WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 08:10 AM GMT

PDB ID : 2A2F
Title : Crystal Structure of Sec15 C-terminal domain
Authors : Wu, S.; Mehta, S.Q.; Pichaud, F.; Bellen, H.J.; Quiocho, F.A.
Deposited on : 2005-06-22
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/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 2.50 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		0.281
Clashscore		25
Ramachandran outliers		2.1%
Sidechain outliers		4.9%
RSRZ outliers		3.4%

Worse *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
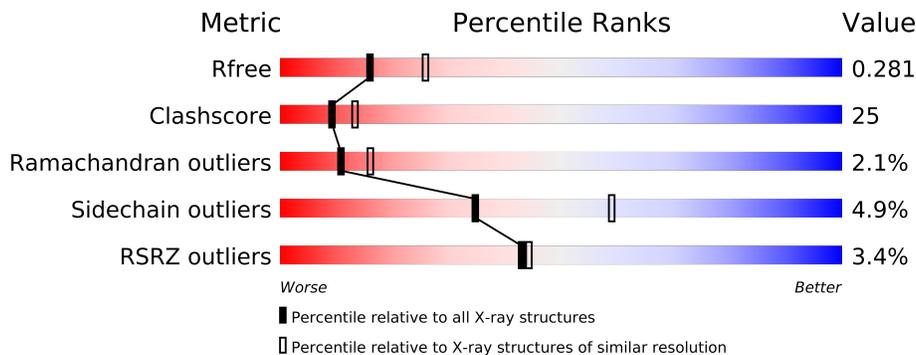
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	X	325	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2511 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 Exocyst complex component Sec15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	296	2424	1569	397	440	18	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	CLONING ARTIFACT	UNP Q9VDE6
X	320	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	321	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	322	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	323	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	324	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	325	HIS	-	EXPRESSION TAG	UNP Q9VDE6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	X	87	87	87	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: Exocyst complex component Sec15

Chain X:
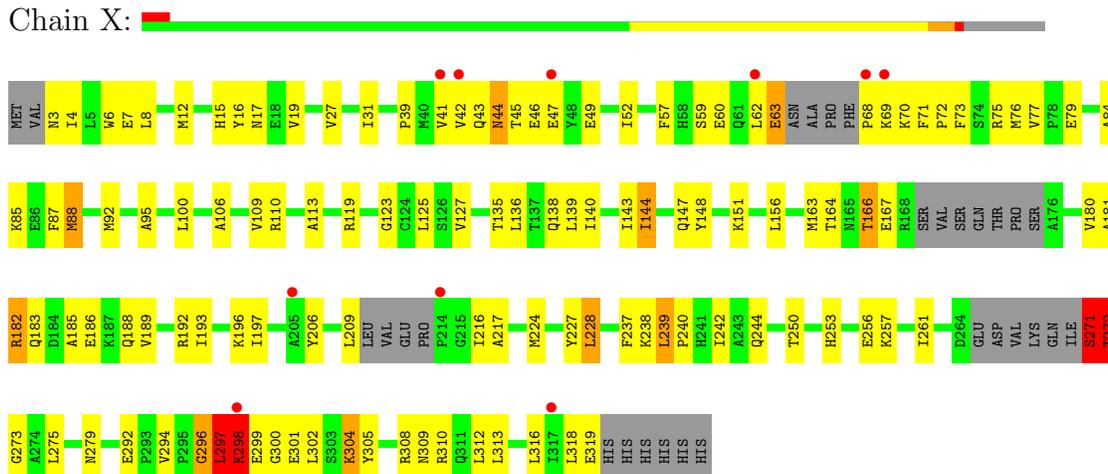
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	80.50Å 93.90Å 123.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.50 43.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.50) 92.6 (43.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.276 0.246 , 0.281	Depositor DCC
R_{free} test set	740 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	1 of 16292 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2511	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	X	0.66	5/2478 (0.2%)	0.89	12/3343 (0.4%)

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	X	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	272	THR	C-N	-15.94	1.04	1.33
1	X	298	LYS	C-N	-13.21	1.03	1.34
1	X	275	LEU	C-N	-8.94	1.13	1.34
1	X	297	LEU	CB-CG	8.34	1.76	1.52
1	X	271	SER	C-N	-7.90	1.15	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	298	LYS	O-C-N	-20.21	90.37	122.70
1	X	298	LYS	CA-C-N	16.42	153.33	117.20
1	X	298	LYS	C-N-CA	14.56	158.11	121.70
1	X	271	SER	O-C-N	-13.29	101.44	122.70
1	X	272	THR	CA-C-N	8.71	133.62	116.20
1	X	297	LEU	O-C-N	-7.74	110.32	122.70
1	X	275	LEU	CA-C-O	-6.43	106.61	120.10
1	X	275	LEU	CA-C-N	6.23	130.91	117.20
1	X	296	GLY	O-C-N	-6.14	112.87	122.70
1	X	272	THR	C-N-CA	5.99	134.88	122.30
1	X	272	THR	CA-C-O	-5.36	108.84	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	297	LEU	CB-CG-CD2	-5.13	102.28	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	271	SER	Mainchain,Peptide
1	X	296	GLY	Mainchain
1	X	297	LEU	Mainchain
1	X	298	LYS	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	X	2424	0	2387	120	0
2	X	87	0	0	2	0
All	All	2511	0	2387	120	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 25.

All (120) close contacts within the same asymmetric unit are listed below:

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:297:LEU:CB	1:X:297:LEU:CG	1.76	1.57
1:X:42:VAL:HG11	1:X:47:GLU:HB2	1.41	1.03
1:X:292:GLU:OE2	1:X:298:LYS:HE2	1.71	0.90
1:X:88:MET:CE	1:X:156:LEU:HG	2.04	0.87
1:X:297:LEU:CB	1:X:297:LEU:CD2	2.55	0.83
1:X:92:MET:HG2	1:X:109:VAL:HG21	1.61	0.83
1:X:279:ASN:ND2	1:X:310:ARG:HH12	1.81	0.78
1:X:297:LEU:HB3	1:X:301:GLU:OE2	1.83	0.78
1:X:297:LEU:CG	1:X:297:LEU:CA	2.62	0.77
1:X:297:LEU:CB	1:X:297:LEU:CD1	2.63	0.77
1:X:292:GLU:OE2	1:X:298:LYS:CE	2.33	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:135:THR:H	1:X:138:GLN:NE2	1.84	0.74
1:X:42:VAL:O	1:X:70:LYS:HE2	1.86	0.74
1:X:88:MET:HE2	1:X:156:LEU:HG	1.68	0.74
1:X:181:ALA:C	1:X:183:GLN:H	1.90	0.74
1:X:41:VAL:HA	1:X:70:LYS:CB	2.18	0.73
1:X:297:LEU:N	1:X:297:LEU:CG	2.51	0.72
1:X:42:VAL:HG11	1:X:47:GLU:CB	2.19	0.72
1:X:123:GLY:O	1:X:127:VAL:HG23	1.88	0.72
1:X:41:VAL:HA	1:X:70:LYS:HB2	1.74	0.69
1:X:41:VAL:HG13	1:X:70:LYS:HB2	1.75	0.69
1:X:292:GLU:OE2	1:X:298:LYS:CD	2.42	0.67
1:X:271:SER:O	1:X:273:GLY:N	2.27	0.67
1:X:139:LEU:O	1:X:143:ILE:HG12	1.94	0.67
1:X:3:ASN:O	1:X:7:GLU:HG2	1.96	0.66
1:X:92:MET:CG	1:X:109:VAL:HG21	2.26	0.65
1:X:41:VAL:HG22	1:X:70:LYS:N	2.12	0.64
1:X:297:LEU:HG	1:X:297:LEU:N	2.13	0.64
1:X:135:THR:HG22	1:X:138:GLN:CD	2.19	0.63
1:X:182:ARG:C	1:X:182:ARG:HD2	2.18	0.63
1:X:299:GLU:O	1:X:301:GLU:N	2.32	0.63
1:X:279:ASN:HD21	1:X:310:ARG:HH12	1.44	0.62
1:X:206:TYR:HE1	1:X:261:ILE:HD13	1.66	0.60
1:X:125:LEU:HD13	1:X:180:VAL:HG22	1.82	0.60
1:X:60:GLU:OE1	1:X:60:GLU:HA	2.01	0.60
1:X:185:ALA:O	1:X:189:VAL:HG23	2.01	0.60
1:X:196:LYS:HG2	1:X:227:TYR:CZ	2.36	0.60
1:X:41:VAL:HG13	1:X:70:LYS:HD3	1.83	0.60
1:X:181:ALA:C	1:X:183:GLN:N	2.56	0.59
1:X:140:ILE:O	1:X:144:ILE:HG23	2.03	0.59
1:X:135:THR:HG23	1:X:138:GLN:H	1.67	0.59
1:X:42:VAL:CG1	1:X:47:GLU:HB2	2.27	0.57
1:X:135:THR:HG22	1:X:138:GLN:CG	2.35	0.56
1:X:181:ALA:O	1:X:183:GLN:N	2.38	0.56
1:X:297:LEU:H	1:X:297:LEU:HG	1.71	0.56
1:X:299:GLU:OE1	1:X:299:GLU:HA	2.05	0.56
1:X:182:ARG:O	1:X:182:ARG:HD2	2.06	0.56
1:X:41:VAL:HA	1:X:70:LYS:HB3	1.88	0.56
1:X:209:LEU:O	1:X:209:LEU:HG	2.06	0.55
1:X:41:VAL:HG21	1:X:69:LYS:N	2.22	0.55
1:X:8:LEU:O	1:X:12:MET:HG3	2.06	0.55
1:X:106:ALA:O	1:X:110:ARG:HB2	2.08	0.54
1:X:73:PHE:HB2	1:X:77:VAL:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:292:GLU:OE2	1:X:298:LYS:HD3	2.09	0.52
1:X:244:GLN:HG2	1:X:297:LEU:HD21	1.90	0.51
1:X:17:ASN:OD1	1:X:119:ARG:HD3	2.10	0.51
1:X:206:TYR:CE1	1:X:261:ILE:HD13	2.44	0.51
1:X:257:LYS:O	1:X:261:ILE:HG13	2.11	0.51
1:X:224:MET:HG2	1:X:228:LEU:HD22	1.93	0.50
1:X:49:GLU:HA	1:X:52:ILE:HB	1.95	0.49
1:X:45:THR:C	1:X:47:GLU:H	2.14	0.49
1:X:164:THR:OG1	1:X:166:THR:HB	2.12	0.49
1:X:43:GLN:HE22	1:X:63:GLU:C	2.15	0.48
1:X:271:SER:O	1:X:272:THR:C	2.48	0.48
1:X:135:THR:HG22	1:X:138:GLN:NE2	2.29	0.48
1:X:41:VAL:O	1:X:42:VAL:HG23	2.14	0.48
1:X:4:ILE:N	1:X:4:ILE:HD12	2.29	0.47
1:X:31:ILE:CD1	1:X:76:MET:HA	2.44	0.47
1:X:318:LEU:O	1:X:319:GLU:HG3	2.15	0.47
1:X:253:HIS:O	1:X:256:GLU:HG2	2.15	0.47
1:X:239:LEU:HB3	1:X:242:ILE:HB	1.95	0.47
1:X:238:LYS:C	1:X:240:PRO:HD3	2.34	0.47
1:X:87:PHE:HE2	1:X:113:ALA:HA	1.78	0.47
1:X:182:ARG:O	1:X:186:GLU:HG3	2.15	0.46
1:X:253:HIS:HA	1:X:256:GLU:HG2	1.96	0.46
1:X:88:MET:HE3	1:X:156:LEU:HG	1.94	0.46
1:X:92:MET:CE	1:X:163:MET:SD	3.04	0.45
1:X:308:ARG:HG3	1:X:309:ASN:N	2.32	0.45
1:X:301:GLU:O	1:X:304:LYS:CD	2.65	0.45
1:X:72:PRO:O	1:X:144:ILE:HD11	2.16	0.45
1:X:239:LEU:HG	1:X:242:ILE:HD12	1.99	0.45
1:X:84:ALA:O	1:X:88:MET:HG2	2.17	0.45
1:X:72:PRO:HB2	1:X:148:TYR:CE2	2.51	0.45
1:X:16:TYR:CE2	1:X:87:PHE:HE1	2.35	0.45
1:X:43:GLN:O	1:X:44:ASN:HB2	2.16	0.44
1:X:31:ILE:HD13	1:X:76:MET:N	2.32	0.44
1:X:62:LEU:HB3	1:X:63:GLU:OE2	2.18	0.44
1:X:3:ASN:HB3	1:X:6:TRP:HB3	1.99	0.44
1:X:147:GLN:O	1:X:151:LYS:HG3	2.17	0.44
1:X:166:THR:HG23	1:X:167:GLU:N	2.32	0.44
1:X:39:PRO:HB3	1:X:71:PHE:O	2.18	0.43
1:X:43:GLN:HA	1:X:43:GLN:OE1	2.19	0.43
1:X:139:LEU:HD12	1:X:192:ARG:CZ	2.49	0.43
1:X:136:LEU:O	1:X:140:ILE:HD13	2.19	0.43
1:X:139:LEU:HD12	1:X:192:ARG:NE	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:192:ARG:HH11	1:X:192:ARG:HG3	1.84	0.42
1:X:302:LEU:O	1:X:305:TYR:HD2	2.01	0.42
1:X:312:LEU:O	1:X:316:LEU:HD23	2.19	0.42
1:X:297:LEU:O	1:X:298:LYS:C	2.57	0.42
1:X:41:VAL:HG22	1:X:70:LYS:HB2	2.02	0.42
1:X:193:ILE:O	1:X:197:ILE:HG13	2.20	0.42
1:X:197:ILE:HD11	1:X:250:THR:HG23	2.01	0.42
1:X:216:ILE:HG23	1:X:217:ALA:N	2.34	0.42
1:X:63:GLU:HB3	2:X:386:HOH:O	2.19	0.42
1:X:294:VAL:O	1:X:294:VAL:HG23	2.18	0.42
1:X:43:GLN:NE2	1:X:63:GLU:O	2.53	0.42
1:X:42:VAL:CG1	1:X:43:GLN:N	2.82	0.42
1:X:301:GLU:O	1:X:304:LYS:HD2	2.20	0.42
1:X:75:ARG:HE	1:X:75:ARG:HB2	1.65	0.41
1:X:156:LEU:HA	1:X:156:LEU:HD12	1.94	0.41
1:X:41:VAL:CA	1:X:70:LYS:HB2	2.48	0.41
1:X:237:PHE:CE1	1:X:238:LYS:HG3	2.56	0.41
1:X:95:ALA:HB1	1:X:100:LEU:HD12	2.03	0.41
1:X:44:ASN:HB3	1:X:47:GLU:HG3	2.02	0.41
1:X:62:LEU:O	1:X:63:GLU:C	2.59	0.41
1:X:151:LYS:NZ	2:X:405:HOH:O	2.53	0.41
1:X:57:PHE:HD2	1:X:71:PHE:HE1	1.69	0.41
1:X:15:HIS:O	1:X:19:VAL:HG23	2.20	0.41
1:X:41:VAL:CG1	1:X:70:LYS:HB2	2.48	0.40
1:X:68:PRO:C	1:X:69:LYS:HG3	2.41	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	X	286/325 (88%)	263 (92%)	17 (6%)	6 (2%)	11 16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	300	GLY
1	X	44	ASN
1	X	182	ARG
1	X	46	GLU
1	X	59	SER
1	X	272	THR

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	X	265/295 (90%)	252 (95%)	13 (5%)	35	59

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	27	VAL
1	X	63	GLU
1	X	79	GLU
1	X	85	LYS
1	X	88	MET
1	X	144	ILE
1	X	166	THR
1	X	188	GLN
1	X	228	LEU
1	X	239	LEU
1	X	297	LEU
1	X	304	LYS
1	X	313	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	11	ASN
1	X	36	GLN
1	X	43	GLN
1	X	114	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	138	GLN
1	X	165	ASN
1	X	183	GLN
1	X	279	ASN
1	X	311	GLN

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.

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(Å^2)	Q<0.9
1	X	296/325 (91%)	0.40	10 (3%)	43	44	53, 77, 117, 142	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	68	PRO	6.2
1	X	42	VAL	5.8
1	X	298	LYS	4.4
1	X	62	LEU	3.3
1	X	47	GLU	2.5
1	X	69	LYS	2.4
1	X	317	ILE	2.2
1	X	41	VAL	2.1
1	X	205	ALA	2.0
1	X	214	PRO	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.