



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 04:51 AM GMT

PDB ID : 2FTK
Title : beryllifluoride Spo0F complex with Spo0B
Authors : Varughese, K.I.
Deposited on : 2006-01-24
Resolution : 3.05 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

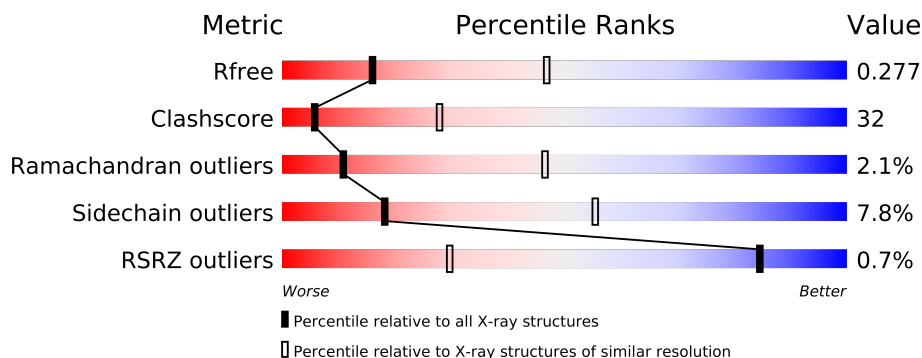
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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}	66092	2079 (3.12-3.00)
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	
1	C	192	
1	D	192	
2	E	124	
2	F	124	
2	G	124	
2	H	124	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	E	2001	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MG	F	2002	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9834 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sporulation initiation phosphotransferase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1497	955	251	284	7			
1	B	182	Total	C	N	O	S	6	0	0
			1505	959	253	286	7			
1	C	181	Total	C	N	O	S	0	0	0
			1497	955	251	284	7			
1	D	182	Total	C	N	O	S	6	0	0
			1505	959	253	286	7			

- Molecule 2 is a protein called Sporulation initiation phosphotransferase F.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	E	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	F	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	G	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	H	119	Total	Be	C	F	N	O	S	0	1	0
			964	1	615	3	159	181	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1213	SER	TYR	ENGINEERED	UNP P06628
E	1254	BFD	ASP	MODIFIED RESIDUE	UNP P06628
F	1013	SER	TYR	ENGINEERED	UNP P06628
F	1054	BFD	ASP	MODIFIED RESIDUE	UNP P06628
G	1613	SER	TYR	ENGINEERED	UNP P06628
G	1654	BFD	ASP	MODIFIED RESIDUE	UNP P06628
H	1413	SER	TYR	ENGINEERED	UNP P06628
H	1454	BFD	ASP	MODIFIED RESIDUE	UNP P06628

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

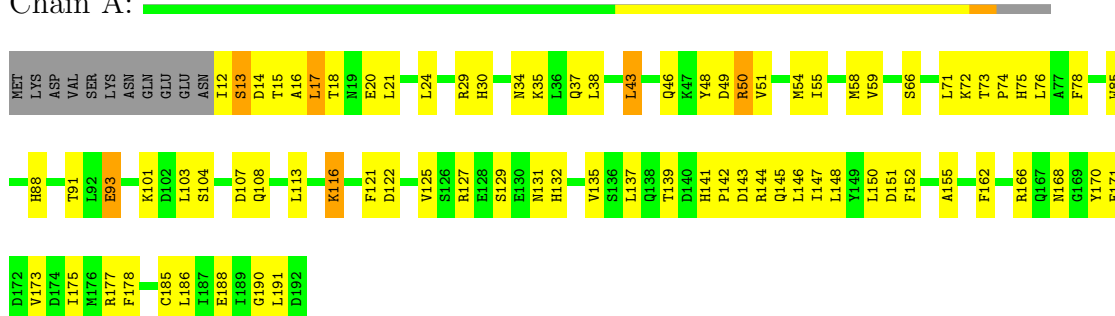
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0

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.

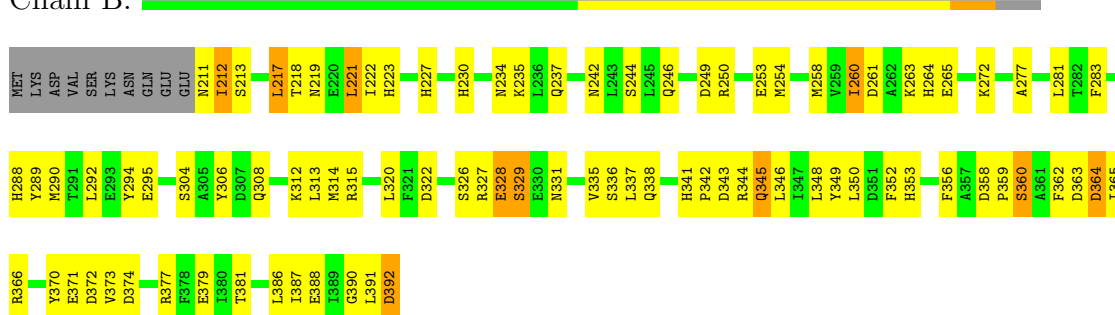
• Molecule 1: Sporulation initiation phosphotransferase B

Chain A:



• Molecule 1: Sporulation initiation phosphotransferase B

Chain B:



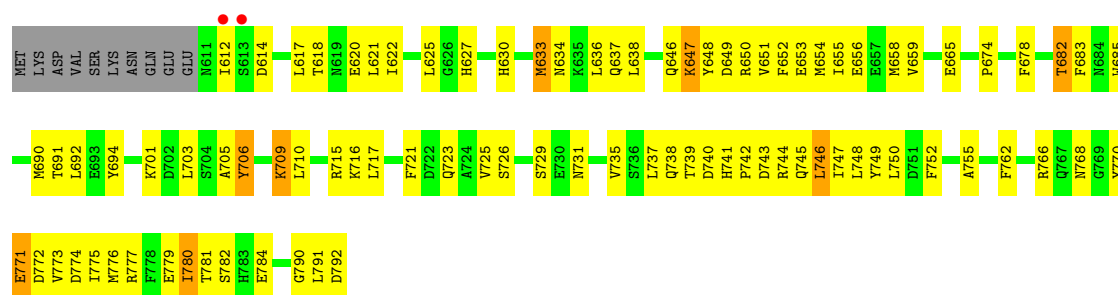
• Molecule 1: Sporulation initiation phosphotransferase B

Chain C:



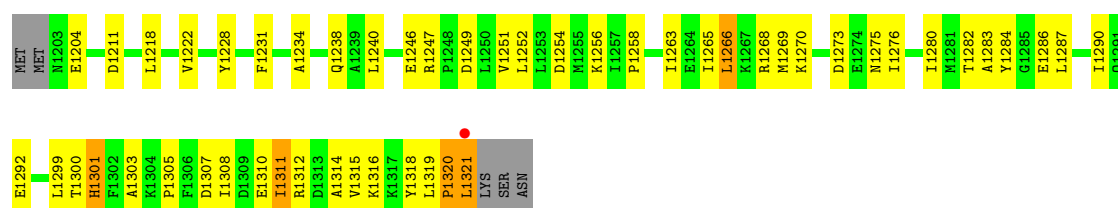
• Molecule 1: Sporulation initiation phosphotransferase B

Chain D:



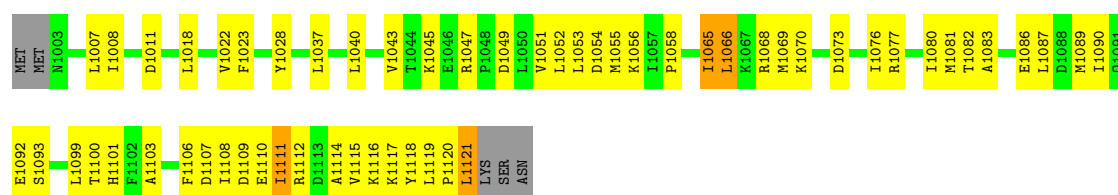
• Molecule 2: Sporulation initiation phosphotransferase F

Chain E:



• Molecule 2: Sporulation initiation phosphotransferase F

Chain F:



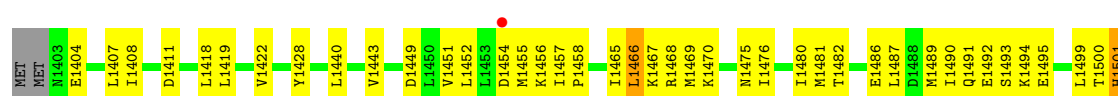
• Molecule 2: Sporulation initiation phosphotransferase F

Chain G:



• Molecule 2: Sporulation initiation phosphotransferase F

Chain H:



F1502	A1503	F1504	P1505	F1506	D1507	I1508	D1509	E1510	I1511	R1512	D1513	A1514	V1515	K1516	K1517	Y1518	L1519	P1520	L1521	LYS	SER	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.47Å 118.33Å 168.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 3.05 19.86 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.86-3.05) 98.7 (19.86-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.282 0.225 , 0.277	Depositor DCC
R_{free} test set	1404 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 28073 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9834	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BFD

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	0.57	0/1530	0.67	0/2064
1	B	0.54	0/1538	0.71	0/2075
1	C	0.45	0/1530	0.66	1/2064 (0.0%)
1	D	0.44	0/1538	0.63	0/2075
2	E	0.38	0/952	0.61	0/1279
2	F	0.46	0/952	0.66	0/1279
2	G	0.32	0/952	0.61	0/1279
2	H	0.35	0/963	0.60	0/1294
All	All	0.46	0/9955	0.65	1/13409 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	489	TYR	Sidechain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1497	0	1457	86	0
1	B	1505	0	1463	80	0
1	C	1497	0	1457	130	0
1	D	1505	0	1463	94	0
2	E	954	0	986	43	0
2	F	954	0	986	43	0
2	G	954	0	986	136	0
2	H	964	0	992	51	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	9834	0	9790	618	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 618 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:1687:LEU:HA	2:G:1690:ILE:HD13	1.26	1.10
2:E:1251:VAL:HG11	2:E:1269:MET:HE1	1.40	1.02
1:C:565:ILE:H	1:C:565:ILE:HD12	1.25	1.01
2:G:1620:ASN:ND2	2:G:1632:GLN:HE21	1.60	0.98
1:B:381:THR:HG23	1:C:581:THR:HG23	1.48	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	179/192 (93%)	165 (92%)	12 (7%)	2 (1%)	21	66
1	B	180/192 (94%)	166 (92%)	13 (7%)	1 (1%)	33	79
1	C	179/192 (93%)	165 (92%)	12 (7%)	2 (1%)	21	66
1	D	180/192 (94%)	168 (93%)	11 (6%)	1 (1%)	33	79
2	E	116/124 (94%)	100 (86%)	15 (13%)	1 (1%)	25	72
2	F	116/124 (94%)	99 (85%)	14 (12%)	3 (3%)	8	39
2	G	116/124 (94%)	84 (72%)	20 (17%)	12 (10%)	1	4
2	H	117/124 (94%)	100 (86%)	14 (12%)	3 (3%)	8	39
All	All	1183/1264 (94%)	1047 (88%)	111 (9%)	25 (2%)	11	46

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1320	PRO
2	F	1120	PRO
2	G	1684	TYR
2	G	1700	THR
2	H	1520	PRO

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	A	166/177 (94%)	155 (93%)	11 (7%)	24	63
1	B	167/177 (94%)	152 (91%)	15 (9%)	14	47
1	C	166/177 (94%)	149 (90%)	17 (10%)	11	38
1	D	167/177 (94%)	151 (90%)	16 (10%)	12	43
2	E	104/109 (95%)	98 (94%)	6 (6%)	28	69
2	F	104/109 (95%)	99 (95%)	5 (5%)	35	78
2	G	104/109 (95%)	97 (93%)	7 (7%)	23	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	105/109 (96%)	97 (92%)	8 (8%)	19	57
All	All	1083/1144 (95%)	998 (92%)	85 (8%)	18	55

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	564	ASP
1	D	647	LYS
2	H	1466	LEU
1	C	566	ARG
1	D	614	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	475	HIS
1	D	630	HIS
2	H	1432	GLN
1	C	488	HIS
1	D	741	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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	BFD	E	1254	3,2	10,11,12	6.02	5 (50%)	5,15,17	3.95	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BFD	F	1054	3,2	10,11,12	5.27	5 (50%)	5,15,17	4.89	2 (40%)
2	BFD	G	1654	3,2	10,11,12	5.69	5 (50%)	5,15,17	4.46	2 (40%)
2	BFD	H	1454	3,2	10,11,12	5.67	5 (50%)	5,15,17	4.57	2 (40%)

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	BFD	E	1254	3,2	-	0/4/11/13	0/0/0/0
2	BFD	F	1054	3,2	-	0/4/11/13	0/0/0/0
2	BFD	G	1654	3,2	-	0/4/11/13	0/0/0/0
2	BFD	H	1454	3,2	-	0/4/11/13	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1254	BFD	O-C	18.02	1.23	1.11
2	G	1654	BFD	O-C	17.16	1.23	1.11
2	H	1454	BFD	O-C	17.07	1.23	1.11
2	F	1054	BFD	O-C	15.60	1.22	1.11
2	E	1254	BFD	F3-BE	-3.38	1.48	1.55

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1054	BFD	C-CA-N	-10.21	103.63	113.83
2	H	1454	BFD	C-CA-N	-9.58	104.26	113.83
2	G	1654	BFD	C-CA-N	-9.32	104.52	113.83
2	E	1254	BFD	C-CA-N	-8.17	105.67	113.83
2	F	1054	BFD	OD2-CG-CB	-3.40	116.98	124.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	181/192 (94%)	-0.34	0	100	100	28, 44, 74, 91	0
1	B	182/192 (94%)	-0.34	0	100	100	24, 46, 75, 96	3 (1%)
1	C	181/192 (94%)	-0.18	1 (0%)	86	33	42, 71, 100, 115	0
1	D	182/192 (94%)	-0.20	2 (1%)	77	21	41, 63, 98, 114	3 (1%)
2	E	119/124 (95%)	-0.13	1 (0%)	83	27	56, 77, 96, 106	0
2	F	119/124 (95%)	-0.29	0	100	100	36, 54, 77, 87	0
2	G	119/124 (95%)	0.08	3 (2%)	54	10	75, 101, 114, 116	1 (0%)
2	H	119/124 (95%)	-0.05	2 (1%)	67	15	56, 87, 112, 121	2 (1%)
All	All	1202/1264 (95%)	-0.20	9 (0%)	84	30	24, 65, 106, 121	9 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1720	PRO	4.5
1	C	412	ILE	3.1
2	H	1521	LEU	3.0
2	G	1721	LEU	2.5
2	E	1321	LEU	2.4

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

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BFD	H	1454	12/13	0.31	1.44	66,68,71,71	4
2	BFD	F	1054	12/13	0.27	1.11	39,41,42,43	4
2	BFD	E	1254	12/13	0.24	0.44	60,62,66,67	4
2	BFD	G	1654	12/13	0.18	-0.67	85,87,88,88	4

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	F	2002	1/1	0.34	5.65	37,37,37,37	0
3	MG	E	2001	1/1	0.31	3.12	37,37,37,37	0
3	MG	H	2003	1/1	0.19	0.53	37,37,37,37	0
3	MG	G	2004	1/1	0.05	-2.00	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.