



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:28 PM UTC

PDB ID : 3AKJ / pdb_00003akj
Title : Crystal structure of A Helicobacter pylori proinflammatory kinase CtkA
Authors : Kim, D.J.; Suh, S.W.
Deposited on : 2010-07-14
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

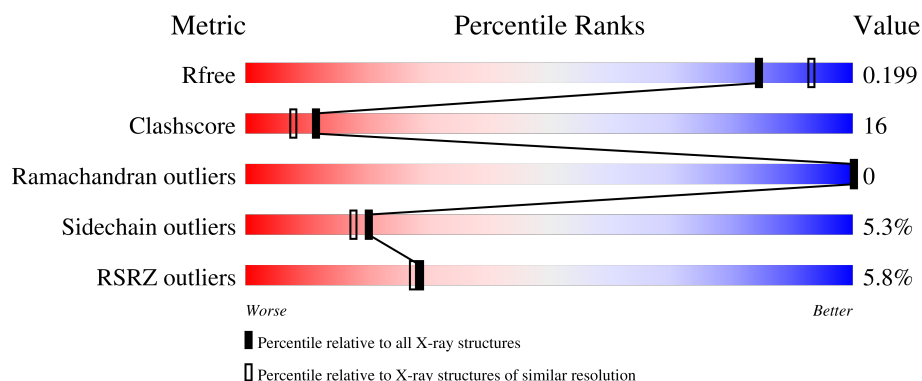
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	325	4% 62% 20% • 15%
1	B	325	6% 61% 21% • • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4814 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 CtkA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2244	1440	367	422	15			
1	B	275	Total	C	N	O	S	0	0	0
			2244	1440	367	422	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	196	Total	O	0	0
			196	196		
2	B	130	Total	O	0	0
			130	130		

- Molecule 1: CtkA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	255.19Å 56.98Å 48.64Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.01Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.5_2	Depositor
R, R_{free}	0.194 , 0.230 0.198 , 0.199	Depositor DCC
R_{free} test set	4750 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4814	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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](#)

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	0.59	0/2293	0.79	3/3102 (0.1%)
1	B	0.58	0/2293	0.78	3/3102 (0.1%)
All	All	0.58	0/4586	0.79	6/6204 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLN	N-CA-C	-8.69	97.23	110.70
1	A	92	THR	N-CA-C	-7.33	99.61	110.23
1	A	93	HIS	N-CA-C	-6.60	101.37	110.35
1	A	282	ILE	CB-CA-C	-6.29	106.36	111.71
1	B	95	TYR	N-CA-C	5.06	117.31	108.76
1	B	91	THR	N-CA-C	-5.05	107.14	113.15

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	2244	0	2202	64	1
1	B	2244	0	2202	86	1
2	A	196	0	0	4	0
2	B	130	0	0	3	0
All	All	4814	0	4404	142	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 16.

All (142) 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:93:HIS:O	1:A:94:GLN:HG2	1.34	1.23
1:B:83:ILE:H	1:B:83:ILE:HD12	1.09	1.10
1:B:83:ILE:HD12	1:B:83:ILE:N	1.71	1.00
1:B:83:ILE:H	1:B:83:ILE:CD1	1.71	1.00
1:B:254:HIS:HD2	1:B:272:HIS:HD2	1.08	0.97
1:B:170:LYS:HD3	1:B:170:LYS:H	1.29	0.97
1:A:157:HIS:HD2	1:A:159:GLY:H	1.13	0.95
1:B:24:LYS:HB2	1:B:35:MET:HE2	1.47	0.93
1:A:254:HIS:HD2	1:A:272:HIS:HD2	1.16	0.92
1:B:157:HIS:HD2	1:B:159:GLY:H	1.19	0.91
1:B:254:HIS:CD2	1:B:272:HIS:HD2	1.91	0.89
1:B:93:HIS:HB3	1:B:95:TYR:CD1	2.08	0.88
1:A:93:HIS:C	1:A:94:GLN:HG2	1.97	0.87
1:B:254:HIS:HD2	1:B:272:HIS:CD2	1.92	0.86
1:B:94:GLN:O	1:B:94:GLN:HG2	1.76	0.84
1:A:254:HIS:CD2	1:A:272:HIS:HD2	1.96	0.84
1:B:93:HIS:CB	1:B:95:TYR:HD1	1.92	0.81
1:B:103:LEU:HD21	1:B:129:GLN:HB3	1.66	0.78
1:B:170:LYS:HD3	1:B:170:LYS:N	1.98	0.77
1:A:254:HIS:HD2	1:A:272:HIS:CD2	2.02	0.75
1:B:94:GLN:O	1:B:94:GLN:CG	2.33	0.75
1:B:143:ASP:OD2	2:B:420:HOH:O	2.05	0.74
1:A:191:VAL:HG12	1:A:195:LYS:HE2	1.72	0.72
1:A:207:ILE:HD13	1:A:281:LYS:HD2	1.69	0.72
1:A:105:ASN:ND2	1:A:114:GLY:H	1.87	0.72
1:B:93:HIS:CB	1:B:95:TYR:CD1	2.70	0.71
1:B:25:ILE:HD11	1:B:79:TYR:CE1	2.26	0.70
1:B:257:ILE:HD11	1:B:275:LEU:HD12	1.74	0.70
1:B:105:ASN:HD21	1:B:114:GLY:H	1.37	0.70
2:A:485:HOH:O	1:B:252:LYS:HD2	1.91	0.70
1:B:24:LYS:O	1:B:24:LYS:HD2	1.90	0.69
1:B:204:ASN:HD21	1:B:281:LYS:NZ	1.92	0.68
1:A:204:ASN:HD21	1:A:281:LYS:HE2	1.58	0.68
1:A:170:LYS:HG2	1:A:170:LYS:O	1.94	0.67
1:A:204:ASN:ND2	1:A:281:LYS:HE2	2.10	0.67
1:B:93:HIS:C	1:B:95:TYR:H	2.03	0.66
1:B:59:VAL:O	1:B:63:ILE:HD13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:HIS:HD1	1:B:95:TYR:HE1	1.40	0.66
1:B:165:ARG:HG3	1:B:172:TYR:CZ	2.31	0.66
1:B:9:CYS:HB2	1:B:27:LEU:HD22	1.77	0.65
1:A:212:GLN:HE21	1:A:224:ASN:HD22	1.44	0.65
1:B:105:ASN:ND2	1:B:114:GLY:H	1.94	0.65
1:A:143:ASP:OD2	2:A:332:HOH:O	2.15	0.64
1:B:109:GLU:H	1:B:109:GLU:CD	2.06	0.64
1:A:93:HIS:O	1:A:94:GLN:CG	2.28	0.64
1:B:157:HIS:CD2	1:B:159:GLY:H	2.10	0.63
1:A:157:HIS:CD2	1:A:159:GLY:H	2.05	0.63
1:A:9:CYS:SG	1:B:2:PRO:HG3	2.39	0.62
1:B:204:ASN:HD21	1:B:281:LYS:HZ3	1.46	0.62
1:A:63:ILE:HD12	1:A:253:ILE:HG12	1.82	0.61
1:A:5:ASP:OD1	1:A:78:THR:HG23	2.00	0.61
1:B:170:LYS:H	1:B:170:LYS:CD	2.03	0.61
1:B:254:HIS:CD2	1:B:272:HIS:CD2	2.77	0.60
1:A:157:HIS:HD2	1:A:159:GLY:N	1.92	0.60
1:B:93:HIS:C	1:B:95:TYR:N	2.58	0.60
1:B:103:LEU:HD11	1:B:129:GLN:HB2	1.85	0.59
1:A:254:HIS:CD2	1:A:272:HIS:CD2	2.82	0.59
1:B:25:ILE:CD1	1:B:79:TYR:CE1	2.86	0.58
1:A:81:ASN:ND2	1:A:81:ASN:H	2.01	0.58
1:B:212:GLN:HE21	1:B:224:ASN:HD22	1.51	0.58
1:B:89:ASP:OD1	1:B:91:THR:HG23	2.04	0.57
1:B:4:ILE:HD12	1:B:4:ILE:N	2.19	0.57
1:B:245:TYR:HB3	1:B:246:PRO:HD3	1.88	0.56
1:A:4:ILE:CD1	1:B:4:ILE:HG13	2.36	0.56
1:A:143:ASP:HA	1:A:244:ILE:HD11	1.88	0.55
1:B:93:HIS:HB2	1:B:95:TYR:HD1	1.67	0.55
1:A:108:ILE:HD12	1:A:109:GLU:N	2.21	0.55
1:A:291:ILE:O	1:A:295:LEU:HG	2.05	0.55
1:A:165:ARG:HB2	1:A:172:TYR:CE1	2.42	0.55
1:B:212:GLN:NE2	1:B:224:ASN:HD22	2.05	0.55
1:A:2:PRO:HG3	1:B:8:PHE:HD2	1.72	0.54
1:B:165:ARG:HG3	1:B:172:TYR:CE1	2.42	0.54
1:B:166:ALA:HB3	1:B:169:SER:O	2.08	0.54
1:B:25:ILE:C	1:B:35:MET:HE3	2.33	0.53
1:A:29:TYR:HE1	1:B:2:PRO:HB2	1.73	0.53
1:B:12:ASN:HB2	1:B:33:LEU:HD11	1.90	0.52
1:B:287:HIS:HE1	2:B:447:HOH:O	1.92	0.52
1:B:288:THR:O	1:B:291:ILE:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:C	1:A:94:GLN:CG	2.75	0.51
1:A:143:ASP:HA	1:A:244:ILE:CD1	2.41	0.51
1:A:245:TYR:HB3	1:A:246:PRO:HD3	1.94	0.50
1:B:257:ILE:HD11	1:B:275:LEU:CD1	2.41	0.50
1:A:108:ILE:HD12	1:A:109:GLU:H	1.77	0.50
1:B:51:THR:N	2:B:440:HOH:O	2.45	0.50
1:A:63:ILE:CD1	1:A:253:ILE:HG23	2.43	0.49
1:B:30:ASN:O	1:B:31:ASN:HB2	2.12	0.49
1:B:103:LEU:HD23	1:B:103:LEU:O	2.13	0.49
1:A:89:ASP:OD1	1:A:91:THR:OG1	2.26	0.48
1:A:192:VAL:HA	1:A:195:LYS:HE3	1.95	0.48
1:A:108:ILE:HD12	1:A:109:GLU:OE2	2.12	0.48
1:A:3:THR:HA	2:A:506:HOH:O	2.14	0.48
1:B:103:LEU:HD21	1:B:129:GLN:CB	2.39	0.47
1:B:203:LEU:HD11	1:B:277:GLU:HG3	1.95	0.47
1:B:92:THR:O	1:B:92:THR:OG1	2.30	0.47
1:A:29:TYR:CE1	1:B:2:PRO:HB2	2.50	0.47
1:B:28:PHE:CE1	1:B:33:LEU:HD13	2.49	0.47
1:B:24:LYS:HD2	1:B:24:LYS:C	2.40	0.46
1:B:200:ILE:HD12	1:B:203:LEU:HD23	1.97	0.46
1:A:109:GLU:H	1:A:109:GLU:CD	2.20	0.46
1:B:103:LEU:HD12	1:B:163:PHE:CE2	2.51	0.46
1:B:216:LYS:NZ	1:B:220:ASP:OD1	2.42	0.46
1:A:103:LEU:HD11	1:A:129:GLN:HB3	1.97	0.45
1:A:126:ILE:HG12	1:A:137:LEU:HD13	1.98	0.45
1:A:212:GLN:NE2	1:A:224:ASN:HD22	2.12	0.45
1:A:270:PHE:O	1:A:274:MET:HG2	2.15	0.45
1:A:29:TYR:OH	1:B:4:ILE:HD11	2.17	0.45
1:B:101:LEU:C	1:B:101:LEU:HD23	2.41	0.45
1:B:103:LEU:HD11	1:B:129:GLN:CB	2.47	0.45
1:A:4:ILE:HD12	1:B:4:ILE:HG13	1.97	0.45
1:B:11:ILE:N	1:B:11:ILE:HD12	2.32	0.45
1:A:263:MET:HE2	1:A:267:HIS:CE1	2.51	0.45
1:A:207:ILE:HD13	1:A:281:LYS:CD	2.44	0.44
1:B:24:LYS:HA	1:B:36:VAL:O	2.16	0.44
1:A:26:SER:HB2	1:A:35:MET:HE1	1.98	0.44
1:A:63:ILE:HD12	1:A:253:ILE:HG23	1.98	0.44
1:A:5:ASP:OD2	1:A:7:THR:HB	2.18	0.44
1:A:4:ILE:HD11	1:B:4:ILE:HG13	1.98	0.44
1:B:93:HIS:ND1	1:B:95:TYR:CE1	2.73	0.44
1:B:203:LEU:HD13	1:B:274:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:O	1:A:244:ILE:HD12	2.18	0.44
1:A:287:HIS:HE1	2:A:434:HOH:O	2.02	0.43
1:B:149:THR:HG21	1:B:229:LEU:CD2	2.49	0.43
1:B:101:LEU:HD23	1:B:101:LEU:O	2.19	0.43
1:B:107:MET:HA	1:B:107:MET:HE2	2.01	0.43
1:B:108:ILE:C	1:B:108:ILE:HD13	2.44	0.43
1:A:92:THR:O	1:A:93:HIS:O	2.37	0.42
1:A:252:LYS:O	1:A:256:ILE:HG12	2.19	0.42
1:B:192:VAL:O	1:B:196:VAL:HG23	2.19	0.42
1:A:206:ARG:HA	1:A:210:PHE:O	2.19	0.42
1:B:260:THR:HG21	1:B:263:MET:HE3	2.01	0.42
1:A:199:ASN:OD1	1:A:201:ASP:HB2	2.19	0.42
1:B:25:ILE:O	1:B:35:MET:HE3	2.20	0.42
1:A:217:ASP:HB3	1:A:223:ILE:HD11	2.02	0.41
1:A:39:PRO:HA	1:A:40:PRO:HD3	1.91	0.41
1:A:83:ILE:HD12	1:A:83:ILE:N	2.35	0.41
1:A:101:LEU:HD13	1:A:115:LYS:HA	2.03	0.41
1:A:94:GLN:HA	1:A:167:SER:HB3	2.03	0.41
1:B:83:ILE:HG23	1:B:262:PHE:CD2	2.56	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.97	0.40
1:B:103:LEU:CD2	1:B:129:GLN:HB3	2.43	0.40
1:B:24:LYS:CB	1:B:35:MET:HE2	2.34	0.40
1:B:9:CYS:O	1:B:11:ILE:HD12	2.21	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:A:113:SER:OG	1:B:96:GLU:OE1[1_554]	2.05	0.15

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	269/325 (83%)	263 (98%)	6 (2%)	0	100	100
1	B	269/325 (83%)	262 (97%)	7 (3%)	0	100	100
All	All	538/650 (83%)	525 (98%)	13 (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	256/299 (86%)	246 (96%)	10 (4%)	28	28
1	B	256/299 (86%)	239 (93%)	17 (7%)	15	12
All	All	512/598 (86%)	485 (95%)	27 (5%)	20	18

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	81	ASN
1	A	94	GLN
1	A	105	ASN
1	A	109	GLU
1	A	137	LEU
1	A	187	GLN
1	A	203	LEU
1	A	241	LEU
1	A	282	ILE
1	B	24	LYS
1	B	67	LEU
1	B	83	ILE
1	B	91	THR
1	B	92	THR
1	B	93	HIS
1	B	94	GLN
1	B	106	THR

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Mol	Chain	Res	Type
1	B	107	MET
1	B	108	ILE
1	B	137	LEU
1	B	170	LYS
1	B	171	GLU
1	B	214	ILE
1	B	221	LYS
1	B	229	LEU
1	B	292	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	31	ASN
1	A	81	ASN
1	A	105	ASN
1	A	120	ASN
1	A	128	ASN
1	A	157	HIS
1	A	168	ASN
1	A	194	GLN
1	A	204	ASN
1	A	212	GLN
1	A	254	HIS
1	A	272	HIS
1	A	287	HIS
1	B	94	GLN
1	B	105	ASN
1	B	120	ASN
1	B	128	ASN
1	B	157	HIS
1	B	168	ASN
1	B	173	GLN
1	B	204	ASN
1	B	212	GLN
1	B	254	HIS
1	B	272	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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	275/325 (84%)	0.01	14 (5%) 33 32	22, 35, 61, 78	0
1	B	275/325 (84%)	0.39	18 (6%) 25 23	29, 43, 72, 85	0
All	All	550/650 (84%)	0.20	32 (5%) 29 27	22, 40, 67, 85	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	THR	4.8
1	B	108	ILE	3.6
1	B	168	ASN	3.5
1	A	51	THR	3.5
1	A	93	HIS	3.2
1	B	11	ILE	3.1
1	B	166	ALA	3.1
1	B	169	SER	3.1
1	A	168	ASN	3.0
1	A	92	THR	3.0
1	B	40	PRO	3.0
1	B	295	LEU	2.9
1	A	2	PRO	2.8
1	A	170	LYS	2.7
1	A	108	ILE	2.7
1	B	79	TYR	2.6
1	A	23	ASN	2.5
1	B	13	PRO	2.5
1	B	171	GLU	2.3
1	B	27	LEU	2.3
1	B	8	PHE	2.3
1	B	191	VAL	2.3
1	B	93	HIS	2.2
1	A	4	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3	THR	2.2
1	A	166	ALA	2.1
1	A	295	LEU	2.0
1	A	81	ASN	2.0
1	B	95	TYR	2.0
1	B	172	TYR	2.0
1	A	169	SER	2.0
1	A	172	TYR	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.