



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:20 AM GMT

PDB ID : 2VRX
Title : STRUCTURE OF AURORA B KINASE IN COMPLEX WITH ZM447439
Authors : Girdler, F.; Sessa, F.; Patercoli, S.; Villa, F.; Ridgway, E.; Musacchio, A.;
Taylor, S.S.
Deposited on : 2008-04-16
Resolution : 1.86 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>

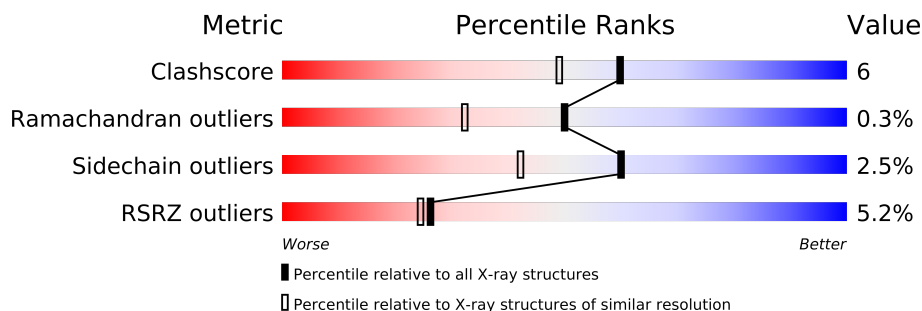
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.86 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))
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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	A	285	
1	B	285	
2	C	43	
2	D	43	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	447	B	1356	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5911 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.

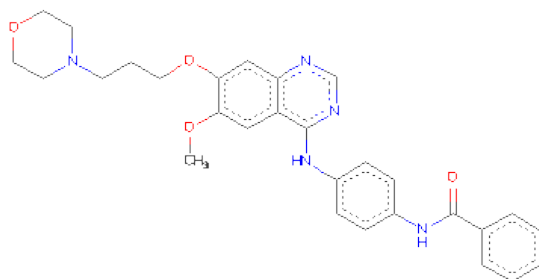
- Molecule 1 is a protein called SERINE/THREONINE-PROTEINKINASE 12-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	P	S	0	4	0
			2272	1454	409	395	1	13			
1	B	275	Total	C	N	O	P	S	0	1	0
			2291	1465	412	399	1	14			

- Molecule 2 is a protein called INNER CENTROMERE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	41	Total	C	N	O	S	0	0	1
			328	212	54	61	1			
2	D	43	Total	C	N	O	S	0	0	0
			350	225	58	66	1			

- Molecule 3 is N-(4-{[6-METHOXY-7-(3-MORPHOLIN-4-YLPROPOXY)QUINAZOLIN-4-YL]AMINO}PHENYL)BENZAMIDE (three-letter code: 447) (formula: C₂₉H₃₁N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			38	29	5	4		
3	B	1	Total	C	N	O	0	0
			38	29	5	4		

- Molecule 4 is water.

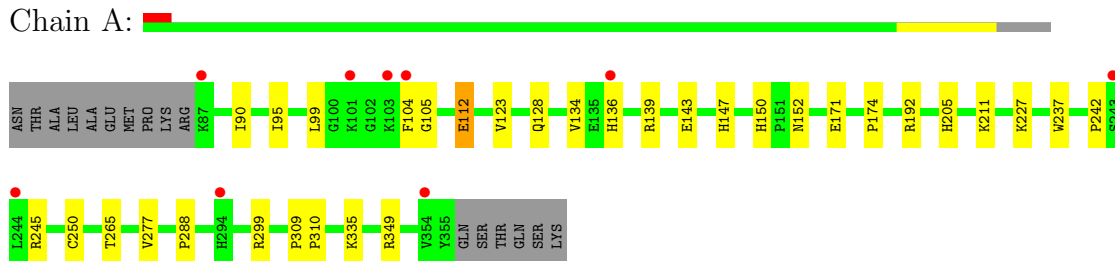
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	261	Total	O	0	0
			261	261		
4	C	30	Total	O	0	0
			30	30		
4	D	36	Total	O	0	0
			36	36		

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.

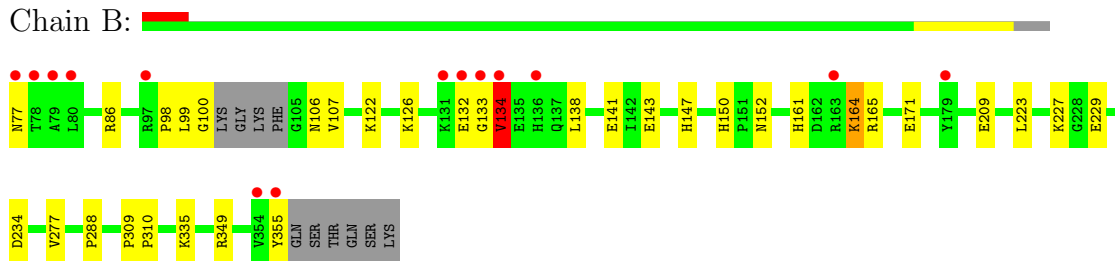
• Molecule 1: SERINE/THREONINE-PROTEINKINASE 12-A

Chain A:



• Molecule 1: SERINE/THREONINE-PROTEINKINASE 12-A

Chain B:



• Molecule 2: INNER CENTROMERE PROTEIN A

Chain C:



• Molecule 2: INNER CENTROMERE PROTEIN A

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.73Å 67.00Å 116.58Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	115.47 – 1.86 28.99 – 1.86	Depositor EDS
% Data completeness (in resolution range)	92.3 (115.47-1.86) 87.9 (28.99-1.86)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.243 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 54800 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5911	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 447

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	0.41	0/2322	0.56	0/3125
1	B	0.42	0/2340	0.57	0/3150
2	C	0.40	0/336	0.55	0/457
2	D	0.35	0/358	0.45	0/485
All	All	0.41	0/5356	0.56	0/7217

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2272	0	2270	25	0
1	B	2291	0	2293	34	0
2	C	328	0	323	3	0
2	D	350	0	347	3	0
3	A	38	0	31	7	0
3	B	38	0	31	8	0
4	A	267	0	0	2	0
4	B	261	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	0	0	0
4	D	36	0	0	1	0
All	All	5911	0	5295	64	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 6.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:GLY:HA2	1:B:134:VAL:HB	1.07	1.05
1:B:133:GLY:CA	1:B:134:VAL:HB	1.94	0.97
1:B:133:GLY:HA2	1:B:134:VAL:CB	2.00	0.91
1:B:107:VAL:HG21	3:B:1356:447:HAK	1.50	0.91
1:A:211:LYS:HD3	1:A:242:PRO:HA	1.52	0.89
1:B:164:LYS:H	1:B:164:LYS:HD2	1.40	0.86
1:B:141:GLU:HB3	3:B:1356:447:HAC	1.62	0.81
1:B:223:LEU:HD11	3:B:1356:447:HAJ	1.70	0.73
1:A:150:HIS:HD2	1:A:152:ASN:H	1.37	0.72
1:B:150:HIS:HD2	1:B:152:ASN:H	1.38	0.70
1:B:229:GLU:HB3	4:B:2256:HOH:O	1.94	0.68
1:A:104:PHE:HA	1:A:128:GLN:OE1	1.94	0.67
1:B:164:LYS:HD3	1:B:165:ARG:NH2	2.11	0.65
1:B:164:LYS:HD2	1:B:164:LYS:N	2.11	0.65
1:B:98:PRO:HB3	1:B:106:ASN:HD21	1.61	0.65
1:A:152:ASN:HD21	1:A:349:ARG:HH21	1.45	0.64
1:A:150:HIS:CD2	1:A:152:ASN:H	2.16	0.63
1:B:227:LYS:NZ	2:C:816:TYR:OH	2.31	0.63
1:A:112:GLU:OE2	4:A:2024:HOH:O	2.16	0.62
1:B:126:LYS:NZ	1:B:161:HIS:HD2	1.97	0.62
1:B:150:HIS:CD2	1:B:152:ASN:H	2.18	0.61
1:B:141:GLU:HB3	3:B:1356:447:CAC	2.30	0.61
1:A:112:GLU:HG2	2:D:825:TYR:OH	2.01	0.60
1:B:234:ASP:HA	3:B:1356:447:HAF	1.85	0.59
1:B:355:TYR:HB2	2:C:818:PRO:O	2.01	0.59
1:B:152:ASN:HD21	1:B:349:ARG:HH21	1.50	0.59
1:B:143:GLU:O	1:B:147:HIS:HD2	1.86	0.59
1:A:237:TRP:CD2	1:A:250:CYS:HB2	2.39	0.57
1:A:174:PRO:O	3:A:1356:447:HAS1	2.04	0.57
1:B:132:GLU:HB2	1:B:133:GLY:HA2	1.86	0.57
1:A:136:HIS:HA	1:A:139:ARG:HG2	1.87	0.56
1:A:245:ARG:NH1	1:A:265:THR:OG1	2.39	0.55
1:B:126:LYS:HZ3	1:B:161:HIS:HD2	1.53	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:GLU:O	3:B:1356:447:H2	2.06	0.55
2:D:832:LYS:O	2:D:835:GLU:HG2	2.07	0.54
1:B:122:LYS:HD3	3:B:1356:447:HAI	1.88	0.54
1:A:105:GLY:HA3	1:A:123:VAL:O	2.09	0.53
1:A:205:HIS:NE2	1:A:335:LYS:HE2	2.25	0.52
1:B:143:GLU:O	1:B:147:HIS:CD2	2.62	0.52
1:B:99:LEU:N	1:B:100:GLY:CA	2.73	0.52
1:A:143:GLU:O	1:A:147:HIS:HD2	1.93	0.51
1:A:152:ASN:ND2	1:A:349:ARG:HH21	2.09	0.51
1:A:237:TRP:CE3	1:A:250:CYS:HB2	2.47	0.50
3:A:1356:447:HAI	3:A:1356:447:OAB	2.11	0.49
1:A:277:VAL:HG13	1:A:288:PRO:HD2	1.97	0.47
1:B:152:ASN:ND2	1:B:349:ARG:HH21	2.13	0.47
1:B:132:GLU:CB	1:B:133:GLY:HA2	2.44	0.46
1:B:132:GLU:HB2	1:B:134:VAL:HB	1.97	0.46
1:A:99:LEU:HB3	3:A:1356:447:HAA3	1.97	0.46
1:A:171:GLU:O	3:A:1356:447:H2	2.16	0.46
2:D:823:ARG:O	2:D:827:THR:HG22	2.16	0.46
1:A:227:LYS:HE3	4:D:2025:HOH:O	2.14	0.46
1:B:277:VAL:HG13	1:B:288:PRO:HD2	1.97	0.46
1:B:107:VAL:CG2	3:B:1356:447:HAK	2.36	0.44
3:A:1356:447:HAA2	3:A:1356:447:OBB	2.17	0.44
1:A:309:PRO:HA	1:A:310:PRO:HD3	1.85	0.43
1:B:355:TYR:HA	2:C:818:PRO:HD2	2.00	0.42
1:A:99:LEU:O	3:A:1356:447:HAA3	2.19	0.42
1:A:90:ILE:HD11	1:A:95:ILE:HD11	2.02	0.42
1:A:349:ARG:NH1	4:A:2262:HOH:O	2.52	0.42
1:B:309:PRO:HA	1:B:310:PRO:HD3	1.93	0.41
3:A:1356:447:CAI	3:A:1356:447:OAB	2.69	0.41
1:B:209:GLU:HG2	4:B:2117:HOH:O	2.21	0.41
1:A:104:PHE:CZ	1:A:134:VAL:HG21	2.56	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	270/285 (95%)	261 (97%)	9 (3%)	0	100	100
1	B	271/285 (95%)	263 (97%)	7 (3%)	1 (0%)	43	24
2	C	39/43 (91%)	36 (92%)	2 (5%)	1 (3%)	8	1
2	D	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	621/656 (95%)	599 (96%)	20 (3%)	2 (0%)	50	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
2	C	804	GLY

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	246/256 (96%)	243 (99%)	3 (1%)	82	75
1	B	248/256 (97%)	242 (98%)	6 (2%)	61	44
2	C	35/38 (92%)	31 (89%)	4 (11%)	8	1
2	D	38/38 (100%)	37 (97%)	1 (3%)	59	41
All	All	567/588 (96%)	553 (98%)	14 (2%)	60	42

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

Mol	Chain	Res	Type
1	A	112	GLU
1	A	192	ARG
1	A	299	ARG
1	B	77	ASN
1	B	86	ARG
1	B	134	VAL
1	B	138	LEU
1	B	164	LYS
1	B	335	LYS
2	C	806	LEU

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Mol	Chain	Res	Type
2	C	817	LYS
2	C	823	ARG
2	C	837	PHE
2	D	827	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	150	HIS
1	A	152	ASN
1	B	106	ASN
1	B	137	GLN
1	B	147	HIS
1	B	150	HIS
1	B	152	ASN
1	B	161	HIS
2	D	809	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	A	248	1	10,10,11	5.75	1 (10%)	12,14,16	1.07	0
1	TPO	B	248	1	10,10,11	5.64	1 (10%)	12,14,16	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	248	1	-	0/9/11/13	0/0/0/0
1	TPO	B	248	1	-	0/9/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	TPO	O-C	18.04	1.23	1.11
1	B	248	TPO	O-C	17.72	1.23	1.11

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	447	A	1356	-	42,42,42	1.55	6 (14%)	56,56,56	2.60	12 (21%)
3	447	B	1356	-	42,42,42	1.61	7 (16%)	56,56,56	2.54	9 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	447	A	1356	-	-	0/21/29/29	0/3/5/5
3	447	B	1356	-	-	0/21/29/29	0/3/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1356	447	CBF-CBC	-4.90	1.39	1.50
3	A	1356	447	CBF-CBC	-4.75	1.40	1.50
3	A	1356	447	C2-N3	4.19	1.40	1.32
3	B	1356	447	C2-N3	4.08	1.40	1.32
3	B	1356	447	CBD-NAX	-3.73	1.34	1.41
3	B	1356	447	C6-C5	-3.72	1.40	1.45
3	A	1356	447	C2-N1	3.56	1.40	1.33
3	A	1356	447	C6-C5	-3.24	1.41	1.45
3	B	1356	447	C2-N1	3.14	1.40	1.33
3	A	1356	447	CBD-NAX	-2.96	1.36	1.41
3	B	1356	447	CBE-NAY	-2.60	1.35	1.40
3	A	1356	447	CAM-CBH	2.09	1.40	1.36
3	B	1356	447	CAN-CBG	2.08	1.40	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1356	447	N3-C2-N1	-11.05	119.47	128.71
3	B	1356	447	N3-C2-N1	-10.93	119.58	128.71
3	B	1356	447	CAN-C5-C6	-6.75	121.36	124.98
3	A	1356	447	C2-N3-C4	6.73	120.58	115.37
3	A	1356	447	CAN-C5-C6	-6.70	121.38	124.98
3	A	1356	447	C6-C5-C4	6.68	119.44	115.63
3	B	1356	447	C2-N3-C4	6.09	120.08	115.37
3	B	1356	447	CBE-NAY-C6	-6.08	116.36	128.67
3	B	1356	447	C6-C5-C4	5.93	119.01	115.63
3	B	1356	447	C2-N1-C6	5.88	120.39	116.69
3	A	1356	447	C2-N1-C6	5.53	120.16	116.69
3	A	1356	447	OAZ-CBG-CAN	-4.11	120.07	125.25
3	A	1356	447	CBE-NAY-C6	-3.87	120.83	128.67
3	A	1356	447	NAY-C6-N1	3.38	122.36	118.92
3	A	1356	447	C5-C4-N3	-2.71	120.08	122.91
3	A	1356	447	OAZ-CBG-CBH	2.68	119.31	115.42
3	A	1356	447	C5-C6-NAY	-2.61	117.36	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1356	447	NAY-C6-N1	2.48	121.45	118.92
3	B	1356	447	CAA-OAZ-CBG	-2.18	114.36	117.59
3	B	1356	447	C5-C4-N3	-2.17	120.65	122.91
3	A	1356	447	CBD-NAX-CBC	-2.02	121.90	126.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	A	269/285 (94%)	0.15	9 (3%) 44 41	11, 21, 39, 42	0
1	B	275/285 (96%)	0.10	14 (5%) 27 25	11, 20, 42, 55	0
2	C	41/43 (95%)	0.35	3 (7%) 15 14	25, 29, 41, 43	0
2	D	43/43 (100%)	1.10	7 (16%) 2 2	30, 42, 54, 56	0
All	All	628/656 (95%)	0.21	33 (5%) 26 23	11, 22, 45, 56	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	GLY	6.7
1	B	355	TYR	5.6
1	B	79	ALA	5.5
1	A	244	LEU	5.0
1	B	131	LYS	4.6
1	A	103	LYS	4.2
2	D	827	THR	4.2
1	B	132	GLU	4.1
1	B	78	THR	4.0
2	D	804	GLY	4.0
2	C	837	PHE	3.3
1	A	243	SER	3.3
1	B	354	VAL	3.3
2	C	838	ASN	3.2
1	B	163	ARG	3.1
2	D	829	ASP	3.0
1	A	294	HIS	3.0
1	A	104	PHE	2.8
2	D	823	ARG	2.7
2	D	834	GLU	2.6
1	A	101	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	80	LEU	2.4
1	B	136	HIS	2.4
1	B	77	ASN	2.4
2	D	837	PHE	2.4
1	A	87	LYS	2.4
1	B	179	TYR	2.3
1	B	134	VAL	2.2
1	A	136	HIS	2.2
1	A	354	VAL	2.2
1	B	97	ARG	2.1
2	C	834	GLU	2.1
2	D	826	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	A	248	11/12	0.10	-0.74	30,33,35,36	0
1	TPO	B	248	11/12	0.05	-2.12	18,20,22,23	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	447	B	1356	38/38	0.29	4.48	55,58,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	447	A	1356	38/38	0.16	0.84	29,33,43,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.