



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:18 PM GMT

PDB ID : 2J4Z
Title : STRUCTURE OF AURORA-2 IN COMPLEX WITH PHA-680626
Authors : Cameron, A.D.; Izzo, G.; Storici, P.; Rusconi, L.; Fancelli, D.; Varasi, M.;
Berta, D.; Bindi, S.; Forte, B.; Severino, D.; Tonani, R.; Vianello, P.
Deposited on : 2006-09-08
Resolution : 2.00 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>

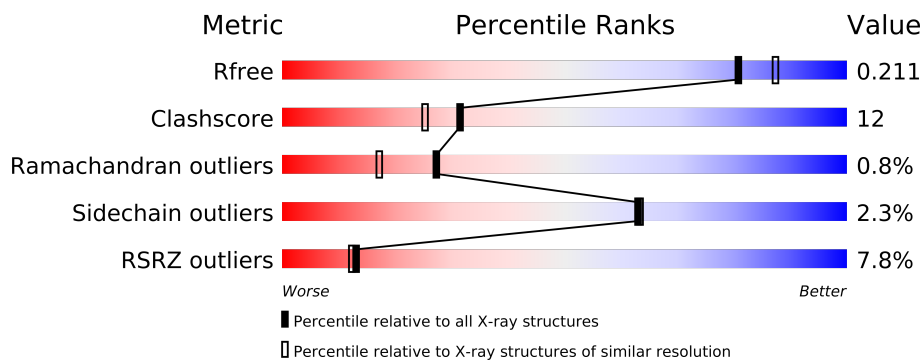
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 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	306	
1	B	306	

2 Entry composition i

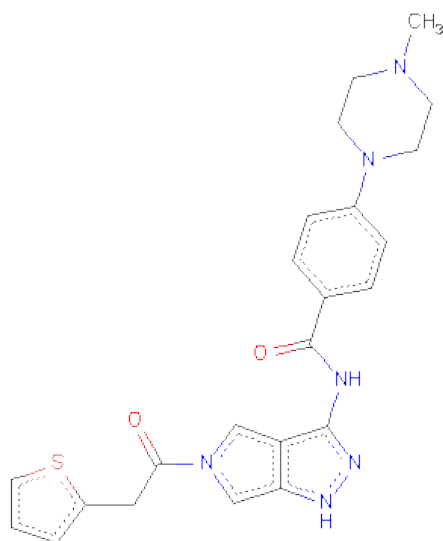
There are 4 unique types of molecules in this entry. The entry contains 4626 atoms, of which 0 are hydrogen and 0 are deuterium.

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-PROTEIN KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	1
			2160	1386	383	385	6			
1	B	270	Total	C	N	O	S	0	0	1
			2205	1412	392	394	7			

- Molecule 2 is 4-(4-METHYLPIPERAZIN-1-YL)-N-[5-(2-THIENYLACETYL)-1,5-DIHYDROPYRROLO[3,4-C]PYRAZOL-3-YL]BENZAMIDE (three-letter code: 626) (formula: C₂₃H₂₄N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	23	6	2	1		
2	B	1	Total	C	N	O	S	0	0
			32	23	6	2	1		

- Molecule 3 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	As 1	0	0
3	A	2	Total 2	As 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total 110	O 110	0	0
4	B	84	Total 84	O 84	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.13Å 89.44Å 94.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.00 29.58 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.58-2.00) 99.3 (29.58-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.00Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.214 , 0.249 0.213 , 0.211	Depositor DCC
R_{free} test set	2086 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.4	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 41440 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4626	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: ARS, 626

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	0.33	0/2214	0.59	0/2994
1	B	0.33	0/2260	0.57	1/3056 (0.0%)
All	All	0.33	0/4474	0.58	1/6050 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	GLY	N-CA-C	5.56	127.00	113.10

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	2160	0	2165	42	0
1	B	2205	0	2208	59	0
2	A	32	0	24	0	0
2	B	32	0	24	1	0
3	A	2	0	0	2	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	110	0	0	1	0
4	B	84	0	0	3	0
All	All	4626	0	4421	101	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 12.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:375:ARG:H	1:B:375:ARG:HD2	0.90	1.03
1:B:375:ARG:N	1:B:375:ARG:HD2	1.75	1.00
1:A:281:ALA:HB3	1:A:282:PRO:HA	1.45	0.97
1:B:375:ARG:CD	1:B:375:ARG:H	1.75	0.96
1:A:162:LYS:HD3	1:A:208:LEU:HD12	1.54	0.89
1:A:281:ALA:CB	1:A:282:PRO:HA	2.11	0.80
1:A:205:ARG:HH11	1:A:205:ARG:HB2	1.46	0.80
1:B:373:MET:HB3	1:B:375:ARG:HH11	1.53	0.71
1:B:299:GLU:HG3	1:B:306:HIS:HB3	1.71	0.71
1:B:380:HIS:HD2	1:B:382:TRP:H	1.37	0.70
1:A:185:GLN:HG3	1:A:275:PHE:CD1	2.27	0.70
1:A:166:LYS:HZ1	1:A:201:HIS:HB2	1.56	0.69
1:B:297:PRO:HG3	1:B:310:VAL:HG13	1.77	0.67
1:B:375:ARG:O	1:B:379:GLU:HG3	1.96	0.66
1:B:204:THR:HB	1:B:205:ARG:NH1	2.10	0.66
1:B:374:LEU:H	1:B:375:ARG:NH1	1.93	0.65
1:B:380:HIS:CD2	1:B:382:TRP:H	2.15	0.64
1:B:204:THR:HB	1:B:205:ARG:HH11	1.63	0.63
1:B:375:ARG:HG3	1:B:393:CYS:SG	2.39	0.63
1:A:281:ALA:HB3	1:A:282:PRO:CA	2.26	0.63
1:A:281:ALA:CB	1:A:282:PRO:CA	2.76	0.63
1:B:358:ASP:OD1	1:B:380:HIS:HE1	1.85	0.60
1:A:166:LYS:NZ	1:A:201:HIS:HB2	2.17	0.60
1:A:353:THR:O	1:A:357:ARG:HG3	2.04	0.58
1:B:373:MET:HB3	1:B:375:ARG:HD3	1.85	0.57
1:A:262:LEU:HB3	1:A:270:LEU:HD11	1.86	0.57
1:B:166:LYS:HG3	1:B:205:ARG:HA	1.87	0.56
1:B:180:ARG:O	1:B:183:GLU:HG2	2.06	0.56
1:A:181:GLU:HG2	1:A:275:PHE:CE1	2.41	0.55
1:B:225:LEU:O	1:B:226:SER:HB3	2.06	0.55
1:A:240:LEU:HD12	1:A:272:ILE:HD11	1.88	0.55
1:A:344:VAL:O	1:A:344:VAL:HG12	2.06	0.54
1:A:162:LYS:HB3	1:A:208:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:164:LEU:O	1:B:205:ARG:HB2	2.08	0.54
1:B:220:ARG:HG2	1:B:220:ARG:HH11	1.73	0.53
1:B:327:PRO:HB2	4:B:2039:HOH:O	2.09	0.52
1:B:187:HIS:HA	1:B:189:ARG:NH1	2.25	0.52
1:B:135:ILE:HD12	1:B:135:ILE:N	2.23	0.52
1:B:205:ARG:HG2	1:B:205:ARG:HH11	1.74	0.51
1:B:185:GLN:HB2	1:B:275:PHE:CD2	2.46	0.51
1:B:248:HIS:CD2	1:B:253:ILE:HG22	2.47	0.50
1:B:306:HIS:HB2	1:B:310:VAL:CG2	2.41	0.50
1:A:185:GLN:HG3	1:A:275:PHE:HD1	1.77	0.50
1:A:375:ARG:HB3	1:A:375:ARG:NH1	2.27	0.49
1:B:306:HIS:HB2	1:B:310:VAL:HG21	1.94	0.49
1:A:339:LYS:HB3	1:A:343:ARG:NH1	2.27	0.49
1:A:339:LYS:HB3	1:A:343:ARG:HH12	1.78	0.49
1:A:309:LYS:CD	1:A:312:LEU:HD12	2.43	0.49
1:A:145:GLY:HA3	1:A:163:VAL:O	2.13	0.49
1:A:178:LEU:O	1:A:182:VAL:HG23	2.13	0.48
1:A:155:SER:O	1:A:156:LYS:HB2	2.14	0.48
1:B:390:PRO:HD3	4:B:2078:HOH:O	2.12	0.48
1:B:374:LEU:H	1:B:375:ARG:HH11	1.59	0.48
1:B:178:LEU:HD23	1:B:178:LEU:C	2.34	0.48
1:B:142:GLY:HA3	1:B:279:VAL:HA	1.95	0.48
1:A:240:LEU:HD23	1:A:315:LEU:CD1	2.43	0.47
1:A:309:LYS:HD2	1:A:312:LEU:HD12	1.96	0.47
1:B:353:THR:O	1:B:357:ARG:HG3	2.15	0.46
1:B:288:THR:HB	4:B:2036:HOH:O	2.14	0.46
1:A:179:ARG:NH1	1:A:183:GLU:HB2	2.29	0.46
1:A:350:ASP:HB2	4:A:2092:HOH:O	2.14	0.46
1:B:343:ARG:HH22	1:B:345:GLU:CD	2.18	0.46
1:B:197:TYR:HE1	1:B:211:GLU:HA	1.80	0.46
1:B:185:GLN:OE1	1:B:196:LEU:HD12	2.16	0.45
1:B:373:MET:HB3	1:B:375:ARG:NH1	2.26	0.45
1:B:185:GLN:HB2	1:B:275:PHE:CE2	2.52	0.45
1:A:375:ARG:CZ	1:A:375:ARG:HB3	2.46	0.45
1:A:205:ARG:HH11	1:A:205:ARG:CB	2.25	0.45
1:B:251:ARG:HG2	1:B:251:ARG:HH11	1.82	0.44
1:A:205:ARG:NH1	1:A:207:TYR:OH	2.51	0.44
1:A:181:GLU:HG2	1:A:275:PHE:HE1	1.81	0.44
1:A:247:CYS:CB	3:A:1390:ARS:AS	3.26	0.44
1:B:373:MET:CB	1:B:375:ARG:HH11	2.28	0.44
1:B:130:LEU:HD13	1:B:207:TYR:CE2	2.52	0.44
1:B:205:ARG:HG2	1:B:205:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:378:LEU:HB3	1:B:391:SER:HB3	1.99	0.43
1:A:179:ARG:HH12	1:A:183:GLU:HB2	1.84	0.43
1:A:196:LEU:HA	1:A:210:LEU:HD23	1.99	0.43
1:B:214:PRO:O	2:B:1395:626:H12	2.18	0.43
1:A:301:ILE:HD12	1:A:341:ILE:HB	2.01	0.42
1:A:285:ARG:HD2	1:A:292:THR:HG21	2.01	0.42
1:B:178:LEU:HA	1:B:277:TRP:CZ3	2.54	0.42
1:B:375:ARG:N	1:B:375:ARG:CD	2.54	0.42
1:A:312:LEU:HD13	1:A:372:PRO:O	2.20	0.42
1:A:301:ILE:HD12	1:A:341:ILE:CG2	2.49	0.42
1:B:267:ALA:N	1:B:269:GLU:OE2	2.50	0.42
1:B:169:LEU:HD13	1:B:178:LEU:HD12	2.01	0.42
1:B:287:THR:CG2	1:B:288:THR:N	2.83	0.42
1:A:250:LYS:O	1:A:251:ARG:HB2	2.20	0.42
1:B:221:GLU:HG2	1:B:232:ARG:NH2	2.35	0.41
1:B:257:ILE:HG22	1:B:272:ILE:HD12	2.03	0.41
1:A:240:LEU:HD22	1:A:318:LEU:HD12	2.01	0.41
1:B:166:LYS:NZ	1:B:201:HIS:HD2	2.19	0.41
1:B:154:GLN:HA	1:B:154:GLN:OE1	2.21	0.41
1:B:374:LEU:N	1:B:375:ARG:HH11	2.18	0.41
1:B:145:GLY:HA3	1:B:163:VAL:O	2.21	0.41
1:B:373:MET:HB3	1:B:375:ARG:CD	2.48	0.41
1:A:290:CYS:SG	3:A:1391:ARS:AS	3.39	0.41
1:A:246:TYR:O	1:A:250:LYS:HG2	2.21	0.41
1:B:163:VAL:CG1	1:B:205:ARG:HD2	2.51	0.40
1:B:215:LEU:HB2	1:B:264:LEU:HB2	2.04	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	262/306 (86%)	249 (95%)	12 (5%)	1 (0%)	43	36
1	B	268/306 (88%)	255 (95%)	10 (4%)	3 (1%)	21	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	530/612 (87%)	504 (95%)	22 (4%)	4 (1%)	27	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
1	B	276	GLY
1	B	154	GLN
1	B	277	TRP

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	232/271 (86%)	226 (97%)	6 (3%)	59	58
1	B	238/271 (88%)	233 (98%)	5 (2%)	66	67
All	All	470/542 (87%)	459 (98%)	11 (2%)	63	63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	178	LEU
1	A	205	ARG
1	A	251	ARG
1	A	282	PRO
1	A	318	LEU
1	B	168	GLN
1	B	181	GLU
1	B	269	GLU
1	B	293	LEU
1	B	375	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	254	HIS
1	A	261	ASN
1	B	201	HIS
1	B	380	HIS

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 ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
2	626	A	1389	-	36,36,36	2.96	18 (50%)	47,51,51	2.55	12 (25%)
2	626	B	1395	-	36,36,36	2.97	19 (52%)	47,51,51	2.39	7 (14%)

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
2	626	A	1389	-	-	0/13/30/30	0/3/5/5
2	626	B	1395	-	-	0/13/30/30	0/3/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1389	626	C18-N3	7.01	1.50	1.39
2	B	1395	626	C17-N3	6.91	1.50	1.39
2	A	1389	626	C17-N3	6.88	1.50	1.39
2	B	1395	626	C18-N3	6.62	1.49	1.39
2	A	1389	626	C5-C16	-4.89	1.33	1.45
2	B	1395	626	C5-N6	-4.72	1.28	1.34
2	A	1389	626	C5-N7	4.65	1.46	1.36
2	B	1395	626	C26-N19	4.60	1.51	1.38
2	B	1395	626	C5-C16	-4.60	1.34	1.45
2	A	1389	626	C18-C15	4.55	1.50	1.40
2	B	1395	626	C18-C15	4.51	1.50	1.40
2	A	1389	626	C26-N19	4.36	1.50	1.38
2	A	1389	626	C20-N19	4.34	1.53	1.46
2	A	1389	626	C24-N19	4.27	1.53	1.46
2	B	1395	626	C20-N19	4.26	1.53	1.46
2	B	1395	626	C5-N7	4.23	1.45	1.36
2	A	1389	626	C5-N6	-4.10	1.28	1.34
2	A	1389	626	C17-C16	4.05	1.49	1.40
2	B	1395	626	C24-N19	3.95	1.52	1.46
2	A	1389	626	C32-C31	3.84	1.55	1.51
2	B	1395	626	C17-C16	3.68	1.48	1.40
2	B	1395	626	C32-C1	3.51	1.56	1.52
2	B	1395	626	C32-C31	3.41	1.54	1.51
2	A	1389	626	C32-C1	2.74	1.55	1.52
2	B	1395	626	C1-N3	-2.73	1.38	1.44
2	A	1389	626	C1-N3	-2.62	1.38	1.44
2	B	1395	626	C14-C9	2.52	1.43	1.39
2	A	1389	626	C14-C9	2.36	1.43	1.39
2	B	1395	626	C23-N22	2.33	1.51	1.46
2	B	1395	626	C12-C26	2.32	1.44	1.39
2	A	1389	626	C11-C9	2.30	1.43	1.39
2	B	1395	626	C21-N22	2.28	1.51	1.46
2	B	1395	626	C11-C9	2.27	1.43	1.39
2	A	1389	626	C12-C26	2.24	1.43	1.39
2	B	1395	626	C13-C26	2.08	1.43	1.39
2	A	1389	626	C13-C26	2.05	1.43	1.39
2	A	1389	626	C23-N22	2.03	1.51	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1389	626	C18-N3-C17	12.80	113.31	108.13
2	B	1395	626	C18-N3-C17	12.55	113.21	108.13
2	B	1395	626	C23-N22-C21	4.15	115.32	109.54
2	A	1389	626	C23-N22-C21	4.11	115.27	109.54
2	A	1389	626	C5-C16-C15	-3.88	101.91	106.89
2	B	1395	626	C5-C16-C15	-3.81	102.00	106.89
2	A	1389	626	C24-C23-N22	3.72	114.93	110.82
2	A	1389	626	C21-C20-N19	3.14	116.53	110.62
2	A	1389	626	C31-C32-C1	-3.06	107.93	112.07
2	A	1389	626	C24-N19-C20	2.82	117.46	111.67
2	B	1395	626	C24-C23-N22	2.70	113.80	110.82
2	A	1389	626	C23-C24-N19	2.58	115.48	110.62
2	A	1389	626	C16-C17-N3	-2.28	104.58	107.37
2	B	1395	626	C16-C17-N3	-2.24	104.62	107.37
2	A	1389	626	C9-C8-N7	2.15	119.96	115.86
2	A	1389	626	C20-C21-N22	2.13	113.17	110.82
2	A	1389	626	C27-S29-C31	-2.12	90.55	91.96
2	B	1395	626	C32-C1-N3	2.06	120.53	117.89
2	B	1395	626	C21-C20-N19	2.01	114.41	110.62

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	264/306 (86%)	0.38	15 (5%) 23 22	20, 34, 56, 73	0
1	B	270/306 (88%)	0.59	27 (10%) 8 7	20, 39, 62, 75	0
All	All	534/612 (87%)	0.49	42 (7%) 13 12	20, 36, 60, 75	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	MET	4.4
1	A	127	GLN	4.3
1	B	171	LYS	4.2
1	B	154	GLN	4.1
1	A	144	PHE	4.0
1	B	126	ARG	4.0
1	A	251	ARG	3.9
1	B	172	ALA	3.9
1	A	281	ALA	3.9
1	A	126	ARG	3.8
1	B	281	ALA	3.6
1	B	157	PHE	3.5
1	B	394	GLN	3.4
1	A	143	LYS	2.9
1	B	168	GLN	2.9
1	A	154	GLN	2.7
1	A	275	PHE	2.7
1	B	134	GLU	2.6
1	B	350	ASP	2.6
1	B	167	ALA	2.5
1	B	187	HIS	2.5
1	B	257	ILE	2.5
1	B	332	ASN	2.5
1	B	156	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	304	ARG	2.4
1	A	170	GLU	2.4
1	B	155	SER	2.4
1	A	282	PRO	2.3
1	A	257	ILE	2.3
1	B	318	LEU	2.3
1	B	284	SER	2.3
1	B	302	GLU	2.3
1	A	177	GLN	2.2
1	B	395	ASN	2.2
1	B	131	GLU	2.2
1	A	157	PHE	2.1
1	A	280	HIS	2.1
1	B	282	PRO	2.1
1	A	199	TYR	2.1
1	B	339	LYS	2.1
1	B	189	ARG	2.0
1	B	275	PHE	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 ⓘ

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
2	626	A	1389	32/32	0.16	0.79	23,31,44,46	0
2	626	B	1395	32/32	0.15	0.15	25,36,52,55	0
3	ARS	A	1391	1/1	0.14	-0.42	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ARS	B	1396	1/1	0.07	-1.46	43,43,43,43	0
3	ARS	A	1390	1/1	0.06	-1.98	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.