



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2017 – 01:33 PM EST

PDB ID : 5WE1
Title : Structural Basis for Shelterin Bridge Assembly
Authors : Kim, J.-K.; Liu, J.; Hu, X.; Yu, C.; Roskamp, K.; Sankaran, B.; Huang, L.; Komives, E.-A.; Qiao, F.
Deposited on : unknown
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

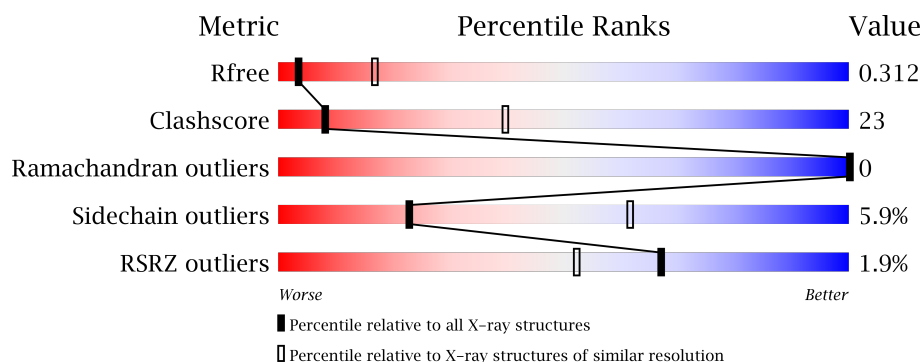
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 $\leq 5\%$. 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	214	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>39%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	214	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	33	<div> <div></div> <div> <div>33%</div> <div>52%</div> <div>•</div> <div>12%</div> </div> </div>
2	D	33	<div> <div></div> <div> <div>55%</div> <div>36%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3513 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 Protection of telomeres protein poz1, Protection of telomeres protein poz1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1496	961	257	263	15			
1	C	180	Total	C	N	O	S	0	0	0
			1510	970	259	266	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	-	expression tag	UNP O13852
A	83	GLY	-	linker	UNP O13852
A	84	GLY	-	linker	UNP O13852
A	85	ALA	-	linker	UNP O13852
A	120	SER	VAL	conflict	UNP O13852
A	125	SER	GLU	conflict	UNP O13852
C	29	SER	-	expression tag	UNP O13852
C	83	GLY	-	linker	UNP O13852
C	84	GLY	-	linker	UNP O13852
C	85	ALA	-	linker	UNP O13852
C	120	SER	VAL	conflict	UNP O13852
C	125	SER	GLU	conflict	UNP O13852

- Molecule 2 is a protein called Protection of telomeres protein tpz1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	S	0	0	0
			250	161	45	41	3			
2	D	30	Total	C	N	O	S	0	0	0
			255	164	46	42	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0

SER	GLU	A478	C479	E480	R483	L486	P487	H488	R496	D497	H498	K499	K500	I501	E502	R505	H506	K507	SER
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	66.11Å 66.11Å 123.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.92 – 3.20 51.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.92-3.20) 99.4 (51.92-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.266 , 0.317 0.267 , 0.312	Depositor DCC
R_{free} test set	514 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l 0.458 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3513	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN

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	0.42	0/1528	0.64	0/2047
1	C	0.42	0/1542	0.65	0/2066
2	B	0.29	0/256	0.54	0/339
2	D	0.28	0/261	0.51	0/346
All	All	0.40	0/3587	0.63	0/4798

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	1496	0	1488	75	0
1	C	1510	0	1504	77	1
2	B	250	0	246	18	0
2	D	255	0	250	7	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	3513	0	3488	164	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 23.

All (164) 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:167:PHE:HE2	1:A:186:GLN:HG2	1.28	0.98
1:A:167:PHE:CE2	1:A:186:GLN:HG2	2.04	0.92
1:A:171:LEU:HB3	1:A:175:GLY:HA3	1.52	0.92
1:A:171:LEU:CB	1:A:175:GLY:HA3	2.01	0.91
1:C:182:MET:HA	1:C:185:LEU:HD23	1.54	0.87
1:A:110:ARG:HH22	1:A:138:LEU:HD23	1.45	0.81
1:C:150:ARG:NH2	1:C:207:MET:SD	2.52	0.81
1:C:196:ARG:CZ	1:C:200:VAL:CG2	2.60	0.79
1:C:196:ARG:CZ	1:C:200:VAL:HG23	2.12	0.78
1:C:171:LEU:HB3	1:C:182:MET:SD	2.24	0.77
1:C:196:ARG:NE	1:C:200:VAL:HG23	2.00	0.77
1:C:203:HIS:HA	1:C:206:LYS:HB3	1.75	0.67
1:C:196:ARG:HA	1:C:199:TYR:HB2	1.77	0.67
1:C:181:GLU:O	1:C:184:ALA:HB3	1.94	0.67
1:A:160:GLU:OE1	1:A:196:ARG:NH2	2.28	0.67
1:A:56:MET:HE2	1:C:40:TYR:HB2	1.75	0.67
1:A:214:SER:OG	1:A:218:ARG:NH1	2.28	0.66
2:D:498:TRP:HE3	2:D:499:LYS:HG2	1.61	0.66
1:C:193:ILE:HG13	1:C:197:LEU:HD11	1.79	0.65
1:A:130:LYS:HD2	1:A:133:LEU:HD12	1.79	0.64
1:A:190:LYS:O	1:A:190:LYS:HG2	1.98	0.63
1:C:185:LEU:O	1:C:189:SER:N	2.32	0.62
1:C:54:ILE:HD11	1:C:106:ILE:HG23	1.81	0.62
2:B:499:LYS:HD2	2:B:499:LYS:O	2.00	0.62
1:C:185:LEU:HA	1:C:188:LEU:HG	1.82	0.61
1:C:196:ARG:NH2	1:C:200:VAL:HG22	2.16	0.61
2:B:486:LEU:O	2:B:488:HIS:ND1	2.33	0.60
1:A:66:ASN:OD1	2:B:505:ARG:NH2	2.34	0.60
1:C:128:LEU:HD13	1:C:230:PHE:CZ	2.35	0.59
1:C:182:MET:O	1:C:185:LEU:HB2	2.02	0.59
1:A:40:TYR:HE1	1:A:47:MET:HG2	1.67	0.59
1:C:164:HIS:HA	1:C:167:PHE:HB3	1.84	0.58
1:C:196:ARG:CZ	1:C:200:VAL:HG22	2.32	0.58
1:A:171:LEU:HB3	1:A:175:GLY:CA	2.29	0.58
1:C:128:LEU:HD13	1:C:230:PHE:CE1	2.38	0.58
1:A:94:SER:O	1:A:98:ASN:ND2	2.22	0.58
1:C:196:ARG:NE	1:C:200:VAL:CG2	2.66	0.58
2:B:496:ARG:O	2:B:500:LYS:HG3	2.04	0.57
1:C:69:LEU:O	1:C:69:LEU:HD12	2.04	0.57
1:C:62:GLU:HA	1:C:67:LEU:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HB2	1:A:175:GLY:HA3	1.86	0.56
1:C:222:CYS:O	1:C:226:GLN:HG3	2.06	0.56
1:A:37:CYS:HB3	1:C:41:LEU:HD11	1.87	0.56
2:B:497:ASP:O	2:B:501:ILE:HG13	2.05	0.55
1:A:222:CYS:SG	1:A:226:GLN:NE2	2.80	0.55
1:A:130:LYS:HG3	1:A:230:PHE:CZ	2.42	0.55
1:A:52:MET:HE1	2:B:494:LEU:HD13	1.89	0.55
1:A:168:THR:HA	1:A:186:GLN:OE1	2.07	0.55
1:A:193:ILE:HA	1:A:196:ARG:HE	1.71	0.55
1:A:154:PHE:O	1:A:158:GLU:HG3	2.07	0.55
1:A:95:LEU:HD21	2:B:501:ILE:HG12	1.90	0.54
1:C:129:ASN:OD1	1:C:132:THR:OG1	2.26	0.54
1:A:110:ARG:HG3	1:A:223:THR:HG23	1.88	0.54
1:A:41:LEU:HD21	1:C:41:LEU:HD21	1.90	0.54
2:B:480:GLU:HA	2:B:483:ARG:HG2	1.89	0.54
1:A:234:ASP:OD1	1:A:235:PHE:N	2.41	0.54
1:A:222:CYS:O	1:A:226:GLN:HG3	2.07	0.54
1:C:102:ARG:O	1:C:106:ILE:HG13	2.07	0.54
1:C:141:TYR:HB2	1:C:219:TYR:CE1	2.43	0.53
1:A:32:SER:OG	1:A:33:ILE:N	2.38	0.53
1:A:60:PHE:HB2	2:B:494:LEU:HD11	1.90	0.53
1:C:145:LYS:NZ	1:C:177:HIS:ND1	2.57	0.53
1:C:206:LYS:HG3	1:C:207:MET:HG3	1.89	0.53
1:C:148:ILE:HD11	1:C:216:LEU:HD11	1.90	0.53
1:C:185:LEU:HD13	1:C:188:LEU:HD11	1.90	0.53
1:A:198:ILE:O	1:A:202:GLN:HB2	2.08	0.52
1:A:57:ASP:O	1:A:61:ILE:HG12	2.10	0.52
2:D:497:ASP:O	2:D:501:ILE:HG13	2.09	0.52
1:A:102:ARG:O	1:A:106:ILE:HG13	2.10	0.51
1:C:181:GLU:O	1:C:184:ALA:CB	2.57	0.51
1:C:234:ASP:OD1	1:C:235:PHE:N	2.44	0.51
1:C:58:ILE:O	1:C:62:GLU:HG3	2.11	0.51
1:C:188:LEU:HD13	1:C:196:ARG:CZ	2.41	0.51
1:C:222:CYS:SG	1:C:226:GLN:NE2	2.81	0.50
1:C:95:LEU:HD21	2:D:501:ILE:HG12	1.93	0.50
2:B:489:GLY:O	2:B:493:GLU:HG2	2.11	0.50
1:C:216:LEU:O	1:C:220:ILE:HG12	2.11	0.50
1:A:35:ASN:HA	1:A:38:LEU:HD12	1.93	0.50
2:B:480:GLU:H	2:B:480:GLU:CD	2.15	0.50
1:A:178:ASN:ND2	1:A:181:GLU:HG2	2.26	0.50
1:A:202:GLN:O	1:A:206:LYS:HD3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:HG3	1:C:230:PHE:CE1	2.47	0.49
2:D:496:ARG:O	2:D:500:LYS:HG3	2.12	0.49
1:C:164:HIS:O	1:C:168:THR:HG22	2.13	0.49
1:C:193:ILE:O	1:C:197:LEU:HD12	2.13	0.48
1:A:148:ILE:HD11	1:A:216:LEU:HD11	1.94	0.48
1:A:40:TYR:OH	1:C:50:GLU:OE2	2.31	0.48
1:C:157:LEU:CD1	1:C:196:ARG:HH21	2.26	0.48
1:C:211:LYS:O	1:C:215:VAL:HG23	2.14	0.48
1:A:164:HIS:NE2	1:A:168:THR:CG2	2.77	0.48
1:A:191:HIS:CD2	1:A:192:LYS:H	2.31	0.48
1:C:202:GLN:N	1:C:202:GLN:OE1	2.40	0.48
2:B:495:LEU:O	2:B:498:TRP:HB3	2.14	0.48
1:C:186:GLN:O	1:C:189:SER:HB3	2.14	0.48
1:C:236:LYS:HD2	1:C:236:LYS:HA	1.49	0.47
1:A:104:GLU:O	1:A:108:LEU:HG	2.15	0.47
1:C:58:ILE:HD13	1:C:106:ILE:HD13	1.97	0.47
1:A:211:LYS:O	1:A:215:VAL:HG23	2.14	0.47
1:C:131:GLU:O	1:C:135:ASN:OD1	2.33	0.47
1:A:186:GLN:C	1:A:189:SER:H	2.18	0.47
1:C:168:THR:O	1:C:172:GLN:HG3	2.14	0.47
1:A:91:TRP:HB3	1:A:152:MET:SD	2.55	0.46
1:C:193:ILE:HG13	1:C:197:LEU:CD1	2.45	0.46
1:A:140:LEU:HD22	1:A:215:VAL:HG13	1.98	0.46
1:C:104:GLU:O	1:C:108:LEU:HG	2.16	0.46
1:C:224:LYS:O	1:C:228:GLU:HB2	2.16	0.46
1:A:182:MET:HA	1:A:185:LEU:HB2	1.97	0.46
1:C:188:LEU:HD13	1:C:196:ARG:NE	2.30	0.46
2:D:486:LEU:O	2:D:488:HIS:ND1	2.42	0.46
1:A:195:LYS:HD3	1:A:195:LYS:HA	1.76	0.45
1:A:196:ARG:HA	1:A:199:TYR:HB3	1.97	0.45
1:A:58:ILE:O	1:A:62:GLU:HG3	2.16	0.45
1:A:63:TYR:OH	2:B:502:GLU:HB2	2.17	0.45
1:A:177:HIS:ND1	1:A:177:HIS:O	2.50	0.45
1:A:110:ARG:HD3	1:A:226:GLN:OE1	2.16	0.45
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.64	0.44
1:A:170:PHE:O	1:A:170:PHE:CD1	2.70	0.44
1:C:128:LEU:CD1	1:C:230:PHE:HZ	2.30	0.44
2:B:493:GLU:OE1	2:B:496:ARG:NH2	2.49	0.44
1:C:200:VAL:HG12	1:C:204:LYS:NZ	2.32	0.44
1:C:57:ASP:O	1:C:61:ILE:HG12	2.17	0.44
1:A:141:TYR:HB2	1:A:219:TYR:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLU:O	1:C:184:ALA:N	2.51	0.44
1:A:54:ILE:HD12	1:A:109:GLU:HB3	1.99	0.43
1:A:35:ASN:O	1:A:39:ARG:N	2.47	0.43
2:B:494:LEU:HD23	2:B:495:LEU:HD12	2.00	0.43
1:A:227:LEU:O	1:A:233:TYR:HB2	2.19	0.43
1:C:45:LYS:HG3	1:C:46:SER:N	2.33	0.43
1:A:57:ASP:HB3	1:A:102:ARG:HB3	2.01	0.43
1:C:201:SER:HA	1:C:204:LYS:NZ	2.33	0.43
1:C:128:LEU:HG	1:C:128:LEU:H	1.72	0.43
1:A:95:LEU:HD13	2:B:500:LYS:HE2	2.01	0.43
1:A:130:LYS:HG3	1:A:230:PHE:CE1	2.54	0.43
1:A:196:ARG:H	1:A:196:ARG:HG2	1.65	0.43
1:C:183:GLU:O	1:C:186:GLN:HB2	2.18	0.43
1:A:135:ASN:HA	1:A:138:LEU:HG	2.01	0.42
1:A:196:ARG:O	1:A:200:VAL:HG13	2.20	0.42
1:A:205:LYS:HD2	1:A:205:LYS:HA	1.77	0.42
1:C:154:PHE:O	1:C:158:GLU:HG3	2.20	0.42
1:A:193:ILE:O	1:A:197:LEU:HG	2.20	0.42
1:A:63:TYR:CZ	2:B:498:TRP:HD1	2.38	0.42
1:A:190:LYS:CG	1:A:190:LYS:O	2.65	0.42
1:C:157:LEU:HD13	1:C:196:ARG:HH21	1.85	0.42
1:C:180:LYS:O	1:C:183:GLU:HG2	2.20	0.41
2:D:502:GLU:O	2:D:505:ARG:HB3	2.20	0.41
1:A:129:ASN:N	1:A:130:LYS:HZ3	2.18	0.41
1:C:110:ARG:HH21	1:C:134:ASN:HA	1.85	0.41
1:C:183:GLU:O	1:C:184:ALA:C	2.58	0.41
1:C:90:LEU:HD23	1:C:95:LEU:HD22	2.03	0.41
1:C:67:LEU:HA	1:C:67:LEU:HD23	1.90	0.41
1:C:93:TYR:O	1:C:97:SER:OG	2.18	0.41
1:A:171:LEU:HG	1:A:171:LEU:H	1.50	0.41
1:A:90:LEU:HD13	2:B:504:PHE:CD1	2.56	0.41
1:C:130:LYS:HE3	1:C:226:GLN:HA	2.03	0.41
1:A:186:GLN:O	1:A:189:SER:CB	2.68	0.41
2:D:480:GLU:HA	2:D:483:ARG:HB3	2.02	0.41
1:C:35:ASN:O	1:C:39:ARG:HB2	2.21	0.41
1:A:170:PHE:C	1:A:172:GLN:H	2.25	0.40
1:A:216:LEU:O	1:A:220:ILE:HG12	2.21	0.40
1:C:144:ALA:O	1:C:148:ILE:HG13	2.22	0.40
1:A:164:HIS:O	1:A:168:THR:HG23	2.21	0.40
1:A:225:LEU:O	1:A:229:VAL:HG23	2.21	0.40
1:C:196:ARG:NH2	1:C:200:VAL:CG2	2.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:SER:O	1:C:218:ARG:HG3	2.20	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)
1:C:131:GLU:OE1	2:D:496:ARG:NH2[3_674]	2.14	0.06

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	172/214 (80%)	160 (93%)	12 (7%)	0	100	100
1	C	174/214 (81%)	166 (95%)	8 (5%)	0	100	100
2	B	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
2	D	28/33 (85%)	27 (96%)	1 (4%)	0	100	100
All	All	401/494 (81%)	379 (94%)	22 (6%)	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	166/199 (83%)	154 (93%)	12 (7%)	17	53
1	C	168/199 (84%)	159 (95%)	9 (5%)	26	65
2	B	27/30 (90%)	25 (93%)	2 (7%)	16	52
2	D	27/30 (90%)	27 (100%)	0	100	100
All	All	388/458 (85%)	365 (94%)	23 (6%)	23	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	47	MET
1	A	128	LEU
1	A	162	ILE
1	A	169	LYS
1	A	171	LEU
1	A	177	HIS
1	A	178	ASN
1	A	181	GLU
1	A	187	ARG
1	A	194	ARG
1	A	195	LYS
2	B	499	LYS
2	B	503	GLU
1	C	50	GLU
1	C	51	LYS
1	C	110	ARG
1	C	127	LEU
1	C	128	LEU
1	C	130	LYS
1	C	164	HIS
1	C	203	HIS
1	C	224	LYS

Some 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 [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 2 ligands modelled in this entry, 2 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.

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	178/214 (83%)	0.23	4 (2%) 62 48	62, 88, 128, 151	0
1	C	180/214 (84%)	0.17	4 (2%) 62 48	63, 85, 127, 145	0
2	B	29/33 (87%)	-0.15	0 100 100	68, 83, 99, 101	0
2	D	30/33 (90%)	-0.10	0 100 100	68, 82, 102, 107	0
All	All	417/494 (84%)	0.15	8 (1%) 67 52	62, 86, 126, 151	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	GLU	6.1
1	A	205	LYS	3.0
1	A	189	SER	2.8
1	C	128	LEU	2.4
1	A	128	LEU	2.3
1	C	180	LYS	2.2
1	C	182	MET	2.2
1	A	206	LYS	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(\AA^2)	Q<0.9
3	ZN	C	601	1/1	0.91	0.16	-0.70	88,88,88,88	0
3	ZN	A	601	1/1	0.97	0.10	-2.09	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.