Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 04:11 pm GMT

PDB ID	:	5MDL
Title	:	Crystal structure of an O2-tolerant [NiFe]-hydrogenase from Ralstonia eutropha in its O2-derivatized form by a "soak-and-freeze" derivatization method
Authors	:	Kalms, J.; Schmidt, A.; Scheerer, P.
Deposited on	:	2016-11-11
Resolution	:	1.41 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:

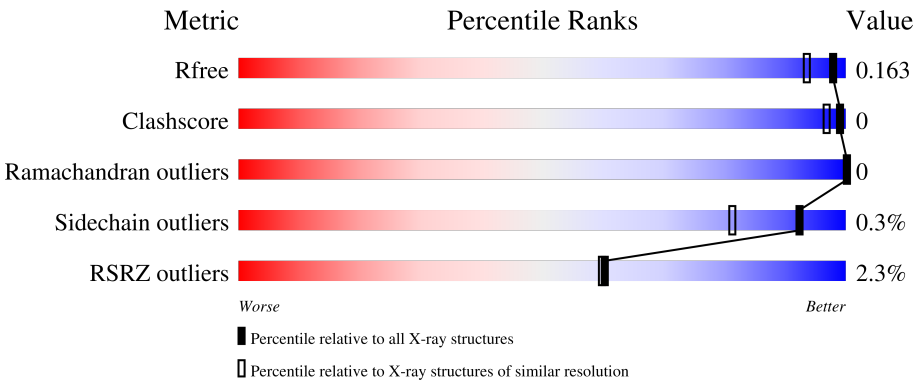
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	L	603	2% 99%
2	S	328	2% 81% 18%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 7551 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 Uptake hydrogenase large subunit;HOXG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	600	4774	3032	841	878	23	0	15	0

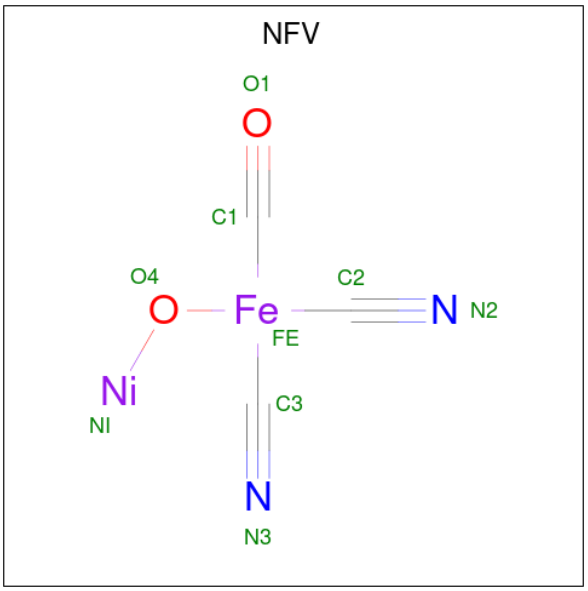
- Molecule 2 is a protein called Uptake hydrogenase small subunit;HOXK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	269	2117	1350	357	389	21	0	7	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	318	ARG	-	expression tag	UNP P31892
S	319	SER	-	expression tag	UNP P31892
S	320	ALA	-	expression tag	UNP P31892
S	321	TRP	-	expression tag	UNP P31892
S	322	SER	-	expression tag	UNP P31892
S	323	HIS	-	expression tag	UNP P31892
S	324	PRO	-	expression tag	UNP P31892
S	325	GLN	-	expression tag	UNP P31892
S	326	PHE	-	expression tag	UNP P31892
S	327	GLU	-	expression tag	UNP P31892
S	328	LYS	-	expression tag	UNP P31892

- Molecule 3 is NI-FE OXIDIZED ACTIVE CENTER (three-letter code: NFV) (formula: $C_3FeN_2NiO_2$).

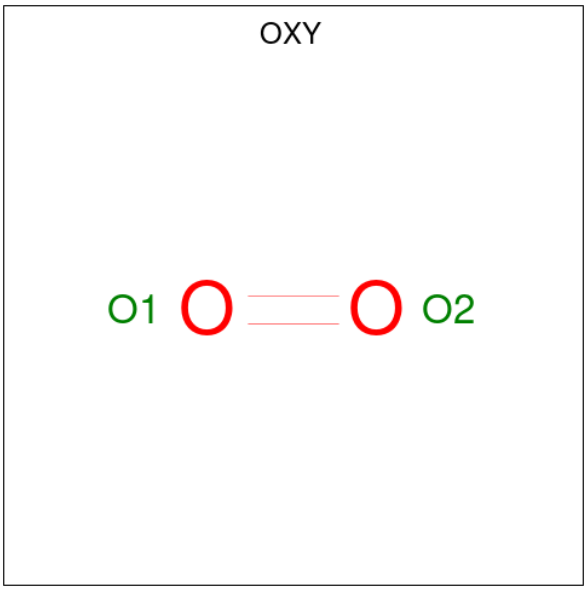


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	N	Ni	O		
3	L	1	9	3	1	2	1	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

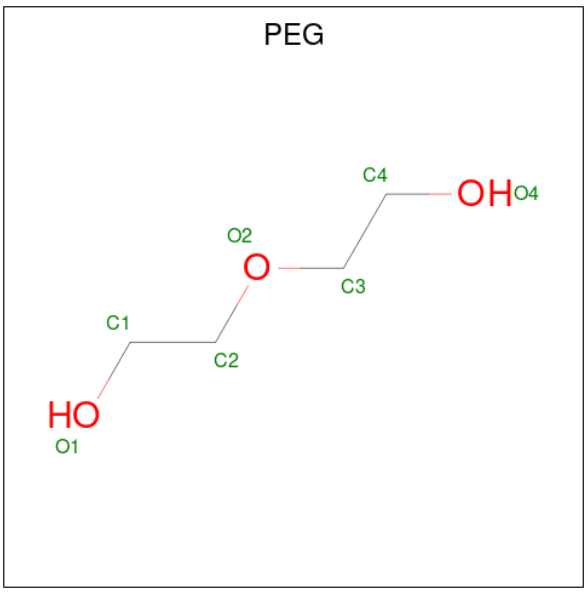
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	L	1	1	1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



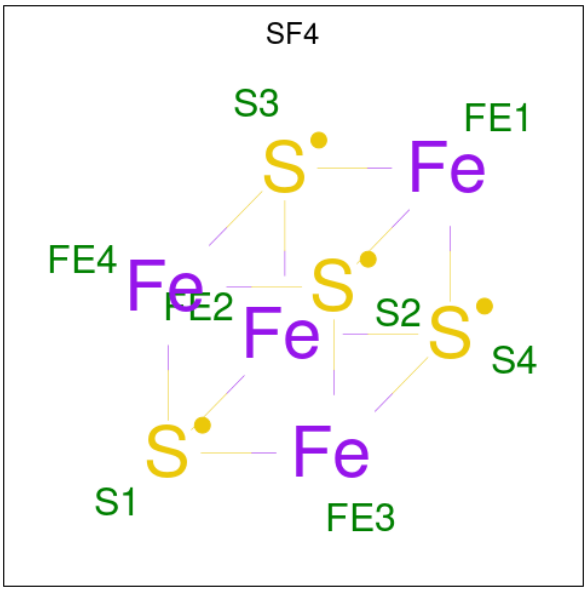
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total O 2 2	0	0
5	L	1	Total O 2 2	0	0
5	L	1	Total O 2 2	0	0
5	S	1	Total O 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



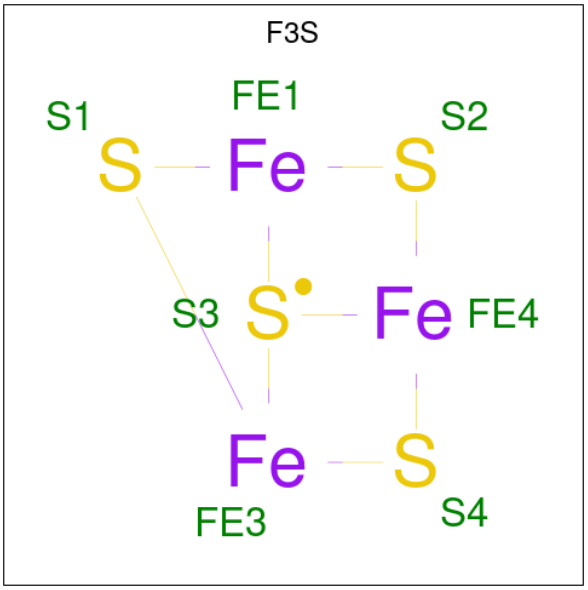
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 7 4 3	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



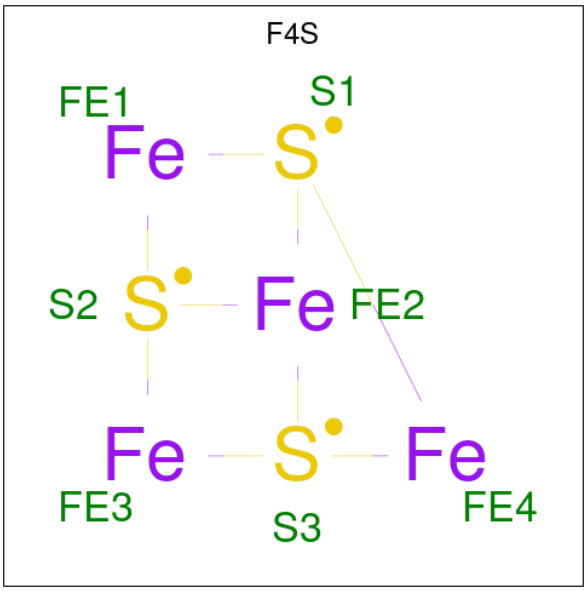
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	S	1	8	4	4	0	0

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	S	1	7	3	4	0	0

- Molecule 9 is FE4-S3 CLUSTER (three-letter code: F4S) (formula: Fe_4S_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	S	1	Total Fe S 7 4 3	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	S	1	Total Cl 1 1	0	0

- Molecule 11 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	S	1	Total O 1 1	0	0

- Molecule 12 is water.

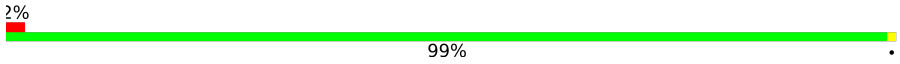
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	414	Total O 420 420	0	6
12	S	189	Total O 191 191	0	2

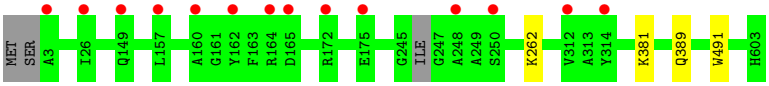
3 Residue-property plots (i)

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: Uptake hydrogenase large subunit;HOXG

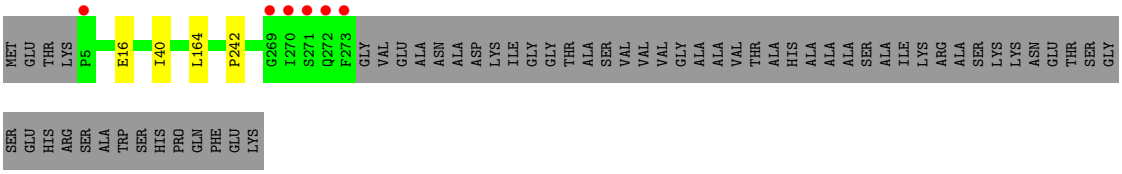
Chain L:





• Molecule 2: Uptake hydrogenase small subunit;HOXK

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.13Å 95.57Å 119.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 1.41 47.78 – 1.41	Depositor EDS
% Data completeness (in resolution range)	96.1 (47.78-1.41) 96.1 (47.78-1.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.132 , 0.163 0.132 , 0.163	Depositor DCC
R_{free} test set	7824 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7551	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: PEG, F3S, SF4, F4S, O, OXY, MG, NFV, CL

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	L	0.40	0/4937	0.61	0/6725
2	S	0.40	0/2195	0.59	0/2975
All	All	0.40	0/7132	0.61	0/9700

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	L	4774	0	4677	2	0
2	S	2117	0	2072	2	0
3	L	9	0	0	0	0
4	L	1	0	0	0	0
5	L	6	0	0	0	0
5	S	2	0	0	0	0
6	L	7	0	10	0	0
7	S	8	0	0	0	0
8	S	7	0	0	0	0
9	S	7	0	0	0	0
10	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	S	1	0	0	0	0
12	L	420	0	0	0	0
12	S	191	0	0	0	0
All	All	7551	0	6759	4	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 0.

All (4) 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)
1:L:381[B]:LYS:HB2	1:L:389[B]:GLN:HB3	1.97	0.47
2:S:40:ILE:CG2	2:S:164:LEU:HD11	2.48	0.44
1:L:262:LYS:HB2	1:L:491:TRP:CE2	2.52	0.43
2:S:40:ILE:HG23	2:S:164:LEU:HD11	2.02	0.41

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	L	612/603 (102%)	599 (98%)	13 (2%)	0	100	100
2	S	274/328 (84%)	265 (97%)	9 (3%)	0	100	100
All	All	886/931 (95%)	864 (98%)	22 (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	L	505/498 (101%)	505 (100%)	0	100	100
2	S	231/269 (86%)	228 (99%)	3 (1%)	69	41
All	All	736/767 (96%)	733 (100%)	3 (0%)	92	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	16[A]	GLU
2	S	16[B]	GLU
2	S	242	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	PEG	L	706	-	6,6,6	0.44	0	5,5,5	0.33	0
9	F4S	S	1003	2,11	0,9,9	-	-	-		
5	OXY	S	1004	-	1,1,1	0.13	0	-		
8	F3S	S	1002	2	0,9,9	-	-	-		
5	OXY	L	704	-	1,1,1	0.13	0	-		
5	OXY	L	703	-	1,1,1	0.08	0	-		
7	SF4	S	1001	2	0,12,12	-	-	-		
3	NFV	L	701	1	3,8,8	6.68	1 (33%)	-		
5	OXY	L	705	-	1,1,1	0.16	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
7	SF4	S	1001	2	-	-	0/6/5/5
6	PEG	L	706	-	-	3/4/4/4	-
8	F3S	S	1002	2	-	-	0/3/3/3
9	F4S	S	1003	2,11	-	-	0/4/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	701	NFV	O1-C1	11.45	1.36	1.16

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	706	PEG	O1-C1-C2-O2
6	L	706	PEG	C4-C3-O2-C2
6	L	706	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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	L	600/603 (99%)	-0.09	14 (2%)	60	60	11, 18, 32, 41	3 (0%)
2	S	269/328 (82%)	-0.22	6 (2%)	62	61	12, 19, 28, 38	5 (1%)
All	All	869/931 (93%)	-0.13	20 (2%)	60	60	11, 18, 31, 41	8 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	272	GLN	5.0
2	S	271	SER	3.7
2	S	269	GLY	3.6
2	S	270	ILE	3.4
1	L	250	SER	3.0
1	L	162	TYR	2.9
2	S	5	PRO	2.8
1	L	149	GLN	2.7
1	L	160	ALA	2.6
2	S	273	PHE	2.6
1	L	165	ASP	2.5
1	L	172	ARG	2.4
1	L	3	ALA	2.3
1	L	175	GLU	2.3
1	L	164[A]	ARG	2.1
1	L	248	ALA	2.1
1	L	314	TYR	2.1
1	L	157	LEU	2.1
1	L	312	VAL	2.0
1	L	26	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
6	PEG	L	706	7/7	0.82	0.23	26,27,31,32	7
5	OXY	L	704	2/2	0.93	0.29	26,26,26,28	2
11	O	S	1006	1/1	0.93	0.33	19,19,19,19	1
5	OXY	S	1004	2/2	0.96	0.18	30,30,30,30	2
5	OXY	L	705	2/2	0.97	0.21	28,28,28,29	2
5	OXY	L	703	2/2	0.98	0.16	27,27,27,29	0
3	NFV	L	701	9/9	0.99	0.10	12,13,15,16	0
4	MG	L	702	1/1	0.99	0.07	14,14,14,14	0
8	F3S	S	1002	7/7	1.00	0.07	13,13,14,14	0
9	F4S	S	1003	7/7	1.00	0.05	13,14,15,20	0
10	CL	S	1005	1/1	1.00	0.04	21,21,21,21	0
7	SF4	S	1001	8/8	1.00	0.05	16,17,18,19	0

6.5 Other polymers (i)

There are no such residues in this entry.