Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:13 PM GMT

PDB ID	:	2R25
Title	:	Complex of YPD1 and SLN1-R1 with bound Mg2+ and BeF3-
Authors	:	Copeland, D.M.; Zhao, X.; Soares, A.S.; West, A.H.
Deposited on	:	2007-08-24
Resolution	:	1.70 Å(reported)

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		18
Ramachandran outliers		1.7%
Sidechain outliers		7.5%
RSRZ outliers		16.6%

Worse — *Better*

∎ Percentile relative to all X-ray structures

❏ Percentile relative to X-ray structures of similar resolution
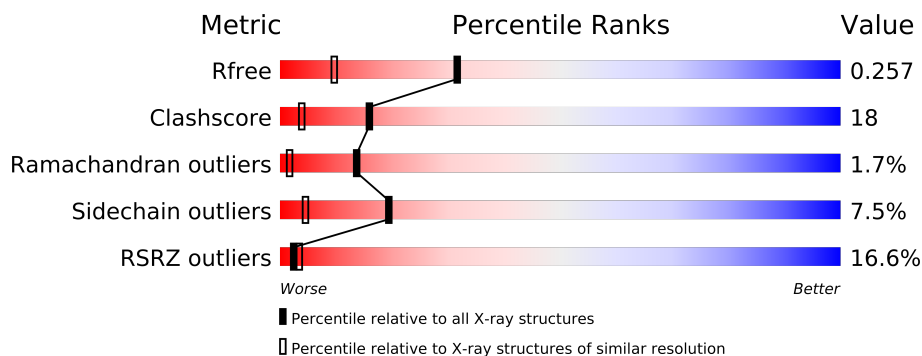
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	167	
2	B	133	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NA	B	5	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 2723 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 Phosphorelay intermediate protein YPD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	6	0
			1383	871	232	275	5			

- Molecule 2 is a protein called Osmosensing histidine protein kinase SLN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	8	0
			1096	694	182	210	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF$_3$).
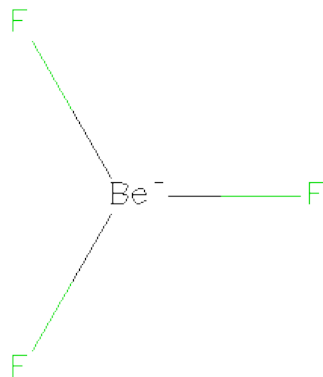
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	Be 1	F 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total 157	O 157	0	0
6	B	81	Total 81	O 81	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: Phosphorelay intermediate protein YPD1

Chain A:
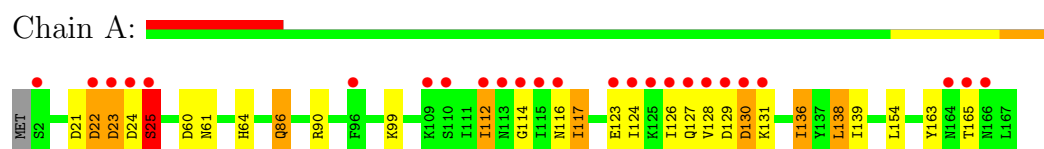
- Molecule 2: Osmosensing histidine protein kinase SLN1

Chain B:
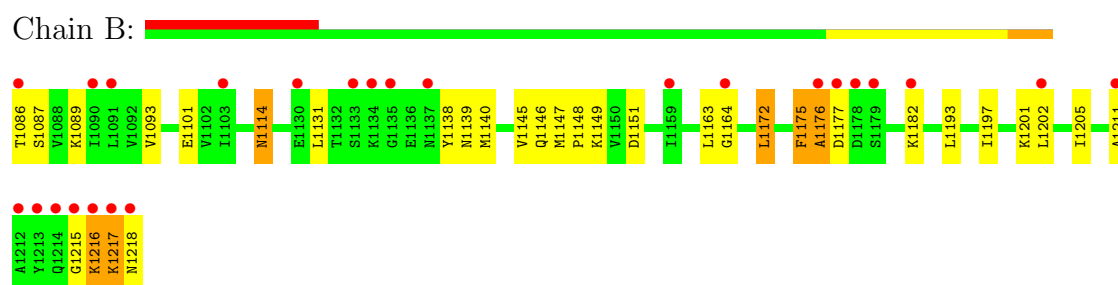
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants $a, b, c, \alpha, \beta, \gamma$	52.01Å 75.54Å 98.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.75 – 1.70 17.75 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (17.75-1.70) 99.2 (17.75-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.240 0.230 , 0.257	Depositor DCC
R_{free} test set	2166 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 42989 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2723	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: NA, MG, BEF

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	0.87	0/1406	0.87	2/1894 (0.1%)
2	B	0.76	1/1111 (0.1%)	0.80	2/1490 (0.1%)
All	All	0.82	1/2517 (0.0%)	0.84	4/3384 (0.1%)

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
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1138	TYR	C-O	5.41	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1140	MET	CB-CG-SD	-6.49	92.92	112.40
1	A	138	LEU	CB-CG-CD1	6.11	121.39	111.00
1	A	138	LEU	CA-CB-CG	5.64	128.26	115.30
2	B	1138	TYR	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1164	GLY	Peptide
2	B	1175	PHE	Peptide

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	1383	0	1377	33	0
2	B	1096	0	1124	60	1
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	B	4	0	0	0	0
6	A	157	0	0	11	1
6	B	81	0	0	2	0
All	All	2723	0	2501	92	1

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 18.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1216:LYS:CB	2:B:1217:LYS:HB2	1.24	1.63
2:B:1216:LYS:HA	2:B:1217:LYS:CD	1.34	1.58
2:B:1216:LYS:CA	2:B:1217:LYS:HD3	1.51	1.37
2:B:1216:LYS:HB3	2:B:1217:LYS:CB	1.59	1.28
2:B:1216:LYS:CB	2:B:1217:LYS:CB	2.19	1.15
1:A:128:VAL:H	1:A:129:ASP:HB2	0.99	1.14
2:B:1172:LEU:CD2	2:B:1197[B]:ILE:HD11	1.81	1.10
2:B:1216:LYS:CA	2:B:1217:LYS:HB2	1.81	1.09
2:B:1172:LEU:HD21	2:B:1197[B]:ILE:HD11	1.33	1.08
1:A:128:VAL:N	1:A:129:ASP:HB2	1.80	0.96
1:A:24:ASP:O	1:A:25:SER:HB3	1.68	0.94
2:B:1172:LEU:HD21	2:B:1197[B]:ILE:CD1	1.96	0.94
2:B:1216:LYS:HA	2:B:1217:LYS:CG	2.00	0.92
2:B:1216:LYS:HB2	2:B:1217:LYS:HB2	1.50	0.91
2:B:1216:LYS:CA	2:B:1217:LYS:CB	2.44	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:VAL:H	1:A:129:ASP:CB	1.86	0.88
2:B:1216:LYS:HB3	2:B:1217:LYS:HB2	0.88	0.86
1:A:22:ASP:HA	6:A:314:HOH:O	1.73	0.86
2:B:1175:PHE:HB3	2:B:1176:ALA:HB3	1.63	0.81
2:B:1175:PHE:HA	2:B:1176:ALA:HB2	1.63	0.80
2:B:1086[A]:THR:HG22	2:B:1087[A]:SER:H	1.47	0.79
1:A:124:ILE:HD11	6:A:270:HOH:O	1.82	0.79
2:B:1216:LYS:CA	2:B:1217:LYS:CD	2.31	0.78
1:A:86:GLN:HE22	1:A:90:ARG:HD2	1.49	0.76
2:B:1172:LEU:HD23	2:B:1197[B]:ILE:HD11	1.69	0.75
2:B:1217:LYS:O	2:B:1218:ASN:OD1	2.05	0.75
2:B:1172:LEU:HD21	2:B:1197[B]:ILE:CG1	2.18	0.73
2:B:1086[B]:THR:HG23	2:B:1087[B]:SER:N	2.04	0.72
6:A:292:HOH:O	2:B:1176:ALA:HA	1.88	0.72
2:B:1086[A]:THR:O	2:B:1087[A]:SER:CB	2.41	0.69
2:B:1215:GLY:O	2:B:1217:LYS:CE	2.41	0.69
2:B:1216:LYS:HA	2:B:1217:LYS:CB	2.17	0.68
1:A:23:ASP:HB3	6:A:296:HOH:O	1.94	0.68
1:A:117:ILE:HG22	6:A:282:HOH:O	1.93	0.67
2:B:1101[A]:GLU:OE1	6:B:238:HOH:O	2.13	0.67
1:A:112:ILE:CD1	1:A:154:LEU:HD21	2.25	0.66
2:B:1215:GLY:O	2:B:1217:LYS:HE2	1.97	0.65
2:B:1216:LYS:HB3	2:B:1217:LYS:CG	2.26	0.65
2:B:1215:GLY:O	2:B:1217:LYS:HD3	1.97	0.64
2:B:1216:LYS:HA	2:B:1217:LYS:HD3	0.67	0.64
1:A:99:LYS:HD3	1:A:117:ILE:CG1	2.28	0.62
2:B:1193:LEU:HD21	2:B:1205:ILE:HG13	1.80	0.62
2:B:1217:LYS:C	2:B:1218:ASN:OD1	2.39	0.61
1:A:116:ASN:HA	6:A:282:HOH:O	1.99	0.61
1:A:86:GLN:NE2	1:A:90:ARG:HD2	2.15	0.60
2:B:1216:LYS:N	2:B:1217:LYS:HD3	2.16	0.60
2:B:1175:PHE:CA	2:B:1176:ALA:CB	2.80	0.59
2:B:1175:PHE:CA	2:B:1176:ALA:HB2	2.31	0.59
1:A:22:ASP:OD1	1:A:23:ASP:N	2.38	0.56
2:B:1215:GLY:O	2:B:1217:LYS:CD	2.53	0.55
2:B:1086[B]:THR:HG23	2:B:1087[B]:SER:H	1.69	0.55
2:B:1175:PHE:CB	2:B:1176:ALA:HB3	2.37	0.54
1:A:21:ASP:O	1:A:22:ASP:CG	2.46	0.54
6:A:292:HOH:O	2:B:1176:ALA:CB	2.55	0.54
1:A:112:ILE:HD11	1:A:154:LEU:HD21	1.89	0.54
1:A:21:ASP:O	1:A:22:ASP:OD1	2.26	0.53
1:A:99:LYS:HD3	1:A:117:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:GLY:CA	6:A:294:HOH:O	2.57	0.52
2:B:1193:LEU:CD2	2:B:1201:LYS:HE2	2.40	0.52
2:B:1197[B]:ILE:N	2:B:1197[B]:ILE:HD13	2.24	0.51
2:B:1172:LEU:HD21	2:B:1197[B]:ILE:HG13	1.93	0.51
2:B:1175:PHE:CB	2:B:1176:ALA:CB	2.90	0.50
2:B:1175:PHE:HD1	2:B:1176:ALA:HB2	1.77	0.50
1:A:64:HIS:HB2	1:A:86:GLN:HG3	1.94	0.50
2:B:1175:PHE:HB3	2:B:1176:ALA:CB	2.38	0.49
2:B:1217:LYS:O	2:B:1218:ASN:CG	2.51	0.49
2:B:1215:GLY:C	2:B:1217:LYS:HD3	2.32	0.49
1:A:21:ASP:OD2	1:A:25:SER:HA	2.12	0.49
1:A:86:GLN:HE22	1:A:90:ARG:CD	2.22	0.49
1:A:112:ILE:O	1:A:112:ILE:HG23	2.14	0.47
2:B:1145:VAL:O	2:B:1151:ASP:HB2	2.15	0.47
2:B:1086[A]:THR:HG22	2:B:1087[A]:SER:N	2.22	0.47
6:A:292:HOH:O	2:B:1176:ALA:HB2	2.14	0.46
2:B:1089:LYS:H	2:B:1139:ASN:ND2	2.13	0.45
1:A:163:TYR:HB3	1:A:165:THR:HG22	1.99	0.45
1:A:127:GLN:HB2	1:A:130:ASP:HB2	1.99	0.45
1:A:99:LYS:HD3	1:A:117:ILE:HG13	1.98	0.45
1:A:24:ASP:O	1:A:25:SER:CB	2.50	0.45
2:B:1086[B]:THR:CG2	2:B:1087[B]:SER:N	2.71	0.44
2:B:1172:LEU:CD2	2:B:1197[B]:ILE:CD1	2.66	0.44
1:A:114:GLY:N	6:A:294:HOH:O	2.46	0.44
2:B:1148:PRO:O	2:B:1149:LYS:HB2	2.18	0.43
1:A:136[A]:ILE:H	1:A:136[A]:ILE:HG13	1.62	0.43
2:B:1175:PHE:CD1	2:B:1176:ALA:HB2	2.53	0.43
1:A:86:GLN:C	1:A:86:GLN:HE21	2.22	0.43
2:B:1177:ASP:HB2	6:B:228:HOH:O	2.18	0.43
2:B:1093:VAL:HG12	2:B:1147:MET:SD	2.59	0.42
2:B:1139:ASN:HD22	2:B:1139:ASN:H	1.66	0.42
1:A:114:GLY:HA3	6:A:294:HOH:O	2.17	0.42
2:B:1089:LYS:HE2	2:B:1114:ASN:OD1	2.20	0.41
1:A:61:ASN:HA	2:B:1146:GLN:HE22	1.84	0.41
1:A:112:ILE:HD12	1:A:112:ILE:HA	1.56	0.41

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	Distance(Å)	Clash(Å)
2:B:1101[B]:GLU:OE2	6:A:203:HOH:O[4_455]	2.07	0.13

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	170/167 (102%)	160 (94%)	8 (5%)	2 (1%)	19	3
2	B	138/133 (104%)	131 (95%)	4 (3%)	3 (2%)	10	1
All	All	308/300 (103%)	291 (94%)	12 (4%)	5 (2%)	14	2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1176	ALA
2	B	1211	ALA
2	B	1217	LYS
1	A	25	SER
1	A	22	ASP

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	156/152 (103%)	142 (91%)	14 (9%)	14	3
2	B	124/118 (105%)	117 (94%)	7 (6%)	30	10
All	All	280/270 (104%)	259 (92%)	21 (8%)	19	4

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	25	SER
1	A	60	ASP
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	112	ILE
1	A	117	ILE
1	A	123	GLU
1	A	126	ILE
1	A	130	ASP
1	A	131	LYS
1	A	136[A]	ILE
1	A	136[B]	ILE
1	A	138	LEU
1	A	139	ILE
2	B	1114	ASN
2	B	1131	LEU
2	B	1163	LEU
2	B	1172	LEU
2	B	1182	LYS
2	B	1202	LEU
2	B	1216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	86	GLN
1	A	94	HIS
1	A	113	ASN
2	B	1139	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

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5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	BEF	B	2	2	0,3,3	0.00	-	0,3,3	0.00	-

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
5	BEF	B	2	2	-	0/0/0/0	0/0/0/0

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	166/167 (99%)	0.97	25 (15%)	3	4	22, 30, 57, 78	5 (3%)
2	B	133/133 (100%)	1.20	25 (18%)	2	3	21, 37, 68, 78	5 (3%)
All	All	299/300 (99%)	1.07	50 (16%)	2	3	21, 33, 67, 78	10 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ILE	12.3
2	B	1218	ASN	12.2
1	A	128	VAL	10.4
2	B	1217	LYS	8.1
1	A	130	ASP	7.3
2	B	1135	GLY	7.2
1	A	129	ASP	6.7
1	A	125	LYS	6.6
2	B	1086[A]	THR	6.1
2	B	1212	ALA	6.0
1	A	124	ILE	5.7
2	B	1215	GLY	5.7
1	A	24	ASP	5.3
2	B	1211	ALA	5.1
1	A	127	GLN	4.9
1	A	23	ASP	4.8
2	B	1216	LYS	4.5
1	A	113	ASN	4.4
1	A	22	ASP	4.2
2	B	1179	SER	4.2
2	B	1177	ASP	4.0
2	B	1130	GLU	4.0
1	A	115	ILE	3.9
2	B	1214	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	110	SER	3.6
1	A	131	LYS	3.3
2	B	1164	GLY	3.3
1	A	164	ASN	3.2
2	B	1178	ASP	3.1
2	B	1134	LYS	3.0
2	B	1091	LEU	2.9
2	B	1213	TYR	2.9
1	A	109	LYS	2.8
1	A	114	GLY	2.6
1	A	165	THR	2.6
1	A	25	SER	2.4
1	A	116	ASN	2.3
1	A	112	ILE	2.3
2	B	1103	ILE	2.3
2	B	1176	ALA	2.2
1	A	166[A]	ASN	2.2
1	A	96	PHE	2.2
2	B	1090	ILE	2.1
1	A	123	GLU	2.1
2	B	1202	LEU	2.1
2	B	1133	SER	2.1
2	B	1137	ASN	2.0
2	B	1159	ILE	2.0
2	B	1182	LYS	2.0
1	A	2	SER	2.0

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

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

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(Å^2)	Q<0.9
4	NA	B	5	1/1	0.22	3.95	39,39,39,39	1
5	BEF	B	2	4/4	0.08	-1.17	25,25,26,28	0
3	MG	B	1	1/1	0.02	-4.49	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.