



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:44 PM GMT

PDB ID : 4ACC
Title : GSK3b in complex with inhibitor
Authors : Xue, Y.; Ormo, M.
Deposited on : 2011-12-14
Resolution : 2.21 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

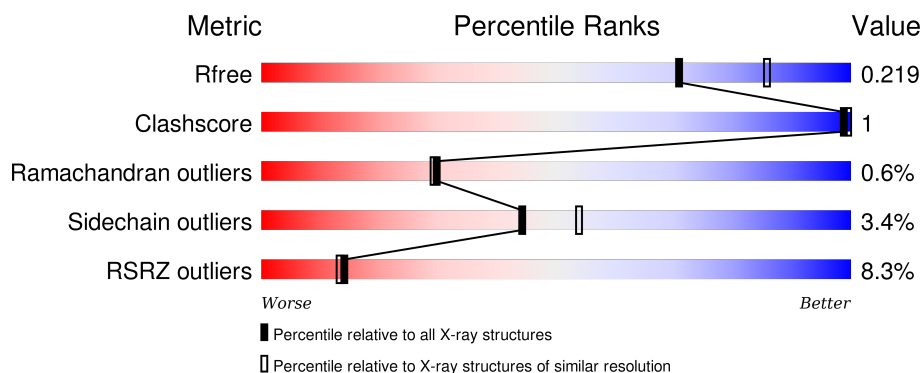
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 $\leq 5\%$. 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	465	<div> <div>5%</div> <div>71%</div> <div>25%</div> </div>
1	B	465	<div> <div>7%</div> <div>71%</div> <div>25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	A	1385	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6196 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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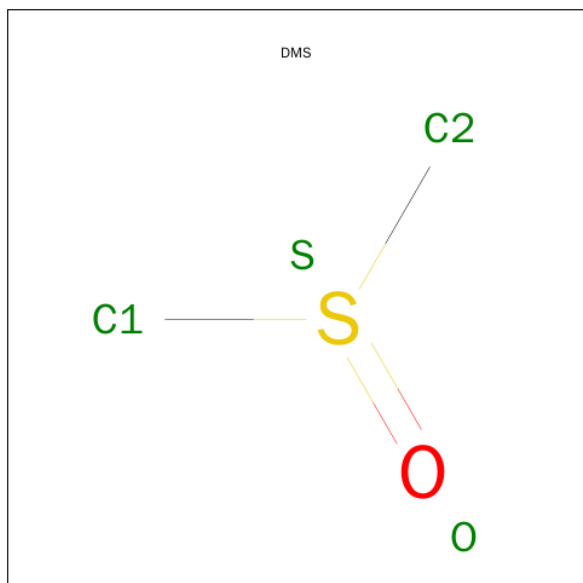
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P49841
A	-18	GLY	-	EXPRESSION TAG	UNP P49841
A	-17	SER	-	EXPRESSION TAG	UNP P49841
A	-16	SER	-	EXPRESSION TAG	UNP P49841
A	-15	HIS	-	EXPRESSION TAG	UNP P49841
A	-14	HIS	-	EXPRESSION TAG	UNP P49841
A	-13	HIS	-	EXPRESSION TAG	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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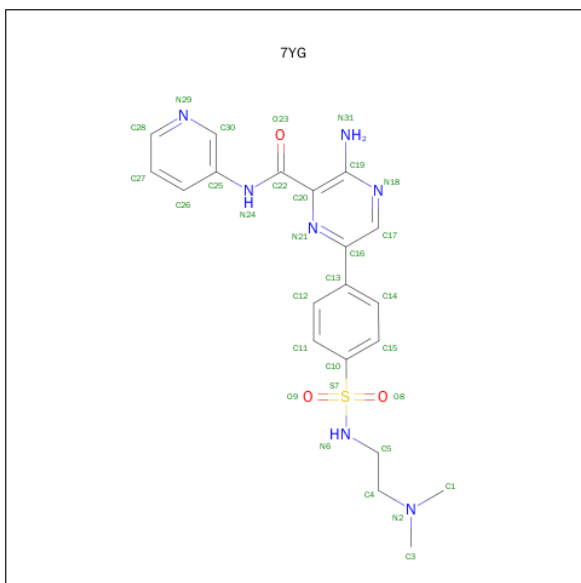
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLN	-	EXPRESSION TAG	UNP P49841
B	-21	GLY	-	EXPRESSION TAG	UNP P49841
B	-20	ALA	-	EXPRESSION TAG	UNP P49841
B	-19	MET	-	EXPRESSION TAG	UNP P49841
B	-18	GLY	-	EXPRESSION TAG	UNP P49841
B	-17	SER	-	EXPRESSION TAG	UNP P49841
B	-16	SER	-	EXPRESSION TAG	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 DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 3-AMINO-6-(4-{[2-(DIMETHYLAMINO)ETHYL]SULFAMOYL}PHENYL)-N-PYRIDIN-3-YLPIRAZINE-2-CARBOXAMIDE (three-letter code: 7YG) (formula: $C_{20}H_{23}N_7O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	20	7	3	1		
3	B	1	Total	C	N	O	S	0	0
			31	20	7	3	1		

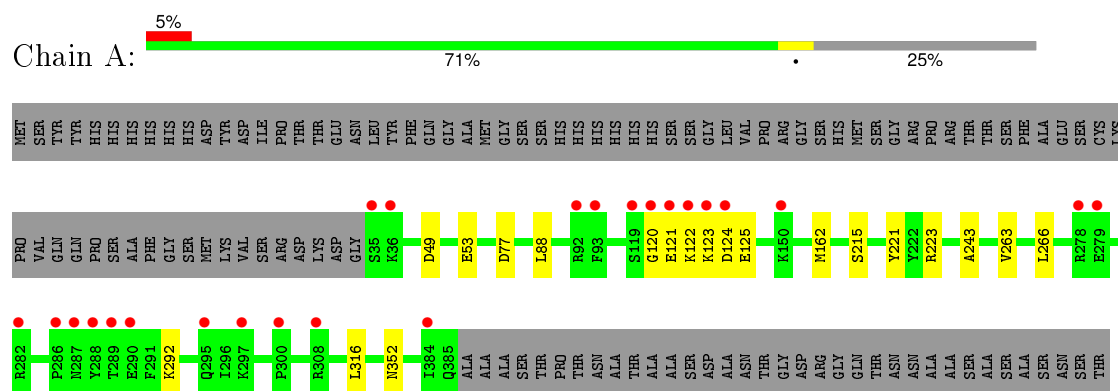
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	245	Total	O	0	0
			245	245		

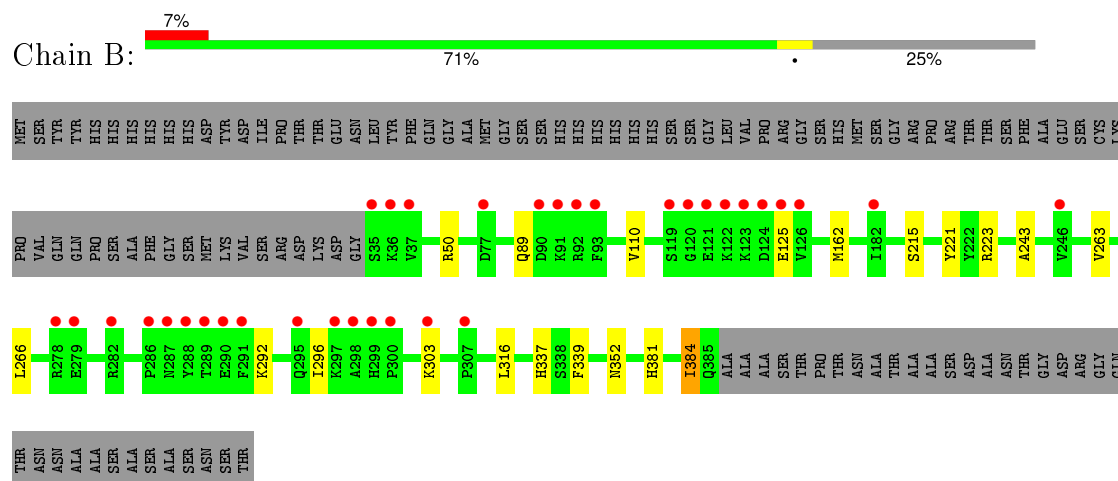
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: GLYCOGEN SYNTHASE KINASE-3 BETA



• Molecule 1: GLYCOGEN SYNTHASE KINASE-3 BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.08Å 85.81Å 177.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.20 – 2.21 42.02 – 2.21	Depositor EDS
% Data completeness (in resolution range)	90.2 (44.20-2.21) 90.2 (42.02-2.21)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.189 , 0.219 0.188 , 0.219	Depositor DCC
R_{free} test set	2946 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.8	EDS
Estimated twinning fraction	0.026 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58051 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6196	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 7YG, DMS

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	0.51	0/2876	0.66	0/3913
1	B	0.49	0/2876	0.68	0/3913
All	All	0.50	0/5752	0.67	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	5	0
1	B	2805	0	2833	4	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0
3	A	31	0	23	0	0
3	B	31	0	23	0	0
4	A	267	0	0	0	0
4	B	245	0	0	0	0
All	All	6196	0	5730	9	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 1.

All (9) 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:215:SER:O	1:B:223:ARG:NH2	2.37	0.58
1:A:215:SER:O	1:A:223:ARG:NH2	2.38	0.57
1:A:88:LEU:HD11	1:A:125:GLU:HB3	1.89	0.55
1:B:381:HIS:HA	1:B:384:ILE:HD12	1.92	0.51
1:A:122:LYS:HB2	1:A:125:GLU:HB2	1.95	0.48
1:B:337:HIS:HD2	1:B:339:PHE:H	1.60	0.48
1:A:121:GLU:C	1:A:122:LYS:HG2	2.40	0.41
1:A:162:MET:HE1	1:A:243:ALA:O	2.20	0.41
1:B:162:MET:HE1	1:B:243:ALA:O	2.21	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%)	331 (95%)	16 (5%)	2 (1%)	30	29
1	B	349/465 (75%)	338 (97%)	9 (3%)	2 (1%)	30	29
All	All	698/930 (75%)	669 (96%)	25 (4%)	4 (1%)	30	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	ILE
1	A	221	TYR
1	B	221	TYR
1	A	120	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	312/404 (77%)	302 (97%)	10 (3%)	46	57
1	B	312/404 (77%)	301 (96%)	11 (4%)	43	52
All	All	624/808 (77%)	603 (97%)	21 (3%)	44	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	53	GLU
1	A	77	ASP
1	A	123	LYS
1	A	124	ASP
1	A	263	VAL
1	A	266	LEU
1	A	292	LYS
1	A	316	LEU
1	A	352	ASN
1	B	50	ARG
1	B	89	GLN
1	B	110	VAL
1	B	125	GLU
1	B	263	VAL
1	B	266	LEU
1	B	292	LYS
1	B	296	ILE
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	145	HIS

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Mol	Chain	Res	Type
1	A	295	GLN
1	A	352	ASN
1	A	381	HIS
1	B	52	GLN
1	B	337	HIS
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 ⓘ

5 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	DMS	A	1385	-	3,3,3	0.88	0	3,3,3	0.79	0
2	DMS	A	1386	-	3,3,3	0.80	0	3,3,3	1.41	0
3	7YG	A	1387	-	32,33,33	1.67	4 (12%)	44,46,46	1.47	7 (15%)
2	DMS	B	1385	-	3,3,3	0.75	0	3,3,3	1.22	0
3	7YG	B	1386	-	32,33,33	1.70	4 (12%)	44,46,46	1.36	4 (9%)

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	DMS	A	1385	-	-	0/0/0/0	0/0/0/0
2	DMS	A	1386	-	-	0/0/0/0	0/0/0/0
3	7YG	A	1387	-	-	0/25/25/25	0/3/3/3
2	DMS	B	1385	-	-	0/0/0/0	0/0/0/0
3	7YG	B	1386	-	-	0/25/25/25	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1387	7YG	O8-S7	2.02	1.45	1.43
3	B	1386	7YG	O8-S7	2.14	1.45	1.43
3	A	1387	7YG	C19-N31	2.28	1.39	1.34
3	B	1386	7YG	C10-S7	2.56	1.80	1.76
3	B	1386	7YG	C19-N31	2.61	1.40	1.34
3	A	1387	7YG	C10-S7	3.30	1.81	1.76
3	A	1387	7YG	S7-N6	7.43	1.71	1.61
3	B	1386	7YG	S7-N6	7.86	1.71	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1386	7YG	C10-S7-N6	-6.41	99.40	107.49
3	A	1387	7YG	C10-S7-N6	-5.21	100.91	107.49
3	A	1387	7YG	C17-N18-C19	-2.54	115.94	118.88
3	B	1386	7YG	O9-S7-C10	-2.14	105.25	107.96
3	A	1387	7YG	O9-S7-C10	-2.01	105.41	107.96
3	B	1386	7YG	C17-N18-C19	-2.00	116.56	118.88
3	A	1387	7YG	C1-N2-C4	2.08	119.06	110.79
3	A	1387	7YG	O9-S7-O8	2.08	122.30	119.54
3	B	1386	7YG	C19-C20-N21	2.56	122.59	120.46
3	A	1387	7YG	C19-C20-N21	2.87	122.84	120.46
3	A	1387	7YG	O9-S7-N6	4.08	113.59	107.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	351/465 (75%)	0.11	24 (6%) 20 19	29, 44, 98, 129	0
1	B	351/465 (75%)	0.27	34 (9%) 10 9	29, 48, 103, 119	0
All	All	702/930 (75%)	0.19	58 (8%) 14 13	29, 46, 102, 129	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	PRO	6.3
1	A	124	ASP	5.8
1	A	289	THR	5.8
1	A	290	GLU	5.7
1	B	289	THR	5.6
1	A	120	GLY	5.4
1	B	93	PHE	5.1
1	A	35	SER	5.0
1	B	124	ASP	4.9
1	A	286	PRO	4.8
1	B	297	LYS	4.7
1	B	121	GLU	4.7
1	A	278	ARG	4.7
1	A	384	ILE	4.6
1	B	290	GLU	4.5
1	B	120	GLY	4.4
1	B	288	TYR	4.4
1	B	122	LYS	4.4
1	B	300	PRO	4.4
1	B	35	SER	4.2
1	A	92	ARG	4.1
1	B	123	LYS	4.0
1	A	123	LYS	3.7
1	B	278	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	90	ASP	3.6
1	A	93	PHE	3.6
1	B	295	GLN	3.6
1	A	288	TYR	3.6
1	A	282	ARG	3.3
1	B	282	ARG	3.2
1	A	297	LYS	3.2
1	A	287	ASN	3.2
1	B	119	SER	3.1
1	B	92	ARG	3.1
1	A	36	LYS	3.0
1	B	298	ALA	3.0
1	A	121	GLU	2.9
1	B	303	LYS	2.8
1	B	126	VAL	2.8
1	B	299	HIS	2.7
1	B	125	GLU	2.7
1	A	279	GLU	2.7
1	A	295	GLN	2.7
1	B	77	ASP	2.6
1	B	91	LYS	2.5
1	B	36	LYS	2.4
1	B	37	VAL	2.3
1	B	279	GLU	2.3
1	A	300	PRO	2.3
1	A	308	ARG	2.3
1	B	307	PRO	2.3
1	B	291	PHE	2.2
1	A	122	LYS	2.2
1	A	119	SER	2.2
1	B	287	ASN	2.1
1	B	246	VAL	2.1
1	B	182	ILE	2.1
1	A	150	LYS	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 [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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DMS	A	1385	4/4	0.92	0.16	2.97	74,76,87,90	0
3	7YG	A	1387	31/31	0.94	0.12	0.19	32,40,71,71	0
3	7YG	B	1386	31/31	0.94	0.13	-0.34	36,46,77,78	0
2	DMS	A	1386	4/4	0.91	0.09	-0.45	85,85,90,98	0
2	DMS	B	1385	4/4	0.90	0.10	-0.60	83,86,92,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.