wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 02:33 pm BST

PDB ID	:	4UCW
Title	:	Structure of the T18V small subunit mutant of D. fructosovorans NiFe- hydrogenase
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Deposited on	:	2014-12-04
Resolution	:	2.30 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:

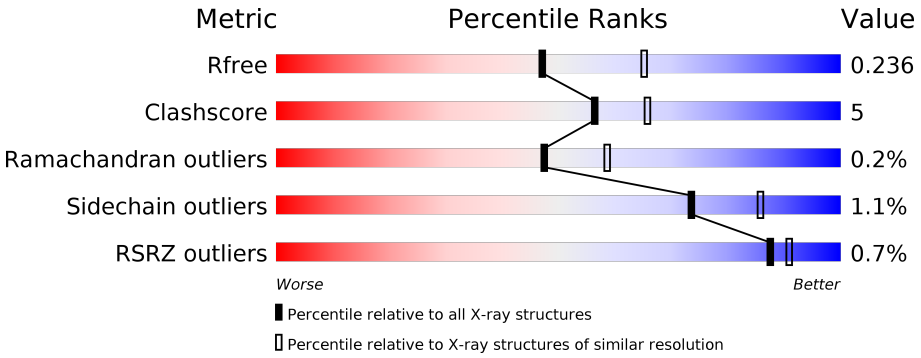
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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 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	88% 12%
1	B	264	87% 11% •
1	C	264	5% 80% 19% •
2	Q	563	86% 11% •
2	R	563	85% 12% •
2	S	563	% 84% 13% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19144 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	263	Total	C	N	O	S	0	1	0
			1981	1261	331	374	15			
1	B	260	Total	C	N	O	S	0	2	0
			1968	1253	327	373	15			
1	C	261	Total	C	N	O	S	0	1	0
			1970	1255	330	370	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	VAL	THR	engineered mutation	UNP E1K248
B	18	VAL	THR	engineered mutation	UNP E1K248
C	18	VAL	THR	engineered mutation	UNP E1K248

- 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	5	0
			4183	2665	724	772	22			
2	R	545	Total	C	N	O	S	0	1	0
			4174	2659	724	769	22			
2	S	545	Total	C	N	O	S	0	1	0
			4174	2657	725	770	22			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-13	ALA	-	expression tag	UNP E1K247
Q	-12	SER	-	expression tag	UNP E1K247
Q	-11	TRP	-	expression tag	UNP E1K247
Q	-10	SER	-	expression tag	UNP E1K247

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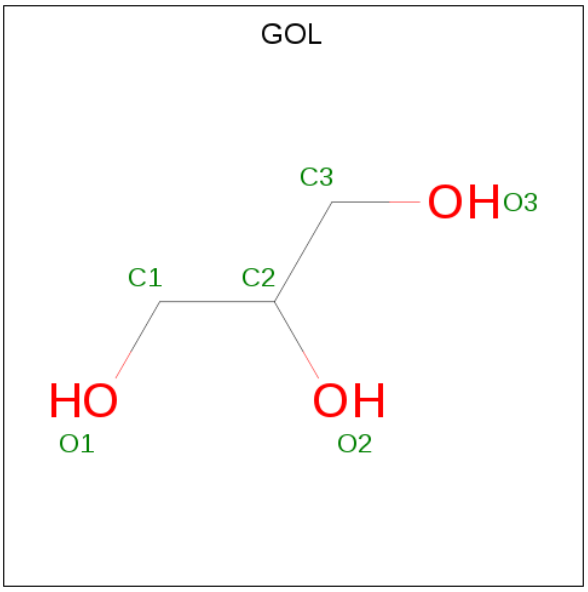
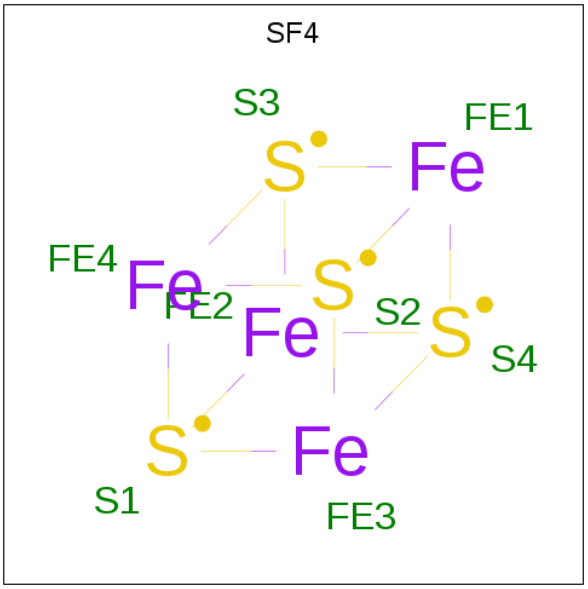
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-9	HIS	-	expression tag	UNP E1K247
Q	-8	PRO	-	expression tag	UNP E1K247
Q	-7	GLN	-	expression tag	UNP E1K247
Q	-6	PHE	-	expression tag	UNP E1K247
Q	-5	GLU	-	expression tag	UNP E1K247
Q	-4	LYS	-	expression tag	UNP E1K247
Q	-3	GLY	-	expression tag	UNP E1K247
Q	-2	ALA	-	expression tag	UNP E1K247
Q	-1	SER	-	expression tag	UNP E1K247
Q	0	GLY	-	expression tag	UNP E1K247
Q	1	ALA	-	expression tag	UNP E1K247
R	-13	ALA	-	expression tag	UNP E1K247
R	-12	SER	-	expression tag	UNP E1K247
R	-11	TRP	-	expression tag	UNP E1K247
R	-10	SER	-	expression tag	UNP E1K247
R	-9	HIS	-	expression tag	UNP E1K247
R	-8	PRO	-	expression tag	UNP E1K247
R	-7	GLN	-	expression tag	UNP E1K247
R	-6	PHE	-	expression tag	UNP E1K247
R	-5	GLU	-	expression tag	UNP E1K247
R	-4	LYS	-	expression tag	UNP E1K247
R	-3	GLY	-	expression tag	UNP E1K247
R	-2	ALA	-	expression tag	UNP E1K247
R	-1	SER	-	expression tag	UNP E1K247
R	0	GLY	-	expression tag	UNP E1K247
R	1	ALA	-	expression tag	UNP E1K247
S	-13	ALA	-	expression tag	UNP E1K247
S	-12	SER	-	expression tag	UNP E1K247
S	-11	TRP	-	expression tag	UNP E1K247
S	-10	SER	-	expression tag	UNP E1K247
S	-9	HIS	-	expression tag	UNP E1K247
S	-8	PRO	-	expression tag	UNP E1K247
S	-7	GLN	-	expression tag	UNP E1K247
S	-6	PHE	-	expression tag	UNP E1K247
S	-5	GLU	-	expression tag	UNP E1K247
S	-4	LYS	-	expression tag	UNP E1K247
S	-3	GLY	-	expression tag	UNP E1K247
S	-2	ALA	-	expression tag	UNP E1K247
S	-1	SER	-	expression tag	UNP E1K247
S	0	GLY	-	expression tag	UNP E1K247
S	1	ALA	-	expression tag	UNP E1K247

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



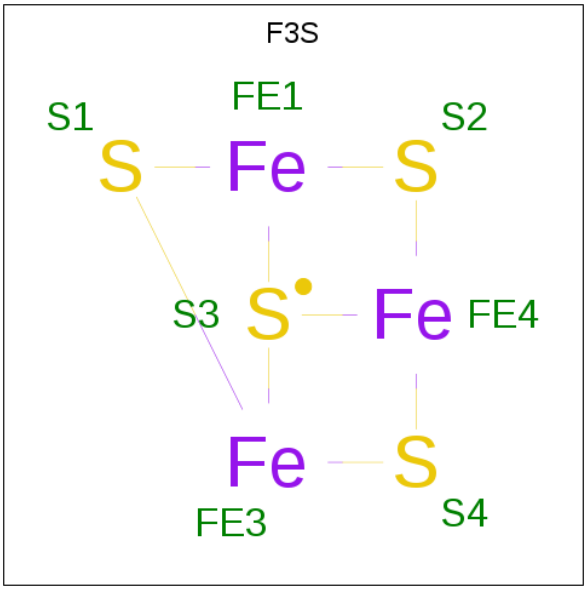
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	Q	1	Total C O 6 3 3	0	0
3	Q	1	Total C O 6 3 3	0	0
3	R	1	Total C O 6 3 3	0	0
3	S	1	Total C O 6 3 3	0	0

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



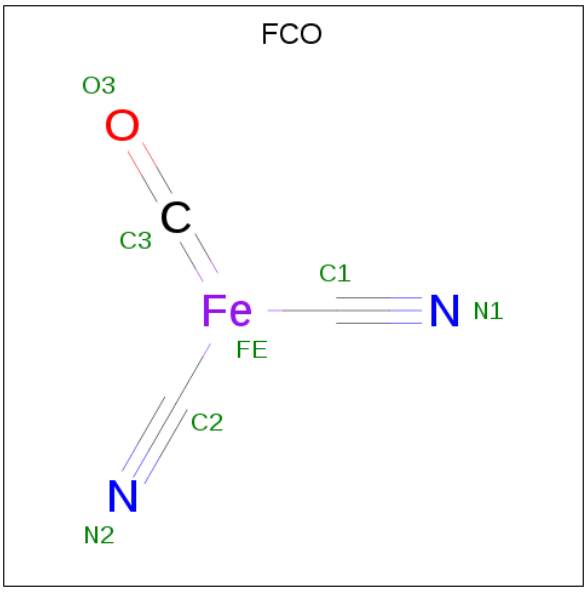
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	C	1	Total Fe S 8 4 4	0	0
4	C	1	Total Fe S 8 4 4	0	0

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



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

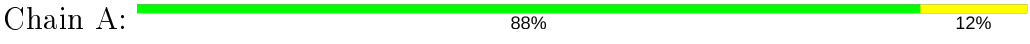
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	95	Total O 95 95	0	0
9	B	77	Total O 77 77	0	0
9	C	57	Total O 57 57	0	0
9	Q	141	Total O 141 141	0	0
9	R	102	Total O 102 102	0	0
9	S	96	Total O 96 96	0	0

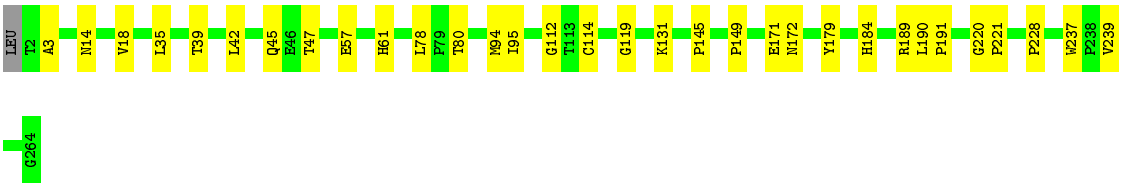
3 Residue-property plots (i)

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

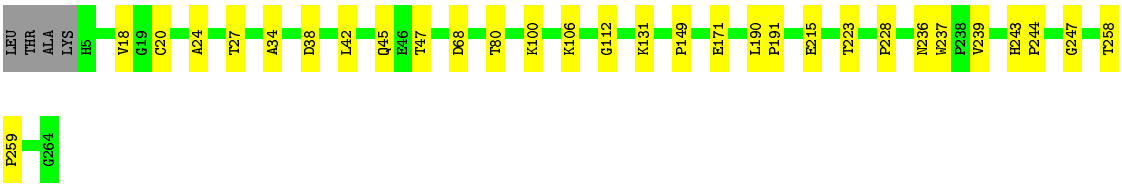
Chain A:





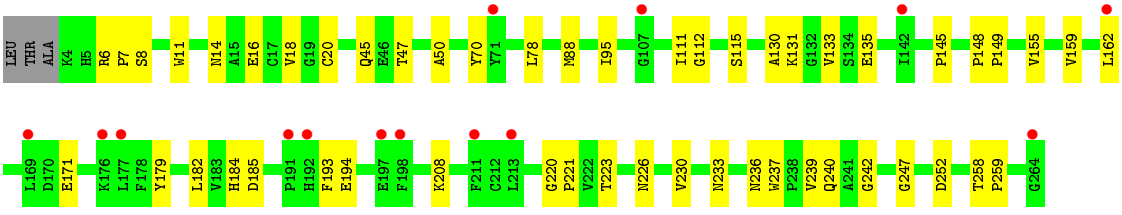
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

Chain B:



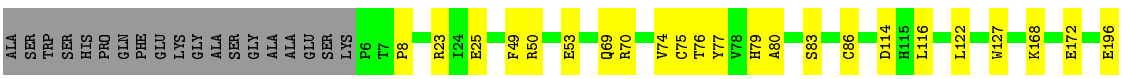
- Molecule 1: HYDROGENASE (NIFE) SMALL SUBUNIT HYDA

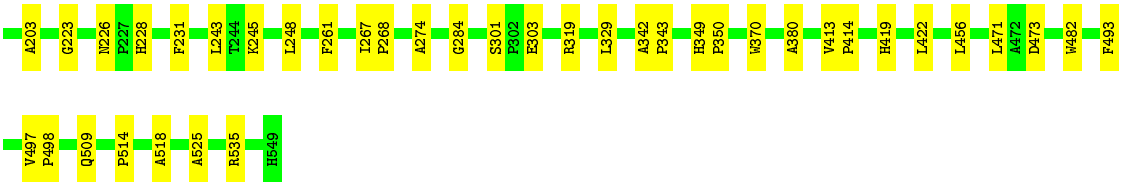
Chain C:



- Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

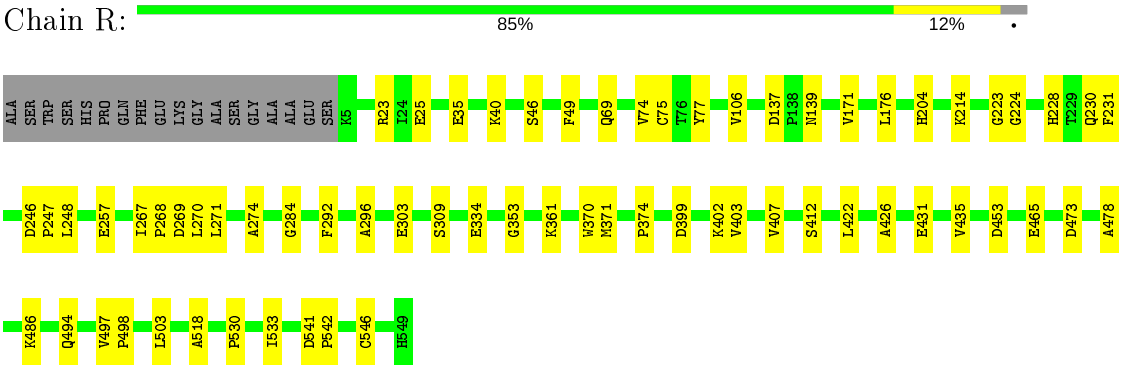
Chain Q:





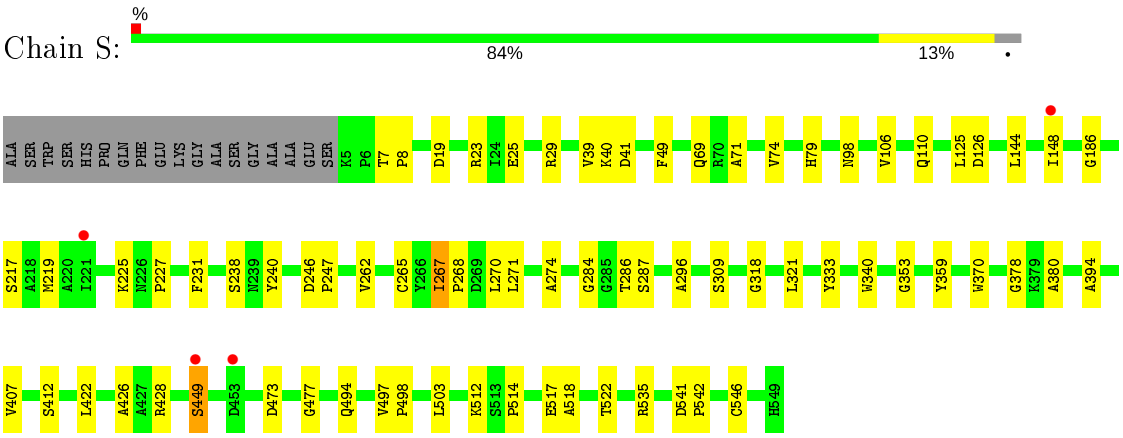
• Molecule 2: NICKEL-DEPENDENT HYDROGENASE LARGE SUBUNIT

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	62.20Å 99.59Å 181.84Å 90.00° 92.47° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 39.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (25.00-2.30) 93.5 (39.06-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.192 , 0.236 0.192 , 0.236	Depositor DCC
R_{free} test set	4583 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 9.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19144	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 3.54% 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	0.68	0/2040	0.73	1/2776 (0.0%)
1	B	0.61	0/2032	0.70	0/2767
1	C	0.57	0/2030	0.67	0/2765
2	Q	0.66	0/4303	0.75	3/5839 (0.1%)
2	R	0.57	0/4275	0.71	0/5802
2	S	0.59	0/4276	0.71	0/5804
All	All	0.61	0/18956	0.72	4/25753 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	114	ASP	CB-CG-OD1	6.98	124.58	118.30
2	Q	50	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	Q	70	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	189	ARG	NE-CZ-NH2	-5.06	117.77	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	1981	0	1916	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1968	0	1903	16	0
1	C	1970	0	1904	34	0
2	Q	4183	0	4159	38	0
2	R	4174	0	4145	40	0
2	S	4174	0	4141	47	0
3	A	6	0	8	0	0
3	Q	12	0	16	1	0
3	R	6	0	8	0	0
3	S	6	0	8	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	1	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
5	C	7	0	0	1	0
6	Q	7	0	0	1	0
6	R	7	0	0	1	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	95	0	0	1	0
9	B	77	0	0	1	0
9	C	57	0	0	2	0
9	Q	141	0	0	2	0
9	R	102	0	0	0	0
9	S	96	0	0	2	0
All	All	19144	0	18208	183	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 5.

The worst 5 of 183 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:S:186:GLY:HA3	9:S:2045:HOH:O	1.74	0.86
2:R:214:LYS:HE3	2:R:257:GLU:OE2	1.79	0.82
2:R:25:GLU:CG	2:R:74:VAL:HG21	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:267:ILE:HG23	2:S:268:PRO:HD3	1.71	0.71
2:R:25:GLU:HG3	2:R:74:VAL:HG21	1.75	0.69

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	262/264 (99%)	252 (96%)	8 (3%)	2 (1%)	19 23
1	B	260/264 (98%)	251 (96%)	8 (3%)	1 (0%)	34 42
1	C	260/264 (98%)	243 (94%)	16 (6%)	1 (0%)	34 42
2	Q	546/563 (97%)	531 (97%)	15 (3%)	0	100 100
2	R	543/563 (96%)	525 (97%)	18 (3%)	0	100 100
2	S	543/563 (96%)	523 (96%)	20 (4%)	0	100 100
All	All	2414/2481 (97%)	2325 (96%)	85 (4%)	4 (0%)	47 58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	18	VAL
1	B	18	VAL
1	C	18	VAL

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	209/210 (100%)	207 (99%)	2 (1%)	76	87
1	C	208/210 (99%)	205 (99%)	3 (1%)	67	81
2	Q	439/447 (98%)	436 (99%)	3 (1%)	84	92
2	R	435/447 (97%)	429 (99%)	6 (1%)	67	81
2	S	435/447 (97%)	428 (98%)	7 (2%)	62	78
All	All	1935/1971 (98%)	1914 (99%)	21 (1%)	73	86

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	402	LYS
2	R	453	ASP
2	S	449	SER
2	R	361	LYS
2	S	473	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
2	S	123	HIS
1	C	172	ASN
1	A	172	ASN
2	R	123	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	R	75	2,7,6	3,6,7	1.18	0	0,6,8	0.00	-
2	CSO	S	75	2,7,6	3,6,7	0.87	0	0,6,8	0.00	-
2	CSO	Q	75	2,7,6	3,6,7	0.46	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	75	2,7,6	-	0/1/5/7	-
2	CSO	S	75	2,7,6	-	0/1/5/7	-
2	CSO	Q	75	2,7,6	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	75	CSO	1	0
2	Q	75	CSO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
6	FCO	R	1550	2	0,6,6	0.00	-	-		
3	GOL	R	1563	-	5,5,5	0.58	0	5,5,5	0.47	0
4	SF4	B	1267	1	0,12,12	0.00	-	-		
4	SF4	C	1265	1	0,12,12	0.00	-	-		
4	SF4	A	1265	1	0,12,12	0.00	-	-		
4	SF4	A	1267	1	0,12,12	0.00	-	-		
5	F3S	A	1266	1	0,9,9	0.00	-	-		
5	F3S	C	1266	1	0,9,9	0.00	-	-		
5	F3S	B	1266	1	0,9,9	0.00	-	-		
3	GOL	S	1561	-	5,5,5	0.45	0	5,5,5	0.65	0
3	GOL	Q	1561	-	5,5,5	0.37	0	5,5,5	0.57	0
4	SF4	C	1267	1	0,12,12	0.00	-	-		
3	GOL	Q	1562	-	5,5,5	0.34	0	5,5,5	0.37	0
6	FCO	S	1550	2	0,6,6	0.00	-	-		
4	SF4	B	1265	1	0,12,12	0.00	-	-		
6	FCO	Q	1550	2	0,6,6	0.00	-	-		
3	GOL	A	271	-	5,5,5	0.51	0	5,5,5	1.53	1 (20%)

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	GOL	R	1563	-	-	0/4/4/4	-
4	SF4	B	1267	1	-	-	0/6/5/5
4	SF4	C	1265	1	-	-	0/6/5/5
4	SF4	A	1265	1	-	-	0/6/5/5
4	SF4	A	1267	1	-	-	0/6/5/5
5	F3S	A	1266	1	-	-	0/3/3/3
5	F3S	C	1266	1	-	-	0/3/3/3
5	F3S	B	1266	1	-	-	0/3/3/3
3	GOL	S	1561	-	-	4/4/4/4	-
3	GOL	Q	1561	-	-	0/4/4/4	-
4	SF4	C	1267	1	-	-	0/6/5/5
3	GOL	Q	1562	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	1265	1	-	-	0/6/5/5
3	GOL	A	271	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	271	GOL	O1-C1-C2	-2.15	99.88	110.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	271	GOL	O1-C1-C2-C3
3	A	271	GOL	C1-C2-C3-O3
3	S	1561	GOL	O1-C1-C2-C3
3	S	1561	GOL	C1-C2-C3-O3
3	S	1561	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	1550	FCO	1	0
4	C	1265	SF4	1	0
5	C	1266	F3S	1	0
3	Q	1562	GOL	1	0
6	Q	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

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	263/264 (99%)	-0.56	0 100 100	10, 20, 34, 66	7 (2%)
1	B	260/264 (98%)	-0.53	0 100 100	14, 22, 35, 61	7 (2%)
1	C	261/264 (98%)	0.21	14 (5%) 25 32	21, 46, 81, 102	5 (1%)
2	Q	543/563 (96%)	-0.61	0 100 100	9, 19, 31, 43	12 (2%)
2	R	544/563 (96%)	-0.42	0 100 100	14, 28, 47, 69	12 (2%)
2	S	544/563 (96%)	-0.18	4 (0%) 87 91	15, 32, 59, 82	14 (2%)
All	All	2415/2481 (97%)	-0.37	18 (0%) 87 91	9, 25, 56, 102	57 (2%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	PRO	4.5
1	C	176	LYS	4.5
1	C	197	GLU	3.6
2	S	449	SER	3.6
1	C	177	LEU	3.4

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	Q	75	7/8	0.96	0.11	8,9,11,13	0
2	CSO	R	75	7/8	0.98	0.08	13,14,15,15	0
2	CSO	S	75	7/8	0.99	0.06	19,21,24,25	0

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
3	GOL	A	271	6/6	0.91	0.18	23,26,28,30	0
3	GOL	S	1561	6/6	0.93	0.15	20,24,26,29	0
3	GOL	Q	1562	6/6	0.94	0.13	20,22,25,25	0
8	MG	R	1553	1/1	0.94	0.08	17,17,17,17	0
4	SF4	C	1265	8/8	0.96	0.07	66,70,75,76	0
3	GOL	Q	1561	6/6	0.97	0.10	16,17,18,19	0
3	GOL	R	1563	6/6	0.97	0.09	14,17,18,19	0
8	MG	Q	1553	1/1	0.97	0.07	13,13,13,13	0
4	SF4	A	1265	8/8	0.98	0.09	20,21,22,22	0
5	F3S	C	1266	7/7	0.98	0.05	42,44,47,49	0
8	MG	S	1553	1/1	0.98	0.03	19,19,19,19	0
5	F3S	B	1266	7/7	0.99	0.06	16,17,17,18	0
7	NI	S	1551	1/1	0.99	0.05	23,23,23,23	0
4	SF4	B	1265	8/8	0.99	0.08	18,19,20,20	0
4	SF4	A	1267	8/8	0.99	0.09	10,11,11,13	0
7	NI	Q	1551	1/1	0.99	0.05	13,13,13,13	0
5	F3S	A	1266	7/7	0.99	0.06	14,15,17,17	0
4	SF4	C	1267	8/8	0.99	0.07	27,30,34,36	0
6	FCO	Q	1550	7/7	0.99	0.08	11,12,15,18	0
6	FCO	S	1550	7/7	0.99	0.07	16,17,17,17	0
6	FCO	R	1550	7/7	0.99	0.09	14,15,16,16	0
7	NI	R	1551	1/1	0.99	0.06	17,17,17,17	0
4	SF4	B	1267	8/8	0.99	0.08	14,15,16,17	0

6.5 Other polymers (i)

There are no such residues in this entry.