wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 07:43 am BST

PDB ID	:	4UD6
Title	:	Structure of methylviologen-treated anaerobically purified D. fructosovorans NiFe-hydrogenase
Authors	:	Volbeda, A.; Martin, L.; Liebgott, P.-P.; Fontecilla-Camps, J.C.
Deposited on	:	2014-12-08
Resolution	:	2.12 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

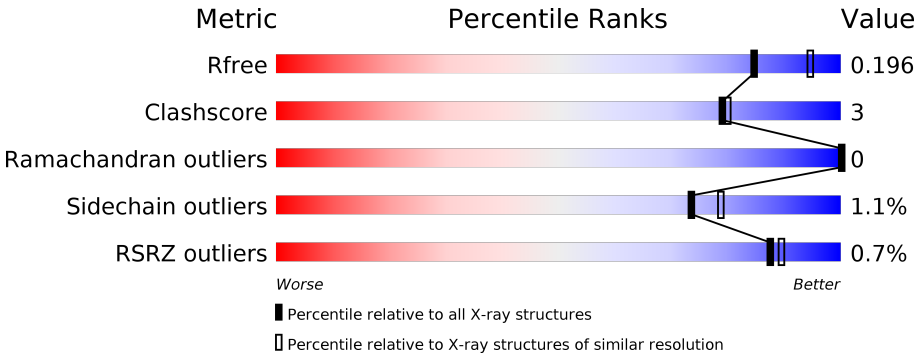
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 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	89% 10%
1	B	264	2% 93% 6%
1	C	264	93% 5%
2	Q	549	92% 7%
2	R	549	93% 6%
2	S	549	% 95%

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	Q	1563	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20531 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.

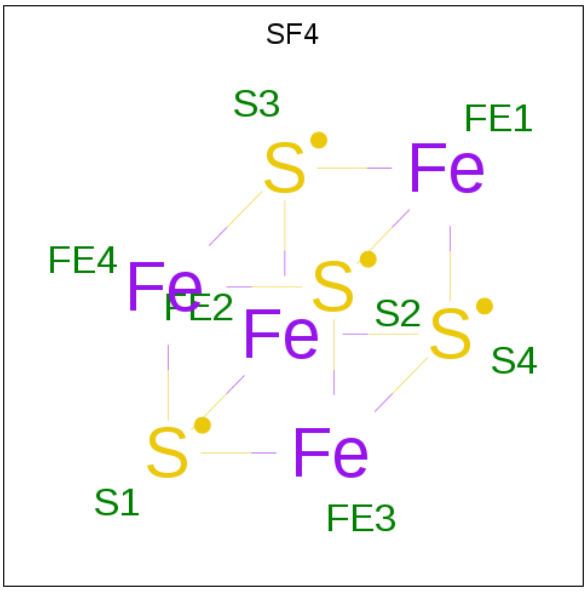
- Molecule 1 is a protein called HYDROGENASE (NIFE) SMALL SUBUNIT HYDA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1973	1256	330	372	15			
1	B	262	Total	C	N	O	S	0	2	0
			1980	1260	330	375	15			
1	C	260	Total	C	N	O	S	0	1	0
			1964	1251	328	370	15			

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

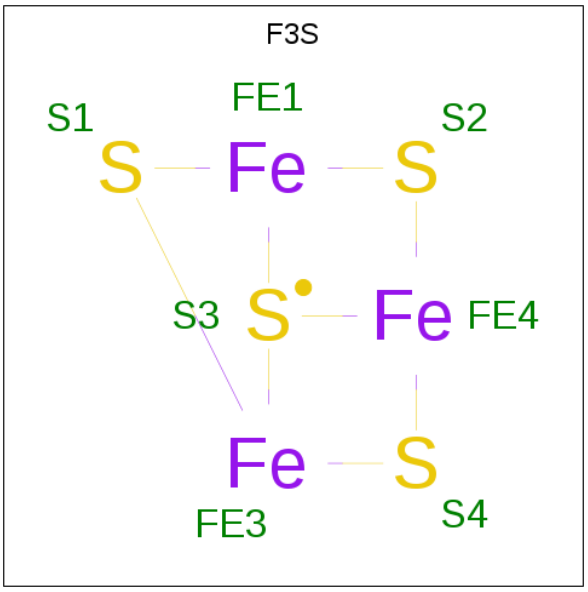
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	544	Total	C	N	O	S	0	9	0
			4195	2676	728	769	22			
2	R	545	Total	C	N	O	S	0	3	0
			4178	2663	724	769	22			
2	S	544	Total	C	N	O	S	0	1	0
			4166	2653	724	767	22			

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



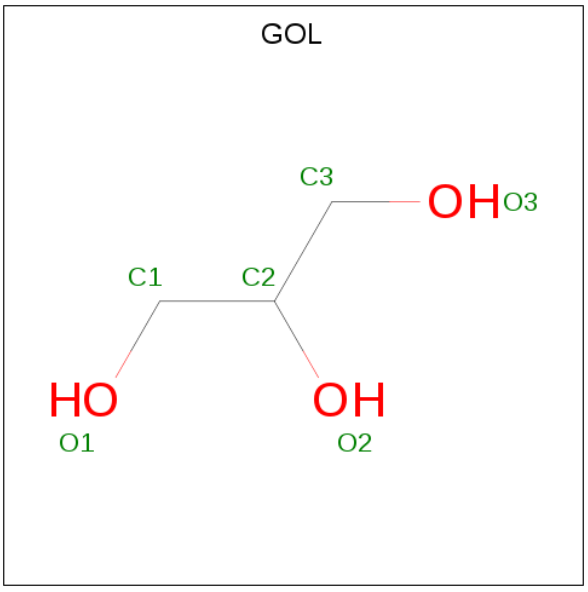
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0

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



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

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



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

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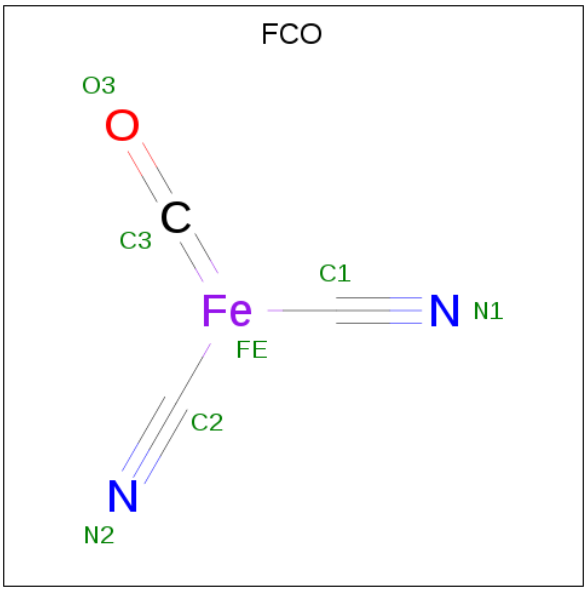
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0
5	R	1	Total C O 6 3 3	0	0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

- Molecule 9 is water.

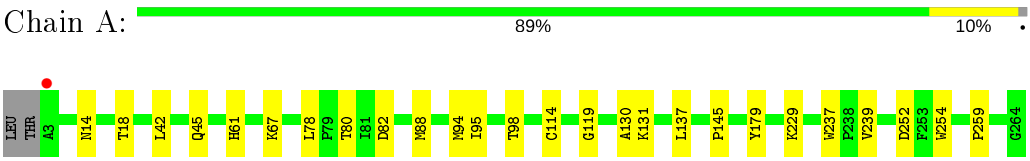
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	325	Total O 325 325	0	0
9	B	210	Total O 210 210	0	0
9	C	242	Total O 242 242	0	0
9	Q	444	Total O 444 444	0	0
9	R	389	Total O 389 389	0	0
9	S	279	Total O 279 279	0	0

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 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.

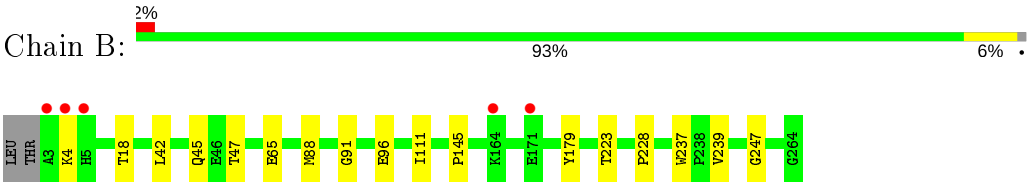
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain A:



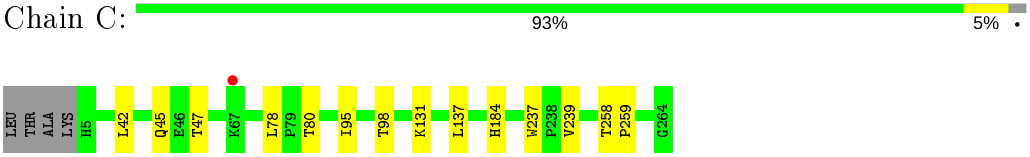
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:



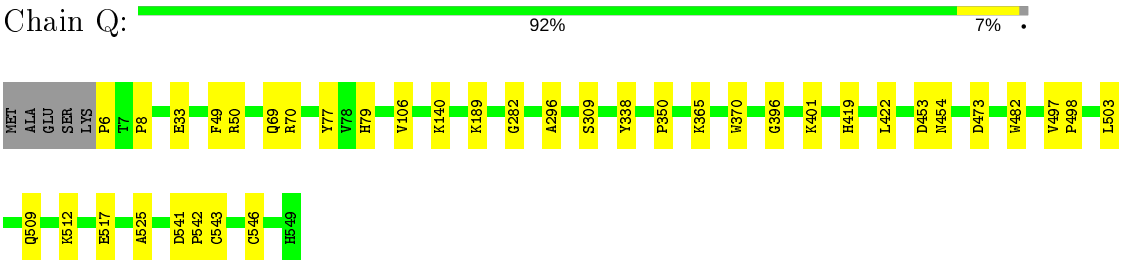
• Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain C:



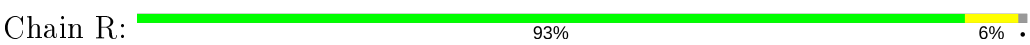
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

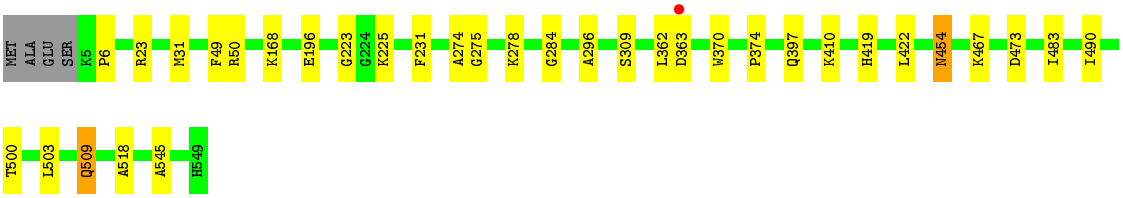
Chain Q:



• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

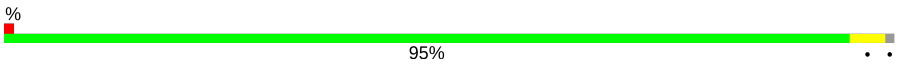
Chain R:

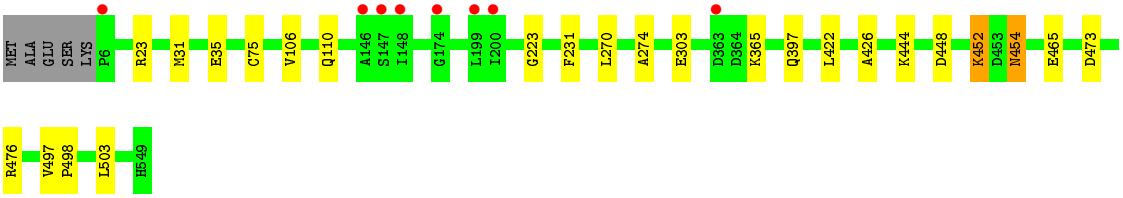




- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

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	64.94Å 99.56Å 183.94Å 90.00° 91.31° 90.00°	Depositor
Resolution (Å)	19.99 – 2.12 19.80 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.99-2.12) 99.2 (19.80-2.12)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.152 , 0.196 0.153 , 0.196	Depositor DCC
R_{free} test set	6657 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20531	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, NI, SF4, MG, F3S, 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	0.59	0/2027	0.68	1/2759 (0.0%)
1	B	0.50	0/2043	0.58	0/2781
1	C	0.50	0/2023	0.59	0/2754
2	Q	0.54	0/4335	0.65	1/5880 (0.0%)
2	R	0.52	0/4289	0.67	0/5821
2	S	0.47	0/4268	0.61	0/5792
All	All	0.52	0/18985	0.64	2/25787 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ASP	CB-CG-OD1	6.30	123.97	118.30
2	Q	50	ARG	NE-CZ-NH2	-5.38	117.61	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	1973	0	1911	16	0
1	B	1980	0	1918	12	0
1	C	1964	0	1906	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	4195	0	4192	23	0
2	R	4178	0	4152	26	0
2	S	4166	0	4138	14	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	1	0
4	A	7	0	0	0	0
4	B	7	0	0	1	0
4	C	7	0	0	0	0
5	A	18	0	24	1	0
5	Q	24	0	32	5	0
5	R	42	0	56	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	1	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	325	0	0	5	0
9	B	210	0	0	2	0
9	C	242	0	0	2	0
9	Q	444	0	0	10	0
9	R	389	0	0	9	0
9	S	279	0	0	2	0
All	All	20531	0	18337	102	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.

The worst 5 of 102 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)
9:Q:2291:HOH:O	2:R:6:PRO:HB3	1.75	0.86
5:R:1001:GOL:H11	9:R:2259:HOH:O	1.76	0.84
2:R:196:GLU:HG2	9:R:2172:HOH:O	1.81	0.81
1:B:65:GLU:HG3	9:B:2074:HOH:O	1.82	0.79
1:A:61:HIS:HE1	9:A:2093:HOH:O	1.70	0.74

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	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	C	259/264 (98%)	251 (97%)	8 (3%)	0	100	100
2	Q	550/549 (100%)	538 (98%)	12 (2%)	0	100	100
2	R	545/549 (99%)	531 (97%)	14 (3%)	0	100	100
2	S	542/549 (99%)	525 (97%)	17 (3%)	0	100	100
All	All	2418/2439 (99%)	2354 (97%)	64 (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%)	206 (99%)	2 (1%)	76	81
1	B	210/210 (100%)	208 (99%)	2 (1%)	76	81
1	C	208/210 (99%)	208 (100%)	0	100	100
2	Q	442/438 (101%)	438 (99%)	4 (1%)	78	83
2	R	436/438 (100%)	431 (99%)	5 (1%)	73	79
2	S	434/438 (99%)	425 (98%)	9 (2%)	53	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1938/1944 (100%)	1916 (99%)	22 (1%)	73 79

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	454	ASN
2	R	509	GLN
2	S	473	ASP
2	R	473	ASP
2	R	503	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	172	ASN
2	S	454	ASN
2	Q	509	GLN
1	A	172	ASN
2	Q	454	ASN

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	0.95	0	0,6,8	0.00	-
2	CSO	Q	543	2,7	3,6,7	0.85	0	0,6,8	0.00	-
2	CSO	S	543	2,7	3,6,7	0.72	0	0,6,8	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
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	R	543	CSO	N-CA-CB-SG
2	Q	543	CSO	N-CA-CB-SG
2	S	543	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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	1267	1	0,12,12	0.00	-	-		
5	GOL	Q	1564	-	5,5,5	0.43	0	5,5,5	0.45	0
5	GOL	R	1561	-	5,5,5	0.37	0	5,5,5	0.44	0
5	GOL	S	1561	-	5,5,5	0.49	0	5,5,5	0.29	0
5	GOL	R	1002	-	5,5,5	0.25	0	5,5,5	0.39	0
5	GOL	R	1004	-	5,5,5	0.41	0	5,5,5	0.58	0
3	SF4	B	1267	1	0,12,12	0.00	-	-		
3	SF4	C	1265	1	0,12,12	0.00	-	-		
3	SF4	A	1265	1	0,12,12	0.00	-	-		
6	FCO	Q	1550	2,7	0,6,6	0.00	-	-		
5	GOL	R	1563	-	5,5,5	0.44	0	5,5,5	0.40	0
5	GOL	Q	1563	-	5,5,5	0.26	0	5,5,5	0.27	0
3	SF4	C	1267	1	0,12,12	0.00	-	-		
5	GOL	Q	1561	-	5,5,5	0.21	0	5,5,5	0.32	0
5	GOL	Q	1562	-	5,5,5	0.30	0	5,5,5	0.28	0
5	GOL	R	1003	-	5,5,5	0.39	0	5,5,5	0.21	0
6	FCO	R	1550	2,7	0,6,6	0.00	-	-		
4	F3S	C	1266	1	0,9,9	0.00	-	-		
4	F3S	A	1266	1	0,9,9	0.00	-	-		
3	SF4	B	1265	1	0,12,12	0.00	-	-		
5	GOL	A	1273	-	5,5,5	0.59	0	5,5,5	0.85	0
6	FCO	S	1550	2,7	0,6,6	0.00	-	-		
5	GOL	R	1562	-	5,5,5	0.29	0	5,5,5	0.16	0
5	GOL	R	1001	-	5,5,5	0.37	0	5,5,5	0.24	0
5	GOL	A	1271	-	5,5,5	0.27	0	5,5,5	0.63	0
4	F3S	B	1266	1	0,9,9	0.00	-	-		
5	GOL	A	1272	-	5,5,5	0.54	0	5,5,5	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	1267	1	-	-	0/6/5/5
5	GOL	Q	1564	-	-	1/4/4/4	-
5	GOL	R	1561	-	-	0/4/4/4	-
5	GOL	S	1561	-	-	0/4/4/4	-
5	GOL	R	1002	-	-	0/4/4/4	-
3	SF4	B	1265	1	-	-	0/6/5/5
3	SF4	B	1267	1	-	-	0/6/5/5
3	SF4	C	1265	1	-	-	0/6/5/5
3	SF4	A	1265	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	1563	-	-	0/4/4/4	-
5	GOL	Q	1563	-	-	0/4/4/4	-
3	SF4	C	1267	1	-	-	0/6/5/5
5	GOL	Q	1561	-	-	0/4/4/4	-
5	GOL	Q	1562	-	-	0/4/4/4	-
5	GOL	R	1003	-	-	2/4/4/4	-
4	F3S	C	1266	1	-	-	0/3/3/3
4	F3S	A	1266	1	-	-	0/3/3/3
5	GOL	R	1004	-	-	1/4/4/4	-
5	GOL	A	1273	-	-	2/4/4/4	-
5	GOL	R	1562	-	-	2/4/4/4	-
5	GOL	R	1001	-	-	2/4/4/4	-
5	GOL	A	1271	-	-	0/4/4/4	-
4	F3S	B	1266	1	-	-	0/3/3/3
5	GOL	A	1272	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	1003	GOL	O1-C1-C2-O2
5	R	1003	GOL	O1-C1-C2-C3
5	R	1562	GOL	O2-C2-C3-O3
5	R	1004	GOL	C1-C2-C3-O3
5	A	1273	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1564	GOL	1	0
5	R	1004	GOL	2	0
3	C	1265	SF4	1	0
5	Q	1563	GOL	4	0
6	S	1550	FCO	1	0
5	R	1562	GOL	1	0
5	R	1001	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1271	GOL	1	0
4	B	1266	F3S	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.73	1 (0%) 92 93	14, 20, 31, 55	4 (1%)
1	B	262/264 (99%)	-0.35	5 (1%) 66 71	20, 30, 48, 63	6 (2%)
1	C	260/264 (98%)	-0.53	1 (0%) 92 93	19, 28, 44, 58	4 (1%)
2	Q	543/549 (98%)	-0.67	0 100 100	13, 22, 35, 47	6 (1%)
2	R	544/549 (99%)	-0.59	1 (0%) 95 95	16, 25, 38, 53	5 (0%)
2	S	543/549 (98%)	-0.30	8 (1%) 73 77	19, 34, 53, 68	6 (1%)
All	All	2414/2439 (98%)	-0.53	16 (0%) 87 89	13, 26, 46, 68	31 (1%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	5.0
1	A	3	ALA	3.3
1	B	4	LYS	3.0
2	S	200	ILE	2.9
2	S	174	GLY	2.6

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. The B-factors column lists the minimum, median, 95^{th} 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	0.98	0.07	20,21,23,23	1
2	CSO	Q	543	7/8	0.98	0.07	16,18,19,22	1
2	CSO	S	543	7/8	0.99	0.05	23,23,24,25	1

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. The B-factors column lists the minimum, median, 95^{th} 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	R	1002	6/6	0.80	0.20	51,55,56,58	0
5	GOL	R	1004	6/6	0.80	0.22	49,58,61,65	0
5	GOL	R	1562	6/6	0.82	0.35	62,67,69,72	0
5	GOL	A	1273	6/6	0.84	0.32	51,58,58,59	0
5	GOL	A	1271	6/6	0.84	0.20	42,46,51,55	0
5	GOL	Q	1563	6/6	0.86	0.24	48,49,51,58	0
5	GOL	R	1001	6/6	0.86	0.25	39,47,50,51	0
5	GOL	Q	1564	6/6	0.86	0.20	37,49,49,50	0
5	GOL	A	1272	6/6	0.86	0.17	46,47,48,50	0
5	GOL	R	1003	6/6	0.87	0.21	52,55,58,65	0
5	GOL	S	1561	6/6	0.96	0.07	24,25,27,28	0
5	GOL	Q	1561	6/6	0.96	0.12	23,24,25,28	0
5	GOL	Q	1562	6/6	0.96	0.09	22,27,28,29	0
8	MG	Q	1553	1/1	0.97	0.04	15,15,15,15	0
5	GOL	R	1563	6/6	0.97	0.08	26,27,28,29	0
4	F3S	C	1266	7/7	0.99	0.04	18,20,21,22	0
4	F3S	A	1266	7/7	0.99	0.05	15,15,16,17	0
8	MG	R	1553	1/1	0.99	0.02	19,19,19,19	0
3	SF4	B	1265	8/8	0.99	0.05	35,37,38,40	0
3	SF4	C	1267	8/8	0.99	0.04	17,19,19,20	0
3	SF4	C	1265	8/8	0.99	0.06	20,21,22,22	0
5	GOL	R	1561	6/6	0.99	0.06	23,24,24,25	0
3	SF4	B	1267	8/8	0.99	0.03	22,23,24,24	0
4	F3S	B	1266	7/7	0.99	0.05	28,30,30,31	0
8	MG	S	1553	1/1	0.99	0.03	25,25,25,25	0
7	NI	Q	1551	1/1	1.00	0.02	18,18,18,18	0
7	NI	R	1551	1/1	1.00	0.03	20,20,20,20	0
6	FCO	S	1550	7/7	1.00	0.05	22,22,23,24	0
6	FCO	R	1550	7/7	1.00	0.04	16,17,18,18	0
3	SF4	A	1265	8/8	1.00	0.05	17,18,18,20	0
6	FCO	Q	1550	7/7	1.00	0.05	15,16,17,18	0
3	SF4	A	1267	8/8	1.00	0.04	14,14,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NI	S	1551	1/1	1.00	0.03	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.