



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2014 – 08:36 PM EDT

PDB ID : 4UQP
Title : High-resolution structure of the D. fructosovorans NiFe-hydrogenase L122A mutant after exposure to air
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 : 1.42 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

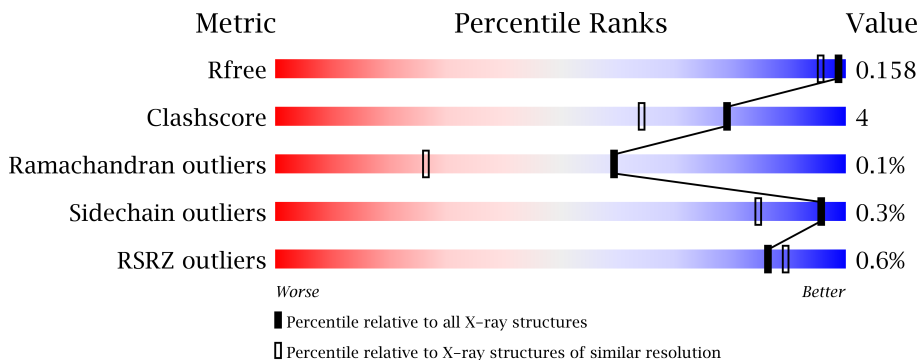
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 1.42 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}	66092	1110 (1.44-1.40)
Clashscore	79885	1263 (1.44-1.40)
Ramachandran outliers	78287	1226 (1.44-1.40)
Sidechain outliers	78261	1225 (1.44-1.40)
RSRZ outliers	66119	1110 (1.44-1.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
2	Q	563	
2	R	563	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	GLY	Q	1555	-	X
11	GLY	R	1558	-	X
5	GOL	A	1268	-	X
5	GOL	Q	1551	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	R	1551	-	X
5	GOL	R	1552[A]	-	X
5	GOL	R	1552[B]	-	X
5	GOL	R	1553	-	X
5	GOL	R	1554	-	X
6	SOT	B	1268[A]	-	X
6	SOT	B	1268[B]	-	X
7	H2S	B	1269	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14563 atoms, of which 0 are hydrogen and 0 are deuterium.

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	11	0
			2026	1291	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 PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT.

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	33	0
			4320	2760	742	793	25			

There are 32 discrepancies between the modelled and reference sequences:

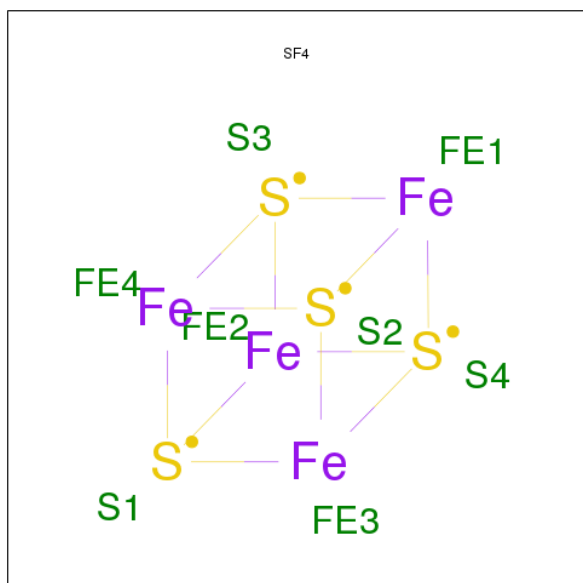
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	EXPRESSION TAG	UNP P18188
Q	-12	SER	-	EXPRESSION TAG	UNP P18188
Q	-11	TRP	-	EXPRESSION TAG	UNP P18188
Q	-10	SER	-	EXPRESSION TAG	UNP P18188
Q	-9	HIS	-	EXPRESSION TAG	UNP P18188
Q	-8	PRO	-	EXPRESSION TAG	UNP P18188
Q	-7	GLN	-	EXPRESSION TAG	UNP P18188
Q	-6	PHE	-	EXPRESSION TAG	UNP P18188
Q	-5	GLU	-	EXPRESSION TAG	UNP P18188
Q	-4	LYS	-	EXPRESSION TAG	UNP P18188
Q	-3	GLY	-	EXPRESSION TAG	UNP P18188
Q	-2	ALA	-	EXPRESSION TAG	UNP P18188
Q	-1	SER	-	EXPRESSION TAG	UNP P18188
Q	0	GLY	-	EXPRESSION TAG	UNP P18188
Q	1	ALA	-	EXPRESSION TAG	UNP P18188
Q	122	ALA	LEU	ENGINEERED MUTATION	UNP P18188

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-13	ALA	-	EXPRESSION TAG	UNP P18188
R	-12	SER	-	EXPRESSION TAG	UNP P18188
R	-11	TRP	-	EXPRESSION TAG	UNP P18188
R	-10	SER	-	EXPRESSION TAG	UNP P18188
R	-9	HIS	-	EXPRESSION TAG	UNP P18188
R	-8	PRO	-	EXPRESSION TAG	UNP P18188
R	-7	GLN	-	EXPRESSION TAG	UNP P18188
R	-6	PHE	-	EXPRESSION TAG	UNP P18188
R	-5	GLU	-	EXPRESSION TAG	UNP P18188
R	-4	LYS	-	EXPRESSION TAG	UNP P18188
R	-3	GLY	-	EXPRESSION TAG	UNP P18188
R	-2	ALA	-	EXPRESSION TAG	UNP P18188
R	-1	SER	-	EXPRESSION TAG	UNP P18188
R	0	GLY	-	EXPRESSION TAG	UNP P18188
R	1	ALA	-	EXPRESSION TAG	UNP P18188
R	122	ALA	LEU	ENGINEERED MUTATION	UNP P18188

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



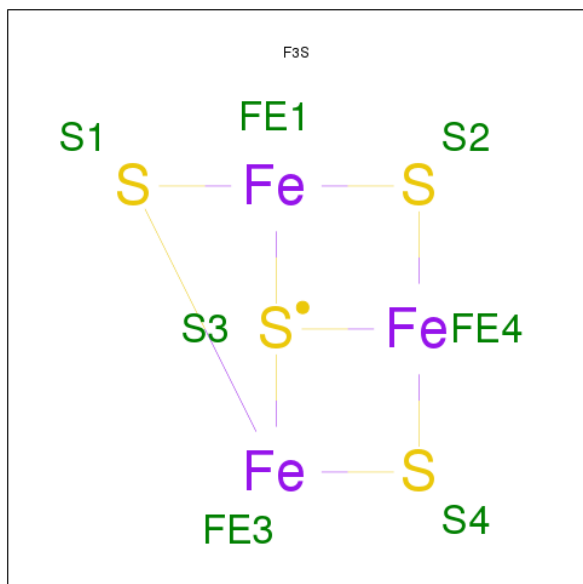
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

Continued on next page...

Continued from previous page...

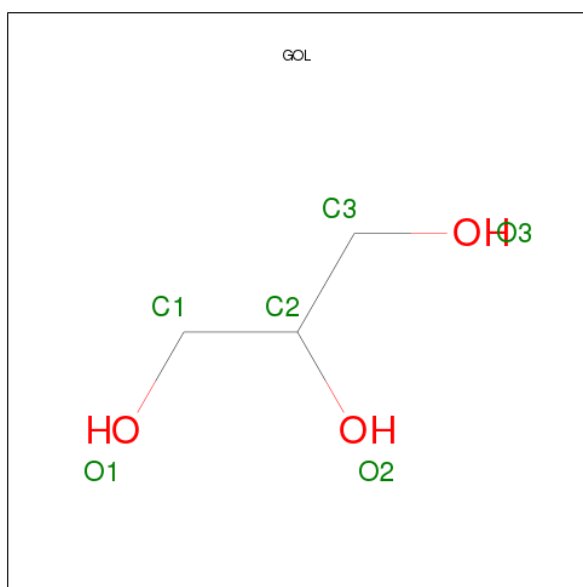
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Fe	S	0	0
			8	4	4		

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



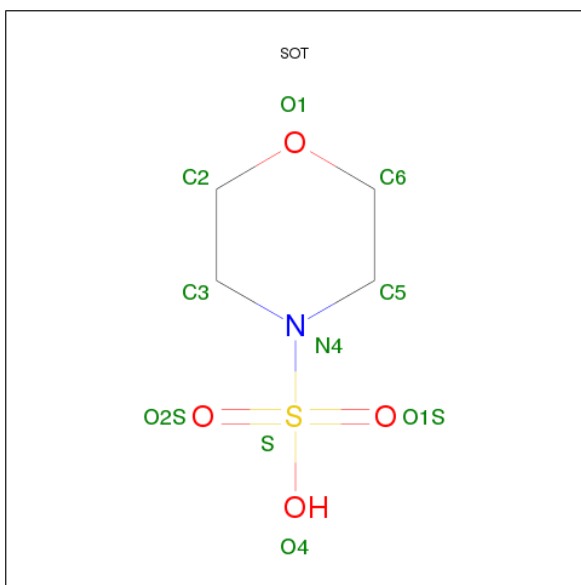
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

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



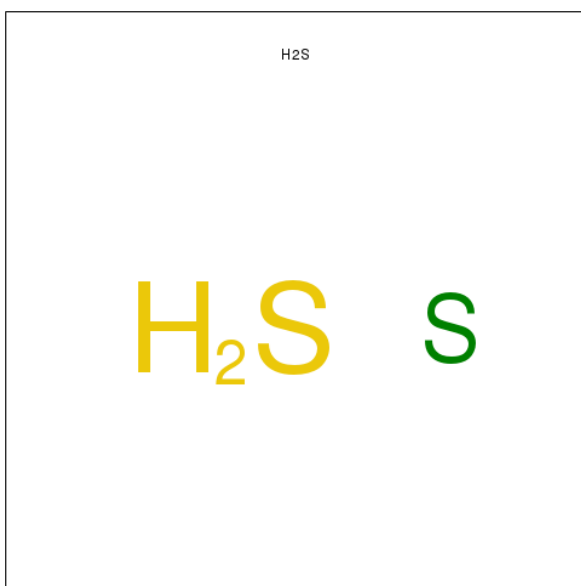
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	1
			7	3	4		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MORPHOLINE-4-SULFONICACID (three-letter code: SOT) (formula: $C_4H_9NO_4S$).



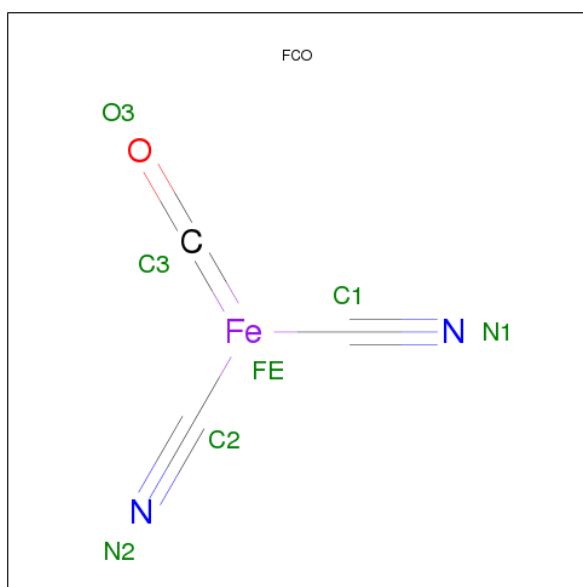
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	1
			18	8	2	6	2		

- Molecule 7 is HYDROSULFURIC ACID (three-letter code: H₂S) (formula: H₂S).



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

- Molecule 8 is CARBONMONOXIDE-(DICYANO)IRON (three-letter code: FCO) (formula: C₃FeN₂O).



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

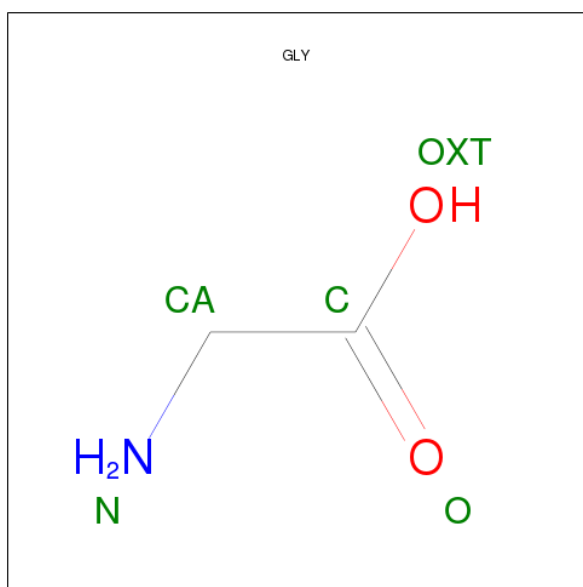
- Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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

- Molecule 12 is water.

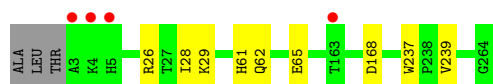
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	272	Total	O	0	5
			277	277		
12	B	310	Total	O	0	4
			314	314		
12	Q	531	Total	O	0	5
			536	536		
12	R	575	Total	O	0	10
			585	585		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



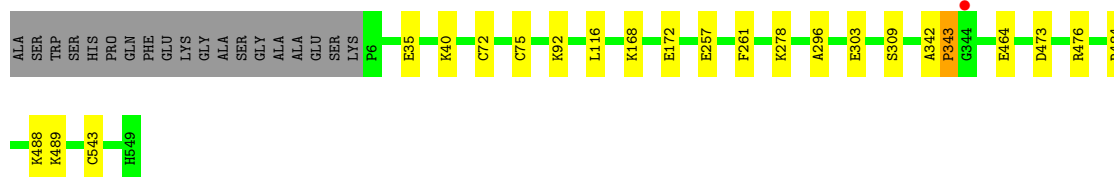
- Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain B: 



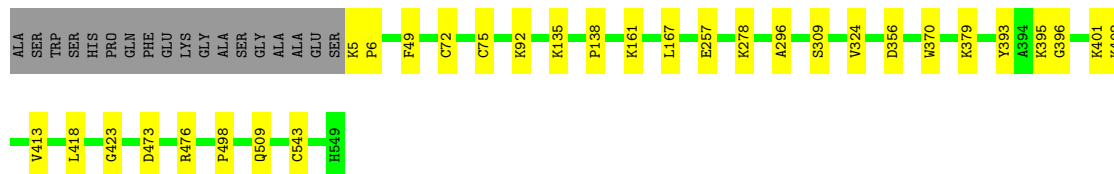
- Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT

Chain Q: 



- Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.70Å 100.90Å 116.70Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	30.00 – 1.42 44.09 – 1.42	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.42) 97.5 (44.09-1.42)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.120 , 0.156 0.122 , 0.158	Depositor DCC
R_{free} test set	13409 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	8.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 264128 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14563	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NI, SOT, SF4, H2S, F3S, CSX, CSS, 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	0/2129	0.66	1/2893 (0.0%)
1	B	0.49	0/2181	0.67	2/2958 (0.1%)
2	Q	0.51	0/4495	0.71	0/6081
2	R	0.52	0/4540	0.73	0/6146
All	All	0.51	0/13345	0.70	3/18078 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	26	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	26	ARG	NE-CZ-NH2	-5.25	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2026	0	1960	5	1
1	B	2061	0	1998	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	4300	0	4316	20	0
2	R	4320	0	4313	36	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	6	0	8	0	0
5	Q	12	0	16	0	0
5	R	31	0	38	2	0
6	B	18	0	16	0	0
7	B	1	0	0	2	0
8	Q	7	0	0	0	0
8	R	7	0	0	1	0
9	Q	2	0	0	0	0
9	R	2	0	0	0	0
10	Q	1	0	0	0	0
10	R	1	0	0	0	0
11	Q	5	0	2	2	0
11	R	5	0	2	3	0
12	A	277	0	0	3	0
12	B	314	0	0	17	0
12	Q	536	0	0	14	1
12	R	585	0	0	22	0
All	All	14563	0	12669	90	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:5:HIS:HE1	7:B:1269:H2S:S	1.19	1.62
11:Q:1555:GLY:N	12:Q:2706:HOH:O	1.58	1.26
2:Q:489[B]:LYS:HE2	12:Q:3141:HOH:O	1.14	1.24
1:B:194[A]:GLU:HG2	12:B:2573:HOH:O	1.43	1.17
2:R:278[B]:LYS:HE3	12:R:3162:HOH:O	1.47	1.15
2:R:92[A]:LYS:HE2	12:R:3254:HOH:O	0.99	1.14
11:R:1558:GLY:N	12:R:2708:HOH:O	1.80	1.13
2:Q:92[B]:LYS:HE2	12:Q:2973:HOH:O	1.48	1.12
2:Q:172[A]:GLU:HG2	12:Q:3209:HOH:O	1.49	1.11
1:B:209[A]:LYS:NZ	12:B:2613:HOH:O	1.87	1.07
11:R:1558:GLY:N	12:R:2706:HOH:O	1.88	1.06
2:R:395[B]:LYS:NZ	5:R:1551:GOL:O1	1.89	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:40[A]:LYS:HE3	12:Q:3104:HOH:O	1.57	1.03
2:Q:257[A]:GLU:OE2	12:Q:3219:HOH:O	1.76	1.03
1:B:4[B]:LYS:HE3	12:B:2622:HOH:O	1.58	1.01
2:R:402[B]:LYS:HE3	12:R:3239:HOH:O	1.58	1.01
2:R:92[A]:LYS:CE	12:R:3254:HOH:O	1.66	1.01
2:R:278[B]:LYS:HG2	12:R:3141:HOH:O	1.69	0.92
1:B:61[A]:HIS:HE1	12:B:2588:HOH:O	1.55	0.89
2:R:356[B]:ASP:OD2	12:R:3201:HOH:O	1.93	0.87
1:B:194[A]:GLU:OE1	12:B:2681:HOH:O	1.93	0.87
2:Q:303[B]:GLU:OE2	12:Q:3224:HOH:O	1.92	0.87
1:B:100:LYS:NZ	12:B:2596:HOH:O	2.08	0.85
1:B:61[A]:HIS:CE1	12:B:2576:HOH:O	2.30	0.83
1:B:4[B]:LYS:CE	12:B:2622:HOH:O	2.18	0.81
1:B:4[B]:LYS:NZ	12:B:2622:HOH:O	2.14	0.80
2:R:402[B]:LYS:CE	12:R:3239:HOH:O	2.20	0.79
2:R:92[A]:LYS:NZ	12:R:3254:HOH:O	2.00	0.76
1:B:61[A]:HIS:ND1	12:B:2576:HOH:O	2.19	0.75
2:R:257[B]:GLU:OE2	12:R:3240:HOH:O	2.09	0.70
2:R:393:TYR:O	2:R:401[A]:LYS:HE2	1.93	0.69
2:Q:303[B]:GLU:OE1	12:Q:3205:HOH:O	0.70	0.69
2:R:396:GLY:HA2	2:R:401[A]:LYS:HE3	1.77	0.67
2:R:72:CYS:HB3	2:R:75:CSX:OD	1.97	0.65
2:Q:489[B]:LYS:CE	12:Q:3141:HOH:O	1.95	0.64
1:A:65[B]:GLU:OE2	12:A:2595:HOH:O	2.15	0.63
2:R:402[B]:LYS:NZ	12:R:3239:HOH:O	2.27	0.63
2:R:324:VAL:HG11	2:R:395[B]:LYS:HE2	1.80	0.63
5:R:1552[A]:GOL:O1	12:R:3260:HOH:O	2.15	0.63
2:R:135[A]:LYS:HD3	12:R:3253:HOH:O	1.98	0.62
1:B:106[A]:LYS:HE3	12:B:2631:HOH:O	1.99	0.62
2:Q:72:CYS:HB3	2:Q:75:CSX:OD	1.99	0.61
2:Q:92[B]:LYS:CE	12:Q:2973:HOH:O	2.25	0.60
1:B:61[A]:HIS:CE1	12:B:2588:HOH:O	2.40	0.59
2:Q:172[B]:GLU:HB3	12:Q:3149:HOH:O	2.02	0.59
1:B:62[A]:GLN:HG3	12:B:2570:HOH:O	2.03	0.58
2:R:138:PRO:HG3	2:R:161[A]:LYS:HG2	1.85	0.58
2:R:257[B]:GLU:CG	12:R:3240:HOH:O	2.52	0.57
11:R:1558:GLY:CA	12:R:2706:HOH:O	2.48	0.55
2:R:509[A]:GLN:HG3	12:R:2839:HOH:O	2.06	0.55
1:B:194[A]:GLU:CG	12:B:2573:HOH:O	2.23	0.54
1:A:61[A]:HIS:HE1	12:A:2555:HOH:O	1.91	0.52
1:A:62[A]:GLN:OE1	12:A:2507:HOH:O	0.53	0.52
2:Q:464[B]:GLU:OE2	2:Q:488:LYS:HE3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194[A]:GLU:OE2	12:B:2693:HOH:O	2.19	0.52
2:R:278[A]:LYS:HE3	2:R:413:VAL:HG12	1.90	0.52
2:R:257[B]:GLU:CD	12:R:3240:HOH:O	2.45	0.51
7:B:1269:H2S:S	12:B:2491:HOH:O	2.60	0.51
2:R:379[A]:LYS:HD2	12:R:3257:HOH:O	2.11	0.51
11:Q:1555:GLY:CA	12:Q:2706:HOH:O	2.34	0.50
1:B:4[B]:LYS:HD2	12:B:2644:HOH:O	2.12	0.50
2:R:401[A]:LYS:HE3	12:R:3181:HOH:O	2.11	0.50
2:R:5:LYS:N	2:R:6:PRO:CD	2.75	0.49
2:R:278[A]:LYS:HE3	2:R:413:VAL:CG1	2.43	0.48
1:A:28:ILE:HG13	1:A:29[B]:LYS:HG3	1.96	0.48
2:Q:342[A]:ALA:HB1	2:Q:343[A]:PRO:HD2	1.96	0.48
2:Q:484[A]:ARG:HD2	12:Q:3166:HOH:O	2.15	0.47
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.50	0.47
2:Q:168:LYS:O	2:Q:172[A]:GLU:HG3	2.16	0.46
2:R:393:TYR:O	2:R:401[A]:LYS:CE	2.62	0.46
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.51	0.45
1:B:106[B]:LYS:HB3	1:B:106[B]:LYS:HE3	1.82	0.45
2:Q:116[B]:LEU:HD11	2:Q:261:PHE:CE2	2.52	0.45
1:B:258:THR:HA	1:B:259:PRO:C	2.38	0.44
2:Q:296:ALA:HA	2:Q:309:SER:HA	1.99	0.44
2:R:257[B]:GLU:HG3	12:R:3240:HOH:O	2.16	0.44
1:B:4[B]:LYS:HB3	1:B:4[B]:LYS:HE3	1.77	0.43
2:R:296:ALA:HA	2:R:309:SER:HA	1.99	0.43
2:R:138:PRO:HG3	2:R:161[A]:LYS:CG	2.48	0.43
2:R:401[A]:LYS:CE	12:R:3181:HOH:O	2.68	0.42
2:R:135[A]:LYS:HE2	2:R:135[A]:LYS:HB3	1.95	0.42
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.54	0.42
2:R:476:ARG:HD2	2:R:543[S]:CSS:SD	2.60	0.41
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.55	0.41
2:R:476:ARG:HD2	8:R:1555:FCO:C2	2.51	0.41
2:Q:476:ARG:HD2	2:Q:543[S]:CSS:SD	2.60	0.41
2:Q:35:GLU:HB2	2:Q:40[A]:LYS:HD3	2.02	0.40
2:R:418:LEU:HA	2:R:423:GLY:HA3	2.03	0.40
2:Q:278[B]:LYS:HE3	12:Q:3042:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168[B]:ASP:OD1	12:Q:3193:HOH:O[2_556]	1.65	0.55

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	272/265 (103%)	265 (97%)	7 (3%)	0	100	100
1	B	277/265 (104%)	270 (98%)	7 (2%)	0	100	100
2	Q	570/563 (101%)	552 (97%)	16 (3%)	2 (0%)	43	16
2	R	574/563 (102%)	564 (98%)	10 (2%)	0	100	100
All	All	1693/1656 (102%)	1651 (98%)	40 (2%)	2 (0%)	59	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Q	343[A]	PRO
2	Q	343[B]	PRO

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	220/210 (105%)	220 (100%)	0	100	100
1	B	225/210 (107%)	223 (99%)	2 (1%)	87	66
2	Q	459/445 (103%)	458 (100%)	1 (0%)	96	85
2	R	465/445 (104%)	463 (100%)	2 (0%)	95	83
All	All	1369/1310 (104%)	1364 (100%)	5 (0%)	96	83

All (5) 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
2	R	498	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	5	HIS
1	B	14	ASN
1	B	172	ASN
2	Q	250	ASN
2	Q	509	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	Q	543[A]	9	5,5,7	8.18	2 (40%)	2,5,8	3.94	1 (50%)
2	CSS	Q	543[S]	9	5,6,7	8.10	1 (20%)	4,6,8	2.81	1 (25%)
2	CSX	Q	75	9,8,2	4,6,7	10.07	1 (25%)	3,6,8	4.30	2 (66%)
2	CSS	R	543[A]	9	5,5,7	8.11	1 (20%)	2,5,8	4.57	1 (50%)
2	CSS	R	543[S]	9	5,6,7	8.06	1 (20%)	4,6,8	3.33	1 (25%)
2	CSX	R	75	9,8,2	4,6,7	8.81	1 (25%)	3,6,8	3.19	2 (66%)

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	Q	543[A]	9	-	0/2/4/7	0/0/0/0
2	CSS	Q	543[S]	9	-	0/2/5/7	0/0/0/0
2	CSX	Q	75	9,8,2	-	0/2/5/7	0/0/0/0
2	CSS	R	543[A]	9	-	0/2/4/7	0/0/0/0
2	CSS	R	543[S]	9	-	0/2/5/7	0/0/0/0
2	CSX	R	75	9,8,2	-	0/2/5/7	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	75	CSX	O-C	20.07	1.25	1.11
2	Q	543[S]	CSS	O-C	17.97	1.23	1.11
2	Q	543[A]	CSS	O-C	17.97	1.23	1.11
2	R	543[S]	CSS	O-C	17.95	1.23	1.11
2	R	543[A]	CSS	O-C	17.95	1.23	1.11
2	R	75	CSX	O-C	17.55	1.23	1.11
2	Q	543[A]	CSS	CB-SG	-2.32	1.76	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	75	CSX	C-CA-N	-6.74	107.09	113.83
2	R	543[S]	CSS	C-CA-N	-6.43	107.41	113.83
2	R	543[A]	CSS	C-CA-N	-6.43	107.41	113.83
2	Q	543[S]	CSS	C-CA-N	-5.37	108.46	113.83
2	Q	543[A]	CSS	C-CA-N	-5.37	108.46	113.83
2	R	75	CSX	C-CA-N	-4.40	109.43	113.83
2	R	75	CSX	CA-CB-SG	2.77	114.63	110.82
2	Q	75	CSX	CA-CB-SG	2.61	114.42	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 1 is modelled with single atom and 6 are monoatomic - leaving 21 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	A	1265	1	12,12,12	6.59	11 (91%)	0,24,24	0.00	-
4	F3S	A	1266	1	3,9,9	5.86	3 (100%)	0,15,15	0.00	-
3	SF4	A	1267	1	12,12,12	6.93	8 (66%)	0,24,24	0.00	-
5	GOL	A	1268	-	5,5,5	0.25	0	5,5,5	0.57	0
3	SF4	B	1265	1	12,12,12	6.00	8 (66%)	0,24,24	0.00	-
4	F3S	B	1266	1	3,9,9	6.78	3 (100%)	0,15,15	0.00	-
3	SF4	B	1267	1	12,12,12	6.00	9 (75%)	0,24,24	0.00	-
6	SOT	B	1268[A]	1	9,9,10	0.79	0	9,11,14	3.70	6 (66%)
6	SOT	B	1268[B]	-	9,9,10	1.43	2 (22%)	9,11,14	2.20	4 (44%)
5	GOL	Q	1550	-	5,5,5	0.36	0	5,5,5	0.41	0
5	GOL	Q	1551	-	5,5,5	0.32	0	5,5,5	0.28	0
8	FCO	Q	1552	12,2	2,6,6	0.26	0	0,6,6	0.00	-
11	GLY	Q	1555	-	4,4,4	1.02	0	4,4,4	0.80	0
5	GOL	R	1550	-	5,5,5	0.47	0	5,5,5	0.17	0
5	GOL	R	1551	-	5,5,5	0.41	0	5,5,5	0.51	0
5	GOL	R	1552[A]	-	5,5,5	0.38	0	5,5,5	0.44	0
5	GOL	R	1552[B]	-	5,5,5	0.39	0	5,5,5	0.46	0
5	GOL	R	1553	-	5,5,5	0.28	0	5,5,5	0.43	0
5	GOL	R	1554	-	5,5,5	0.20	0	5,5,5	0.90	0
8	FCO	R	1555	12,2	2,6,6	0.48	0	0,6,6	0.00	-
11	GLY	R	1558	-	4,4,4	1.05	0	4,4,4	0.73	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
3	SF4	A	1265	1	-	0/0/48/48	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F3S	A	1266	1	-	0/0/24/24	0/0/3/3
3	SF4	A	1267	1	-	0/0/48/48	0/6/5/5
5	GOL	A	1268	-	-	0/4/4/4	0/0/0/0
3	SF4	B	1265	1	-	0/0/48/48	0/6/5/5
4	F3S	B	1266	1	-	0/0/24/24	0/0/3/3
3	SF4	B	1267	1	-	0/0/48/48	0/6/5/5
6	SOT	B	1268[A]	1	-	0/4/12/14	0/1/1/1
6	SOT	B	1268[B]	-	-	0/4/12/14	0/1/1/1
5	GOL	Q	1550	-	-	0/4/4/4	0/0/0/0
5	GOL	Q	1551	-	-	0/4/4/4	0/0/0/0
8	FCO	Q	1552	12,2	-	0/0/6/6	0/0/0/0
11	GLY	Q	1555	-	-	0/2/2/2	0/0/0/0
5	GOL	R	1550	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1551	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1552[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1552[B]	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1553	-	-	0/4/4/4	0/0/0/0
5	GOL	R	1554	-	-	0/4/4/4	0/0/0/0
8	FCO	R	1555	12,2	-	0/0/6/6	0/0/0/0
11	GLY	R	1558	-	-	0/2/2/2	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1267	SF4	S3-FE4	-15.29	2.23	2.33
3	A	1267	SF4	S4-FE3	-12.70	2.24	2.33
3	B	1267	SF4	S4-FE2	-12.53	2.24	2.33
3	A	1265	SF4	S4-FE1	-11.60	2.25	2.33
3	A	1265	SF4	S1-FE4	-11.16	2.25	2.33
3	B	1265	SF4	S2-FE3	-9.82	2.26	2.33
3	B	1267	SF4	S3-FE1	-9.34	2.27	2.33
3	B	1265	SF4	S4-FE1	-9.26	2.27	2.33
3	B	1267	SF4	S2-FE4	-8.78	2.27	2.33
3	A	1265	SF4	S3-FE2	-8.73	2.27	2.33
3	A	1267	SF4	S2-FE1	-8.09	2.27	2.33
4	A	1266	F3S	S3-FE3	-8.06	2.27	2.33
4	B	1266	F3S	S3-FE3	-7.98	2.27	2.33
3	B	1265	SF4	S1-FE4	-7.86	2.28	2.33
3	B	1265	SF4	S1-FE3	-7.71	2.28	2.33
3	A	1267	SF4	S1-FE2	-6.98	2.28	2.33
3	A	1265	SF4	S2-FE3	-6.88	2.28	2.33
3	A	1265	SF4	S4-FE2	-6.71	2.28	2.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1267	SF4	S3-FE2	-6.58	2.28	2.33
3	B	1265	SF4	S3-FE2	-6.56	2.28	2.33
4	B	1266	F3S	S3-FE1	-6.26	2.29	2.33
4	B	1266	F3S	S3-FE4	-5.92	2.29	2.33
3	B	1267	SF4	S4-FE3	-5.83	2.29	2.33
3	A	1265	SF4	S3-FE1	-5.73	2.29	2.33
3	B	1267	SF4	S2-FE1	-5.65	2.29	2.33
3	B	1265	SF4	S2-FE4	-5.47	2.29	2.33
3	B	1265	SF4	S4-FE2	-5.25	2.29	2.33
3	B	1267	SF4	S1-FE3	-4.92	2.29	2.33
3	A	1265	SF4	S1-FE3	-4.61	2.30	2.33
4	A	1266	F3S	S3-FE1	-4.59	2.30	2.33
3	B	1265	SF4	S3-FE1	-4.53	2.30	2.33
4	A	1266	F3S	S3-FE4	-4.10	2.30	2.33
3	A	1265	SF4	S2-FE4	-3.77	2.30	2.33
3	A	1265	SF4	S4-FE3	-3.58	2.30	2.33
6	B	1268[B]	SOT	S-N4	-2.98	1.61	1.68
3	A	1267	SF4	S1-FE4	2.77	2.35	2.33
3	A	1265	SF4	S1-FE2	-2.70	2.31	2.33
3	A	1267	SF4	S4-FE1	-2.66	2.31	2.33
3	B	1267	SF4	S4-FE1	2.55	2.35	2.33
3	B	1267	SF4	S2-FE3	-2.51	2.31	2.33
3	A	1265	SF4	S3-FE4	-2.40	2.31	2.33
3	B	1267	SF4	S3-FE4	-2.26	2.31	2.33
6	B	1268[B]	SOT	O2S-S	-2.25	1.43	1.45
3	A	1267	SF4	S4-FE2	-2.16	2.31	2.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1268[A]	SOT	C2-C3-N4	6.84	116.70	108.44
6	B	1268[A]	SOT	C6-C5-N4	6.22	115.95	108.44
6	B	1268[B]	SOT	O2S-S-O1S	3.94	116.48	113.03
6	B	1268[A]	SOT	C6-O1-C2	3.67	122.37	109.90
6	B	1268[B]	SOT	C6-C5-N4	2.89	111.93	108.44
6	B	1268[A]	SOT	O1-C6-C5	2.75	118.28	111.87
6	B	1268[A]	SOT	O1-C2-C3	2.56	117.85	111.87
6	B	1268[A]	SOT	O2S-S-O1S	2.55	115.27	113.03
6	B	1268[B]	SOT	C5-N4-S	-2.55	106.88	115.14
6	B	1268[B]	SOT	C2-C3-N4	2.46	111.41	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	262/265 (98%)	-0.54	4 (1%) 70 74	7, 11, 21, 47	4 (1%)
1	B	263/265 (99%)	-0.52	4 (1%) 70 74	6, 10, 20, 36	3 (1%)
2	Q	544/563 (96%)	-0.52	1 (0%) 93 94	6, 11, 21, 34	7 (1%)
2	R	545/563 (96%)	-0.56	0 100 100	6, 10, 18, 42	4 (0%)
All	All	1614/1656 (97%)	-0.54	9 (0%) 86 89	6, 10, 20, 47	18 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	6.3
1	A	4	LYS	3.3
1	A	163	THR	2.9
1	B	4[A]	LYS	2.7
1	A	5	HIS	2.5
1	B	3	ALA	2.4
2	Q	344[A]	GLY	2.2
1	B	264[A]	GLY	2.1
1	B	2	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CSS	Q	543[S]	7/8	0.08	0.21	7,8,10,12	3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSS	Q	543[A]	6/8	0.08	0.21	7,8,9,11	2
2	CSS	R	543[A]	6/8	0.08	0.19	6,6,8,11	2
2	CSS	R	543[S]	7/8	0.08	-0.06	6,6,9,10	3
2	CSX	Q	75	7/8	0.06	-1.42	7,8,8,9	1
2	CSX	R	75	7/8	0.06	-1.50	6,7,8,8	1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	R	1552[B]	6/6	0.11	33.00	13,22,26,27	1
5	GOL	A	1268	6/6	0.24	32.15	29,31,36,37	0
11	GLY	R	1558	5/5	0.38	15.68	11,11,14,17	5
5	GOL	Q	1551	6/6	0.23	14.06	19,26,34,44	0
11	GLY	Q	1555	5/5	0.27	11.72	13,15,18,22	5
5	GOL	R	1553	6/6	0.20	9.05	22,24,31,39	0
5	GOL	R	1551	6/6	0.21	8.00	20,21,23,27	1
5	GOL	R	1552[A]	6/6	0.11	7.77	13,22,26,29	1
5	GOL	R	1554	6/6	0.17	5.90	23,29,33,37	0
6	SOT	B	1268[A]	9/10	0.11	3.79	9,11,15,15	9
6	SOT	B	1268[B]	9/10	0.11	3.43	16,17,21,21	9
7	H2S	B	1269	1/1	0.16	2.35	20,20,20,20	1
5	GOL	R	1550	6/6	0.05	0.27	8,9,11,11	0
5	GOL	Q	1550	6/6	0.04	-0.67	9,9,9,11	0
10	MG	R	1557	1/1	0.05	-0.69	6,6,6,6	0
4	F3S	B	1266	7/7	0.03	-1.33	7,7,7,8	0
4	F3S	A	1266	7/7	0.03	-1.40	7,7,7,7	0
3	SF4	B	1267	8/8	0.04	-1.44	6,7,7,7	0
8	FCO	R	1555	7/7	0.05	-1.62	6,7,8,8	0
8	FCO	Q	1552	7/7	0.05	-1.62	8,8,9,9	0
3	SF4	A	1265	8/8	0.02	-1.72	7,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	NI	Q	1553[S]	1/1	0.03	-1.82	11,11,11,11	1
3	SF4	B	1265	8/8	0.03	-2.08	7,7,8,8	0
9	NI	Q	1553[A]	1/1	0.03	-2.11	11,11,11,11	1
10	MG	Q	1554	1/1	0.03	-2.16	6,6,6,6	0
3	SF4	A	1267	8/8	0.04	-2.21	7,7,7,7	0
9	NI	R	1556[A]	1/1	0.02	-3.26	10,10,10,10	1
9	NI	R	1556[S]	1/1	0.02	-3.78	10,10,10,10	1

6.5 Other polymers

There are no such residues in this entry.