Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 10:31 pm GMT

PDB ID	:	4UE2
Title	:	Structure of air-treated anaerobically purified D. fructosovorans NiFe-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on	:	2014-12-15
Resolution	:	2.02 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:

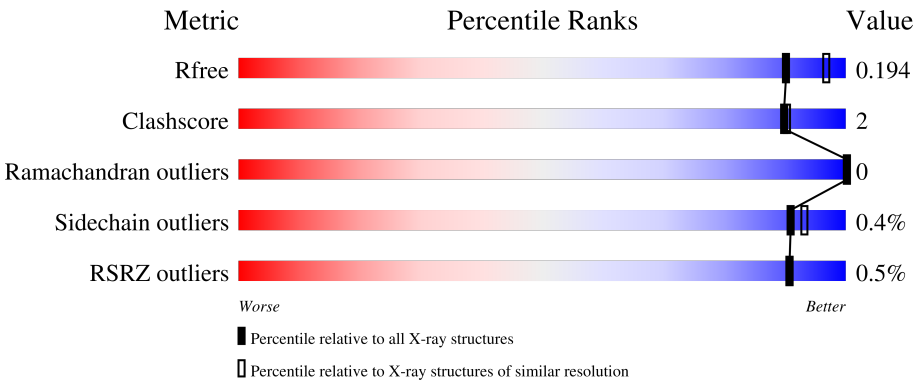
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	% 94% 6% •
1	B	264	3% 95% 5% •
1	C	264	94% 5% •
2	Q	549	96% • •
2	R	549	95% • •

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Mol	Chain	Length	Quality of chain
2	S	549	96%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20366 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.

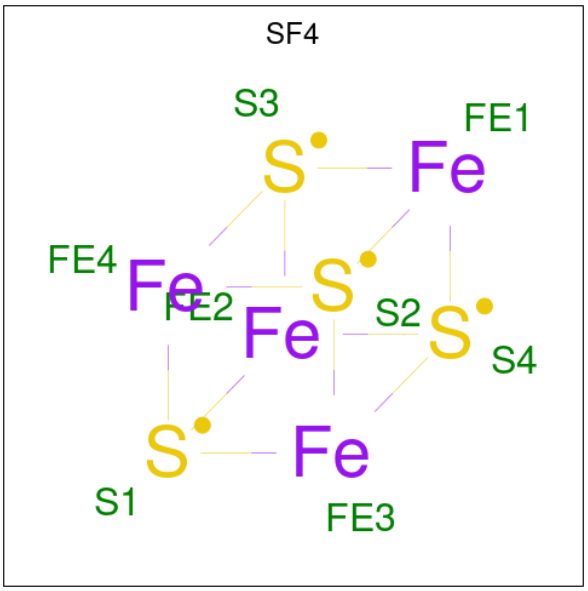
- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	1979	1260	330	374	15	0	1	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.

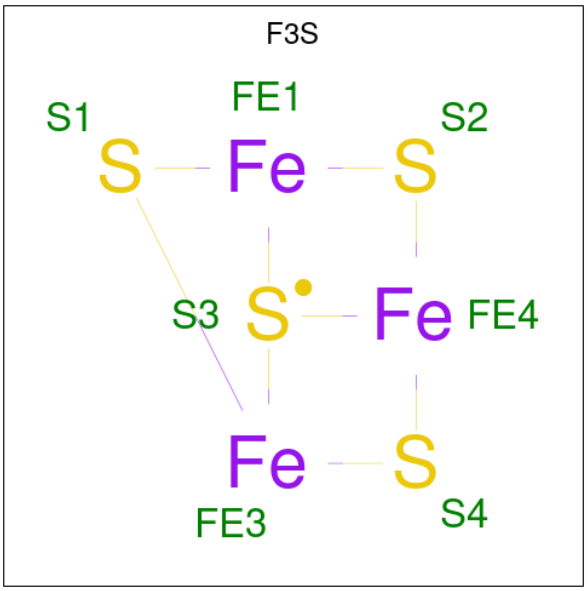
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Q	545	4171	2656	724	769	22	0	0	0
2	R	544	4178	2659	724	773	22	0	3	0
2	S	544	4181	2662	723	774	22	0	3	0

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



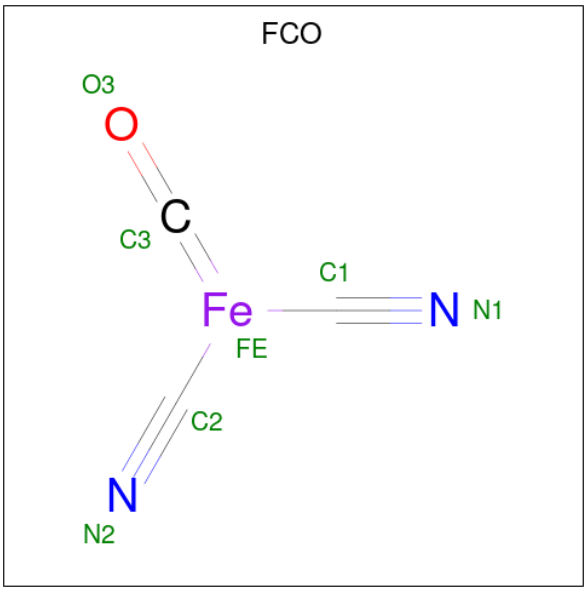
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	B	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0
			Total	Fe	S		
3	C	1	8	4	4	0	0

- 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
			Total	Fe	S		
4	B	1	7	3	4	0	0
			Total	Fe	S		
4	C	1	7	3	4	0	0

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



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

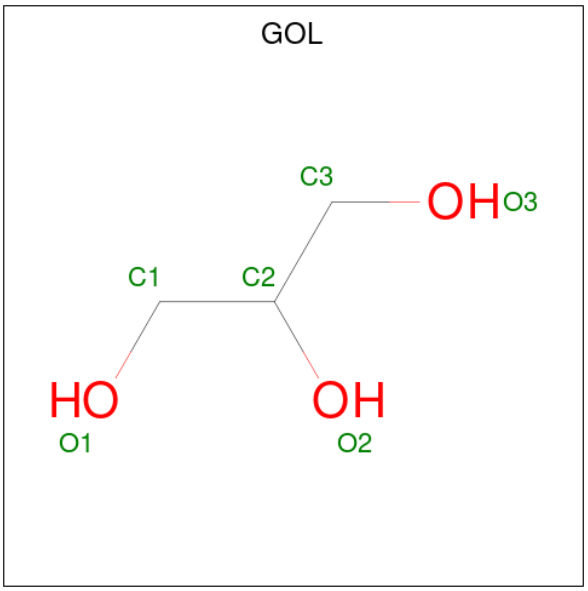
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	Q	1	1	1	0	0
7	R	2	2	2	0	0
7	S	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

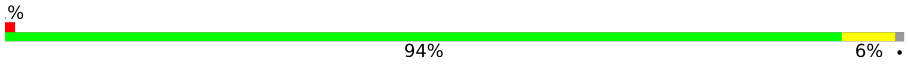
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	287	287	287	0	0
			Total	O		
9	B	195	195	195	0	0
			Total	O		
9	C	245	245	245	0	0
			Total	O		
9	Q	398	398	398	0	0
			Total	O		
9	R	366	366	366	0	0
			Total	O		
9	S	305	305	305	0	0

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.

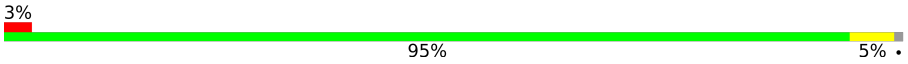
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

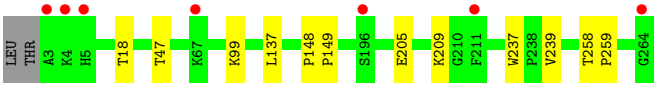
Chain A:



• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

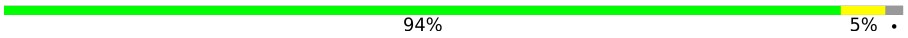
Chain B:

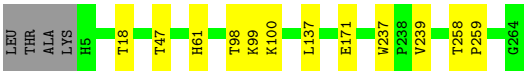




• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

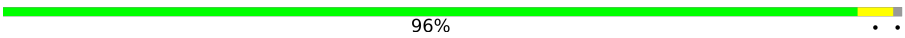
Chain C:





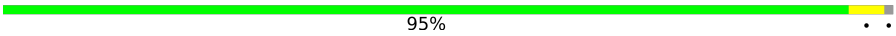
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

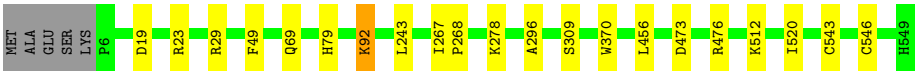
Chain Q:



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

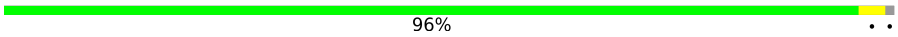
Chain R:

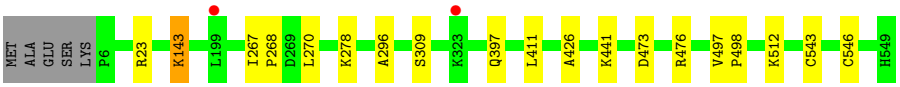




• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

Chain S:


96%


MET
ALA
GLU
SER
LYS
P6
R23
K143
L199
I267
P268
D269
L270
K278
A296
S309
K323
Q397
L411
A426
K441
D473
R476
V497
P498
K512
C543
C546
H549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.09Å 99.65Å 184.17Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	19.91 – 2.02 19.91 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.91-2.02) 97.5 (19.91-2.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.164 , 0.191 0.167 , 0.194	Depositor DCC
R_{free} test set	7604 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20366	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CSO, MG, NI, FCO, F3S, GOL, SF4

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	0.54	0/2036	0.61	0/2772
1	B	0.44	0/2028	0.56	0/2761
1	C	0.50	0/2014	0.58	0/2743
2	Q	0.53	0/4268	0.62	0/5793
2	R	0.49	0/4290	0.60	0/5821
2	S	0.46	0/4290	0.59	0/5821
All	All	0.50	0/18926	0.60	0/25711

There are no bond length outliers.

There are no bond angle outliers.

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	1979	0	1919	11	0
1	B	1974	0	1915	8	0
1	C	1960	0	1897	9	0
2	Q	4171	0	4139	15	0
2	R	4178	0	4146	12	0
2	S	4181	0	4148	14	0
3	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	Q	7	0	0	0	0
5	R	7	0	0	0	0
5	S	7	0	0	1	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
7	Q	1	0	0	0	0
7	R	2	0	0	0	0
7	S	1	0	0	0	0
8	Q	12	0	16	1	0
8	R	12	0	16	0	0
8	S	6	0	8	0	0
9	A	287	0	0	2	0
9	B	195	0	0	0	0
9	C	245	0	0	3	0
9	Q	398	0	0	4	0
9	R	366	0	0	4	0
9	S	305	0	0	3	0
All	All	20366	0	18204	66	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 2.

All (66) 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:5:LYS:CB	2:Q:6:PRO:HA	2.25	0.66
2:R:512:LYS:HE2	2:R:520:ILE:HD11	1.78	0.65
1:B:205:GLU:HG3	1:B:209:LYS:HE3	1.80	0.63
1:C:99:LYS:HG2	1:C:137:LEU:HD22	1.81	0.62
1:A:61:HIS:HE1	9:A:2082:HOH:O	1.83	0.62
1:C:47:THR:O	2:S:23:ARG:HA	2.02	0.60
2:R:278:LYS:HG2	9:R:2205:HOH:O	2.05	0.56
2:Q:529:ARG:HD3	8:Q:1562:GOL:H31	1.86	0.55
1:C:171:GLU:HG2	9:C:2158:HOH:O	2.09	0.51
1:A:98:THR:HG22	1:A:137:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:TRP:CZ2	1:C:239:VAL:HB	2.46	0.50
1:A:61:HIS:HB3	9:A:2084:HOH:O	2.11	0.50
1:B:99:LYS:HG3	1:B:137:LEU:HD22	1.94	0.49
2:Q:12:PHE:HB2	2:Q:527:PRO:HG3	1.95	0.49
1:B:47:THR:O	2:R:23:ARG:HA	2.13	0.48
1:A:47:THR:O	2:Q:23:ARG:HA	2.13	0.48
2:S:270:LEU:HD21	2:S:426:ALA:HA	1.94	0.48
2:S:267:ILE:HB	2:S:268:PRO:HD3	1.96	0.48
2:Q:497:VAL:CG1	2:Q:498:PRO:HD2	2.44	0.47
1:C:258:THR:HA	1:C:259:PRO:C	2.35	0.47
2:S:497:VAL:HG13	2:S:498:PRO:HD2	1.97	0.47
2:Q:278:LYS:HE2	9:Q:2229:HOH:O	2.14	0.47
1:C:18:THR:HG22	1:C:18:THR:O	2.16	0.46
2:R:92:LYS:HD2	9:R:2073:HOH:O	2.14	0.46
2:Q:395:LYS:HE3	9:Q:2259:HOH:O	2.14	0.46
2:Q:284:GLY:HA2	2:Q:518:ALA:O	2.15	0.46
2:S:497:VAL:CG1	2:S:498:PRO:HD2	2.45	0.46
2:R:267:ILE:HB	2:R:268:PRO:HD3	1.97	0.46
1:B:18:THR:HG22	1:B:18:THR:O	2.16	0.46
2:S:476:ARG:HD2	9:S:2050:HOH:O	2.16	0.45
2:R:49:PHE:HB2	2:R:370:TRP:CD2	2.51	0.45
1:B:237:TRP:CZ2	1:B:239:VAL:HB	2.52	0.45
2:R:243:LEU:HD11	2:R:456:LEU:HD13	1.98	0.45
2:S:296:ALA:HA	2:S:309:SER:HA	1.98	0.45
2:R:296:ALA:HA	2:R:309:SER:HA	1.98	0.44
2:S:497:VAL:HG11	2:S:546:CYS:HB3	1.99	0.44
2:S:476:ARG:HD2	5:S:1550:FCO:C2	2.48	0.44
2:Q:497:VAL:HG13	2:Q:498:PRO:HD2	1.99	0.44
1:A:237:TRP:CH2	1:A:239:VAL:HB	2.53	0.44
1:C:61:HIS:HB3	9:C:2063:HOH:O	2.18	0.44
2:R:476:ARG:HD2	9:R:2066:HOH:O	2.17	0.44
2:R:543:CSO:CB	9:R:2066:HOH:O	2.66	0.44
2:S:512:LYS:HD3	9:S:2021:HOH:O	2.17	0.44
1:A:78:LEU:O	1:A:130:ALA:HA	2.18	0.43
1:B:258:THR:HA	1:B:259:PRO:C	2.39	0.43
2:Q:497:VAL:HG11	2:Q:546:CYS:HB3	2.00	0.43
1:A:18:THR:HG22	1:A:18:THR:O	2.18	0.43
1:B:148:PRO:HB2	1:B:149:PRO:HD2	1.99	0.43
2:Q:296:ALA:HA	2:Q:309:SER:HA	1.99	0.43
2:Q:476:ARG:HD2	9:Q:2074:HOH:O	2.18	0.43
1:C:100:LYS:HG3	9:C:2104:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:CZ2	1:A:239:VAL:HB	2.54	0.42
2:S:278:LYS:NZ	2:S:411:LEU:O	2.48	0.42
2:Q:543:CSO:CB	9:Q:2074:HOH:O	2.67	0.42
1:A:258:THR:HA	1:A:259:PRO:C	2.40	0.41
1:A:14:ASN:ND2	1:A:94:MET:HB3	2.34	0.41
2:R:19:ASP:HB2	2:R:29:ARG:HG3	2.03	0.41
1:A:114:CYS:HA	1:A:119:GLY:HA3	2.02	0.41
1:B:237:TRP:CH2	1:B:239:VAL:HB	2.55	0.41
2:Q:541:ASP:N	2:Q:542:PRO:HD3	2.36	0.41
2:Q:5:LYS:CB	2:Q:6:PRO:CA	2.96	0.41
2:S:441:LYS:HE2	2:S:441:LYS:HB3	1.84	0.41
2:S:143:LYS:HA	2:S:143:LYS:HD2	1.92	0.40
1:C:98:THR:HG22	1:C:137:LEU:HD11	2.03	0.40
2:R:69:GLN:HA	2:R:79:HIS:HB2	2.03	0.40
2:S:543:CSO:CB	9:S:2050:HOH:O	2.70	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	261/264 (99%)	254 (97%)	7 (3%)	0	100	100
1	B	260/264 (98%)	253 (97%)	7 (3%)	0	100	100
1	C	258/264 (98%)	251 (97%)	7 (3%)	0	100	100
2	Q	542/549 (99%)	527 (97%)	15 (3%)	0	100	100
2	R	544/549 (99%)	533 (98%)	11 (2%)	0	100	100
2	S	544/549 (99%)	531 (98%)	13 (2%)	0	100	100
All	All	2409/2439 (99%)	2349 (98%)	60 (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	209/210 (100%)	209 (100%)	0	100	100
1	B	208/210 (99%)	208 (100%)	0	100	100
1	C	207/210 (99%)	207 (100%)	0	100	100
2	Q	434/438 (99%)	433 (100%)	1 (0%)	93	95
2	R	437/438 (100%)	434 (99%)	3 (1%)	84	87
2	S	437/438 (100%)	434 (99%)	3 (1%)	84	87
All	All	1932/1944 (99%)	1925 (100%)	7 (0%)	91	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	473	ASP
2	R	92	LYS
2	R	473	ASP
2	R	546	CYS
2	S	143	LYS
2	S	397	GLN
2	S	473	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	B	14	ASN
1	C	14	ASN
2	Q	509	GLN
2	R	367	HIS

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	2,6	3,6,7	0.76	0	0,6,8	-	-
2	CSO	Q	543	2,6	3,6,7	0.86	0	0,6,8	-	-
2	CSO	R	543	2,6	3,6,7	0.65	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	2,6	-	1/1/5/7	-
2	CSO	Q	543	2,6	-	1/1/5/7	-
2	CSO	R	543	2,6	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	543	CSO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	543	CSO	1	0
2	R	543	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 7 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
8	GOL	Q	1561	-	5,5,5	0.35	0	5,5,5	0.41	0
3	SF4	C	1267	1	0,12,12	-	-	-		
8	GOL	S	1561	-	5,5,5	0.47	0	5,5,5	0.21	0
8	GOL	Q	1562	-	5,5,5	0.30	0	5,5,5	0.41	0
3	SF4	C	1265	1	0,12,12	-	-	-		
4	F3S	B	1266	1	0,9,9	-	-	-		
5	FCO	Q	1550	2,6,9	0,6,6	-	-	-		
4	F3S	C	1266	1	0,9,9	-	-	-		
8	GOL	R	1561	-	5,5,5	0.41	0	5,5,5	0.22	0
3	SF4	B	1265	1	0,12,12	-	-	-		
3	SF4	B	1267	1	0,12,12	-	-	-		
3	SF4	A	1265	1	0,12,12	-	-	-		
3	SF4	A	1267	1	0,12,12	-	-	-		
4	F3S	A	1266	1	0,9,9	-	-	-		
5	FCO	R	1550	2,6,9	0,6,6	-	-	-		
8	GOL	R	1562	-	5,5,5	0.50	0	5,5,5	0.61	0
5	FCO	S	1550	2,6,9	0,6,6	-	-	-		

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
8	GOL	Q	1561	-	-	0/4/4/4	-
8	GOL	S	1561	-	-	0/4/4/4	-
3	SF4	C	1267	1	-	-	0/6/5/5
8	GOL	Q	1562	-	-	2/4/4/4	-
3	SF4	C	1265	1	-	-	0/6/5/5
4	F3S	B	1266	1	-	-	0/3/3/3
8	GOL	R	1561	-	-	0/4/4/4	-
4	F3S	C	1266	1	-	-	0/3/3/3
3	SF4	B	1265	1	-	-	0/6/5/5
8	GOL	R	1562	-	-	0/4/4/4	-
3	SF4	A	1265	1	-	-	0/6/5/5
3	SF4	A	1267	1	-	-	0/6/5/5
3	SF4	B	1267	1	-	-	0/6/5/5
4	F3S	A	1266	1	-	-	0/3/3/3

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
8	Q	1562	GOL	C1-C2-C3-O3
8	Q	1562	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Q	1562	GOL	1	0
5	S	1550	FCO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	262/264 (99%)	-0.60	3 (1%)	80	80	10, 17, 27, 54	11 (4%)
1	B	262/264 (99%)	-0.18	7 (2%)	54	54	14, 30, 50, 69	11 (4%)
1	C	260/264 (98%)	-0.49	0	100	100	14, 22, 38, 59	14 (5%)
2	Q	544/549 (99%)	-0.63	0	100	100	10, 18, 28, 57	25 (4%)
2	R	543/549 (98%)	-0.54	0	100	100	12, 21, 34, 52	22 (4%)
2	S	543/549 (98%)	-0.33	2 (0%)	92	92	13, 28, 44, 58	18 (3%)
All	All	2414/2439 (98%)	-0.47	12 (0%)	91	91	10, 21, 41, 69	101 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	4.6
1	B	264	GLY	3.4
1	A	3	ALA	3.3
1	B	4	LYS	3.1
1	A	4	LYS	2.8
1	B	5	HIS	2.7
1	A	163	THR	2.5
1	B	196	SER	2.4
1	B	67	LYS	2.3
2	S	323	LYS	2.1
1	B	211	PHE	2.1
2	S	199	LEU	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	0.97	0.08	14,14,18,20	1
2	CSO	R	543	7/8	0.98	0.08	14,15,19,20	1
2	CSO	S	543	7/8	0.98	0.09	17,18,21,22	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
8	GOL	R	1561	6/6	0.92	0.12	24,26,27,29	0
8	GOL	Q	1562	6/6	0.94	0.14	24,31,38,39	0
7	MG	R	1560	1/1	0.94	0.15	46,46,46,46	0
8	GOL	S	1561	6/6	0.95	0.09	27,28,29,29	0
8	GOL	R	1562	6/6	0.96	0.08	21,24,25,28	0
7	MG	Q	1553	1/1	0.96	0.05	12,12,12,12	0
8	GOL	Q	1561	6/6	0.97	0.10	19,20,21,22	0
4	F3S	B	1266	7/7	0.98	0.06	28,31,32,33	0
3	SF4	B	1265	8/8	0.98	0.06	37,39,40,42	0
7	MG	R	1553	1/1	0.98	0.04	16,16,16,16	0
7	MG	S	1553	1/1	0.99	0.04	18,18,18,18	0
5	FCO	R	1550	7/7	0.99	0.05	14,14,15,16	0
5	FCO	S	1550	7/7	0.99	0.06	16,16,17,18	0
3	SF4	C	1265	8/8	0.99	0.05	17,18,19,19	0
3	SF4	B	1267	8/8	0.99	0.04	18,19,19,21	0
4	F3S	C	1266	7/7	0.99	0.04	18,18,20,20	0
3	SF4	A	1265	8/8	1.00	0.04	13,14,14,15	0
5	FCO	Q	1550	7/7	1.00	0.04	10,11,12,12	0
3	SF4	C	1267	8/8	1.00	0.03	13,14,14,16	0
4	F3S	A	1266	7/7	1.00	0.03	13,14,16,17	0
6	NI	Q	1551	1/1	1.00	0.01	12,12,12,12	0
6	NI	R	1551	1/1	1.00	0.03	15,15,15,15	0
6	NI	S	1551	1/1	1.00	0.02	18,18,18,18	0
3	SF4	A	1267	8/8	1.00	0.04	10,10,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.