



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:03 PM GMT

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 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

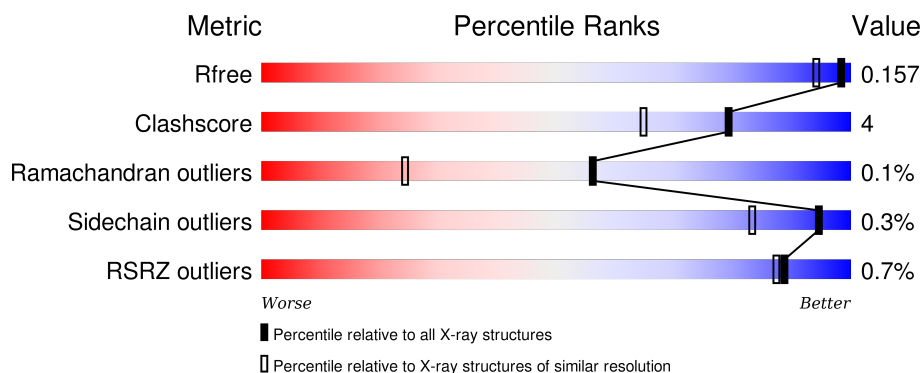
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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}	91344	1632 (1.44-1.40)
Clashscore	102246	1743 (1.44-1.40)
Ramachandran outliers	100387	1698 (1.44-1.40)
Sidechain outliers	100360	1697 (1.44-1.40)
RSRZ outliers	91569	1632 (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. 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>96%</div> <div>• •</div> </div>
1	B	265	<div> <div>2%</div> <div>94%</div> <div>5% •</div> </div>
2	Q	563	<div> <div>93%</div> <div>• •</div> </div>
2	R	563	<div> <div>91%</div> <div>6% •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GLY	Q	1555	-	-	-	X
11	GLY	R	1558	-	-	-	X
5	GOL	A	1268	-	-	-	X
5	GOL	R	1551	-	-	-	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 [i](#)

There are 12 unique types of molecules in this entry. The entry contains 14563 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	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:

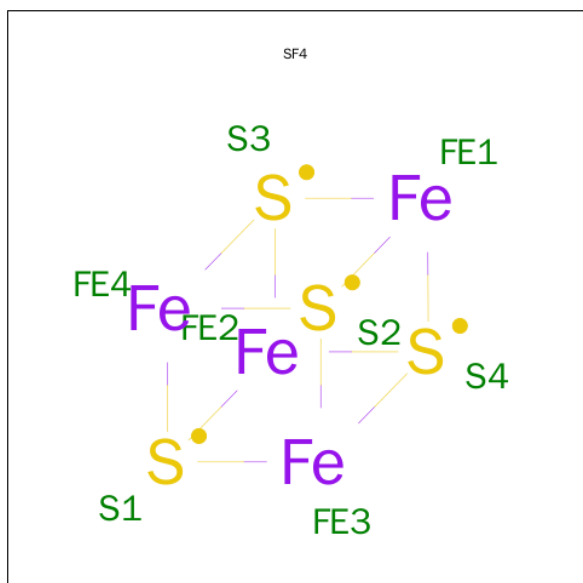
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	EXPRESSION TAG	UNP P18188
Q	-12	SER	-	EXPRESSION TAG	UNP P18188
Q	-11	TRP	-	EXPRESSION TAG	UNP P18188
Q	-10	SER	-	EXPRESSION TAG	UNP P18188
Q	-9	HIS	-	EXPRESSION TAG	UNP P18188
Q	-8	PRO	-	EXPRESSION TAG	UNP P18188
Q	-7	GLN	-	EXPRESSION TAG	UNP 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

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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).



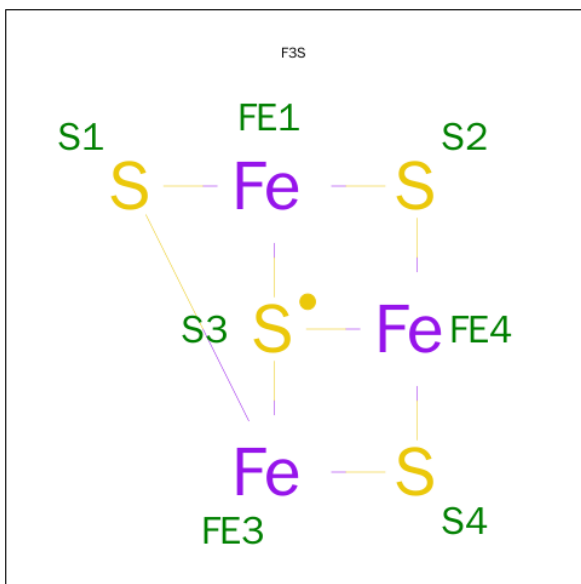
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

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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).



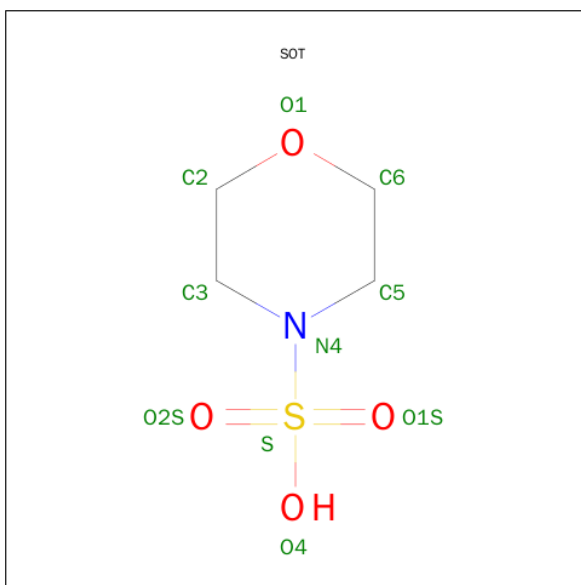
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	B	1	Total	Fe	S	0	0
			7	3	4		

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



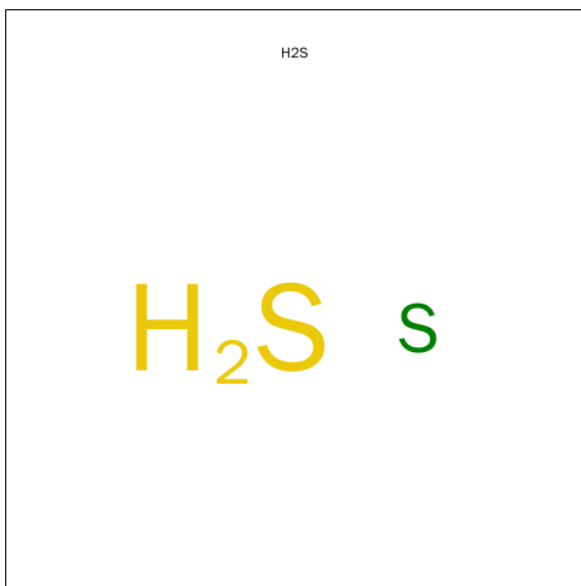
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	1
			7	3	4		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		

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



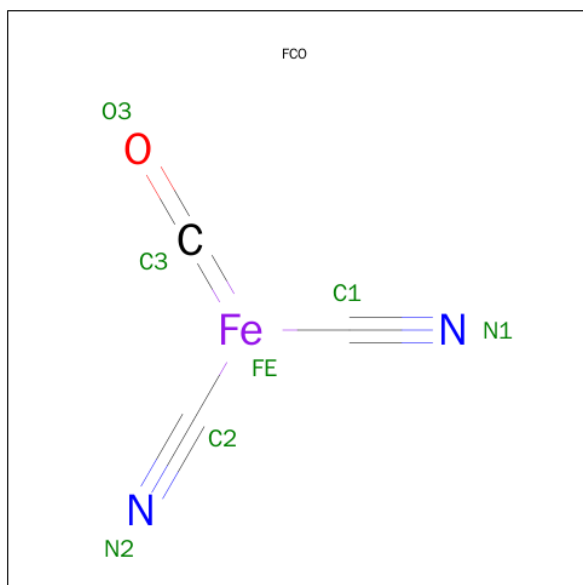
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	1
			18	8	2	6	2		

- 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		

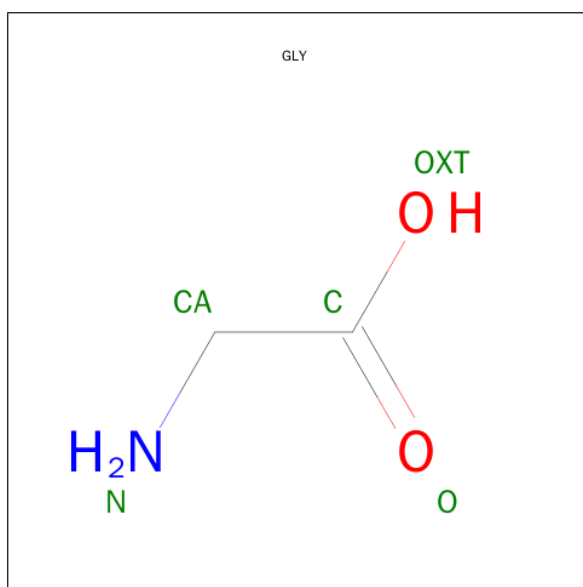
- Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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 [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 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.

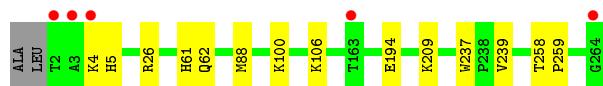
- Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain A: 



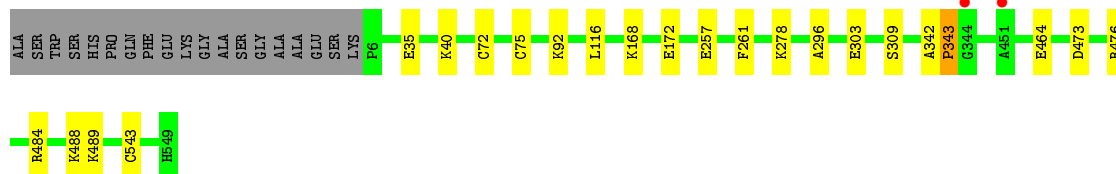
- Molecule 1: PERIPLASMIC [NIFE] HYDROGENASE SMALL SUBUNIT

Chain B: 



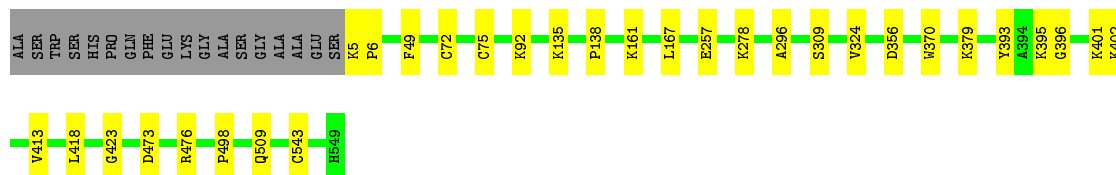
- Molecule 2: PERIPLASMIC [NIFE] HYDROGENASE LARGE SUBUNIT

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	64.70 Å 100.90 Å 116.70 Å 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 1.42 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.120 , 0.156 0.120 , 0.157	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)	0.36 , 56.2	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NI, 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 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	2026	0	1960	5	0
1	B	2061	0	1998	22	0
2	Q	4300	0	4316	20	0
2	R	4320	0	4313	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0
12	R	585	0	0	22	0
All	All	14563	0	12669	90	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 (90) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
2:R:402[B]:LYS:NZ	12:R:3239:HOH:O	2.27	0.63
1:A:65[B]:GLU:OE2	12:A:2595:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:464[B]:GLU:OE2	2:Q:488:LYS:HE3	2.08	0.52
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
2:Q:342[A]:ALA:HB1	2:Q:343[A]:PRO:HD2	1.96	0.48
1:A:28:ILE:HG13	1:A:29[B]:LYS:HG3	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:HE3	1:B:106[B]:LYS:HB3	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

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	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%)	39	14
2	R	574/563 (102%)	564 (98%)	10 (2%)	0	100	100
All	All	1693/1656 (102%)	1651 (98%)	40 (2%)	2 (0%)	56	24

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/210 (105%)	220 (100%)	0	100	100
1	B	225/210 (107%)	223 (99%)	2 (1%)	84	62
2	Q	459/445 (103%)	458 (100%)	1 (0%)	95	84
2	R	465/445 (104%)	463 (100%)	2 (0%)	93	81
All	All	1369/1310 (104%)	1364 (100%)	5 (0%)	94	81

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 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	Q	543[A]	9	4,5,7	1.63	1 (25%)	3,5,8	1.56	1 (33%)
2	CSS	Q	543[S]	9	4,6,7	0.97	0	3,6,8	1.08	0
2	CSX	Q	75	9,8,2	3,6,7	0.76	0	3,6,8	0.81	0
2	CSS	R	543[A]	9	4,5,7	1.18	0	3,5,8	1.55	1 (33%)
2	CSS	R	543[S]	9	4,6,7	0.72	0	3,6,8	1.18	0
2	CSX	R	75	9,8,2	3,6,7	0.53	0	3,6,8	0.84	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	Q	543[A]	9	-	0/1/4/7	0/0/0/0
2	CSS	Q	543[S]	9	-	0/1/5/7	0/0/0/0
2	CSX	Q	75	9,8,2	-	0/1/5/7	0/0/0/0
2	CSS	R	543[A]	9	-	0/1/4/7	0/0/0/0
2	CSS	R	543[S]	9	-	0/1/5/7	0/0/0/0
2	CSX	R	75	9,8,2	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	543[A]	CSS	CB-SG	-2.40	1.76	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	543[A]	CSS	CA-CB-SG	-2.12	109.63	114.48
2	Q	543[A]	CSS	CA-CB-SG	-2.07	109.74	114.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	A	1266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	A	1267	1	0,12,12	0.00	-	0,24,24	0.00	-
5	GOL	A	1268	-	5,5,5	0.26	0	5,5,5	0.55	0
3	SF4	B	1265	1	0,12,12	0.00	-	0,24,24	0.00	-
4	F3S	B	1266	1	0,9,9	0.00	-	0,15,15	0.00	-
3	SF4	B	1267	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SOT	B	1268[A]	1	6,9,10	0.51	0	5,11,14	7.86	5 (100%)
6	SOT	B	1268[B]	-	6,9,10	0.31	0	5,11,14	3.33	2 (40%)
5	GOL	Q	1550	-	5,5,5	0.38	0	5,5,5	0.40	0
5	GOL	Q	1551	-	5,5,5	0.33	0	5,5,5	0.23	0
8	FCO	Q	1552	12,2	0,6,6	0.00	-	0,6,6	0.00	-
11	GLY	Q	1555	-	1,4,4	0.84	0	0,4,4	0.00	-
5	GOL	R	1550	-	5,5,5	0.48	0	5,5,5	0.15	0
5	GOL	R	1551	-	5,5,5	0.43	0	5,5,5	0.51	0
5	GOL	R	1552[A]	-	5,5,5	0.40	0	5,5,5	0.41	0
5	GOL	R	1552[B]	-	5,5,5	0.41	0	5,5,5	0.43	0
5	GOL	R	1553	-	5,5,5	0.28	0	5,5,5	0.42	0
5	GOL	R	1554	-	5,5,5	0.19	0	5,5,5	0.81	0
8	FCO	R	1555	12,2	0,6,6	0.00	-	0,6,6	0.00	-
11	GLY	R	1558	-	1,4,4	0.86	0	0,4,4	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	1265	1	-	0/0/48/48	0/6/5/5
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SOT	B	1268[A]	1	-	0/0/12/14	0/1/1/1
6	SOT	B	1268[B]	-	-	0/0/12/14	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	-	-	0/0/2/2	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	-	-	0/0/2/2	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1268[A]	SOT	O1-C2-C3	2.62	117.85	111.84
6	B	1268[A]	SOT	O1-C6-C5	2.81	118.28	111.84
6	B	1268[A]	SOT	C6-O1-C2	3.71	122.37	109.89
6	B	1268[B]	SOT	C2-C3-N4	4.68	111.41	108.19
6	B	1268[B]	SOT	C6-C5-N4	5.44	111.93	108.19
6	B	1268[A]	SOT	C6-C5-N4	11.29	115.95	108.19
6	B	1268[A]	SOT	C2-C3-N4	12.38	116.70	108.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	1555	GLY	2	0
5	R	1551	GOL	1	0
5	R	1552[A]	GOL	1	0
8	R	1555	FCO	1	0
11	R	1558	GLY	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/265 (98%)	-0.47	5 (1%) 70 68	7, 11, 21, 47	4 (1%)
1	B	263/265 (99%)	-0.44	5 (1%) 70 68	6, 10, 20, 36	3 (1%)
2	Q	542/563 (96%)	-0.46	2 (0%) 93 92	6, 11, 21, 34	7 (1%)
2	R	543/563 (96%)	-0.47	0 100 100	6, 10, 18, 42	4 (0%)
All	All	1610/1656 (97%)	-0.46	12 (0%) 89 87	6, 10, 20, 47	18 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	7.6
1	A	4	LYS	3.6
1	A	163	THR	3.4
1	B	4[A]	LYS	3.1
2	Q	344[A]	GLY	2.7
1	A	164[A]	LYS	2.5
1	A	5	HIS	2.5
1	B	3	ALA	2.3
2	Q	451	ALA	2.3
1	B	264[A]	GLY	2.2
1	B	163	THR	2.0
1	B	2	THR	2.0

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CSS	Q	543[S]	7/8	0.99	0.08	-	7,8,10,12	3
2	CSX	Q	75	7/8	0.99	0.07	-	7,8,8,9	1
2	CSS	R	543[S]	7/8	0.98	0.09	-	6,6,9,10	3
2	CSS	Q	543[A]	6/8	0.99	0.08	-	7,8,9,11	2
2	CSX	R	75	7/8	0.99	0.07	-	6,7,8,8	1
2	CSS	R	543[A]	6/8	0.98	0.09	-	6,6,8,11	2

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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	1268	6/6	0.72	0.23	33.97	29,31,36,37	0
11	GLY	R	1558	5/5	0.96	0.37	13.56	11,11,14,17	5
11	GLY	Q	1555	5/5	0.95	0.29	11.42	13,15,18,22	5
5	GOL	R	1553	6/6	0.92	0.21	9.40	22,24,31,39	0
5	GOL	R	1551	6/6	0.90	0.23	9.23	20,21,23,27	1
5	GOL	R	1554	6/6	0.90	0.20	7.15	23,29,33,37	0
6	SOT	B	1268[A]	9/10	0.96	0.12	4.25	9,11,15,15	9
6	SOT	B	1268[B]	9/10	0.96	0.12	3.98	16,17,21,21	9
7	H2S	B	1269	1/1	0.97	0.16	1.52	20,20,20,20	1
5	GOL	R	1550	6/6	0.98	0.06	0.46	8,9,11,11	0
5	GOL	Q	1550	6/6	0.98	0.06	0.04	9,9,9,11	0
10	MG	R	1557	1/1	1.00	0.06	-0.24	6,6,6,6	0
4	F3S	B	1266	7/7	1.00	0.05	-0.78	7,7,7,8	0
4	F3S	A	1266	7/7	1.00	0.05	-0.88	7,7,7,7	0
3	SF4	B	1267	8/8	1.00	0.06	-1.17	6,7,7,7	0
8	FCO	R	1555	7/7	1.00	0.06	-1.31	6,7,8,8	0
3	SF4	A	1265	8/8	1.00	0.04	-1.35	7,8,8,8	0
10	MG	Q	1554	1/1	1.00	0.05	-1.37	6,6,6,6	0
3	SF4	A	1267	8/8	1.00	0.05	-1.54	7,7,7,7	0
8	FCO	Q	1552	7/7	1.00	0.06	-1.67	8,8,9,9	0
3	SF4	B	1265	8/8	1.00	0.04	-1.71	7,7,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	NI	R	1556[S]	1/1	1.00	0.03	-	10,10,10,10	1
9	NI	Q	1553[A]	1/1	1.00	0.04	-	11,11,11,11	1
5	GOL	R	1552[A]	6/6	0.96	0.11	-	13,22,26,29	1
9	NI	Q	1553[S]	1/1	1.00	0.04	-	11,11,11,11	1
5	GOL	Q	1551	6/6	0.94	0.22	-	19,26,34,44	0
9	NI	R	1556[A]	1/1	1.00	0.03	-	10,10,10,10	1
5	GOL	R	1552[B]	6/6	0.96	0.11	-	13,22,26,27	1

6.5 Other polymers [i](#)

There are no such residues in this entry.