Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 07:17 pm GMT

PDB ID	:	4UD2
Title	:	Structure of anaerobically purified D. fructosovorans NiFe- hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on	:	2014-12-05
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:

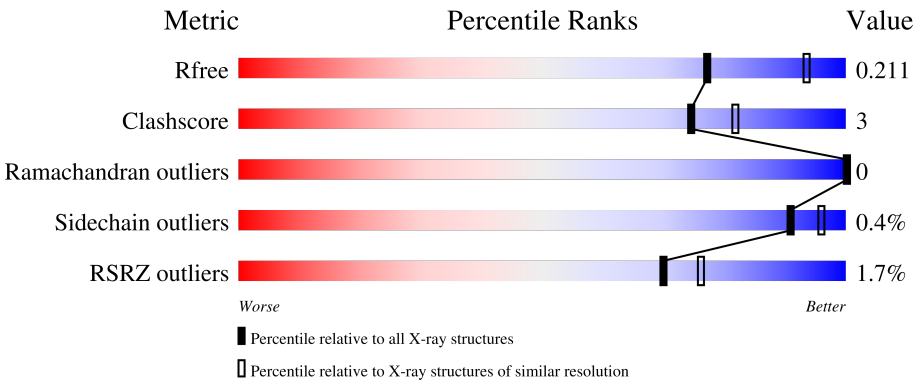
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	.% 91% 8% •
1	B	264	3% 92% 7% •
1	C	264	.% 89% 9% •
2	Q	549	93% 6% •
2	R	549	92% 7% •

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Mol	Chain	Length	Quality of chain
2	S	549	5% 89% 10%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19572 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.

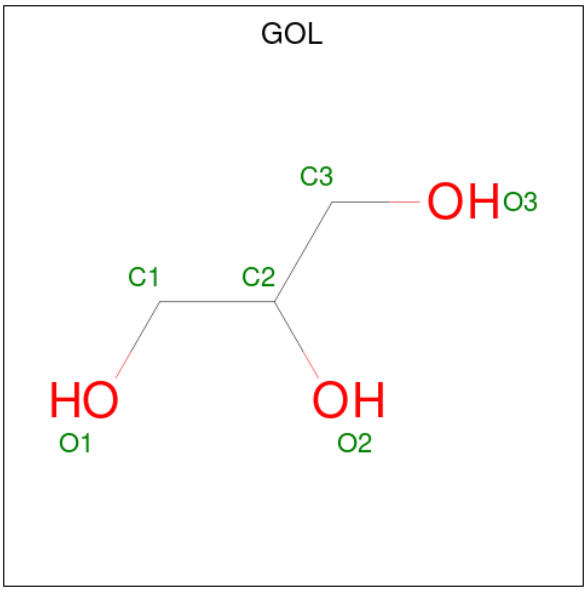
- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

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	1983	1262	331	375	15	0	1	0
1	C	260	1960	1248	327	370	15	0	0	0

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

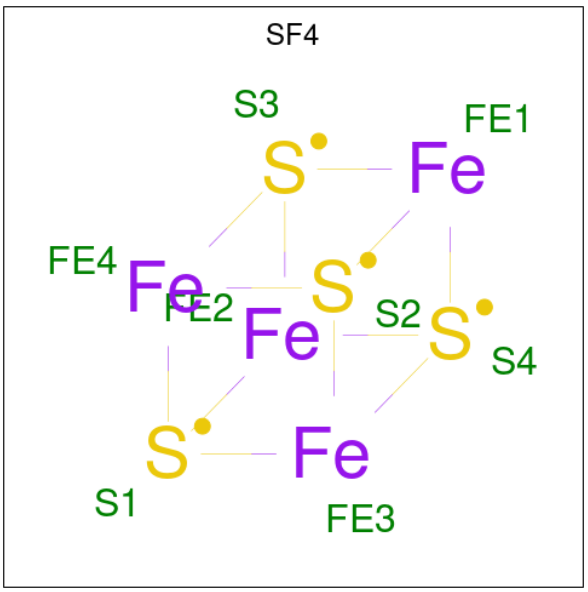
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Q	544	4163	2652	723	766	22	0	0	0
2	R	544	4168	2655	724	767	22	0	1	0
2	S	544	4163	2652	723	766	22	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



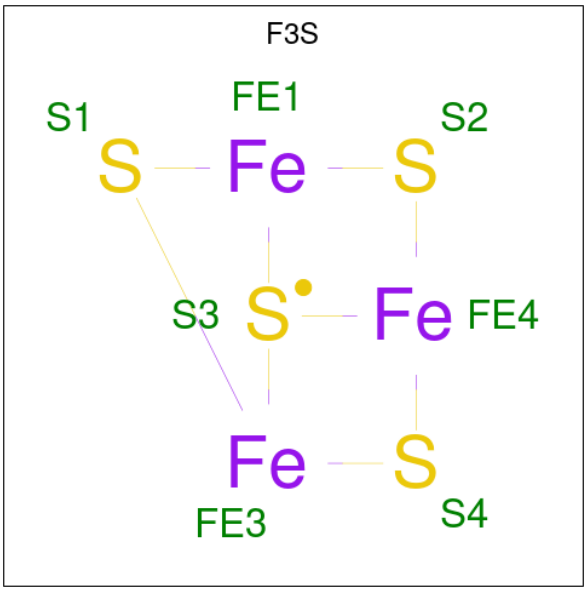
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	Q	1	6	3	3	0	0
			Total	C	O		
3	Q	1	6	3	3	0	0
			Total	C	O		
3	Q	1	6	3	3	0	0
			Total	C	O		
3	Q	1	6	3	3	0	0
			Total	C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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



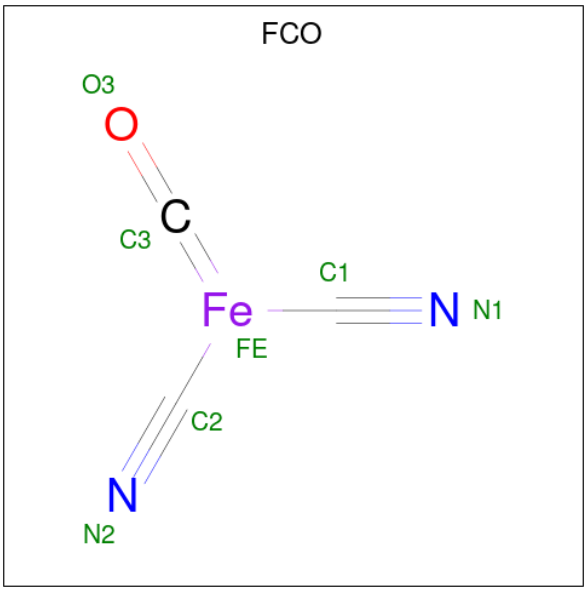
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	C	1	8	4	4	0	0
			Total	Fe	S		
4	C	1	8	4	4	0	0

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	A	1	7	3	4	0	0
5	B	1	7	3	4	0	0
5	C	1	7	3	4	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
6	R	1	7	3	1	2	1	0	0
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
			Total	Ni		
7	Q	1	1	1	0	0
7	R	1	1	1	0	0
7	S	1	1	1	0	0

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

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

- Molecule 9 is water.

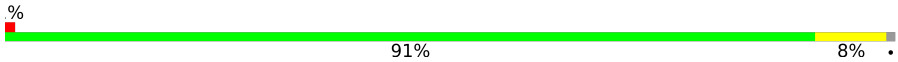
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	184	184	184	0	0
9	B	115	115	115	0	0
9	C	122	122	122	0	0
9	Q	239	239	239	0	0
9	R	206	206	206	0	0
9	S	116	116	116	0	0

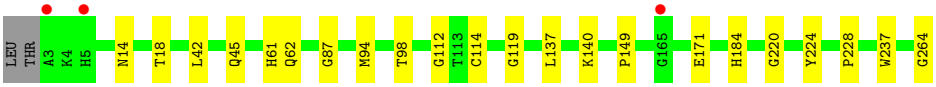
3 Residue-property plots (i)

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

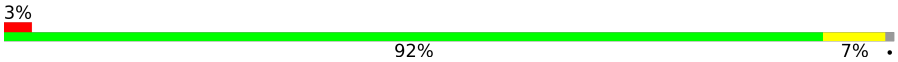
Chain A:

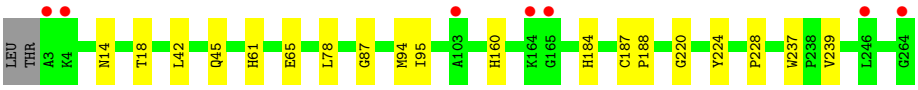




• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:



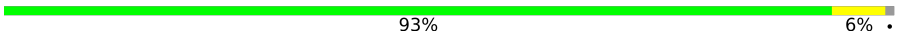


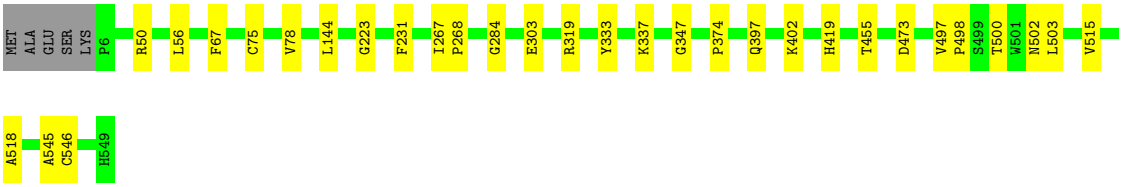
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain C:

• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

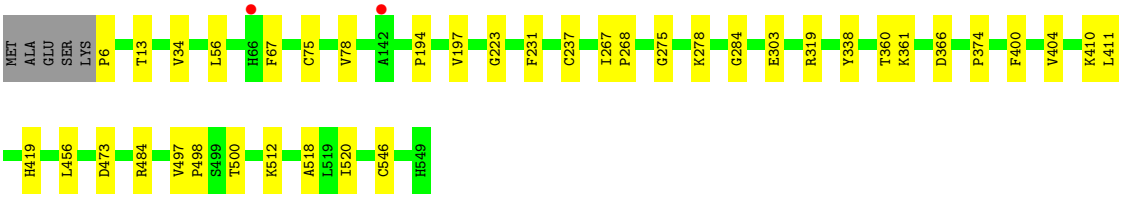
Chain Q:





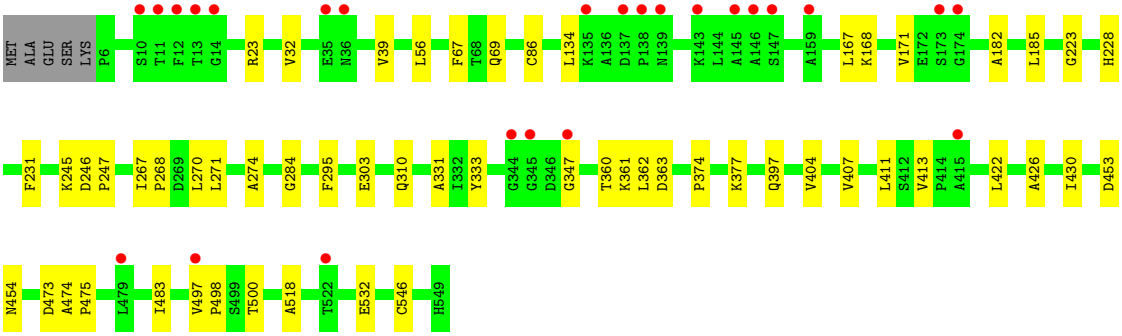
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

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	65.01Å 100.17Å 183.98Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 29.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.7 (25.00-2.30) 88.7 (29.81-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.173 , 0.207 0.176 , 0.211	Depositor DCC
R_{free} test set	4631 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19572	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: NI, CSO, SF4, MG, FCO, GOL, F3S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.63	4/2027 (0.2%)	0.63	0/2759
1	B	0.48	1/2037 (0.0%)	0.56	0/2773
1	C	0.50	1/2014 (0.0%)	0.57	0/2743
2	Q	0.52	1/4260 (0.0%)	0.61	0/5781
2	R	0.48	1/4268 (0.0%)	0.60	0/5792
2	S	0.48	3/4260 (0.1%)	0.59	1/5781 (0.0%)
All	All	0.51	11/18866 (0.1%)	0.59	1/25629 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TYR	CE1-CZ	-8.78	1.27	1.38
2	S	532	GLU	CD-OE2	-8.14	1.16	1.25
1	A	224	TYR	CG-CD1	-7.99	1.28	1.39
2	S	532	GLU	CD-OE1	-7.76	1.17	1.25
1	A	224	TYR	CG-CD2	-7.01	1.30	1.39
1	A	224	TYR	CE2-CZ	-6.73	1.29	1.38
1	C	224	TYR	CE1-CZ	-5.83	1.30	1.38
1	B	224	TYR	CE1-CZ	-5.50	1.31	1.38
2	S	303	GLU	CB-CG	-5.31	1.42	1.52
2	R	303	GLU	CB-CG	-5.21	1.42	1.52
2	Q	303	GLU	CB-CG	-5.15	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	532	GLU	OE1-CD-OE2	-10.16	111.11	123.30

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	1983	0	1920	12	0
1	C	1960	0	1897	16	0
2	Q	4163	0	4136	20	0
2	R	4168	0	4142	23	0
2	S	4163	0	4136	34	0
3	A	24	0	32	1	0
3	Q	24	0	32	3	0
3	R	24	0	32	2	0
3	S	12	0	16	2	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
5	C	7	0	0	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	184	0	0	4	0
9	B	115	0	0	1	0
9	C	122	0	0	4	0
9	Q	239	0	0	2	0
9	R	206	0	0	2	0
9	S	116	0	0	1	0
All	All	19572	0	18254	118	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 (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:503:LEU:HG	2:Q:515:VAL:HG21	1.66	0.77
2:S:134:LEU:HD22	2:S:168:LYS:HG2	1.71	0.71
2:S:361:LYS:HG2	2:S:362:LEU:O	1.93	0.68
2:R:410:LYS:HG2	3:R:605:GOL:H12	1.78	0.65
2:Q:319:ARG:HH22	3:Q:606:GOL:H2	1.65	0.61
2:S:271:LEU:HD21	2:S:407:VAL:HG22	1.82	0.61
2:Q:337:LYS:HE2	3:Q:607:GOL:H2	1.81	0.61
2:S:333:TYR:CD2	2:S:347:GLY:HA2	2.38	0.59
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.86	0.57
1:A:140:LYS:HE3	3:A:305:GOL:H11	1.85	0.57
2:R:6:PRO:N	9:R:2002:HOH:O	2.36	0.57
1:C:62:GLN:HG2	9:C:2026:HOH:O	2.04	0.56
1:A:61:HIS:HE1	9:A:2046:HOH:O	1.89	0.55
1:A:42:LEU:HD21	1:A:45:GLN:HG3	1.88	0.55
1:C:99:LYS:HG3	1:C:137:LEU:HD22	1.89	0.55
1:B:160:HIS:HE1	9:B:2085:HOH:O	1.90	0.54
2:R:319:ARG:HG2	2:R:419:HIS:CE1	2.42	0.54
2:S:333:TYR:HD2	2:S:347:GLY:HA2	1.72	0.54
1:C:98:THR:HG22	1:C:137:LEU:HD11	1.90	0.53
2:R:194:PRO:HG2	2:R:197:VAL:HG23	1.89	0.52
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.39	0.52
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.39	0.52
1:C:140:LYS:HE3	9:C:2060:HOH:O	2.10	0.52
2:S:246:ASP:HB2	2:S:247:PRO:HD3	1.90	0.52
2:S:274:ALA:HA	2:S:422:LEU:HD11	1.92	0.51
2:S:497:VAL:HG11	2:S:546:CYS:HB3	1.91	0.51
1:A:62:GLN:NE2	9:A:2052:HOH:O	2.44	0.51
1:C:18:THR:HG22	1:C:18:THR:O	2.11	0.51
2:R:497:VAL:HG13	2:R:498:PRO:HD2	1.93	0.51
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.91	0.51
1:B:14:ASN:ND2	1:B:94:MET:HB3	2.27	0.50
1:C:42:LEU:HD21	1:C:45:GLN:HG3	1.93	0.50
2:R:275:GLY:O	2:R:278:LYS:HG3	2.12	0.50
2:S:362:LEU:O	2:S:363:ASP:HB2	2.11	0.49
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.92	0.49
2:Q:267:ILE:HB	2:Q:268:PRO:HD3	1.93	0.49
1:A:171:GLU:HG3	9:A:2120:HOH:O	2.12	0.48
2:S:454:ASN:H	3:S:605:GOL:H31	1.78	0.48
2:Q:333:TYR:CD1	2:Q:347:GLY:HA2	2.47	0.48
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	1.96	0.48
2:R:278:LYS:NZ	2:R:411:LEU:O	2.30	0.48
2:Q:75:CYS:O	2:Q:78:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:400:PHE:O	2:R:404:VAL:HG23	2.13	0.48
1:B:18:THR:HG22	1:B:18:THR:O	2.14	0.47
2:Q:402:LYS:NZ	9:Q:2200:HOH:O	2.47	0.47
2:S:69:GLN:OE1	2:S:228:HIS:HA	2.14	0.47
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.97	0.47
1:C:95:ILE:O	1:C:99:LYS:HB2	2.14	0.47
2:R:497:VAL:CG1	2:R:498:PRO:HD2	2.44	0.47
2:Q:223:GLY:HA2	2:Q:231:PHE:CD1	2.50	0.47
1:C:237:TRP:CH2	1:C:239:VAL:HB	2.49	0.46
2:R:223:GLY:HA2	2:R:231:PHE:CD1	2.50	0.46
2:S:134:LEU:HD22	2:S:168:LYS:CG	2.41	0.46
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.31	0.46
1:B:61:HIS:O	1:B:65:GLU:HG2	2.15	0.46
1:C:47:THR:O	2:S:23:ARG:HA	2.14	0.46
2:R:284:GLY:HA2	2:R:518:ALA:O	2.15	0.46
2:S:167:LEU:O	2:S:171:VAL:HG23	2.16	0.46
2:R:512:LYS:HE2	2:R:520:ILE:HD11	1.98	0.45
1:C:86:TRP:HB2	9:C:2033:HOH:O	2.17	0.45
2:S:404:VAL:HG22	2:S:430:ILE:HD13	1.99	0.45
2:R:410:LYS:HA	3:R:605:GOL:H31	1.98	0.45
2:R:13:THR:HA	2:R:34:VAL:O	2.17	0.45
2:R:338:TYR:HA	2:R:366:ASP:O	2.17	0.45
1:B:42:LEU:HD21	1:B:45:GLN:HG3	1.99	0.44
1:A:184:HIS:HB2	1:A:220:GLY:C	2.37	0.44
1:C:236:ASN:OD1	1:C:240:GLN:HB3	2.17	0.44
2:R:75:CYS:O	2:R:78:VAL:HG22	2.16	0.44
1:C:5:HIS:ND1	1:C:5:HIS:C	2.71	0.44
2:S:270:LEU:HD21	2:S:426:ALA:HA	2.00	0.44
1:B:78:LEU:HD22	1:B:95:ILE:HA	2.00	0.44
1:A:264:GLY:HA3	9:A:2178:HOH:O	2.18	0.44
2:Q:502:ASN:O	2:Q:515:VAL:HG23	2.18	0.44
2:Q:319:ARG:HD3	2:Q:419:HIS:CD2	2.53	0.44
1:A:18:THR:HG22	1:A:18:THR:O	2.18	0.44
2:R:267:ILE:HB	2:R:268:PRO:HD3	1.99	0.43
2:S:454:ASN:N	3:S:605:GOL:H31	2.33	0.43
1:C:145:PRO:HG3	1:C:174:ARG:HD3	2.01	0.43
2:Q:337:LYS:HE2	3:Q:607:GOL:C2	2.47	0.43
2:Q:374:PRO:HD3	2:Q:500:THR:HG22	2.00	0.43
2:S:182:ALA:HB3	2:S:185:LEU:HG	2.00	0.43
1:B:187:CYS:HA	1:B:188:PRO:HD3	1.83	0.43
2:S:223:GLY:HA2	2:S:231:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.01	0.43
1:C:14:ASN:ND2	1:C:94:MET:HB3	2.34	0.43
2:R:56:LEU:HD21	2:R:67:PHE:HB2	2.01	0.43
2:S:331:ALA:HB1	2:S:377:LYS:HG3	2.01	0.43
2:R:237:CYS:HB2	2:R:456:LEU:HG	2.01	0.43
2:R:278:LYS:HE2	9:R:2112:HOH:O	2.18	0.43
2:R:497:VAL:HG11	2:R:546:CYS:HB3	2.00	0.43
2:S:86:CYS:SG	2:S:483:ILE:HG22	2.59	0.42
1:B:87:GLY:O	1:B:94:MET:HG3	2.19	0.42
2:S:284:GLY:HA2	2:S:518:ALA:O	2.19	0.42
2:R:360:THR:OG1	2:R:361:LYS:N	2.50	0.42
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.54	0.42
2:R:374:PRO:HD3	2:R:500:THR:HG22	2.01	0.42
1:A:87:GLY:O	1:A:94:MET:HG3	2.19	0.42
1:A:228:PRO:HB3	1:A:237:TRP:CZ2	2.54	0.42
1:B:14:ASN:HD22	1:B:94:MET:HB3	1.84	0.42
1:B:228:PRO:HB3	1:B:237:TRP:CZ2	2.55	0.42
2:Q:144:LEU:HD23	2:Q:144:LEU:O	2.19	0.41
2:S:374:PRO:HD3	2:S:500:THR:HG22	2.01	0.41
2:S:411:LEU:O	2:S:413:VAL:HG13	2.20	0.41
2:Q:284:GLY:HA2	2:Q:518:ALA:O	2.20	0.41
2:S:474:ALA:HB1	2:S:475:PRO:HD2	2.02	0.41
2:Q:50:ARG:NH2	2:Q:545:ALA:HB1	2.34	0.41
2:S:295:PHE:O	2:S:310:GLN:HG3	2.21	0.41
2:S:360:THR:OG1	2:S:361:LYS:N	2.52	0.41
1:C:114:CYS:HB2	9:C:2032:HOH:O	2.19	0.41
2:Q:56:LEU:HD21	2:Q:67:PHE:HB2	2.03	0.41
2:S:32:VAL:HB	2:S:39:VAL:HG13	2.02	0.41
2:S:56:LEU:HD21	2:S:67:PHE:HB2	2.02	0.41
2:S:453:ASP:HB3	9:S:2031:HOH:O	2.21	0.41
2:S:134:LEU:CD2	2:S:167:LEU:HD23	2.51	0.40
1:B:184:HIS:HB2	1:B:220:GLY:C	2.42	0.40
2:Q:455:THR:HG23	9:Q:2215:HOH:O	2.21	0.40
1:A:112:GLY:HA2	1:A:149:PRO:HD3	2.02	0.40
1:C:184:HIS:HB2	1:C:220:GLY:C	2.42	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%)	252 (97%)	8 (3%)	0	100	100
1	B	261/264 (99%)	251 (96%)	10 (4%)	0	100	100
1	C	258/264 (98%)	251 (97%)	7 (3%)	0	100	100
2	Q	541/549 (98%)	527 (97%)	14 (3%)	0	100	100
2	R	542/549 (99%)	527 (97%)	15 (3%)	0	100	100
2	S	541/549 (98%)	523 (97%)	18 (3%)	0	100	100
All	All	2403/2439 (98%)	2331 (97%)	72 (3%)	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%)	208 (100%)	0	100	100
1	B	209/210 (100%)	209 (100%)	0	100	100
1	C	207/210 (99%)	206 (100%)	1 (0%)	88	95
2	Q	433/438 (99%)	431 (100%)	2 (0%)	88	95
2	R	434/438 (99%)	432 (100%)	2 (0%)	88	95
2	S	433/438 (99%)	430 (99%)	3 (1%)	84	92
All	All	1924/1944 (99%)	1916 (100%)	8 (0%)	91	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	HIS
2	Q	397	GLN
2	Q	473	ASP
2	R	473	ASP
2	R	484	ARG
2	S	245	LYS
2	S	397	GLN
2	S	473	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	234	GLN
1	B	14	ASN
1	B	172	ASN
1	C	14	ASN
1	C	62	GLN
2	Q	509	GLN
2	R	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	R	543	2,7	3,6,7	0.99	0	0,6,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	Q	543	2,7	3,6,7	0.80	0	0,6,8	-	-
2	CSO	S	543	2,7	3,6,7	0.72	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	R	543	2,7	-	1/1/5/7	-
2	CSO	Q	543	2,7	-	1/1/5/7	-
2	CSO	S	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 (3) 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
2	S	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 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	SF4	A	1267	1	0,12,12	-	-	-		
5	F3S	A	1266	1	0,9,9	-	-	-		
3	GOL	A	306	-	5,5,5	0.37	0	5,5,5	0.30	0
6	FCO	R	1550	2,7	0,6,6	-	-	-		
3	GOL	A	305	-	5,5,5	0.40	0	5,5,5	0.67	0
3	GOL	R	606	-	5,5,5	0.43	0	5,5,5	0.32	0
3	GOL	A	307	-	5,5,5	0.44	0	5,5,5	0.26	0
4	SF4	B	1265	1	0,12,12	-	-	-		
6	FCO	Q	1550	2,7	0,6,6	-	-	-		
3	GOL	Q	605	-	5,5,5	0.19	0	5,5,5	0.25	0
4	SF4	A	1265	1	0,12,12	-	-	-		
6	FCO	S	1550	2,7	0,6,6	-	-	-		
3	GOL	S	604	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	Q	604	-	5,5,5	0.25	0	5,5,5	0.15	0
3	GOL	R	604	-	5,5,5	0.35	0	5,5,5	0.32	0
4	SF4	C	1267	1	0,12,12	-	-	-		
5	F3S	C	1266	1	0,9,9	-	-	-		
3	GOL	A	304	-	5,5,5	0.25	0	5,5,5	0.39	0
4	SF4	C	1265	1	0,12,12	-	-	-		
5	F3S	B	1266	1	0,9,9	-	-	-		
3	GOL	Q	606	-	5,5,5	0.46	0	5,5,5	0.67	0
4	SF4	B	1267	1	0,12,12	-	-	-		
3	GOL	R	607	-	5,5,5	0.30	0	5,5,5	0.26	0
3	GOL	S	605	-	5,5,5	0.24	0	5,5,5	0.30	0
3	GOL	Q	607	-	5,5,5	0.34	0	5,5,5	0.20	0
3	GOL	R	605	-	5,5,5	0.27	0	5,5,5	0.17	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
4	SF4	A	1267	1	-	-	0/6/5/5
5	F3S	A	1266	1	-	-	0/3/3/3
3	GOL	A	306	-	-	4/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	R	606	-	-	0/4/4/4	-
3	GOL	A	307	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	1265	1	-	-	0/6/5/5
3	GOL	Q	605	-	-	2/4/4/4	-
4	SF4	A	1265	1	-	-	0/6/5/5
3	GOL	S	604	-	-	1/4/4/4	-
3	GOL	Q	604	-	-	0/4/4/4	-
3	GOL	R	604	-	-	0/4/4/4	-
4	SF4	C	1267	1	-	-	0/6/5/5
5	F3S	C	1266	1	-	-	0/3/3/3
3	GOL	A	304	-	-	2/4/4/4	-
4	SF4	C	1265	1	-	-	0/6/5/5
5	F3S	B	1266	1	-	-	0/3/3/3
3	GOL	Q	606	-	-	3/4/4/4	-
4	SF4	B	1267	1	-	-	0/6/5/5
3	GOL	R	607	-	-	2/4/4/4	-
3	GOL	S	605	-	-	4/4/4/4	-
3	GOL	Q	607	-	-	2/4/4/4	-
3	GOL	R	605	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	GOL	C1-C2-C3-O3
3	A	304	GOL	O2-C2-C3-O3
3	A	305	GOL	C1-C2-C3-O3
3	A	306	GOL	C1-C2-C3-O3
3	A	307	GOL	O1-C1-C2-C3
3	Q	606	GOL	C1-C2-C3-O3
3	R	605	GOL	O1-C1-C2-C3
3	R	605	GOL	C1-C2-C3-O3
3	A	306	GOL	O2-C2-C3-O3
3	R	605	GOL	O1-C1-C2-O2
3	A	306	GOL	O1-C1-C2-C3
3	A	307	GOL	C1-C2-C3-O3
3	Q	605	GOL	C1-C2-C3-O3
3	Q	607	GOL	C1-C2-C3-O3
3	R	607	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	S	605	GOL	C1-C2-C3-O3
3	A	305	GOL	O2-C2-C3-O3
3	A	307	GOL	O1-C1-C2-O2
3	Q	606	GOL	O2-C2-C3-O3
3	R	605	GOL	O2-C2-C3-O3
3	R	607	GOL	O2-C2-C3-O3
3	S	605	GOL	O2-C2-C3-O3
3	A	306	GOL	O1-C1-C2-O2
3	A	307	GOL	O2-C2-C3-O3
3	S	604	GOL	C1-C2-C3-O3
3	S	605	GOL	O1-C1-C2-O2
3	Q	606	GOL	O1-C1-C2-C3
3	Q	607	GOL	O2-C2-C3-O3
3	S	605	GOL	O1-C1-C2-C3
3	Q	605	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	GOL	1	0
3	Q	606	GOL	1	0
3	S	605	GOL	2	0
3	Q	607	GOL	2	0
3	R	605	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%)	-0.38	3 (1%)	80	85	17, 26, 40, 69	9 (3%)
1	B	262/264 (99%)	0.10	7 (2%)	54	62	24, 39, 60, 73	10 (3%)
1	C	260/264 (98%)	-0.11	3 (1%)	79	83	21, 37, 58, 81	8 (3%)
2	Q	543/549 (98%)	-0.36	0	100	100	16, 29, 46, 60	15 (2%)
2	R	543/549 (98%)	-0.16	2 (0%)	92	95	18, 34, 50, 67	11 (2%)
2	S	543/549 (98%)	0.29	25 (4%)	32	39	22, 47, 70, 87	21 (3%)
All	All	2413/2439 (98%)	-0.09	40 (1%)	70	76	16, 35, 61, 87	74 (3%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	12	PHE	5.3
2	S	344	GLY	3.9
1	B	3	ALA	3.6
1	B	264	GLY	3.6
2	S	11	THR	3.2
2	S	36	ASN	3.2
2	S	174	GLY	3.1
1	C	163	THR	3.0
2	S	146	ALA	3.0
2	S	173	SER	2.9
2	S	14	GLY	2.9
2	S	137	ASP	2.9
2	S	135	LYS	2.9
1	C	69	GLY	2.8
2	S	147	SER	2.7
2	S	13	THR	2.7
2	S	345	GLY	2.7
1	B	246	LEU	2.7
1	B	103	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	S	138	PRO	2.6
2	S	497	VAL	2.6
2	S	159	ALA	2.5
1	B	4	LYS	2.5
2	S	479	LEU	2.4
1	A	3	ALA	2.3
2	S	139	ASN	2.3
2	S	347	GLY	2.3
2	S	35	GLU	2.2
2	S	522	THR	2.2
2	S	145	ALA	2.2
1	C	67	LYS	2.2
1	A	5	HIS	2.2
2	S	143	LYS	2.2
1	B	165	GLY	2.2
2	R	142	ALA	2.1
1	B	164	LYS	2.1
1	A	165	GLY	2.0
2	S	10	SER	2.0
2	R	66	HIS	2.0
2	S	415	ALA	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	R	543	7/8	0.97	0.13	20,22,26,27	1
2	CSO	Q	543	7/8	0.98	0.09	20,21,22,25	1
2	CSO	S	543	7/8	0.98	0.15	30,31,36,36	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
3	GOL	Q	606	6/6	0.76	0.20	56,62,65,69	0
3	GOL	R	607	6/6	0.82	0.20	51,57,58,64	0
3	GOL	A	305	6/6	0.83	0.20	54,55,61,65	0
3	GOL	A	307	6/6	0.85	0.22	57,66,68,77	0
3	GOL	Q	607	6/6	0.86	0.32	62,67,70,73	0
3	GOL	A	304	6/6	0.86	0.19	47,56,71,76	0
3	GOL	R	605	6/6	0.87	0.20	58,60,69,72	0
8	MG	R	1553	1/1	0.87	0.06	23,23,23,23	0
3	GOL	A	306	6/6	0.90	0.16	58,61,68,75	0
3	GOL	R	606	6/6	0.90	0.16	38,41,42,42	0
8	MG	Q	1553	1/1	0.92	0.05	21,21,21,21	0
3	GOL	S	605	6/6	0.93	0.20	56,59,64,72	0
3	GOL	S	604	6/6	0.95	0.11	36,38,39,39	0
3	GOL	Q	604	6/6	0.97	0.10	32,35,38,41	0
4	SF4	B	1265	8/8	0.97	0.04	40,42,48,52	0
8	MG	S	1553	1/1	0.97	0.06	32,32,32,32	0
4	SF4	B	1267	8/8	0.98	0.06	25,26,28,28	0
5	F3S	A	1266	7/7	0.98	0.06	16,19,20,22	0
5	F3S	B	1266	7/7	0.98	0.06	35,37,39,39	0
3	GOL	Q	605	6/6	0.98	0.13	31,32,36,38	0
4	SF4	A	1265	8/8	0.98	0.04	18,20,22,23	0
3	GOL	R	604	6/6	0.98	0.11	29,30,32,32	0
5	F3S	C	1266	7/7	0.99	0.04	23,23,25,27	0
6	FCO	Q	1550	7/7	0.99	0.09	15,17,19,20	0
6	FCO	R	1550	7/7	0.99	0.10	17,19,21,23	0
6	FCO	S	1550	7/7	0.99	0.14	25,29,32,33	0
7	NI	Q	1551	1/1	0.99	0.05	18,18,18,18	0
7	NI	R	1551	1/1	0.99	0.06	24,24,24,24	0
7	NI	S	1551	1/1	0.99	0.07	28,28,28,28	0
4	SF4	C	1267	8/8	0.99	0.04	22,23,24,26	0
4	SF4	A	1267	8/8	0.99	0.06	15,16,17,18	0
4	SF4	C	1265	8/8	0.99	0.04	22,24,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.