



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:27 PM GMT

PDB ID : 1TPZ  
Title : Crystal Structure of IIGP1: a paradigm for interferon inducible p47 resistance GTPases  
Authors : Ghosh, A.; Uthaiiah, R.; Howard, J.; Herrmann, C.; Wolf, E.  
Deposited on : 2004-06-16  
Resolution : 2.00 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

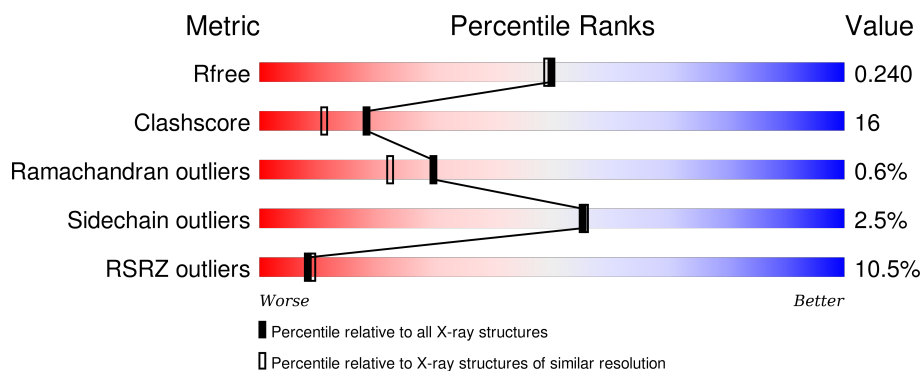
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	422	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>• 6%</div> </div> </div>
1	B	422	<div> <div>10%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>• 7%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	2000	-	-	-	X
5	MPD	B	1000	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7034 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 interferon-inducible GTPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3200	2065	524	597	14			
1	B	392	Total	C	N	O	S	0	0	0
			3175	2047	520	594	14			

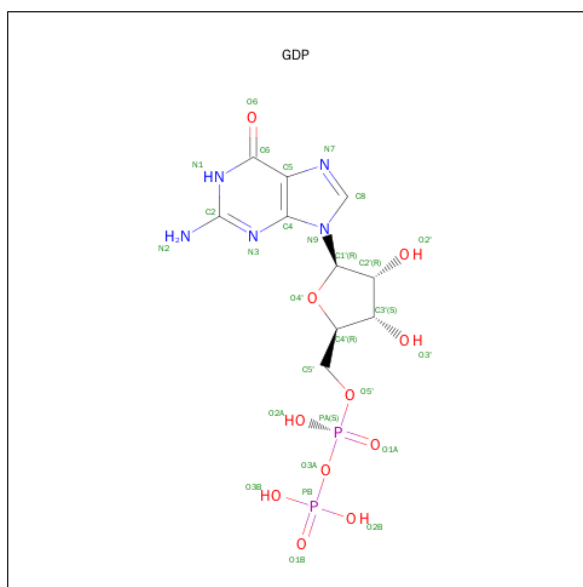
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	LYS	-	CLONING ARTIFACT	UNP Q9QZ85
A	413	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
A	414	GLY	-	CLONING ARTIFACT	UNP Q9QZ85
A	415	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	416	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
A	417	GLU	-	CLONING ARTIFACT	UNP Q9QZ85
A	418	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	419	PRO	-	CLONING ARTIFACT	UNP Q9QZ85
A	420	HIS	-	CLONING ARTIFACT	UNP Q9QZ85
A	421	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	422	ASP	-	CLONING ARTIFACT	UNP Q9QZ85
B	412	LYS	-	CLONING ARTIFACT	UNP Q9QZ85
B	413	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
B	414	GLY	-	CLONING ARTIFACT	UNP Q9QZ85
B	415	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	416	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
B	417	GLU	-	CLONING ARTIFACT	UNP Q9QZ85
B	418	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	419	PRO	-	CLONING ARTIFACT	UNP Q9QZ85
B	420	HIS	-	CLONING ARTIFACT	UNP Q9QZ85
B	421	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	422	ASP	-	CLONING ARTIFACT	UNP Q9QZ85

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



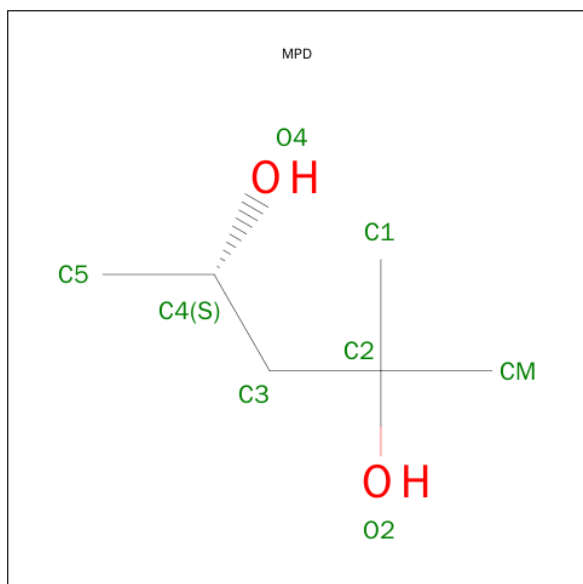
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 28 10 5 11 2	0	0
3	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

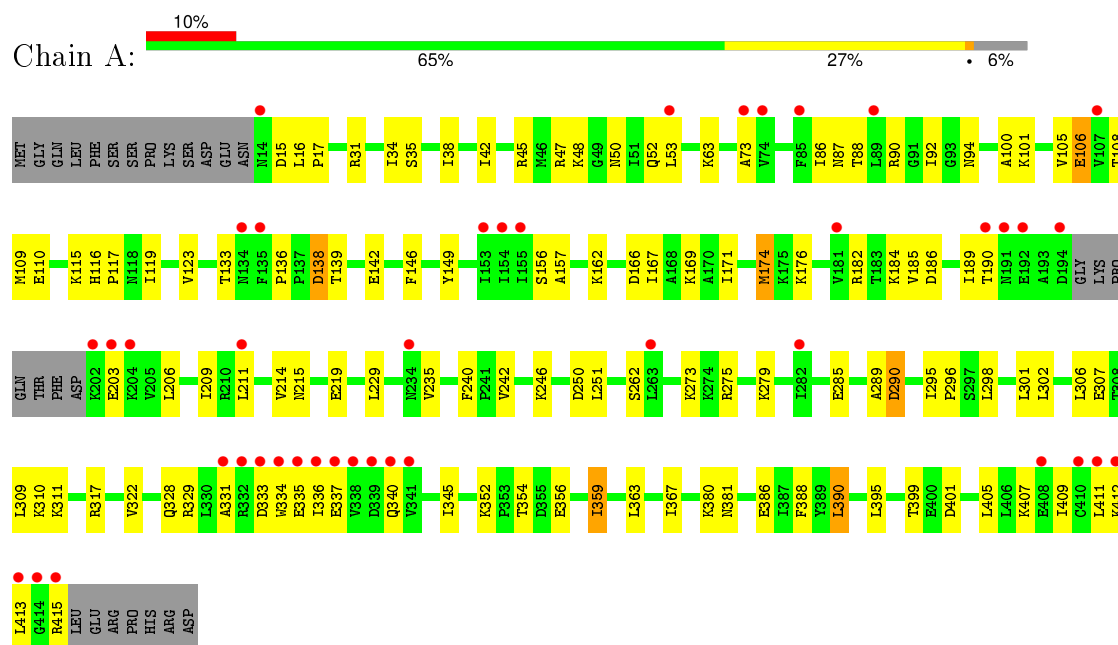
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	274	Total 274	O 274	0	0
6	B	315	Total 315	O 315	0	0

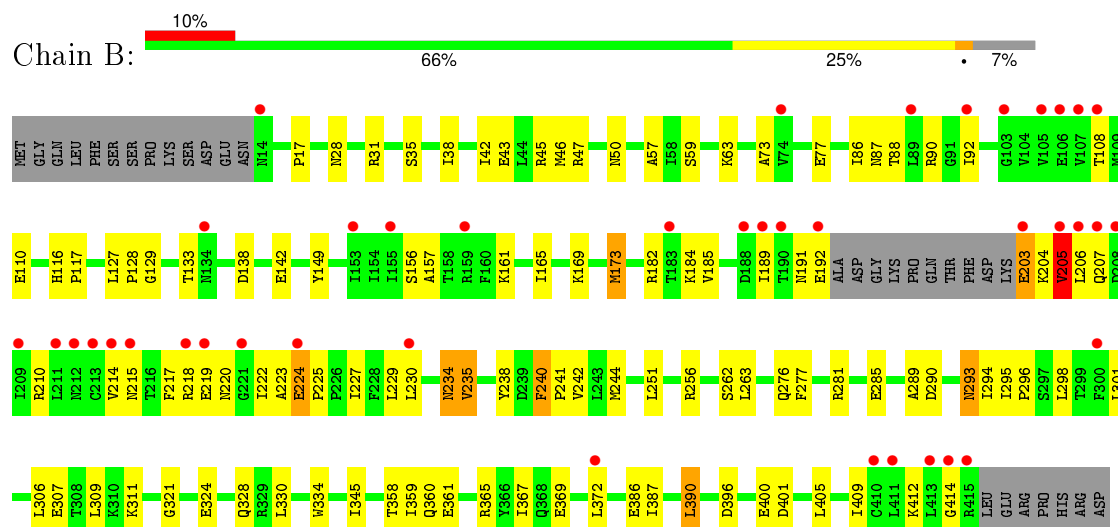
### 3 Residue-property plots

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: interferon-inducible GTPase



#### • Molecule 1: interferon-inducible GTPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.54Å 91.89Å 143.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.00) 96.9 (29.95-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.241 0.208 , 0.240	Depositor DCC
$R_{free}$ test set	5742 reflections (8.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70334 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, MG, MPD, EDO

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	0.32	0/3264	0.56	0/4404
1	B	0.33	0/3239	0.55	0/4371
All	All	0.33	0/6503	0.56	0/8775

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3200	0	3235	101	0
1	B	3175	0	3198	102	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
4	B	4	0	6	0	0
5	B	8	0	14	2	0
6	A	274	0	0	8	0
6	B	315	0	0	10	0
All	All	7034	0	6477	202	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 16.

All (202) 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:87:ASN:HD21	1:A:100:ALA:H	0.99	0.97
1:A:189:ILE:HD11	1:A:206:LEU:HD11	1.61	0.83
1:B:214:VAL:HG13	1:B:224:GLU:HB2	1.61	0.82
1:B:17:PRO:HB2	1:B:47:ARG:NH1	1.95	0.81
1:A:174:MET:HB3	6:A:1654:HOH:O	1.80	0.80
1:B:28:ASN:HB3	6:B:2762:HOH:O	1.80	0.79
1:A:169:LYS:HD3	1:B:169:LYS:HD3	1.65	0.79
1:A:295:ILE:H	1:A:295:ILE:HD12	1.47	0.79
1:B:92:ILE:HD11	1:B:117:PRO:HG2	1.64	0.78
1:A:88:THR:HG23	1:A:235:VAL:HG12	1.67	0.77
1:A:87:ASN:ND2	1:A:100:ALA:H	1.81	0.76
1:A:182:ARG:NH1	1:A:209:ILE:HG23	2.02	0.75
1:A:174:MET:CE	1:A:176:LYS:HG3	2.17	0.75
1:A:306:LEU:HD11	1:A:310:LYS:HE3	1.70	0.74
1:A:354:THR:HG22	1:A:356:GLU:H	1.52	0.74
1:A:174:MET:HE2	1:A:176:LYS:HG3	1.70	0.73
1:A:211:LEU:O	1:A:214:VAL:HG12	1.89	0.72
1:A:52:GLN:H	1:A:52:GLN:CD	1.92	0.72
1:A:359:ILE:HD12	1:A:363:LEU:HG	1.69	0.72
1:A:88:THR:HG23	1:A:235:VAL:CG1	2.19	0.72
1:B:204:LYS:O	1:B:205:VAL:HG22	1.90	0.72
1:B:365:ARG:O	1:B:369:GLU:HG3	1.90	0.71
1:A:235:VAL:HG13	6:A:1764:HOH:O	1.91	0.70
1:B:298:LEU:HD11	1:B:301:LEU:HD13	1.71	0.70
1:B:293:ASN:HD22	1:B:293:ASN:C	1.94	0.70
1:A:185:VAL:HG11	1:A:229:LEU:HB3	1.75	0.68
1:A:246:LYS:HE2	1:A:250:ASP:OD1	1.94	0.68
1:A:45:ARG:HD3	1:A:53:LEU:HB3	1.75	0.67
1:A:87:ASN:HD21	1:A:100:ALA:N	1.82	0.66
1:A:88:THR:CG2	1:A:235:VAL:HG12	2.25	0.66
1:B:330:LEU:HD21	1:B:334:TRP:CZ3	2.30	0.65
1:B:330:LEU:HD21	1:B:334:TRP:CE3	2.33	0.64
1:B:295:ILE:HG13	6:B:2765:HOH:O	1.98	0.63
1:B:321:GLY:O	5:B:1000:MPD:H4	1.97	0.63
1:B:108:THR:HG22	1:B:110:GLU:H	1.62	0.63
1:B:386:GLU:HG3	6:B:2624:HOH:O	1.98	0.63
1:B:214:VAL:HG22	1:B:224:GLU:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:HD21	1:A:101:LYS:HA	1.63	0.63
1:B:210:ARG:O	1:B:214:VAL:HG23	1.99	0.63
1:B:157:ALA:HB1	1:B:184:LYS:HD2	1.80	0.62
1:B:173:MET:HG3	6:B:2709:HOH:O	1.99	0.62
1:B:204:LYS:HG2	1:B:205:VAL:HG13	1.81	0.62
1:A:92:ILE:HG21	1:A:117:PRO:HG2	1.81	0.61
1:A:48:LYS:HE3	1:A:50:ASN:HD21	1.64	0.61
1:B:281:ARG:HH11	1:B:281:ARG:HG2	1.65	0.61
1:B:296:PRO:HA	1:B:386:GLU:HG2	1.83	0.61
1:B:242:VAL:HG23	6:B:2778:HOH:O	1.99	0.60
1:A:162:LYS:HG2	1:A:166:ASP:OD2	2.02	0.60
1:B:217:PHE:HE2	1:B:227:ILE:HD11	1.67	0.60
1:B:87:ASN:HB3	1:B:92:ILE:O	2.02	0.60
1:B:396:ASP:O	1:B:400:GLU:HG3	2.02	0.59
1:B:217:PHE:CE2	1:B:227:ILE:HD11	2.37	0.59
1:B:324:GLU:O	1:B:328:GLN:HG3	2.02	0.59
1:B:59:SER:O	1:B:63:LYS:HG3	2.02	0.59
1:B:215:ASN:ND2	1:B:218:ARG:HH22	2.00	0.59
1:A:295:ILE:N	1:A:295:ILE:HD12	2.17	0.58
1:B:50:ASN:HB2	6:B:2712:HOH:O	2.04	0.58
1:A:411:LEU:HD12	1:A:412:LYS:N	2.18	0.58
1:B:185:VAL:HG21	1:B:229:LEU:HB3	1.84	0.58
1:B:367:ILE:HG13	1:B:390:LEU:HD13	1.85	0.58
1:A:242:VAL:HG13	6:A:1607:HOH:O	2.03	0.57
1:A:307:GLU:O	1:A:311:LYS:HG3	2.04	0.57
1:A:295:ILE:H	1:A:295:ILE:CD1	2.17	0.57
1:A:157:ALA:HB1	1:A:184:LYS:HD2	1.84	0.57
1:A:352:LYS:HB2	1:A:352:LYS:NZ	2.20	0.57
1:A:289:ALA:O	1:A:290:ASP:HB2	2.04	0.56
1:A:395:LEU:O	1:A:399:THR:HG23	2.05	0.56
1:A:317:ARG:HD2	1:A:322:VAL:O	2.04	0.56
1:A:108:THR:HG22	1:A:110:GLU:H	1.70	0.56
1:B:43:GLU:OE2	1:B:47:ARG:NH1	2.39	0.56
1:A:15:ASP:OD2	1:A:17:PRO:HD2	2.06	0.56
1:B:289:ALA:O	1:B:290:ASP:HB2	2.05	0.56
1:B:165:ILE:HG22	1:B:169:LYS:HE3	1.88	0.55
1:B:214:VAL:HG12	1:B:218:ARG:NH1	2.21	0.55
1:B:222:ILE:O	1:B:223:ALA:HB3	2.07	0.55
1:B:185:VAL:O	1:B:189:ILE:HG12	2.06	0.55
1:A:167:ILE:O	1:A:171:ILE:HG13	2.08	0.54
1:B:367:ILE:CG1	1:B:390:LEU:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HG3	1:B:205:VAL:HG11	1.90	0.54
1:B:358:THR:OG1	1:B:361:GLU:HG3	2.08	0.53
1:B:330:LEU:C	1:B:330:LEU:HD23	2.29	0.53
1:B:31:ARG:HD3	1:B:276:GLN:OE1	2.09	0.53
1:B:293:ASN:ND2	1:B:293:ASN:C	2.62	0.53
1:A:336:ILE:HG13	1:A:337:GLU:N	2.23	0.53
1:B:281:ARG:NH1	1:B:285:GLU:OE2	2.42	0.53
1:A:73:ALA:HB2	1:A:149:TYR:CG	2.43	0.53
1:A:171:ILE:HG23	1:A:176:LYS:HB2	1.91	0.53
1:B:218:ARG:C	1:B:220:ASN:H	2.12	0.52
1:B:345:ILE:HB	1:B:401:ASP:CG	2.30	0.52
1:B:35:SER:OG	1:B:38:ILE:HG12	2.09	0.52
1:A:86:ILE:O	1:A:90:ARG:HD3	2.09	0.52
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.75	0.51
1:B:203:GLU:O	1:B:207:GLN:HG2	2.11	0.51
1:A:367:ILE:CG1	1:A:390:LEU:HD13	2.39	0.51
1:B:372:LEU:HD12	6:B:2553:HOH:O	2.10	0.51
1:B:244:MET:HE3	1:B:263:LEU:HD13	1.93	0.51
1:A:115:LYS:HG2	1:A:123:VAL:HG22	1.93	0.51
1:A:336:ILE:HD11	1:A:340:GLN:HG3	1.92	0.51
1:B:309:LEU:HD21	1:B:387:ILE:HG13	1.92	0.51
1:B:129:GLY:O	1:B:133:THR:HG23	2.11	0.50
1:B:86:ILE:O	1:B:90:ARG:HD3	2.11	0.50
1:A:306:LEU:HD11	1:A:310:LYS:CE	2.39	0.50
1:A:306:LEU:HD13	1:A:306:LEU:C	2.32	0.50
1:A:386:GLU:HG3	6:A:1661:HOH:O	2.11	0.50
1:B:161:LYS:O	1:B:165:ILE:HG12	2.12	0.50
1:B:182:ARG:HB3	1:B:229:LEU:HD23	1.94	0.50
1:B:405:LEU:O	1:B:409:ILE:HG13	2.12	0.50
1:B:138:ASP:O	1:B:142:GLU:HG3	2.13	0.49
1:A:285:GLU:HG2	1:A:388:PHE:CE2	2.47	0.49
1:A:407:LYS:O	1:A:411:LEU:HG	2.12	0.49
1:A:105:VAL:HG23	6:A:1724:HOH:O	2.12	0.49
1:B:73:ALA:HB2	1:B:149:TYR:CG	2.48	0.48
1:A:215:ASN:O	1:A:219:GLU:HB2	2.13	0.48
1:A:186:ASP:O	1:A:190:THR:HG23	2.14	0.48
1:B:281:ARG:HG2	1:B:281:ARG:NH1	2.29	0.48
1:A:182:ARG:HB3	1:A:229:LEU:HD22	1.96	0.48
1:B:189:ILE:HD13	1:B:205:VAL:CG2	2.43	0.48
1:B:256:ARG:HB3	1:B:277:PHE:HE2	1.79	0.48
1:A:31:ARG:HD2	1:A:273:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:O	1:B:46:MET:HG3	2.13	0.47
1:A:38:ILE:O	1:A:42:ILE:HG13	2.13	0.47
1:A:302:LEU:HD12	1:A:302:LEU:N	2.29	0.47
1:B:234:ASN:HD22	1:B:234:ASN:C	2.16	0.47
1:A:109:MET:SD	1:A:133:THR:HG22	2.55	0.47
1:A:35:SER:OG	1:A:38:ILE:HG12	2.14	0.47
1:A:34:ILE:HD11	1:A:38:ILE:CG2	2.44	0.47
1:A:146:PHE:HB2	1:A:174:MET:HE1	1.97	0.47
1:B:306:LEU:HD11	1:B:359:ILE:CD1	2.45	0.46
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.80	0.46
1:A:405:LEU:O	1:A:409:ILE:HG13	2.15	0.46
1:B:43:GLU:HG2	1:B:47:ARG:HH11	1.80	0.46
1:B:110:GLU:HG3	6:B:2663:HOH:O	2.14	0.46
1:B:116:HIS:CD2	1:B:262:SER:HB2	2.50	0.46
1:B:17:PRO:CB	1:B:47:ARG:NH1	2.73	0.46
1:A:174:MET:HE3	1:A:176:LYS:HG3	1.95	0.46
1:B:45:ARG:NH1	1:B:57:ALA:HB2	2.30	0.46
1:A:345:ILE:HB	1:A:401:ASP:CG	2.35	0.46
1:A:285:GLU:HG2	1:A:388:PHE:HE2	1.80	0.46
1:A:116:HIS:CD2	1:A:262:SER:HB2	2.51	0.46
1:A:119:ILE:HG23	6:A:1715:HOH:O	2.15	0.46
1:A:90:ARG:NH1	1:A:92:ILE:HD11	2.31	0.45
1:B:359:ILE:HG23	1:B:360:GLN:N	2.31	0.45
1:A:334:TRP:O	1:A:336:ILE:N	2.44	0.45
1:B:238:TYR:N	1:B:238:TYR:CD2	2.83	0.45
1:B:225:PRO:O	1:B:227:ILE:HG13	2.17	0.45
1:A:411:LEU:HD12	1:A:411:LEU:C	2.37	0.45
1:A:367:ILE:HG12	1:A:390:LEU:HD13	1.98	0.45
1:B:17:PRO:HB2	1:B:47:ARG:HH12	1.76	0.45
1:A:309:LEU:HD11	1:A:390:LEU:HD23	1.98	0.45
1:B:189:ILE:HD11	1:B:206:LEU:CD2	2.47	0.45
1:B:110:GLU:N	1:B:110:GLU:OE2	2.49	0.45
1:B:281:ARG:O	1:B:285:GLU:HG3	2.17	0.45
1:A:298:LEU:HB2	1:A:367:ILE:HD12	1.98	0.45
1:B:295:ILE:HB	6:B:2766:HOH:O	2.15	0.45
1:B:306:LEU:HD11	1:B:359:ILE:HD11	1.98	0.45
1:A:182:ARG:HH11	1:A:209:ILE:HG23	1.79	0.44
1:B:108:THR:HG23	6:B:2769:HOH:O	2.16	0.44
1:A:92:ILE:CG2	1:A:117:PRO:HG2	2.47	0.44
1:A:106:GLU:N	1:A:106:GLU:OE1	2.50	0.44
1:B:215:ASN:HD22	1:B:218:ARG:HH12	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LYS:C	1:B:414:GLY:H	2.21	0.44
1:A:136:PRO:HD2	1:A:139:THR:HB	1.99	0.44
1:A:302:LEU:HD12	1:A:302:LEU:H	1.83	0.44
1:B:230:LEU:C	1:B:230:LEU:HD12	2.38	0.44
1:B:215:ASN:O	1:B:219:GLU:HG2	2.19	0.43
1:B:240:PHE:N	1:B:241:PRO:CD	2.82	0.43
1:A:73:ALA:HB2	1:A:149:TYR:CD1	2.53	0.43
1:B:45:ARG:HB3	1:B:50:ASN:OD1	2.19	0.43
1:B:204:LYS:C	1:B:206:LEU:H	2.22	0.43
1:A:171:ILE:CG2	1:A:176:LYS:HB2	2.48	0.43
1:B:334:TRP:CD2	1:B:412:LYS:HE3	2.54	0.43
1:B:372:LEU:O	1:B:372:LEU:HD13	2.19	0.43
1:A:119:ILE:CG2	6:A:1715:HOH:O	2.66	0.43
1:B:127:LEU:HA	1:B:128:PRO:HD3	1.91	0.42
1:A:413:LEU:C	1:A:415:ARG:H	2.23	0.42
1:A:90:ARG:HB3	1:A:117:PRO:HD3	2.01	0.42
1:A:328:GLN:O	1:A:331:ALA:HB3	2.18	0.42
1:A:367:ILE:HG13	1:A:390:LEU:HD13	2.01	0.42
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.34	0.42
1:B:88:THR:HG23	1:B:235:VAL:HG22	2.01	0.42
1:A:295:ILE:HA	1:A:296:PRO:HD3	1.94	0.42
1:B:156:SER:O	1:B:182:ARG:HA	2.19	0.42
1:B:293:ASN:HD22	1:B:294:ILE:N	2.17	0.41
1:B:330:LEU:HD12	5:B:1000:MPD:C5	2.50	0.41
1:A:156:SER:O	1:A:182:ARG:HD2	2.20	0.41
1:B:203:GLU:N	1:B:203:GLU:OE1	2.54	0.41
1:A:301:LEU:CD2	1:A:359:ILE:HG23	2.49	0.41
1:B:157:ALA:CB	1:B:184:LYS:HD2	2.49	0.41
1:A:275:ARG:O	1:A:279:LYS:HG3	2.20	0.41
1:A:301:LEU:HD21	1:A:306:LEU:HD23	2.02	0.41
1:A:380:LYS:O	1:A:381:ASN:HB2	2.20	0.41
1:B:295:ILE:HA	1:B:296:PRO:HD3	1.92	0.41
1:B:372:LEU:C	1:B:372:LEU:HD13	2.42	0.41
1:A:94:ASN:ND2	1:A:101:LYS:HA	2.32	0.41
1:A:138:ASP:O	1:A:142:GLU:HG3	2.21	0.41
1:A:45:ARG:HD3	1:A:53:LEU:CB	2.47	0.40
1:B:191:ASN:N	1:B:191:ASN:HD22	2.20	0.40
1:A:63:LYS:HG3	6:A:1772:HOH:O	2.22	0.40
1:A:16:LEU:HB2	1:A:17:PRO:HD3	2.04	0.40
1:A:329:ARG:HG3	1:A:329:ARG:NH1	2.35	0.40
1:B:307:GLU:O	1:B:311:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:O	1:B:224:GLU:C	2.60	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	391/422 (93%)	372 (95%)	16 (4%)	3 (1%)	24	15
1	B	388/422 (92%)	369 (95%)	17 (4%)	2 (0%)	34	26
All	All	779/844 (92%)	741 (95%)	33 (4%)	5 (1%)	30	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	VAL
1	A	203	GLU
1	B	224	GLU
1	A	290	ASP
1	A	335	GLU

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/386 (93%)	351 (98%)	8 (2%)	60	62
1	B	356/386 (92%)	346 (97%)	10 (3%)	51	50
All	All	715/772 (93%)	697 (98%)	18 (2%)	55	55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	138	ASP
1	A	174	MET
1	A	240	PHE
1	A	251	LEU
1	A	333	ASP
1	A	359	ILE
1	A	390	LEU
1	B	77	GLU
1	B	173	MET
1	B	203	GLU
1	B	205	VAL
1	B	234	ASN
1	B	235	VAL
1	B	240	PHE
1	B	251	LEU
1	B	293	ASN
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	87	ASN
1	A	94	ASN
1	A	191	ASN
1	A	215	ASN
1	A	293	ASN
1	A	328	GLN
1	B	134	ASN
1	B	163	ASN

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Mol	Chain	Res	Type
1	B	191	ASN
1	B	215	ASN
1	B	234	ASN
1	B	237	HIS
1	B	258	ASN
1	B	293	ASN
1	B	368	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GDP	A	1500	2	23,30,30	1.89	5 (21%)	30,47,47	2.69	11 (36%)
5	MPD	B	1000	-	6,7,7	0.74	0	7,10,10	0.76	0
4	EDO	B	2000	-	3,3,3	0.78	0	2,2,2	0.42	0
3	GDP	B	2500	2	23,30,30	1.88	5 (21%)	30,47,47	2.64	11 (36%)

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	GDP	A	1500	2	-	0/12/32/32	0/3/3/3
5	MPD	B	1000	-	-	0/5/5/5	0/0/0/0
4	EDO	B	2000	-	-	0/1/1/1	0/0/0/0
3	GDP	B	2500	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	2500	GDP	C8-N7	-2.15	1.30	1.34
3	A	1500	GDP	C8-N7	-2.06	1.30	1.34
3	B	2500	GDP	C6-C5	2.23	1.45	1.41
3	A	1500	GDP	C6-C5	2.42	1.46	1.41
3	A	1500	GDP	C4-N3	2.54	1.39	1.35
3	B	2500	GDP	C4-N3	2.54	1.39	1.35
3	A	1500	GDP	C2-N1	2.81	1.40	1.35
3	B	2500	GDP	C2-N1	2.92	1.40	1.35
3	B	2500	GDP	C6-N1	6.36	1.44	1.33
3	A	1500	GDP	C6-N1	6.55	1.45	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1500	GDP	C5-C6-N1	-7.66	113.12	123.59
3	B	2500	GDP	C5-C6-N1	-7.61	113.18	123.59
3	A	1500	GDP	C1'-N9-C4	-4.69	119.86	126.94
3	B	2500	GDP	C1'-N9-C4	-3.86	121.11	126.94
3	A	1500	GDP	C6-C5-C4	-3.48	116.74	120.90
3	B	2500	GDP	PA-O3A-PB	-3.35	121.43	132.67
3	A	1500	GDP	N3-C2-N1	-3.31	122.40	127.44
3	B	2500	GDP	N3-C2-N1	-3.27	122.46	127.44
3	B	2500	GDP	C6-C5-C4	-3.22	117.04	120.90
3	A	1500	GDP	PA-O3A-PB	-3.05	122.45	132.67
3	A	1500	GDP	O3'-C3'-C4'	-2.34	104.03	111.05
3	A	1500	GDP	O4'-C4'-C3'	-2.33	100.45	105.15
3	B	2500	GDP	O3'-C3'-C4'	-2.13	104.66	111.05
3	B	2500	GDP	O4'-C4'-C3'	-2.07	100.97	105.15
3	B	2500	GDP	O2A-PA-O5'	2.33	120.21	108.46
3	A	1500	GDP	O2A-PA-O5'	2.38	120.44	108.46
3	B	2500	GDP	O2A-PA-O3A	3.03	118.82	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	1500	GDP	O2A-PA-O3A	3.20	119.59	105.09
3	A	1500	GDP	C4'-O4'-C1'	3.28	113.32	109.72
3	B	2500	GDP	C4'-O4'-C1'	3.43	113.49	109.72
3	B	2500	GDP	C6-N1-C2	6.53	125.00	115.94
3	A	1500	GDP	C6-N1-C2	6.56	125.04	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1000	MPD	2	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

### 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	395/422 (93%)	0.55	42 (10%) 8 9	24, 40, 76, 81	0
1	B	392/422 (92%)	0.51	41 (10%) 8 9	22, 38, 79, 81	0
All	All	787/844 (93%)	0.53	83 (10%) 8 9	22, 39, 79, 81	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	9.9
1	A	414	GLY	8.2
1	A	411	LEU	7.7
1	A	194	ASP	7.7
1	A	413	LEU	5.6
1	B	189	ILE	5.5
1	A	415	ARG	5.2
1	B	192	GLU	5.0
1	A	332	ARG	4.8
1	B	414	GLY	4.6
1	A	334	TRP	4.3
1	B	205	VAL	4.2
1	B	415	ARG	4.2
1	B	215	ASN	4.1
1	B	190	THR	3.8
1	A	335	GLU	3.8
1	A	192	GLU	3.7
1	B	153	ILE	3.6
1	A	134	ASN	3.5
1	A	412	LYS	3.5
1	A	410	CYS	3.4
1	B	207	GLN	3.4
1	A	336	ILE	3.3
1	A	107	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	221	GLY	3.3
1	A	337	GLU	3.2
1	A	89	LEU	3.1
1	B	206	LEU	3.1
1	B	203	GLU	3.1
1	B	208	ASP	3.1
1	B	219	GLU	3.1
1	A	338	VAL	3.1
1	B	413	LEU	3.1
1	A	333	ASP	3.0
1	A	181	VAL	2.9
1	B	155	ILE	2.9
1	B	188	ASP	2.9
1	B	218	ARG	2.9
1	B	105	VAL	2.9
1	A	203	GLU	2.9
1	A	339	ASP	2.8
1	A	331	ALA	2.8
1	B	89	LEU	2.8
1	A	190	THR	2.8
1	B	14	ASN	2.8
1	A	204	LYS	2.8
1	A	155	ILE	2.7
1	A	135	PHE	2.7
1	B	410	CYS	2.6
1	B	106	GLU	2.6
1	A	154	ILE	2.6
1	B	300	PHE	2.6
1	B	211	LEU	2.6
1	B	372	LEU	2.6
1	A	153	ILE	2.5
1	A	282	ILE	2.5
1	A	85	PHE	2.5
1	A	73	ALA	2.4
1	B	183	THR	2.4
1	B	230	LEU	2.4
1	A	53	LEU	2.4
1	A	211	LEU	2.4
1	B	213	CYS	2.4
1	B	212	ASN	2.4
1	B	134	ASN	2.3
1	A	408	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	224	GLU	2.3
1	B	107	VAL	2.3
1	A	340	GLN	2.3
1	B	411	LEU	2.3
1	A	234	ASN	2.3
1	B	159	ARG	2.3
1	A	263	LEU	2.2
1	B	108	THR	2.2
1	B	74	VAL	2.2
1	A	191	ASN	2.2
1	A	74	VAL	2.2
1	B	214	VAL	2.1
1	B	92	ILE	2.1
1	A	14	ASN	2.1
1	A	341	VAL	2.1
1	B	103	GLY	2.0
1	B	209	ILE	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	EDO	B	2000	4/4	0.89	0.31	4.23	66,67,67,67	0
5	MPD	B	1000	8/8	0.87	0.21	2.17	41,47,54,56	0
3	GDP	A	1500	28/28	0.96	0.12	-0.62	34,41,45,46	0
3	GDP	B	2500	28/28	0.95	0.13	-0.98	39,55,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	1501	1/1	0.96	0.39	-	29,29,29,29	0
2	MG	B	2501	1/1	0.99	0.18	-	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.