



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:12 pm BST

PDB ID : 4UQL
Title : High-resolution structure of a Ni-A Ni-Sox mixture of the D. fructosovorans NiFe-hydrogenase L122A mutant
Authors : Volbeda, A.; Martin, L.; Barbier, E.; Gutierrez-Sanz, O.; DeLacey, A.L.; Liebgott, P.P.; Dementin, S.; Rousset, M.; Fontecilla-Camps, J.C.
Deposited on : 2014-06-24
Resolution : 1.22 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

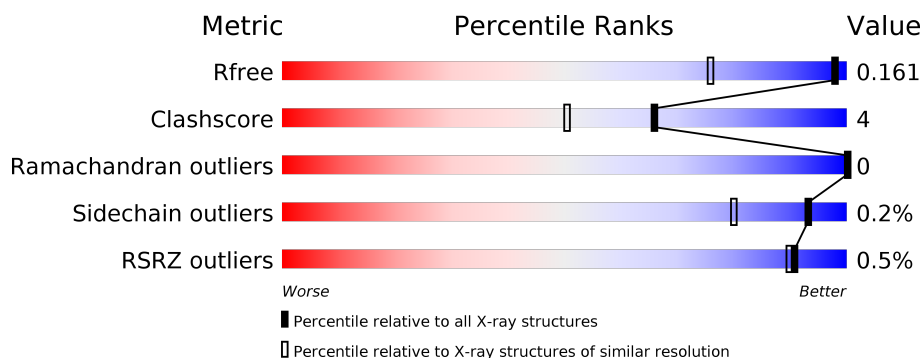
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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	1232 (1.24-1.20)
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

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	265	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> <div></div> </div> <div>• •</div> </div>
1	B	265	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div></div> </div> <div>•</div> </div>
2	Q	563	<div> <div></div> <div> <div>91%</div> <div>6%</div> <div></div> </div> <div>•</div> </div>
2	R	563	<div> <div></div> <div> <div>91%</div> <div>6%</div> <div></div> </div> <div>•</div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14688 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 HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	12	0
			2031	1296	336	383	16			
1	B	263	Total	C	N	O	S	0	16	0
			2061	1316	339	390	16			

- Molecule 2 is a protein called NICKEL-DEPENDENT HYDROGENASE LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	31	0
			4300	2748	744	783	25			
2	R	545	Total	C	N	O	S	0	35	0
			4328	2765	742	796	25			

There are 32 discrepancies between the modelled and reference sequences:

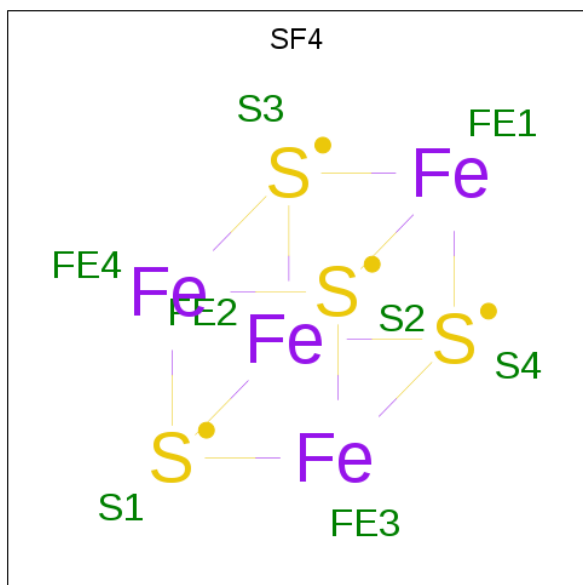
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	expression tag	UNP E1K247
Q	-12	SER	-	expression tag	UNP E1K247
Q	-11	TRP	-	expression tag	UNP E1K247
Q	-10	SER	-	expression tag	UNP E1K247
Q	-9	HIS	-	expression tag	UNP E1K247
Q	-8	PRO	-	expression tag	UNP E1K247
Q	-7	GLN	-	expression tag	UNP E1K247
Q	-6	PHE	-	expression tag	UNP E1K247
Q	-5	GLU	-	expression tag	UNP E1K247
Q	-4	LYS	-	expression tag	UNP E1K247
Q	-3	GLY	-	expression tag	UNP E1K247
Q	-2	ALA	-	expression tag	UNP E1K247
Q	-1	SER	-	expression tag	UNP E1K247
Q	0	GLY	-	expression tag	UNP E1K247
Q	1	ALA	-	expression tag	UNP E1K247
Q	122	ALA	LEU	engineered mutation	UNP E1K247

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-13	ALA	-	expression tag	UNP E1K247
R	-12	SER	-	expression tag	UNP E1K247
R	-11	TRP	-	expression tag	UNP E1K247
R	-10	SER	-	expression tag	UNP E1K247
R	-9	HIS	-	expression tag	UNP E1K247
R	-8	PRO	-	expression tag	UNP E1K247
R	-7	GLN	-	expression tag	UNP E1K247
R	-6	PHE	-	expression tag	UNP E1K247
R	-5	GLU	-	expression tag	UNP E1K247
R	-4	LYS	-	expression tag	UNP E1K247
R	-3	GLY	-	expression tag	UNP E1K247
R	-2	ALA	-	expression tag	UNP E1K247
R	-1	SER	-	expression tag	UNP E1K247
R	0	GLY	-	expression tag	UNP E1K247
R	1	ALA	-	expression tag	UNP E1K247
R	122	ALA	LEU	engineered mutation	UNP E1K247

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



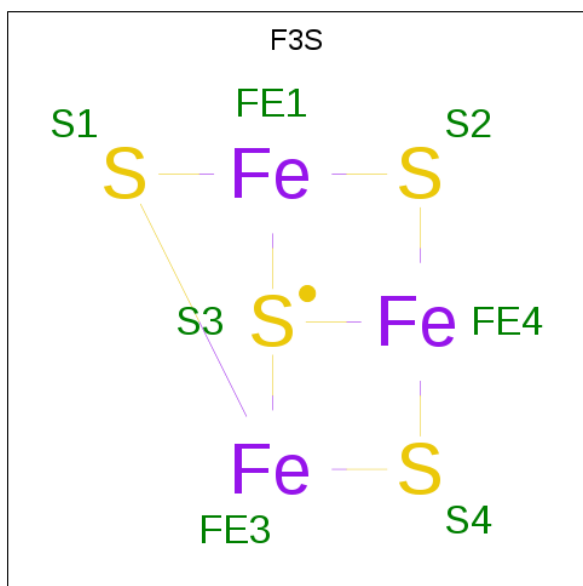
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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).



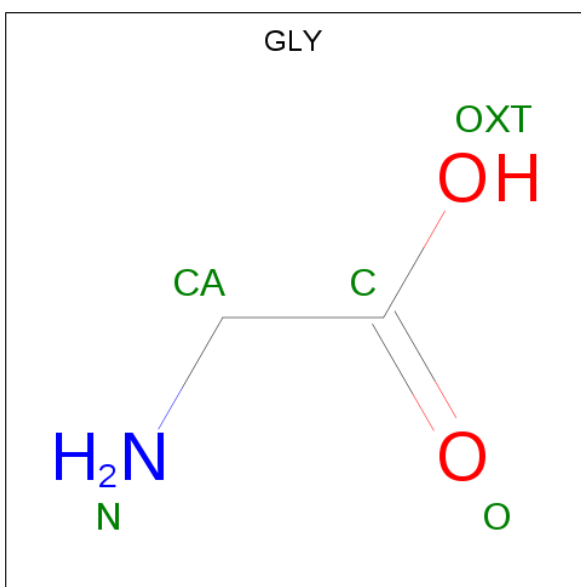
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



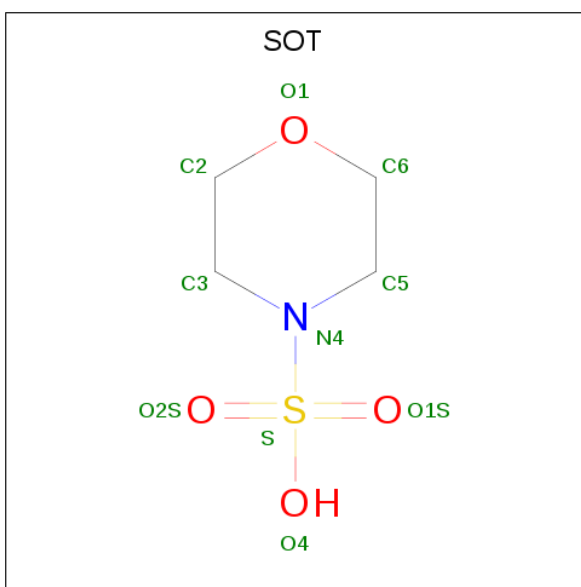
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	1
			7	3	4		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



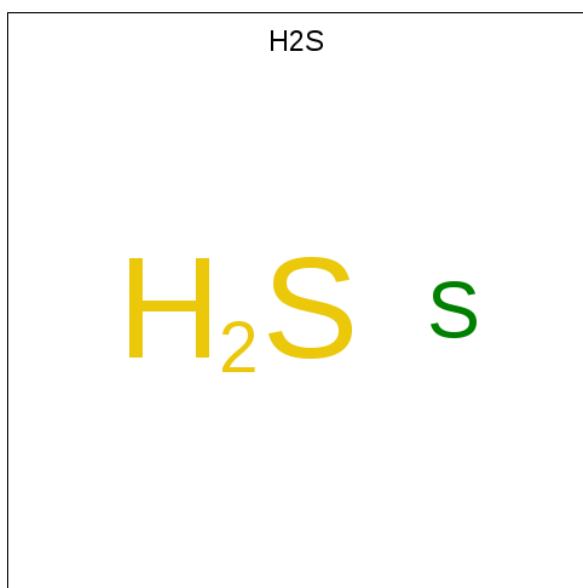
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			5	2	1	2		
6	Q	1	Total	C	N	O	0	0
			5	2	1	2		
6	R	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 7 is morpholine-4-sulfonic acid (three-letter code: SOT) (formula: C₄H₉NO₄S).



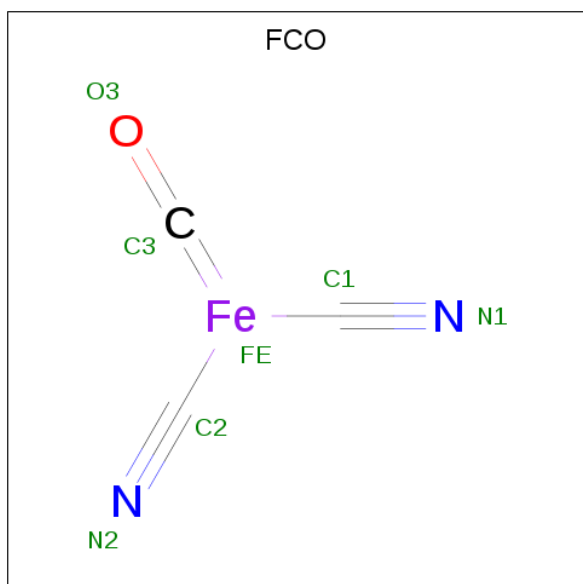
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	1
			18	8	2	6	2		

- Molecule 8 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	S	0	0
			1	1		

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C₃FeN₂O).



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

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

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	R	1	Total	Ni	0	1
			2	2		
10	Q	1	Total	Ni	0	1
			2	2		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	Q	1	Total	Cl	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	283	Total	O	0	12
			295	295		
13	B	307	Total	O	0	9
			316	316		
13	Q	544	Total	O	0	13
			557	557		
13	R	618	Total	O	0	14
			632	632		

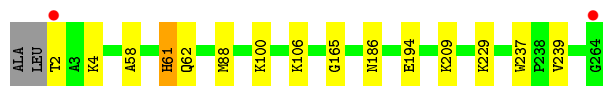
3 Residue-property plots [i](#)

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.

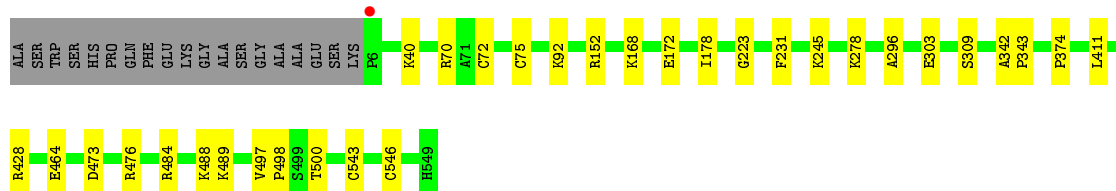
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA



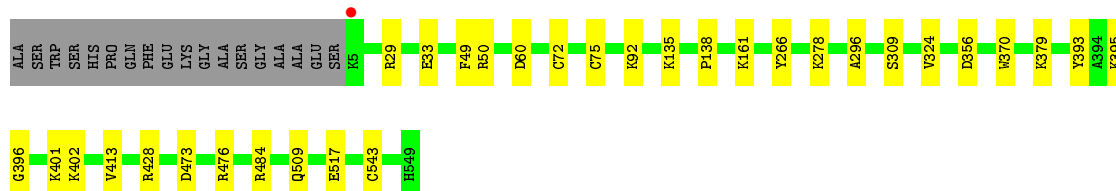
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA



- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT



- Molecule 2: NICKEL-DEPENDENT 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	64.69Å 100.85Å 116.70Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	30.00 – 1.22 45.99 – 1.15	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-1.22) 95.9 (45.99-1.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.15Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.120 , 0.152 0.132 , 0.161	Depositor DCC
R_{free} test set	24508 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	6.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14688	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 4.76% 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: NI, MG, GOL, CL, SF4, H2S, F3S, CSX, FCO, CSS, SOT

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	0/2137	0.75	1/2904 (0.0%)
1	B	0.63	0/2181	0.79	2/2958 (0.1%)
2	Q	0.63	0/4495	0.80	3/6081 (0.0%)
2	R	0.63	0/4555	0.84	5/6166 (0.1%)
All	All	0.63	0/13368	0.81	11/18109 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	428	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	R	50	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	Q	152	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	Q	428	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	R	266	TYR	CB-CG-CD1	5.75	124.45	121.00
1	B	61[A]	HIS	CB-CA-C	5.49	121.38	110.40
1	B	61[B]	HIS	CB-CA-C	5.49	121.38	110.40
2	Q	70	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	R	29	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	252	ASP	CB-CG-OD1	5.16	122.94	118.30
2	R	60	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ARG	Sidechain

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	2031	0	1971	10	0
1	B	2061	0	1998	21	0
2	Q	4300	0	4316	31	0
2	R	4328	0	4320	37	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	12	0	16	0	0
5	B	18	0	24	2	0
5	Q	6	0	8	0	0
5	R	31	0	38	5	0
6	B	5	0	2	0	0
6	Q	5	0	2	1	0
6	R	5	0	2	1	0
7	B	18	0	16	0	0
8	B	1	0	0	0	0
9	Q	7	0	0	0	0
9	R	7	0	0	0	0
10	Q	2	0	0	0	0
10	R	2	0	0	0	0
11	Q	1	0	0	0	0
11	R	1	0	0	0	0
12	Q	1	0	0	0	0
13	A	295	0	0	4	0
13	B	316	0	0	18	0
13	Q	557	0	0	17	0
13	R	632	0	0	27	0
All	All	14688	0	12713	103	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 4.

All (103) 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:245[B]:LYS:HE2	13:Q:2510:HOH:O	1.16	1.25
2:R:92[B]:LYS:HE3	13:R:2558:HOH:O	1.11	1.25
5:B:1269:GOL:O3	13:B:2305:HOH:O	1.52	1.25
2:Q:489[B]:LYS:HE2	13:Q:2441:HOH:O	1.13	1.24
2:Q:92[B]:LYS:HE2	13:Q:2272:HOH:O	1.41	1.18
6:R:601:GLY:N	13:R:2006:HOH:O	1.72	1.18
6:Q:601:GLY:N	13:Q:2006:HOH:O	1.75	1.17
2:R:92[A]:LYS:HE2	13:R:2566:HOH:O	1.00	1.17
2:R:278[B]:LYS:HE3	13:R:2466:HOH:O	1.44	1.14
2:R:395[B]:LYS:NZ	5:R:1554:GOL:O1	1.78	1.13
2:R:517[B]:GLU:OE1	13:R:2617:HOH:O	1.69	1.10
2:R:92[B]:LYS:CE	13:R:2558:HOH:O	1.75	1.07
2:Q:245[B]:LYS:CE	13:Q:2510:HOH:O	1.81	1.06
2:R:484[A]:ARG:NH2	13:R:2486:HOH:O	1.90	1.04
2:R:278[B]:LYS:HG2	13:R:2443:HOH:O	1.63	0.98
1:B:61[A]:HIS:ND1	13:B:2172:HOH:O	1.97	0.98
5:R:1555[A]:GOL:O1	13:R:2584:HOH:O	1.81	0.98
5:R:1556:GOL:H2	13:R:2385:HOH:O	0.77	0.94
2:Q:303[B]:GLU:OE2	13:Q:2535:HOH:O	1.86	0.92
1:A:48[B]:ILE:HD11	2:Q:178:ILE:HG21	1.50	0.92
2:Q:172[A]:GLU:HG2	13:Q:2513:HOH:O	1.70	0.92
2:R:92[A]:LYS:CE	13:R:2566:HOH:O	1.74	0.91
2:R:402[B]:LYS:HE3	13:R:2547:HOH:O	1.76	0.85
1:B:61[A]:HIS:HE1	13:B:2182:HOH:O	1.61	0.83
1:B:209[A]:LYS:NZ	13:B:2206:HOH:O	2.13	0.81
5:R:1557:GOL:O3	13:R:2555:HOH:O	1.98	0.81
1:A:29[B]:LYS:NZ	13:A:2266:HOH:O	2.14	0.79
1:B:61[A]:HIS:CE1	13:B:2172:HOH:O	2.35	0.79
2:Q:40[A]:LYS:HE3	13:Q:2405:HOH:O	1.81	0.78
1:B:194[A]:GLU:CG	13:B:2169:HOH:O	2.32	0.78
2:R:401[A]:LYS:NZ	13:R:2549:HOH:O	1.77	0.75
1:B:194[A]:GLU:OE1	13:B:2271:HOH:O	2.05	0.75
1:B:194[A]:GLU:OE2	13:B:2285:HOH:O	2.05	0.74
1:B:194[A]:GLU:HG2	13:B:2169:HOH:O	1.88	0.72
2:Q:303[B]:GLU:OE1	13:Q:2509:HOH:O	0.71	0.71
1:B:106[A]:LYS:HE3	13:B:2224:HOH:O	1.90	0.69
1:A:65[B]:GLU:OE2	13:A:2197:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61[A]:HIS:CE1	13:B:2182:HOH:O	2.39	0.67
2:Q:72:CYS:HB3	2:Q:75:CSX:OD	1.95	0.65
2:R:356[B]:ASP:OD2	13:R:2507:HOH:O	2.16	0.64
2:Q:72:CYS:CB	2:Q:75:CSX:OD	2.46	0.63
2:R:379[A]:LYS:HD2	13:R:2568:HOH:O	1.99	0.63
2:R:402[B]:LYS:CE	13:R:2547:HOH:O	2.41	0.62
1:B:194[A]:GLU:HG3	13:B:2169:HOH:O	1.97	0.62
2:R:324:VAL:HG11	2:R:395[B]:LYS:HE2	1.82	0.61
1:A:61[A]:HIS:HE1	13:A:2156:HOH:O	1.83	0.60
2:Q:92[B]:LYS:CE	13:Q:2272:HOH:O	2.18	0.59
2:R:396:GLY:HA2	2:R:401[A]:LYS:HE3	1.86	0.58
2:R:138:PRO:HG3	2:R:161[A]:LYS:HG2	1.84	0.58
2:R:72:CYS:HB3	2:R:75:CSX:OD	2.04	0.57
2:R:484[A]:ARG:HD2	13:R:2370:HOH:O	2.03	0.57
2:R:402[B]:LYS:NZ	13:R:2547:HOH:O	2.37	0.56
2:Q:342[A]:ALA:HB1	2:Q:343[A]:PRO:HD2	1.88	0.55
1:A:48[B]:ILE:CD1	2:Q:178:ILE:HG21	2.33	0.55
2:Q:464[B]:GLU:OE2	2:Q:488:LYS:HE3	2.07	0.55
1:A:48[B]:ILE:CD1	2:Q:178:ILE:HD13	2.37	0.54
2:R:92[A]:LYS:NZ	13:R:2566:HOH:O	2.11	0.54
1:B:62[A]:GLN:HG3	13:B:2166:HOH:O	2.07	0.54
2:Q:489[B]:LYS:CE	13:Q:2441:HOH:O	1.97	0.53
1:A:28:ILE:HG13	1:A:29[B]:LYS:HG3	1.90	0.53
2:R:509[A]:GLN:HG3	13:R:2140:HOH:O	2.07	0.53
2:Q:172[B]:GLU:HB3	13:Q:2450:HOH:O	2.09	0.53
2:R:135[A]:LYS:HD3	13:R:2565:HOH:O	2.10	0.51
2:R:92[A]:LYS:HE2	13:R:2558:HOH:O	2.10	0.51
1:B:165:GLY:HA2	13:B:2264:HOH:O	2.10	0.50
2:Q:168:LYS:O	2:Q:172[A]:GLU:HG3	2.12	0.50
2:Q:245[B]:LYS:HE3	13:Q:2510:HOH:O	1.80	0.50
1:B:4[B]:LYS:HE3	13:B:2215:HOH:O	2.12	0.49
1:A:62[A]:GLN:OE1	13:A:2107:HOH:O	0.49	0.49
2:Q:92[B]:LYS:NZ	13:Q:2272:HOH:O	2.42	0.48
2:R:278[A]:LYS:HE3	2:R:413:VAL:HG12	1.94	0.48
2:R:393:TYR:O	2:R:401[A]:LYS:CE	2.61	0.48
2:R:92[B]:LYS:HE2	13:R:2558:HOH:O	1.73	0.47
1:B:100:LYS:HE3	13:B:2300:HOH:O	2.15	0.47
2:R:509[A]:GLN:CD	13:R:2512:HOH:O	2.54	0.47
2:R:278[A]:LYS:HE3	2:R:413:VAL:CG1	2.46	0.46
5:B:1269:GOL:C3	13:B:2305:HOH:O	2.38	0.46
2:R:296:ALA:HA	2:R:309:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:278[B]:LYS:CE	13:R:2466:HOH:O	2.28	0.46
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.51	0.46
1:B:186:ASN:ND2	1:B:229[A]:LYS:HD2	2.30	0.45
1:B:58:ALA:O	1:B:62[A]:GLN:HG3	2.16	0.45
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.51	0.45
2:R:138:PRO:HG3	2:R:161[A]:LYS:CG	2.46	0.45
1:B:4[B]:LYS:CE	13:B:2215:HOH:O	2.66	0.44
2:R:509[A]:GLN:CD	13:R:2457:HOH:O	2.56	0.43
1:B:2:THR:CG2	1:B:4[A]:LYS:HE3	2.48	0.43
2:Q:245[A]:LYS:NZ	13:Q:2230:HOH:O	2.31	0.43
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.53	0.43
2:R:476:ARG:CZ	2:R:543[B]:CSS:SD	3.07	0.42
2:Q:278[B]:LYS:HE3	13:Q:2342:HOH:O	2.19	0.42
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.50	0.42
2:Q:484[A]:ARG:HD2	13:Q:2467:HOH:O	2.20	0.41
2:R:33[A]:GLU:HG2	5:R:1557:GOL:O1	2.21	0.41
2:Q:278[B]:LYS:HE2	2:Q:411:LEU:O	2.20	0.41
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	2.03	0.41
2:R:476:ARG:HD2	2:R:543[B]:CSS:SD	2.61	0.41
2:Q:296:ALA:HA	2:Q:309:SER:HA	2.02	0.41
2:Q:476:ARG:CZ	2:Q:543[B]:CSS:SD	3.09	0.40
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.57	0.40
2:Q:374:PRO:HD3	2:Q:500:THR:HG22	2.03	0.40
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.56	0.40
2:Q:223:GLY:HA2	2:Q:231:PHE:CD1	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	273/265 (103%)	266 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	277/265 (104%)	271 (98%)	6 (2%)	0	100	100
2	Q	570/563 (101%)	554 (97%)	16 (3%)	0	100	100
2	R	576/563 (102%)	566 (98%)	10 (2%)	0	100	100
All	All	1696/1656 (102%)	1657 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	221/210 (105%)	221 (100%)	0	100	100
1	B	225/210 (107%)	223 (99%)	2 (1%)	78	50
2	Q	459/445 (103%)	458 (100%)	1 (0%)	93	80
2	R	467/445 (105%)	466 (100%)	1 (0%)	93	80
All	All	1372/1310 (105%)	1368 (100%)	4 (0%)	93	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88[A]	MET
1	B	88[B]	MET
2	Q	473	ASP
2	R	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	5	HIS
2	Q	250	ASN
2	Q	509	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	CSS	R	543[B]	10	4,6,7	1.09	0	1,6,8	0.36	0
2	CSS	Q	543[B]	10	4,6,7	0.73	0	1,6,8	0.13	0
2	CSX	R	75	9,10,2	3,6,7	0.67	0	1,6,8	1.37	0
2	CSX	Q	75	9,10,2	3,6,7	0.51	0	1,6,8	0.55	0
2	CSS	R	543[A]	10	4,5,7	1.53	1 (25%)	1,5,8	1.09	0
2	CSS	Q	543[A]	10	4,5,7	1.55	1 (25%)	1,5,8	1.60	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
2	CSS	R	543[B]	10	-	0/1/5/7	-
2	CSS	Q	543[B]	10	-	0/1/5/7	-
2	CSX	R	75	9,10,2	-	0/1/5/7	-
2	CSX	Q	75	9,10,2	-	0/1/5/7	-
2	CSS	R	543[A]	10	-	0/1/4/7	-
2	CSS	Q	543[A]	10	-	0/1/4/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	543[A]	CSS	CB-SG	-2.73	1.72	1.81
2	R	543[A]	CSS	CB-SG	-2.32	1.74	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	543[B]	CSS	2	0
2	Q	543[B]	CSS	1	0
2	R	75	CSX	1	0
2	Q	75	CSX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 1 is modelled with single atom and 7 are monoatomic - leaving 25 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	R	1554	-	5,5,5	0.73	0	5,5,5	0.21	0
4	F3S	A	1266	1	0,9,9	0.00	-	-		
4	F3S	B	1266	1	0,9,9	0.00	-	-		
5	GOL	R	1555[B]	-	5,5,5	0.52	0	5,5,5	1.24	1 (20%)
5	GOL	R	1556	-	5,5,5	0.31	0	5,5,5	0.87	0
9	FCO	Q	1550	13,2	0,6,6	0.00	-	-		
3	SF4	B	1267	1	0,12,12	0.00	-	-		
5	GOL	B	1272	-	5,5,5	0.36	0	5,5,5	0.79	0
5	GOL	A	1269	-	5,5,5	0.56	0	5,5,5	0.69	0
3	SF4	A	1265	1	0,12,12	0.00	-	-		
5	GOL	B	1270	-	5,5,5	0.26	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	R	1557	-	5,5,5	0.16	0	5,5,5	0.69	0
5	GOL	R	1553	-	5,5,5	0.43	0	5,5,5	0.33	0
3	SF4	A	1267	1	0,12,12	0.00	-	-		
9	FCO	R	1550	13,2	0,6,6	0.00	-	-		
5	GOL	B	1269	-	5,5,5	0.49	0	5,5,5	0.68	0
5	GOL	Q	1553	-	5,5,5	0.35	0	5,5,5	0.29	0
7	SOT	B	1268[A]	1	6,9,10	0.70	0	3,11,14	3.73	3 (100%)
3	SF4	B	1265	1	0,12,12	0.00	-	-		
5	GOL	A	1268	-	5,5,5	0.16	0	5,5,5	0.90	0
5	GOL	R	1555[A]	-	5,5,5	0.44	0	5,5,5	0.85	0
7	SOT	B	1268[B]	-	6,9,10	0.50	0	3,11,14	1.36	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	1554	-	-	0/4/4/4	-
5	GOL	B	1270	-	-	0/4/4/4	-
4	F3S	A	1266	1	-	-	0/3/3/3
3	SF4	B	1267	1	-	-	0/6/5/5
5	GOL	R	1557	-	-	1/4/4/4	-
5	GOL	R	1555[B]	-	-	0/4/4/4	-
4	F3S	B	1266	1	-	-	0/3/3/3
5	GOL	R	1553	-	-	0/4/4/4	-
5	GOL	Q	1553	-	-	0/4/4/4	-
7	SOT	B	1268[A]	1	-	0/0/12/14	0/1/1/1
3	SF4	B	1265	1	-	-	0/6/5/5
5	GOL	A	1268	-	-	0/4/4/4	-
5	GOL	R	1556	-	-	1/4/4/4	-
5	GOL	B	1272	-	-	0/4/4/4	-
7	SOT	B	1268[B]	-	-	0/0/12/14	0/1/1/1
5	GOL	R	1555[A]	-	-	2/4/4/4	-
3	SF4	A	1267	1	-	-	0/6/5/5
5	GOL	B	1269	-	-	1/4/4/4	-
5	GOL	A	1269	-	-	4/4/4/4	-
3	SF4	A	1265	1	-	-	0/6/5/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1268[A]	SOT	O1-C2-C3	4.23	121.10	111.80
7	B	1268[A]	SOT	C6-O1-C2	3.47	121.46	109.89
7	B	1268[A]	SOT	O1-C6-C5	3.44	119.38	111.80
5	R	1555[B]	GOL	O1-C1-C2	-2.64	97.56	110.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1269	GOL	O1-C1-C2-C3
5	R	1555[A]	GOL	O1-C1-C2-C3
5	R	1556	GOL	C1-C2-C3-O3
5	B	1269	GOL	O1-C1-C2-C3
5	R	1555[A]	GOL	O1-C1-C2-O2
5	A	1269	GOL	O1-C1-C2-O2
5	A	1269	GOL	O2-C2-C3-O3
5	R	1557	GOL	C1-C2-C3-O3
5	A	1269	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1554	GOL	1	0
5	R	1556	GOL	1	0
5	R	1557	GOL	2	0
5	B	1269	GOL	2	0
5	R	1555[A]	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	262/265 (98%)	-0.46	4 (1%) 73 71	4, 8, 20, 48	4 (1%)
1	B	263/265 (99%)	-0.53	2 (0%) 86 85	4, 7, 17, 32	3 (1%)
2	Q	542/563 (96%)	-0.49	1 (0%) 95 94	4, 9, 19, 37	6 (1%)
2	R	543/563 (96%)	-0.51	1 (0%) 95 94	4, 7, 15, 40	4 (0%)
All	All	1610/1656 (97%)	-0.50	8 (0%) 91 90	4, 8, 18, 48	17 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	8.1
1	A	163	THR	3.4
1	B	264[A]	GLY	2.8
1	A	164[A]	LYS	2.7
1	A	4	LYS	2.7
1	B	2	THR	2.6
2	Q	6	PRO	2.4
2	R	5	LYS	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSS	R	543[B]	7/8	0.99	0.08	3,4,7,8	3
2	CSS	Q	543[B]	7/8	0.99	0.07	5,5,8,9	3
2	CSS	R	543[A]	6/8	0.99	0.08	3,4,5,7	2
2	CSS	Q	543[A]	6/8	0.99	0.07	5,5,6,8	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CSX	R	75	7/8	1.00	0.06	3,4,5,5	1
2	CSX	Q	75	7/8	1.00	0.06	4,4,5,6	1

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(\AA^2)	Q<0.9
5	GOL	B	1269	6/6	0.75	0.15	20,22,27,28	1
5	GOL	R	1557	6/6	0.83	0.25	14,23,25,26	6
5	GOL	B	1270	6/6	0.84	0.16	20,22,27,33	6
5	GOL	A	1268	6/6	0.85	0.16	26,27,30,33	0
6	GLY	B	301	5/5	0.87	0.15	14,16,16,18	5
12	CL	Q	1554	1/1	0.92	0.07	32,32,32,32	1
8	H2S	B	1271	1/1	0.93	0.18	18,18,18,18	1
5	GOL	B	1272	6/6	0.94	0.15	17,20,25,37	0
5	GOL	A	1269	6/6	0.94	0.13	18,27,30,32	0
6	GLY	R	601	5/5	0.94	0.31	9,10,12,14	5
5	GOL	R	1556	6/6	0.95	0.10	11,14,15,17	6
6	GLY	Q	601	5/5	0.96	0.29	12,12,14,16	5
7	SOT	B	1268[A]	9/10	0.96	0.11	11,12,14,16	9
5	GOL	R	1554	6/6	0.96	0.10	14,15,17,20	1
7	SOT	B	1268[B]	9/10	0.96	0.11	15,17,22,22	9
5	GOL	R	1555[A]	6/6	0.98	0.09	11,18,22,24	1
5	GOL	R	1555[B]	6/6	0.98	0.09	11,18,22,24	1
5	GOL	R	1553	6/6	0.99	0.06	6,6,7,8	0
5	GOL	Q	1553	6/6	0.99	0.04	6,7,8,8	0
10	NI	R	1551[B]	1/1	1.00	0.02	8,8,8,8	1
10	NI	R	1551[A]	1/1	1.00	0.02	7,7,7,7	1
3	SF4	A	1267	8/8	1.00	0.04	4,4,4,4	0
10	NI	Q	1551[B]	1/1	1.00	0.02	7,7,7,7	1
9	FCO	R	1550	7/7	1.00	0.04	5,5,5,6	0
4	F3S	B	1266	7/7	1.00	0.03	4,4,5,5	0
4	F3S	A	1266	7/7	1.00	0.03	4,4,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NI	Q	1551[A]	1/1	1.00	0.02	8,8,8,8	1
3	SF4	A	1265	8/8	1.00	0.03	5,5,5,6	0
9	FCO	Q	1550	7/7	1.00	0.05	5,5,6,7	0
3	SF4	B	1265	8/8	1.00	0.03	5,5,5,5	0
11	MG	Q	1552	1/1	1.00	0.03	4,4,4,4	0
11	MG	R	1552	1/1	1.00	0.05	4,4,4,4	0
3	SF4	B	1267	8/8	1.00	0.04	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.