



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:52 PM UTC

PDB ID : 5MDL / pdb_00005mdl
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

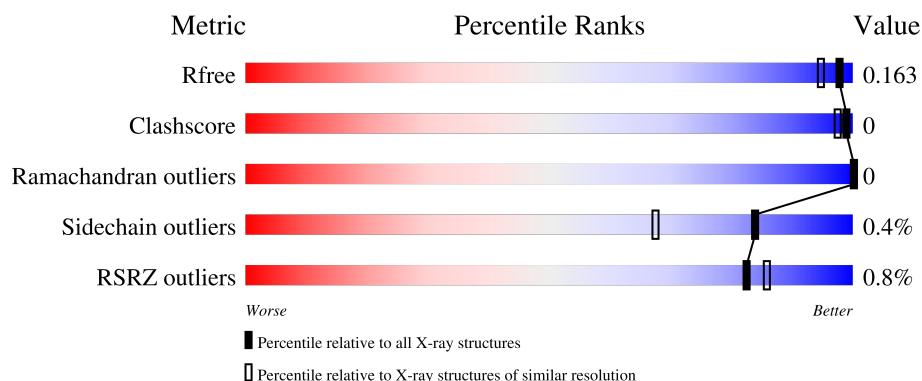
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

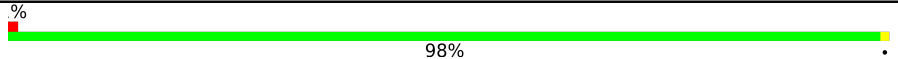
The reported resolution of this entry is 1.41 Å.

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}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (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 $\leq 5\%$. 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	 98%
2	S	328	 81% 18%

2 Entry composition

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
1	L	600	Total	C	N	O	S	0	15	0
			4774	3032	841	878	23			

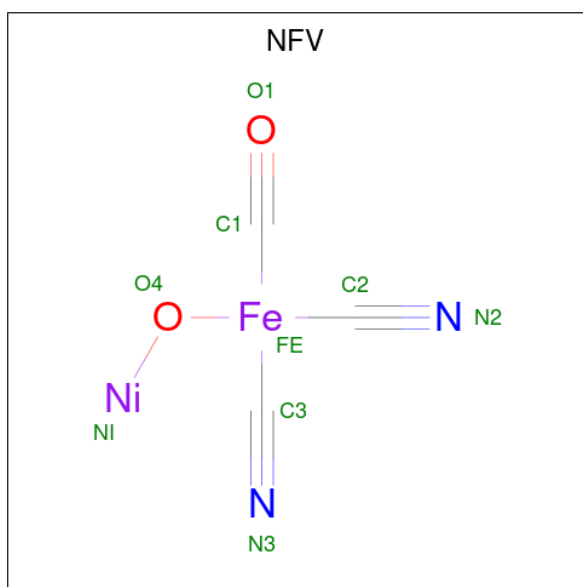
- Molecule 2 is a protein called Uptake hydrogenase small subunit;HOXK.

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

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 (CCD ID: NFV) (formula: C₃FeN₂NiO₂).

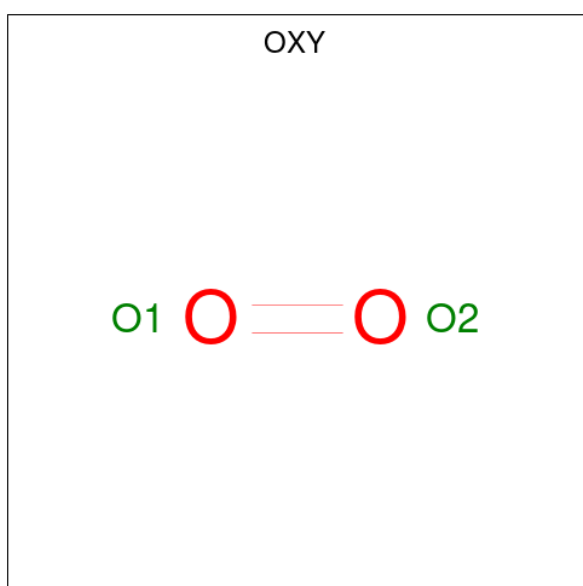


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	L	1	Total	C	Fe	N	Ni	O	0	0
			9	3	1	2	1	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

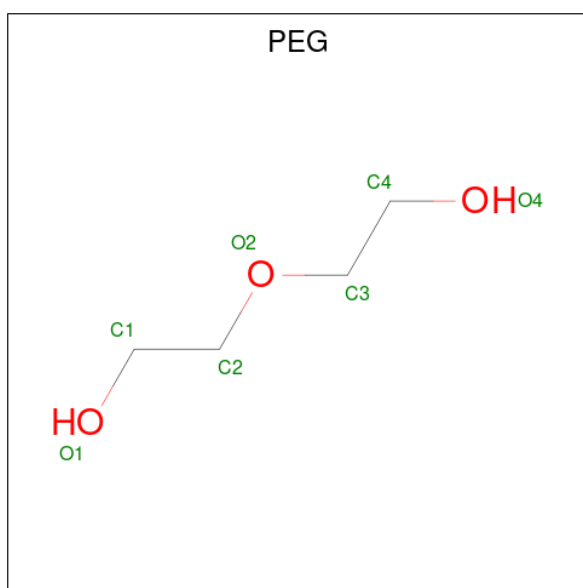
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Mg	0	0
			1	1		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



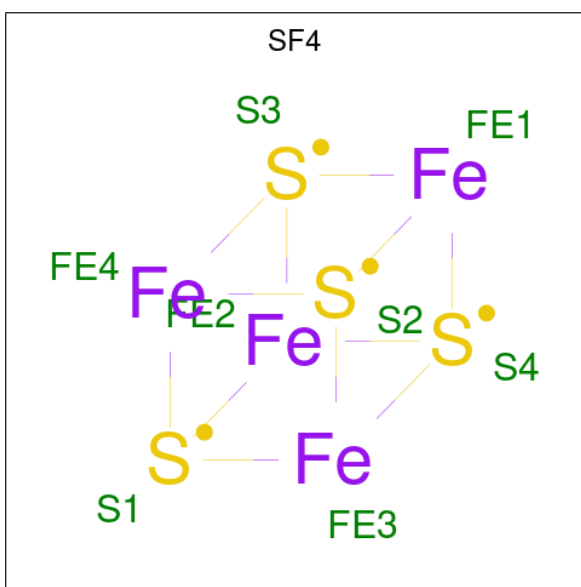
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total O 2 2	0	0
5	L	1	Total O 2 2	0	0
5	L	1	Total O 2 2	0	0
5	S	1	Total O 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



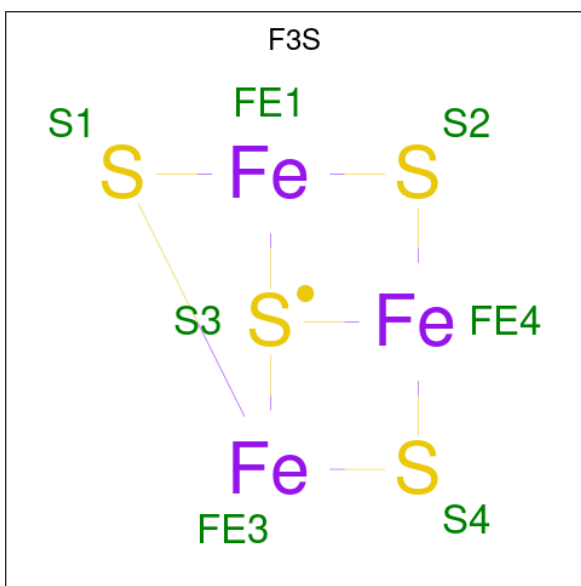
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 7 4 3	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



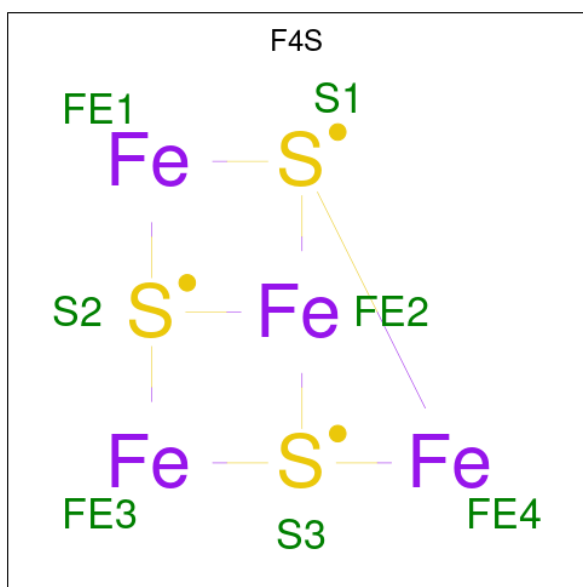
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	S	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 9 is FE4-S3 CLUSTER (CCD ID: F4S) (formula: Fe_4S_3).



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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 11 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 12 is water.

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

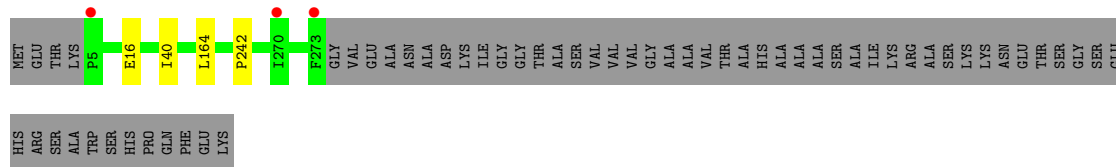
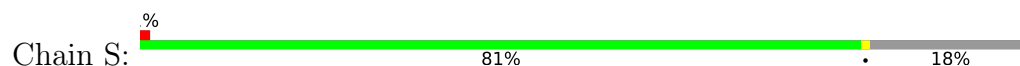
3 Residue-property plots [i](#)

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



- Molecule 2: Uptake hydrogenase small subunit;HOXK



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.84%)	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)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SF4, MG, NFV, F4S, CL, O, OXY, F3S, PEG

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	0.54	0/4937	0.69	0/6725
2	S	0.56	0/2195	0.71	0/2975
All	All	0.55	0/7132	0.70	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	3	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	5	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 (5) 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
1:L:244:ASP:O	1:L:245:GLY:C	2.60	0.44
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 ⓘ

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%)	504 (100%)	1 (0%)	87	73
2	S	231/269 (86%)	228 (99%)	3 (1%)	61	29
All	All	736/767 (96%)	732 (100%)	4 (0%)	84	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	390	ILE
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. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	343	GLN
1	L	443	GLN
1	L	497	ASN
2	S	54	HIS
2	S	184	GLN
2	S	272	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
5	OXY	S	1004	-	1,1,1	0.15	0	-		
8	F3S	S	1002	2	0,9,9	-	-	-		
7	SF4	S	1001	2	0,12,12	-	-	-		
5	OXY	L	703	-	1,1,1	0.11	0	-		
5	OXY	L	705	-	1,1,1	0.18	0	-		
5	OXY	L	704	-	1,1,1	0.15	0	-		
3	NFV	L	701	1	3,8,8	5.80	1 (33%)	-		
6	PEG	L	706	-	6,6,6	0.45	0	5,5,5	0.33	0
9	F4S	S	1003	11,2	0,9,9	-	-	-		

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
6	PEG	L	706	-	-	3/4/4/4	-
8	F3S	S	1002	2	-	-	0/3/3/3
7	SF4	S	1001	2	-	-	0/6/5/5
9	F4S	S	1003	11,2	-	-	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	9.91	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%)	-0.27	4 (0%) 84 87	8, 17, 31, 41	18 (3%)
2	S	269/328 (82%)	-0.21	3 (1%) 78 81	10, 18, 28, 36	12 (4%)
All	All	869/931 (93%)	-0.25	7 (0%) 82 86	8, 18, 30, 41	30 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	243	LEU	4.1
2	S	273	PHE	3.6
1	L	245	GLY	3.5
2	S	270	ILE	2.8
2	S	5	PRO	2.5
1	L	247	GLY	2.2
1	L	311	ASN	2.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
6	PEG	L	706	7/7	0.82	0.14	26,27,31,32	7
5	OXY	L	704	2/2	0.91	0.40	26,26,26,28	2
5	OXY	S	1004	2/2	0.92	0.18	30,30,30,30	2
5	OXY	L	705	2/2	0.93	0.21	28,28,28,29	2
11	O	S	1006	1/1	0.95	0.22	19,19,19,19	1
5	OXY	L	703	2/2	0.97	0.23	27,27,27,29	0
3	NFV	L	701	9/9	0.99	0.05	12,13,15,16	0
4	MG	L	702	1/1	0.99	0.02	14,14,14,14	0
8	F3S	S	1002	7/7	1.00	0.02	13,13,14,14	0
9	F4S	S	1003	7/7	1.00	0.02	13,14,15,20	0
10	CL	S	1005	1/1	1.00	0.06	21,21,21,21	0
7	SF4	S	1001	8/8	1.00	0.02	16,17,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.