Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 03:49 pm GMT

PDB ID	:	4UE6
Title	:	Structure of methylene blue-treated anaerobically purified D. fructosovorans NiFe-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on	:	2014-12-16
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

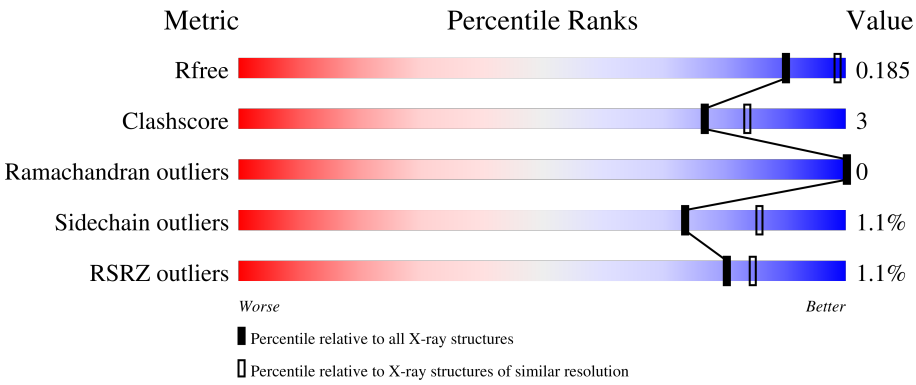
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	2%, 89%, 10%
1	B	264	4%, 92%, 7%
1	C	264	2%, 89%, 9%
2	Q	549	93%, 5%
2	R	549	92%, 7%

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Mol	Chain	Length	Quality of chain
2	S	549	% 93% 6%

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
5	GOL	R	1562	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19601 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.

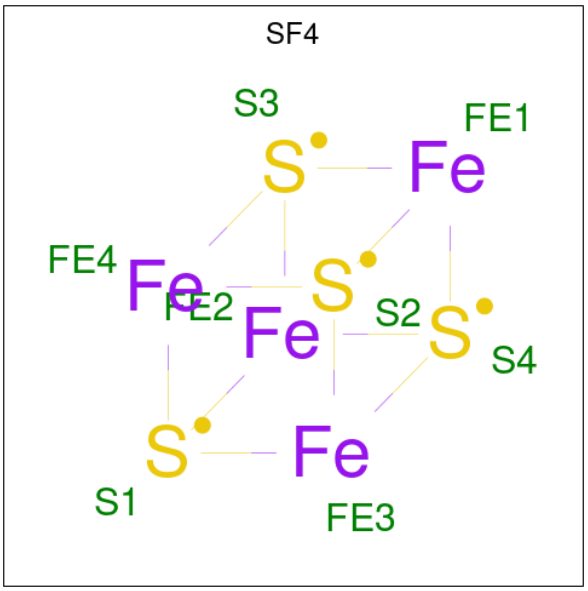
- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	1973	1256	330	372	15	0	0	0
1	B	262	1974	1257	330	372	15	0	0	0
1	C	260	1960	1248	327	370	15	0	0	0

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

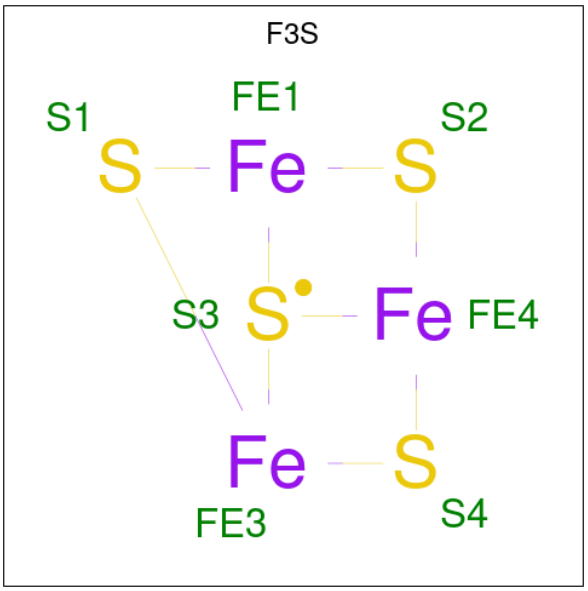
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Q	545	4167	2654	724	767	22	0	0	0
2	R	544	4166	2653	723	768	22	0	0	0
2	S	544	4163	2652	723	766	22	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



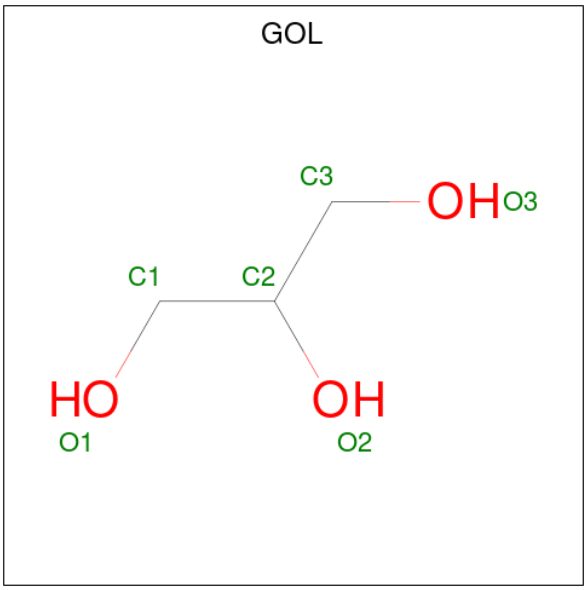
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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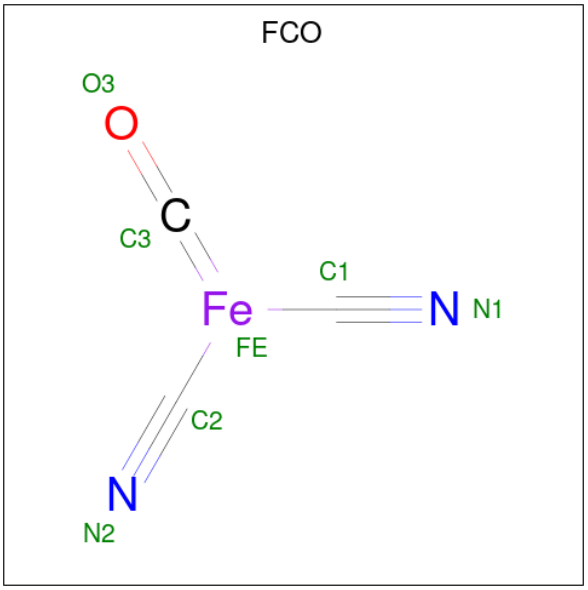
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	Q	1	6	3	3		0	0
			Total	C	O			
5	Q	1	6	3	3		0	0
			Total	C	O			
5	R	1	6	3	3		0	0
			Total	C	O			
5	R	1	6	3	3		0	0
			Total	C	O			
5	R	1	6	3	3		0	0
			Total	C	O			
5	R	1	6	3	3		0	0
			Total	C	O			
5	S	1	6	3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

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	185	Total O 185 185	0	0
9	B	111	Total O 111 111	0	0
9	C	154	Total O 154 154	0	0
9	Q	234	Total O 234 234	0	0
9	R	205	Total O 205 205	0	0
9	S	159	Total O 159 159	0	0

3 Residue-property plots (i)

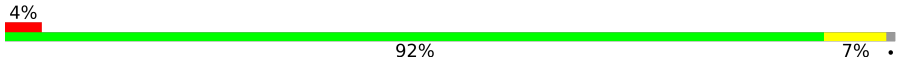
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

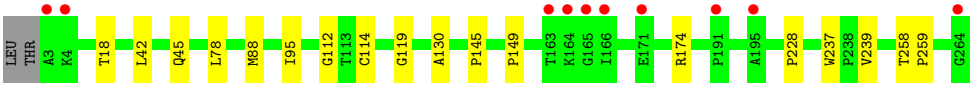
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain A:

• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

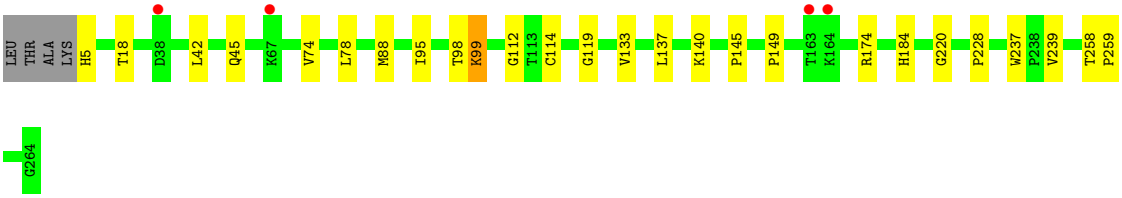
Chain B:





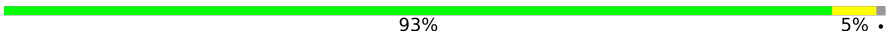
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

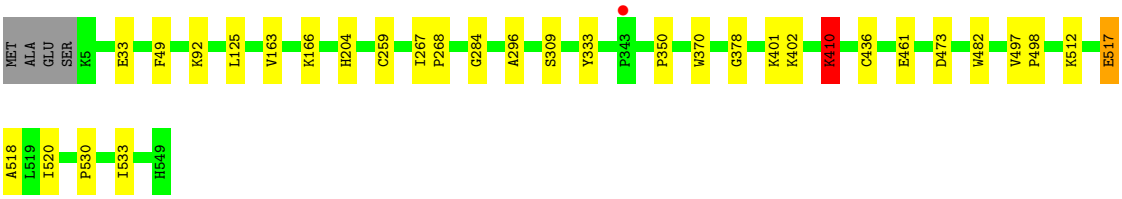
Chain C:



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

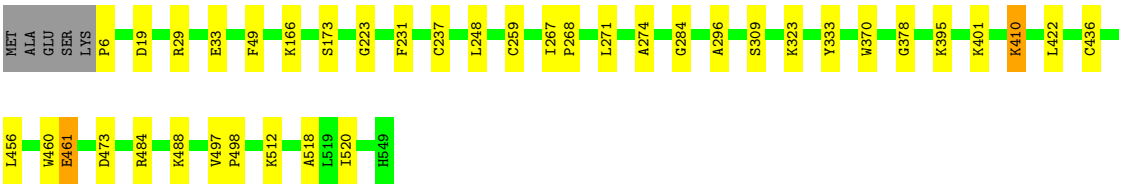
Chain Q:





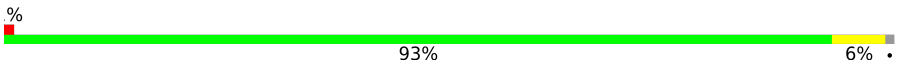
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

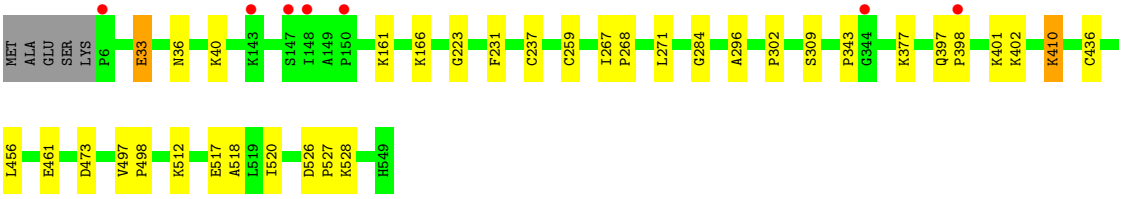
Chain R:



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain S:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.28Å 99.55Å 184.02Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	23.90 – 2.30 23.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (23.90-2.30) 95.0 (23.94-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.151 , 0.181 0.155 , 0.185	Depositor DCC
R_{free} test set	4971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19601	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FCO, F3S, NI, GOL, CSO, SF4, MG

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	0.51	0/2027	0.61	0/2759
1	B	0.48	0/2028	0.57	0/2761
1	C	0.49	0/2014	0.58	0/2743
2	Q	0.56	3/4264 (0.1%)	0.67	4/5787 (0.1%)
2	R	0.55	2/4263 (0.0%)	0.69	2/5785 (0.0%)
2	S	0.52	2/4260 (0.0%)	0.66	4/5781 (0.1%)
All	All	0.53	7/18856 (0.0%)	0.64	10/25616 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	461	GLU	CD-OE1	-11.99	1.12	1.25
2	S	461	GLU	CD-OE1	-11.42	1.13	1.25
2	Q	461	GLU	CD-OE1	-11.14	1.13	1.25
2	R	33	GLU	CD-OE1	-7.36	1.17	1.25
2	Q	33	GLU	CD-OE1	-6.32	1.18	1.25
2	S	33	GLU	CD-OE2	-5.55	1.19	1.25
2	Q	517	GLU	CB-CG	-5.49	1.41	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	461	GLU	OE1-CD-OE2	-18.54	101.06	123.30
2	S	33	GLU	CG-CD-OE1	11.31	140.92	118.30
2	R	461	GLU	CG-CD-OE2	9.80	137.90	118.30
2	S	33	GLU	CG-CD-OE2	-7.61	103.08	118.30
2	S	33	GLU	OE1-CD-OE2	-7.26	114.59	123.30
2	Q	461	GLU	CA-CB-CG	-6.23	99.70	113.40
2	Q	402	LYS	CD-CE-NZ	6.22	126.01	111.70
2	S	461	GLU	CA-CB-CG	-5.41	101.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	410	LYS	CD-CE-NZ	5.26	123.79	111.70
2	Q	517	GLU	CG-CD-OE2	-5.08	108.14	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1973	0	1911	14	0
1	B	1974	0	1915	11	0
1	C	1960	0	1897	15	0
2	Q	4167	0	4138	16	0
2	R	4166	0	4140	33	0
2	S	4163	0	4138	20	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
5	A	12	0	16	0	0
5	Q	12	0	16	0	0
5	R	24	0	32	6	0
5	S	6	0	8	0	0
6	Q	7	0	0	0	0
6	R	7	0	0	0	0
6	S	7	0	0	0	0
7	Q	1	0	0	0	0
7	R	1	0	0	0	0
7	S	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
8	S	1	0	0	0	0
9	A	185	0	0	2	0
9	B	111	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	154	0	0	1	0
9	Q	234	0	0	3	0
9	R	205	0	0	7	0
9	S	159	0	0	7	0
All	All	19601	0	18211	109	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:488:LYS:HE2	9:R:2194:HOH:O	1.48	1.10
2:R:484:ARG:HH11	5:R:1564:GOL:H32	1.31	0.91
2:Q:163:VAL:HG22	9:Q:2044:HOH:O	1.79	0.82
2:R:395:LYS:HZ3	5:R:1562:GOL:C2	1.96	0.79
1:A:61:HIS:HB2	9:A:2051:HOH:O	1.85	0.76
2:R:395:LYS:HZ3	5:R:1562:GOL:H2	1.49	0.76
2:R:323:LYS:HD3	9:R:2136:HOH:O	1.86	0.75
2:R:395:LYS:NZ	5:R:1562:GOL:H2	2.04	0.72
2:S:40:LYS:HE3	9:S:2011:HOH:O	1.91	0.70
2:S:343:PRO:HD3	9:S:2107:HOH:O	1.91	0.70
2:S:36:ASN:HB3	9:S:2010:HOH:O	1.94	0.67
2:R:484:ARG:NH1	5:R:1564:GOL:H32	2.09	0.66
1:C:99:LYS:HG2	1:C:137:LEU:HD22	1.79	0.65
2:R:259:CYS:HG	2:R:436:CYS:HG	1.40	0.64
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.82	0.62
2:S:271:LEU:HD13	2:S:410:LYS:HG2	1.84	0.60
2:Q:259:CYS:HG	2:Q:436:CYS:HG	1.53	0.56
2:Q:530:PRO:HB2	2:Q:533:ILE:HD12	1.88	0.56
2:R:395:LYS:NZ	5:R:1562:GOL:C2	2.64	0.56
2:R:271:LEU:HD13	2:R:410:LYS:HG3	1.88	0.54
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.89	0.53
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.43	0.52
2:Q:512:LYS:HE2	2:Q:520:ILE:HD11	1.92	0.52
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.46	0.50
2:S:259:CYS:HG	2:S:436:CYS:HG	1.51	0.50
1:A:145:PRO:HG3	1:A:174:ARG:HD3	1.93	0.50
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.94	0.49
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.47	0.49
2:S:302:PRO:HD2	9:S:2087:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:6:PRO:N	9:R:2002:HOH:O	2.48	0.47
1:B:145:PRO:HG3	1:B:174:ARG:HD3	1.96	0.47
2:S:284:GLY:HA2	2:S:518:ALA:O	2.13	0.47
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.45	0.47
2:R:267:ILE:HB	2:R:268:PRO:HD3	1.96	0.47
1:C:78:LEU:HD22	1:C:95:ILE:HA	1.97	0.47
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.96	0.47
1:C:145:PRO:HG3	1:C:174:ARG:HD3	1.97	0.47
2:R:6:PRO:N	9:R:2003:HOH:O	2.48	0.47
2:S:512:LYS:HE2	2:S:520:ILE:HD11	1.97	0.47
2:R:259:CYS:SG	2:R:436:CYS:SG	3.00	0.47
2:R:6:PRO:HD2	9:R:2002:HOH:O	2.13	0.46
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.51	0.46
2:Q:267:ILE:HB	2:Q:268:PRO:HD3	1.96	0.46
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.50	0.46
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.96	0.46
1:C:74:VAL:HG11	1:C:133:VAL:HG21	1.98	0.46
1:C:228:PRO:HB3	1:C:237:TRP:CZ2	2.49	0.45
2:Q:49:PHE:HB2	2:Q:370:TRP:CD2	2.51	0.45
2:Q:284:GLY:HA2	2:Q:518:ALA:O	2.17	0.45
2:R:19:ASP:HB2	2:R:29:ARG:HG3	1.98	0.45
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.47	0.45
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.99	0.45
2:Q:296:ALA:HA	2:Q:309:SER:HA	1.98	0.45
1:A:114:CYS:HA	1:A:119:GLY:HA3	1.99	0.45
2:R:296:ALA:HA	2:R:309:SER:HA	1.99	0.44
2:R:512:LYS:HE2	2:R:520:ILE:HD11	1.98	0.44
2:S:161:LYS:HB3	9:S:2057:HOH:O	2.16	0.44
2:S:296:ALA:HA	2:S:309:SER:HA	1.98	0.44
2:R:223:GLY:HA2	2:R:231:PHE:CD1	2.53	0.44
1:C:114:CYS:HA	1:C:119:GLY:HA3	2.00	0.43
2:Q:125:LEU:HG	9:Q:2074:HOH:O	2.17	0.43
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.48	0.43
1:C:42:LEU:HD21	1:C:45:GLN:HG3	2.00	0.43
2:R:333:TYR:OH	2:R:378:GLY:HA2	2.18	0.43
1:A:184:HIS:HB2	1:A:220:GLY:C	2.39	0.43
1:B:112:GLY:HA2	1:B:149:PRO:HD3	2.01	0.43
1:C:112:GLY:HA2	1:C:149:PRO:HD3	2.00	0.43
1:C:184:HIS:HB2	1:C:220:GLY:C	2.39	0.43
2:Q:350:PRO:HB2	2:Q:482:TRP:CG	2.54	0.43
1:C:18:THR:HG22	1:C:18:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:6:PRO:CD	9:R:2002:HOH:O	2.67	0.42
2:R:284:GLY:HA2	2:R:518:ALA:O	2.18	0.42
2:R:484:ARG:NH2	9:R:2161:HOH:O	2.50	0.42
2:R:460:TRP:O	2:R:461:GLU:HG2	2.19	0.42
1:A:78:LEU:HD22	1:A:95:ILE:HA	2.02	0.42
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.54	0.42
2:R:259:CYS:HA	2:R:436:CYS:HG	1.84	0.42
1:A:99:LYS:NZ	9:A:2083:HOH:O	2.53	0.42
2:S:377:LYS:HA	9:S:2098:HOH:O	2.19	0.42
1:C:140:LYS:HE3	9:C:2045:HOH:O	2.18	0.42
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.54	0.42
1:B:78:LEU:HD22	1:B:95:ILE:HA	2.01	0.42
2:R:237:CYS:HB2	2:R:456:LEU:HG	2.00	0.42
2:S:497:VAL:HG13	2:S:498:PRO:HD2	2.02	0.42
2:R:410:LYS:HD3	2:R:410:LYS:HA	1.76	0.42
2:S:237:CYS:HB2	2:S:456:LEU:HG	2.01	0.41
2:S:410:LYS:HA	2:S:410:LYS:HD2	1.77	0.41
1:A:112:GLY:HA2	1:A:149:PRO:HD3	2.01	0.41
2:Q:204:HIS:CE1	9:Q:2092:HOH:O	2.73	0.41
2:S:402:LYS:NZ	9:S:2129:HOH:O	2.53	0.41
1:A:18:THR:HG22	1:A:18:THR:O	2.19	0.41
1:B:78:LEU:O	1:B:130:ALA:HA	2.20	0.41
2:R:274:ALA:HA	2:R:422:LEU:HD11	2.02	0.41
1:B:114:CYS:HA	1:B:119:GLY:HA3	2.02	0.41
1:B:258:THR:HA	1:B:259:PRO:C	2.41	0.41
1:B:18:THR:HG22	1:B:18:THR:O	2.21	0.41
2:Q:92:LYS:HA	2:Q:92:LYS:HD3	1.94	0.41
2:S:223:GLY:HA2	2:S:231:PHE:CD1	2.56	0.41
2:Q:333:TYR:OH	2:Q:378:GLY:HA2	2.21	0.41
2:S:397:GLN:HA	2:S:398:PRO:HD3	1.93	0.41
1:A:71:TYR:CE1	1:A:106:LYS:HD2	2.56	0.41
2:Q:410:LYS:HA	2:Q:410:LYS:HD3	1.69	0.41
9:B:2001:HOH:O	2:R:173:SER:HB2	2.21	0.40
1:C:258:THR:HA	1:C:259:PRO:C	2.42	0.40
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.56	0.40
2:S:526:ASP:HA	2:S:527:PRO:HD3	1.94	0.40
1:A:74:VAL:HG11	1:A:133:VAL:HG21	2.03	0.40
2:R:248:LEU:HD23	2:R:248:LEU:HA	1.93	0.40
2:R:497:VAL:HG13	2:R:498:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	B	260/264 (98%)	253 (97%)	7 (3%)	0	100	100
1	C	258/264 (98%)	253 (98%)	5 (2%)	0	100	100
2	Q	542/549 (99%)	533 (98%)	9 (2%)	0	100	100
2	R	541/549 (98%)	535 (99%)	6 (1%)	0	100	100
2	S	541/549 (98%)	531 (98%)	10 (2%)	0	100	100
All	All	2402/2439 (98%)	2359 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	208/210 (99%)	206 (99%)	2 (1%)	76	87
1	B	208/210 (99%)	207 (100%)	1 (0%)	88	95
1	C	207/210 (99%)	204 (99%)	3 (1%)	67	81
2	Q	433/438 (99%)	428 (99%)	5 (1%)	71	84
2	R	434/438 (99%)	430 (99%)	4 (1%)	78	89
2	S	433/438 (99%)	426 (98%)	7 (2%)	62	78
All	All	1923/1944 (99%)	1901 (99%)	22 (1%)	73	86

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

Mol	Chain	Res	Type
1	A	88	MET
1	A	229	LYS
1	B	88	MET
1	C	5	HIS
1	C	88	MET
1	C	99	LYS
2	Q	166	LYS
2	Q	401	LYS
2	Q	410	LYS
2	Q	473	ASP
2	Q	517	GLU
2	R	166	LYS
2	R	401	LYS
2	R	410	LYS
2	R	473	ASP
2	S	33	GLU
2	S	166	LYS
2	S	401	LYS
2	S	410	LYS
2	S	473	ASP
2	S	517	GLU
2	S	528	LYS

Sometimes 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	14	ASN
1	B	172	ASN
1	C	14	ASN
1	C	62	GLN
2	Q	509	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	CSO	S	543	2,7	3,6,7	0.72	0	0,6,8	-	-
2	CSO	Q	543	2,7	3,6,7	0.74	0	0,6,8	-	-
2	CSO	R	543	2,7	3,6,7	0.78	0	0,6,8	-	-

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	CSO	S	543	2,7	-	0/1/5/7	-
2	CSO	Q	543	2,7	-	1/1/5/7	-
2	CSO	R	543	2,7	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	543	CSO	N-CA-CB-SG
2	R	543	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 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	$\#\|Z\| > 2$
4	F3S	A	1266	1	0,9,9	-	-	-		
3	SF4	B	1265	1	0,12,12	-	-	-		
4	F3S	B	1266	1	0,9,9	-	-	-		
5	GOL	R	1561	-	5,5,5	0.33	0	5,5,5	0.29	0
3	SF4	A	1267	1	0,12,12	-	-	-		
3	SF4	B	1267	1	0,12,12	-	-	-		
5	GOL	Q	1562	-	5,5,5	0.62	0	5,5,5	0.80	0
5	GOL	Q	1561	-	5,5,5	0.39	0	5,5,5	0.45	0
6	FCO	R	1550	2,7	0,6,6	-	-	-		
5	GOL	R	1562	-	5,5,5	0.48	0	5,5,5	0.25	0
3	SF4	A	1265	1	0,12,12	-	-	-		
3	SF4	C	1265	1	0,12,12	-	-	-		
5	GOL	A	1271	-	5,5,5	0.23	0	5,5,5	0.25	0
4	F3S	C	1266	1	0,9,9	-	-	-		
5	GOL	S	1561	-	5,5,5	0.29	0	5,5,5	0.37	0
6	FCO	S	1550	2,7	0,6,6	-	-	-		
5	GOL	R	1563	-	5,5,5	0.29	0	5,5,5	0.39	0
5	GOL	A	1272	-	5,5,5	0.62	0	5,5,5	0.63	0
6	FCO	Q	1550	2,7	0,6,6	-	-	-		
3	SF4	C	1267	1	0,12,12	-	-	-		
5	GOL	R	1564	-	5,5,5	0.54	0	5,5,5	1.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	1561	-	-	0/4/4/4	-
3	SF4	A	1265	1	-	-	0/6/5/5
5	GOL	A	1272	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	1267	1	-	-	0/6/5/5
3	SF4	C	1265	1	-	-	0/6/5/5
3	SF4	B	1267	1	-	-	0/6/5/5
3	SF4	B	1265	1	-	-	0/6/5/5
4	F3S	A	1266	1	-	-	0/3/3/3
5	GOL	Q	1562	-	-	2/4/4/4	-
5	GOL	Q	1561	-	-	0/4/4/4	-
5	GOL	A	1271	-	-	0/4/4/4	-
3	SF4	C	1267	1	-	-	0/6/5/5
4	F3S	B	1266	1	-	-	0/3/3/3
4	F3S	C	1266	1	-	-	0/3/3/3
5	GOL	S	1561	-	-	0/4/4/4	-
5	GOL	R	1564	-	-	4/4/4/4	-
5	GOL	R	1563	-	-	0/4/4/4	-
5	GOL	R	1562	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	1562	GOL	O1-C1-C2-C3
5	R	1562	GOL	C1-C2-C3-O3
5	R	1562	GOL	O2-C2-C3-O3
5	R	1564	GOL	O1-C1-C2-O2
5	R	1564	GOL	O1-C1-C2-C3
5	A	1272	GOL	O1-C1-C2-C3
5	Q	1562	GOL	C1-C2-C3-O3
5	R	1564	GOL	C1-C2-C3-O3
5	R	1562	GOL	O1-C1-C2-O2
5	R	1564	GOL	O2-C2-C3-O3
5	A	1272	GOL	O1-C1-C2-O2
5	Q	1562	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1562	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	1564	GOL	2	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	262/264 (99%)	-0.51	4 (1%) 73 79	17, 26, 39, 67	19 (7%)
1	B	262/264 (99%)	-0.15	10 (3%) 40 47	23, 35, 54, 76	19 (7%)
1	C	260/264 (98%)	-0.32	4 (1%) 73 79	20, 30, 46, 71	15 (5%)
2	Q	544/549 (99%)	-0.46	1 (0%) 95 96	18, 28, 41, 54	22 (4%)
2	R	543/549 (98%)	-0.37	0 100 100	19, 30, 46, 66	23 (4%)
2	S	543/549 (98%)	-0.14	7 (1%) 77 81	21, 38, 60, 70	28 (5%)
All	All	2414/2439 (98%)	-0.32	26 (1%) 80 85	17, 31, 51, 76	126 (5%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	3.9
2	S	143	LYS	3.5
1	B	3	ALA	3.1
1	C	163	THR	3.1
1	C	67	LYS	3.0
1	A	163	THR	2.8
1	B	164	LYS	2.8
1	B	165	GLY	2.7
1	B	264	GLY	2.7
1	B	4	LYS	2.7
1	B	166	ILE	2.5
2	S	344	GLY	2.5
1	A	4	LYS	2.5
2	S	150	PRO	2.5
2	S	6	PRO	2.3
1	A	164	LYS	2.3
2	S	148	ILE	2.3
2	S	147	SER	2.2
1	B	195	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	164	LYS	2.2
2	Q	343	PRO	2.2
2	S	398	PRO	2.2
1	B	191	PRO	2.2
1	B	171	GLU	2.1
1	B	163	THR	2.1
1	C	38	ASP	2.0

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	CSO	Q	543	7/8	0.99	0.07	20,20,24,26	1
2	CSO	R	543	7/8	0.99	0.06	22,24,25,26	1
2	CSO	S	543	7/8	0.99	0.10	25,25,27,29	1

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
5	GOL	Q	1562	6/6	0.80	0.23	47,52,55,55	0
5	GOL	R	1564	6/6	0.83	0.19	47,50,51,56	0
5	GOL	A	1272	6/6	0.87	0.25	46,56,60,65	0
5	GOL	R	1562	6/6	0.94	0.18	47,51,52,59	0
8	MG	Q	1553	1/1	0.94	0.14	24,24,24,24	0
5	GOL	Q	1561	6/6	0.96	0.10	32,34,36,40	0
5	GOL	S	1561	6/6	0.96	0.10	35,38,39,41	0
5	GOL	R	1563	6/6	0.96	0.10	33,36,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	1271	6/6	0.97	0.09	29,34,36,38	0
5	GOL	R	1561	6/6	0.98	0.07	29,32,33,34	0
4	F3S	B	1266	7/7	0.98	0.08	37,37,39,40	0
8	MG	R	1553	1/1	0.98	0.09	30,30,30,30	0
3	SF4	C	1265	8/8	0.99	0.07	27,28,29,29	0
3	SF4	C	1267	8/8	0.99	0.06	26,26,28,29	0
4	F3S	A	1266	7/7	0.99	0.08	24,25,27,28	0
3	SF4	A	1265	8/8	0.99	0.08	23,25,27,27	0
4	F3S	C	1266	7/7	0.99	0.07	26,27,28,29	0
3	SF4	A	1267	8/8	0.99	0.07	23,23,25,25	0
6	FCO	Q	1550	7/7	0.99	0.07	21,22,24,24	0
6	FCO	S	1550	7/7	0.99	0.08	27,28,29,29	0
3	SF4	B	1265	8/8	0.99	0.06	44,48,48,52	0
3	SF4	B	1267	8/8	0.99	0.07	28,30,31,33	0
8	MG	S	1553	1/1	0.99	0.13	30,30,30,30	0
7	NI	S	1551	1/1	1.00	0.04	29,29,29,29	0
6	FCO	R	1550	7/7	1.00	0.08	23,25,25,26	0
7	NI	Q	1551	1/1	1.00	0.05	25,25,25,25	0
7	NI	R	1551	1/1	1.00	0.05	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.