W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:02 PM GMT

PDB ID : 3GC9
Title : The structure of p38beta C119S, C162S in complex with a dihydroquinazoli-
none inhibitor
Authors : Scapin, G.; Patel, S.B.
Deposited on : 2009-02-21
Resolution : 2.05 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.05 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		0.272
Clashscore		6
Ramachandran outliers		1.1%
Sidechain outliers		2.1%
RSRZ outliers		6.2%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
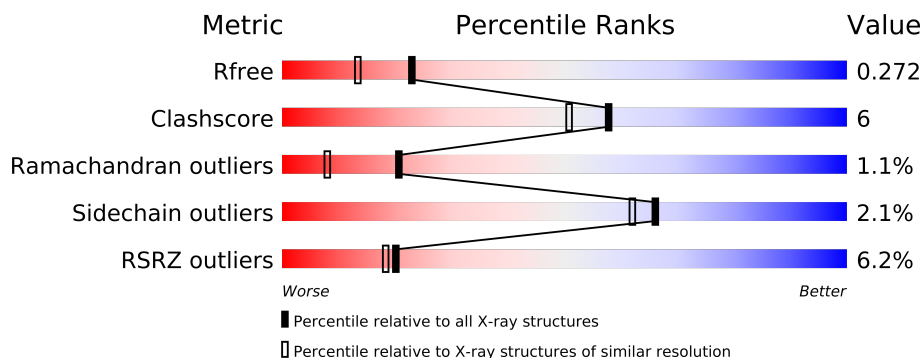
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	370	
1	B	370	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NA	A	601	-	X
2	NA	B	602	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5805 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 Mitogen-activated protein kinase 11.

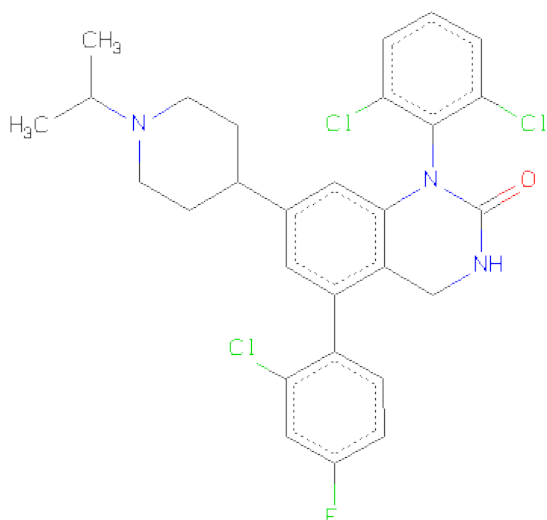| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total 2687	C 1712	N 466	O 500	S 9	0	0	0
1	B	339	Total 2697	C 1718	N 465	O 505	S 9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q15759
A	-4	SER	-	EXPRESSION TAG	UNP Q15759
A	-3	HIS	-	EXPRESSION TAG	UNP Q15759
A	-2	MET	-	EXPRESSION TAG	UNP Q15759
A	-1	LEU	-	EXPRESSION TAG	UNP Q15759
A	0	GLU	-	EXPRESSION TAG	UNP Q15759
A	119	SER	CYS	ENGINEERED	UNP Q15759
A	162	SER	CYS	ENGINEERED	UNP Q15759
B	-5	GLY	-	EXPRESSION TAG	UNP Q15759
B	-4	SER	-	EXPRESSION TAG	UNP Q15759
B	-3	HIS	-	EXPRESSION TAG	UNP Q15759
B	-2	MET	-	EXPRESSION TAG	UNP Q15759
B	-1	LEU	-	EXPRESSION TAG	UNP Q15759
B	0	GLU	-	EXPRESSION TAG	UNP Q15759
B	119	SER	CYS	ENGINEERED	UNP Q15759
B	162	SER	CYS	ENGINEERED	UNP Q15759

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is 5-(2-CHLORO-4-FLUOROPHENYL)-1-(2,6-DICHLOROPHENYL)-7-[1-(1-METHYLETHYL)PIPERIDIN-4-YL]-3,4-DIHYDROQUINAZOLIN-2(1H)-ONE (three-letter code: B45) (formula: $C_{28}H_{27}Cl_3FN_3O$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			36	28	3	1	3	1		
3	B	1	Total	C	Cl	F	N	O	0	0
			36	28	3	1	3	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	181	Total	O	0	0
			181	181		
5	B	165	Total	O	0	0
			165	165		

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.
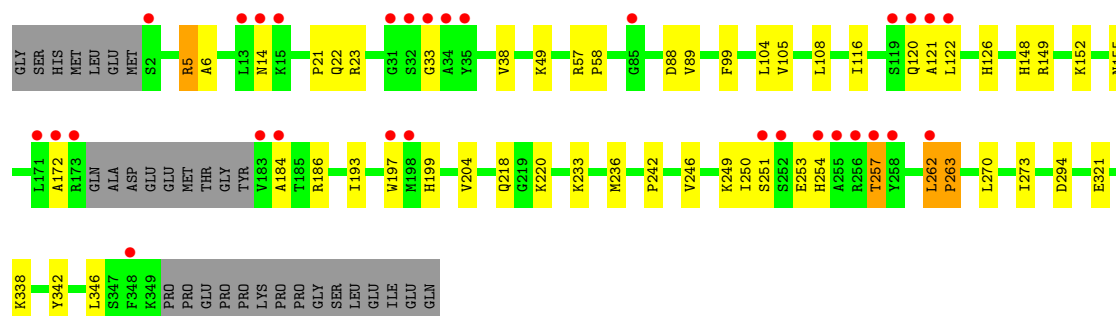
• Molecule 1: Mitogen-activated protein kinase 11

Chain A:
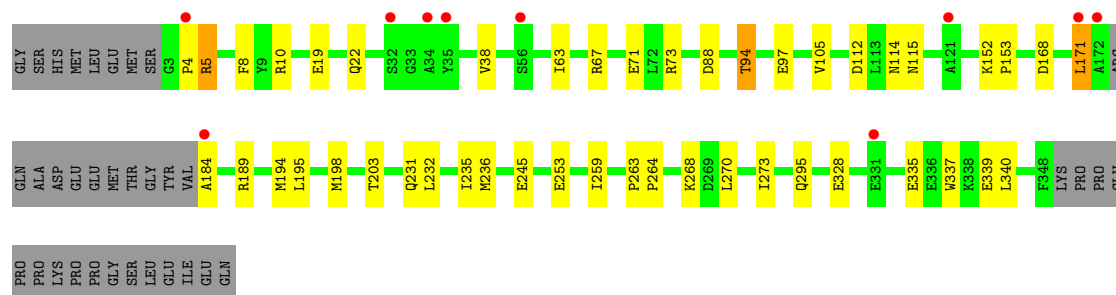
• Molecule 1: Mitogen-activated protein kinase 11

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.18Å 158.82Å 60.87Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.05) 90.8 (29.88-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.275 0.218 , 0.272	Depositor DCC
R_{free} test set	2309 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.9	EDS
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 45713 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5805	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: B45, NA, ZN

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	0.53	0/2747	0.62	1/3725 (0.0%)
1	B	0.53	0/2756	0.65	1/3739 (0.0%)
All	All	0.53	0/5503	0.64	2/7464 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	294	ASP	CB-CG-OD1	5.37	123.13	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ALA	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	A	2687	0	2675	33	0
1	B	2697	0	2670	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	27	2	0
3	B	36	0	27	1	0
4	B	1	0	0	0	0
5	A	181	0	0	10	0
5	B	165	0	0	6	0
All	All	5805	0	5399	68	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 (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:THR:HG22	5:A:609:HOH:O	1.56	1.03
1:B:262:LEU:HB2	1:B:263:PRO:HD3	1.53	0.91
1:B:242:PRO:HB3	1:B:246:VAL:HG22	1.54	0.90
1:A:295:GLN:HG2	5:A:606:HOH:O	1.87	0.74
1:B:321:GLU:HG2	5:B:620:HOH:O	1.93	0.68
1:B:218:GLN:HG3	1:B:220:LYS:HG2	1.75	0.68
1:A:112:ASP:H	1:A:115:ASN:HD22	1.43	0.67
1:B:270:LEU:HD23	1:B:273:ILE:HD13	1.76	0.67
1:A:22:GLN:NE2	5:A:647:HOH:O	2.24	0.66
1:B:242:PRO:HB3	1:B:246:VAL:CG2	2.27	0.63
1:A:335:GLU:O	1:A:339:GLU:HG3	2.02	0.60
1:B:197:TRP:HB3	1:B:253:GLU:HG3	1.85	0.59
1:B:270:LEU:HA	1:B:273:ILE:CD1	2.33	0.58
1:B:89:VAL:HG13	1:B:104:LEU:HD23	1.85	0.58
1:A:189:ARG:HE	1:A:194:MET:HE1	1.67	0.58
1:B:22:GLN:NE2	5:B:553:HOH:O	2.36	0.58
1:B:249:LYS:O	1:B:253:GLU:HG2	2.04	0.57
1:B:23:ARG:NH1	5:B:550:HOH:O	2.37	0.57
1:A:67:ARG:O	1:A:71:GLU:HG3	2.06	0.56
1:B:122:LEU:HD13	1:B:126:HIS:HD2	1.71	0.56
1:B:262:LEU:HB2	1:B:263:PRO:CD	2.31	0.55
1:A:73:ARG:NH2	5:A:425:HOH:O	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:250:ILE:HG23	1:B:254:HIS:CE1	2.43	0.54
1:A:5:ARG:HD3	1:A:94:THR:CG2	2.37	0.54
1:A:5:ARG:HG2	1:A:8:PHE:CD1	2.43	0.53
1:B:251:SER:HB2	1:B:257:THR:HG21	1.90	0.52
1:A:195:LEU:HD11	1:A:259:ILE:HD11	1.91	0.52
1:A:5:ARG:HD3	1:A:94:THR:HG23	1.92	0.51
1:A:194:MET:HA	1:A:194:MET:CE	2.40	0.50
1:A:38:VAL:HG21	3:A:365:B45:H33A	1.93	0.50
1:B:21:PRO:HG3	1:B:23:ARG:NH1	2.26	0.50
1:B:270:LEU:HA	1:B:273:ILE:HD13	1.95	0.49
1:B:193:ILE:HD11	1:B:204:VAL:HB	1.95	0.49
1:B:184:ALA:HA	5:B:403:HOH:O	2.13	0.49
1:B:148:HIS:O	1:B:149:ARG:HB2	2.12	0.49
1:B:57:ARG:N	1:B:58:PRO:HD3	2.28	0.48
1:B:270:LEU:HA	1:B:273:ILE:HD12	1.95	0.48
1:B:21:PRO:CG	1:B:23:ARG:NH1	2.77	0.48
1:A:112:ASP:H	1:A:115:ASN:ND2	2.11	0.48
1:A:194:MET:HE2	1:A:194:MET:HA	1.94	0.48
1:A:184:ALA:HB1	5:A:384:HOH:O	2.14	0.48
1:A:245:GLU:HG3	5:A:627:HOH:O	2.13	0.48
1:A:253:GLU:HG3	5:B:459:HOH:O	2.14	0.47
1:B:49:LYS:HD2	1:B:108:LEU:HD23	1.95	0.47
1:A:270:LEU:HD23	1:A:273:ILE:HD13	1.96	0.47
1:B:120:GLN:HB2	1:B:122:LEU:HD23	1.96	0.46
1:A:328:GLU:HA	1:A:337:TRP:HH2	1.80	0.46
1:B:88:ASP:HB3	1:B:105:VAL:HB	1.97	0.46
1:A:268:LYS:HE3	5:A:605:HOH:O	2.16	0.45
1:A:198:MET:HE1	5:A:481:HOH:O	2.15	0.45
1:A:71:GLU:HG2	1:A:171:LEU:HD13	1.99	0.45
1:A:71:GLU:HG2	1:A:171:LEU:HD22	1.98	0.45
1:B:38:VAL:HG21	3:B:365:B45:H33A	1.99	0.44
1:A:231:GLN:O	1:A:235:ILE:HG13	2.18	0.44
1:A:10:ARG:HG2	1:A:19:GLU:HG3	1.99	0.43
1:B:122:LEU:HD13	1:B:126:HIS:CD2	2.53	0.42
1:B:342:TYR:CE2	1:B:346:LEU:HD11	2.55	0.42
1:A:232:LEU:O	1:A:236:MET:HG2	2.19	0.42
1:B:99:PHE:O	1:B:338:LYS:HE3	2.19	0.41
1:A:88:ASP:HB3	1:A:105:VAL:HB	2.02	0.41
1:A:112:ASP:OD1	1:A:114:ASN:HB2	2.20	0.41
1:B:152:LYS:NZ	1:B:155:ASN:HD21	2.17	0.41
1:A:263:PRO:HA	1:A:264:PRO:HD3	1.85	0.41
3:A:365:B45:H22	5:A:626:HOH:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:5:ARG:HG3	1:B:6:ALA:N	2.36	0.41
1:B:218:GLN:HB3	5:B:622:HOH:O	2.20	0.40
1:A:152:LYS:HB2	1:A:153:PRO:HD2	2.03	0.40
1:A:295:GLN:NE2	5:A:436:HOH:O	2.54	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	331/370 (90%)	320 (97%)	9 (3%)	2 (1%)	33	20
1	B	335/370 (90%)	314 (94%)	16 (5%)	5 (2%)	15	4
All	All	666/740 (90%)	634 (95%)	25 (4%)	7 (1%)	21	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	B	33	GLY
1	B	199	HIS
1	A	168	ASP
1	B	172	ALA
1	B	262	LEU
1	B	263	PRO

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	291/322 (90%)	286 (98%)	5 (2%)	73	71
1	B	290/322 (90%)	283 (98%)	7 (2%)	61	57
All	All	581/644 (90%)	569 (98%)	12 (2%)	66	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	63	ILE
1	A	94	THR
1	A	97	GLU
1	A	171	LEU
1	B	5	ARG
1	B	14	ASN
1	B	116	ILE
1	B	186	ARG
1	B	233	LYS
1	B	236	MET
1	B	257	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	155	ASN
1	A	295	GLN
1	B	22	GLN
1	B	48	GLN
1	B	126	HIS
1	B	155	ASN
1	B	254	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	#$|Z| > 2$
3	B45	A	365	-	40,40,40	0.85	1 (2%)	59,59,59	1.18	7 (11%)
3	B45	B	365	-	40,40,40	0.75	1 (2%)	59,59,59	1.12	5 (8%)

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	B45	A	365	-	-	0/16/39/39	0/3/5/5
3	B45	B	365	-	-	0/16/39/39	0/3/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	365	B45	C16-C20	-2.52	1.45	1.49
3	B	365	B45	C16-C20	-2.48	1.45	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	365	B45	C32-N31-C30	3.33	115.31	109.16
3	A	365	B45	C29-C28-C18	-2.80	106.79	112.89
3	B	365	B45	C29-C28-C18	-2.60	107.24	112.89
3	A	365	B45	C16-C13-C14	2.55	121.02	118.26
3	B	365	B45	C16-C13-C14	2.50	120.97	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	365	B45	C29-C30-N31	-2.46	107.52	111.49
3	A	365	B45	C4-C3-N9	-2.31	119.51	121.22
3	B	365	B45	C19-C14-C13	-2.18	118.85	123.36
3	A	365	B45	C3-C4-CL7	-2.18	117.35	119.93
3	A	365	B45	C32-N31-C30	2.15	113.13	109.16
3	B	365	B45	C25-C24-C23	2.15	119.28	117.75
3	A	365	B45	C24-C25-CL26	-2.05	115.32	118.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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	335/370 (90%)	0.41	10 (2%)	48	48	24, 32, 42, 52	0
1	B	339/370 (91%)	0.60	30 (8%)	10	9	23, 32, 49, 59	0
All	All	674/740 (91%)	0.50	40 (5%)	20	20	23, 32, 46, 59	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	8.4
1	B	252	SER	7.1
1	B	184	ALA	6.4
1	B	35	TYR	5.8
1	B	258	TYR	5.7
1	A	32	SER	5.7
1	B	32	SER	5.0
1	B	257	THR	4.9
1	A	171	LEU	4.7
1	A	56	SER	4.2
1	A	184	ALA	4.2
1	B	13	LEU	4.0
1	B	85	GLY	3.9
1	B	255	ALA	3.9
1	B	33	GLY	3.7
1	B	173	ARG	3.6
1	B	121	ALA	3.4
1	B	172	ALA	3.4
1	B	198	MET	3.4
1	A	35	TYR	3.4
1	A	34	ALA	3.4
1	B	171	LEU	3.3
1	B	197	TRP	3.3
1	B	2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	119	SER	2.9
1	B	348	PHE	2.9
1	B	34	ALA	2.8
1	B	122	LEU	2.7
1	B	256	ARG	2.7
1	A	172	ALA	2.5
1	B	183	VAL	2.4
1	B	254	HIS	2.4
1	B	251	SER	2.3
1	B	120	GLN	2.3
1	B	14	ASN	2.2
1	A	4	PRO	2.2
1	A	331	GLU	2.1
1	A	121	ALA	2.1
1	B	31	GLY	2.0
1	B	15	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

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	NA	B	602	1/1	0.46	7.47	48,48,48,48	0
2	NA	A	601	1/1	0.40	5.29	32,32,32,32	0
3	B45	B	365	36/36	0.21	0.88	24,27,34,35	0
3	B45	A	365	36/36	0.19	0.76	26,29,33,35	0
4	ZN	B	603	1/1	0.13	-0.38	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.