



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2QA5  
Title : Crystal structure of Sept2 G-domain  
Authors : Sirajuddin, M.; Wittinghofer, A.  
Deposited on : 2007-06-14  
Resolution : 3.40 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

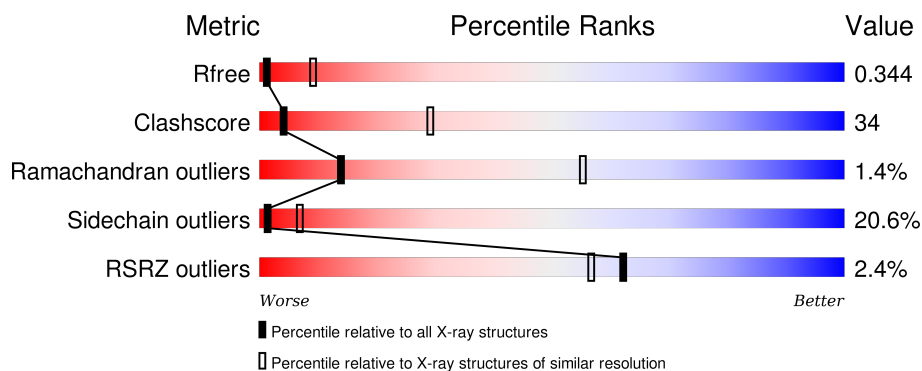
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	315	
1	B	315	

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	GDP	B	316	-	-	X	-

## 2 Entry composition [i](#)

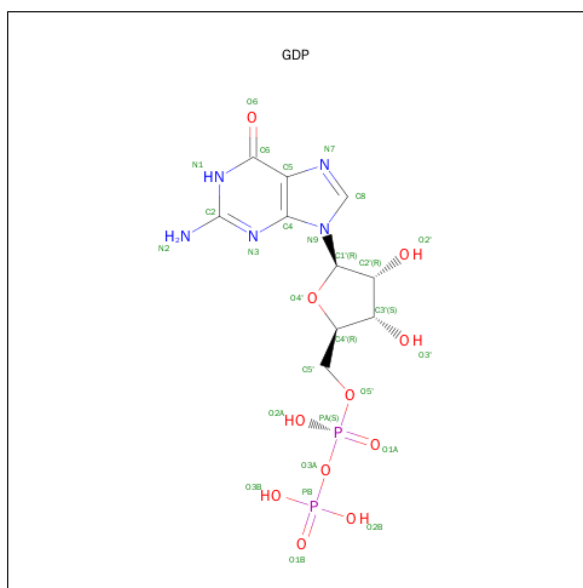
There are 2 unique types of molecules in this entry. The entry contains 3620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Septin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	Se	0	0	0
			1747	1122	292	327	2	4			
1	B	234	Total	C	N	O	S	Se	0	0	0
			1817	1169	306	336	2	4			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

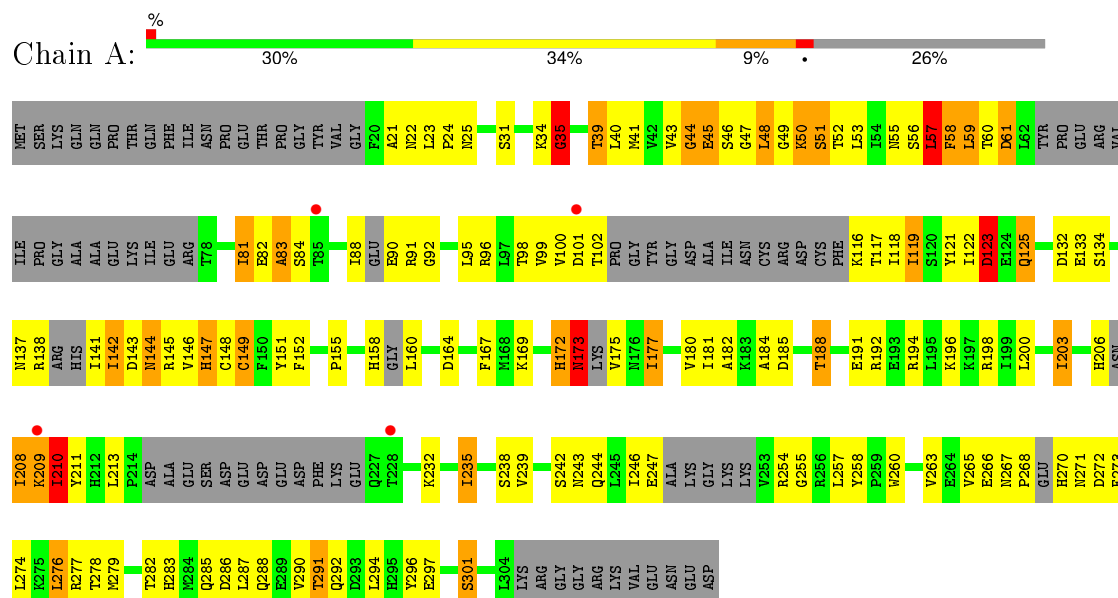


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

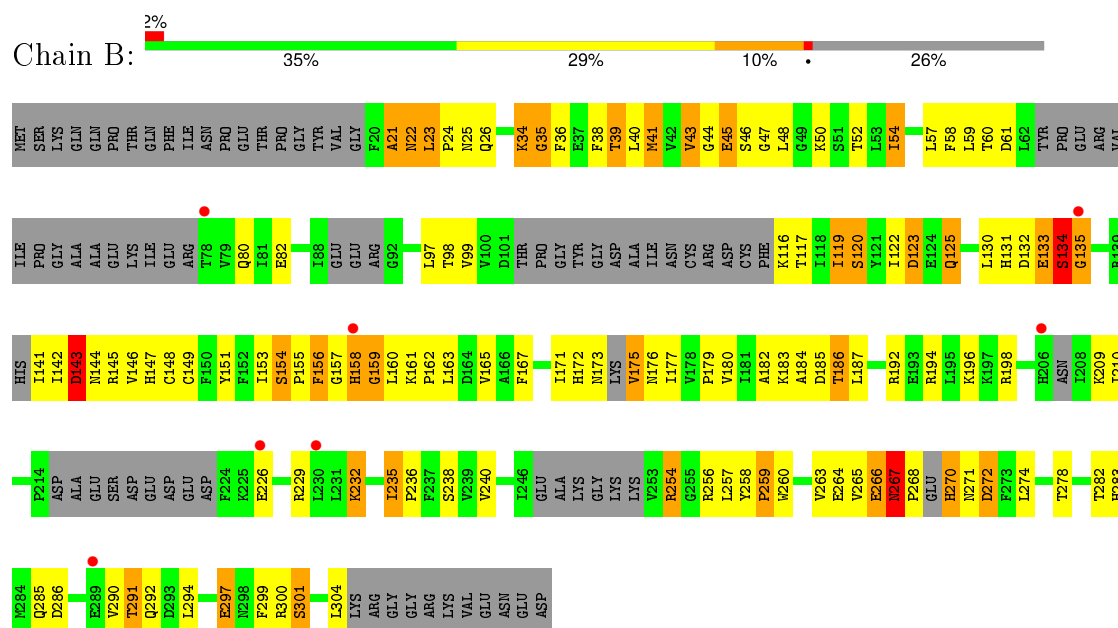
### 3 Residue-property plots

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: Septin-2



#### • Molecule 1: Septin-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.96Å 53.92Å 110.27Å 90.00° 128.37° 90.00°	Depositor
Resolution (Å)	19.79 – 3.40 19.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.79-3.40) 99.1 (19.79-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.13 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.280 , 0.314 0.307 , 0.344	Depositor DCC
$R_{free}$ test set	501 reflections (4.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 30.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 10430 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

### 5.1 Standard geometry

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

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	0.50	3/1766 (0.2%)	1.05	19/2389 (0.8%)
1	B	0.49	1/1840 (0.1%)	1.01	12/2482 (0.5%)
All	All	0.50	4/3606 (0.1%)	1.03	31/4871 (0.6%)

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	4
1	B	0	8
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ASP	C-O	6.94	1.36	1.23
1	B	133	GLU	CD-OE2	6.49	1.32	1.25
1	A	123	ASP	C-N	-5.81	1.20	1.34
1	A	188	THR	C-O	5.07	1.32	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLY	N-CA-C	9.38	136.56	113.10
1	B	23	LEU	CA-CB-CG	7.74	133.10	115.30
1	A	59	LEU	N-CA-CB	7.38	125.16	110.40
1	B	82	GLU	N-CA-CB	-7.10	97.82	110.60
1	A	263	VAL	CB-CA-C	-7.02	98.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ASP	CB-CA-C	6.81	124.02	110.40
1	A	50	LYS	CB-CA-C	-6.75	96.90	110.40
1	A	84	SER	CB-CA-C	6.58	122.60	110.10
1	A	209	LYS	CB-CA-C	6.45	123.29	110.40
1	B	232	LYS	CB-CA-C	6.41	123.23	110.40
1	A	81	ILE	CB-CA-C	-6.31	98.99	111.60
1	B	134	SER	N-CA-C	-6.30	94.00	111.00
1	B	254	ARG	CB-CA-C	-6.05	98.30	110.40
1	A	92	GLY	N-CA-C	-5.87	98.44	113.10
1	A	58	PHE	N-CA-C	5.63	126.20	111.00
1	A	59	LEU	N-CA-C	5.54	125.96	111.00
1	A	57	LEU	N-CA-C	5.52	125.90	111.00
1	A	83	ALA	N-CA-CB	5.44	117.72	110.10
1	B	120	SER	N-CA-CB	-5.44	102.34	110.50
1	B	301	SER	N-CA-C	5.34	125.41	111.00
1	B	21	ALA	CB-CA-C	5.31	118.06	110.10
1	B	297	GLU	CB-CA-C	5.25	120.90	110.40
1	B	123	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	123	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	49	GLY	N-CA-C	5.14	125.95	113.10
1	A	173	ASN	N-CA-C	5.12	124.82	111.00
1	A	210	ILE	N-CA-C	-5.08	97.27	111.00
1	A	91	ARG	CB-CA-C	5.08	120.56	110.40
1	A	147	HIS	CB-CA-C	5.06	120.52	110.40
1	A	184	ALA	CB-CA-C	-5.01	102.58	110.10
1	A	82	GLU	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	HIS	Peptide
1	A	21	ALA	Peptide
1	A	34	LYS	Peptide
1	A	35	GLY	Peptide
1	B	134	SER	Peptide
1	B	158	HIS	Peptide
1	B	159	GLY	Peptide
1	B	254	ARG	Peptide
1	B	267	ASN	Peptide
1	B	34	LYS	Peptide
1	B	35	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	43	VAL	Peptide

## 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	1747	0	1637	110	0
1	B	1817	0	1759	128	0
2	A	28	0	12	7	0
2	B	28	0	12	9	0
All	All	3620	0	3420	238	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 34.

All (238) 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:48:LEU:HD22	1:B:182:ALA:CB	1.45	1.46
1:A:188:THR:HG22	1:A:191:GLU:CD	1.57	1.22
1:B:130:LEU:HD12	1:B:299:PHE:HD1	1.07	1.17
1:B:238:SER:O	1:B:272:ASP:HB2	1.46	1.14
1:B:48:LEU:CD2	1:B:182:ALA:HB1	1.81	1.10
1:B:183:LYS:O	1:B:186:THR:HG22	1.55	1.07
1:B:130:LEU:HD12	1:B:299:PHE:CD1	1.94	1.03
1:A:31:SER:O	1:A:35:GLY:HA2	1.59	1.03
1:B:48:LEU:CD2	1:B:182:ALA:CB	2.40	1.00
1:B:125:GLN:HG2	1:B:144:ASN:O	1.61	1.00
1:A:278:THR:O	1:A:282:THR:HG22	1.61	0.99
1:B:268:PRO:HG3	1:B:271:ASN:O	1.64	0.96
1:A:81:ILE:HG13	1:A:81:ILE:O	1.61	0.95
1:B:48:LEU:HD12	1:B:154:SER:HB2	1.49	0.94
2:B:316:GDP:H8	2:B:316:GDP:H5'	1.34	0.92
1:B:48:LEU:HD22	1:B:182:ALA:HB3	1.47	0.92
1:B:48:LEU:HD22	1:B:182:ALA:HB1	0.91	0.90
1:B:48:LEU:CD1	1:B:154:SER:HB2	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA3	2:A:316:GDP:O1B	1.75	0.87
1:A:133:GLU:O	1:A:138:ARG:CZ	2.23	0.86
1:B:226:GLU:HA	1:B:229:ARG:NH1	1.90	0.86
1:B:238:SER:O	1:B:272:ASP:CB	2.24	0.85
1:A:57:LEU:HD12	1:A:57:LEU:O	1.75	0.85
1:B:48:LEU:HD11	1:B:155:PRO:HD3	1.59	0.84
1:A:188:THR:CG2	1:A:191:GLU:CD	2.44	0.84
1:B:21:ALA:O	1:B:24:PRO:HD2	1.78	0.84
2:B:316:GDP:C8	2:B:316:GDP:H5'	2.13	0.82
1:A:282:THR:HG23	1:A:283:HIS:HD2	1.46	0.80
1:A:147:HIS:HA	1:A:290:VAL:HG21	1.61	0.80
1:B:226:GLU:HA	1:B:229:ARG:HH12	1.47	0.80
1:B:116:LYS:HA	1:B:119:ILE:HD11	1.64	0.79
1:A:169:LYS:O	1:A:172:HIS:CE1	2.37	0.78
1:B:130:LEU:CD1	1:B:299:PHE:HD1	1.94	0.78
1:A:282:THR:HG23	1:A:283:HIS:CD2	2.18	0.78
1:A:172:HIS:HB3	1:A:177:ILE:HD11	1.67	0.77
1:A:23:LEU:N	1:A:24:PRO:HD2	2.00	0.76
1:B:232:LYS:O	1:B:235:ILE:CG2	2.33	0.76
1:A:132:ASP:HB3	1:A:141:ILE:HG22	1.68	0.76
1:B:130:LEU:CD1	1:B:299:PHE:CD1	2.70	0.75
1:B:48:LEU:CD1	1:B:154:SER:HA	2.17	0.74
1:B:48:LEU:HD11	1:B:155:PRO:CD	2.17	0.74
1:A:100:VAL:HG11	1:A:118:ILE:HD11	1.68	0.74
1:B:268:PRO:HA	1:B:270:HIS:N	2.05	0.72
1:A:210:ILE:HG12	1:A:211:TYR:N	2.03	0.72
1:B:278:THR:O	1:B:282:THR:HG22	1.89	0.72
1:B:232:LYS:O	1:B:235:ILE:HG22	1.88	0.72
1:A:194:ARG:O	1:A:198:ARG:HG3	1.90	0.72
1:B:48:LEU:HD13	1:B:154:SER:HA	1.73	0.71
1:B:54:ILE:HG12	1:B:97:LEU:HD22	1.72	0.70
1:B:268:PRO:CG	1:B:271:ASN:O	2.39	0.70
1:A:297:GLU:O	1:A:301:SER:HB2	1.93	0.68
1:A:210:ILE:HG12	1:A:211:TYR:H	1.57	0.67
1:A:188:THR:HG22	1:A:191:GLU:OE2	1.95	0.67
1:A:116:LYS:HA	1:A:119:ILE:HD11	1.75	0.67
1:B:291:THR:HG22	1:B:292:GLN:HG3	1.77	0.67
1:A:188:THR:HG22	1:A:191:GLU:OE1	1.95	0.66
1:B:22:ASN:O	1:B:25:ASN:HB2	1.95	0.66
1:B:48:LEU:CD1	1:B:154:SER:CB	2.74	0.65
1:B:185:ASP:CG	2:B:316:GDP:HN21	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:CG	1:A:144:ASN:O	2.44	0.65
1:B:116:LYS:HA	1:B:119:ILE:CD1	2.27	0.65
1:B:256:ARG:CB	1:B:263:VAL:HB	2.27	0.64
1:B:35:GLY:O	1:B:36:PHE:CD2	2.51	0.64
1:B:267:ASN:HB3	1:B:270:HIS:HB2	1.79	0.63
1:B:185:ASP:OD2	2:B:316:GDP:N2	2.31	0.63
1:B:125:GLN:CG	1:B:144:ASN:O	2.43	0.63
1:A:266:GLU:HB2	1:A:274:LEU:HG	1.81	0.62
1:A:125:GLN:HG3	1:A:144:ASN:O	1.99	0.62
1:B:240:VAL:HB	1:B:271:ASN:HD22	1.65	0.62
1:B:297:GLU:O	1:B:301:SER:HB2	2.00	0.61
1:B:161:LYS:HB3	1:B:162:PRO:HD2	1.84	0.60
1:B:194:ARG:O	1:B:198:ARG:HG3	2.02	0.60
1:B:155:PRO:HG3	1:B:182:ALA:O	2.00	0.60
1:B:48:LEU:CD2	1:B:182:ALA:HB3	2.21	0.60
1:B:265:VAL:HG12	1:B:266:GLU:N	2.15	0.60
1:A:47:GLY:CA	2:A:316:GDP:O1B	2.49	0.60
1:A:265:VAL:O	1:A:266:GLU:HG2	2.01	0.60
1:B:175:VAL:HA	1:B:294:LEU:HD13	1.84	0.59
1:A:88:ILE:C	1:A:90:GLU:N	2.55	0.59
1:B:240:VAL:CG2	1:B:271:ASN:ND2	2.66	0.59
1:B:116:LYS:HA	1:B:119:ILE:CG1	2.33	0.59
1:A:119:ILE:H	1:A:119:ILE:HD13	1.67	0.58
1:A:239:VAL:HG11	1:A:276:LEU:HD12	1.84	0.58
1:B:282:THR:HG23	1:B:283:HIS:CD2	2.38	0.58
1:B:48:LEU:HD23	1:B:48:LEU:O	2.03	0.58
1:B:48:LEU:CD2	1:B:48:LEU:O	2.52	0.58
1:A:188:THR:HG22	1:A:191:GLU:CG	2.32	0.57
1:A:81:ILE:CG1	1:A:81:ILE:O	2.43	0.57
1:A:41:MSE:HB2	1:A:146:VAL:HG11	1.85	0.57
1:B:176:ASN:ND2	1:B:290:VAL:HG23	2.19	0.57
1:A:255:GLY:HA2	1:A:265:VAL:HG23	1.87	0.57
1:A:48:LEU:O	1:A:182:ALA:HB1	2.05	0.57
1:B:41:MSE:HE1	1:B:171:ILE:HD11	1.87	0.57
1:A:278:THR:O	1:A:282:THR:CG2	2.45	0.56
1:B:268:PRO:HG3	1:B:271:ASN:C	2.26	0.56
1:B:300:ARG:O	1:B:304:LEU:HG	2.04	0.56
1:A:267:ASN:HB3	1:A:270:HIS:HB3	1.88	0.56
1:A:31:SER:O	1:A:35:GLY:CA	2.45	0.56
2:B:316:GDP:C8	2:B:316:GDP:C5'	2.86	0.55
1:A:192:ARG:O	1:A:196:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:HIS:O	1:B:134:SER:O	2.25	0.55
1:A:52:THR:HG22	2:A:316:GDP:O1A	2.06	0.55
1:B:52:THR:HG21	2:B:316:GDP:C8	2.42	0.55
1:A:270:HIS:HE1	1:B:260:TRP:HB3	1.71	0.55
1:A:141:ILE:HG13	1:A:141:ILE:O	2.05	0.54
1:A:267:ASN:O	1:A:268:PRO:C	2.46	0.54
1:A:134:SER:OG	1:A:134:SER:O	2.25	0.54
1:B:264:GLU:HB3	1:B:270:HIS:CD2	2.42	0.54
1:A:158:HIS:O	1:A:198:ARG:HD3	2.08	0.54
1:A:291:THR:HG22	1:A:292:GLN:HG3	1.90	0.54
1:B:266:GLU:HA	1:B:274:LEU:HG	1.90	0.53
1:B:133:GLU:O	1:B:135:GLY:HA3	2.08	0.53
1:B:265:VAL:HG12	1:B:266:GLU:H	1.74	0.53
1:A:119:ILE:HA	1:A:122:ILE:HG12	1.91	0.53
1:B:21:ALA:O	1:B:24:PRO:CD	2.55	0.53
1:A:188:THR:CG2	1:A:191:GLU:OE2	2.54	0.52
1:A:288:GLN:HB3	1:A:292:GLN:NE2	2.24	0.52
1:B:183:LYS:O	1:B:186:THR:CG2	2.44	0.52
1:A:143:ASP:OD2	1:A:145:ARG:HD3	2.09	0.52
1:B:48:LEU:CD1	1:B:154:SER:CA	2.86	0.52
1:A:57:LEU:HD12	1:A:57:LEU:C	2.29	0.52
1:B:268:PRO:HG3	1:B:272:ASP:HA	1.91	0.52
1:A:52:THR:HG21	2:A:316:GDP:H8	1.74	0.52
1:A:100:VAL:CG1	1:A:118:ILE:HD11	2.40	0.52
1:B:179:PRO:HG3	1:B:210:ILE:HD11	1.90	0.52
1:B:240:VAL:HB	1:B:271:ASN:ND2	2.24	0.52
1:B:196:LYS:HD3	1:B:236:PRO:O	2.10	0.52
1:B:268:PRO:CD	1:B:271:ASN:O	2.57	0.52
1:B:157:GLY:C	1:B:159:GLY:N	2.63	0.52
1:B:258:TYR:HB3	1:B:260:TRP:CE2	2.46	0.51
1:A:133:GLU:O	1:A:138:ARG:NH1	2.44	0.51
1:B:265:VAL:C	1:B:266:GLU:HG3	2.31	0.51
1:A:83:ALA:HA	1:A:96:ARG:HA	1.92	0.51
1:A:188:THR:CG2	1:A:191:GLU:CG	2.89	0.51
1:A:155:PRO:HG3	1:A:182:ALA:O	2.11	0.51
1:A:23:LEU:N	1:A:24:PRO:CD	2.68	0.51
1:B:274:LEU:O	1:B:278:THR:HG23	2.10	0.51
1:A:203:ILE:HG23	1:A:208:ILE:HG22	1.92	0.51
1:B:132:ASP:HB3	1:B:141:ILE:HG22	1.91	0.50
1:B:133:GLU:C	1:B:135:GLY:HA3	2.32	0.50
1:A:151:TYR:HE1	1:A:167:PHE:CD2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ALA:HB2	1:B:238:SER:HB2	1.92	0.50
1:B:264:GLU:HB3	1:B:270:HIS:HD2	1.77	0.50
1:A:52:THR:HG21	2:A:316:GDP:C8	2.46	0.50
1:A:243:ASN:OD1	1:A:254:ARG:NH2	2.45	0.50
1:B:43:VAL:HG21	1:B:167:PHE:CZ	2.47	0.50
1:A:286:ASP:O	1:A:290:VAL:HG23	2.12	0.49
1:A:43:VAL:HG22	1:A:100:VAL:HG11	1.93	0.49
1:A:22:ASN:O	1:A:25:ASN:N	2.46	0.49
1:B:179:PRO:HG2	1:B:236:PRO:HB3	1.94	0.49
1:A:100:VAL:HG11	1:A:118:ILE:CD1	2.40	0.49
1:A:246:ILE:HG22	1:A:247:GLU:N	2.28	0.48
1:B:268:PRO:O	1:B:270:HIS:N	2.46	0.48
1:A:41:MSE:HB2	1:A:146:VAL:CG1	2.42	0.48
1:A:41:MSE:HB3	1:A:149:CYS:HB2	1.94	0.48
1:A:260:TRP:CE2	1:B:263:VAL:HG22	2.48	0.48
1:A:41:MSE:HE2	1:A:149:CYS:SG	2.53	0.48
1:A:292:GLN:O	1:A:296:TYR:CB	2.61	0.48
1:A:238:SER:O	1:A:271:ASN:O	2.32	0.48
1:B:57:LEU:HB3	1:B:58:PHE:CD2	2.49	0.48
1:B:48:LEU:O	1:B:182:ALA:HB1	2.12	0.48
1:B:268:PRO:HD3	1:B:271:ASN:O	2.13	0.48
1:A:148:CYS:SG	1:A:149:CYS:N	2.86	0.48
1:B:48:LEU:HD12	1:B:154:SER:CB	2.30	0.48
1:B:43:VAL:CG1	1:B:151:TYR:CE1	2.97	0.47
1:A:137:ASN:O	1:A:138:ARG:HG3	2.14	0.47
1:B:172:HIS:HD2	1:B:209:LYS:HB2	1.80	0.47
1:B:155:PRO:CG	1:B:182:ALA:O	2.62	0.47
1:B:240:VAL:HG21	1:B:271:ASN:ND2	2.30	0.47
1:A:151:TYR:OH	1:A:164:ASP:HA	2.14	0.47
1:A:39:THR:H	1:A:147:HIS:HD2	1.63	0.47
1:B:52:THR:HB	2:B:316:GDP:O1A	2.15	0.47
1:A:45:GLU:H	1:A:50:LYS:CE	2.28	0.46
1:A:143:ASP:O	1:A:143:ASP:CG	2.53	0.46
1:A:121:TYR:CD1	1:A:121:TYR:C	2.89	0.46
1:A:173:ASN:HA	1:A:294:LEU:HD22	1.98	0.46
1:B:282:THR:HG23	1:B:283:HIS:HD2	1.79	0.46
1:B:46:SER:HA	1:B:47:GLY:HA2	1.60	0.46
1:A:133:GLU:O	1:A:138:ARG:NH2	2.48	0.46
1:B:265:VAL:CG1	1:B:266:GLU:N	2.79	0.46
1:A:268:PRO:O	1:A:270:HIS:HB2	2.15	0.45
1:B:173:ASN:O	1:B:175:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:N	1:B:24:PRO:HD2	2.32	0.45
1:B:59:LEU:HD23	1:B:59:LEU:N	2.31	0.45
1:A:51:SER:HB3	2:A:316:GDP:O3B	2.16	0.45
1:B:123:ASP:O	1:B:123:ASP:OD1	2.34	0.45
1:A:46:SER:HA	1:A:47:GLY:HA2	1.63	0.45
1:A:232:LYS:O	1:A:235:ILE:CG2	2.65	0.45
1:B:43:VAL:HG11	1:B:151:TYR:CE1	2.52	0.44
1:B:39:THR:OG1	1:B:146:VAL:HA	2.17	0.44
1:A:173:ASN:O	1:A:175:VAL:N	2.51	0.44
1:A:142:ILE:HD12	1:A:142:ILE:O	2.17	0.44
1:B:41:MSE:CE	1:B:122:ILE:HG21	2.48	0.44
1:A:206:HIS:C	1:A:208:ILE:N	2.71	0.44
1:A:101:ASP:O	1:A:102:THR:CB	2.64	0.44
1:B:141:ILE:O	1:B:141:ILE:HG13	2.17	0.44
1:B:59:LEU:O	1:B:60:THR:HG23	2.18	0.44
1:A:57:LEU:HA	1:A:273:PHE:HZ	1.83	0.44
1:B:258:TYR:C	1:B:260:TRP:H	2.20	0.44
1:B:48:LEU:HD11	1:B:154:SER:HA	1.99	0.44
1:B:116:LYS:HA	1:B:119:ILE:HG12	2.00	0.43
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.87	0.43
1:A:268:PRO:HA	1:A:270:HIS:N	2.32	0.43
1:B:41:MSE:HB2	1:B:146:VAL:HG11	2.01	0.43
1:B:265:VAL:CG1	1:B:266:GLU:H	2.31	0.43
1:A:53:LEU:HD23	1:A:152:PHE:HZ	1.84	0.43
1:B:35:GLY:C	1:B:36:PHE:CG	2.92	0.43
1:B:179:PRO:HD3	1:B:210:ILE:HD11	2.01	0.43
1:B:160:LEU:CD2	1:B:165:VAL:HG23	2.49	0.42
1:B:48:LEU:CD1	1:B:155:PRO:HD3	2.38	0.42
1:A:268:PRO:O	1:A:270:HIS:N	2.52	0.42
1:B:148:CYS:SG	1:B:149:CYS:N	2.91	0.42
1:A:267:ASN:HB3	1:A:270:HIS:CD2	2.54	0.42
1:A:246:ILE:HG22	1:A:247:GLU:H	1.84	0.42
1:B:45:GLU:H	1:B:50:LYS:HE2	1.83	0.42
1:B:54:ILE:HG12	1:B:97:LEU:CD2	2.47	0.42
1:B:258:TYR:O	1:B:260:TRP:N	2.49	0.41
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.56	0.41
1:A:149:CYS:HB3	1:A:175:VAL:CG1	2.50	0.41
1:B:47:GLY:HA3	2:B:316:GDP:O1B	2.20	0.41
1:B:185:ASP:OD1	2:B:316:GDP:N1	2.45	0.41
1:A:185:ASP:OD2	2:A:316:GDP:N1	2.43	0.41
1:B:192:ARG:HD2	1:B:238:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:O	1:A:123:ASP:HB2	2.20	0.41
1:A:40:LEU:HD12	1:A:148:CYS:O	2.20	0.41
1:A:22:ASN:O	1:A:25:ASN:HB2	2.20	0.41
1:B:156:PHE:CD1	1:B:156:PHE:N	2.85	0.41
1:B:143:ASP:OD2	1:B:145:ARG:HD3	2.21	0.41
1:B:43:VAL:HG12	1:B:151:TYR:CE1	2.56	0.41
1:A:44:GLY:O	1:A:45:GLU:HG3	2.21	0.41
1:B:160:LEU:HD22	1:B:165:VAL:HG23	2.03	0.41
1:A:188:THR:CG2	1:A:191:GLU:HG3	2.51	0.40
1:A:258:TYR:CE1	1:B:185:ASP:O	2.74	0.40
1:A:239:VAL:HG12	1:A:273:PHE:HA	2.03	0.40
1:B:259:PRO:HG2	1:B:260:TRP:CE3	2.57	0.40
1:A:55:ASN:CG	1:A:61:ASP:HA	2.42	0.40
1:A:169:LYS:O	1:A:172:HIS:HE1	1.97	0.40
1:B:38:PHE:HA	1:B:147:HIS:HD2	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	211/315 (67%)	196 (93%)	13 (6%)	2 (1%)	21	65
1	B	214/315 (68%)	195 (91%)	15 (7%)	4 (2%)	10	49
All	All	425/630 (68%)	391 (92%)	28 (7%)	6 (1%)	14	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
1	A	35	GLY
1	B	267	ASN

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Mol	Chain	Res	Type
1	B	44	GLY
1	B	259	PRO
1	A	44	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	179/280 (64%)	137 (76%)	42 (24%)	1	4
1	B	195/280 (70%)	160 (82%)	35 (18%)	2	11
All	All	374/560 (67%)	297 (79%)	77 (21%)	1	7

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	45	GLU
1	A	48	LEU
1	A	51	SER
1	A	56	SER
1	A	57	LEU
1	A	58	PHE
1	A	59	LEU
1	A	60	THR
1	A	61	ASP
1	A	95	LEU
1	A	98	THR
1	A	99	VAL
1	A	117	THR
1	A	119	ILE
1	A	123	ASP
1	A	125	GLN
1	A	142	ILE
1	A	144	ASN
1	A	149	CYS

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	173	ASN
1	A	177	ILE
1	A	180	VAL
1	A	181	ILE
1	A	200	LEU
1	A	203	ILE
1	A	208	ILE
1	A	210	ILE
1	A	213	LEU
1	A	235	ILE
1	A	242	SER
1	A	244	GLN
1	A	257	LEU
1	A	272	ASP
1	A	276	LEU
1	A	277	ARG
1	A	279	MSE
1	A	285	GLN
1	A	287	LEU
1	A	291	THR
1	A	301	SER
1	B	22	ASN
1	B	26	GLN
1	B	34	LYS
1	B	39	THR
1	B	40	LEU
1	B	41	MSE
1	B	45	GLU
1	B	54	ILE
1	B	61	ASP
1	B	80	GLN
1	B	98	THR
1	B	99	VAL
1	B	117	THR
1	B	119	ILE
1	B	120	SER
1	B	125	GLN
1	B	142	ILE
1	B	143	ASP
1	B	153	ILE
1	B	154	SER

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Mol	Chain	Res	Type
1	B	156	PHE
1	B	163	LEU
1	B	175	VAL
1	B	177	ILE
1	B	180	VAL
1	B	186	THR
1	B	187	LEU
1	B	235	ILE
1	B	257	LEU
1	B	266	GLU
1	B	270	HIS
1	B	272	ASP
1	B	285	GLN
1	B	286	ASP
1	B	291	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	25	ASN
1	A	147	HIS
1	A	244	GLN
1	A	267	ASN
1	A	283	HIS
1	B	26	GLN
1	B	28	HIS
1	B	137	ASN
1	B	172	HIS
1	B	176	ASN
1	B	270	HIS
1	B	271	ASN
1	B	283	HIS
1	B	285	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 ⓘ

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	GDP	A	316	-	23,30,30	1.16	2 (8%)	30,47,47	1.84	7 (23%)
2	GDP	B	316	-	23,30,30	1.10	2 (8%)	30,47,47	1.60	6 (20%)

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	GDP	A	316	-	-	0/12/32/32	0/3/3/3
2	GDP	B	316	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	316	GDP	C5-C4	2.91	1.47	1.40
2	B	316	GDP	C5-C4	3.05	1.47	1.40
2	B	316	GDP	C6-C5	3.07	1.47	1.41
2	A	316	GDP	C6-C5	3.61	1.48	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	316	GDP	C5-C6-N1	-4.21	117.83	123.59
2	A	316	GDP	C5-C6-N1	-4.07	118.03	123.59
2	A	316	GDP	PA-O3A-PB	-3.74	120.12	132.67
2	B	316	GDP	PA-O3A-PB	-3.63	120.51	132.67
2	A	316	GDP	N3-C2-N1	-3.10	122.72	127.44
2	A	316	GDP	C6-C5-C4	-2.94	117.38	120.90
2	A	316	GDP	C4-C5-N7	-2.80	106.90	109.48
2	B	316	GDP	N3-C2-N1	-2.36	123.85	127.44
2	A	316	GDP	C2'-C1'-N9	-2.35	110.69	114.29
2	B	316	GDP	C4-C5-N7	-2.17	107.48	109.48
2	B	316	GDP	C6-C5-C4	-2.13	118.36	120.90
2	B	316	GDP	C6-N1-C2	4.32	121.93	115.94
2	A	316	GDP	C6-N1-C2	4.49	122.17	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	316	GDP	7	0
2	B	316	GDP	9	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, 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	229/315 (72%)	-0.09	4 (1%) 73 67	25, 78, 95, 104	0
1	B	230/315 (73%)	0.11	7 (3%) 54 49	20, 81, 101, 130	0
All	All	459/630 (72%)	0.01	11 (2%) 62 57	20, 80, 100, 130	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	THR	5.5
1	A	228	THR	3.2
1	B	230	LEU	2.8
1	A	85	THR	2.7
1	A	101	ASP	2.4
1	B	158	HIS	2.4
1	A	209	LYS	2.4
1	B	135	GLY	2.3
1	B	226	GLU	2.2
1	B	289	GLU	2.2
1	B	206	HIS	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
2	GDP	A	316	28/28	0.95	0.13	-1.29	57,60,62,62	0
2	GDP	B	316	28/28	0.94	0.15	-1.44	63,71,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.