Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 11:41 AM EDT

PDB ID	:	7K02
Title	:	The crystal structure of a BAK dimer activated by detergent
Authors	:	Birkinshaw, R.W.; Czabotar, P.E.
Deposited on	:	2020-09-02
Resolution	:	3.40 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:

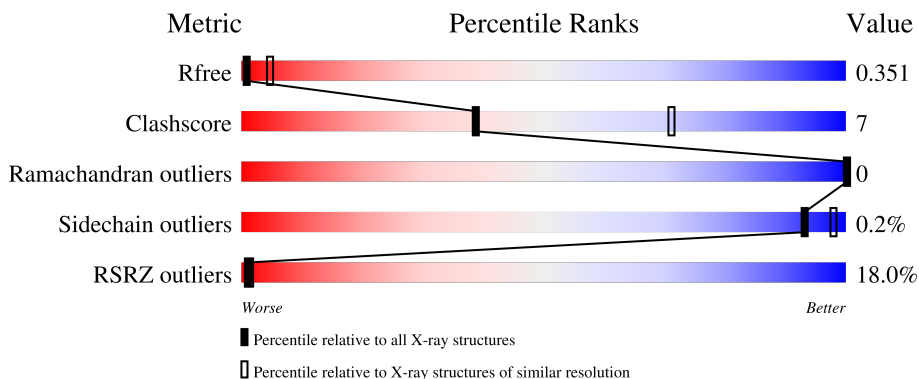|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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		0.351
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.2%
RSRZ outliers		18.0%

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$_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	122	18% / 70% 16% 14%
1	B	122	14% / 78% 17% • •
1	C	122	10% / 87% 9% •
1	D	122	18% / 71% 14% 15%
1	E	122	21% / 69% 18% 13%

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Mol	Chain	Length	Quality of chain
1	F	122	

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 5225 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 Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			848	546	150	149	3			
1	B	117	Total	C	N	O	S	0	0	0
			932	599	167	163	3			
1	C	117	Total	C	N	O	S	0	0	0
			935	602	167	163	3			
1	D	104	Total	C	N	O	S	0	0	0
			840	541	148	148	3			
1	E	106	Total	C	N	O	S	0	0	0
			859	552	154	150	3			
1	F	102	Total	C	N	O	S	0	0	0
			811	520	142	146	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	expression tag	UNP Q16611
A	66	SER	-	expression tag	UNP Q16611
A	166	SER	CYS	engineered mutation	UNP Q16611
B	65	GLY	-	expression tag	UNP Q16611
B	66	SER	-	expression tag	UNP Q16611
B	166	SER	CYS	engineered mutation	UNP Q16611
C	65	GLY	-	expression tag	UNP Q16611
C	66	SER	-	expression tag	UNP Q16611
C	166	SER	CYS	engineered mutation	UNP Q16611
D	65	GLY	-	expression tag	UNP Q16611
D	66	SER	-	expression tag	UNP Q16611
D	166	SER	CYS	engineered mutation	UNP Q16611
E	65	GLY	-	expression tag	UNP Q16611
E	66	SER	-	expression tag	UNP Q16611
E	166	SER	CYS	engineered mutation	UNP Q16611
F	65	GLY	-	expression tag	UNP Q16611
F	66	SER	-	expression tag	UNP Q16611

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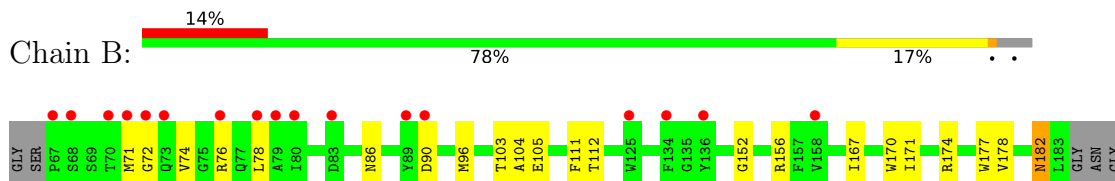| Chain	Residue	Modelled	Actual	Comment	Reference
F	166	SER	CYS	engineered mutation	UNP Q16611

3 Residue-property plots ⓘ

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.
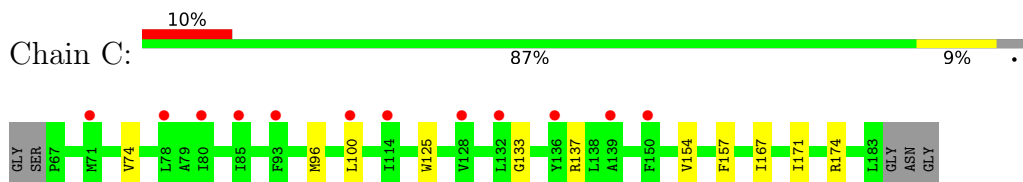
• Molecule 1: Bcl-2 homologous antagonist/killer
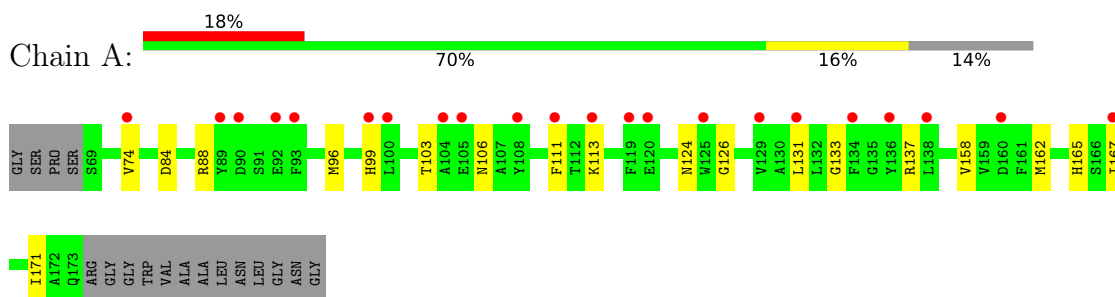
Chain A:
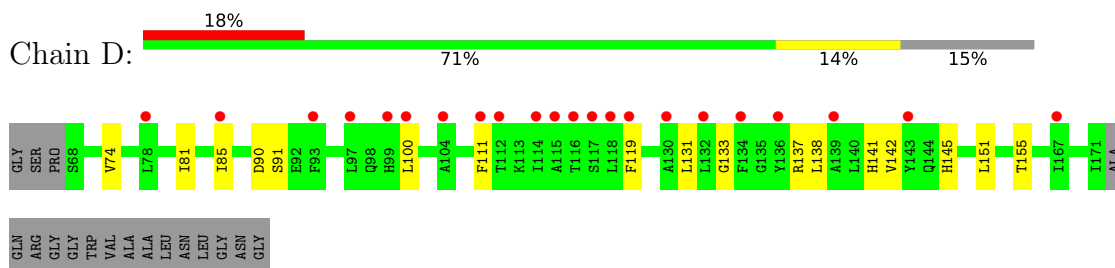

• Molecule 1: Bcl-2 homologous antagonist/killer

Chain B:

• Molecule 1: Bcl-2 homologous antagonist/killer

Chain C:

• Molecule 1: Bcl-2 homologous antagonist/killer

Chain D:

• Molecule 1: Bcl-2 homologous antagonist/killer

Chain E:

GLY SER PRO SER S69 T70 M71 G72 Q73 V74 G75 R76 Q77 L78 I85 N86 R87 D90 S91 E92 F93 Q94 T95 M96 L97 Q98 H99 L100 Y110 F111 T112 K113 I114 A115 T116 S117 L118 F119 E120 S121 G122 I123 N124 W125 G126 R127 V128 V129 A130 L131 F134 L138 L147

F150 Q153 V154 V158 F161 R174 GLY GLY TRP VAL ALA ALA LEU ASN LEU GLY ASN GLY

• Molecule 1: Bcl-2 homologous antagonist/killer

Chain F:

15%

72%　　　11%　　　16%

GLY SER P67 S68 S69 T70 M71 V74 L78 R87 R88 Y89 D90 S91 E92 F93 M96 L100 Y108 E109 Y110 F111 T112 K113 I114 A115 T116 S117 S121 G122 I123 N124 R127 V128 V129 A130 T155 A168 ARG TRP ILE ALA GLN ARG GLY GLY TRP VAL ALA ALA

LEU ASN LEU GLY ASN GLY
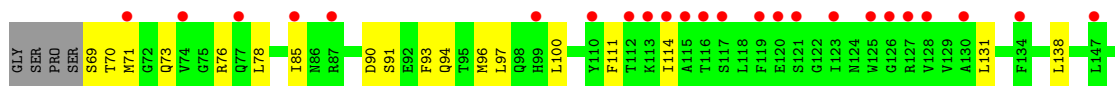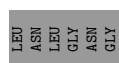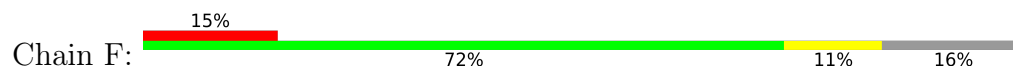
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.32Å　115.61Å　44.53Å 90.00°　90.06°　90.00°	Depositor
Resolution (Å)	39.33 – 3.40 47.76 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.33-3.40) 99.6 (47.76-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.296 , 0.343 0.296 , 0.351	Depositor DCC
R_{free} test set	555 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	154.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 155.1	EDS
L-test for twinning [2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.419 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5225	wwPDB-VP
Average B, all atoms (Å^2)	202.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.28	0/869	0.46	0/1176
1	B	0.28	0/956	0.40	0/1295
1	C	0.24	0/959	0.38	0/1299
1	D	0.24	0/861	0.38	0/1165
1	E	0.27	0/880	0.43	0/1190
1	F	0.25	0/830	0.42	0/1122
All	All	0.26	0/5355	0.41	0/7247

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	A	848	0	827	17	0
1	B	932	0	907	21	0
1	C	935	0	916	9	0
1	D	840	0	819	14	0
1	E	859	0	840	23	0
1	F	811	0	786	18	0
All	All	5225	0	5095	77	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 7.

All (77) 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:178:VAL:O	1:B:182:ASN:HB2	1.63	0.98
1:F:96:MET:O	1:F:100:LEU:HD13	1.67	0.94
1:A:158:VAL:O	1:A:162:MET:HG2	1.66	0.92
1:A:126:GLY:N	1:B:86:ASN:OD1	2.22	0.71
1:E:69:SER:O	1:E:73:GLN:HG2	1.92	0.69
1:E:71:MET:HB2	1:F:114:ILE:HG12	1.74	0.69
1:B:105:GLU:N	1:B:105:GLU:OE1	2.24	0.69
1:F:123:ILE:HA	1:F:127:ARG:HD2	1.76	0.67
1:F:96:MET:O	1:F:100:LEU:CD1	2.41	0.66
1:E:114:ILE:HG22	1:F:71:MET:HG2	1.79	0.63
1:D:111:PHE:CE2	1:E:154:VAL:HG13	2.34	0.62
1:A:124:ASN:CG	1:B:86:ASN:HD21	2.04	0.61
1:C:100:LEU:HD11	1:D:74:VAL:HG21	1.83	0.61
1:E:71:MET:HB2	1:F:114:ILE:HA	1.82	0.60
1:B:86:ASN:O	1:B:90:ASP:HB2	2.04	0.57
1:D:90:ASP:OD1	1:D:91:SER:N	2.38	0.57
1:E:90:ASP:HA	1:E:93:PHE:CZ	2.41	0.56
1:B:105:GLU:H	1:B:105:GLU:CD	2.06	0.55
1:F:90:ASP:OD1	1:F:91:SER:N	2.39	0.55
1:D:141:HIS:O	1:D:145:HIS:HB2	2.07	0.54
1:E:71:MET:CB	1:F:114:ILE:HG12	2.38	0.53
1:E:114:ILE:HG22	1:F:71:MET:CG	2.38	0.53
1:C:74:VAL:HG21	1:D:100:LEU:HD11	1.89	0.53
1:E:78:LEU:HD22	1:F:130:ALA:HB1	1.89	0.53
1:B:71:MET:HA	1:B:74:VAL:HG22	1.89	0.53
1:C:96:MET:SD	1:D:74:VAL:HG13	2.49	0.52
1:F:68:SER:HA	1:F:71:MET:CE	2.40	0.51
1:E:97:LEU:HD11	1:E:138:LEU:HA	1.93	0.50
1:E:71:MET:HB2	1:F:114:ILE:CG1	2.41	0.50
1:A:113:LYS:HD3	1:B:71:MET:SD	2.53	0.49
1:A:84:ASP:O	1:A:88:ARG:HB2	2.13	0.49
1:A:133:GLY:O	1:A:137:ARG:HG2	2.14	0.47
1:E:70:THR:HA	1:E:73:GLN:NE2	2.29	0.47
1:A:103:THR:N	1:A:106:ASN:OD1	2.48	0.47
1:A:162:MET:O	1:A:165:HIS:HB3	2.15	0.47
1:D:111:PHE:CE1	1:D:131:LEU:HG	2.50	0.47
1:D:119:PHE:HB2	1:E:161:PHE:HE2	1.79	0.46
1:B:152:GLY:O	1:B:156:ARG:HG3	2.15	0.46
1:E:111:PHE:CE1	1:E:131:LEU:HD11	2.51	0.46
1:B:170:TRP:O	1:B:174:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:O	1:B:171:ILE:HG12	2.16	0.45
1:A:126:GLY:CA	1:B:86:ASN:OD1	2.65	0.45
1:B:74:VAL:O	1:B:78:LEU:HG	2.16	0.45
1:E:85:ILE:HG12	1:F:89:TYR:CZ	2.51	0.45
1:E:150:PHE:O	1:E:153:GLN:HG2	2.16	0.45
1:F:108:TYR:O	1:F:112:THR:HG23	2.16	0.45
1:A:158:VAL:O	1:A:162:MET:CG	2.53	0.45
1:D:133:GLY:O	1:D:137:ARG:HG2	2.16	0.45
1:B:171:ILE:HG21	1:B:177:TRP:CG	2.51	0.45
1:C:125:TRP:CZ3	1:D:85:ILE:HG22	2.52	0.45
1:B:171:ILE:HG21	1:B:177:TRP:CD1	2.52	0.45
1:A:96:MET:SD	1:B:74:VAL:HG12	2.58	0.44
1:B:72:GLY:O	1:B:76:ARG:HG3	2.18	0.44
1:C:174:ARG:O	1:C:174:ARG:HG3	2.18	0.44
1:E:100:LEU:HD11	1:F:74:VAL:HG21	1.99	0.44
1:E:91:SER:HA	1:E:94:GLN:HG2	1.99	0.44
1:A:111:PHE:CE1	1:A:131:LEU:HD11	2.53	0.43
1:C:133:GLY:O	1:C:137:ARG:HG2	2.18	0.43
1:D:81:ILE:O	1:D:85:ILE:HG13	2.17	0.43
1:C:167:ILE:O	1:C:171:ILE:HG12	2.19	0.43
1:E:96:MET:SD	1:F:74:VAL:HG22	2.59	0.43
1:A:167:ILE:O	1:A:171:ILE:HG12	2.18	0.43
1:D:151:LEU:O	1:D:155:THR:OG1	2.24	0.43
1:A:162:MET:O	1:A:165:HIS:N	2.52	0.42
1:B:111:PHE:CZ	1:C:154:VAL:HG13	2.55	0.42
1:F:68:SER:HA	1:F:71:MET:HE3	2.01	0.42
1:A:111:PHE:CE1	1:A:131:LEU:CD1	3.03	0.41
1:A:74:VAL:HG13	1:B:96:MET:SD	2.61	0.41
1:B:112:THR:HG23	1:C:157:PHE:CE1	2.56	0.41
1:D:119:PHE:HB2	1:E:161:PHE:CE2	2.56	0.41
1:B:103:THR:HG22	1:B:104:ALA:N	2.37	0.40
1:D:138:LEU:O	1:D:142:VAL:HG22	2.21	0.40
1:E:76:ARG:HE	1:E:76:ARG:HB2	1.66	0.40
1:E:111:PHE:HE1	1:E:131:LEU:HD11	1.85	0.40
1:A:99:HIS:ND1	1:A:99:HIS:O	2.54	0.40
1:E:150:PHE:O	1:E:154:VAL:HG23	2.22	0.40
1:F:68:SER:HA	1:F:71:MET:HE2	2.03	0.40

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	103/122 (84%)	99 (96%)	4 (4%)	0	100	100
1	B	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
1	C	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
1	D	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
1	E	104/122 (85%)	103 (99%)	1 (1%)	0	100	100
1	F	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
All	All	639/732 (87%)	627 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	87/97 (90%)	87 (100%)	0	100	100
1	B	94/97 (97%)	93 (99%)	1 (1%)	73	86
1	C	95/97 (98%)	95 (100%)	0	100	100
1	D	87/97 (90%)	87 (100%)	0	100	100
1	E	88/97 (91%)	88 (100%)	0	100	100
1	F	84/97 (87%)	84 (100%)	0	100	100
All	All	535/582 (92%)	534 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	105/122 (86%)	1.01	22 (20%)	1	1	132, 199, 252, 298	0
1	B	117/122 (95%)	0.71	17 (14%)	2	3	94, 129, 263, 298	0
1	C	117/122 (95%)	0.47	12 (10%)	6	8	92, 130, 211, 262	0
1	D	104/122 (85%)	0.90	22 (21%)	0	1	134, 197, 242, 284	0
1	E	106/122 (86%)	1.05	26 (24%)	0	0	211, 276, 311, 371	0
1	F	102/122 (83%)	1.12	18 (17%)	1	1	205, 274, 315, 349	0
All	All	651/732 (88%)	0.87	117 (17%)	1	1	92, 203, 300, 371	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	117	SER	7.8
1	F	114	ILE	6.8
1	F	130	ALA	6.4
1	A	89	TYR	6.3
1	F	128	VAL	6.3
1	F	116	THR	6.2
1	D	97	LEU	6.1
1	F	71	MET	6.1
1	D	111	PHE	5.8
1	A	134	PHE	5.7
1	E	130	ALA	5.4
1	B	78	LEU	5.3
1	C	71	MET	5.3
1	A	131	LEU	5.2
1	D	112	THR	5.1
1	E	112	THR	5.0
1	A	90	ASP	5.0
1	E	119	PHE	4.9
1	F	100	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	155	THR	4.5
1	E	128	VAL	4.5
1	B	79	ALA	4.4
1	E	116	THR	4.4
1	F	124	ASN	4.3
1	A	105	GLU	4.2
1	D	119	PHE	4.1
1	A	92	GLU	4.1
1	E	114	ILE	4.1
1	B	89	TYR	4.1
1	C	78	LEU	4.0
1	A	167	ILE	3.9
1	B	90	ASP	3.9
1	B	70	THR	3.8
1	E	134	PHE	3.8
1	A	108	TYR	3.8
1	F	127	ARG	3.8
1	F	113	LYS	3.7
1	D	100	LEU	3.6
1	E	120	GLU	3.5
1	E	71	MET	3.5
1	E	126	GLY	3.5
1	A	129	VAL	3.5
1	A	160	ASP	3.5
1	D	99	HIS	3.5
1	F	121	SER	3.5
1	C	100	LEU	3.5
1	D	118	LEU	3.4
1	B	76	ARG	3.4
1	B	68	SER	3.4
1	B	67	PRO	3.4
1	A	120	GLU	3.4
1	D	93	PHE	3.3
1	F	117	SER	3.3
1	B	134	PHE	3.3
1	E	123	ILE	3.3
1	D	139	ALA	3.3
1	E	110	TYR	3.2
1	A	119	PHE	3.2
1	E	121	SER	3.2
1	E	127	ARG	3.2
1	B	73	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	PHE	3.1
1	C	80	ILE	3.1
1	D	134	PHE	3.1
1	A	136	TYR	3.0
1	D	116	THR	3.0
1	E	87	ARG	3.0
1	C	85	ILE	3.0
1	C	128	VAL	2.9
1	E	113	LYS	2.9
1	D	167	ILE	2.9
1	B	136	TYR	2.9
1	F	110	TYR	2.9
1	D	114	ILE	2.8
1	A	100	LEU	2.8
1	E	115	ALA	2.8
1	A	74	VAL	2.8
1	D	117	SER	2.8
1	F	69	SER	2.8
1	B	125	TRP	2.7
1	F	87	ARG	2.7
1	D	132	LEU	2.7
1	E	125	TRP	2.7
1	A	104	ALA	2.7
1	A	138	LEU	2.6
1	E	77	GLN	2.6
1	F	109	GLU	2.6
1	B	71	MET	2.6
1	C	132	LEU	2.6
1	A	125	TRP	2.5
1	F	78	LEU	2.5
1	D	115	ALA	2.5
1	E	74	VAL	2.4
1	D	104	ALA	2.4
1	C	150	PHE	2.4
1	E	85	ILE	2.4
1	E	158	VAL	2.4
1	B	72	GLY	2.4
1	D	85	ILE	2.4
1	D	136	TYR	2.3
1	B	80	ILE	2.3
1	A	93	PHE	2.3
1	A	99	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	114	ILE	2.2
1	B	83	ASP	2.2
1	F	93	PHE	2.1
1	D	143	TYR	2.1
1	A	113	LYS	2.1
1	E	147	LEU	2.1
1	C	93	PHE	2.1
1	E	154	VAL	2.1
1	D	78	LEU	2.0
1	C	139	ALA	2.0
1	C	136	TYR	2.0
1	B	158	VAL	2.0
1	E	99	HIS	2.0
1	D	130	ALA	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.