



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2018 – 02:03 PM EDT

PDB ID : 6B0Y
Title : Crystal Structure of small molecule ARS-917 covalently bound to K-Ras G12C
Authors : Hansen, R.; Peters, U.; Babbar, A.; Chen, Y.; Feng, J.; Janes, M.R.; Li, L.-S.; Ren, P.; Liu, Y.; Zarrinkar, P.P.
Deposited on : 2017-09-15
Resolution : 1.43 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

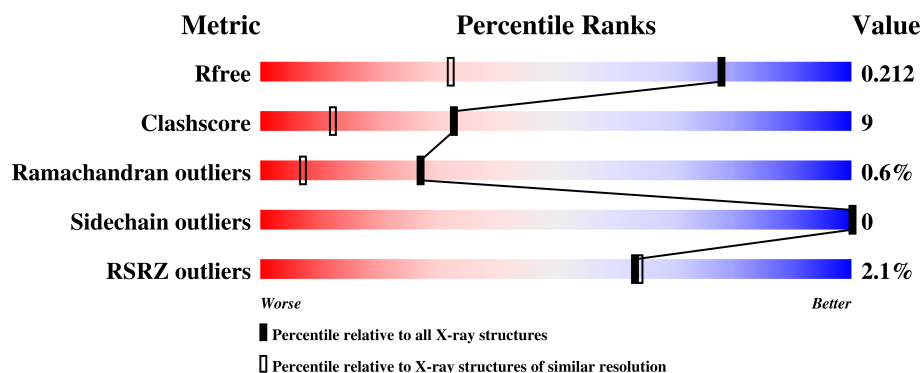
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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}	111664	1592 (1.46-1.42)
Clashscore	122126	1643 (1.46-1.42)
Ramachandran outliers	120053	1618 (1.46-1.42)
Sidechain outliers	120020	1618 (1.46-1.42)
RSRZ outliers	108989	1566 (1.46-1.42)

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	170	 2% 79% 19% ..
1	B	170	 2% 84% 14% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3230 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 GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	7	0
			1367	864	234	265	4			
1	B	167	Total	C	N	O	S	0	9	0
			1379	867	237	270	5			

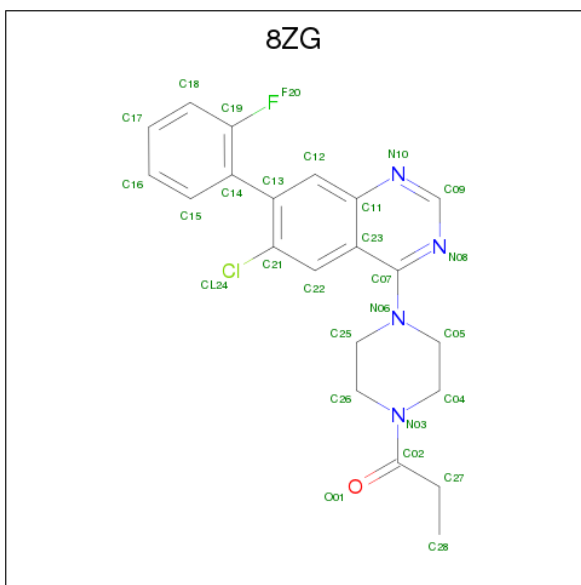
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	CYS	GLY	engineered mutation	UNP P01116
A	51	SER	CYS	engineered mutation	UNP P01116
A	80	LEU	CYS	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	12	CYS	GLY	engineered mutation	UNP P01116
B	51	SER	CYS	engineered mutation	UNP P01116
B	80	LEU	CYS	engineered mutation	UNP P01116
B	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

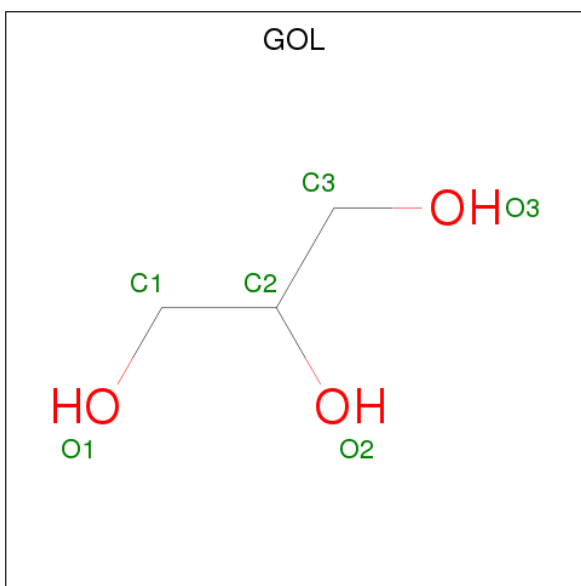
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 1-{4-[6-chloro-7-(2-fluorophenyl)quinazolin-4-yl]piperazin-1-yl}propan-1-one (three-letter code: 8ZG) (formula: C₂₁H₂₀ClFN₄O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 28	C 21	Cl 1	F 1	N 4	O 1	0	0
3	B	1	Total 28	C 21	Cl 1	F 1	N 4	O 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



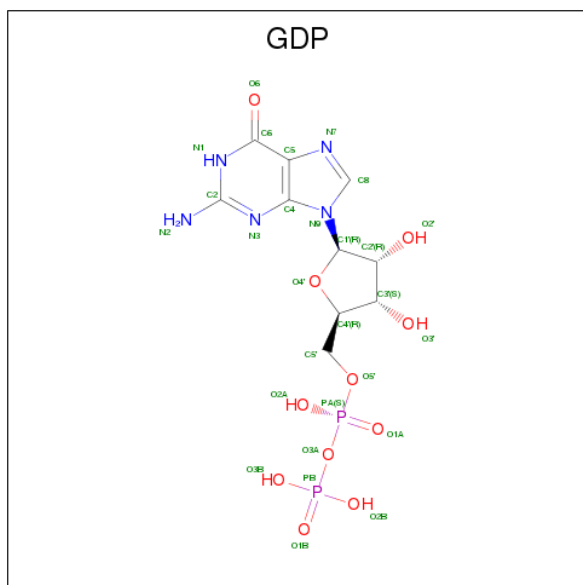
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

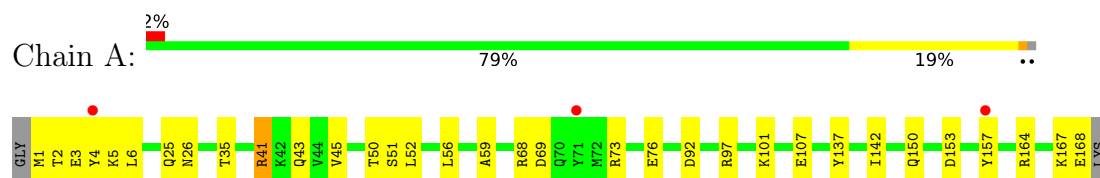
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	164	Total	O	0	5
			169	169		
6	B	165	Total	O	0	16
			181	181		

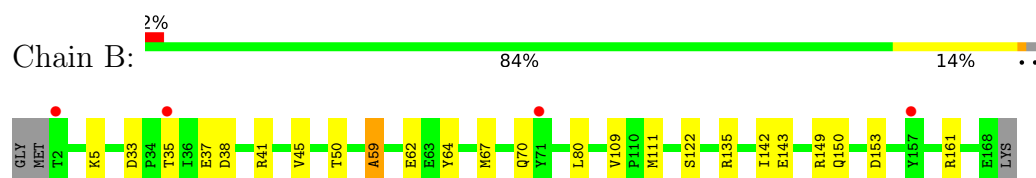
3 Residue-property plots [i](#)

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: GTPase KRas



- Molecule 1: GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	33.43Å 39.66Å 61.85Å 77.45° 81.71° 77.12°	Depositor
Resolution (Å)	37.94 – 1.43 37.94 – 1.43	Depositor EDS
% Data completeness (in resolution range)	92.7 (37.94-1.43) 92.7 (37.94-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.174 , 0.207 0.183 , 0.212	Depositor DCC
R_{free} test set	2501 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3230	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.71% 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, 0.333 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: GDP, GOL, CA, 8ZG

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	1.05	0/1401	1.21	14/1892 (0.7%)
1	B	1.10	2/1415 (0.1%)	1.17	8/1910 (0.4%)
All	All	1.08	2/2816 (0.1%)	1.19	22/3802 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143[A]	GLU	CG-CD	5.88	1.60	1.51
1	B	143[B]	GLU	CG-CD	5.88	1.60	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	B	135	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	157	TYR	CB-CG-CD2	-8.39	115.97	121.00
1	B	33	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	68	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	153	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	73	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	64	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	B	135	ARG	CG-CD-NE	6.71	125.88	111.80
1	A	69	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	153	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	137	TYR	CB-CG-CD1	6.08	124.65	121.00
1	A	41	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	153	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	92	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	161	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	6	LEU	CB-CG-CD2	5.91	121.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	137	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	A	97	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	73	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	38	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1367	0	1345	27	0
1	B	1379	0	1364	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	28	0	0	1	0
3	B	28	0	0	0	0
4	A	6	0	8	1	0
4	B	12	0	16	1	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
6	A	169	0	0	9	0
6	B	181	0	0	12	0
All	All	3230	0	2757	53	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 9.

All (53) 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:35[B]:THR:HB	6:B:371[B]:HOH:O	1.46	1.13
1:B:35[A]:THR:O	6:B:301[A]:HOH:O	1.66	1.12
1:B:5[B]:LYS:NZ	1:B:5[B]:LYS:HB2	1.64	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122[A]:SER:OG	6:B:302[A]:HOH:O	1.85	0.94
1:B:5[B]:LYS:HZ2	1:B:5[B]:LYS:HB2	1.22	0.91
1:A:26:ASN:HB3	6:A:313:HOH:O	1.74	0.87
1:B:150:GLN:CB	6:B:437:HOH:O	2.23	0.86
1:B:41:ARG:HD2	6:B:430:HOH:O	1.79	0.81
1:A:5[A]:LYS:NZ	1:A:56:LEU:HB2	2.00	0.76
1:B:5[B]:LYS:NZ	1:B:5[B]:LYS:CB	2.44	0.76
1:B:45:VAL:HG22	1:B:50:THR:HG22	1.69	0.75
1:B:80:LEU:HD11	1:B:111[B]:MET:CE	2.18	0.73
1:A:168:GLU:CB	6:A:441:HOH:O	2.39	0.70
1:B:5[B]:LYS:HZ3	1:B:5[B]:LYS:HB2	1.56	0.70
1:A:2:THR:HG23	1:A:4[A]:TYR:CE2	2.27	0.70
1:B:35[B]:THR:CB	6:B:371[B]:HOH:O	2.21	0.68
1:A:51:SER:OG	1:A:164:ARG:NH2	2.32	0.62
1:A:45:VAL:HG22	1:A:50:THR:HG22	1.83	0.61
1:A:101:LYS:HD3	1:A:107:GLU:HG2	1.83	0.61
1:A:41:ARG:NH2	1:A:52:LEU:HD21	2.16	0.60
1:B:80:LEU:HD11	1:B:111[B]:MET:HE3	1.83	0.60
1:B:80:LEU:HD11	1:B:111[B]:MET:HE1	1.82	0.60
1:A:150:GLN:NE2	6:A:304:HOH:O	2.32	0.60
1:A:26:ASN:CB	6:A:313:HOH:O	2.42	0.60
1:A:25:GLN:OE1	4:A:204:GOL:H2	2.02	0.59
1:A:1:MET:CB	6:A:429:HOH:O	2.50	0.59
1:A:5[A]:LYS:HZ1	1:A:56:LEU:HB2	1.67	0.58
1:B:62:GLU:HG2	4:B:201:GOL:O1	2.05	0.56
1:A:76[B]:GLU:OE2	1:A:167:LYS:HE2	2.06	0.55
1:B:142:ILE:CD1	6:B:410[A]:HOH:O	2.56	0.53
1:A:43:GLN:HG2	1:A:52:LEU:HD13	1.92	0.52
1:B:142:ILE:HD13	6:B:410[A]:HOH:O	2.09	0.52
1:B:37:GLU:CD	6:B:315[A]:HOH:O	2.48	0.52
1:A:3:GLU:O	1:A:4[B]:TYR:CD1	2.63	0.52
1:A:5[A]:LYS:HZ3	1:A:56:LEU:HB2	1.76	0.49
1:B:41:ARG:NH1	6:B:305:HOH:O	2.44	0.49
3:A:203:8ZG:C25	3:A:203:8ZG:C22	2.91	0.48
1:A:35:THR:CB	6:A:430:HOH:O	2.60	0.48
1:A:35:THR:HA	6:A:430:HOH:O	2.13	0.48
1:A:2:THR:HG23	1:A:4[A]:TYR:HE2	1.76	0.48
1:A:35:THR:CA	6:A:430:HOH:O	2.62	0.47
1:B:41:ARG:HG3	6:B:361:HOH:O	2.15	0.46
1:A:2:THR:HG21	1:A:4[A]:TYR:OH	2.15	0.45
1:A:76[B]:GLU:OE2	1:A:167:LYS:CE	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5[B]:LYS:HE3	1:A:5[B]:LYS:HB2	1.64	0.45
1:B:37:GLU:HG2	1:B:59:ALA:N	2.32	0.43
1:A:142[B]:ILE:HD11	6:A:456:HOH:O	2.19	0.43
1:B:67:MET:O	1:B:70:GLN:HG2	2.19	0.42
1:B:109:VAL:O	1:B:111[B]:MET:HG3	2.21	0.41
1:B:149[B]:ARG:HG3	6:B:438:HOH:O	2.20	0.41
1:A:4[B]:TYR:HA	1:A:76[B]:GLU:OE1	2.21	0.41
1:A:76[B]:GLU:OE2	1:A:167:LYS:NZ	2.53	0.41
1:B:5[B]:LYS:HZ3	1:B:5[B]:LYS:CB	2.27	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	173/170 (102%)	171 (99%)	1 (1%)	1 (1%)	27	7
1	B	174/170 (102%)	171 (98%)	2 (1%)	1 (1%)	27	7
All	All	347/340 (102%)	342 (99%)	3 (1%)	2 (1%)	27	7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	B	59	ALA

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	148/150 (99%)	148 (100%)	0	100	100
1	B	153/150 (102%)	153 (100%)	0	100	100
All	All	301/300 (100%)	301 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN

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 ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	8ZG	A	203	1	30,31,31	1.43	5 (16%)	42,44,44	2.41	15 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	204	-	5,5,5	0.68	0	5,5,5	0.89	0
5	GDP	A	205	2	25,30,30	1.24	1 (4%)	27,47,47	1.73	5 (18%)
4	GOL	B	201	-	5,5,5	0.56	0	5,5,5	0.39	0
3	8ZG	B	204	1	30,31,31	1.16	2 (6%)	42,44,44	2.10	14 (33%)
4	GOL	B	205	-	5,5,5	0.65	0	5,5,5	1.14	0
5	GDP	B	206	2	25,30,30	1.17	2 (8%)	27,47,47	1.87	6 (22%)

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	8ZG	A	203	1	-	0/14/24/24	0/4/4/4
4	GOL	A	204	-	-	0/4/4/4	0/0/0/0
5	GDP	A	205	2	-	0/12/32/32	0/3/3/3
4	GOL	B	201	-	-	0/4/4/4	0/0/0/0
3	8ZG	B	204	1	-	0/14/24/24	0/4/4/4
4	GOL	B	205	-	-	0/4/4/4	0/0/0/0
5	GDP	B	206	2	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	204	8ZG	C23-C11	-3.03	1.37	1.42
3	A	203	8ZG	C15-C14	-2.94	1.35	1.39
3	A	203	8ZG	C22-C21	-2.58	1.32	1.36
3	A	203	8ZG	C23-C11	-2.44	1.38	1.42
3	B	204	8ZG	C09-N10	2.03	1.35	1.32
5	B	206	GDP	PB-O3A	2.10	1.63	1.60
5	A	205	GDP	C2-N2	2.41	1.38	1.33
3	A	203	8ZG	C21-CL24	2.78	1.80	1.73
3	A	203	8ZG	C09-N10	2.81	1.36	1.32
5	B	206	GDP	C6-C5	3.38	1.47	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	8ZG	N10-C09-N08	-8.43	121.65	128.86
5	A	205	GDP	C5-C6-N1	-5.88	115.10	123.47
5	B	206	GDP	C5-C6-N1	-5.40	115.79	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	204	8ZG	N10-C09-N08	-4.78	124.78	128.86
3	A	203	8ZG	C22-C21-CL24	-3.51	115.80	119.15
5	B	206	GDP	C6-C5-C4	-3.45	117.46	120.85
5	B	206	GDP	N2-C2-N3	-3.28	111.75	117.75
3	B	204	8ZG	C23-C11-N10	-3.23	119.44	122.88
3	A	203	8ZG	C04-C05-N06	-3.07	104.64	110.67
3	B	204	8ZG	C22-C23-C07	-2.83	122.53	124.90
5	A	205	GDP	C4-C5-N7	-2.71	106.79	109.41
3	A	203	8ZG	C18-C19-C14	-2.66	119.92	123.26
3	A	203	8ZG	O01-C02-N03	-2.52	116.87	122.05
3	B	204	8ZG	C13-C21-CL24	-2.41	117.26	120.87
3	A	203	8ZG	C23-C11-N10	-2.21	120.52	122.88
5	B	206	GDP	C4-C5-N7	-2.17	107.31	109.41
5	A	205	GDP	O3'-C3'-C2'	-2.14	104.98	111.83
3	A	203	8ZG	C22-C23-C11	-2.10	116.23	118.93
3	B	204	8ZG	C26-N03-C02	-2.06	116.05	122.82
3	A	203	8ZG	C23-C07-N06	2.26	125.62	121.04
3	B	204	8ZG	C27-C02-N03	2.29	121.82	117.94
3	B	204	8ZG	C07-C23-C11	2.43	119.97	117.34
3	A	203	8ZG	C22-C23-C07	2.53	127.03	124.90
5	A	205	GDP	O2'-C2'-C3'	2.54	119.97	111.83
3	B	204	8ZG	C04-C05-N06	2.58	115.72	110.67
3	B	204	8ZG	C09-N08-C07	2.61	118.16	111.81
5	B	206	GDP	N2-C2-N1	2.64	121.39	117.25
3	B	204	8ZG	C23-C07-N06	2.97	127.06	121.04
3	A	203	8ZG	C25-N06-C05	3.26	118.55	111.54
3	A	203	8ZG	C09-N08-C07	3.55	120.43	111.81
3	B	204	8ZG	C09-N10-C11	3.69	118.94	115.24
3	B	204	8ZG	C14-C13-C21	3.78	126.93	123.05
5	A	205	GDP	C6-N1-C2	3.82	121.56	116.06
3	A	203	8ZG	C27-C02-N03	3.85	124.47	117.94
3	A	203	8ZG	C22-C21-C13	3.91	124.65	121.89
3	A	203	8ZG	C15-C14-C19	4.05	120.46	115.98
5	B	206	GDP	C6-N1-C2	4.09	121.94	116.06
3	B	204	8ZG	C26-N03-C04	4.54	121.19	112.61
3	B	204	8ZG	C26-C25-N06	4.77	120.02	110.67
3	A	203	8ZG	C09-N10-C11	4.78	120.04	115.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	203	8ZG	1	0
4	A	204	GOL	1	0
4	B	201	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	168/170 (98%)	0.40	3 (1%) 68 68	5, 13, 25, 35	0
1	B	167/170 (98%)	0.36	4 (2%) 59 59	5, 11, 26, 32	0
All	All	335/340 (98%)	0.38	7 (2%) 63 64	5, 12, 26, 35	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	TYR	3.0
1	A	71	TYR	3.0
1	B	157	TYR	2.3
1	B	35[A]	THR	2.1
1	A	4[A]	TYR	2.1
1	B	2	THR	2.1
1	A	157	TYR	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. 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	B-factors(\AA^2)	Q<0.9
4	GOL	A	204	6/6	0.89	0.13	23,24,25,25	0
4	GOL	B	201	6/6	0.89	0.12	20,23,23,23	0
3	8ZG	B	204	28/28	0.95	0.10	10,12,14,15	0
4	GOL	B	205	6/6	0.95	0.11	15,17,18,19	0
3	8ZG	A	203	28/28	0.96	0.10	9,11,13,13	0
5	GDP	A	205	28/28	0.98	0.08	7,9,12,14	0
5	GDP	B	206	28/28	0.98	0.08	6,8,10,12	0
2	CA	A	202	1/1	0.99	0.09	11,11,11,11	0
2	CA	A	201	1/1	1.00	0.07	7,7,7,7	0
2	CA	B	203	1/1	1.00	0.08	8,8,8,8	0
2	CA	B	202	1/1	1.00	0.07	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.