Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2018 – 11:07 PM EST

PDB ID	:	4ACD
Title	:	GSK3b in complex with inhibitor
Authors	:	Xue, Y.; Ormo, M.
Deposited on	:	2011-12-15
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

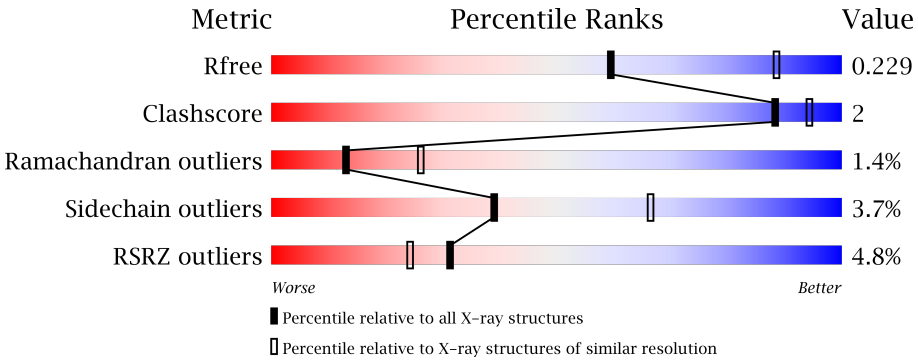
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	465	4% 68% 7% 25%
1	B	465	3% 67% 8% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6005 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 GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	1
			2805	1804	482	508	11			
1	B	351	Total	C	N	O	S	0	0	1
			2805	1804	482	508	11			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	expression tag	UNP P49841
A	-43	SER	-	expression tag	UNP P49841
A	-42	TYR	-	expression tag	UNP P49841
A	-41	TYR	-	expression tag	UNP P49841
A	-40	HIS	-	expression tag	UNP P49841
A	-39	HIS	-	expression tag	UNP P49841
A	-38	HIS	-	expression tag	UNP P49841
A	-37	HIS	-	expression tag	UNP P49841
A	-36	HIS	-	expression tag	UNP P49841
A	-35	HIS	-	expression tag	UNP P49841
A	-34	ASP	-	expression tag	UNP P49841
A	-33	TYR	-	expression tag	UNP P49841
A	-32	ASP	-	expression tag	UNP P49841
A	-31	ILE	-	expression tag	UNP P49841
A	-30	PRO	-	expression tag	UNP P49841
A	-29	THR	-	expression tag	UNP P49841
A	-28	THR	-	expression tag	UNP P49841
A	-27	GLU	-	expression tag	UNP P49841
A	-26	ASN	-	expression tag	UNP P49841
A	-25	LEU	-	expression tag	UNP P49841
A	-24	TYR	-	expression tag	UNP P49841
A	-23	PHE	-	expression tag	UNP P49841
A	-22	GLN	-	expression tag	UNP P49841
A	-21	GLY	-	expression tag	UNP P49841
A	-20	ALA	-	expression tag	UNP P49841

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P49841
A	-18	GLY	-	expression tag	UNP P49841
A	-17	SER	-	expression tag	UNP P49841
A	-16	SER	-	expression tag	UNP P49841
A	-15	HIS	-	expression tag	UNP P49841
A	-14	HIS	-	expression tag	UNP P49841
A	-13	HIS	-	expression tag	UNP P49841
A	-12	HIS	-	expression tag	UNP P49841
A	-11	HIS	-	expression tag	UNP P49841
A	-10	HIS	-	expression tag	UNP P49841
A	-9	SER	-	expression tag	UNP P49841
A	-8	SER	-	expression tag	UNP P49841
A	-7	GLY	-	expression tag	UNP P49841
A	-6	LEU	-	expression tag	UNP P49841
A	-5	VAL	-	expression tag	UNP P49841
A	-4	PRO	-	expression tag	UNP P49841
A	-3	ARG	-	expression tag	UNP P49841
A	-2	GLY	-	expression tag	UNP P49841
A	-1	SER	-	expression tag	UNP P49841
A	0	HIS	-	expression tag	UNP P49841
B	-44	MET	-	expression tag	UNP P49841
B	-43	SER	-	expression tag	UNP P49841
B	-42	TYR	-	expression tag	UNP P49841
B	-41	TYR	-	expression tag	UNP P49841
B	-40	HIS	-	expression tag	UNP P49841
B	-39	HIS	-	expression tag	UNP P49841
B	-38	HIS	-	expression tag	UNP P49841
B	-37	HIS	-	expression tag	UNP P49841
B	-36	HIS	-	expression tag	UNP P49841
B	-35	HIS	-	expression tag	UNP P49841
B	-34	ASP	-	expression tag	UNP P49841
B	-33	TYR	-	expression tag	UNP P49841
B	-32	ASP	-	expression tag	UNP P49841
B	-31	ILE	-	expression tag	UNP P49841
B	-30	PRO	-	expression tag	UNP P49841
B	-29	THR	-	expression tag	UNP P49841
B	-28	THR	-	expression tag	UNP P49841
B	-27	GLU	-	expression tag	UNP P49841
B	-26	ASN	-	expression tag	UNP P49841
B	-25	LEU	-	expression tag	UNP P49841
B	-24	TYR	-	expression tag	UNP P49841
B	-23	PHE	-	expression tag	UNP P49841

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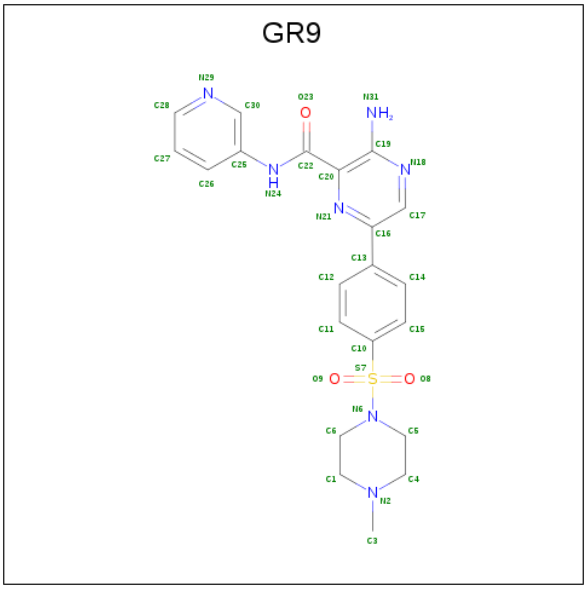
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLN	-	expression tag	UNP P49841
B	-21	GLY	-	expression tag	UNP P49841
B	-20	ALA	-	expression tag	UNP P49841
B	-19	MET	-	expression tag	UNP P49841
B	-18	GLY	-	expression tag	UNP P49841
B	-17	SER	-	expression tag	UNP P49841
B	-16	SER	-	expression tag	UNP P49841
B	-15	HIS	-	expression tag	UNP P49841
B	-14	HIS	-	expression tag	UNP P49841
B	-13	HIS	-	expression tag	UNP P49841
B	-12	HIS	-	expression tag	UNP P49841
B	-11	HIS	-	expression tag	UNP P49841
B	-10	HIS	-	expression tag	UNP P49841
B	-9	SER	-	expression tag	UNP P49841
B	-8	SER	-	expression tag	UNP P49841
B	-7	GLY	-	expression tag	UNP P49841
B	-6	LEU	-	expression tag	UNP P49841
B	-5	VAL	-	expression tag	UNP P49841
B	-4	PRO	-	expression tag	UNP P49841
B	-3	ARG	-	expression tag	UNP P49841
B	-2	GLY	-	expression tag	UNP P49841
B	-1	SER	-	expression tag	UNP P49841
B	0	HIS	-	expression tag	UNP P49841

- Molecule 2 is 3-AMINO-6-{4-[(4-METHYLPIPERAZIN-1-YL)SULFONYL]PHENYL} -N-PYRIDIN-3-YLPYRAZINE-2-CARBOXAMIDE (three-letter code: GR9) (formula: $C_{21}H_{23}N_7O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	7	3	1		
2	B	1	Total	C	N	O	S	0	0
			32	21	7	3	1		

- Molecule 3 is water.

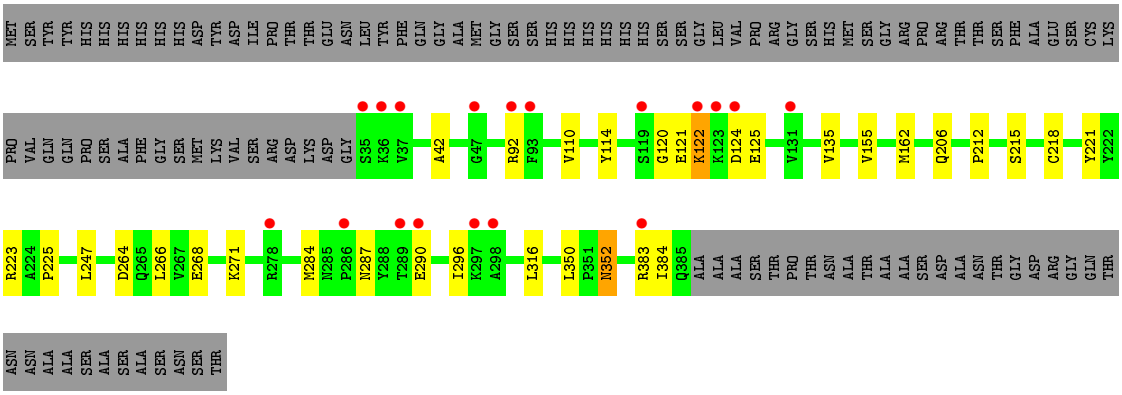
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	157	Total	O	0	0
			157	157		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

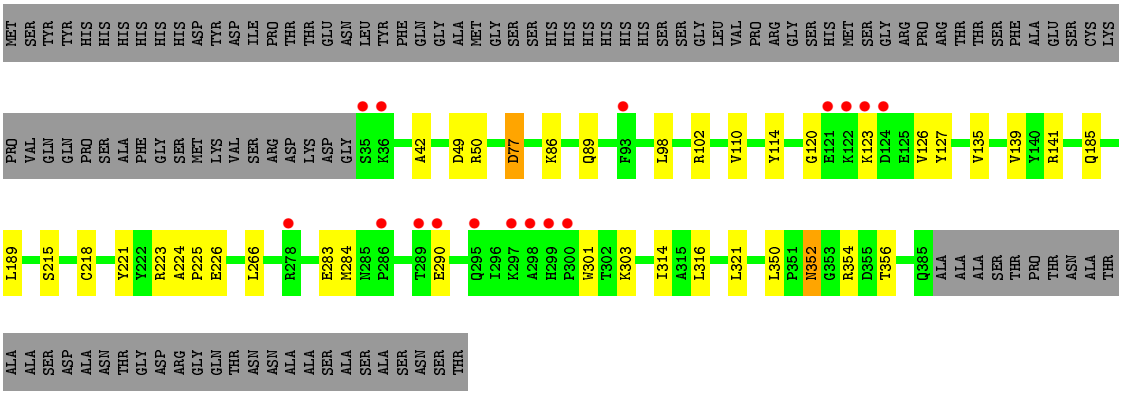
- Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA

Chain A:



- Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.32Å 84.99Å 177.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.22 – 2.60 21.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.2 (21.22-2.60) 86.3 (21.19-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.60Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.178 , 0.226 0.180 , 0.229	Depositor DCC
R_{free} test set	1726 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6005	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GR9

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	0.52	0/2876	0.73	0/3913
1	B	0.51	0/2876	0.71	0/3913
All	All	0.51	0/5752	0.72	0/7826

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	2805	0	2833	9	0
1	B	2805	0	2833	17	0
2	A	32	0	23	1	0
2	B	32	0	23	1	0
3	A	174	0	0	0	0
3	B	157	0	0	3	0
All	All	6005	0	5712	26	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 2.

All (26) 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:B:49:ASP:OD2	3:B:2006:HOH:O	2.03	0.75
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.82	0.61
1:A:135:VAL:O	2:A:1385:GR9:H12	2.04	0.57
1:B:98:LEU:O	1:B:102:ARG:HG3	2.07	0.55
1:B:185:GLN:HG2	3:B:2082:HOH:O	2.07	0.54
1:B:225:PRO:HB2	1:B:284:MET:SD	2.47	0.53
1:A:225:PRO:HB2	1:A:284:MET:SD	2.48	0.53
1:A:350:LEU:HB3	1:A:352:ASN:ND2	2.28	0.48
1:A:121:GLU:O	1:A:125:GLU:HB2	2.14	0.48
1:B:290:GLU:HB2	3:B:2116:HOH:O	2.14	0.47
1:B:120:GLY:HA3	1:B:127:TYR:CD1	2.49	0.47
1:B:86:LYS:HE2	1:B:120:GLY:HA2	1.97	0.47
1:B:350:LEU:HB3	1:B:352:ASN:ND2	2.30	0.46
1:B:301:TRP:HB3	1:B:314:ILE:HG23	1.99	0.44
1:B:139:VAL:HG22	1:B:189:LEU:HD11	2.00	0.44
1:B:135:VAL:O	2:B:1385:GR9:H12	2.18	0.43
1:B:350:LEU:HD13	1:B:356:THR:HA	1.99	0.43
1:A:264:ASP:O	1:A:268:GLU:HG2	2.19	0.43
1:A:271:LYS:HA	1:A:296:ILE:HG21	2.02	0.42
1:A:215:SER:O	1:A:223:ARG:NH2	2.54	0.41
1:B:301:TRP:HH2	1:B:321:LEU:HD12	1.85	0.41
1:B:224:ALA:HB1	1:B:226:GLU:OE2	2.21	0.40
1:A:42:ALA:HB1	1:A:114:TYR:HB3	2.02	0.40
1:A:162:MET:HG3	1:A:247:LEU:HD13	2.03	0.40
1:B:215:SER:O	1:B:223:ARG:NH2	2.54	0.40
1:B:352:ASN:HD21	1:B:354:ARG:HB2	1.87	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	349/465 (75%)	327 (94%)	15 (4%)	7 (2%)	9 17
1	B	349/465 (75%)	333 (95%)	13 (4%)	3 (1%)	20 40
All	All	698/930 (75%)	660 (95%)	28 (4%)	10 (1%)	13 26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	ARG
1	A	122	LYS
1	A	221	TYR
1	B	221	TYR
1	B	77	ASP
1	A	124	ASP
1	A	120	GLY
1	B	218	CYS
1	A	218	CYS
1	A	384	ILE

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	312/404 (77%)	301 (96%)	11 (4%)	41 68
1	B	312/404 (77%)	300 (96%)	12 (4%)	38 66
All	All	624/808 (77%)	601 (96%)	23 (4%)	39 66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	110	VAL
1	A	122	LYS
1	A	155	VAL
1	A	206	GLN
1	A	212	PRO

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Mol	Chain	Res	Type
1	A	266	LEU
1	A	287	ASN
1	A	290	GLU
1	A	316	LEU
1	A	352	ASN
1	B	50	ARG
1	B	77	ASP
1	B	89	GLN
1	B	110	VAL
1	B	123	LYS
1	B	126	VAL
1	B	141	ARG
1	B	266	LEU
1	B	283	GLU
1	B	303	LYS
1	B	316	LEU
1	B	352	ASN

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

Mol	Chain	Res	Type
1	A	129	ASN
1	A	145	HIS
1	A	265	GLN
1	A	352	ASN
1	A	381	HIS
1	B	129	ASN
1	B	352	ASN

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 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	$\#\|Z\| > 2$
2	GR9	A	1385	-	34,35,35	0.90	2 (5%)	46,50,50	1.98	9 (19%)
2	GR9	B	1385	-	34,35,35	0.97	1 (2%)	46,50,50	1.79	9 (19%)

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	GR9	A	1385	-	-	0/24/34/34	0/4/4/4
2	GR9	B	1385	-	-	0/24/34/34	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1385	GR9	C10-S7	2.04	1.79	1.76
2	A	1385	GR9	C6-N6	2.13	1.50	1.47
2	B	1385	GR9	S7-N6	2.76	1.67	1.63

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1385	GR9	C16-C17-N18	-2.69	118.78	122.38
2	A	1385	GR9	C5-C4-N2	-2.40	108.03	110.79
2	A	1385	GR9	C17-N18-C19	2.11	121.19	118.84
2	A	1385	GR9	C20-N21-C16	2.26	121.81	118.16
2	B	1385	GR9	C6-N6-S7	2.30	121.41	117.06
2	B	1385	GR9	C20-N21-C16	2.41	122.05	118.16
2	B	1385	GR9	O9-S7-N6	2.48	109.03	106.69
2	A	1385	GR9	C13-C16-N21	2.54	119.54	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1385	GR9	C22-C20-N21	2.58	118.29	116.04
2	B	1385	GR9	C4-C5-N6	2.66	111.02	108.94
2	B	1385	GR9	C17-N18-C19	2.93	122.10	118.84
2	A	1385	GR9	C28-N29-C30	3.02	122.12	116.83
2	B	1385	GR9	C28-N29-C30	3.28	122.57	116.83
2	A	1385	GR9	C4-N2-C1	3.38	113.98	109.47
2	A	1385	GR9	C1-C6-N6	3.99	112.06	108.94
2	B	1385	GR9	C4-N2-C1	4.49	115.46	109.47
2	B	1385	GR9	C6-N6-C5	5.96	118.88	112.11
2	A	1385	GR9	C6-N6-C5	8.90	122.21	112.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1385	GR9	1	0
2	B	1385	GR9	1	0

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, 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	351/465 (75%)	-0.20	18 (5%)	29	22	38, 57, 111, 136	0
1	B	351/465 (75%)	-0.08	16 (4%)	33	26	38, 59, 116, 144	0
All	All	702/930 (75%)	-0.14	34 (4%)	31	24	38, 58, 114, 144	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	GLU	5.0
1	A	290	GLU	4.8
1	B	286	PRO	4.7
1	A	123	LYS	4.1
1	B	93	PHE	3.9
1	B	297	LYS	3.6
1	A	289	THR	3.5
1	B	124	ASP	3.3
1	B	289	THR	3.3
1	A	93	PHE	3.3
1	A	297	LYS	3.3
1	A	35	SER	3.1
1	B	121	GLU	3.1
1	B	122	LYS	3.1
1	B	35	SER	3.1
1	A	36	LYS	3.1
1	A	124	ASP	2.9
1	B	36	LYS	2.9
1	A	92	ARG	2.8
1	A	298	ALA	2.8
1	B	295	GLN	2.8
1	A	286	PRO	2.7
1	B	300	PRO	2.7
1	A	278	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	383	ARG	2.5
1	A	122	LYS	2.4
1	A	119	SER	2.4
1	B	123	LYS	2.3
1	A	47	GLY	2.3
1	B	298	ALA	2.2
1	A	37	VAL	2.2
1	B	278	ARG	2.1
1	B	299	HIS	2.1
1	A	131	VAL	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, 95^{th} 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GR9	B	1385	32/32	0.95	0.14	-0.22	45,60,80,83	0
2	GR9	A	1385	32/32	0.96	0.13	-0.57	45,50,70,74	0

6.5 Other polymers (i)

There are no such residues in this entry.