



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:06 am BST

PDB ID : 1YQW
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 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

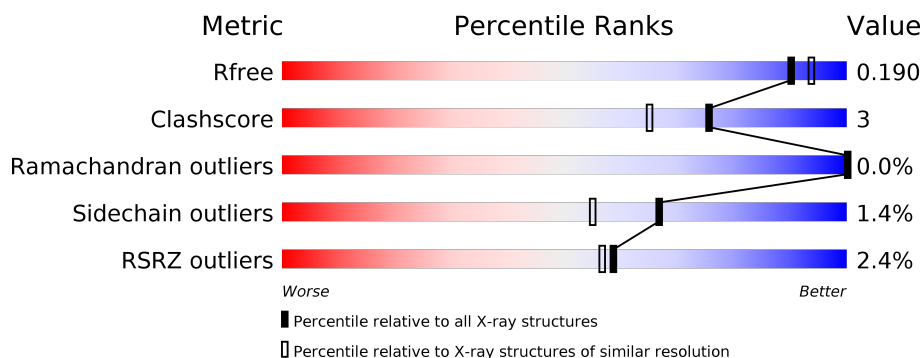
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	B	264	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	C	264	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	Q	549	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	R	549	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
2	S	549	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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			

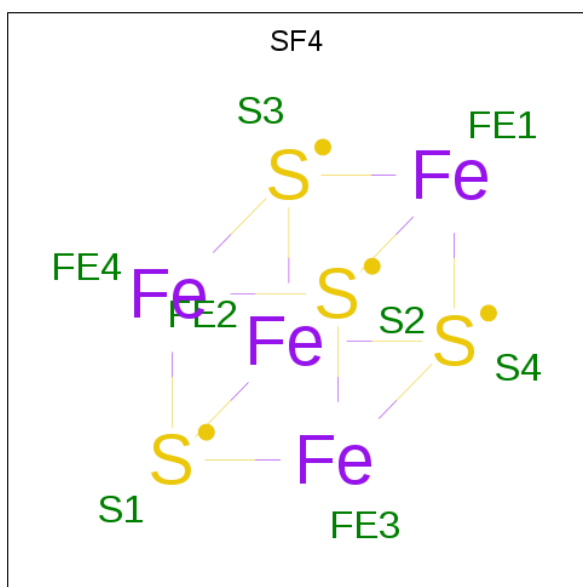
- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

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:

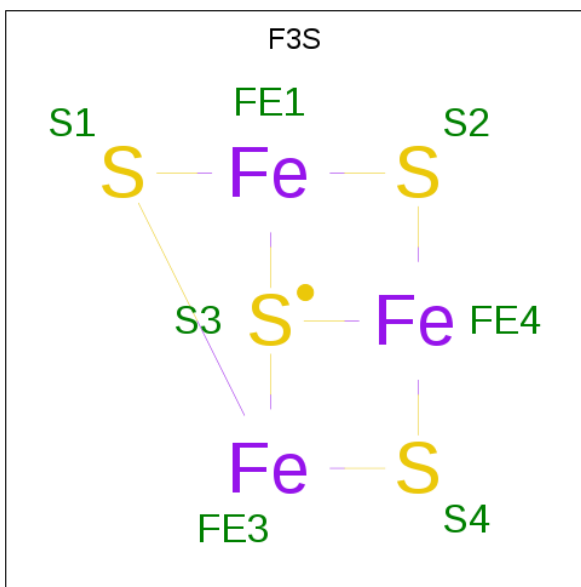
Chain	Residue	Modelled	Actual	Comment	Reference
Q	198	ASN	ASP	conflict	UNP P18188
Q	303	SER	GLU	conflict	UNP P18188
Q	499	ALA	SER	engineered mutation	UNP P18188
R	198	ASN	ASP	conflict	UNP P18188
R	303	SER	GLU	conflict	UNP P18188
R	499	ALA	SER	engineered mutation	UNP P18188
S	198	ASN	ASP	conflict	UNP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

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



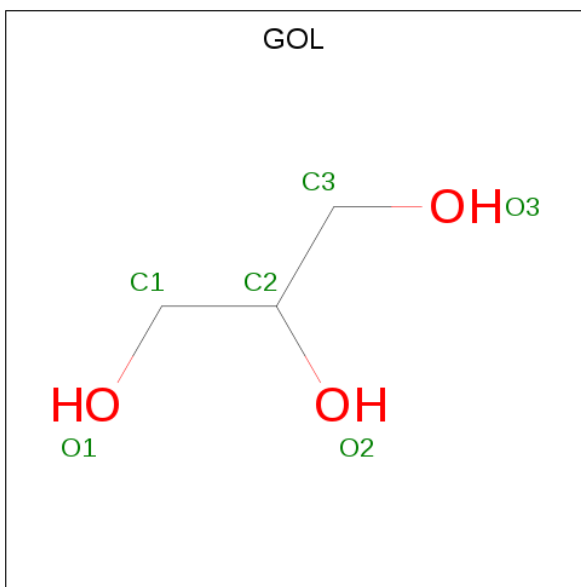
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

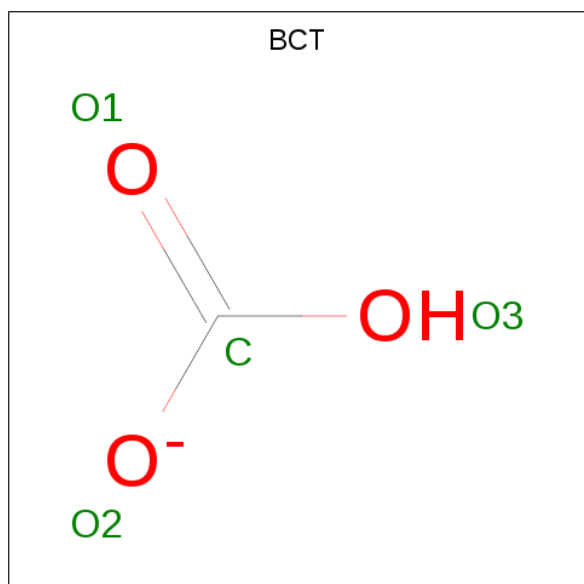
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 8 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

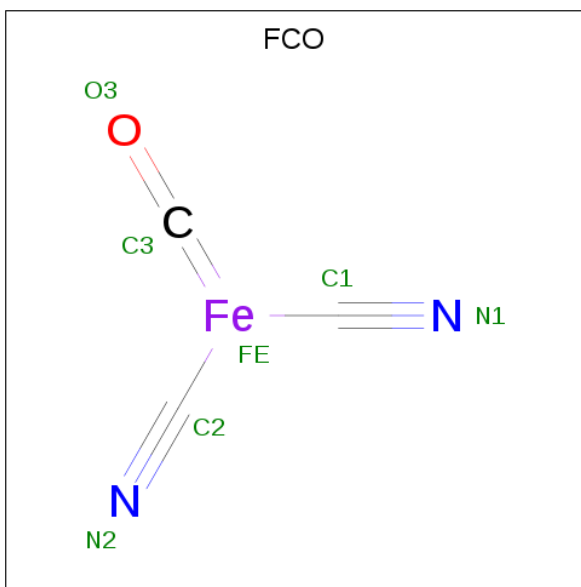


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	Q	1	Total	C	O	0	0
			4	1	3		

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

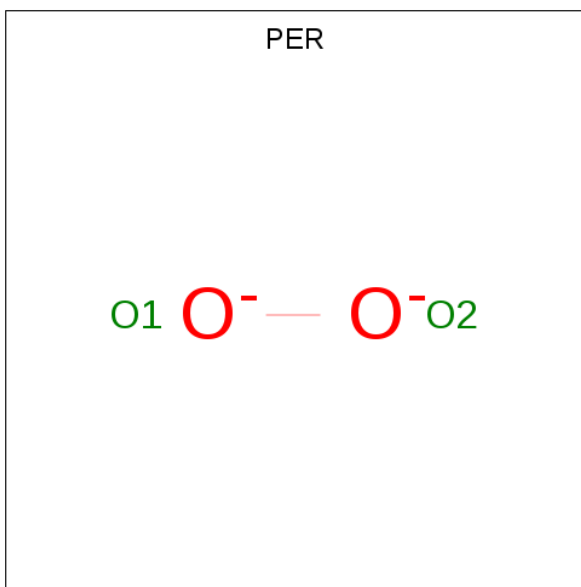
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	R	1	Total	Mg	0	0
			1	1		
9	Q	2	Total	Mg	0	0
			2	2		

- Molecule 10 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: 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 (three-letter code: PER) (formula: O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 12 is water.

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

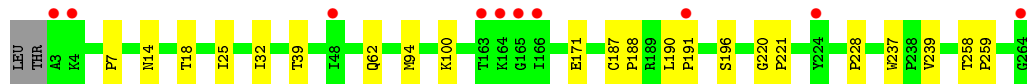
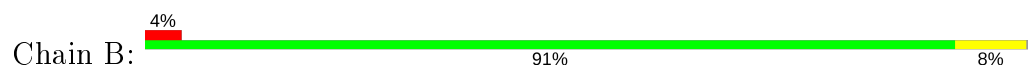
3 Residue-property plots [i](#)

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



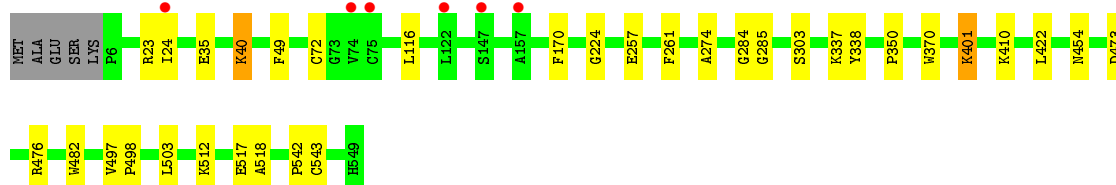
- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit



- Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

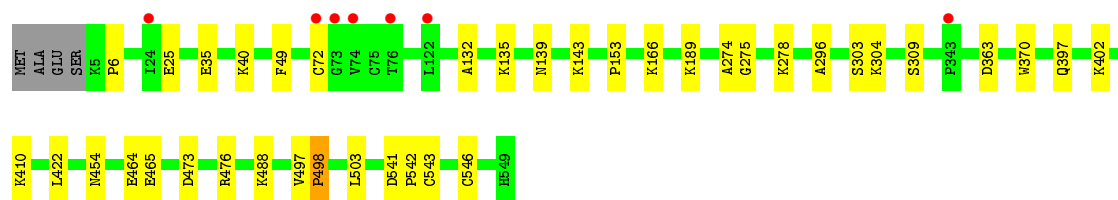


- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

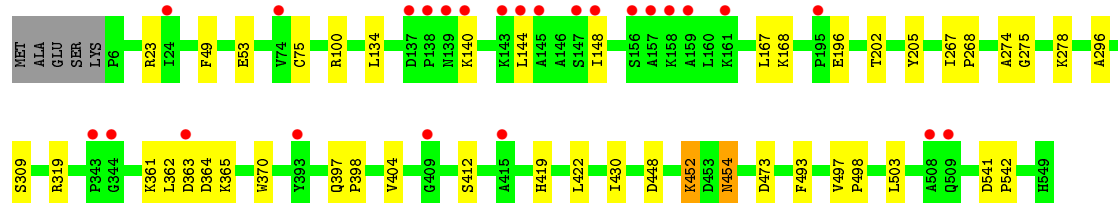
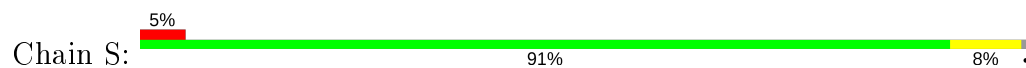


- Molecule 2: Periplasmic [NiFe] hydrogenase large subunit





• 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 46.98 – 1.78	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-1.83) 81.0 (46.98-1.78)	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 (4.74%)	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)	0.36 , 55.6	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	0.96	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: GOL, MG, NI, SF4, PER, F3S, FE2, BCT, 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	0.50	0/2027	0.60	0/2759
1	B	0.42	0/2043	0.55	0/2781
1	C	0.41	0/2014	0.53	0/2743
2	Q	0.48	0/4330	0.60	0/5876
2	R	0.45	0/4292	0.58	0/5827
2	S	0.40	0/4280	0.55	0/5810
All	All	0.44	0/18986	0.57	0/25796

There are no bond length outliers.

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	16	0
1	B	1980	0	1918	11	0
1	C	1960	0	1897	8	0
2	Q	4187	0	4180	25	0
2	R	4173	0	4154	31	0
2	S	4165	0	4142	26	0
3	A	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	1	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	113	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 (113) 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:Q:543[B]:CYS:SG	11:Q:552:PER:O2	2.11	1.08
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:S:134:LEU:CD2	2:S:167:LEU:HD23	2.28	0.62
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.80	0.62
2:Q:35:GLU:HB2	2:Q:40:LYS:HE2	1.82	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:171:GLU:H	1:A:171:GLU:CD	2.06	0.58
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
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: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
1:B:258:THR:HA	1:B:259:PRO:C	2.32	0.50
2:S:75:CYS:N	12:S:557:HOH:O	2.38	0.50
2:Q:410:LYS:HD3	2:Q:410:LYS:O	2.12	0.49
2:Q:285:GLY:HA3	5:Q:559:GOL:H2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Q:35:GLU:HB2	2:Q:40:LYS:CE	2.45	0.45
2:R:410:LYS:HA	5:R:1302:GOL:C1	2.46	0.45
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.52	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:HA	2:R:304:LYS:HD3	1.75	0.45
2:R:153:PRO:HD2	12:R:1437:HOH:O	2.16	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
2:S:267:ILE:HB	2:S:268:PRO:HD3	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.01	0.41
2:Q:476:ARG:HD2	10:Q:550:FCO:C2	2.50	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
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:228:PRO:HB3	1:B:237:TRP:CZ2	2.56	0.41
1:B:25:ILE:HG22	1:B:32:ILE:HG12	2.03	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
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
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.55	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:HD3	2:S:100:ARG:HH11	1.77	0.40
2:S:454:ASN:N	2:S:454:ASN:HD22	2.18	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 [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	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%)	47	33
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%)	207 (100%)	1 (0%)	88	85
1	B	210/210 (100%)	207 (99%)	3 (1%)	67	55
1	C	207/210 (99%)	205 (99%)	2 (1%)	76	68
2	Q	442/438 (101%)	436 (99%)	6 (1%)	67	55
2	R	437/438 (100%)	430 (98%)	7 (2%)	62	49
2	S	436/438 (100%)	429 (98%)	7 (2%)	62	49
All	All	1940/1944 (100%)	1914 (99%)	26 (1%)	67	58

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

Mol	Chain	Res	Type
1	A	88	MET
2	Q	40	LYS
2	Q	303	SER
2	Q	401	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	454	ASN
2	Q	473	ASP
2	Q	503	LEU
1	B	100	LYS
1	B	171	GLU
1	B	196	SER
2	R	166	LYS
2	R	397	GLN
2	R	402	LYS
2	R	454	ASN
2	R	473	ASP
2	R	498	PRO
2	R	503	LEU
1	C	88	MET
1	C	95	ILE
2	S	168	LYS
2	S	365	LYS
2	S	412	SER
2	S	452	LYS
2	S	454	ASN
2	S	473	ASP
2	S	503	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	62	GLN
1	A	172	ASN
2	Q	181	ASN
2	Q	454	ASN
2	Q	509	GLN
1	B	14	ASN
1	B	62	GLN
2	R	139	ASN
2	R	181	ASN
2	R	367	HIS
2	R	454	ASN
2	R	509	GLN
1	C	14	ASN
2	S	454	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SF4	C	265	1	0,12,12	0.00	-	-		
8	BCT	Q	554	-	0,3,3	0.00	-	0,3,3	0.00	-
4	F3S	A	266	1	0,9,9	0.00	-	-		
4	F3S	B	266	1	0,9,9	0.00	-	-		
3	SF4	B	267	1	0,12,12	0.00	-	-		
11	PER	S	552	10,6	0,1,1	0.00	-	-		
11	PER	Q	552	10,6	0,1,1	0.00	-	-		
5	GOL	R	1301	-	5,5,5	0.41	0	5,5,5	0.35	0
10	FCO	R	550	11,2	0,6,6	0.00	-	-		
5	GOL	R	1305	-	5,5,5	0.43	0	5,5,5	0.33	0
3	SF4	B	265	1	0,12,12	0.00	-	-		
5	GOL	Q	558	-	5,5,5	0.47	0	5,5,5	0.31	0
5	GOL	R	1303	-	5,5,5	0.29	0	5,5,5	0.37	0
3	SF4	C	267	1	0,12,12	0.00	-	-		
5	GOL	R	1307	-	5,5,5	0.29	0	5,5,5	0.30	0
11	PER	R	552	10,6	0,1,1	0.00	-	-		
5	GOL	A	269	-	5,5,5	0.26	0	5,5,5	0.67	0
3	SF4	A	265	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	R	1302	-	5,5,5	0.40	0	5,5,5	0.23	0
5	GOL	S	2301	-	5,5,5	0.44	0	5,5,5	0.16	0
5	GOL	R	1304	-	5,5,5	0.37	0	5,5,5	0.17	0
3	SF4	A	267	1	0,12,12	0.00	-	-	-	-
5	GOL	A	270	-	5,5,5	0.41	0	5,5,5	0.95	0
5	GOL	S	2303	-	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	R	1306	-	5,5,5	0.38	0	5,5,5	0.29	0
10	FCO	Q	550	11,2	0,6,6	0.00	-	-	-	-
10	FCO	S	550	11,2	0,6,6	0.00	-	-	-	-
5	GOL	Q	560	-	5,5,5	0.44	0	5,5,5	0.37	0
5	GOL	Q	557	-	5,5,5	0.38	0	5,5,5	0.24	0
4	F3S	C	266	1	0,9,9	0.00	-	-	-	-
5	GOL	A	268	-	5,5,5	0.47	0	5,5,5	0.71	0
5	GOL	Q	559	-	5,5,5	0.40	0	5,5,5	0.18	0
5	GOL	S	2302	-	5,5,5	0.42	0	5,5,5	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	1306	-	-	4/4/4/4	-
4	F3S	A	266	1	-	-	0/3/3/3
4	F3S	B	266	1	-	-	0/3/3/3
3	SF4	B	267	1	-	-	0/6/5/5
5	GOL	R	1301	-	-	1/4/4/4	-
3	SF4	C	265	1	-	-	0/6/5/5
5	GOL	R	1307	-	-	0/4/4/4	-
5	GOL	Q	557	-	-	0/4/4/4	-
3	SF4	B	265	1	-	-	0/6/5/5
5	GOL	Q	558	-	-	0/4/4/4	-
5	GOL	R	1303	-	-	0/4/4/4	-
3	SF4	C	267	1	-	-	0/6/5/5
5	GOL	R	1305	-	-	0/4/4/4	-
5	GOL	A	269	-	-	3/4/4/4	-
3	SF4	A	265	1	-	-	0/6/5/5
5	GOL	R	1302	-	-	4/4/4/4	-
5	GOL	S	2301	-	-	0/4/4/4	-
5	GOL	R	1304	-	-	2/4/4/4	-
3	SF4	A	267	1	-	-	0/6/5/5
5	GOL	A	270	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	S	2303	-	-	4/4/4/4	-
5	GOL	Q	560	-	-	2/4/4/4	-
4	F3S	C	266	1	-	-	0/3/3/3
5	GOL	A	268	-	-	2/4/4/4	-
5	GOL	Q	559	-	-	0/4/4/4	-
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 (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	269	GOL	O1-C1-C2-C3
5	R	1302	GOL	C1-C2-C3-O3
5	A	270	GOL	C1-C2-C3-O3
5	S	2303	GOL	O1-C1-C2-C3
5	S	2303	GOL	C1-C2-C3-O3
5	R	1306	GOL	O1-C1-C2-C3
5	R	1306	GOL	C1-C2-C3-O3
5	Q	560	GOL	C1-C2-C3-O3
5	A	268	GOL	C1-C2-C3-O3
5	A	268	GOL	O2-C2-C3-O3
5	S	2302	GOL	C1-C2-C3-O3
5	R	1304	GOL	C1-C2-C3-O3
5	A	270	GOL	O1-C1-C2-C3
5	A	269	GOL	O1-C1-C2-O2
5	R	1302	GOL	O2-C2-C3-O3
5	A	270	GOL	O2-C2-C3-O3
5	S	2303	GOL	O1-C1-C2-O2
5	S	2303	GOL	O2-C2-C3-O3
5	R	1306	GOL	O1-C1-C2-O2
5	R	1306	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	R	1302	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	269	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	552	PER	1	0
5	R	1307	GOL	1	0
11	R	552	PER	1	0
5	A	269	GOL	1	0
5	R	1302	GOL	3	0
5	A	270	GOL	1	0
5	R	1306	GOL	1	0
10	Q	550	FCO	1	0
5	Q	560	GOL	2	0
5	Q	559	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(Å²)	Q<0.9	
1	A	262/264 (99%)	-0.17	4 (1%)	73	73	4, 9, 16, 32	8 (3%)
1	B	262/264 (99%)	0.07	10 (3%)	40	37	5, 10, 17, 29	9 (3%)
1	C	260/264 (98%)	-0.07	7 (2%)	54	52	6, 11, 20, 28	6 (2%)
2	Q	544/549 (99%)	-0.25	6 (1%)	80	80	4, 9, 15, 22	12 (2%)
2	R	545/549 (99%)	-0.19	7 (1%)	77	77	5, 9, 16, 40	13 (2%)
2	S	544/549 (99%)	0.11	25 (4%)	32	29	6, 11, 18, 28	15 (2%)
All	All	2417/2439 (99%)	-0.09	59 (2%)	59	57	4, 10, 17, 40	63 (2%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	5.3
1	B	3	ALA	5.2
1	C	67	LYS	3.7
1	A	48	ILE	3.7
2	S	157	ALA	3.7
1	C	162	LEU	3.6
2	S	158	LYS	3.5
2	R	74	VAL	3.3
2	S	344	GLY	3.2
2	Q	24	ILE	3.2
2	S	148	ILE	3.2
1	B	4	LYS	3.2
2	S	147	SER	3.2
2	S	137	ASP	3.0
2	S	363	ASP	3.0
2	S	138	PRO	2.9
2	S	145	ALA	2.9
1	C	5	HIS	2.8
2	S	144	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	157	ALA	2.8
1	B	163	THR	2.8
2	S	74	VAL	2.8
2	S	343	PRO	2.7
2	S	139	ASN	2.7
1	C	163	THR	2.7
2	R	24	ILE	2.7
1	B	264	GLY	2.7
2	S	409	GLY	2.7
2	S	159	ALA	2.6
2	R	122	LEU	2.6
2	S	161	LYS	2.6
1	B	165	GLY	2.6
1	B	48	ILE	2.6
1	A	18	THR	2.6
1	B	224	TYR	2.6
2	S	143	LYS	2.6
2	R	343	PRO	2.5
1	C	66	GLY	2.5
2	S	415	ALA	2.5
1	B	164	LYS	2.4
2	Q	122	LEU	2.4
2	Q	147	SER	2.3
1	B	191	PRO	2.3
2	R	72	CYS	2.3
2	S	24	ILE	2.3
2	S	140	LYS	2.3
2	S	509	GLN	2.3
2	Q	74	VAL	2.2
2	S	508	ALA	2.2
1	C	48	ILE	2.2
2	R	73	GLY	2.2
1	C	164	LYS	2.2
2	S	156	SER	2.2
2	S	393	TYR	2.2
2	R	76	THR	2.1
1	A	4	LYS	2.1
1	B	166	ILE	2.1
2	S	195	PRO	2.0
2	Q	75	CYS	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
5	GOL	R	1302	6/6	0.78	0.13	27,28,30,33	0
5	GOL	R	1307	6/6	0.85	0.21	28,31,32,36	0
5	GOL	S	2303	6/6	0.85	0.14	34,35,36,38	6
5	GOL	S	2302	6/6	0.85	0.12	32,35,35,35	6
5	GOL	Q	560	6/6	0.86	0.23	25,38,41,47	0
5	GOL	A	269	6/6	0.87	0.14	21,27,28,36	0
5	GOL	R	1306	6/6	0.87	0.22	30,37,39,41	0
5	GOL	R	1304	6/6	0.89	0.19	28,31,33,36	0
5	GOL	R	1305	6/6	0.90	0.16	21,23,25,26	0
5	GOL	Q	559	6/6	0.90	0.26	29,31,33,35	0
5	GOL	A	270	6/6	0.90	0.25	17,29,31,34	0
5	GOL	A	268	6/6	0.92	0.16	16,20,24,28	0
5	GOL	R	1303	6/6	0.94	0.09	9,10,11,13	0
8	BCT	Q	554	4/4	0.96	0.10	24,29,31,32	0
9	MG	Q	555	1/1	0.96	0.13	29,29,29,29	0
9	MG	R	1308	1/1	0.97	0.13	30,30,30,30	0
5	GOL	R	1301	6/6	0.97	0.09	7,8,9,10	0
9	MG	Q	556	1/1	0.97	0.08	35,35,35,35	0
5	GOL	Q	557	6/6	0.98	0.09	8,9,11,12	0
3	SF4	B	265	8/8	0.98	0.13	8,10,11,11	0
5	GOL	Q	558	6/6	0.98	0.08	8,10,11,12	0
5	GOL	S	2301	6/6	0.98	0.07	7,10,11,12	0
4	F3S	B	266	7/7	0.98	0.10	9,9,11,12	0
11	PER	Q	552	2/2	0.98	0.09	14,14,14,15	1
11	PER	R	552	2/2	0.98	0.09	14,14,14,16	1
7	FE2	S	553	1/1	0.98	0.10	9,9,9,9	1
3	SF4	C	267	8/8	0.99	0.03	9,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	PER	S	552	2/2	0.99	0.04	12,12,12,12	1
4	F3S	A	266	7/7	0.99	0.04	9,9,10,10	0
10	FCO	R	550	7/7	0.99	0.05	5,7,9,11	0
7	FE2	Q	553	1/1	0.99	0.03	9,9,9,9	1
10	FCO	Q	550	7/7	0.99	0.07	7,8,9,10	0
10	FCO	S	550	7/7	0.99	0.05	8,11,13,13	0
3	SF4	A	265	8/8	0.99	0.04	7,8,8,10	0
4	F3S	C	266	7/7	0.99	0.04	10,10,11,12	0
7	FE2	R	553	1/1	0.99	0.04	9,9,9,9	1
6	NI	S	551	1/1	0.99	0.03	15,15,15,15	0
3	SF4	C	265	8/8	0.99	0.05	8,9,10,11	0
6	NI	R	551	1/1	0.99	0.02	14,14,14,14	0
3	SF4	B	267	8/8	0.99	0.04	9,9,11,12	0
6	NI	Q	551	1/1	1.00	0.04	14,14,14,14	0
3	SF4	A	267	8/8	1.00	0.07	8,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.