Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:50 AM EDT

PDB ID	:	4IUC
Title	:	Crystal structure of an O2-tolerant [NiFe]-hydrogenase from Ralstonia eutropha in its as-isolated form - oxidized state 2
Authors	:	Frielingsdorf, S.; Schmidt, A.; Fritsch, J.; Lenz, O.; Scheerer, P.
Deposited on	:	2013-01-20
Resolution	:	1.45 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:

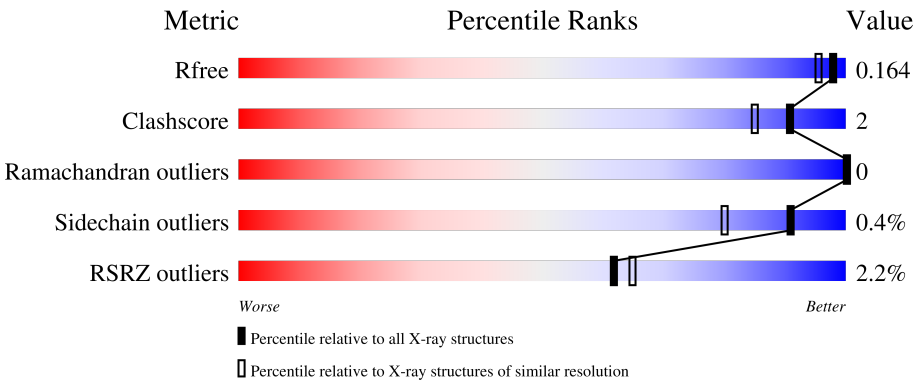
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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% 96% .
2	S	339	% 74% . 22%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8113 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	601	4861	3096	852	890	23	0	25	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	265	2126	1356	357	391	22	0	12	0

There are 22 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
S	329	ARG	-	expression tag	UNP P31892
S	330	SER	-	expression tag	UNP P31892
S	331	ALA	-	expression tag	UNP P31892
S	332	TRP	-	expression tag	UNP P31892
S	333	SER	-	expression tag	UNP P31892
S	334	HIS	-	expression tag	UNP P31892
S	335	PRO	-	expression tag	UNP P31892
S	336	GLN	-	expression tag	UNP P31892
S	337	PHE	-	expression tag	UNP P31892

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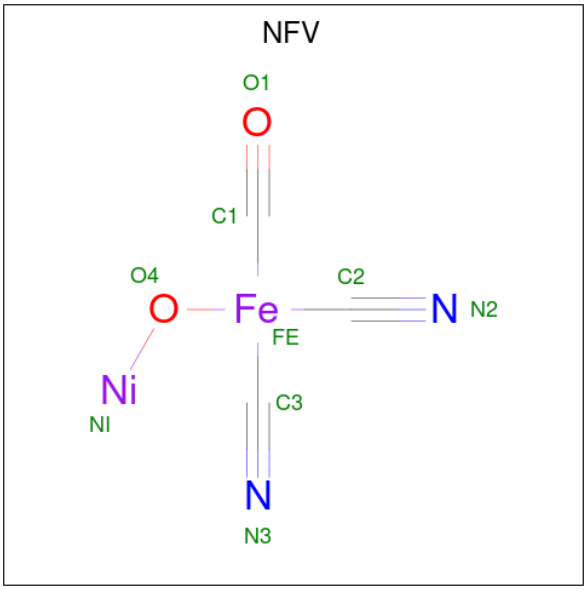
Chain	Residue	Modelled	Actual	Comment	Reference
S	338	GLU	-	expression tag	UNP P31892
S	339	LYS	-	expression tag	UNP P31892

- 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

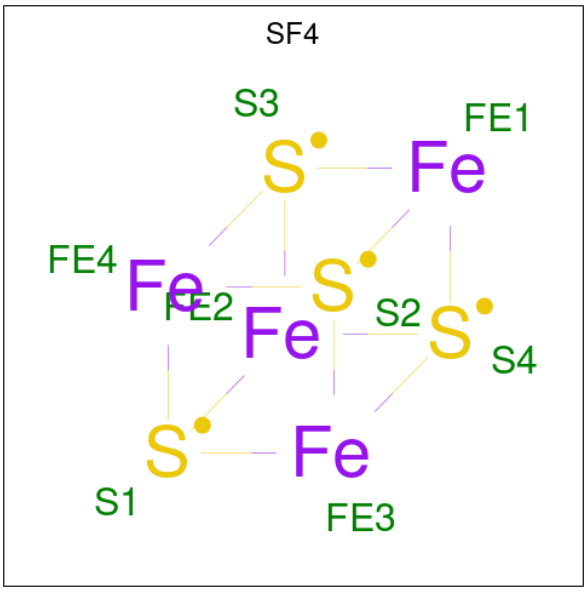
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

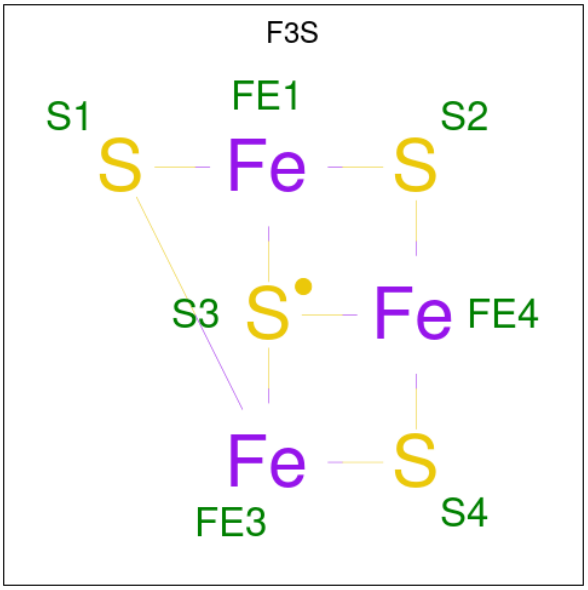
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	L	1	1	1	0	0
			Total	Cl		
5	S	1	1	1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



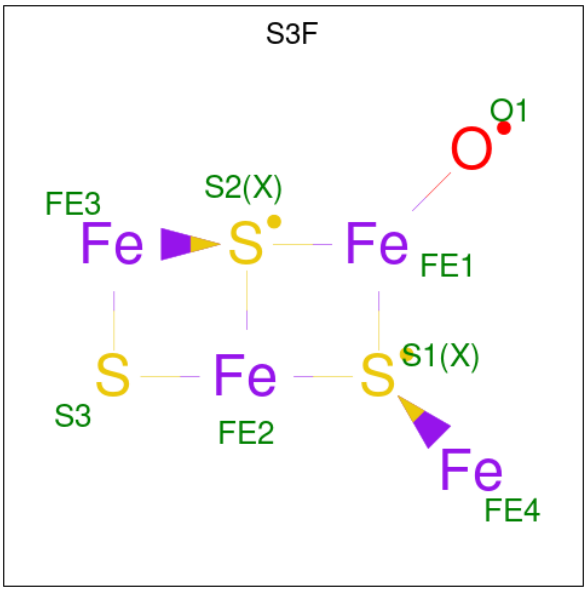
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	S	1	8	4	4	0	0

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

- Molecule 8 is oxidized [Fe4-S3] cluster (three-letter code: S3F) (formula: Fe_4OS_3).



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

- Molecule 9 is water.

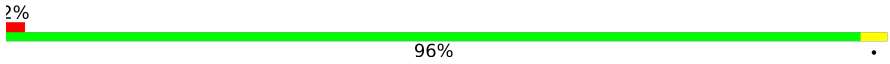
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	L	717	747	747	0	29
			Total	O		
9	S	329	344	344	0	15

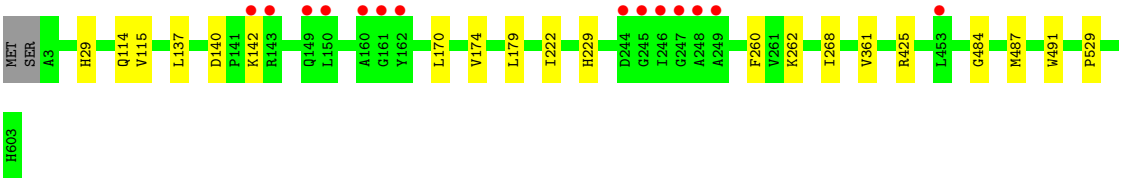
3 Residue-property plots (i)

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

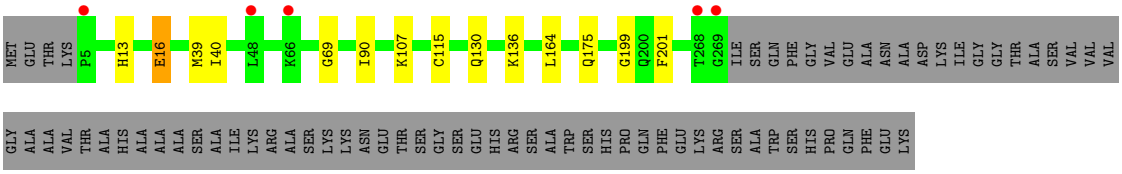
Chain L:





- Molecule 2: Uptake hydrogenase small subunit

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	73.62Å 95.74Å 120.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.36 – 1.45 34.36 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.36-1.45) 99.4 (34.36-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.125 , 0.157 0.139 , 0.164	Depositor DCC
R_{free} test set	7516 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8113	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: SF4, F3S, MG, S3F, CL, NFV

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	0.57	0/5064	0.53	0/6891
2	S	0.55	0/2218	0.52	0/3001
All	All	0.56	0/7282	0.53	0/9892

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	4861	0	4836	11	0
2	S	2126	0	2105	14	0
3	L	9	0	0	0	0
4	L	1	0	0	0	0
5	L	1	0	0	0	0
5	S	1	0	0	0	0
6	S	8	0	0	0	0
7	S	7	0	0	0	0
8	S	8	0	0	1	0
9	L	747	0	0	0	0
9	S	344	0	0	5	0
All	All	8113	0	6941	24	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 (24) 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:140:ASP:OD2	1:L:142:LYS:HG3	1.82	0.78
2:S:39[B]:MET:HG2	2:S:164:LEU:HD13	1.77	0.66
2:S:136:LYS:HE2	9:S:1294:HOH:O	1.98	0.63
2:S:39[B]:MET:SD	2:S:164:LEU:HD12	2.39	0.62
2:S:69:GLY:O	2:S:107[A]:LYS:HB3	2.02	0.59
2:S:40:ILE:CG2	2:S:164:LEU:HD11	2.34	0.57
2:S:13:HIS:HD2	9:S:1157:HOH:O	1.88	0.57
2:S:130[A]:GLN:NE2	9:S:1196:HOH:O	2.41	0.52
1:L:174:VAL:HG13	1:L:179[A]:LEU:HD21	1.91	0.52
1:L:229:HIS:NE2	8:S:1003:S3F:O1	2.40	0.51
2:S:40:ILE:HG22	2:S:164:LEU:HD11	1.94	0.49
1:L:29:HIS:CE1	2:S:90:ILE:HD11	2.48	0.49
2:S:13:HIS:HD1	2:S:16[B]:GLU:CD	2.18	0.47
1:L:222[A]:ILE:HD11	1:L:260:PHE:CD1	2.50	0.47
1:L:484:GLY:O	1:L:487[B]:MET:HG2	2.14	0.46
2:S:115:CYS:HB2	9:S:1117:HOH:O	2.15	0.46
1:L:262:LYS:HB2	1:L:491:TRP:CE2	2.50	0.46
1:L:115:VAL:HG11	1:L:268:ILE:HG23	1.97	0.45
1:L:140:ASP:OD2	1:L:142:LYS:CG	2.59	0.43
2:S:40:ILE:HG23	2:S:164:LEU:HD11	2.01	0.42
1:L:114:GLN:OE1	1:L:529:PRO:HA	2.21	0.41
1:L:137:LEU:HD21	1:L:170[A]:LEU:HG	2.03	0.41
2:S:175:GLN:NE2	9:S:1221:HOH:O	2.54	0.41
2:S:199:GLY:HA2	2:S:201:PHE:CE2	2.57	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	L	626/603 (104%)	614 (98%)	12 (2%)	0	100	100
2	S	275/339 (81%)	269 (98%)	6 (2%)	0	100	100
All	All	901/942 (96%)	883 (98%)	18 (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	523/498 (105%)	520 (99%)	3 (1%)	86	69
2	S	235/279 (84%)	233 (99%)	2 (1%)	78	57
All	All	758/777 (98%)	753 (99%)	5 (1%)	91	65

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	361[A]	VAL
1	L	361[B]	VAL
1	L	425	ARG
2	S	16[A]	GLU
2	S	16[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	10	ASN
2	S	29	HIS
2	S	175	GLN

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	SF4	S	1001	2	0,12,12	-	-	-		
8	S3F	S	1003	2	0,9,9	-	-	-		
7	F3S	S	1002	2	0,9,9	-	-	-		
3	NFV	L	701	1	3,8,8	1.60	1 (33%)	-		

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	SF4	S	1001	2	-	-	0/6/5/5
8	S3F	S	1003	2	-	-	0/2/2/2
7	F3S	S	1002	2	-	-	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	701	NFV	O1-C1	-2.69	1.12	1.16

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	1003	S3F	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	L	601/603 (99%)	-0.08	14 (2%)	60	63	7, 11, 23, 50	0
2	S	265/339 (78%)	-0.25	5 (1%)	66	68	7, 11, 20, 35	0
All	All	866/942 (91%)	-0.13	19 (2%)	62	65	7, 11, 22, 50	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	246	ILE	12.4
1	L	248	ALA	8.8
2	S	269	GLY	7.0
1	L	247	GLY	6.2
1	L	249	ALA	5.3
2	S	5	PRO	3.5
1	L	245	GLY	3.3
1	L	142	LYS	3.2
1	L	453	LEU	3.1
1	L	244[A]	ASP	3.1
2	S	268	THR	2.9
1	L	160	ALA	2.7
2	S	48[A]	LEU	2.7
1	L	143	ARG	2.5
1	L	149[A]	GLN	2.5
2	S	66	LYS	2.4
1	L	150	LEU	2.4
1	L	162	TYR	2.2
1	L	161	GLY	2.1

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
5	CL	L	703	1/1	0.99	0.06	29,29,29,29	1
6	SF4	S	1001	8/8	0.99	0.04	8,8,9,9	0
8	S3F	S	1003	8/8	0.99	0.04	5,8,8,15	1
5	CL	S	1004	1/1	1.00	0.07	15,15,15,15	1
4	MG	L	702	1/1	1.00	0.04	6,6,6,6	0
7	F3S	S	1002	7/7	1.00	0.03	6,6,6,7	0
3	NFV	L	701	9/9	1.00	0.04	4,4,5,6	0

6.5 Other polymers (i)

There are no such residues in this entry.