



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:37 am BST

PDB ID : 1YQ9
Title : Structure of the unready oxidized form of [NiFe] hydrogenase
Authors : Volbeda, A.; Martin, L.; Cavazza, C.; Matho, M.; Faber, B.W.; Roseboom, W.; Albracht, S.P.; Garcin, E.; Rousset, M.; Fontecilla-Camps, J.C.
Deposited on : 2005-02-01
Resolution : 2.35 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
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

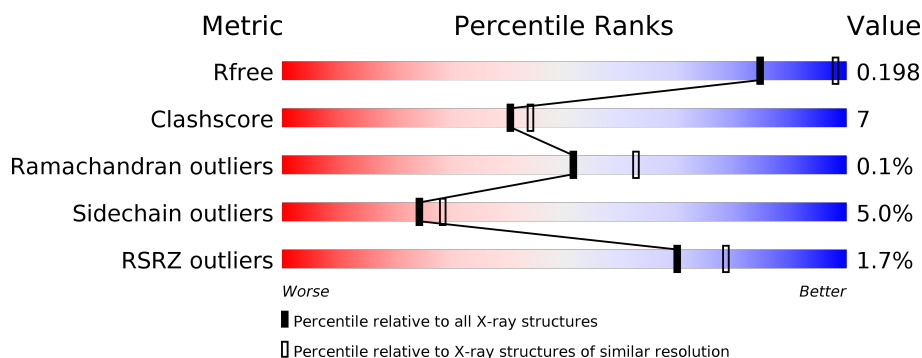
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	264	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 82%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 82% 16% .. </div> </div>
1	B	264	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 78%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 78% 19% .. </div> </div>
2	H	536	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 82% 15% .. </div> </div>
2	I	536	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 15%, green 82%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 3% 82% 15% .. </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12882 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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	2	0
			1972	1252	330	371	19			
1	B	260	Total	C	N	O	S	0	1	0
			1959	1244	328	368	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	LEU	SEE REMARK 999	UNP P12943
A	89	GLY	ARG	SEE REMARK 999	UNP P12943
B	24	VAL	LEU	SEE REMARK 999	UNP P12943
B	89	GLY	ARG	SEE REMARK 999	UNP P12943

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	530	Total	C	N	O	S	0	1	0
			4164	2658	730	759	17			
2	I	530	Total	C	N	O	S	0	0	0
			4158	2655	727	759	17			

There are 6 discrepancies between the modelled and reference sequences:

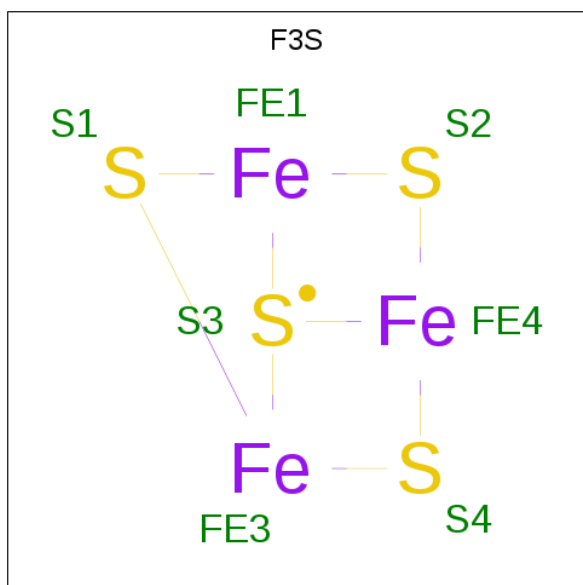
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	INITIATING METHIONINE	UNP P12944
H	482	LEU	HIS	SEE REMARK 999	UNP P12944
H	497	GLY	ARG	SEE REMARK 999	UNP P12944
I	1	MET	-	INITIATING METHIONINE	UNP P12944
I	482	LEU	HIS	SEE REMARK 999	UNP P12944
I	497	GLY	ARG	SEE REMARK 999	UNP P12944

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



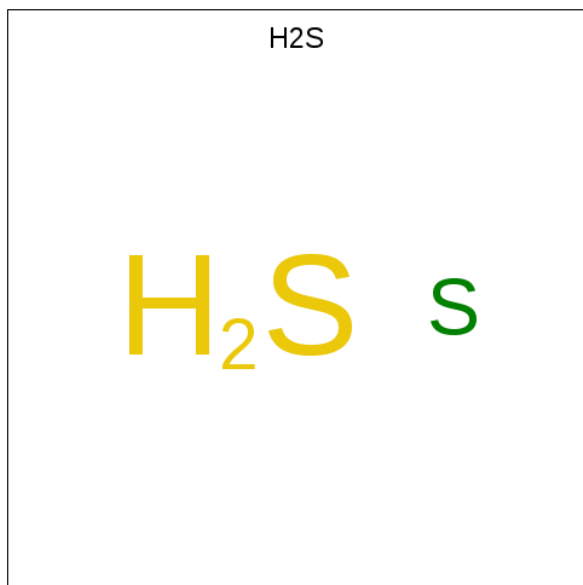
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	S	0	0
			1	1		
5	H	1	Total	S	0	0
			1	1		
5	B	1	Total	S	0	0
			1	1		
5	I	1	Total	S	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

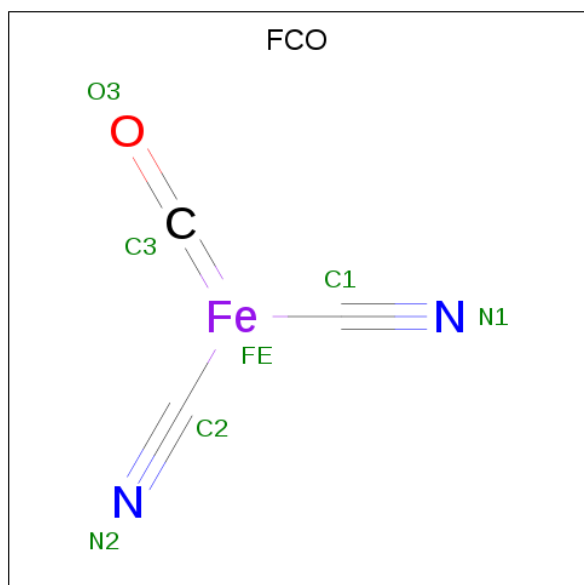
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ni	0	0
			1	1		
7	I	1	Total	Ni	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

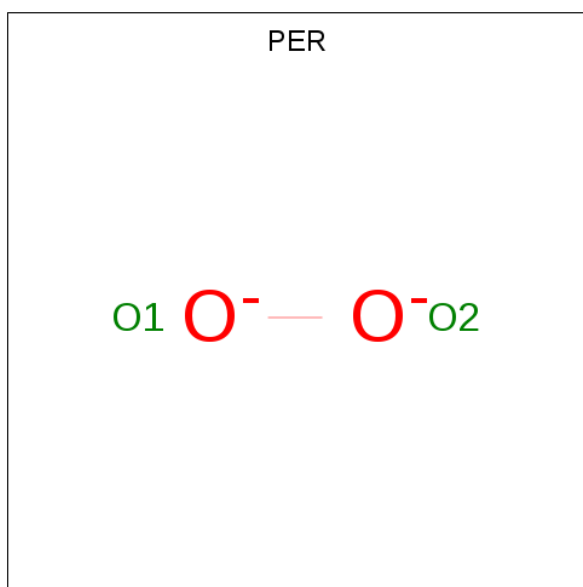
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total Mg 1 1	0	0
8	I	1	Total Mg 1 1	0	0

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C Fe N O 7 3 1 2 1	0	0
9	I	1	Total C Fe N O 7 3 1 2 1	0	0

- Molecule 10 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total O 2 2	0	0
10	I	1	Total O 2 2	0	0

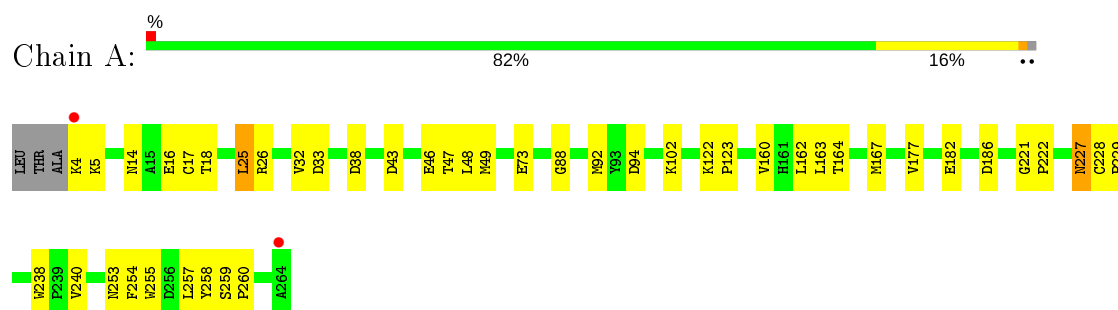
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	117	Total O 117 117	0	0
11	H	167	Total O 167 167	0	0
11	B	94	Total O 94 94	0	0
11	I	137	Total O 137 137	0	0

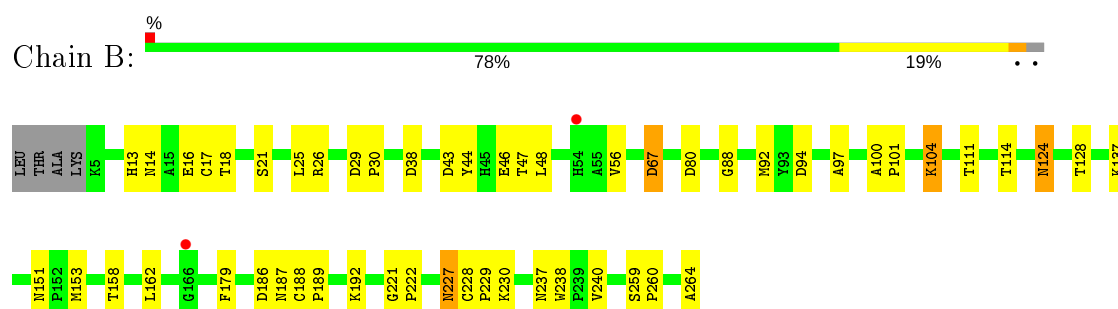
3 Residue-property plots [i](#)

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.

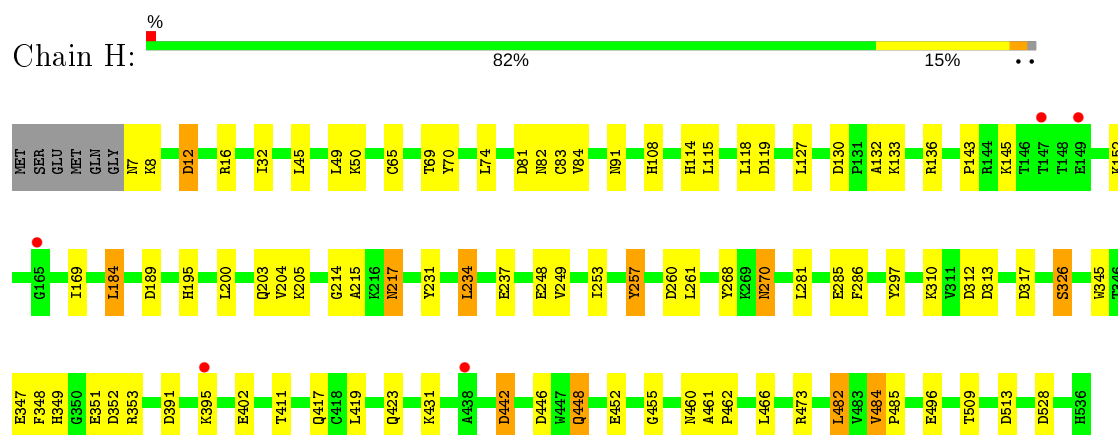
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



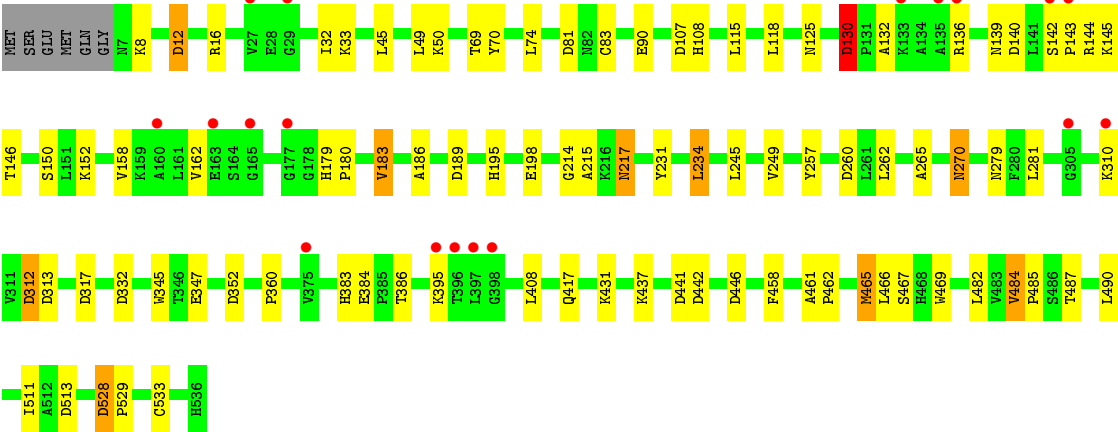
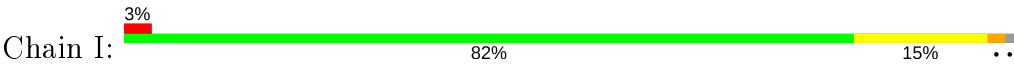
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.75Å 93.44Å 69.03Å 89.33° 102.41° 90.95°	Depositor
Resolution (Å)	13.00 – 2.35 19.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.2 (13.00-2.35) 91.7 (19.82-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.46 (at 2.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.132 , 0.183 0.150 , 0.198	Depositor DCC
R_{free} test set	2967 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12882	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 4.88% 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: GOL, MG, NI, SF4, H2S, F3S, PER, FCO

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	0.48	0/2035	0.69	5/2765 (0.2%)
1	B	0.41	0/2017	0.68	6/2742 (0.2%)
2	H	0.43	0/4274	0.71	13/5809 (0.2%)
2	I	0.38	0/4263	0.69	16/5795 (0.3%)
All	All	0.42	0/12589	0.69	40/17111 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	442	ASP	CB-CG-OD2	7.60	125.14	118.30
2	H	528	ASP	CB-CG-OD2	7.47	125.03	118.30
2	I	107	ASP	CB-CG-OD2	7.17	124.75	118.30
2	I	81	ASP	CB-CG-OD2	6.94	124.54	118.30
1	A	43	ASP	CB-CG-OD2	6.85	124.47	118.30
2	I	446	ASP	CB-CG-OD2	6.62	124.26	118.30
2	H	446	ASP	CB-CG-OD2	6.54	124.18	118.30
2	H	130	ASP	CB-CG-OD2	6.49	124.14	118.30
2	H	119	ASP	CB-CG-OD2	6.40	124.06	118.30
2	H	81	ASP	CB-CG-OD2	6.29	123.96	118.30
2	H	317	ASP	CB-CG-OD2	6.19	123.87	118.30
2	I	352	ASP	CB-CG-OD2	6.16	123.84	118.30
2	I	313	ASP	CB-CG-OD2	6.10	123.79	118.30
2	I	12	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	94	ASP	CB-CG-OD2	5.79	123.51	118.30
2	H	189	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	38	ASP	CB-CG-OD2	5.73	123.45	118.30
2	H	313	ASP	CB-CG-OD2	5.67	123.40	118.30
2	I	189	ASP	CB-CG-OD2	5.67	123.40	118.30
2	I	442	ASP	CB-CG-OD2	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	317	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	33	ASP	CB-CG-OD2	5.49	123.24	118.30
2	I	528	ASP	CB-CG-OD2	5.41	123.17	118.30
2	I	513	ASP	CB-CG-OD2	5.41	123.17	118.30
2	H	513	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	80	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	186	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	38	ASP	CB-CG-OD2	5.35	123.11	118.30
2	H	391	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	94	ASP	CB-CG-OD2	5.33	123.10	118.30
2	I	130	ASP	CB-CG-OD2	5.33	123.09	118.30
2	H	12	ASP	CB-CG-OD2	5.30	123.07	118.30
2	I	312	ASP	CB-CG-OD2	5.28	123.05	118.30
2	H	312	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	67	ASP	CB-CG-OD2	5.19	122.97	118.30
2	I	332	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	43	ASP	CB-CG-OD2	5.12	122.91	118.30
2	I	441	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	186	ASP	CB-CG-OD2	5.09	122.88	118.30
2	I	140	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1972	0	1899	27	0
1	B	1959	0	1884	39	1
2	H	4164	0	4124	57	0
2	I	4158	0	4115	66	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	A	24	0	32	1	1
6	B	6	0	8	0	0
6	H	12	0	16	3	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
9	H	7	0	0	0	0
9	I	7	0	0	1	0
10	H	2	0	0	0	0
10	I	2	0	0	0	0
11	A	117	0	0	3	0
11	B	94	0	0	5	0
11	H	167	0	0	1	0
11	I	137	0	0	1	0
All	All	12882	0	12078	176	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 7.

All (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:270:ASN:H	2:H:270:ASN:HD22	1.14	0.96
2:I:139:ASN:HD21	2:I:146:THR:N	1.64	0.96
2:I:108:HIS:HE1	2:I:417:GLN:HE21	1.13	0.94
2:I:139:ASN:ND2	2:I:146:THR:H	1.67	0.92
2:I:484:VAL:HG23	2:I:485:PRO:HD2	1.56	0.87
2:I:108:HIS:CE1	2:I:417:GLN:HE21	1.93	0.86
2:I:195:HIS:ND1	2:I:260:ASP:OD1	2.09	0.85
1:A:26:ARG:HH21	2:H:217:ASN:HD21	1.21	0.81
2:H:484:VAL:HG23	2:H:485:PRO:HD2	1.62	0.81
2:I:270:ASN:HD22	2:I:270:ASN:H	1.30	0.80
1:B:67:ASP:HA	11:B:322:HOH:O	1.81	0.79
2:H:237:GLU:OE1	2:H:237:GLU:N	2.11	0.79
2:H:348:PHE:CG	6:H:1543:GOL:H31	2.22	0.73
2:I:139:ASN:HD21	2:I:146:THR:H	0.83	0.73
1:B:26:ARG:HH21	2:I:217:ASN:HD21	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:270:ASN:HD22	2:I:270:ASN:N	1.87	0.72
1:A:229:PRO:HD2	11:A:1559:HOH:O	1.89	0.72
1:B:124:ASN:HD21	1:B:128:THR:H	1.34	0.71
1:B:44:TYR:HE1	1:B:56:VAL:HG13	1.55	0.70
2:H:419:LEU:O	2:H:423:GLN:HG3	1.92	0.69
2:I:158:VAL:O	2:I:162:VAL:HG23	1.92	0.68
1:A:253[B]:ASN:OD1	11:A:1634:HOH:O	2.13	0.67
1:B:227:ASN:HD22	1:B:227:ASN:H	1.43	0.66
2:H:270:ASN:N	2:H:270:ASN:HD22	1.91	0.65
1:B:44:TYR:CE1	1:B:56:VAL:HG13	2.32	0.65
2:I:136:ARG:HH11	2:I:136:ARG:HG3	1.62	0.65
2:I:458:PHE:HD1	2:I:465:MET:HE3	1.63	0.64
2:H:452:GLU:HG3	2:H:473:ARG:HG3	1.80	0.63
1:B:26:ARG:HE	2:I:217:ASN:ND2	1.96	0.62
1:A:46:GLU:OE1	11:A:1588:HOH:O	2.16	0.62
2:H:402:GLU:H	2:H:402:GLU:CD	2.03	0.62
2:I:145:LYS:HA	2:I:145:LYS:HE2	1.80	0.62
2:I:195:HIS:HD1	2:I:260:ASP:CG	2.01	0.62
2:H:270:ASN:ND2	2:H:270:ASN:H	1.91	0.61
1:B:13:HIS:HD2	11:B:312:HOH:O	1.83	0.61
2:H:214:GLY:O	2:H:215:ALA:HB3	2.00	0.61
2:I:139:ASN:ND2	2:I:145:LYS:HA	2.15	0.60
1:B:259:SER:HA	1:B:260:PRO:C	2.22	0.60
2:H:108:HIS:CE1	2:H:417:GLN:HE21	2.19	0.60
2:I:484:VAL:HG23	2:I:485:PRO:CD	2.30	0.59
2:I:130:ASP:OD2	2:I:130:ASP:C	2.42	0.58
2:I:265:ALA:HB1	2:I:408:LEU:HD11	1.86	0.58
2:I:345:TRP:CZ2	2:I:347:GLU:HA	2.39	0.57
2:I:484:VAL:HG21	2:I:533:CYS:HB3	1.86	0.57
2:H:205:LYS:NZ	2:H:248:GLU:OE2	2.39	0.56
2:I:383:HIS:HD2	2:I:386:THR:OG1	1.90	0.55
2:I:528:ASP:N	2:I:529:PRO:HD3	2.21	0.55
2:H:108:HIS:HE1	2:H:417:GLN:HE21	1.53	0.55
2:I:125:ASN:ND2	2:I:186:ALA:HA	2.22	0.55
1:A:259:SER:HA	1:A:260:PRO:C	2.26	0.55
1:B:13:HIS:HE1	1:B:21:SER:OG	1.90	0.55
2:H:217:ASN:C	2:H:217:ASN:HD22	2.10	0.55
2:H:132:ALA:O	2:H:136[A]:ARG:HG3	2.06	0.54
2:I:465:MET:HE1	2:I:466:LEU:C	2.28	0.54
1:A:227:ASN:HD22	1:A:227:ASN:H	1.56	0.53
1:B:187:ASN:OD1	1:B:230:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:TYR:HE1	1:B:56:VAL:CG1	2.20	0.53
2:H:351:GLU:O	2:H:352:ASP:HB2	2.08	0.53
2:I:90:GLU:OE2	2:I:431:LYS:HE2	2.09	0.53
1:A:88:GLY:HA2	2:H:12:ASP:CG	2.29	0.53
1:A:257:LEU:HD23	1:A:258:TYR:CE2	2.45	0.52
2:H:69:THR:O	2:H:70:TYR:HB3	2.10	0.51
2:I:231:TYR:O	2:I:234:LEU:HB2	2.11	0.51
1:B:192:LYS:HG2	11:B:319:HOH:O	2.11	0.51
2:H:484:VAL:HG23	2:H:485:PRO:CD	2.37	0.51
1:A:160:VAL:O	1:A:164:THR:HG23	2.11	0.51
2:H:82:ASN:HD22	2:H:455:GLY:HA2	1.74	0.51
2:I:270:ASN:ND2	2:I:270:ASN:N	2.58	0.51
2:I:310:LYS:HE3	2:I:312:ASP:OD2	2.11	0.50
2:H:348:PHE:CD1	6:H:1543:GOL:H31	2.46	0.50
2:I:458:PHE:CD1	2:I:465:MET:HE3	2.45	0.50
1:B:221:GLY:N	1:B:222:PRO:CD	2.75	0.49
2:H:452:GLU:OE1	2:H:473:ARG:HD2	2.12	0.49
2:H:32:ILE:HD12	2:H:509:THR:HB	1.92	0.49
2:I:281:LEU:HD12	2:I:281:LEU:C	2.32	0.49
1:A:25:LEU:HD12	1:A:32:VAL:HG21	1.93	0.48
1:B:88:GLY:HA2	2:I:12:ASP:CG	2.33	0.48
1:B:88:GLY:HA2	2:I:12:ASP:OD1	2.14	0.48
2:H:270:ASN:ND2	2:H:270:ASN:N	2.57	0.48
2:I:217:ASN:C	2:I:217:ASN:HD22	2.17	0.48
1:A:221:GLY:N	1:A:222:PRO:CD	2.77	0.48
1:B:227:ASN:ND2	1:B:227:ASN:H	2.10	0.48
2:H:345:TRP:CZ2	2:H:347:GLU:HA	2.49	0.47
1:A:26:ARG:HE	2:H:217:ASN:ND2	2.13	0.47
2:I:179:HIS:ND1	2:I:180:PRO:HD2	2.29	0.47
2:H:249:VAL:O	2:H:253:ILE:HG13	2.14	0.47
1:B:104:LYS:HA	1:B:104:LYS:HE3	1.95	0.47
1:B:227:ASN:HD22	1:B:227:ASN:N	2.05	0.47
2:I:136:ARG:NH1	2:I:136:ARG:HG3	2.26	0.47
1:A:18:THR:HG22	1:A:18:THR:O	2.15	0.46
2:I:245:LEU:O	2:I:249:VAL:HG23	2.15	0.46
1:B:18:THR:O	1:B:18:THR:HG22	2.16	0.46
2:I:132:ALA:HB1	2:I:136:ARG:HH12	1.80	0.46
2:I:183:VAL:O	2:I:183:VAL:HG23	2.16	0.46
2:H:482:LEU:N	2:H:482:LEU:HD23	2.31	0.45
2:H:91:ASN:HB2	2:H:442:ASP:O	2.17	0.45
2:H:448:GLN:H	6:H:1544:GOL:H11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:484:VAL:CG2	2:H:485:PRO:HD2	2.41	0.45
2:I:461:ALA:HB1	2:I:462:PRO:CD	2.46	0.45
2:H:214:GLY:O	2:H:215:ALA:CB	2.65	0.45
2:I:108:HIS:HD2	11:I:5033:HOH:O	1.99	0.45
2:I:125:ASN:HD22	2:I:186:ALA:HA	1.81	0.45
1:B:14:ASN:OD1	1:B:92:MET:HB3	2.17	0.45
2:I:270:ASN:ND2	2:I:270:ASN:H	2.07	0.45
1:A:238:TRP:CH2	1:A:240:VAL:HB	2.52	0.45
1:A:254:PHE:CZ	1:A:255:TRP:CE2	3.04	0.45
1:B:158:THR:O	1:B:162:LEU:HB2	2.16	0.45
2:H:326:SER:O	2:H:353:ARG:HD3	2.16	0.45
2:H:466:LEU:HD13	2:H:484:VAL:HB	1.97	0.45
1:B:47:THR:O	2:I:16:ARG:HA	2.17	0.45
2:H:281:LEU:C	2:H:281:LEU:HD12	2.37	0.45
1:A:238:TRP:CZ2	1:A:240:VAL:HB	2.52	0.45
2:H:231:TYR:O	2:H:234:LEU:HB2	2.17	0.44
1:A:17:CYS:HB2	2:H:65:CYS:HA	1.99	0.44
2:I:461:ALA:HB1	2:I:462:PRO:HD2	1.99	0.44
2:I:214:GLY:O	2:I:215:ALA:HB3	2.16	0.44
2:I:484:VAL:CG2	2:I:485:PRO:HD2	2.36	0.44
2:H:257:TYR:CD1	2:H:257:TYR:C	2.89	0.44
1:B:26:ARG:NH2	2:I:217:ASN:HD21	2.10	0.44
1:B:153:MET:CE	1:B:179:PHE:CE2	3.01	0.44
2:I:262:LEU:HD23	2:I:262:LEU:HA	1.81	0.44
1:B:238:TRP:CH2	1:B:240:VAL:HB	2.53	0.44
1:A:49:MET:HG2	2:H:169:ILE:HA	1.99	0.43
1:B:100:ALA:N	1:B:101:PRO:CD	2.80	0.43
2:I:257:TYR:C	2:I:257:TYR:CD1	2.90	0.43
1:B:228:CYS:HB2	1:B:229:PRO:HD3	2.01	0.43
1:A:227:ASN:ND2	1:A:227:ASN:H	2.16	0.43
1:B:104:LYS:HA	1:B:104:LYS:CE	2.47	0.43
1:B:153:MET:HE3	1:B:179:PHE:CE2	2.54	0.43
2:H:461:ALA:HB1	2:H:462:PRO:HD2	2.01	0.43
1:B:17:CYS:O	1:B:18:THR:HB	2.18	0.43
1:B:97:ALA:O	1:B:101:PRO:HG2	2.19	0.43
1:B:29:ASP:HA	1:B:30:PRO:HA	1.84	0.42
2:H:195:HIS:ND1	2:H:260:ASP:OD1	2.45	0.42
2:H:348:PHE:O	2:H:349:HIS:HB2	2.19	0.42
2:I:33:LYS:HG2	2:I:33:LYS:O	2.19	0.42
1:A:228:CYS:N	1:A:229:PRO:CD	2.82	0.42
2:H:83:CYS:HB3	2:H:455:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:108:HIS:HE1	2:I:417:GLN:NE2	1.97	0.42
1:A:227:ASN:HD22	1:A:227:ASN:N	2.16	0.42
1:A:47:THR:O	2:H:16:ARG:HA	2.18	0.42
2:I:69:THR:O	2:I:70:TYR:HB3	2.19	0.42
1:A:14:ASN:OD1	1:A:92:MET:HB3	2.19	0.42
1:A:18:THR:HA	1:A:73:GLU:OE2	2.20	0.42
1:A:122:LYS:HA	1:A:123:PRO:HA	1.79	0.42
1:B:188:CYS:HA	1:B:189:PRO:HD3	1.91	0.42
2:H:217:ASN:ND2	2:H:217:ASN:C	2.72	0.42
2:H:184:LEU:HD13	2:H:268:TYR:CE1	2.55	0.42
2:H:143:PRO:O	2:H:145:LYS:HE2	2.20	0.42
1:B:111:THR:HA	1:B:114:THR:OG1	2.20	0.41
1:B:151:ASN:HB2	11:B:308:HOH:O	2.19	0.41
2:I:360:PRO:HD3	2:I:487:THR:HG22	2.01	0.41
2:I:469:TRP:N	2:I:469:TRP:CD1	2.88	0.41
2:H:184:LEU:HB2	11:H:5108:HOH:O	2.21	0.41
2:I:217:ASN:C	2:I:217:ASN:ND2	2.73	0.41
2:H:82:ASN:HD22	2:H:455:GLY:CA	2.34	0.41
2:I:485:PRO:HG2	9:I:537:FCO:N1	2.35	0.41
1:B:46:GLU:OE1	11:B:370:HOH:O	2.22	0.41
2:H:127:LEU:HD23	2:H:127:LEU:HA	1.88	0.41
2:H:114:HIS:CE1	2:H:200:LEU:HD23	2.55	0.41
1:B:237:ASN:HB3	2:I:215:ALA:O	2.20	0.41
2:I:32:ILE:CG1	2:I:511:ILE:HD11	2.51	0.41
2:H:145:LYS:HA	2:H:145:LYS:HD3	1.78	0.41
2:H:285:GLU:HB2	2:H:460:ASN:HB3	2.02	0.41
2:H:261:LEU:HD11	2:H:411:THR:HG22	2.02	0.41
2:H:203:GLN:NE2	2:H:204:VAL:HG23	2.36	0.41
2:I:465:MET:CE	2:I:467:SER:HB3	2.52	0.40
1:B:227:ASN:ND2	1:B:227:ASN:N	2.68	0.40
2:I:142:SER:HA	2:I:143:PRO:HD3	1.94	0.40
2:I:144:ARG:NH2	2:I:198:GLU:OE2	2.42	0.40
2:I:484:VAL:CG2	2:I:533:CYS:HB3	2.51	0.40
1:A:102:LYS:HE3	6:A:1273:GOL:H2	2.04	0.40
2:H:286:PHE:HB2	2:H:297:TYR:HB3	2.03	0.40
2:I:310:LYS:CE	2:I:312:ASP:OD2	2.70	0.40
2:I:465:MET:HE3	2:I:467:SER:HB3	2.03	0.40
1:A:17:CYS:O	1:A:18:THR:HB	2.21	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)
1:B:264:ALA:OXT	6:A:1273:GOL:O1[1_454]	2.11	0.09

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	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	B	259/264 (98%)	251 (97%)	8 (3%)	0	100	100
2	H	529/536 (99%)	514 (97%)	15 (3%)	0	100	100
2	I	528/536 (98%)	514 (97%)	13 (2%)	1 (0%)	47	56
All	All	1577/1600 (99%)	1533 (97%)	43 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	279	ASN

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	210/210 (100%)	199 (95%)	11 (5%)	23	27
1	B	208/210 (99%)	201 (97%)	7 (3%)	37	46
2	H	436/440 (99%)	412 (94%)	24 (6%)	21	24
2	I	435/440 (99%)	413 (95%)	22 (5%)	24	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1289/1300 (99%)	1225 (95%)	64 (5%)	24	28

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	16	GLU
1	A	25	LEU
1	A	48	LEU
1	A	162	LEU
1	A	163	LEU
1	A	167	MET
1	A	177	VAL
1	A	182	GLU
1	A	227	ASN
2	H	7	ASN
2	H	8	LYS
2	H	45	LEU
2	H	49	LEU
2	H	50	LYS
2	H	74	LEU
2	H	84	VAL
2	H	115	LEU
2	H	118	LEU
2	H	133	LYS
2	H	152	LYS
2	H	184	LEU
2	H	217	ASN
2	H	234	LEU
2	H	257	TYR
2	H	270	ASN
2	H	310	LYS
2	H	326	SER
2	H	395	LYS
2	H	431	LYS
2	H	448	GLN
2	H	482	LEU
2	H	484	VAL
2	H	496	GLU
1	B	16	GLU
1	B	25	LEU

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Mol	Chain	Res	Type
1	B	48	LEU
1	B	104	LYS
1	B	124	ASN
1	B	137	LYS
1	B	227	ASN
2	I	8	LYS
2	I	45	LEU
2	I	49	LEU
2	I	50	LYS
2	I	74	LEU
2	I	83	CYS
2	I	115	LEU
2	I	118	LEU
2	I	130	ASP
2	I	150	SER
2	I	152	LYS
2	I	183	VAL
2	I	217	ASN
2	I	234	LEU
2	I	270	ASN
2	I	384	GLU
2	I	395	LYS
2	I	437	LYS
2	I	465	MET
2	I	482	LEU
2	I	484	VAL
2	I	490	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	227	ASN
2	H	82	ASN
2	H	108	HIS
2	H	217	ASN
2	H	270	ASN
2	H	383	HIS
2	H	448	GLN
2	H	460	ASN
2	H	481	GLN
1	B	13	HIS

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Mol	Chain	Res	Type
1	B	45	HIS
1	B	61	HIS
1	B	124	ASN
1	B	154	ASN
1	B	227	ASN
1	B	231	GLN
2	I	82	ASN
2	I	108	HIS
2	I	116	HIS
2	I	125	ASN
2	I	128	ASN
2	I	139	ASN
2	I	217	ASN
2	I	270	ASN
2	I	383	HIS
2	I	423	GLN
2	I	481	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	A	1542	-	5,5,5	0.41	0	5,5,5	0.22	0
6	GOL	B	2542	-	5,5,5	0.30	0	5,5,5	0.43	0
3	SF4	A	267	1	0,12,12	0.00	-	-		
3	SF4	B	267	1	0,12,12	0.00	-	-		
10	PER	H	539	9,7	0,1,1	0.00	-	-		
3	SF4	A	265	1	0,12,12	0.00	-	-		
10	PER	I	539	9,7	0,1,1	0.00	-	-		
6	GOL	A	1273	-	5,5,5	0.32	0	5,5,5	0.32	0
4	F3S	B	266	1	0,9,9	0.00	-	-		
9	FCO	I	537	10,2	0,6,6	0.00	-	-		
9	FCO	H	537	10,2	0,6,6	0.00	-	-		
6	GOL	H	1543	-	5,5,5	0.33	0	5,5,5	0.64	0
6	GOL	H	1544	-	5,5,5	0.41	0	5,5,5	0.58	0
6	GOL	A	1272	-	5,5,5	0.49	0	5,5,5	0.24	0
4	F3S	A	266	1	0,9,9	0.00	-	-		
6	GOL	A	1271	-	5,5,5	0.36	0	5,5,5	0.33	0
3	SF4	B	265	1	0,12,12	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
3	SF4	A	267	1	-	-	0/6/5/5
6	GOL	A	1272	-	-	2/4/4/4	-
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	B	265	1	-	-	0/6/5/5
6	GOL	A	1273	-	-	2/4/4/4	-
4	F3S	B	266	1	-	-	0/3/3/3
3	SF4	B	267	1	-	-	0/6/5/5
6	GOL	A	1542	-	-	2/4/4/4	-
6	GOL	H	1544	-	-	4/4/4/4	-
6	GOL	B	2542	-	-	2/4/4/4	-
4	F3S	A	266	1	-	-	0/3/3/3
6	GOL	A	1271	-	-	2/4/4/4	-
6	GOL	H	1543	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1542	GOL	C1-C2-C3-O3
6	A	1542	GOL	O2-C2-C3-O3
6	H	1543	GOL	O1-C1-C2-C3
6	A	1273	GOL	C1-C2-C3-O3
6	H	1544	GOL	O1-C1-C2-O2
6	H	1544	GOL	O1-C1-C2-C3
6	H	1543	GOL	O1-C1-C2-O2
6	A	1273	GOL	O2-C2-C3-O3
6	A	1272	GOL	C1-C2-C3-O3
6	A	1271	GOL	O1-C1-C2-C3
6	H	1544	GOL	C1-C2-C3-O3
6	A	1271	GOL	O1-C1-C2-O2
6	H	1544	GOL	O2-C2-C3-O3
6	A	1272	GOL	O2-C2-C3-O3
6	B	2542	GOL	C1-C2-C3-O3
6	B	2542	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1273	GOL	1	1
9	I	537	FCO	1	0
6	H	1543	GOL	2	0
6	H	1544	GOL	1	0

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	261/264 (98%)	-0.29	2 (0%)	86 91	5, 13, 20, 37	17 (6%)
1	B	260/264 (98%)	-0.06	2 (0%)	86 91	8, 14, 22, 33	17 (6%)
2	H	530/536 (98%)	-0.24	5 (0%)	84 90	7, 13, 21, 28	43 (8%)
2	I	530/536 (98%)	0.03	18 (3%)	45 57	7, 14, 23, 31	38 (7%)
All	All	1581/1600 (98%)	-0.13	27 (1%)	70 78	5, 14, 22, 37	115 (7%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	177	GLY	4.4
2	I	395	LYS	3.5
2	I	396	THR	3.2
1	B	54	HIS	3.1
2	I	305	GLY	3.1
2	I	135	ALA	3.0
1	A	264	ALA	2.9
1	A	4	LYS	2.9
2	I	27	VAL	2.9
2	I	142	SER	2.9
1	B	166	GLY	2.7
2	H	165	GLY	2.7
2	I	397	LEU	2.6
2	I	398	GLY	2.5
2	I	136	ARG	2.5
2	I	143	PRO	2.4
2	H	438	ALA	2.4
2	I	310	LYS	2.4
2	I	165	GLY	2.3
2	I	133	LYS	2.3
2	I	163	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	149	GLU	2.1
2	I	29	GLY	2.1
2	I	375	VAL	2.1
2	H	395	LYS	2.1
2	I	160	ALA	2.0
2	H	147	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MG	I	540	1/1	0.85	0.11	8,8,8,8	0
6	GOL	A	1271	6/6	0.89	0.28	41,46,47,48	6
6	GOL	H	1544	6/6	0.89	0.18	25,30,32,33	0
8	MG	H	540	1/1	0.89	0.05	9,9,9,9	0
6	GOL	H	1543	6/6	0.93	0.17	25,27,29,31	0
6	GOL	A	1542	6/6	0.93	0.15	25,31,33,35	6
6	GOL	A	1272	6/6	0.94	0.22	37,39,40,41	0
6	GOL	A	1273	6/6	0.94	0.12	23,25,25,29	0
6	GOL	B	2542	6/6	0.96	0.22	34,39,40,41	0
5	H2S	B	2268	1/1	0.98	0.09	27,27,27,27	0
3	SF4	A	267	8/8	0.99	0.04	10,11,11,11	0
9	FCO	I	537	7/7	0.99	0.10	11,12,13,17	0
5	H2S	I	2541	1/1	0.99	0.09	20,20,20,20	0
3	SF4	A	265	8/8	0.99	0.04	7,9,10,10	0
10	PER	H	539	2/2	0.99	0.14	18,18,18,24	1
4	F3S	A	266	7/7	0.99	0.06	10,11,12,13	0
7	NI	H	538	1/1	0.99	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SF4	B	267	8/8	0.99	0.04	9,11,11,12	0
9	FCO	H	537	7/7	0.99	0.12	10,11,13,15	0
4	F3S	B	266	7/7	0.99	0.06	10,10,12,13	0
5	H2S	A	1268	1/1	0.99	0.08	21,21,21,21	0
5	H2S	H	1541	1/1	0.99	0.09	13,13,13,13	0
3	SF4	B	265	8/8	0.99	0.05	6,9,10,12	0
7	NI	I	538	1/1	1.00	0.03	16,16,16,16	0
10	PER	I	539	2/2	1.00	0.13	18,18,18,24	1

6.5 Other polymers [i](#)

There are no such residues in this entry.