Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2024 – 09:19 pm GMT

PDB ID	:	5JT1
Title	:	The 3D structure of Ni-reconstituted U489C variant of [NiFeSe] hydrogenase from Desulfovibrio vulgaris Hildenborough in the oxidized state at 1.35 Angstrom resolution
Authors	:	Marques, M.C.; Pereira, I.A.C.; Matias, P.M.
Deposited on	:	2016-05-09
Resolution	:	1.35 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:

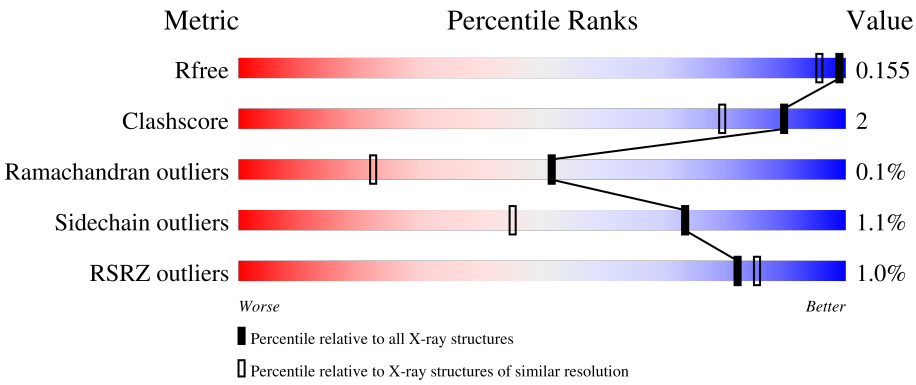
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	A	317	2% 86% • 11%
2	B	509	% 91% • 5%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13001 atoms, of which 6094 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 Periplasmic [NiFeSe] hydrogenase, small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	283	4394	1419	2179	366	409	21	0	20	0

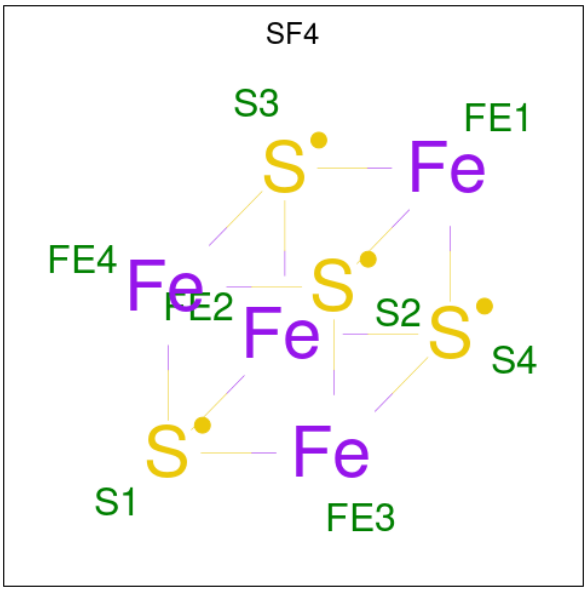
- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	483	7792	2481	3913	671	701	26	0	23	0

There are 9 discrepancies between the modelled and reference sequences:

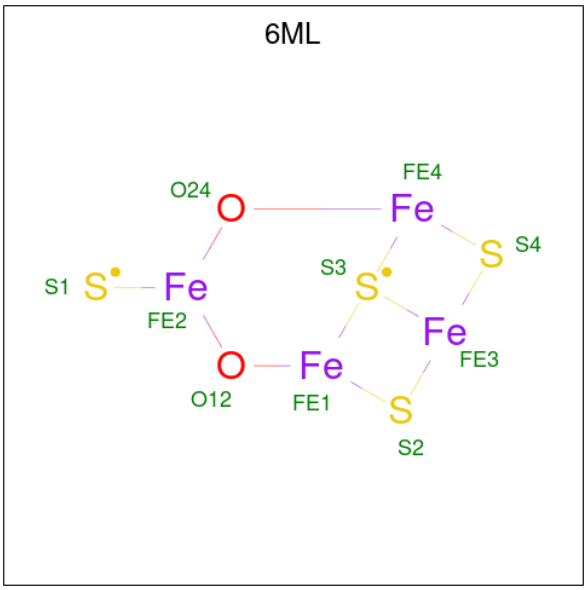
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	TRP	-	expression tag	UNP Q72AS3
B	5	SER	-	expression tag	UNP Q72AS3
B	6	HIS	-	expression tag	UNP Q72AS3
B	7	PRO	-	expression tag	UNP Q72AS3
B	8	GLN	-	expression tag	UNP Q72AS3
B	9	PHE	-	expression tag	UNP Q72AS3
B	10	GLU	-	expression tag	UNP Q72AS3
B	11	LYS	-	expression tag	UNP Q72AS3
B	489	CYS	SEC	engineered mutation	UNP Q72AS3

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



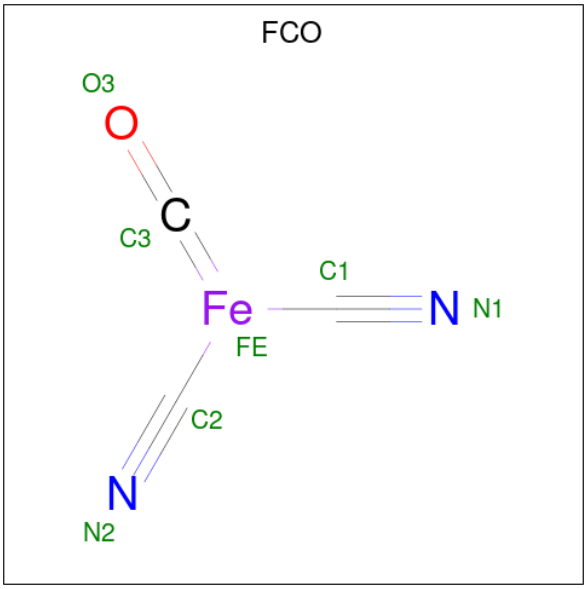
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	0
			Total	Fe	S		
3	A	1	8	4	4	0	1

- Molecule 4 is oxygen-damaged SF4 (three-letter code: 6ML) (formula: $Fe_4O_2S_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	O	S		
4	A	1	10	4	2	4	0	1

- Molecule 5 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	B	1	7	3	1	2	1	0	0

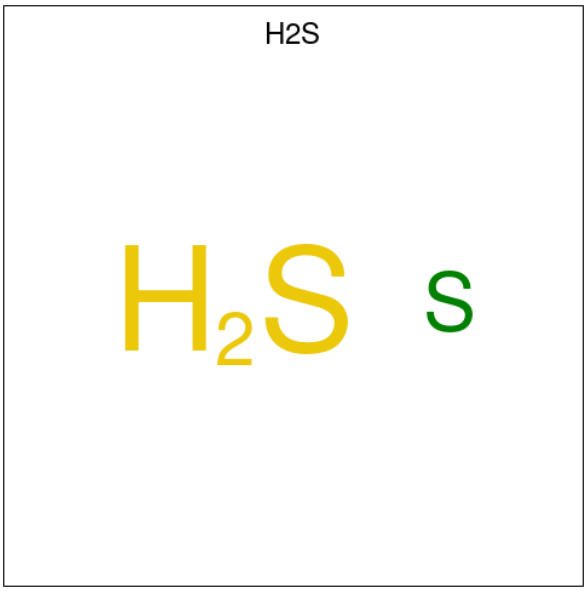
- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
6	B	1	1	1	0	1

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	B	1	1	1	0	0

- Molecule 8 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	S		
8	B	1	3	2	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	286	290	290	0	4
			Total	O		
9	B	472	479	479	0	8

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: Periplasmic [NiFeSe] hydrogenase, small subunit

Chain A: 2% 86% • 11%

MET SER LEU THR ARG ARG ASP PHE VAL LYS LEU CYS THR GLY THR VAL ALA GLY PHE GLY ILE SER GLN MET PHE HIS PRO ALA VAL HIS GLU ALA LEU ALA G1 T2 L3 T4 C21 T24 W52 E77 G78 H97 M101 I127 M242 Q261 N262 A263

A283

• Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing

Chain B: % 91% • 5%

TRP SER HIS PRO GLN PHE GLU LYS GLY A13 T14 G15 R16 T17 E28 G29 H30 V37 R46 R73 I74 C75 C75 T80 Q116 V224 K243 K281 P319 E366 V403 L446 R458 D471 D472 I473 L482 C489 C489 H495 VAL LEU

HIS ALA GLU SER GLY LYS VAL ALA VAL ILE GLU VAL LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.78Å 63.18Å 110.66Å 90.00° 105.27° 90.00°	Depositor
Resolution (Å)	45.63 – 1.35 45.63 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.63-1.35) 97.5 (45.63-1.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.35Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.116 , 0.145 0.129 , 0.155	Depositor DCC
R_{free} test set	7575 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13001	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: CSX, SF4, 6ML, FE2, NI, CSD, FCO, H2S

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	0.45	0/2329	0.63	0/3167
2	B	0.46	0/4007	0.67	2/5412 (0.0%)
All	All	0.46	0/6336	0.65	2/8579 (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})
2	B	458	ARG	NE-CZ-NH1	6.23	123.41	120.30
2	B	458	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	A	2215	2179	2160	5	0
2	B	3879	3913	3913	16	0
3	A	24	0	0	0	0
4	A	10	0	0	0	0
5	B	7	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	2	0	0	0
9	A	290	0	0	4	2
9	B	479	0	0	7	1
All	All	6907	6094	6073	20	2

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 (20) 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:A:2:THR:OG1	9:A:401:HOH:O	2.10	0.69
2:B:281:LYS:NZ	9:B:703:HOH:O	2.29	0.63
9:A:639[A]:HOH:O	2:B:30[A]:HIS:HD2	1.92	0.52
2:B:46[A]:ARG:NH2	9:B:707:HOH:O	2.43	0.50
2:B:243:LYS:HE3	9:B:1005:HOH:O	2.13	0.49
2:B:30[B]:HIS:CE1	9:B:1052:HOH:O	2.68	0.47
1:A:21[B]:CYS:O	1:A:24:THR:HG22	2.15	0.47
2:B:471:ASP:OD1	9:B:701:HOH:O	2.21	0.44
1:A:77[B]:GLU:HG2	1:A:78[B]:GLY:N	2.32	0.44
9:A:639[A]:HOH:O	2:B:30[A]:HIS:CD2	2.70	0.44
1:A:127:ILE:HD12	2:B:73:ARG:HG2	2.00	0.43
2:B:28:GLU:OE1	2:B:489[A]:CYS:SG	2.77	0.43
2:B:489[A]:CYS:CB	9:B:1056[A]:HOH:O	2.66	0.43
1:A:242:MET:HG2	9:A:628:HOH:O	2.19	0.42
2:B:17:THR:HG21	2:B:473[B]:ILE:HG21	2.01	0.42
2:B:319:PRO:HG3	2:B:446:LEU:HG	2.02	0.41
2:B:366:GLU:HG2	9:B:1063:HOH:O	2.21	0.40
2:B:482:LEU:HD13	2:B:482:LEU:C	2.41	0.40
2:B:16:ARG:HA	2:B:37:VAL:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:605:HOH:O	9:A:605:HOH:O[2_658]	1.50	0.70
9:A:401:HOH:O	9:B:1053:HOH:O[3_545]	2.08	0.12

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	301/317 (95%)	293 (97%)	7 (2%)	1 (0%)	41	18
2	B	500/509 (98%)	492 (98%)	8 (2%)	0	100	100
All	All	801/826 (97%)	785 (98%)	15 (2%)	1 (0%)	51	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ALA

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	244/253 (96%)	240 (98%)	4 (2%)	62	30
2	B	414/413 (100%)	410 (99%)	4 (1%)	76	49
All	All	658/666 (99%)	650 (99%)	8 (1%)	73	42

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TRP
1	A	101[A]	MET
1	A	101[B]	MET
1	A	261	GLN
2	B	80	THR

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Mol	Chain	Res	Type
2	B	116	GLN
2	B	224	VAL
2	B	403	VAL

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)

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	CSD	B	489[B]	2	3,7,8	1.02	0	1,8,10	0.91	0
2	CSX	B	75[A]	2,6	3,6,7	0.98	0	1,6,8	0.26	0
2	CSX	B	75[B]	2	3,6,7	1.06	0	1,6,8	0.42	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
2	CSD	B	489[B]	2	-	0/2/6/8	-
2	CSX	B	75[A]	2,6	-	0/1/5/7	-
2	CSX	B	75[B]	2	-	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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 5 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	$\#\|Z\| > 2$
4	6ML	A	304[B]	1	0,12,12	-	-	-		
3	SF4	A	303[A]	1	0,12,12	-	-	-		
3	SF4	A	302	1	0,12,12	-	-	-		
5	FCO	B	601	2,9	0,6,6	-	-	-		
3	SF4	A	301	1	0,12,12	-	-	-		

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
4	6ML	A	304[B]	1	-	-	0/2/3/3
3	SF4	A	303[A]	1	-	-	0/6/5/5
3	SF4	A	302	1	-	-	0/6/5/5
3	SF4	A	301	1	-	-	0/6/5/5

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.

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	A	283/317 (89%)	-0.32	5 (1%)	68	73	9, 14, 27, 69	1 (0%)
2	B	481/509 (94%)	-0.40	2 (0%)	92	93	9, 14, 24, 47	3 (0%)
All	All	764/826 (92%)	-0.37	7 (0%)	82	87	9, 14, 25, 69	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	13	ALA	6.8
1	A	3	LEU	6.1
1	A	2	THR	3.9
1	A	1	GLY	3.8
1	A	4	THR	3.1
1	A	97	HIS	2.2
2	B	14	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	CSX	B	75[A]	7/8	0.97	0.15	11,13,17,17	11
2	CSX	B	75[B]	7/8	0.97	0.15	11,13,17,17	11
2	CSD	B	489[B]	8/9	0.98	0.10	10,13,18,19	11

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	NI	B	602[A]	1/1	0.99	0.14	16,16,16,16	1
3	SF4	A	302	8/8	1.00	0.07	9,10,10,10	0
3	SF4	A	303[A]	8/8	1.00	0.07	9,9,11,11	8
4	6ML	A	304[B]	10/10	1.00	0.08	9,11,12,12	10
5	FCO	B	601	7/7	1.00	0.08	11,12,14,16	0
3	SF4	A	301	8/8	1.00	0.06	11,11,12,12	0
7	FE2	B	603	1/1	1.00	0.05	11,11,11,11	0
8	H2S	B	604	1/1	1.00	0.07	11,11,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.