Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:01 PM GMT

PDB ID : 5BYR

Title : Semisynthetic [FeFe]-hydrogenase CpI with propane-dithiolato-bridged [2Fe] cofactor

Authors : Esselborn, J.; Muraki, N.; Engelbrecht, V.; Hofmann, E.; Kurisu, G.; Happe, T.

Deposited on : 2015-06-10

Resolution : 1.82 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.82 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.
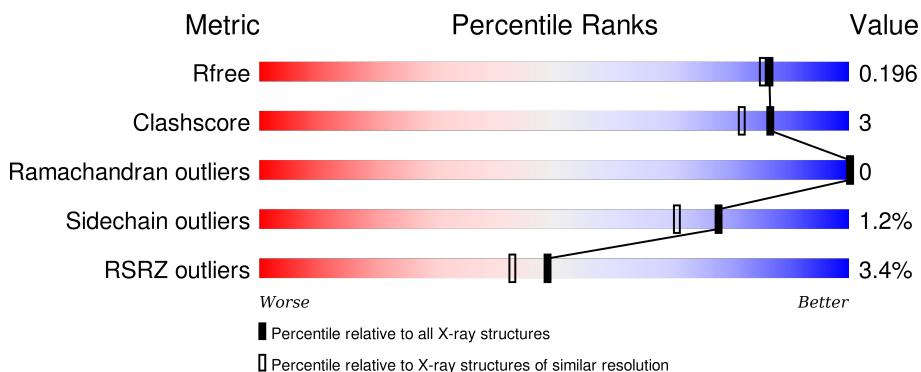
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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. 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	584	
1	B	584	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18690 atoms, of which 8831 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 Iron hydrogenase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	571	Total 8838	C 2782	H 4396	N 764	O 857	S 39	0	1	0
1	B	572	Total 8870	C 2789	H 4419	N 767	O 856	S 39	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP P29166
A	576	ALA	-	expression tag	UNP P29166
A	577	TRP	-	expression tag	UNP P29166
A	578	SER	-	expression tag	UNP P29166
A	579	HIS	-	expression tag	UNP P29166
A	580	PRO	-	expression tag	UNP P29166
A	581	GLN	-	expression tag	UNP P29166
A	582	PHE	-	expression tag	UNP P29166
A	583	GLU	-	expression tag	UNP P29166
A	584	LYS	-	expression tag	UNP P29166
B	575	SER	-	expression tag	UNP P29166
B	576	ALA	-	expression tag	UNP P29166
B	577	TRP	-	expression tag	UNP P29166
B	578	SER	-	expression tag	UNP P29166
B	579	HIS	-	expression tag	UNP P29166
B	580	PRO	-	expression tag	UNP P29166
B	581	GLN	-	expression tag	UNP P29166
B	582	PHE	-	expression tag	UNP P29166
B	583	GLU	-	expression tag	UNP P29166
B	584	LYS	-	expression tag	UNP P29166

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
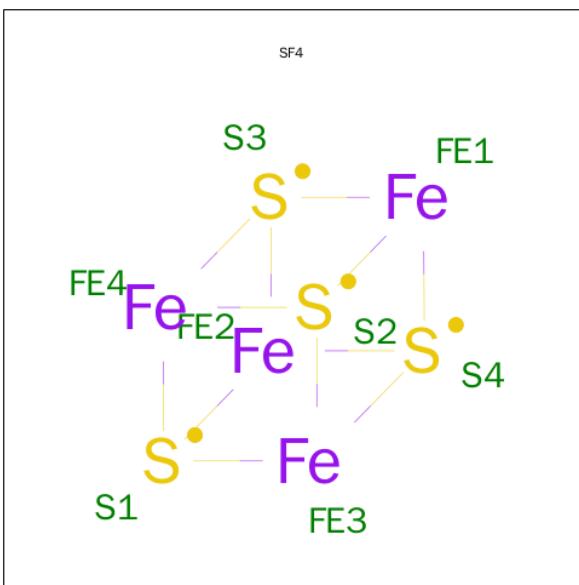
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

FES
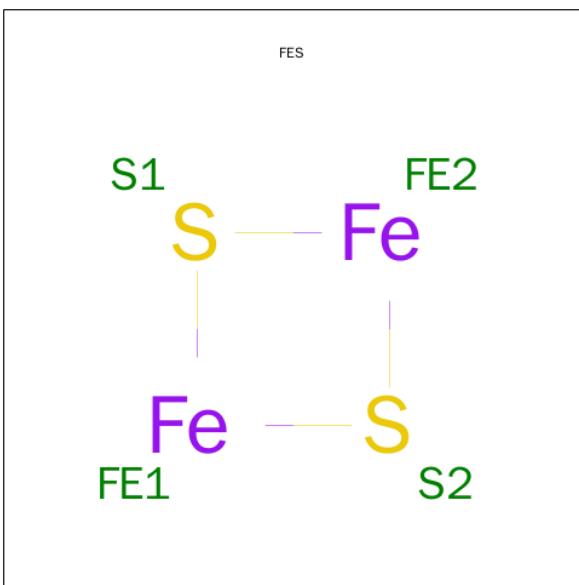
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is bis(cyanido-kappaC)(dicarbonyl)-mu-(oxomethylidene)[mu-propane-1,3-bis(thiolate)-1kappa 2 S 1 ,S 3 :2kappa 2 S 1 ,S 3]diiron(2+) (three-letter code: 4WW) (formula: $C_8H_6Fe_2N_2O_3S_2$).
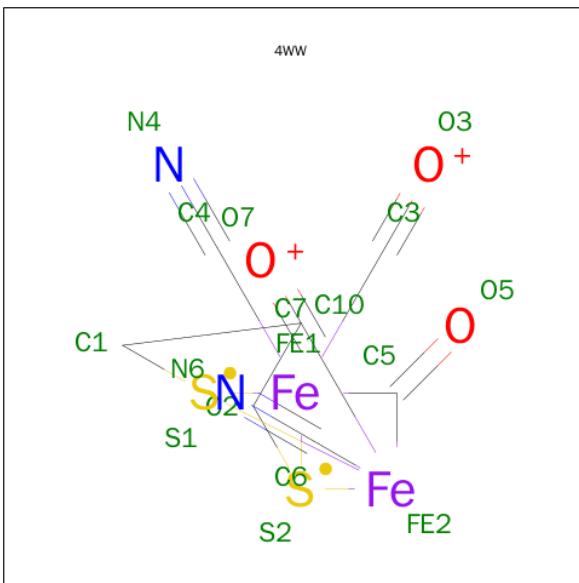
4WW

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	S	0	0
			17	8	2	2	3	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 17	C 8	Fe 2	N 2	O 3	S 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Mg 2	0	0
5	A	3	Total 3	Mg 3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
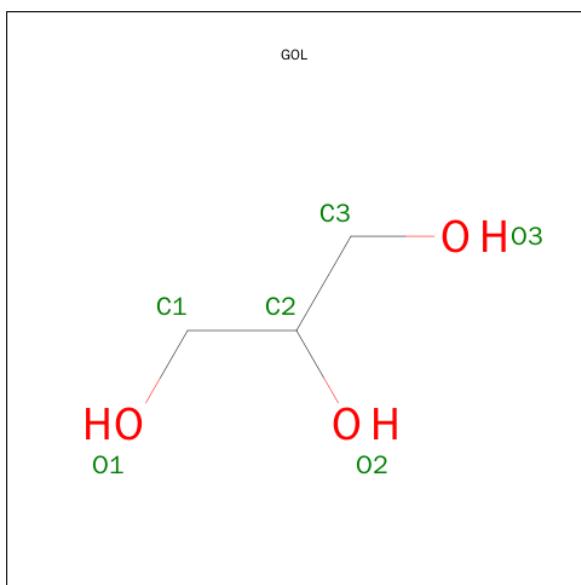
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 3	H 8	O 3	0	0
6	A	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	427	Total 427	O 427	0	0
7	B	416	Total 416	O 416	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Iron hydrogenase 1
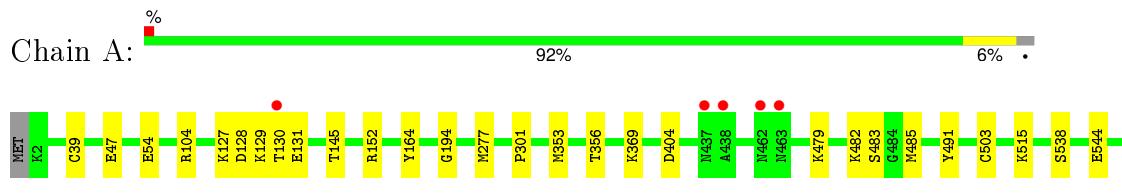
• Molecule 1: Iron hydrogenase 1
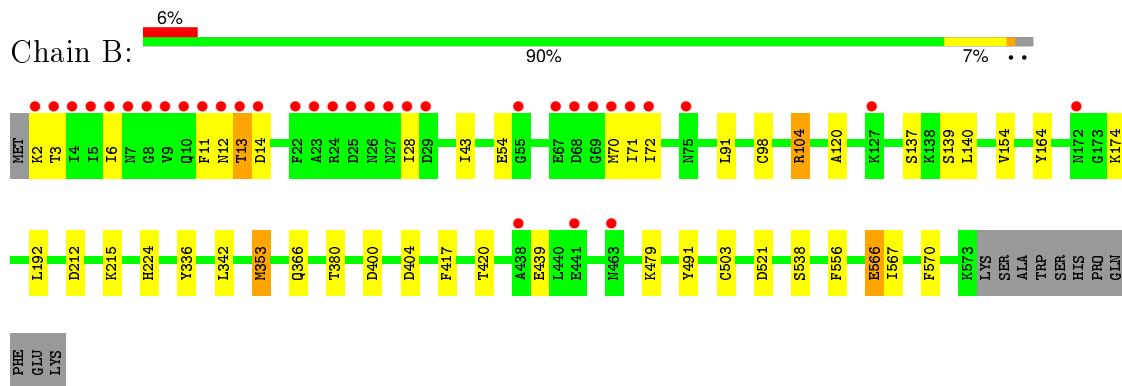
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	87.47Å 72.07Å 102.71Å	Depositor
a, b, c, α, β, γ	90.00° 100.86° 90.00°	
Resolution (Å)	47.58 – 1.82	Depositor
	47.58 – 1.82	EDS
% Data completeness	99.9 (47.58-1.82)	Depositor
(in resolution range)	99.8 (47.58-1.82)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.58 (at 1.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.155 , 0.192	Depositor
	0.166 , 0.196	DCC
R_{free} test set	1186 reflections (1.07%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 112346 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18690	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, SF4, 4WW, FES

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	0.79	1/4515 (0.0%)	0.75	4/6082 (0.1%)
1	B	0.81	2/4527 (0.0%)	0.75	3/6096 (0.0%)
All	All	0.80	3/9042 (0.0%)	0.75	7/12178 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	CYS	CB-SG	-6.54	1.71	1.82
1	B	491	TYR	CD1-CE1	-5.13	1.31	1.39
1	B	98	CYS	CB-SG	-5.04	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	353	MET	CG-SD-CE	-6.98	89.03	100.20
1	B	353	MET	CG-SD-CE	-6.82	89.28	100.20
1	B	404	ASP	CB-CG-OD2	6.36	124.03	118.30
1	A	152	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	152	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	400	ASP	CB-CG-OD1	5.24	123.02	118.30

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	4442	4396	4397	22	0
1	B	4451	4419	4418	29	0
2	A	32	0	0	1	0
2	B	32	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	17	0	6	1	0
4	B	17	0	6	1	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	12	16	16	0	0
7	A	427	0	0	9	0
7	B	416	0	0	8	1
All	All	9859	8831	8843	48	1

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 3.

All (48) 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:B:174:LYS:NZ	7:B:701:HOH:O	2.07	0.87
1:B:2:LYS:N	1:B:13:THR:O	2.19	0.75
1:A:194:GLY:HA3	7:A:713:HOH:O	1.87	0.74
1:A:544:GLU:OE2	7:A:701:HOH:O	2.09	0.70
1:B:556:PHE:HE1	1:B:567:ILE:HD11	1.60	0.67
1:A:131:GLU:O	7:A:702:HOH:O	2.14	0.65
1:A:54:GLU:OE1	7:A:703:HOH:O	2.14	0.65
1:A:550:LYS:NZ	7:A:710:HOH:O	2.32	0.62
1:A:356:THR:CG2	7:A:713:HOH:O	2.50	0.59
1:A:129:LYS:HE3	1:A:145:THR:HG21	1.87	0.55
1:A:503:CYS:CB	4:A:606:4WW:C4	2.84	0.55
1:B:566:GLU:HG2	1:B:567:ILE:HG23	1.90	0.53
1:B:215:LYS:NZ	7:B:703:HOH:O	2.36	0.52
1:A:47:GLU:OE2	7:A:704:HOH:O	2.19	0.51
1:B:479:LYS:NZ	7:B:711:HOH:O	2.35	0.51
1:B:174:LYS:CE	7:B:796:HOH:O	2.60	0.49
1:B:70:MET:HE3	1:B:72:ILE:HD11	1.94	0.49
1:B:70:MET:CE	1:B:72:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:CZ	1:A:104:ARG:HB3	2.42	0.49
1:B:503:CYS:CB	4:B:606:4WW:C4	2.90	0.49
1:A:277:MET:HG3	1:A:548:LEU:HD21	1.93	0.49
1:B:521:ASP:OD1	7:B:702:HOH:O	2.19	0.48
1:B:212:ASP:OD1	7:B:703:HOH:O	2.20	0.48
1:A:555:TYR:O	1:A:563:ARG:NH2	2.46	0.48
1:B:139:SER:HB2	1:B:192:LEU:HD22	1.96	0.47
1:B:14:ASP:OD1	1:B:14:ASP:N	2.43	0.47
1:B:566:GLU:CG	1:B:567:ILE:HG23	2.45	0.47
1:B:3:THR:HA	1:B:11:PHE:O	2.14	0.47
1:A:301:PRO:HD2	2:A:601:SF4:S2	2.55	0.47
1:B:224:HIS:CD2	1:B:342:LEU:HD11	2.52	0.45
1:A:485:MET:HE1	7:B:838:HOH:O	2.16	0.45
1:A:566:GLU:HG2	1:A:567:ILE:HG12	1.99	0.44
1:A:479:LYS:NZ	7:B:717:HOH:O	2.50	0.44
1:A:128:ASP:OD1	1:A:130:THR:HB	2.18	0.44
1:A:164:TYR:HA	7:A:753:HOH:O	2.19	0.42
1:B:336:TYR:CE2	1:B:342:LEU:HD12	2.54	0.42
1:B:353:MET:O	1:B:380:THR:HA	2.19	0.42
1:A:491:TYR:OH	1:B:43:ILE:HD12	2.19	0.42
1:A:483:SER:HB2	1:B:154:VAL:CG1	2.48	0.42
1:A:356:THR:HG21	7:A:713:HOH:O	2.18	0.42
1:B:91:LEU:HB3	1:B:120:ALA:HB2	2.03	0.41
1:B:366:GLN:CD	1:B:366:GLN:H	2.24	0.41
1:A:482:LYS:HD3	1:B:164:TYR:CD1	2.56	0.41
1:B:104:ARG:HH11	1:B:104:ARG:HG3	1.86	0.41
1:B:137:SER:HB3	1:B:140:LEU:O	2.20	0.40
1:B:366:GLN:HG3	1:B:570:PHE:CZ	2.57	0.40
1:B:6:ILE:HG21	1:B:28:ILE:HD13	2.03	0.40
1:B:54:GLU:HB2	1:B:71:ILE:HB	2.04	0.40

All (1) 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)
7:B:742:HOH:O	7:B:909:HOH:O[2_555]	2.18	0.02

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	570/584 (98%)	549 (96%)	21 (4%)	0	100	100
1	B	571/584 (98%)	550 (96%)	21 (4%)	0	100	100
All	All	1141/1168 (98%)	1099 (96%)	42 (4%)	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	A	488/499 (98%)	484 (99%)	4 (1%)	86	83
1	B	489/499 (98%)	481 (98%)	8 (2%)	70	59
All	All	977/998 (98%)	965 (99%)	12 (1%)	78	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	369	LYS
1	A	515	LYS
1	A	538	SER
1	B	12	ASN
1	B	13	THR
1	B	104	ARG
1	B	417	PHE

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Mol	Chain	Res	Type
1	B	420	THR
1	B	439	GLU
1	B	538	SER
1	B	566	GLU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\#|Z| > 2$
2	SF4	A	601	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	602	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	603	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	604	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FES	A	605	1	0,4,4	0.00	-	0,4,4	0.00	-
4	4WW	A	606	1	13,19,19	3.03	5 (38%)	1,36,36	1.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	GOL	A	610	-	5,5,5	0.83	0	5,5,5	0.39	0
6	GOL	A	611	-	5,5,5	0.89	0	5,5,5	1.31	0
2	SF4	B	601	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	602	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	603	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	604	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FES	B	605	1	0,4,4	0.00	-	0,4,4	0.00	-
4	4WW	B	606	1	13,19,19	3.46	6 (46%)	1,36,36	2.07	1 (100%)

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	SF4	A	601	1	-	0/0/48/48	0/6/5/5
2	SF4	A	602	1	-	0/0/48/48	0/6/5/5
2	SF4	A	603	1	-	0/0/48/48	0/6/5/5
2	SF4	A	604	1	-	0/0/48/48	0/6/5/5
3	FES	A	605	1	-	0/0/4/4	0/1/1/1
4	4WW	A	606	1	-	0/0/70/70	0/0/3/3
6	GOL	A	610	-	-	0/4/4/4	0/0/0/0
6	GOL	A	611	-	-	0/4/4/4	0/0/0/0
2	SF4	B	601	1	-	0/0/48/48	0/6/5/5
2	SF4	B	602	1	-	0/0/48/48	0/6/5/5
2	SF4	B	603	1	-	0/0/48/48	0/6/5/5
2	SF4	B	604	1	-	0/0/48/48	0/6/5/5
3	FES	B	605	1	-	0/0/4/4	0/1/1/1
4	4WW	B	606	1	-	0/0/70/70	0/0/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	606	4WW	C6-N6	-3.61	1.09	1.15
4	B	606	4WW	C3-FE1	-2.26	1.72	1.79
4	A	606	4WW	C3-FE1	-2.06	1.72	1.79
4	A	606	4WW	O3-C3	2.01	1.20	1.15
4	B	606	4WW	C4-N4	2.14	1.18	1.15
4	A	606	4WW	C4-N4	3.63	1.21	1.15
4	A	606	4WW	S1-FE1	3.71	2.31	2.26
4	B	606	4WW	S1-FE1	4.68	2.33	2.26
4	B	606	4WW	S1-FE2	6.11	2.35	2.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	606	4WW	S2-FE1	8.32	2.38	2.26
4	A	606	4WW	S1-FE2	8.84	2.39	2.26

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	606	4WW	C1-C10-C2	-2.07	108.52	116.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SF4	1	0
4	A	606	4WW	1	0
4	B	606	4WW	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(Å²)	Q<0.9
1	A	571/584 (97%)	-0.27	5 (0%)	85	84	16, 26, 47, 61	0
1	B	572/584 (97%)	0.04	34 (5%)	26	20	15, 24, 63, 81	0
All	All	1143/1168 (97%)	-0.12	39 (3%)	49	43	15, 25, 52, 81	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	9.1
1	B	9	VAL	7.0
1	B	71	ILE	6.9
1	B	10	GLN	6.1
1	B	6	ILE	6.1
1	B	4	ILE	5.9
1	B	8	GLY	5.7
1	B	12	ASN	5.6
1	B	3	THR	5.5
1	B	11	PHE	5.3
1	A	130	THR	4.9
1	B	69	GLY	4.4
1	B	70	MET	4.4
1	B	2	LYS	4.0
1	B	127	LYS	3.7
1	B	27	ASN	3.6
1	B	75	ASN	3.3
1	A	437	ASN	3.3
1	B	72	ILE	3.3
1	B	22	PHE	3.2
1	B	68	ASP	3.2
1	B	7	ASN	3.2
1	B	28	ILE	3.0
1	B	13	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLY	3.0
1	A	463	ASN	2.9
1	B	172	ASN	2.9
1	B	14	ASP	2.8
1	B	25	ASP	2.7
1	A	438	ALA	2.5
1	B	441	GLU	2.5
1	A	462	ASN	2.5
1	B	29	ASP	2.5
1	B	67	GLU	2.4
1	B	26	ASN	2.3
1	B	24[A]	ARG	2.3
1	B	438	ALA	2.2
1	B	23	ALA	2.2
1	B	463	ASN	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	MG	A	608	1/1	0.92	0.13	1.12	45,45,45,45	0
6	GOL	A	611	6/6	0.87	0.15	1.09	37,46,63,63	0
4	4WW	A	606	17/17	0.99	0.11	0.96	15,18,22,23	2
3	FES	A	605	4/4	1.00	0.09	0.63	19,19,21,21	0
5	MG	B	607	1/1	0.98	0.08	0.49	25,25,25,25	0
3	FES	B	605	4/4	0.99	0.10	0.25	22,22,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
6	GOL	A	610	6/6	0.93	0.07	-0.30	22,30,36,42	0
4	4WW	B	606	17/17	0.99	0.10	-0.30	15,17,20,20	5
2	SF4	B	603	8/8	0.99	0.09	-0.33	16,18,18,20	0
2	SF4	A	602	8/8	0.99	0.10	-0.35	16,18,19,20	0
2	SF4	B	601	8/8	0.99	0.11	-0.42	13,14,15,15	0
5	MG	A	607	1/1	0.98	0.07	-0.43	25,25,25,25	0
2	SF4	A	603	8/8	0.99	0.07	-0.47	17,18,19,19	0
2	SF4	A	601	8/8	0.99	0.09	-0.56	15,16,17,18	0
2	SF4	B	602	8/8	0.99	0.11	-0.77	15,17,17,19	0
2	SF4	B	604	8/8	0.99	0.07	-1.00	23,24,25,25	0
5	MG	A	609	1/1	0.98	0.08	-1.36	25,25,25,25	0
2	SF4	A	604	8/8	0.99	0.05	-1.64	22,23,24,25	0
5	MG	B	608	1/1	0.96	0.06	-3.17	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.