



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 AM UTC

PDB ID : 1YQW / pdb_00001yqw
Title : Structure of the Oxidized Unready Form of Ni-Fe Hydrogenase
Authors : Volbeda, A.
Deposited on : 2005-02-02
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

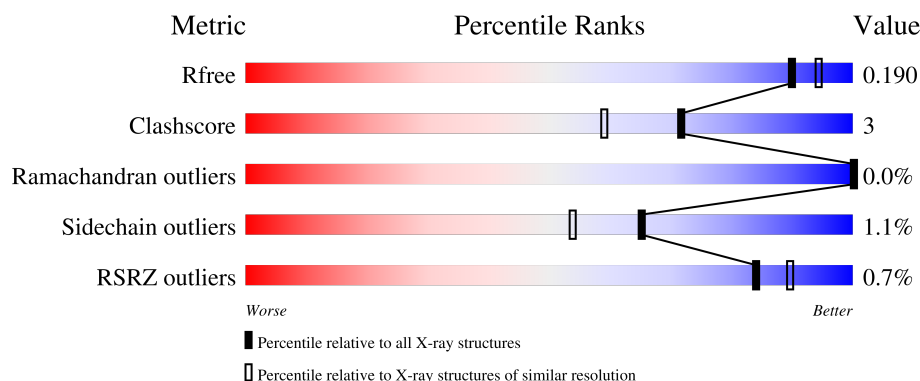
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

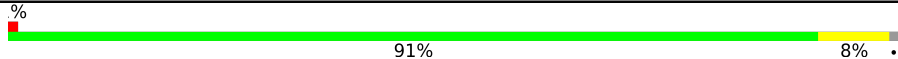
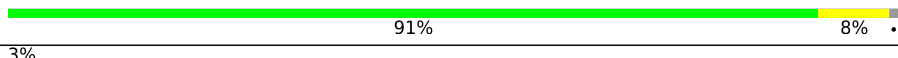
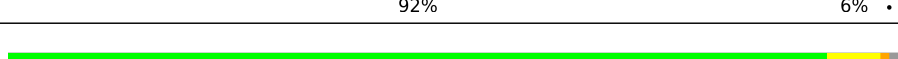
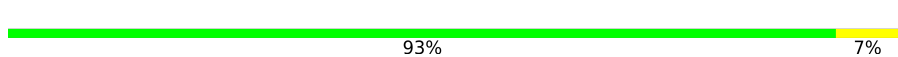
The reported resolution of this entry is 1.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	264	
1	C	264	
2	Q	549	
2	R	549	

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Mol	Chain	Length	Quality of chain
2	S	549	% 90% 8% ..

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 20497 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	262	Total	C	N	O	S	0	0	0
			1973	1256	330	372	15			
1	B	262	Total	C	N	O	S	0	2	0
			1980	1260	330	375	15			
1	C	260	Total	C	N	O	S	0	0	0
			1960	1248	327	370	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	8	0
			4187	2669	728	767	23			
2	R	545	Total	C	N	O	S	0	3	0
			4173	2660	725	765	23			
2	S	544	Total	C	N	O	S	0	2	0
			4165	2652	725	765	23			

There are 9 discrepancies between the modelled and reference sequences:

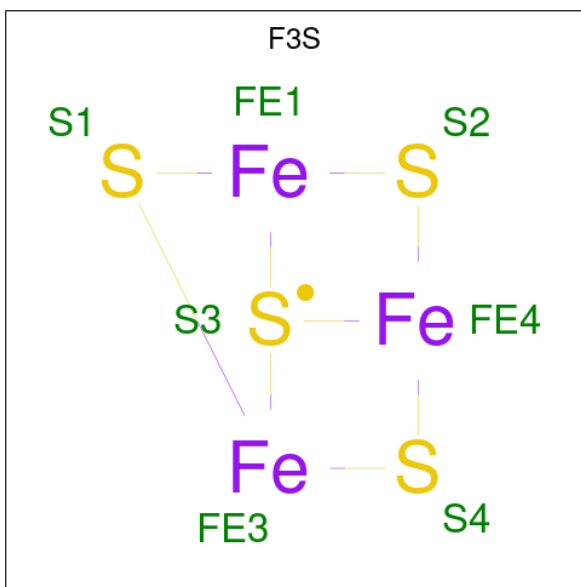
Chain	Residue	Modelled	Actual	Comment	Reference
Q	198	ASN	ASP	conflict	UNP P18188
Q	303	SER	GLU	conflict	UNP P18188
Q	499	ALA	SER	engineered mutation	UNP P18188
R	198	ASN	ASP	conflict	UNP P18188
R	303	SER	GLU	conflict	UNP P18188
R	499	ALA	SER	engineered mutation	UNP P18188
S	198	ASN	ASP	conflict	UNP P18188
S	303	SER	GLU	conflict	UNP P18188
S	499	ALA	SER	engineered mutation	UNP P18188

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



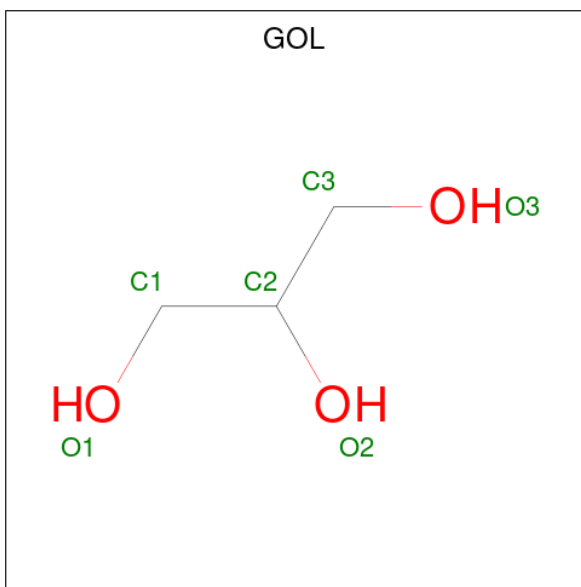
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: 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		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0

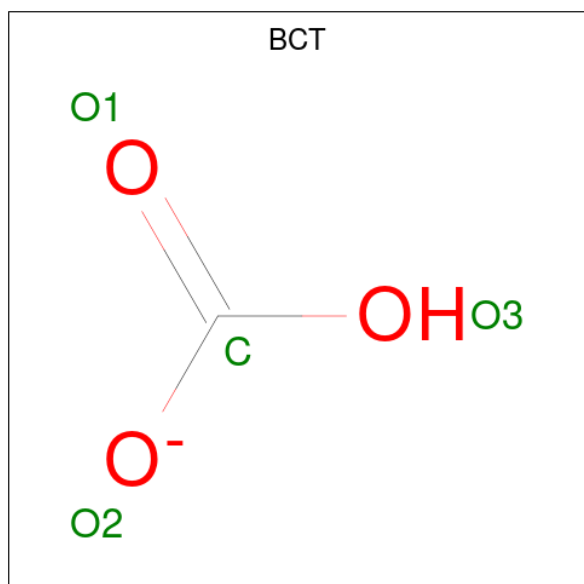
- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	1	Total Ni 1 1	0	0
6	R	1	Total Ni 1 1	0	0
6	S	1	Total Ni 1 1	0	0

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Q	1	Total	Fe	0	0
			1	1		
7	R	1	Total	Fe	0	0
			1	1		
7	S	1	Total	Fe	0	0
			1	1		

- Molecule 8 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

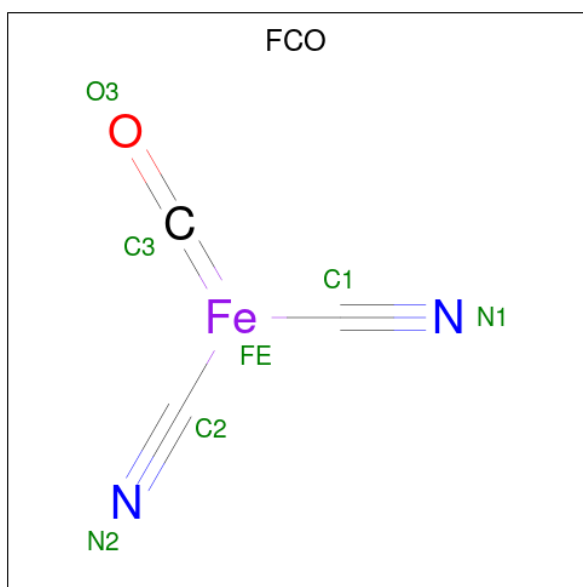


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

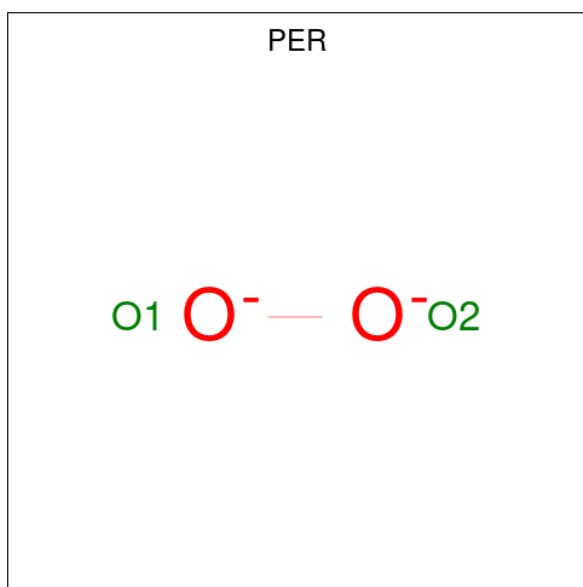
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	Q	2	Total	Mg	0	0
			2	2		
9	R	1	Total	Mg	0	0
			1	1		

- Molecule 10 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	Q	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
10	R	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
10	S	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 11 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	Q	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	R	1	Total O 2 2	0	0
11	S	1	Total O 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	275	Total O 275 275	0	0
12	Q	482	Total O 482 482	0	0
12	B	194	Total O 194 194	0	0
12	R	419	Total O 419 419	0	0
12	C	185	Total O 185 185	0	0
12	S	293	Total O 293 293	0	0

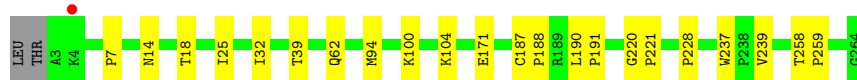
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

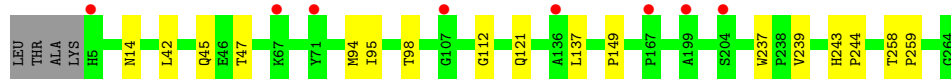
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

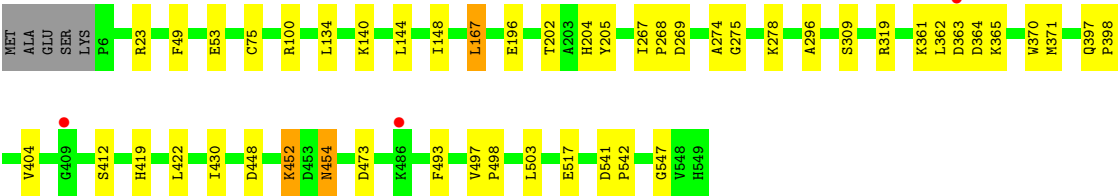
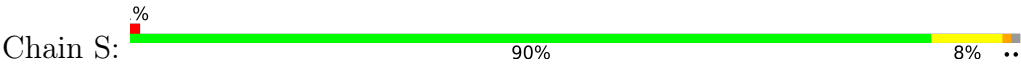


- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit





● Molecule 2: Periplasmic [NiFe] hydrogenase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.41Å 99.70Å 182.83Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	20.00 – 1.83 20.00 – 1.83	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-1.83) 82.9 (20.00-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.146 , 0.185 0.161 , 0.190	Depositor DCC
R_{free} test set	8485 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.910	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20497	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, NI, MG, SF4, PER, F3S, FE2, GOL, 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	0.63	1/2027 (0.0%)	0.76	0/2759
1	B	0.53	0/2043	0.76	0/2781
1	C	0.51	0/2014	0.75	0/2743
2	Q	0.57	0/4330	0.77	0/5876
2	R	0.55	0/4292	0.76	0/5827
2	S	0.49	0/4280	0.76	0/5810
All	All	0.54	1/18986 (0.0%)	0.76	0/25796

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASN	C-O	5.40	1.26	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	1911	18	0
1	B	1980	0	1918	11	0
1	C	1960	0	1897	10	0
2	Q	4187	0	4180	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	4173	0	4154	31	0
2	S	4165	0	4142	28	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
5	A	18	0	24	3	0
5	Q	24	0	32	3	0
5	R	42	0	56	5	0
5	S	18	0	24	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	4	0	0	0	0
9	Q	2	0	0	0	0
9	R	1	0	0	0	0
10	Q	7	0	0	1	0
10	R	7	0	0	0	0
10	S	7	0	0	0	0
11	Q	2	0	0	0	0
11	R	2	0	0	1	0
11	S	2	0	0	0	0
12	A	275	0	0	6	0
12	B	194	0	0	1	0
12	C	185	0	0	0	0
12	Q	482	0	0	3	0
12	R	419	0	0	9	0
12	S	293	0	0	2	0
All	All	20497	0	18338	120	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 3.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:410:LYS:HD3	5:R:1302:GOL:H11	1.59	0.84
2:S:134:LEU:HD21	2:S:167:LEU:HD23	1.68	0.74
12:Q:1038:HOH:O	2:R:6:PRO:HB3	1.88	0.71
1:A:61:HIS:HE1	12:A:469:HOH:O	1.73	0.71
1:B:62:GLN:OE1	12:B:1191:HOH:O	2.08	0.70
2:R:72:CYS:HB3	12:R:557:HOH:O	1.91	0.70
2:S:362:LEU:O	2:S:363:ASP:HB2	1.91	0.70
5:A:270:GOL:H32	2:Q:170:PHE:HA	1.79	0.65
2:R:35:GLU:HB2	2:R:40:LYS:HE2	1.79	0.65
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.26	0.65
2:Q:512[A]:LYS:HE2	2:Q:517[A]:GLU:OE1	1.99	0.63
1:A:171:GLU:H	1:A:171:GLU:CD	2.06	0.62
2:S:134:LEU:CD2	2:S:167:LEU:HD23	2.28	0.62
2:Q:35:GLU:HB2	2:Q:40:LYS:HE2	1.82	0.62
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.80	0.62
2:R:363:ASP:HB2	12:R:1532:HOH:O	2.02	0.59
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.33	0.59
1:A:170:ASP:O	5:A:269:GOL:H11	2.04	0.58
2:S:140:LYS:HG2	2:S:196:GLU:HG2	1.87	0.57
1:C:47:THR:O	2:S:23:ARG:HA	2.04	0.57
2:R:189:LYS:HE2	12:R:1485:HOH:O	2.05	0.57
1:A:99:LYS:HE2	12:A:421:HOH:O	2.03	0.57
2:Q:72:CYS:HB3	12:Q:564:HOH:O	2.05	0.56
2:Q:257:GLU:OE2	12:Q:1041:HOH:O	2.18	0.56
2:R:139:ASN:O	2:R:143:LYS:HG3	2.06	0.55
1:A:264:GLY:HA3	12:A:498:HOH:O	2.07	0.55
1:B:258:THR:HA	1:B:259:PRO:C	2.32	0.55
2:R:278:LYS:HG2	12:R:1478:HOH:O	2.07	0.54
2:R:465:GLU:HG2	5:R:1307:GOL:H11	1.88	0.54
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.38	0.53
2:R:410:LYS:HA	5:R:1302:GOL:H12	1.91	0.53
2:R:497:VAL:HG13	2:R:498:PRO:HD2	1.90	0.53
2:R:275:GLY:O	2:R:278:LYS:HG3	2.10	0.52
2:S:361:LYS:HG3	2:S:362:LEU:O	2.10	0.52
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.91	0.52
1:A:62:GLN:OE1	12:A:399:HOH:O	2.19	0.51
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.92	0.51
2:S:275:GLY:O	2:S:278:LYS:HG3	2.10	0.51
2:Q:371:MET:HE2	2:Q:547:GLY:HA3	1.92	0.51
2:R:72:CYS:CB	12:R:557:HOH:O	2.51	0.51
1:A:47:THR:O	2:Q:23:ARG:HA	2.11	0.51
2:S:75:CYS:N	12:S:557:HOH:O	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:410:LYS:O	2:Q:410:LYS:HD3	2.12	0.49
2:Q:285:GLY:HA3	5:Q:559:GOL:H2	1.94	0.49
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.27	0.49
2:R:497:VAL:HG12	2:R:498:PRO:HD2	1.95	0.48
2:S:278:LYS:HG2	12:S:2533:HOH:O	2.13	0.48
2:Q:274:ALA:CB	2:Q:422:LEU:HD11	2.43	0.48
2:R:274:ALA:HA	2:R:422[A]:LEU:HD11	1.95	0.48
2:R:476:ARG:HD2	11:R:552:PER:O1	2.14	0.48
1:B:14:ASN:ND2	1:B:94:MET:HB3	2.29	0.47
2:Q:401:LYS:HE3	2:Q:401:LYS:HB2	1.72	0.47
2:R:189:LYS:CE	12:R:1485:HOH:O	2.59	0.47
2:S:452:LYS:N	2:S:452:LYS:HD3	2.30	0.47
2:S:53:GLU:HG2	2:S:493:PHE:O	2.15	0.47
2:R:363:ASP:CB	12:R:1532:HOH:O	2.61	0.47
2:S:49:PHE:HB2	2:S:370:TRP:CD2	2.51	0.46
2:R:543[B]:CYS:HB3	2:R:546:CYS:HB2	1.97	0.46
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.51	0.46
1:A:258:THR:HA	1:A:259:PRO:C	2.41	0.46
2:Q:35:GLU:HB2	2:Q:40:LYS:CE	2.45	0.45
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.52	0.45
2:R:410:LYS:HA	5:R:1302:GOL:C1	2.46	0.45
2:R:153:PRO:HA	5:R:1306:GOL:H2	1.97	0.45
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.52	0.45
2:Q:116[B]:LEU:HD11	2:Q:261:PHE:CE2	2.51	0.45
1:A:262:GLU:HB3	12:A:498:HOH:O	2.17	0.45
2:R:304:LYS:HD3	2:R:304:LYS:HA	1.75	0.45
2:R:153:PRO:HD2	12:R:1437:HOH:O	2.16	0.44
1:C:258:THR:HA	1:C:259:PRO:C	2.42	0.44
1:C:42:LEU:HD21	1:C:45:GLN:HG3	2.00	0.44
2:Q:476:ARG:NE	2:Q:543[B]:CYS:SG	2.90	0.44
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.52	0.44
1:C:243:HIS:CG	1:C:244:PRO:HD2	2.52	0.44
1:A:170:ASP:C	5:A:269:GOL:H11	2.42	0.44
2:S:267:ILE:HB	2:S:268:PRO:HD3	2.00	0.43
2:S:371:MET:HE2	2:S:547:GLY:HA3	2.00	0.43
1:A:61:HIS:CE1	12:A:469:HOH:O	2.60	0.43
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.53	0.43
2:R:541:ASP:N	2:R:542:PRO:HD3	2.32	0.43
2:Q:24:ILE:HG22	2:Q:542:PRO:HD2	1.99	0.43
2:Q:337:LYS:HE2	5:Q:560:GOL:O2	2.18	0.43
2:R:296:ALA:HA	2:R:309:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:338:TYR:CE1	5:Q:560:GOL:H31	2.54	0.43
2:S:144:LEU:O	2:S:148:ILE:HG12	2.19	0.42
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.55	0.42
2:S:319:ARG:HG2	2:S:419:HIS:CE1	2.54	0.42
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.34	0.42
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.55	0.42
1:A:98:THR:HG22	1:A:137:LEU:HD11	2.02	0.42
2:R:132:ALA:HA	2:R:135:LYS:HD2	2.02	0.42
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.02	0.41
2:Q:116[B]:LEU:HD11	2:Q:261:PHE:HE2	1.85	0.41
1:B:18:THR:OG1	2:R:25:GLU:HG2	2.20	0.41
2:S:448:ASP:O	2:S:452:LYS:HE2	2.20	0.41
2:Q:476:ARG:HD2	10:Q:550:FCO:C2	2.50	0.41
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.01	0.41
1:B:190:LEU:N	1:B:191:PRO:CD	2.84	0.41
1:B:220:GLY:N	1:B:221:PRO:CD	2.83	0.41
1:C:121:GLN:CD	1:C:121:GLN:H	2.28	0.41
2:S:404:VAL:HG22	2:S:430:ILE:HD13	2.02	0.41
2:S:541:ASP:N	2:S:542:PRO:HD3	2.35	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.03	0.41
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.56	0.41
2:S:202:THR:O	2:S:205:TYR:HB3	2.21	0.41
2:S:397:GLN:HA	2:S:398:PRO:HD3	1.94	0.41
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.55	0.41
2:Q:284:GLY:HA2	2:Q:518:ALA:O	2.21	0.41
2:R:464:GLU:OE2	2:R:488:LYS:HE3	2.21	0.41
2:S:204:HIS:HD1	2:S:269:ASP:CG	2.26	0.41
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.90	0.40
2:S:274:ALA:HA	2:S:422:LEU:HD11	2.02	0.40
1:A:236:ASN:HB3	2:Q:224:GLY:O	2.22	0.40
1:B:7:PRO:HD2	1:B:39:THR:O	2.21	0.40
2:S:296:ALA:HA	2:S:309:SER:HA	2.03	0.40
2:R:303:SER:HB3	12:R:1565:HOH:O	2.20	0.40
2:S:100:ARG:HH11	2:S:100:ARG:HD3	1.77	0.40
2:S:454:ASN:N	2:S:454:ASN:HD22	2.18	0.40
2:Q:81:LEU:HD23	2:Q:107:MET:HE2	2.02	0.40
2:Q:350:PRO:HB2	2:Q:482:TRP:CG	2.56	0.40

There are no symmetry-related clashes.

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	260/264 (98%)	253 (97%)	7 (3%)	0	100	100
1	B	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	C	258/264 (98%)	252 (98%)	6 (2%)	0	100	100
2	Q	550/549 (100%)	539 (98%)	11 (2%)	0	100	100
2	R	546/549 (100%)	529 (97%)	17 (3%)	0	100	100
2	S	544/549 (99%)	525 (96%)	18 (3%)	1 (0%)	43	34
All	All	2420/2439 (99%)	2353 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	364	ASP

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	208/210 (99%)	208 (100%)	0	100	100
1	B	210/210 (100%)	207 (99%)	3 (1%)	59	45
1	C	207/210 (99%)	206 (100%)	1 (0%)	81	75
2	Q	442/438 (101%)	436 (99%)	6 (1%)	59	45
2	R	437/438 (100%)	433 (99%)	4 (1%)	70	60
2	S	436/438 (100%)	428 (98%)	8 (2%)	51	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1940/1944 (100%)	1918 (99%)	22 (1%)	65	54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	40	LYS
2	Q	303	SER
2	Q	401	LYS
2	Q	410	LYS
2	Q	454	ASN
2	Q	473	ASP
1	B	100	LYS
1	B	104	LYS
1	B	171	GLU
2	R	167	LEU
2	R	402	LYS
2	R	454	ASN
2	R	473	ASP
1	C	95	ILE
2	S	167	LEU
2	S	365	LYS
2	S	412	SER
2	S	452	LYS
2	S	454	ASN
2	S	473	ASP
2	S	503	LEU
2	S	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	172	ASN
1	A	234	GLN
1	A	240	GLN
2	Q	164	GLN
2	Q	241	GLN
2	Q	454	ASN
2	Q	509	GLN
1	B	14	ASN
1	B	62	GLN

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Mol	Chain	Res	Type
1	B	240	GLN
2	R	47	GLN
2	R	139	ASN
2	R	181	ASN
2	R	241	GLN
2	R	454	ASN
2	R	509	GLN
1	C	14	ASN
1	C	240	GLN
2	S	241	GLN
2	S	454	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 9 are monoatomic - leaving 33 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	GOL	Q	558	-	5,5,5	0.48	0	5,5,5	0.34	0
5	GOL	A	270	-	5,5,5	0.43	0	5,5,5	0.98	0
3	SF4	A	265	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	S	2302	-	5,5,5	0.43	0	5,5,5	0.26	0
5	GOL	A	268	-	5,5,5	0.48	0	5,5,5	0.75	0
5	GOL	R	1307	-	5,5,5	0.29	0	5,5,5	0.32	0
5	GOL	S	2303	-	5,5,5	0.37	0	5,5,5	0.36	0
5	GOL	Q	560	-	5,5,5	0.45	0	5,5,5	0.38	0
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
3	SF4	B	265	1	0,12,12	-	-	-		
10	FCO	Q	550	2,11	0,6,6	-	-	-		
10	FCO	S	550	2,11	0,6,6	-	-	-		
11	PER	S	552	6,10	1,1,1	0.19	0	-		
5	GOL	R	1301	-	5,5,5	0.42	0	5,5,5	0.37	0
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	B	266	1	0,9,9	-	-	-		
5	GOL	R	1305	-	5,5,5	0.43	0	5,5,5	0.38	0
5	GOL	R	1306	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	Q	557	-	5,5,5	0.39	0	5,5,5	0.27	0
5	GOL	A	269	-	5,5,5	0.26	0	5,5,5	0.71	0
5	GOL	Q	559	-	5,5,5	0.41	0	5,5,5	0.20	0
8	BCT	Q	554	-	3,3,3	0.53	0	2,3,3	0.47	0
5	GOL	R	1302	-	5,5,5	0.40	0	5,5,5	0.26	0
5	GOL	R	1303	-	5,5,5	0.30	0	5,5,5	0.38	0
11	PER	Q	552	6,10	1,1,1	0.11	0	-		
5	GOL	R	1304	-	5,5,5	0.38	0	5,5,5	0.18	0
11	PER	R	552	6,10	1,1,1	0.14	0	-		
4	F3S	A	266	1	0,9,9	-	-	-		
5	GOL	S	2301	-	5,5,5	0.45	0	5,5,5	0.19	0
3	SF4	C	267	1	0,12,12	-	-	-		
10	FCO	R	550	2,11	0,6,6	-	-	-		
3	SF4	B	267	1	0,12,12	-	-	-		

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	GOL	Q	558	-	-	0/4/4/4	-
5	GOL	A	270	-	-	4/4/4/4	-
3	SF4	A	265	1	-	-	0/6/5/5
5	GOL	A	268	-	-	2/4/4/4	-
5	GOL	R	1307	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	S	2303	-	-	4/4/4/4	-
5	GOL	Q	560	-	-	2/4/4/4	-
3	SF4	C	265	1	-	-	0/6/5/5
3	SF4	A	267	1	-	-	0/6/5/5
3	SF4	B	265	1	-	-	0/6/5/5
5	GOL	R	1301	-	-	1/4/4/4	-
5	GOL	R	1305	-	-	0/4/4/4	-
4	F3S	B	266	1	-	-	0/3/3/3
4	F3S	C	266	1	-	-	0/3/3/3
5	GOL	R	1306	-	-	4/4/4/4	-
5	GOL	Q	557	-	-	0/4/4/4	-
5	GOL	A	269	-	-	3/4/4/4	-
5	GOL	Q	559	-	-	0/4/4/4	-
3	SF4	B	267	1	-	-	0/6/5/5
5	GOL	R	1302	-	-	4/4/4/4	-
5	GOL	R	1303	-	-	1/4/4/4	-
5	GOL	R	1304	-	-	2/4/4/4	-
4	F3S	A	266	1	-	-	0/3/3/3
5	GOL	S	2301	-	-	0/4/4/4	-
3	SF4	C	267	1	-	-	0/6/5/5
5	GOL	S	2302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	268	GOL	C1-C2-C3-O3
5	A	268	GOL	O2-C2-C3-O3
5	A	269	GOL	O1-C1-C2-C3
5	A	270	GOL	C1-C2-C3-O3
5	R	1302	GOL	C1-C2-C3-O3
5	R	1306	GOL	O1-C1-C2-C3
5	R	1306	GOL	C1-C2-C3-O3
5	S	2302	GOL	C1-C2-C3-O3
5	S	2303	GOL	O1-C1-C2-C3
5	S	2303	GOL	C1-C2-C3-O3
5	A	270	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	Q	560	GOL	C1-C2-C3-O3
5	R	1304	GOL	C1-C2-C3-O3
5	A	269	GOL	O1-C1-C2-O2
5	A	270	GOL	O2-C2-C3-O3
5	R	1302	GOL	O2-C2-C3-O3
5	R	1306	GOL	O1-C1-C2-O2
5	R	1306	GOL	O2-C2-C3-O3
5	S	2303	GOL	O1-C1-C2-O2
5	S	2303	GOL	O2-C2-C3-O3
5	R	1304	GOL	O2-C2-C3-O3
5	A	270	GOL	O1-C1-C2-O2
5	Q	560	GOL	O2-C2-C3-O3
5	S	2302	GOL	O2-C2-C3-O3
5	R	1301	GOL	O2-C2-C3-O3
5	R	1302	GOL	O1-C1-C2-O2
5	A	269	GOL	O2-C2-C3-O3
5	R	1302	GOL	O1-C1-C2-C3
5	R	1303	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	270	GOL	1	0
5	R	1307	GOL	1	0
5	Q	560	GOL	2	0
10	Q	550	FCO	1	0
5	R	1306	GOL	1	0
5	A	269	GOL	2	0
5	Q	559	GOL	1	0
5	R	1302	GOL	3	0
11	R	552	PER	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/264 (99%)	-0.55	2 (0%)	82 88	4, 9, 15, 32	8 (3%)
1	B	262/264 (99%)	-0.12	1 (0%)	88 93	5, 10, 17, 29	11 (4%)
1	C	260/264 (98%)	0.14	8 (3%)	51 56	6, 11, 20, 28	6 (2%)
2	Q	544/549 (99%)	-0.58	1 (0%)	91 94	4, 9, 15, 22	20 (3%)
2	R	545/549 (99%)	-0.43	1 (0%)	91 94	5, 9, 16, 40	16 (2%)
2	S	544/549 (99%)	-0.03	3 (0%)	85 90	6, 11, 18, 28	17 (3%)
All	All	2417/2439 (99%)	-0.29	16 (0%)	84 90	4, 10, 17, 40	78 (3%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	LYS	4.7
2	S	363	ASP	2.9
2	S	486	LYS	2.6
1	C	136	ALA	2.5
1	C	204	SER	2.4
1	C	107	GLY	2.4
2	S	409	GLY	2.4
1	A	3	ALA	2.4
1	A	165	GLY	2.4
2	Q	147	SER	2.4
1	C	167	PRO	2.2
1	C	71	TYR	2.1
1	B	4	LYS	2.1
1	C	5	HIS	2.1
1	C	199	ALA	2.1
2	R	343	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
5	GOL	S	2303	6/6	0.73	0.13	34,35,36,38	6
5	GOL	R	1302	6/6	0.79	0.13	27,28,30,33	0
5	GOL	R	1306	6/6	0.81	0.11	30,37,39,41	0
5	GOL	S	2302	6/6	0.83	0.14	32,35,35,35	6
5	GOL	R	1307	6/6	0.83	0.10	28,31,32,36	0
5	GOL	Q	560	6/6	0.84	0.12	25,38,41,47	0
5	GOL	A	268	6/6	0.86	0.11	16,20,24,28	0
5	GOL	R	1304	6/6	0.87	0.10	28,31,33,36	0
5	GOL	A	270	6/6	0.88	0.10	17,29,31,34	0
5	GOL	R	1305	6/6	0.88	0.11	21,23,25,26	0
5	GOL	Q	559	6/6	0.88	0.14	29,31,33,35	0
5	GOL	A	269	6/6	0.91	0.09	21,27,28,36	0
8	BCT	Q	554	4/4	0.92	0.08	24,29,31,32	0
5	GOL	R	1303	6/6	0.93	0.07	9,10,11,13	0
9	MG	R	1308	1/1	0.93	0.09	30,30,30,30	0
5	GOL	S	2301	6/6	0.95	0.05	7,10,11,12	0
5	GOL	Q	557	6/6	0.96	0.07	8,9,11,12	0
9	MG	Q	555	1/1	0.96	0.14	29,29,29,29	0
3	SF4	B	265	8/8	0.96	0.18	8,10,11,11	0
5	GOL	R	1301	6/6	0.97	0.05	7,8,9,10	0
5	GOL	Q	558	6/6	0.97	0.10	8,10,11,12	0
9	MG	Q	556	1/1	0.97	0.09	35,35,35,35	0
7	FE2	S	553	1/1	0.97	0.17	9,9,9,9	1
7	FE2	R	553	1/1	0.98	0.13	9,9,9,9	1
4	F3S	C	266	7/7	0.98	0.08	10,10,11,12	0
4	F3S	B	266	7/7	0.98	0.14	9,9,11,12	0
11	PER	Q	552	2/2	0.98	0.09	14,14,14,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	PER	S	552	2/2	0.98	0.07	12,12,12,12	1
7	FE2	Q	553	1/1	0.99	0.08	9,9,9,9	1
3	SF4	A	265	8/8	0.99	0.07	7,8,8,10	0
3	SF4	B	267	8/8	0.99	0.10	9,9,11,12	0
3	SF4	C	265	8/8	0.99	0.09	8,9,10,11	0
3	SF4	C	267	8/8	0.99	0.08	9,10,10,10	0
4	F3S	A	266	7/7	0.99	0.04	9,9,10,10	0
3	SF4	A	267	8/8	0.99	0.03	8,9,9,9	0
10	FCO	R	550	7/7	0.99	0.07	5,7,9,11	0
10	FCO	S	550	7/7	0.99	0.11	8,11,13,13	0
6	NI	R	551	1/1	0.99	0.08	14,14,14,14	0
11	PER	R	552	2/2	0.99	0.07	14,14,14,16	1
6	NI	S	551	1/1	0.99	0.10	15,15,15,15	0
10	FCO	Q	550	7/7	1.00	0.04	7,8,9,10	0
6	NI	Q	551	1/1	1.00	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.