IMD	C	503	-	3,5,5	0.40	0	4,5,5	0.59	0
5	IMD	B	603	-	3,5,5	0.36	0	4,5,5	0.57	0
5	IMD	B	602	-	3,5,5	0.21	0	4,5,5	0.81	0
4	ICE	C	502	1,3,6	12,28,28	2.40	5 (41%)	-	-	-
6	CMO	C	505	-	0,1,1	0.00	-	-	-	-
6	CMO	C	504	4	0,1,1	0.00	-	-	-	-

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	D	603	-	-	-	0/1/1/1
3	HCA	C	501	4	-	0/7/17/17	-
7	CLF	A	507	1,2	-	-	0/12/10/10
5	IMD	A	503	-	-	-	0/1/1/1
7	CLF	C	507	1,2	-	-	0/12/10/10
5	IMD	B	601	-	-	-	0/1/1/1
5	IMD	D	602	-	-	-	0/1/1/1
5	IMD	C	503	-	-	-	0/1/1/1
5	IMD	B	603	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	D	601	-	-	-	0/1/1/1
5	IMD	B	602	-	-	-	0/1/1/1
3	HCA	A	501	4	-	0/7/17/17	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICE	S4B-FE5	-4.70	2.20	2.32
4	C	502	ICE	S4B-FE5	-4.36	2.21	2.32
4	A	502	ICE	S3B-FE7	-4.11	2.22	2.32
4	A	502	ICE	S4B-FE7	-3.81	2.23	2.32
4	C	502	ICE	S3B-FE7	-3.53	2.23	2.32
4	C	502	ICE	S4B-FE7	-3.51	2.23	2.32
4	C	502	ICE	S4A-FE3	-2.70	2.25	2.32
4	A	502	ICE	S4A-FE3	-2.49	2.26	2.32
4	C	502	ICE	S5A-FE7	-2.21	2.19	2.24
4	A	502	ICE	S5A-FE3	-2.03	2.20	2.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	C4-C5-C6	5.85	120.25	111.39
3	C	501	HCA	C4-C5-C6	5.40	119.57	111.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 21 short contacts:

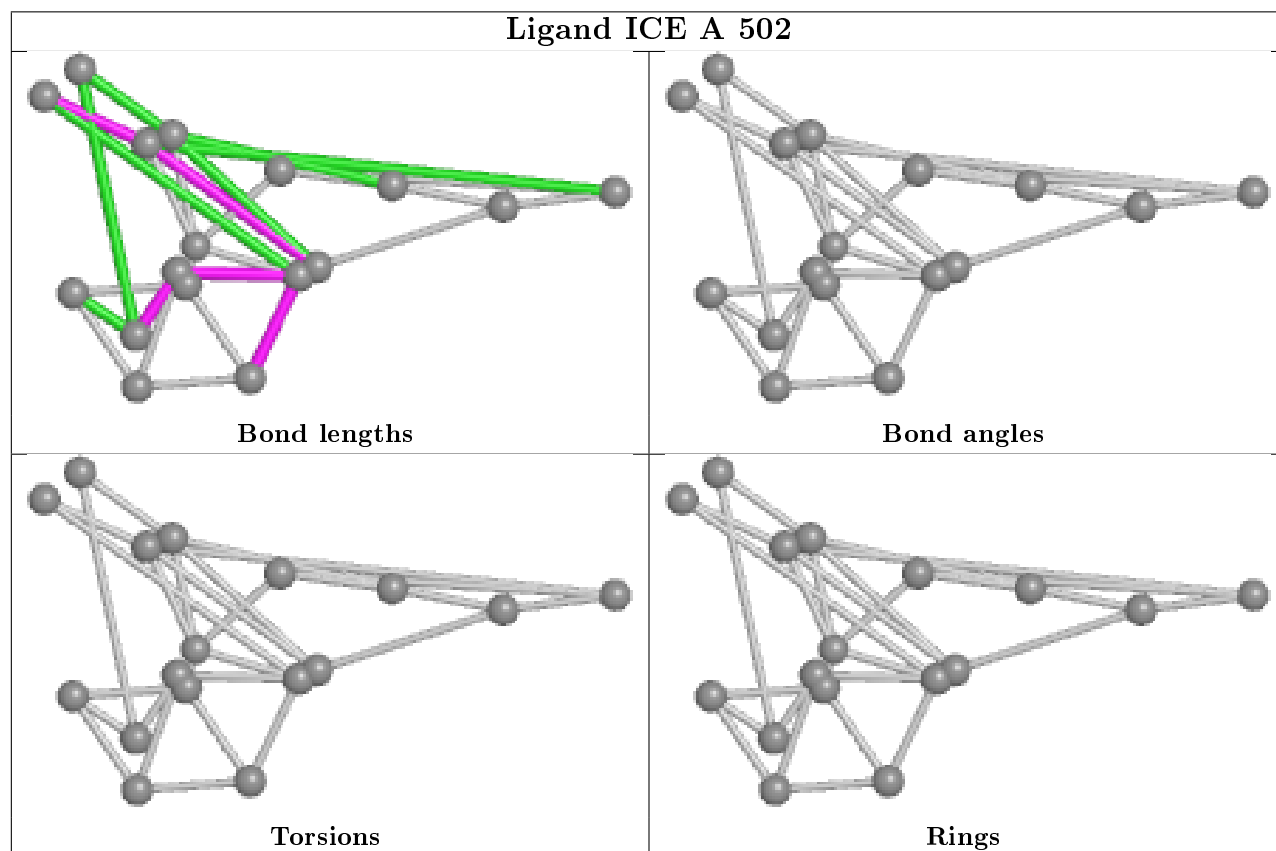
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	2	0
5	D	603	IMD	1	0
3	C	501	HCA	2	0
6	A	505	CMO	2	0
5	D	601	IMD	1	0
6	D	604	CMO	2	0
6	B	604	CMO	3	0
5	B	601	IMD	1	0
4	A	502	ICE	1	0
5	C	503	IMD	2	0

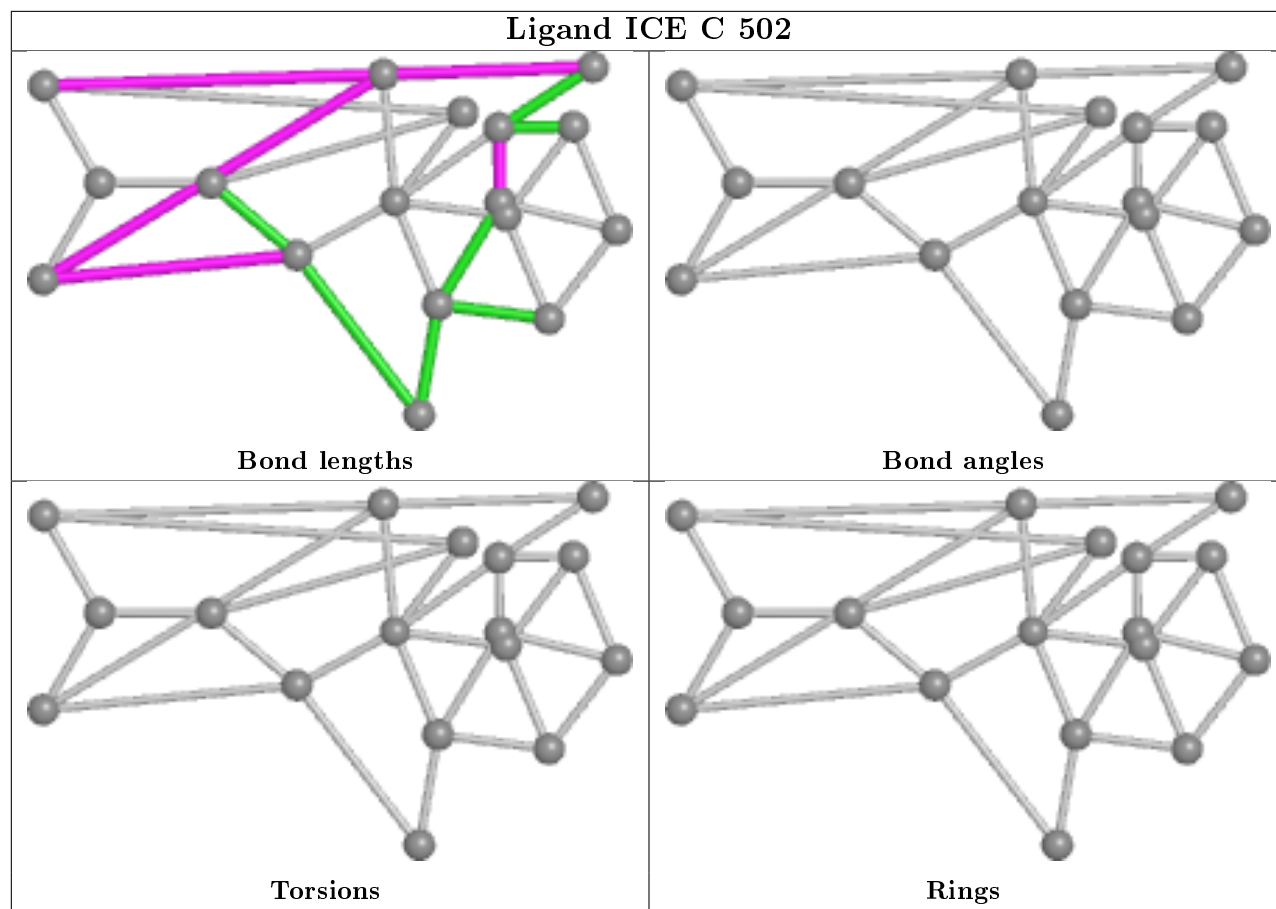
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	603	IMD	1	0
4	C	502	ICE	1	0
6	C	505	CMO	2	0

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	477/492 (96%)	-0.13	4 (0%) 86 89	10, 14, 28, 43	5 (1%)
1	C	477/492 (96%)	-0.13	4 (0%) 86 89	10, 15, 27, 38	8 (1%)
2	B	522/523 (99%)	-0.28	1 (0%) 95 95	10, 14, 23, 33	6 (1%)
2	D	522/523 (99%)	-0.24	5 (0%) 82 85	10, 14, 24, 35	4 (0%)
All	All	1998/2030 (98%)	-0.20	14 (0%) 87 90	10, 14, 25, 43	23 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	5.6
1	A	39	VAL	4.9
1	C	38	ALA	4.9
1	C	39	VAL	4.4
2	D	125	PHE	3.1
2	D	214	ASP	3.1
1	C	480	GLU	2.6
1	C	7	GLU	2.5
1	A	174	LEU	2.5
2	D	124	VAL	2.5
2	B	214	ASP	2.3
2	D	412	ALA	2.2
2	D	58	GLN	2.2
1	A	40	THR	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

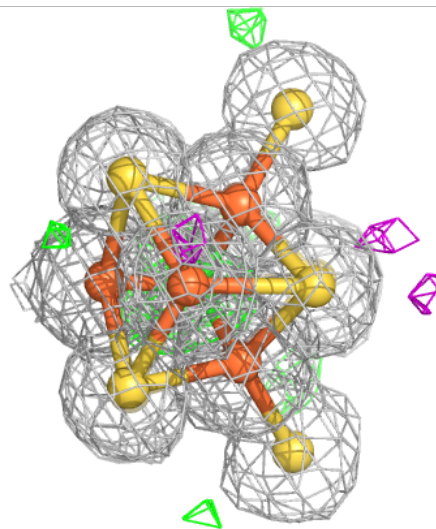
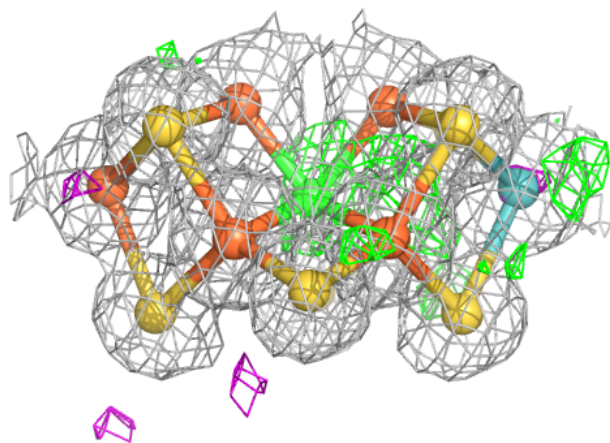
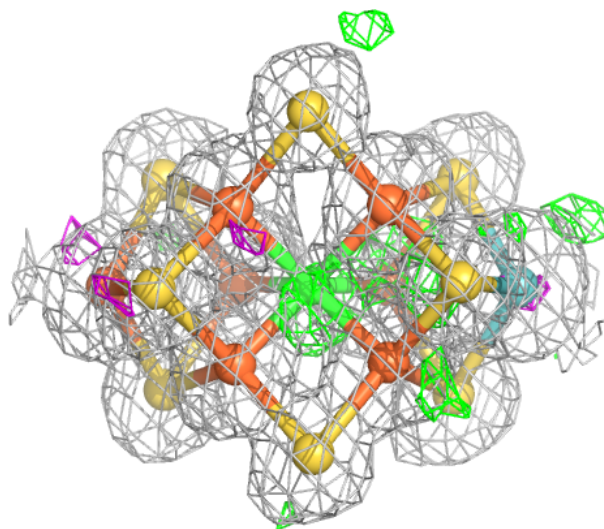
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CMO	A	505	2/2	0.89	0.23	18,18,18,21	2
5	IMD	B	601	5/5	0.90	0.12	26,29,33,34	0
6	CMO	C	505	2/2	0.91	0.25	16,16,16,19	2
6	CMO	B	604	2/2	0.92	0.13	14,14,14,18	2
6	CMO	A	504	2/2	0.94	0.12	11,11,11,13	0
5	IMD	B	603	5/5	0.94	0.08	25,25,27,31	0
6	CMO	D	604	2/2	0.95	0.15	13,13,13,17	2
5	IMD	D	603	5/5	0.95	0.09	25,29,30,32	0
5	IMD	C	503	5/5	0.96	0.12	18,22,24,28	0
5	IMD	B	602	5/5	0.97	0.07	14,14,17,18	0
5	IMD	D	601	5/5	0.97	0.10	12,14,16,18	0
5	IMD	D	602	5/5	0.97	0.08	21,21,24,25	0
5	IMD	A	503	5/5	0.97	0.16	21,26,26,29	0
3	HCA	C	501	14/14	0.97	0.10	9,11,13,14	0
3	HCA	A	501	14/14	0.97	0.11	10,11,13,14	0
6	CMO	C	504	2/2	0.98	0.09	10,10,10,11	0
4	ICE	C	502	17/17	0.99	0.06	11,11,12,12	0
7	CLF	C	507	15/15	0.99	0.06	11,12,12,13	0
4	ICE	A	502	17/17	0.99	0.07	11,11,12,12	0
7	CLF	A	507	15/15	1.00	0.06	11,11,12,12	0
8	FE2	B	606	1/1	1.00	0.05	15,15,15,15	1
4	ICE	C	506	1/17	1.00	0.08	18,18,18,18	0
4	ICE	A	506	1/17	1.00	0.07	18,18,18,18	0
8	FE2	B	605	1/1	1.00	0.04	14,14,14,14	1

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

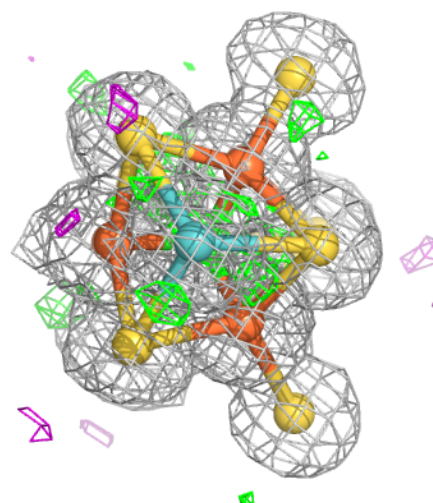
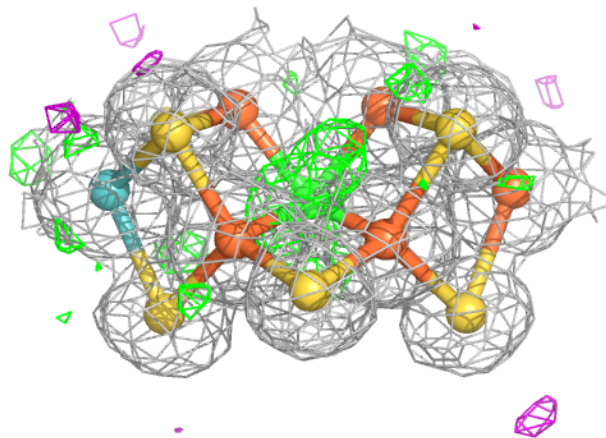
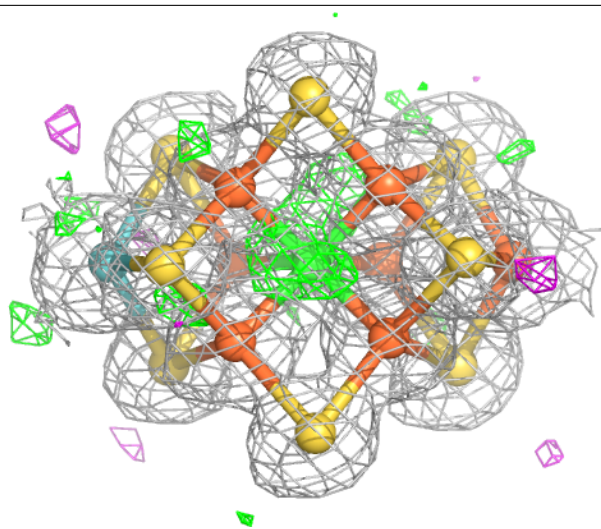
Electron density around ICE C 502:

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



Electron density around ICE 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.