



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:12 PM GMT

PDB ID : 4HDQ  
Title : Crystal Structure of the Ternary Complex of KRIT1 bound to both the Rap1 GTPase and the Heart of Glass (HEG1) cytoplasmic tail  
Authors : Gingras, A.R.  
Deposited on : 2012-10-02  
Resolution : 1.95 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](mailto: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.

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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

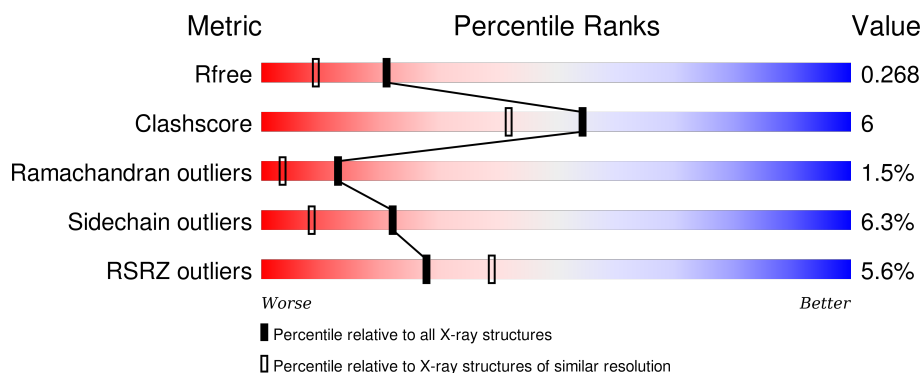
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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  $\geq 3$ , 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	322	<div> <div>7%</div> <div>77%</div> <div>14%</div> <div>5%</div> <div>••</div> </div>
2	B	167	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>
3	C	26	<div> <div>19%</div> <div>81%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4015 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 Krev interaction trapped protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	1	0
			2542	1641	433	454	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	GLY	-	EXPRESSION TAG	UNP O00522
A	416	ALA	-	EXPRESSION TAG	UNP O00522

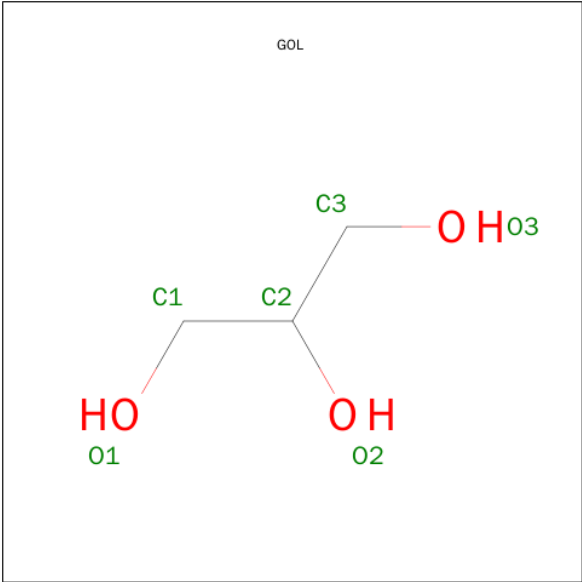
- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1300	813	224	255	8			

- Molecule 3 is a protein called Protein HEG homolog 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			41	28	5	8			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

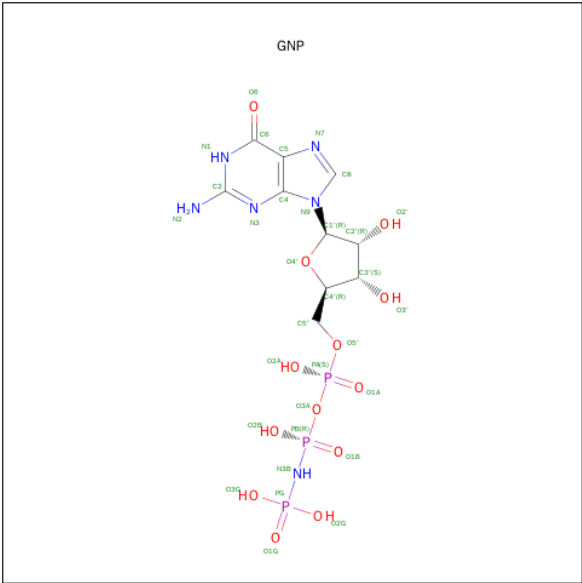


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	67	Total	O	0	0
			67	67		
7	B	25	Total	O	0	0
			25	25		
7	C	1	Total	O	0	0
			1	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.31Å 77.41Å 58.57Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	29.15 – 1.95 29.15 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.15-1.95) 99.2 (29.15-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.200 , 0.263 0.205 , 0.268	Depositor DCC
$R_{free}$ test set	1848 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.0	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36961 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GNP, MG

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	0.97	1/2603 (0.0%)	0.98	9/3519 (0.3%)
2	B	0.96	1/1314 (0.1%)	0.94	0/1768
3	C	1.22	0/42	1.16	0/56
All	All	0.97	2/3959 (0.1%)	0.97	9/5343 (0.2%)

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	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138	TRP	CD2-CE2	5.71	1.48	1.41
1	A	487	TRP	CD2-CE2	5.54	1.48	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	511	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	510	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	623	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	679	ILE	CB-CA-C	-5.76	100.09	111.60
1	A	548	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	623	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	670	LEU	CB-CG-CD1	-5.23	102.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	432	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	452	ARG	Peptide
1	A	648	ALA	Peptide
1	A	651	SER	Peptide

## 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	2542	0	2584	38	0
2	B	1300	0	1291	15	0
3	C	41	0	25	0	0
4	A	6	0	8	0	0
5	B	1	0	0	0	0
6	B	32	0	13	0	0
7	A	67	0	0	1	0
7	B	25	0	0	2	0
7	C	1	0	0	0	0
All	All	4015	0	3921	50	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 6.

All (50) 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:A:519:GLU:O	1:A:522:ILE:HG23	1.52	1.09
1:A:452:ARG:HH21	2:B:29:VAL:HG11	1.36	0.88
1:A:460:TYR:OH	1:A:522:ILE:HB	1.77	0.85
1:A:519:GLU:O	1:A:522:ILE:CG2	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:SER:O	1:A:653:HIS:CB	2.41	0.69
1:A:606:LYS:O	1:A:610:THR:HG23	1.95	0.67
1:A:432:ARG:NH1	7:A:962:HOH:O	2.28	0.67
1:A:660:VAL:HG22	1:A:669:LEU:CD2	2.30	0.61
1:A:459:GLN:NE2	1:A:460:TYR:CZ	2.70	0.59
1:A:652:ASN:N	1:A:653:HIS:HA	2.17	0.58
1:A:567:GLU:H	1:A:571:HIS:HD2	1.50	0.57
1:A:660:VAL:HG22	1:A:669:LEU:HD21	1.86	0.56
1:A:590:LEU:O	1:A:595:PRO:HD3	2.06	0.56
2:B:68:ARG:HD2	7:B:308:HOH:O	2.07	0.55
2:B:133:ASN:HD22	2:B:136:ARG:HH11	1.54	0.55
1:A:452:ARG:HD2	2:B:33:ASP:OD2	2.07	0.53
2:B:68:ARG:NH1	7:B:323:HOH:O	2.42	0.53
1:A:637:ALA:HA	1:A:663:ASN:HB3	1.92	0.52
1:A:703:GLU:O	1:A:704:ASN:HB2	2.09	0.51
1:A:557:LEU:HD21	1:A:624:MET:HE2	1.92	0.51
1:A:646:THR:O	1:A:653:HIS:CB	2.59	0.50
1:A:570:LYS:NZ	2:B:45:GLU:OE1	2.44	0.49
1:A:487:TRP:N	1:A:488:PRO:CD	2.75	0.49
1:A:594:ALA:HB3	1:A:595:PRO:HD3	1.95	0.49
1:A:460:TYR:CZ	1:A:522:ILE:HB	2.48	0.48
1:A:582:LYS:HG2	1:A:582:LYS:O	2.13	0.48
1:A:563:TYR:OH	1:A:580:ASN:ND2	2.47	0.47
1:A:440:ASN:HD22	1:A:440:ASN:C	2.18	0.47
1:A:702:MET:O	1:A:703:GLU:CB	2.62	0.47
1:A:522:ILE:HD12	1:A:524:ASP:H	1.80	0.46
1:A:649:SER:O	1:A:650:PRO:O	2.33	0.46
2:B:108:ASP:OD1	2:B:167:ARG:NH1	2.49	0.46
1:A:464:TRP:CD1	1:A:509:ARG:HB2	2.51	0.45
2:B:83:SER:OG	2:B:85:THR:HB	2.16	0.45
1:A:646:THR:OG1	1:A:653:HIS:CB	2.65	0.45
1:A:660:VAL:HG13	1:A:667:LEU:HD11	1.99	0.44
2:B:46:VAL:HG22	2:B:159:TYR:CD1	2.53	0.44
1:A:452:ARG:O	1:A:452:ARG:CG	2.65	0.43
2:B:99:GLN:HG3	2:B:102:ARG:NH2	2.34	0.43
1:A:529:LEU:HD12	1:A:529:LEU:C	2.38	0.43
1:A:658:VAL:HG11	1:A:669:LEU:HD13	2.01	0.43
1:A:567:GLU:N	1:A:571:HIS:HD2	2.16	0.42
1:A:578:GLU:O	1:A:579:GLU:C	2.58	0.42
1:A:460:TYR:CE1	1:A:522:ILE:HG21	2.54	0.42
2:B:68:ARG:HB3	2:B:99:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ASP:OD1	2:B:163:ARG:NE	2.43	0.41
2:B:2:ARG:HD3	2:B:4:TYR:OH	2.20	0.41
2:B:56:LEU:HD21	2:B:71:TYR:CD1	2.56	0.41
1:A:459:GLN:NE2	1:A:460:TYR:CE2	2.83	0.40
2:B:116:ASN:ND2	2:B:117:LYS:H	2.20	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	310/322 (96%)	290 (94%)	13 (4%)	7 (2%)	8	1
2	B	160/167 (96%)	155 (97%)	5 (3%)	0	100	100
3	C	3/26 (12%)	3 (100%)	0	0	100	100
All	All	473/515 (92%)	448 (95%)	18 (4%)	7 (2%)	13	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	SER
1	A	650	PRO
1	A	703	GLU
1	A	704	ASN
1	A	651	SER
1	A	652	ASN
1	A	705	LYS

### 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	282/293 (96%)	260 (92%)	22 (8%)	16	4
2	B	143/147 (97%)	138 (96%)	5 (4%)	43	29
3	C	3/25 (12%)	3 (100%)	0	100	100
All	All	428/465 (92%)	401 (94%)	27 (6%)	22	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	TYR
1	A	440	ASN
1	A	456	GLU
1	A	458	GLN
1	A	500	GLN
1	A	501	ARG
1	A	522	ILE
1	A	578	GLU
1	A	590	LEU
1	A	595	PRO
1	A	599	ASN
1	A	649	SER
1	A	664	ILE
1	A	669	LEU
1	A	679	ILE
1	A	689	GLN
1	A	693	THR
1	A	694	ASP
1	A	702	MET
1	A	704	ASN
1	A	706	MET
1	A	707	SER
2	B	1	MET
2	B	68	ARG
2	B	85	THR
2	B	87	GLN

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Mol	Chain	Res	Type
2	B	129	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	A	459	GLN
1	A	560	GLN
1	A	565	ASN
1	A	571	HIS
1	A	580	ASN
1	A	627	GLN
1	A	726	ASN
2	B	99	GLN
2	B	116	ASN
2	B	132	GLN
2	B	133	ASN
2	B	137	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 3 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
4	GOL	A	801	-	5,5,5	0.74	0	5,5,5	1.24	1 (20%)
6	GNP	B	201	5	28,34,34	3.48	9 (32%)	33,54,54	2.83	13 (39%)

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
4	GOL	A	801	-	-	0/4/4/4	0/0/0/0
6	GNP	B	201	5	-	0/12/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	GNP	PB-O2B	-2.60	1.49	1.56
6	B	201	GNP	C4-N3	-2.35	1.32	1.35
6	B	201	GNP	PG-O3G	2.27	1.63	1.56
6	B	201	GNP	C6-C5	2.70	1.46	1.41
6	B	201	GNP	C5-C4	3.35	1.48	1.40
6	B	201	GNP	PG-N3B	3.78	1.73	1.63
6	B	201	GNP	PB-N3B	4.42	1.75	1.63
6	B	201	GNP	PG-O1G	11.17	1.59	1.46
6	B	201	GNP	PB-O1B	11.60	1.59	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	201	GNP	O1B-PB-N3B	-7.78	99.97	111.90
6	B	201	GNP	O3G-PG-O1G	-5.12	99.87	113.49
6	B	201	GNP	C5-C6-N1	-4.92	116.87	123.59
6	B	201	GNP	C6-C5-C4	-4.90	115.05	120.90
6	B	201	GNP	C2'-C1'-N9	-3.91	108.31	114.29
6	B	201	GNP	PA-O3A-PB	-2.62	123.88	132.67
6	B	201	GNP	N3-C2-N1	-2.48	123.67	127.44
6	B	201	GNP	O5'-PA-O1A	-2.27	100.82	109.62
6	B	201	GNP	N2-C2-N1	2.01	120.53	117.20
4	A	801	GOL	O3-C3-C2	2.18	120.74	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	B	201	GNP	O2B-PB-O1B	3.57	117.45	110.00
6	B	201	GNP	O1G-PG-N3B	3.65	117.49	111.90
6	B	201	GNP	C4'-O4'-C1'	3.99	114.11	109.72
6	B	201	GNP	C6-N1-C2	5.14	123.07	115.94

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	311/322 (96%)	0.39	22 (7%) 19 29	15, 33, 69, 98	0
2	B	164/167 (98%)	0.36	5 (3%) 54 64	21, 38, 58, 67	0
3	C	5/26 (19%)	0.35	0 100 100	30, 32, 48, 56	0
All	All	480/515 (93%)	0.38	27 (5%) 28 39	15, 35, 67, 98	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	651	SER	8.0
1	A	649	SER	5.2
1	A	648	ALA	4.9
2	B	32	TYR	4.7
1	A	612	GLU	4.7
2	B	29	VAL	4.6
1	A	613	GLY	4.3
1	A	702	MET	3.7
1	A	419	TYR	3.5
1	A	452	ARG	3.4
1	A	614	VAL	3.4
1	A	705	LYS	3.3
1	A	568	SER	3.2
1	A	575	PHE	3.1
1	A	611	SER	2.9
1	A	703	GLU	2.7
1	A	610	THR	2.6
1	A	569	LYS	2.6
1	A	647	LYS	2.6
1	A	706	MET	2.3
1	A	498	ASP	2.2
2	B	105	ASP	2.2
1	A	653	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	9	LEU	2.2
1	A	472	LEU	2.1
2	B	86	ALA	2.1
1	A	693	THR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	A	801	6/6	0.76	0.18	1.48	35,48,49,57	0
6	GNP	B	201	32/32	0.97	0.09	-0.81	25,31,38,40	0
5	MG	B	200	1/1	0.96	0.10	-0.95	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.