



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JWY  
Title : CRYSTAL STRUCTURE OF THE DYNAMIN A GTPASE DOMAIN COM-  
PLEXED WITH GDP, DETERMINED AS MYOSIN FUSION  
Authors : Niemann, H.H.; Knetsch, M.L.W.; Scherer, A.; Manstein, D.J.; Kull, F.J.  
Deposited on : 2001-09-05  
Resolution : 2.30 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

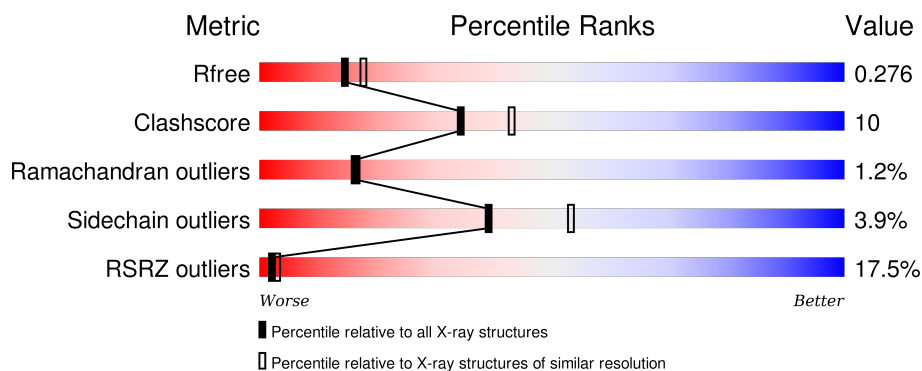
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	776	<div> <div>12%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
2	B	315	<div> <div>28%</div> <div>64%</div> <div>22%</div> <div>• 11%</div> </div>
3	C	9	<div> <div>33%</div> <div>22%</div> <div>44%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8735 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 Myosin II heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	0
			6052	3850	1043	1143	16			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P08799
A	2	HIS	-	EXPRESSION TAG	UNP P08799
A	3	HIS	-	EXPRESSION TAG	UNP P08799
A	4	HIS	-	EXPRESSION TAG	UNP P08799
A	5	HIS	-	EXPRESSION TAG	UNP P08799
A	6	HIS	-	EXPRESSION TAG	UNP P08799
A	7	HIS	-	EXPRESSION TAG	UNP P08799
A	8	HIS	-	EXPRESSION TAG	UNP P08799
A	9	ASP	-	EXPRESSION TAG	UNP P08799
A	10	GLY	-	EXPRESSION TAG	UNP P08799
A	11	THR	-	EXPRESSION TAG	UNP P08799
A	12	GLU	-	EXPRESSION TAG	UNP P08799
A	13	ASP	-	EXPRESSION TAG	UNP P08799
A	260	SER	ASN	SEE REMARK 999	UNP P08799
A	323	CYS	TYR	SEE REMARK 999	UNP P08799

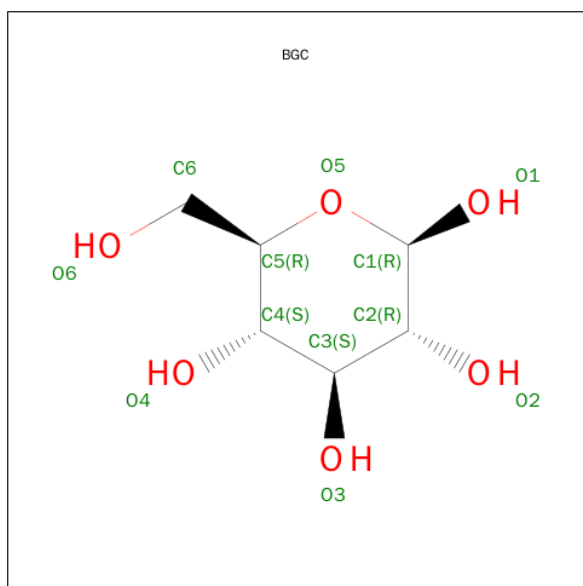
- Molecule 2 is a protein called Dynamin A GTPase domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total	C	N	O	S	0	0	0
			2208	1408	374	419	7			

- Molecule 3 is a protein called Linker Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			37	23	8	6			

- Molecule 4 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).

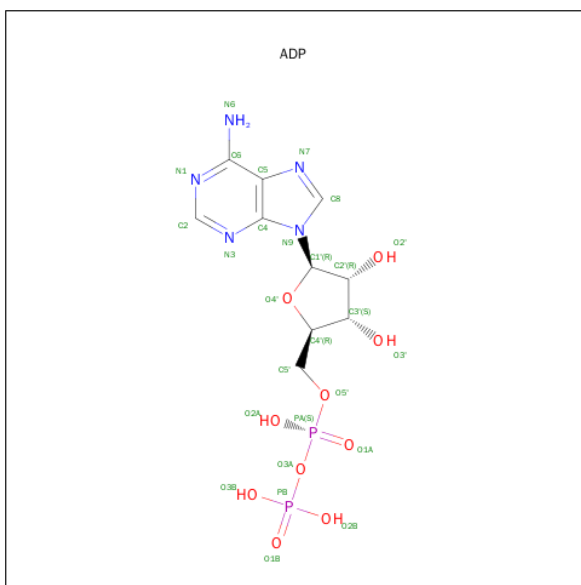


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

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

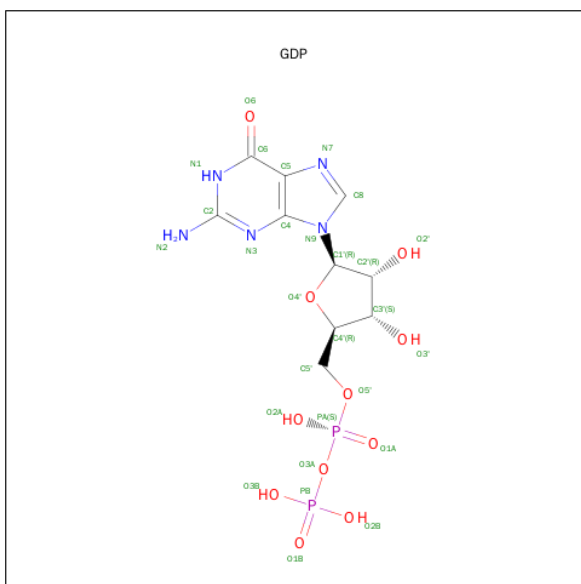
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

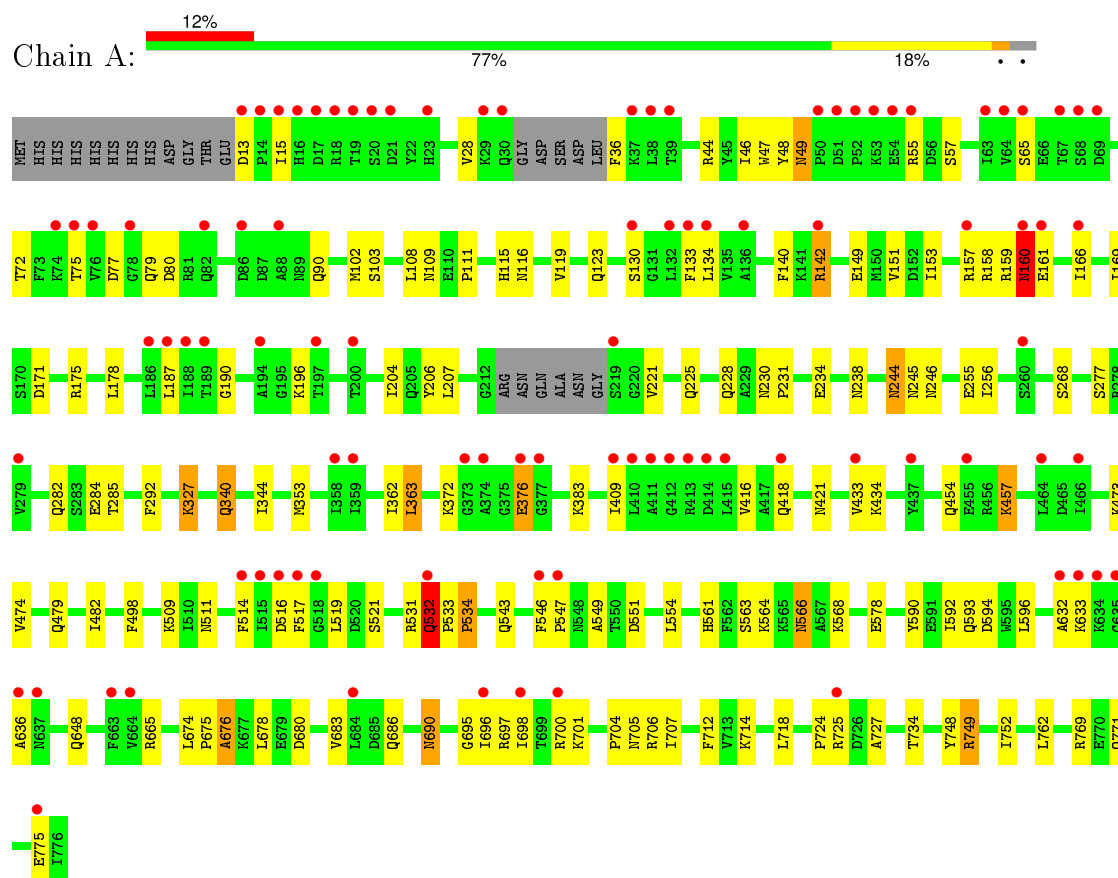
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	343	Total 343	O 343	0	0
8	B	26	Total 26	O 26	0	0

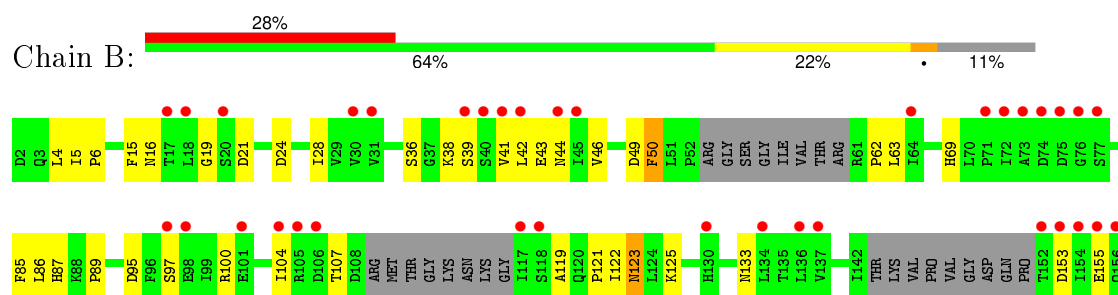
### 3 Residue-property plots

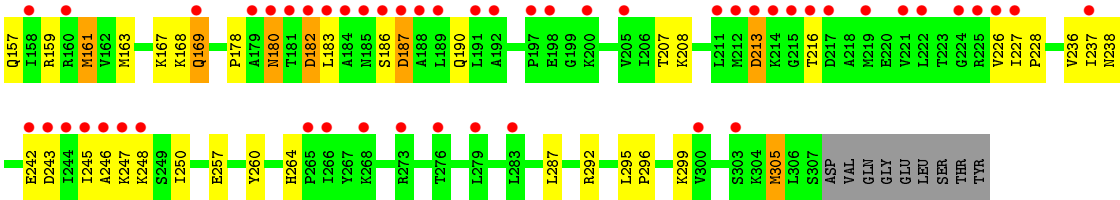
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Myosin II heavy chain

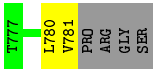
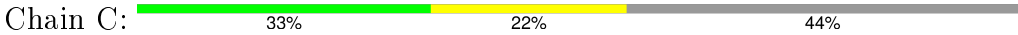


#### • Molecule 2: Dynamitin A GTPase domain





● Molecule 3: Linker Peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.55Å 61.95Å 181.07Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	29.40 – 2.30 29.44 – 2.32	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.40-2.30) 95.4 (29.44-2.32)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.02 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.203 , 0.257 0.233 , 0.276	Depositor DCC
$R_{free}$ test set	3470 reflections (7.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50492 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: GDP, MG, BGC, ADP

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	0.45	0/6170	0.58	0/8324
2	B	0.33	0/2240	0.51	0/3031
3	C	0.26	0/36	0.57	0/47
All	All	0.42	0/8446	0.56	0/11402

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 [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	6052	0	6010	109	0
2	B	2208	0	2291	60	0
3	C	37	0	42	2	0
4	A	12	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	0	0
7	B	28	0	12	1	0
8	A	343	0	0	6	0
8	B	26	0	0	0	0
All	All	8735	0	8379	167	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 10.

All (167) 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:532:GLN:HB3	1:A:533:PRO:HD3	1.38	1.03
1:A:566:ASN:HD22	1:A:568:LYS:H	1.20	0.90
1:A:244:ASN:ND2	1:A:246:ASN:H	1.76	0.82
1:A:566:ASN:ND2	1:A:568:LYS:H	1.82	0.77
2:B:178:PRO:HB3	2:B:208:LYS:HD2	1.66	0.76
1:A:532:GLN:HB3	1:A:533:PRO:CD	2.15	0.73
1:A:13:ASP:OD1	1:A:15:ILE:HG22	1.89	0.73
2:B:28:ILE:HD11	2:B:287:LEU:HB2	1.71	0.73
1:A:665:ARG:HD2	1:A:690:ASN:ND2	2.04	0.72
1:A:65:SER:HB3	1:A:72:THR:HB	1.70	0.72
1:A:748:TYR:O	1:A:749:ARG:HD3	1.91	0.69
2:B:4:LEU:HD11	2:B:292:ARG:HE	1.57	0.69
2:B:69:HIS:H	2:B:133:ASN:ND2	1.90	0.68
1:A:665:ARG:HD2	1:A:690:ASN:HD21	1.59	0.67
1:A:514:PHE:HE1	1:A:701:LYS:HB2	1.58	0.67
1:A:533:PRO:HD2	8:A:1276:HOH:O	1.94	0.66
1:A:632:ALA:HB1	1:A:636:ALA:HB3	1.79	0.65
1:A:166:ILE:HD12	1:A:169:ILE:HD11	1.77	0.64
1:A:532:GLN:CB	1:A:533:PRO:HD3	2.22	0.64
1:A:551:ASP:HB3	1:A:592:ILE:HG23	1.80	0.64
2:B:28:ILE:HG13	2:B:287:LEU:HD13	1.80	0.64
2:B:19:GLY:HA2	2:B:121:PRO:HD3	1.80	0.63
2:B:237:ILE:HD11	2:B:257:GLU:HA	1.81	0.63
2:B:86:LEU:HB2	2:B:123:ASN:HB3	1.82	0.62
1:A:532:GLN:O	1:A:534:PRO:HD3	1.99	0.62
1:A:284:GLU:HG2	1:A:285:THR:HG23	1.82	0.62
1:A:13:ASP:CG	1:A:15:ILE:HG22	2.20	0.61
1:A:140:PHE:O	1:A:675:PRO:HG3	2.00	0.61
2:B:207:THR:HA	2:B:236:VAL:O	2.01	0.60
1:A:700:ARG:HA	1:A:704:PRO:HG3	1.83	0.60
1:A:454:GLN:HB3	8:A:1136:HOH:O	2.01	0.60
1:A:44:ARG:HH21	1:A:90:GLN:HE22	1.47	0.60
1:A:376:GLU:CD	1:A:376:GLU:H	2.05	0.60
1:A:49:ASN:ND2	1:A:55:ARG:HD2	2.17	0.59
1:A:509:LYS:HE2	1:A:752:ILE:HD11	1.85	0.59
2:B:213:ASP:HB2	2:B:216:THR:OG1	2.03	0.58
1:A:244:ASN:HD22	1:A:245:ASN:N	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:GLY:O	1:A:698:ILE:HG12	2.04	0.57
2:B:46:VAL:HG21	2:B:50:PHE:CE2	2.39	0.57
1:A:546:PHE:HB3	1:A:549:ALA:HB2	1.85	0.57
2:B:155:GLU:O	2:B:159:ARG:HG2	2.05	0.57
1:A:566:ASN:HD22	1:A:568:LYS:N	1.99	0.56
2:B:208:LYS:NZ	7:B:901:GDP:C8	2.73	0.56
2:B:207:THR:HG22	2:B:236:VAL:HG23	1.87	0.56
1:A:700:ARG:HD3	1:A:704:PRO:HG2	1.88	0.55
2:B:21:ASP:HB3	2:B:168:LYS:HE3	1.89	0.55
2:B:95:ASP:OD1	2:B:97:SER:HB2	2.07	0.55
2:B:260:TYR:O	2:B:264:HIS:HB2	2.07	0.55
2:B:237:ILE:HG13	2:B:237:ILE:O	2.06	0.55
1:A:102:MET:HG2	1:A:116:ASN:ND2	2.22	0.54
1:A:516:ASP:HB3	1:A:519:LEU:HD13	1.88	0.54
1:A:149:GLU:O	1:A:153:ILE:HG13	2.07	0.54
1:A:204:ILE:HD12	1:A:256:ILE:HD11	1.90	0.54
2:B:39:SER:O	2:B:43:GLU:HG3	2.08	0.53
2:B:38:LYS:O	2:B:41:VAL:HG12	2.09	0.52
2:B:5:ILE:HB	2:B:6:PRO:HD3	1.91	0.52
1:A:724:PRO:HG2	1:A:727:ALA:HB2	1.91	0.52
1:A:36:PHE:CZ	2:B:299:LYS:HD2	2.45	0.52
2:B:295:LEU:HB3	2:B:296:PRO:HD3	1.91	0.52
1:A:498:PHE:HB2	1:A:517:PHE:CD1	2.45	0.51
2:B:242:GLU:HA	2:B:245:ILE:HD12	1.93	0.51
2:B:157:GLN:HA	2:B:157:GLN:HE21	1.76	0.51
1:A:255:GLU:HB2	1:A:268:SER:OG	2.11	0.51
1:A:340:GLN:HE22	1:A:344:ILE:HG12	1.76	0.51
1:A:228:GLN:O	1:A:231:PRO:HD2	2.11	0.50
1:A:648:GLN:NE2	8:A:1310:HOH:O	2.43	0.50
1:A:151:VAL:HG13	1:A:206:TYR:CD1	2.47	0.50
1:A:686:GLN:O	1:A:690:ASN:HB2	2.12	0.50
1:A:102:MET:O	1:A:108:LEU:HD21	2.11	0.50
2:B:295:LEU:HD21	3:C:781:VAL:O	2.11	0.50
2:B:169:GLN:HE21	2:B:169:GLN:H	1.59	0.50
2:B:163:MET:O	2:B:167:LYS:HB2	2.11	0.50
1:A:700:ARG:HA	1:A:704:PRO:CG	2.41	0.49
1:A:340:GLN:HE22	1:A:344:ILE:CG1	2.26	0.49
2:B:169:GLN:NE2	2:B:169:GLN:H	2.09	0.49
1:A:416:VAL:HG13	1:A:418:GLN:NE2	2.28	0.49
1:A:521:SER:HA	8:A:1067:HOH:O	2.13	0.49
1:A:362:ILE:HG23	1:A:433:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:SER:HB2	2:B:178:PRO:HD3	1.95	0.48
1:A:102:MET:HG2	1:A:116:ASN:HD22	1.77	0.48
1:A:28:VAL:HG13	1:A:123:GLN:HE22	1.79	0.48
1:A:327:LYS:HE2	1:A:327:LYS:H	1.78	0.48
1:A:409:ILE:HG12	1:A:418:GLN:HG3	1.95	0.48
2:B:21:ASP:OD2	2:B:24:ASP:HA	2.14	0.48
1:A:593:GLN:O	1:A:594:ASP:HB2	2.13	0.48
1:A:234:GLU:O	1:A:238:ASN:HB2	2.14	0.47
1:A:514:PHE:CE1	1:A:701:LYS:HB2	2.45	0.47
1:A:49:ASN:HB3	1:A:57:SER:O	2.15	0.47
2:B:295:LEU:O	2:B:299:LYS:HG3	2.14	0.47
2:B:87:HIS:C	2:B:89:PRO:HD3	2.35	0.47
1:A:158:ARG:H	1:A:161:GLU:CD	2.18	0.47
2:B:100:ARG:O	2:B:104:ILE:HG13	2.15	0.47
1:A:632:ALA:HB1	1:A:636:ALA:CB	2.46	0.46
2:B:41:VAL:HG13	2:B:42:LEU:N	2.31	0.46
2:B:245:ILE:O	2:B:246:ALA:HB3	2.15	0.46
2:B:180:ASN:HD22	2:B:180:ASN:C	2.19	0.45
1:A:49:ASN:HD21	1:A:55:ARG:HD2	1.81	0.45
2:B:86:LEU:CB	2:B:123:ASN:HB3	2.44	0.45
1:A:115:HIS:O	1:A:119:VAL:HG23	2.17	0.45
2:B:237:ILE:HG12	2:B:257:GLU:HG3	1.99	0.45
1:A:327:LYS:N	1:A:327:LYS:HE2	2.32	0.45
1:A:171:ASP:O	1:A:175:ARG:HG2	2.17	0.45
2:B:104:ILE:O	2:B:107:THR:HG22	2.17	0.45
2:B:180:ASN:OD1	2:B:208:LYS:HD3	2.17	0.44
1:A:695:GLY:C	1:A:697:ARG:H	2.20	0.44
1:A:277:SER:HA	1:A:434:LYS:HD3	2.00	0.44
1:A:75:THR:HG22	1:A:77:ASP:H	1.83	0.44
1:A:531:ARG:O	1:A:532:GLN:C	2.55	0.44
1:A:244:ASN:HD22	1:A:244:ASN:C	2.20	0.44
1:A:292:PHE:CD1	1:A:363:LEU:HD13	2.53	0.44
2:B:226:VAL:C	2:B:228:PRO:HD3	2.38	0.43
1:A:158:ARG:H	1:A:161:GLU:CG	2.31	0.43
1:A:158:ARG:HB2	1:A:158:ARG:NH1	2.33	0.43
2:B:49:ASP:HB2	2:B:100:ARG:NH2	2.33	0.43
2:B:36:SER:HA	2:B:178:PRO:CG	2.49	0.43
1:A:44:ARG:HH21	1:A:90:GLN:NE2	2.14	0.43
1:A:714:LYS:HG2	1:A:725:ARG:HE	1.84	0.43
1:A:554:LEU:HD23	1:A:592:ILE:HG13	2.00	0.43
2:B:243:ASP:O	2:B:248:LYS:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HB3	1:A:231:PRO:HD3	2.01	0.43
1:A:479:GLN:HA	1:A:482:ILE:HG22	1.99	0.43
1:A:700:ARG:HH12	1:A:705:ASN:HD21	1.67	0.43
2:B:62:PRO:O	2:B:122:ILE:HG22	2.19	0.43
1:A:706:ARG:HD2	8:A:1216:HOH:O	2.19	0.42
2:B:123:ASN:ND2	2:B:125:LYS:NZ	2.67	0.42
1:A:372:LYS:NZ	1:A:421:ASN:HB2	2.33	0.42
1:A:674:LEU:HA	1:A:675:PRO:HD3	1.86	0.42
1:A:48:TYR:OH	1:A:75:THR:HG23	2.18	0.42
1:A:563:SER:O	1:A:564:LYS:HB2	2.19	0.42
1:A:159:ARG:O	1:A:159:ARG:HG2	2.19	0.42
1:A:675:PRO:O	1:A:676:ALA:C	2.57	0.42
2:B:42:LEU:O	2:B:46:VAL:HG23	2.18	0.42
2:B:104:ILE:C	2:B:107:THR:HG22	2.40	0.42
1:A:130:SER:O	1:A:133:PHE:HB2	2.18	0.42
1:A:707:ILE:HD11	1:A:762:LEU:HD21	2.00	0.42
1:A:157:ARG:HA	1:A:161:GLU:OE2	2.19	0.42
1:A:714:LYS:HA	1:A:725:ARG:HG3	2.02	0.42
1:A:678:LEU:HD11	1:A:683:VAL:HG21	2.01	0.42
2:B:19:GLY:HA2	2:B:121:PRO:CD	2.49	0.42
1:A:102:MET:CG	1:A:116:ASN:HD22	2.32	0.42
2:B:36:SER:HA	2:B:178:PRO:HG3	2.01	0.42
1:A:190:GLY:N	1:A:196:LYS:HD3	2.35	0.42
1:A:46:ILE:HG12	1:A:47:TRP:N	2.35	0.42
2:B:44:ASN:HD22	2:B:250:ILE:HD12	1.85	0.42
1:A:187:LEU:HD12	1:A:187:LEU:N	2.35	0.42
1:A:109:ASN:OD1	1:A:111:PRO:HG2	2.20	0.42
1:A:142:ARG:HG2	1:A:142:ARG:HH11	1.85	0.42
1:A:158:ARG:H	1:A:161:GLU:HG2	1.85	0.41
2:B:85:PHE:HE2	2:B:122:ILE:HD11	1.84	0.41
1:A:718:LEU:HD12	1:A:769:ARG:NH1	2.35	0.41
2:B:182:ASP:C	2:B:183:LEU:HD22	2.40	0.41
1:A:712:PHE:CD2	1:A:734:THR:HG23	2.55	0.41
1:A:79:GLN:HG2	1:A:80:ASP:N	2.34	0.41
1:A:578:GLU:HA	1:A:590:TYR:O	2.21	0.41
1:A:771:GLN:O	1:A:775:GLU:HG3	2.21	0.41
1:A:160:ASN:HA	1:A:160:ASN:HD22	1.57	0.41
2:B:226:VAL:O	2:B:227:ILE:HD13	2.20	0.41
2:B:305:MET:HG3	2:B:305:MET:O	2.20	0.41
1:A:409:ILE:CG1	1:A:418:GLN:HG3	2.51	0.41
1:A:221:VAL:O	1:A:225:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LYS:HG3	1:A:474:VAL:N	2.37	0.40
1:A:457:LYS:H	1:A:457:LYS:HD3	1.86	0.40
2:B:180:ASN:ND2	2:B:180:ASN:H	2.19	0.40
1:A:718:LEU:HD21	2:B:15:PHE:CE2	2.57	0.40
2:B:299:LYS:HD3	3:C:780:LEU:O	2.22	0.40
2:B:119:ALA:HA	2:B:161:MET:HE1	2.03	0.40
1:A:561:HIS:HE1	8:A:1277:HOH:O	2.05	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	747/776 (96%)	710 (95%)	31 (4%)	6 (1%)	24	27
2	B	273/315 (87%)	239 (88%)	28 (10%)	6 (2%)	8	6
3	C	3/9 (33%)	2 (67%)	1 (33%)	0	100	100
All	All	1023/1100 (93%)	951 (93%)	60 (6%)	12 (1%)	16	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	186	SER
2	B	247	LYS
1	A	160	ASN
2	B	182	ASP
2	B	187	ASP
1	A	547	PRO
2	B	50	PHE
1	A	676	ALA
1	A	696	ILE
2	B	16	ASN

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Mol	Chain	Res	Type
1	A	534	PRO
1	A	532	GLN

### 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	658/679 (97%)	633 (96%)	25 (4%)	40	54
2	B	254/282 (90%)	243 (96%)	11 (4%)	35	47
3	C	4/7 (57%)	4 (100%)	0	100	100
All	All	916/968 (95%)	880 (96%)	36 (4%)	39	53

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	103	SER
1	A	134	LEU
1	A	142	ARG
1	A	160	ASN
1	A	178	LEU
1	A	207	LEU
1	A	244	ASN
1	A	282	GLN
1	A	327	LYS
1	A	340	GLN
1	A	353	MET
1	A	363	LEU
1	A	376	GLU
1	A	383	LYS
1	A	457	LYS
1	A	511	ASN
1	A	532	GLN
1	A	543	GLN
1	A	566	ASN

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Mol	Chain	Res	Type
1	A	596	LEU
1	A	633	LYS
1	A	680	ASP
1	A	690	ASN
1	A	749	ARG
2	B	63	LEU
2	B	123	ASN
2	B	153	ASP
2	B	161	MET
2	B	169	GLN
2	B	180	ASN
2	B	187	ASP
2	B	190	GLN
2	B	213	ASP
2	B	238	ASN
2	B	305	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	90	GLN
1	A	160	ASN
1	A	199	ASN
1	A	244	ASN
1	A	245	ASN
1	A	282	GLN
1	A	294	GLN
1	A	308	HIS
1	A	316	ASN
1	A	320	GLN
1	A	340	GLN
1	A	418	GLN
1	A	450	ASN
1	A	511	ASN
1	A	566	ASN
1	A	605	GLN
1	A	627	ASN
1	A	644	GLN
1	A	648	GLN
1	A	690	ASN
1	A	705	ASN

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Mol	Chain	Res	Type
2	B	9	ASN
2	B	27	GLN
2	B	34	GLN
2	B	80	GLN
2	B	120	GLN
2	B	123	ASN
2	B	133	ASN
2	B	157	GLN
2	B	169	GLN
2	B	180	ASN
2	B	272	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
6	ADP	A	801	5	22,29,29	1.68	5 (22%)	27,45,45	1.29	3 (11%)
4	BGC	A	803	-	12,12,12	0.75	0	17,17,17	0.70	0
7	GDP	B	901	-	23,30,30	1.71	6 (26%)	30,47,47	1.94	3 (10%)

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
6	ADP	A	801	5	-	0/12/32/32	0/3/3/3
4	BGC	A	803	-	-	0/2/22/22	0/1/1/1
7	GDP	B	901	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	ADP	C8-N7	-3.22	1.28	1.34
7	B	901	GDP	C6-C5	-3.09	1.35	1.41
6	A	801	ADP	PB-O2B	-2.98	1.44	1.54
7	B	901	GDP	PB-O2B	-2.29	1.46	1.54
6	A	801	ADP	PA-O2A	-2.13	1.45	1.54
7	B	901	GDP	C2-N2	2.02	1.38	1.34
7	B	901	GDP	C4-N3	2.03	1.38	1.35
7	B	901	GDP	PB-O3B	2.04	1.62	1.54
6	A	801	ADP	C4-N3	2.80	1.39	1.35
6	A	801	ADP	C2-N1	3.48	1.40	1.33
7	B	901	GDP	C6-N1	4.54	1.41	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	901	GDP	C5-C6-N1	-6.43	114.80	123.59
7	B	901	GDP	N3-C2-N1	-3.17	122.62	127.44
6	A	801	ADP	N3-C2-N1	-2.48	126.99	128.89
6	A	801	ADP	O3'-C3'-C2'	2.08	118.59	111.83
6	A	801	ADP	O3'-C3'-C4'	2.72	119.21	111.05
7	B	901	GDP	C6-N1-C2	6.31	124.69	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	901	GDP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	753/776 (97%)	0.77	95 (12%) 5 8	11, 34, 78, 108	0
2	B	281/315 (89%)	1.68	87 (30%) 1 1	28, 62, 103, 123	0
3	C	5/9 (55%)	0.75	0 100 100	43, 49, 59, 68	0
All	All	1039/1100 (94%)	1.02	182 (17%) 2 3	11, 41, 91, 123	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	ILE	8.2
1	A	413	ARG	7.5
1	A	38	LEU	7.5
1	A	635	GLY	7.1
2	B	184	ALA	7.0
1	A	634	LYS	7.0
2	B	216	THR	6.7
1	A	53	LYS	6.1
2	B	215	GLY	6.0
2	B	192	ALA	5.8
1	A	52	PRO	5.8
1	A	636	ALA	5.5
2	B	73	ALA	5.4
2	B	152	THR	5.4
2	B	18	LEU	5.2
2	B	224	GLY	5.1
2	B	186	SER	5.1
2	B	154	ILE	5.0
2	B	185	ASN	4.9
2	B	245	ILE	4.9
2	B	246	ALA	4.9
1	A	29	LYS	4.9
2	B	226	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	4.8
2	B	72	ILE	4.7
1	A	515	ILE	4.6
2	B	42	LEU	4.3
2	B	41	VAL	4.2
2	B	182	ASP	4.2
2	B	265	PRO	4.1
2	B	198	GLU	4.1
2	B	74	ASP	4.1
1	A	19	THR	4.1
1	A	633	LYS	4.0
2	B	179	ALA	4.0
2	B	156	GLN	3.9
1	A	219	SER	3.9
2	B	303	SER	3.9
1	A	75	THR	3.8
2	B	155	GLU	3.8
2	B	214	LYS	3.8
2	B	219	MET	3.8
1	A	664	VAL	3.8
1	A	17	ASP	3.7
1	A	23	HIS	3.7
2	B	136	LEU	3.7
1	A	55	ARG	3.7
1	A	54	GLU	3.7
2	B	188	ALA	3.7
1	A	186	LEU	3.6
2	B	242	GLU	3.6
1	A	69	ASP	3.6
1	A	455	GLU	3.6
1	A	547	PRO	3.5
2	B	118	SER	3.5
1	A	15	ILE	3.5
1	A	37	LYS	3.5
2	B	77	SER	3.5
1	A	374	ALA	3.5
2	B	266	ILE	3.4
2	B	75	ASP	3.4
1	A	411	ALA	3.4
1	A	412	GLY	3.4
1	A	415	LEU	3.4
2	B	200	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	197	PRO	3.4
1	A	188	ILE	3.4
2	B	225	ARG	3.3
1	A	14	PRO	3.3
2	B	98	GLU	3.2
2	B	40	SER	3.2
2	B	300	VAL	3.2
2	B	247	LYS	3.2
2	B	158	ILE	3.2
1	A	546	PHE	3.1
1	A	30	GLN	3.1
2	B	71	PRO	3.1
2	B	105	ARG	3.1
1	A	532	GLN	3.0
1	A	696	ILE	3.0
2	B	244	ILE	3.0
2	B	169	GLN	3.0
2	B	39	SER	3.0
2	B	279	LEU	3.0
1	A	133	PHE	2.9
1	A	698	ILE	2.9
1	A	279	VAL	2.9
1	A	18	ARG	2.9
1	A	409	ILE	2.9
1	A	157	ARG	2.9
1	A	358	ILE	2.9
2	B	213	ASP	2.8
1	A	74	LYS	2.8
1	A	632	ALA	2.8
1	A	433	VAL	2.8
2	B	97	SER	2.8
1	A	684	LEU	2.8
1	A	76	VAL	2.7
1	A	88	ALA	2.7
1	A	39	THR	2.7
1	A	82	GLN	2.7
2	B	181	THR	2.7
2	B	217	ASP	2.7
1	A	134	LEU	2.7
2	B	268	LYS	2.7
1	A	189	THR	2.7
1	A	518	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	227	ILE	2.7
1	A	136	ALA	2.7
1	A	725	ARG	2.7
1	A	65	SER	2.7
1	A	13	ASP	2.7
1	A	51	ASP	2.6
2	B	183	LEU	2.6
2	B	248	LYS	2.6
1	A	418	GLN	2.6
2	B	76	GLY	2.6
1	A	359	ILE	2.6
1	A	376	GLU	2.6
2	B	283	LEU	2.6
2	B	237	ILE	2.6
1	A	466	ILE	2.5
2	B	101	GLU	2.5
1	A	410	LEU	2.5
1	A	161	GLU	2.5
1	A	130	SER	2.5
1	A	373	GLY	2.5
2	B	222	LEU	2.5
2	B	153	ASP	2.5
1	A	260	SER	2.5
1	A	50	PRO	2.5
1	A	637	ASN	2.4
2	B	189	LEU	2.4
2	B	187	ASP	2.4
1	A	20	SER	2.4
1	A	86	ASP	2.4
1	A	68	SER	2.4
2	B	211	LEU	2.4
2	B	212	MET	2.4
1	A	377	GLY	2.4
2	B	106	ASP	2.3
1	A	464	LEU	2.3
1	A	187	LEU	2.3
2	B	20	SER	2.3
1	A	166	ILE	2.3
2	B	243	ASP	2.3
1	A	132	LEU	2.3
2	B	134	LEU	2.3
2	B	45	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	137	VAL	2.3
1	A	700	ARG	2.3
2	B	180	ASN	2.3
2	B	31	VAL	2.2
2	B	130	HIS	2.2
2	B	221	VAL	2.2
1	A	516	ASP	2.2
1	A	64	VAL	2.2
2	B	44	ASN	2.2
1	A	16	HIS	2.2
2	B	205	VAL	2.1
1	A	67	THR	2.1
1	A	200	THR	2.1
1	A	194	ALA	2.1
1	A	517	PHE	2.1
2	B	276	THR	2.1
2	B	104	ILE	2.1
1	A	21	ASP	2.1
1	A	160	ASN	2.1
1	A	514	PHE	2.1
1	A	437	TYR	2.1
2	B	17	THR	2.1
1	A	63	ILE	2.1
1	A	142	ARG	2.1
2	B	64	ILE	2.1
2	B	30	VAL	2.1
1	A	197	THR	2.0
1	A	663	PHE	2.0
1	A	775	GLU	2.0
2	B	160	ARG	2.0
2	B	273	ARG	2.0
1	A	78	GLY	2.0
2	B	191	LEU	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 ⓘ

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	BGC	A	803	12/12	0.91	0.14	0.11	32,41,49,51	0
5	MG	A	802	1/1	0.90	0.19	-0.08	15,15,15,15	0
7	GDP	B	901	28/28	0.79	0.23	-0.32	78,88,92,93	0
6	ADP	A	801	27/27	0.95	0.17	-0.61	14,20,26,28	0
5	MG	B	902	1/1	0.79	0.28	-	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.