Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:28 AM EDT

PDB ID	:	6GRK
Title	:	Structure of the soluble AhlB of the tripartite alpha-pore forming toxin, AHL, from Aeromonas hydrophila.
Authors	:	Churchill-Angus, A.M.; Wilson, J.S.; Baker, P.J.
Deposited on	:	2018-06-11
Resolution	:	2.33 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 ⓘ 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 ⓘ) were used in the production of this report:

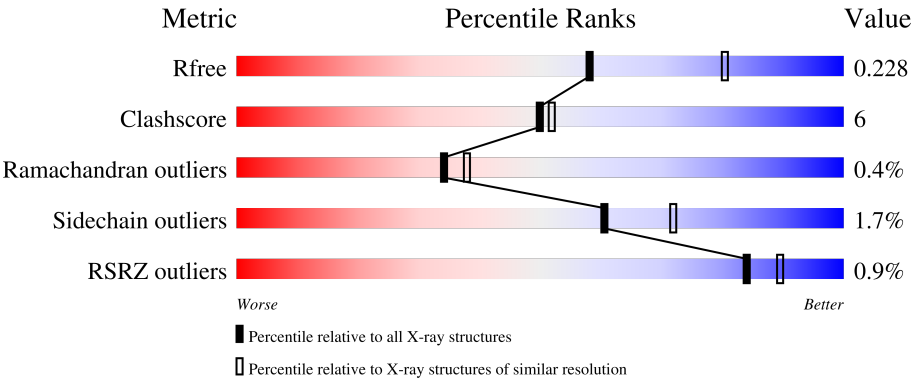
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.33 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	367	% 88% 8%
1	B	367	% 80% 14% 5%
1	I	367	% 83% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7875 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 AhlB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2603	1625	452	518	8			
1	I	354	Total	C	N	O	S	0	0	0
			2607	1627	452	520	8			
1	B	347	Total	C	N	O	S	0	0	0
			2564	1600	445	511	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	LEU	-	expression tag	UNP A0A081US78
A	361	GLU	-	expression tag	UNP A0A081US78
A	362	HIS	-	expression tag	UNP A0A081US78
A	363	HIS	-	expression tag	UNP A0A081US78
A	364	HIS	-	expression tag	UNP A0A081US78
A	365	HIS	-	expression tag	UNP A0A081US78
A	366	HIS	-	expression tag	UNP A0A081US78
A	367	HIS	-	expression tag	UNP A0A081US78
I	360	LEU	-	expression tag	UNP A0A081US78
I	361	GLU	-	expression tag	UNP A0A081US78
I	362	HIS	-	expression tag	UNP A0A081US78
I	363	HIS	-	expression tag	UNP A0A081US78
I	364	HIS	-	expression tag	UNP A0A081US78
I	365	HIS	-	expression tag	UNP A0A081US78
I	366	HIS	-	expression tag	UNP A0A081US78
I	367	HIS	-	expression tag	UNP A0A081US78
B	360	LEU	-	expression tag	UNP A0A081US78
B	361	GLU	-	expression tag	UNP A0A081US78
B	362	HIS	-	expression tag	UNP A0A081US78
B	363	HIS	-	expression tag	UNP A0A081US78
B	364	HIS	-	expression tag	UNP A0A081US78
B	365	HIS	-	expression tag	UNP A0A081US78
B	366	HIS	-	expression tag	UNP A0A081US78

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	367	HIS	-	expression tag	UNP A0A081US78

- Molecule 2 is water.

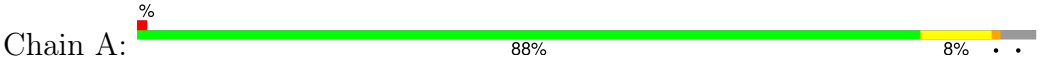
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	49	Total O 49 49	0	0
2	I	39	Total O 39 39	0	0
2	B	13	Total O 13 13	0	0

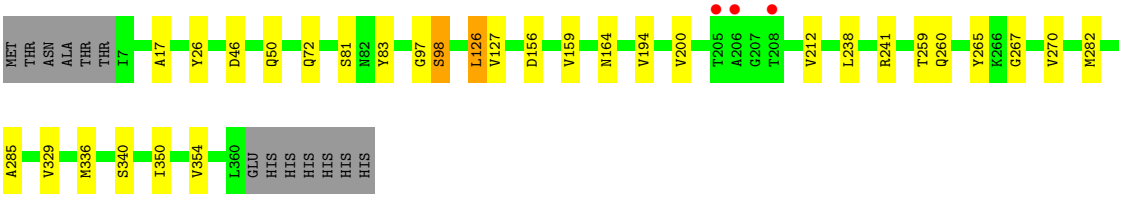
3 Residue-property plots (i)

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: AhlB

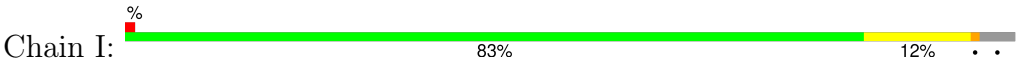
Chain A:

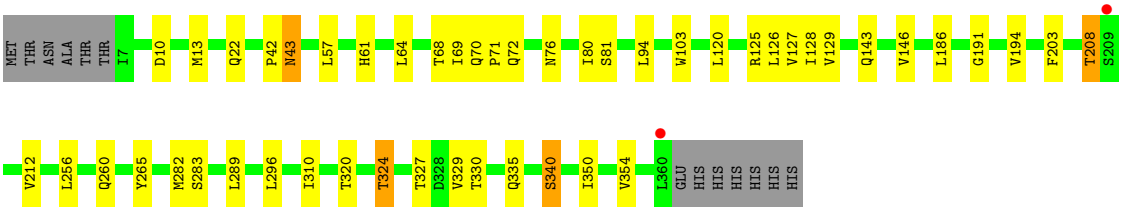




- Molecule 1: AhlB

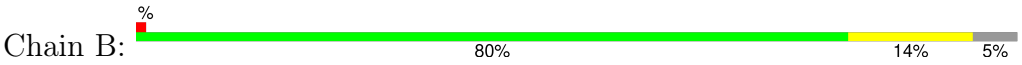
Chain I:

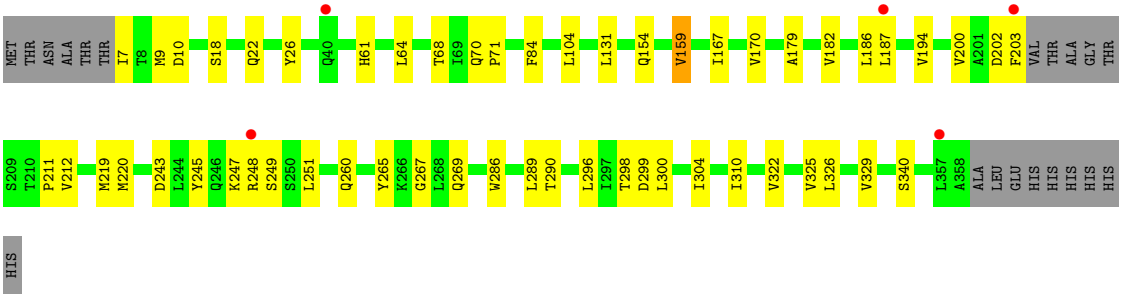




- Molecule 1: AhlB

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.47Å 79.81Å 111.01Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	58.41 – 2.33 58.34 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.41-2.33) 98.0 (58.34-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.222 , 0.254 0.219 , 0.228	Depositor DCC
R_{free} test set	2408 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 13.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.024 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.022 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.059 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.076 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.029 for -h,-k,l	Xtriage
Reported twinning fraction	0.895 for H, K, L 0.105 for -1/2H+3/2K, -1/2H-1/2K, L	Depositor
Outliers	0 of 49042 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7875	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	A	0.54	0/2632	0.72	0/3589
1	B	0.48	0/2592	0.67	0/3531
1	I	0.57	0/2636	0.72	0/3594
All	All	0.53	0/7860	0.71	0/10714

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

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	2603	0	2637	25	0
1	B	2564	0	2593	33	0
1	I	2607	0	2641	33	0
2	A	49	0	0	1	0
2	B	13	0	0	0	0
2	I	39	0	0	1	0
All	All	7875	0	7871	91	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 6.

All (91) 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:I:13:MET:HA	1:I:282:MET:HE1	1.33	1.11
1:B:9:MET:HE1	1:B:286:TRP:HA	1.49	0.93
1:A:81:SER:HB2	1:A:329:VAL:HG11	1.54	0.88
1:I:81:SER:HB3	1:I:329:VAL:HG11	1.62	0.81
1:A:46:ASP:O	1:A:50:GLN:HG2	1.86	0.75
1:A:17:ALA:HA	1:A:336:MET:HE2	1.74	0.69
1:I:42:PRO:O	1:I:43:ASN:CB	2.40	0.68
1:I:13:MET:CA	1:I:282:MET:HE1	2.19	0.67
1:B:202:ASP:O	1:B:203:PHE:CD1	2.51	0.64
1:A:126:LEU:C	1:A:126:LEU:HD23	2.18	0.64
1:A:238:LEU:HD12	1:A:354:VAL:HG21	1.79	0.64
1:I:194:VAL:HA	1:I:340:SER:O	1.97	0.64
1:I:42:PRO:O	1:I:43:ASN:HB3	1.96	0.63
1:I:191:GLY:C	1:I:335:GLN:HE21	2.02	0.63
1:I:327:THR:O	1:I:330:THR:HG22	1.99	0.62
1:I:320:THR:O	1:I:324:THR:HG22	1.99	0.61
1:I:126:LEU:C	1:I:126:LEU:HD23	2.21	0.61
1:B:200:VAL:HG23	1:B:212:VAL:O	2.01	0.60
1:A:17:ALA:HA	1:A:336:MET:CE	2.31	0.59
1:B:18:SER:HB2	1:B:182:VAL:HG23	1.83	0.59
1:I:13:MET:HA	1:I:282:MET:CE	2.22	0.59
1:A:17:ALA:HB1	1:A:336:MET:HE3	1.87	0.57
1:A:17:ALA:HB1	1:A:336:MET:CE	2.35	0.57
1:B:159:VAL:HG13	1:B:251:LEU:HD11	1.87	0.57
1:A:270:VAL:CG2	2:A:434:HOH:O	2.52	0.56
1:B:104:LEU:HD23	1:B:300:LEU:HD23	1.87	0.56
1:A:194:VAL:HA	1:A:340:SER:O	2.06	0.56
1:A:17:ALA:CB	1:A:336:MET:CE	2.83	0.55
1:B:296:LEU:HD11	1:B:310:ILE:HG12	1.89	0.54
1:I:13:MET:SD	1:I:329:VAL:HG22	2.47	0.54
1:I:212:VAL:HG11	1:I:260:GLN:HB3	1.90	0.53
1:I:22:GLN:NE2	2:I:403:HOH:O	2.41	0.53
1:I:203:PHE:O	1:I:208:THR:O	2.27	0.52
1:B:219:MET:O	1:B:220:MET:HG3	2.10	0.51
1:I:289:LEU:C	1:I:289:LEU:HD23	2.31	0.51
1:B:212:VAL:HG11	1:B:260:GLN:HB3	1.93	0.50
1:B:64:LEU:HD23	1:B:131:LEU:HD13	1.92	0.49
1:A:350:ILE:O	1:A:354:VAL:HG13	2.13	0.49
1:I:186:LEU:HA	1:I:335:GLN:OE1	2.12	0.49
1:B:325:VAL:O	1:B:329:VAL:HG12	2.13	0.48
1:B:299:ASP:OD1	1:B:304:ILE:HD12	2.13	0.48
1:A:17:ALA:CA	1:A:336:MET:HE2	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:GLN:HB3	1:I:71:PRO:HD3	1.95	0.47
1:B:167:ILE:O	1:B:170:VAL:N	2.47	0.47
1:B:22:GLN:OE1	1:B:179:ALA:HA	2.15	0.47
1:I:72:GLN:OE1	1:I:120:LEU:HD11	2.14	0.47
1:B:194:VAL:HA	1:B:340:SER:O	2.15	0.47
1:I:296:LEU:HD11	1:I:310:ILE:HG12	1.98	0.46
1:I:350:ILE:O	1:I:354:VAL:HG23	2.14	0.46
1:B:64:LEU:HD12	1:B:68:THR:HB	1.97	0.46
1:A:282:MET:HE3	1:A:285:ALA:HB3	1.97	0.46
1:I:76:ASN:HD21	1:I:282:MET:HG2	1.81	0.46
1:B:248:ARG:NH2	1:B:249:SER:O	2.49	0.45
1:A:238:LEU:CD1	1:A:354:VAL:HG21	2.44	0.45
1:B:9:MET:HE3	1:B:289:LEU:CD2	2.47	0.45
1:B:203:PHE:CE1	1:B:211:PRO:HB3	2.52	0.45
1:B:212:VAL:HG21	1:B:260:GLN:HB2	1.99	0.45
1:I:94:LEU:HD23	1:I:103:TRP:CE2	2.52	0.45
1:I:64:LEU:O	1:I:68:THR:HB	2.17	0.45
1:A:26:TYR:OH	1:A:267:GLY:HA3	2.16	0.45
1:B:186:LEU:O	1:B:187:LEU:HB2	2.15	0.45
1:I:94:LEU:HD23	1:I:103:TRP:CD2	2.52	0.44
1:B:26:TYR:OH	1:B:267:GLY:HA3	2.17	0.44
1:I:126:LEU:HD23	1:I:127:VAL:N	2.32	0.44
1:A:17:ALA:CA	1:A:336:MET:CE	2.94	0.44
1:B:7:ILE:HG23	1:B:7:ILE:O	2.18	0.44
1:B:243:ASP:O	1:B:247:LYS:HG2	2.17	0.44
1:B:9:MET:HE1	1:B:286:TRP:CA	2.34	0.44
1:A:156:ASP:HB3	1:A:159:VAL:HG12	1.99	0.44
1:B:219:MET:C	1:B:220:MET:HG3	2.38	0.43
1:I:57:LEU:O	1:I:61:HIS:CD2	2.71	0.43
1:A:97:GLY:O	1:A:98:SER:O	2.36	0.43
1:I:68:THR:O	1:I:72:GLN:HG2	2.18	0.43
1:B:84:PHE:HB3	1:B:322:VAL:HG13	2.01	0.43
1:A:212:VAL:HG11	1:A:260:GLN:HB3	2.00	0.43
1:B:61:HIS:HB3	1:B:131:LEU:HD11	2.00	0.43
1:B:326:LEU:HA	1:B:329:VAL:HG12	2.01	0.42
1:B:70:GLN:HB3	1:B:71:PRO:HD3	2.00	0.42
1:A:164:ASN:OD1	1:A:259:THR:CG2	2.68	0.42
1:I:125:ARG:NH1	1:I:129:VAL:HG21	2.35	0.42
1:I:143:GLN:O	1:I:146:VAL:HG12	2.20	0.42
1:B:245:TYR:CE1	1:B:260:GLN:HG2	2.55	0.42
1:A:126:LEU:HD23	1:A:127:VAL:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:ILE:HG22	1:I:329:VAL:HG21	2.02	0.41
1:I:13:MET:SD	1:I:329:VAL:CG2	3.08	0.41
1:A:72:GLN:OE1	1:A:72:GLN:HA	2.20	0.41
1:I:69:ILE:HD13	1:I:128:ILE:HG12	2.01	0.41
1:B:9:MET:HE2	1:B:289:LEU:HB2	2.02	0.41
1:B:64:LEU:O	1:B:68:THR:HB	2.21	0.41
1:A:83:TYR:CD2	1:A:83:TYR:C	2.93	0.40
1:A:200:VAL:HG13	1:A:241:ARG:CD	2.51	0.40

There are no symmetry-related clashes.

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	352/367 (96%)	336 (96%)	15 (4%)	1 (0%)	41	47
1	B	343/367 (94%)	329 (96%)	13 (4%)	1 (0%)	41	47
1	I	352/367 (96%)	338 (96%)	12 (3%)	2 (1%)	25	26
All	All	1047/1101 (95%)	1003 (96%)	40 (4%)	4 (0%)	34	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	I	43	ASN
1	B	154	GLN
1	I	208	THR

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	282/295 (96%)	280 (99%)	2 (1%)	84	90
1	B	279/295 (95%)	273 (98%)	6 (2%)	52	63
1	I	283/295 (96%)	277 (98%)	6 (2%)	53	65
All	All	844/885 (95%)	830 (98%)	14 (2%)	60	72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	265	TYR
1	I	10	ASP
1	I	256	LEU
1	I	265	TYR
1	I	283	SER
1	I	324	THR
1	I	340	SER
1	B	10	ASP
1	B	159	VAL
1	B	265	TYR
1	B	269	GLN
1	B	290	THR
1	B	298	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	I	22	GLN
1	I	76	ASN
1	B	40	GLN
1	B	53	GLN
1	B	236	ASN
1	B	271	GLN

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, 95^{th} 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	354/367 (96%)	-0.40	3 (0%)	86	90	29, 45, 69, 109	0
1	B	347/367 (94%)	-0.17	5 (1%)	75	82	29, 55, 81, 104	0
1	I	354/367 (96%)	-0.39	2 (0%)	89	93	26, 43, 73, 107	0
All	All	1055/1101 (95%)	-0.32	10 (0%)	84	89	26, 47, 79, 109	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	ARG	3.7
1	A	206	ALA	3.5
1	A	205	THR	3.1
1	B	357	LEU	3.0
1	I	209	SER	2.9
1	A	208	THR	2.8
1	I	360	LEU	2.7
1	B	40	GLN	2.5
1	B	187	LEU	2.2
1	B	203	PHE	2.1

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.