



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:27 AM GMT

PDB ID : 1TQ2  
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 : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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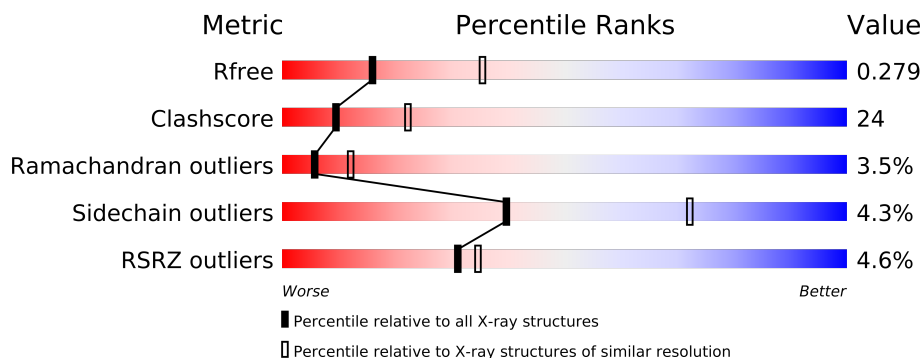
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MPD	B	1000	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6573 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3181	2053	520	594	14			

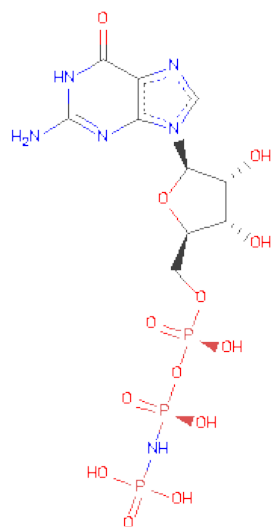
There are 22 discrepancies between the modelled and reference sequences:

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).

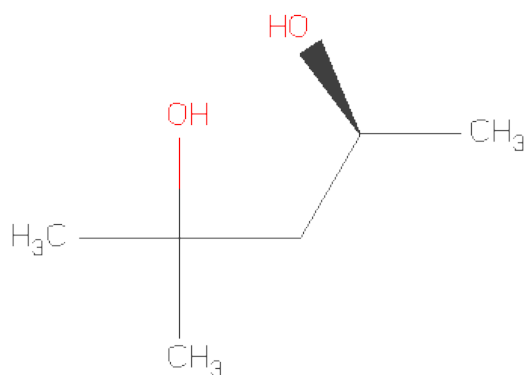
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



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

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



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

- Molecule 5 is water.

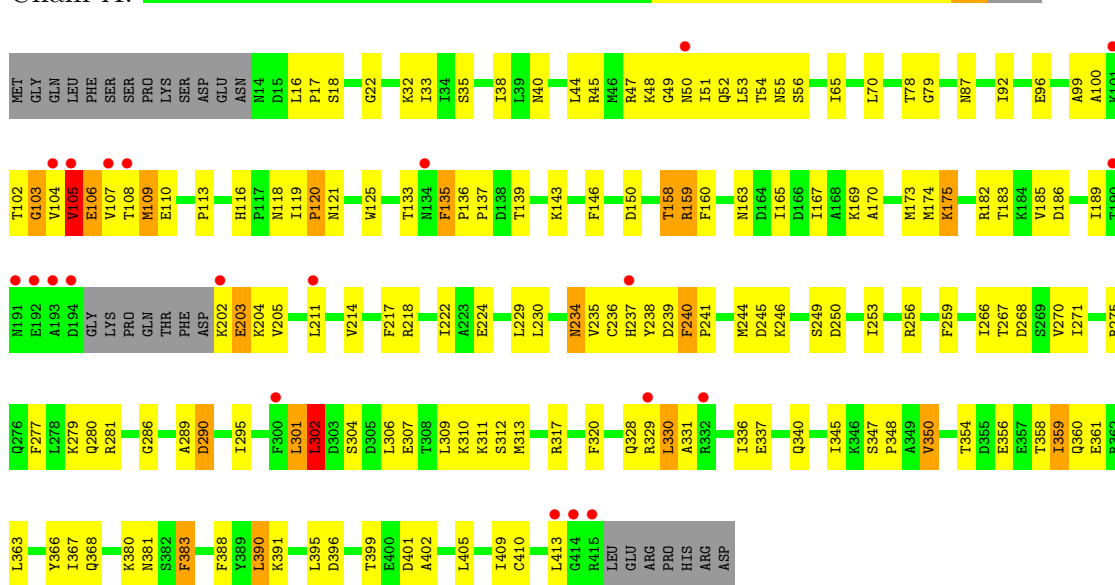
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	69	Total	O	0	0
			69	69		

### 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

Chain A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.86Å 92.67Å 142.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-2.70) 93.4 (19.96-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.280 0.223 , 0.279	Depositor DCC
$R_{free}$ test set	1419 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28362 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/3264	0.61	0/4404
1	B	0.41	0/3245	0.60	0/4379
All	All	0.40	0/6509	0.60	0/8783

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3200	0	3236	172	0
1	B	3181	0	3216	152	0
2	B	1	0	0	0	0
3	A	32	0	13	2	0
3	B	32	0	13	2	0
4	B	8	0	14	7	0
5	A	50	0	0	10	0
5	B	69	0	0	11	0
All	All	6573	0	6492	317	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (317) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:105:VAL:HG12	1:B:106:GLU:H	1.24	1.01
1:A:340:GLN:HG3	5:A:506:HOH:O	1.68	0.90
1:A:45:ARG:HD3	1:A:53:LEU:HB3	1.56	0.88
1:B:159:ARG:HB3	1:B:216:THR:HG21	1.57	0.86
1:A:87:ASN:HD21	1:A:100:ALA:H	1.27	0.82
1:A:306:LEU:HD11	1:A:310:LYS:HE3	1.61	0.82
1:B:94:ASN:HD22	1:B:102:THR:HG21	1.45	0.80
1:A:44:LEU:HD13	1:B:44:LEU:HD13	1.63	0.80
1:A:202:LYS:HG2	1:A:203:GLU:H	1.47	0.80
1:B:365:ARG:O	1:B:369:GLU:HG3	1.82	0.79
1:A:354:THR:HG22	1:A:356:GLU:H	1.47	0.78
1:B:92:ILE:HD11	1:B:117:PRO:HG3	1.63	0.78
1:A:230:LEU:HD22	1:A:240:PHE:CD1	2.18	0.78
1:B:281:ARG:HH11	1:B:281:ARG:HG2	1.50	0.77
1:A:202:LYS:HG2	1:A:203:GLU:HG2	1.67	0.77
1:B:359:ILE:O	1:B:359:ILE:HG12	1.83	0.77
5:A:511:HOH:O	1:B:138:ASP:HB3	1.86	0.76
1:A:301:LEU:O	1:A:302:LEU:HB2	1.85	0.75
1:B:298:LEU:HD11	1:B:301:LEU:HD22	1.69	0.74
1:A:359:ILE:HD13	1:A:363:LEU:HG	1.70	0.74
1:B:253:ILE:HB	4:B:1000:MPD:HM2	1.69	0.74
1:A:367:ILE:HG13	1:A:390:LEU:HD13	1.68	0.73
1:B:289:ALA:O	1:B:290:ASP:HB2	1.88	0.73
1:B:215:ASN:HD22	1:B:218:ARG:HH12	1.34	0.73
1:A:78:THR:HA	3:A:500:GNP:O1G	1.89	0.72
1:B:105:VAL:HG12	1:B:106:GLU:N	2.03	0.72
1:A:302:LEU:HD12	1:A:304:SER:H	1.53	0.72
1:A:92:ILE:HD11	1:A:99:ALA:HA	1.73	0.71
1:A:266:ILE:HG13	1:A:267:THR:N	2.07	0.70
1:A:189:ILE:HD11	1:A:202:LYS:HD3	1.74	0.69
1:B:209:ILE:HA	1:B:212:ASN:HD22	1.56	0.69
1:A:267:THR:HG22	1:A:268:ASP:N	2.08	0.69
1:A:102:THR:HB	1:A:105:VAL:HG22	1.75	0.69
1:A:358:THR:OG1	1:A:361:GLU:HG3	1.92	0.68
1:B:94:ASN:HD22	1:B:102:THR:CG2	2.07	0.68
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.57	0.68
1:A:211:LEU:HA	1:A:214:VAL:HG12	1.77	0.66
1:B:266:ILE:HG13	1:B:267:THR:HG23	1.78	0.66
1:A:202:LYS:CG	1:A:203:GLU:H	2.09	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:246:LYS:HE2	1:B:250:ASP:OD1	1.96	0.65
1:B:296:PRO:HA	1:B:386:GLU:HG2	1.76	0.65
1:A:51:ILE:HA	1:A:54:THR:HG22	1.77	0.65
1:A:214:VAL:HG23	1:A:224:GLU:HG3	1.79	0.65
1:B:358:THR:OG1	1:B:361:GLU:HG3	1.97	0.65
1:B:73:ALA:HB2	1:B:149:TYR:CG	2.32	0.64
1:A:158:THR:OG1	1:A:159:ARG:N	2.31	0.64
1:B:158:THR:HA	1:B:182:ARG:HH21	1.63	0.63
1:B:105:VAL:CG1	1:B:106:GLU:H	2.07	0.63
1:A:238:TYR:O	1:A:241:PRO:HD2	1.99	0.63
1:A:106:GLU:C	1:A:108:THR:H	2.02	0.63
1:A:33:ILE:H	1:A:280:GLN:NE2	1.97	0.62
1:B:108:THR:HG23	1:B:128:PRO:HB3	1.82	0.62
1:A:202:LYS:HG2	1:A:203:GLU:N	2.14	0.62
1:A:51:ILE:HA	1:A:54:THR:CG2	2.30	0.62
1:B:350:VAL:HG23	1:B:351:PHE:CD2	2.35	0.62
1:B:92:ILE:HD11	1:B:117:PRO:CG	2.30	0.61
1:A:236:CYS:HB2	1:A:266:ILE:HD12	1.82	0.61
1:A:211:LEU:O	1:A:214:VAL:HG12	2.01	0.61
1:B:235:VAL:HB	1:B:266:ILE:HG21	1.83	0.61
1:A:51:ILE:N	1:A:51:ILE:HD12	2.16	0.61
1:B:275:ARG:O	1:B:279:LYS:HG3	2.01	0.60
1:A:169:LYS:HD3	1:B:169:LYS:HD3	1.83	0.60
1:B:386:GLU:HG3	5:B:1558:HOH:O	2.01	0.60
1:A:120:PRO:O	1:A:121:ASN:HB2	2.01	0.60
1:A:33:ILE:H	1:A:280:GLN:HE22	1.49	0.60
1:A:301:LEU:O	1:A:302:LEU:CB	2.49	0.59
1:A:313:MET:O	1:A:317:ARG:HG3	2.02	0.59
1:A:135:PHE:HD2	1:A:135:PHE:N	1.99	0.59
1:A:347:SER:HB2	1:A:401:ASP:OD2	2.02	0.59
1:A:405:LEU:O	1:A:409:ILE:HG13	2.03	0.59
1:A:70:LEU:HD12	1:A:150:ASP:OD2	2.02	0.59
1:A:186:ASP:O	1:A:189:ILE:HG22	2.01	0.59
1:B:345:ILE:HB	1:B:401:ASP:CG	2.23	0.59
1:B:16:LEU:HB2	1:B:17:PRO:HD3	1.83	0.59
1:A:189:ILE:HD11	1:A:202:LYS:CD	2.33	0.58
1:A:135:PHE:N	1:A:135:PHE:CD2	2.68	0.58
1:B:159:ARG:HB3	1:B:216:THR:CG2	2.29	0.58
1:B:254:TYR:H	4:B:1000:MPD:HM1	1.68	0.58
1:A:79:GLY:H	3:A:500:GNP:HNB3	1.49	0.58
1:A:337:GLU:O	1:A:340:GLN:HB2	2.03	0.58
1:A:70:LEU:HD22	1:A:259:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:82:LYS:HE3	1:B:127:LEU:O	2.03	0.58
1:B:223:ALA:O	1:B:225:PRO:HD3	2.04	0.58
1:B:297:SER:HB3	1:B:299:THR:HG23	1.85	0.57
1:A:306:LEU:CD1	1:A:310:LYS:HE3	2.32	0.57
1:B:159:ARG:CZ	1:B:212:ASN:HB3	2.35	0.56
1:A:53:LEU:HA	1:A:56:SER:HB3	1.86	0.56
1:B:50:ASN:HD21	1:B:52:GLN:HG2	1.69	0.56
1:B:157:ALA:HB1	1:B:184:LYS:HD2	1.88	0.56
1:A:170:ALA:O	1:A:174:MET:HG2	2.06	0.56
1:B:101:LYS:HD2	1:B:105:VAL:HG13	1.88	0.56
1:A:336:ILE:HG13	5:A:506:HOH:O	2.05	0.56
1:A:256:ARG:HB3	1:A:277:PHE:HE2	1.70	0.56
1:B:136:PRO:HB2	1:B:138:ASP:OD1	2.06	0.55
1:B:159:ARG:NH1	1:B:212:ASN:HB3	2.21	0.55
1:A:320:PHE:CZ	1:A:399:THR:HG22	2.42	0.55
1:B:101:LYS:HD2	1:B:105:VAL:CG1	2.36	0.55
1:B:281:ARG:NH1	1:B:281:ARG:HG2	2.22	0.55
1:A:116:HIS:HB3	1:A:119:ILE:O	2.07	0.55
1:A:51:ILE:H	1:A:51:ILE:HD12	1.72	0.55
1:A:281:ARG:HH11	1:A:281:ARG:HG2	1.72	0.55
1:B:165:ILE:HG23	1:B:222:ILE:HD12	1.89	0.55
1:B:188:ASP:O	1:B:205:VAL:HG11	2.06	0.54
1:B:359:ILE:O	1:B:359:ILE:CG1	2.54	0.54
1:B:298:LEU:C	1:B:300:PHE:H	2.11	0.54
1:A:104:VAL:HG22	5:A:512:HOH:O	2.06	0.54
1:A:312:SER:OG	1:A:391:LYS:HD3	2.08	0.54
1:A:350:VAL:HG13	1:A:366:TYR:HE2	1.73	0.54
1:B:38:ILE:HG13	4:B:1000:MPD:H51	1.89	0.54
1:B:359:ILE:N	5:B:1564:HOH:O	2.37	0.53
1:B:50:ASN:HB3	5:B:1508:HOH:O	2.08	0.53
1:B:78:THR:HA	3:B:1500:GNP:O1G	2.08	0.53
1:A:165:ILE:N	1:A:165:ILE:HD12	2.22	0.53
1:B:367:ILE:HG13	1:B:390:LEU:HD13	1.90	0.53
1:A:32:LYS:HA	1:A:280:GLN:HE22	1.74	0.53
1:B:185:VAL:O	1:B:189:ILE:HG12	2.07	0.53
1:A:320:PHE:CE2	1:A:399:THR:HG22	2.44	0.53
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.73	0.53
1:A:51:ILE:CA	1:A:54:THR:HG22	2.37	0.53
1:A:395:LEU:O	1:A:399:THR:HG23	2.09	0.53
1:A:267:THR:HG22	1:A:268:ASP:H	1.74	0.53
1:B:108:THR:HG22	5:B:1503:HOH:O	2.09	0.52
1:B:136:PRO:HD2	1:B:139:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:LYS:HE3	1:A:250:ASP:OD1	2.10	0.52
1:A:309:LEU:HD11	1:A:390:LEU:HD23	1.92	0.52
1:A:44:LEU:CD1	1:B:44:LEU:HD13	2.36	0.52
1:A:236:CYS:CB	1:A:266:ILE:HD12	2.40	0.52
1:B:254:TYR:H	4:B:1000:MPD:CM	2.22	0.52
1:A:240:PHE:HB3	1:A:241:PRO:HD3	1.91	0.52
1:A:133:THR:HB	1:A:135:PHE:CD2	2.45	0.52
1:A:217:PHE:HB3	1:A:222:ILE:HD11	1.92	0.52
1:A:165:ILE:H	1:A:165:ILE:HD12	1.75	0.52
1:A:249:SER:HA	1:A:256:ARG:HH21	1.73	0.52
1:A:380:LYS:HG2	1:A:381:ASN:ND2	2.25	0.52
1:A:52:GLN:H	1:A:52:GLN:CD	2.12	0.52
1:B:138:ASP:CG	1:B:139:THR:N	2.64	0.51
1:A:40:ASN:O	1:A:44:LEU:HB2	2.10	0.51
1:A:183:THR:HG22	1:A:230:LEU:HD11	1.93	0.51
1:A:345:ILE:HB	1:A:401:ASP:CG	2.31	0.51
1:A:229:LEU:O	1:A:239:ASP:HB2	2.10	0.51
1:B:107:VAL:O	1:B:109:MET:HG3	2.11	0.51
1:B:298:LEU:CD1	1:B:301:LEU:HD13	2.41	0.51
1:A:48:LYS:HE2	1:B:47:ARG:CZ	2.40	0.50
1:A:240:PHE:HD2	1:A:244:MET:CE	2.23	0.50
1:A:175:LYS:O	1:A:175:LYS:HG2	2.12	0.50
1:A:359:ILE:O	1:A:359:ILE:HD13	2.11	0.50
1:A:33:ILE:HG21	1:A:280:GLN:HB3	1.94	0.50
1:A:266:ILE:HG12	1:A:270:VAL:HG21	1.94	0.50
1:B:358:THR:C	1:B:360:GLN:H	2.15	0.50
1:B:94:ASN:ND2	1:B:102:THR:CG2	2.74	0.50
1:B:88:THR:HG21	1:B:235:VAL:HG13	1.94	0.50
1:A:107:VAL:O	1:A:108:THR:HG23	2.11	0.50
1:A:281:ARG:NH1	1:A:281:ARG:HG2	2.27	0.50
1:A:202:LYS:HE2	1:A:203:GLU:OE2	2.12	0.50
1:A:183:THR:HG22	1:A:230:LEU:CD1	2.42	0.50
1:A:146:PHE:CE1	1:A:174:MET:HG3	2.47	0.50
1:A:410:CYS:O	1:A:413:LEU:HG	2.11	0.50
1:B:298:LEU:HD11	1:B:301:LEU:HD13	1.93	0.50
1:A:267:THR:CG2	1:A:268:ASP:N	2.74	0.50
1:B:134:ASN:HA	5:B:1560:HOH:O	2.11	0.50
1:A:133:THR:HA	5:A:513:HOH:O	2.10	0.49
1:B:367:ILE:CG1	1:B:390:LEU:HD13	2.42	0.49
1:A:214:VAL:O	1:A:218:ARG:HD3	2.12	0.49
1:A:113:PRO:HB3	1:A:125:TRP:CZ3	2.47	0.49
1:A:45:ARG:CD	1:A:53:LEU:HB3	2.36	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:ILE:HG23	1:A:320:PHE:CD2	2.48	0.49
1:B:345:ILE:HB	1:B:401:ASP:OD1	2.13	0.49
1:A:102:THR:HB	1:A:105:VAL:CG2	2.41	0.49
1:B:238:TYR:N	1:B:238:TYR:CD2	2.80	0.49
1:A:33:ILE:HG22	1:A:280:GLN:NE2	2.28	0.49
1:B:77:GLU:HG2	1:B:78:THR:N	2.28	0.49
1:A:289:ALA:O	1:A:290:ASP:HB2	2.13	0.49
1:A:103:GLY:HA2	5:A:501:HOH:O	2.12	0.49
1:B:37:GLU:HB2	5:B:1527:HOH:O	2.13	0.49
1:A:48:LYS:HE2	1:B:47:ARG:NH2	2.28	0.48
1:A:173:MET:CE	1:B:169:LYS:HA	2.43	0.48
1:B:380:LYS:O	1:B:381:ASN:HB2	2.13	0.48
1:A:217:PHE:CD2	1:A:222:ILE:HD11	2.49	0.48
1:A:202:LYS:CG	1:A:203:GLU:N	2.73	0.48
1:B:77:GLU:HG2	1:B:78:THR:H	1.79	0.48
1:A:106:GLU:C	1:A:108:THR:N	2.63	0.48
1:B:116:HIS:HB3	1:B:119:ILE:O	2.13	0.48
1:A:136:PRO:HD2	1:A:139:THR:HB	1.95	0.48
1:B:108:THR:CG2	1:B:128:PRO:HB3	2.43	0.48
1:B:302:LEU:H	1:B:302:LEU:HD12	1.79	0.48
1:A:354:THR:HG22	1:A:356:GLU:N	2.23	0.47
1:B:301:LEU:HD21	1:B:306:LEU:HD13	1.96	0.47
1:B:222:ILE:O	1:B:223:ALA:O	2.32	0.47
1:B:138:ASP:OD2	1:B:139:THR:HG23	2.15	0.47
1:A:54:THR:HG23	1:A:55:ASN:N	2.30	0.47
1:A:165:ILE:HG22	1:A:169:LYS:HE3	1.96	0.47
1:B:141:LEU:HD12	1:B:141:LEU:C	2.35	0.47
1:B:28:ASN:HB2	5:B:1561:HOH:O	2.13	0.47
1:A:120:PRO:O	1:A:121:ASN:CB	2.63	0.47
1:A:182:ARG:HB3	1:A:229:LEU:HD23	1.96	0.47
1:B:118:ASN:O	1:B:120:PRO:HD3	2.15	0.47
1:A:106:GLU:OE1	1:A:109:MET:HA	2.15	0.46
1:A:203:GLU:C	1:A:205:VAL:H	2.18	0.46
1:B:215:ASN:HA	1:B:218:ARG:NH1	2.30	0.46
1:A:159:ARG:O	1:A:160:PHE:HB2	2.15	0.46
1:B:334:TRP:HZ3	1:B:344:MET:SD	2.38	0.46
1:B:159:ARG:O	1:B:160:PHE:C	2.53	0.46
1:B:347:SER:N	1:B:348:PRO:CD	2.79	0.46
1:A:301:LEU:HD21	1:A:306:LEU:HD23	1.97	0.46
1:B:254:TYR:HB3	4:B:1000:MPD:H32	1.97	0.46
1:A:113:PRO:HB3	1:A:125:TRP:CH2	2.51	0.46
1:B:254:TYR:HD2	4:B:1000:MPD:HM1	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:338:VAL:O	1:B:342:GLU:HG3	2.16	0.46
1:A:306:LEU:O	1:A:310:LYS:HG3	2.16	0.46
1:B:362:ARG:HB3	1:B:362:ARG:NH1	2.31	0.46
1:B:212:ASN:O	1:B:216:THR:HG23	2.16	0.45
1:B:215:ASN:HA	1:B:218:ARG:HH12	1.80	0.45
1:B:362:ARG:HG3	1:B:365:ARG:HH21	1.81	0.45
1:A:108:THR:C	1:A:110:GLU:H	2.20	0.45
1:B:302:LEU:HD12	1:B:302:LEU:N	2.31	0.45
1:B:210:ARG:O	1:B:214:VAL:HG23	2.16	0.45
1:B:185:VAL:HG21	1:B:229:LEU:HB3	1.98	0.45
1:B:347:SER:N	1:B:348:PRO:HD3	2.31	0.45
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.81	0.45
1:B:229:LEU:O	1:B:238:TYR:HB3	2.16	0.45
1:A:48:LYS:HE2	1:B:47:ARG:NH1	2.32	0.45
1:B:153:ILE:HG23	1:B:181:VAL:HG21	1.98	0.45
1:B:348:PRO:HB3	5:B:1544:HOH:O	2.17	0.45
1:B:234:ASN:OD1	1:B:237:HIS:CE1	2.69	0.45
1:A:367:ILE:HG13	1:A:390:LEU:CD1	2.44	0.45
1:A:214:VAL:HG22	1:A:218:ARG:HD3	1.99	0.45
1:A:301:LEU:HD21	1:A:306:LEU:HB2	1.98	0.45
1:A:133:THR:C	1:A:135:PHE:H	2.21	0.45
1:A:182:ARG:HD3	1:A:182:ARG:C	2.38	0.45
1:A:163:ASN:O	1:A:167:ILE:HG13	2.17	0.45
1:B:298:LEU:C	1:B:300:PHE:N	2.70	0.44
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.22	0.44
1:B:43:GLU:CD	1:B:47:ARG:HH12	2.20	0.44
1:B:246:LYS:HE2	1:B:250:ASP:CG	2.38	0.44
1:A:240:PHE:CB	1:A:241:PRO:HD3	2.48	0.44
1:A:136:PRO:HD2	1:A:139:THR:CB	2.47	0.44
1:B:133:THR:O	1:B:134:ASN:HB2	2.17	0.44
1:B:293:ASN:HD22	1:B:293:ASN:C	2.20	0.44
1:A:87:ASN:ND2	1:A:100:ALA:H	2.04	0.44
1:A:320:PHE:HB3	1:A:402:ALA:HB2	1.99	0.44
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.79	0.44
1:B:66:ASP:OD2	1:B:281:ARG:NH2	2.50	0.44
1:B:187:SER:C	1:B:189:ILE:H	2.21	0.44
1:A:234:ASN:ND2	1:A:237:HIS:CE1	2.86	0.44
1:A:92:ILE:CD1	1:A:99:ALA:HA	2.46	0.44
1:A:50:ASN:O	1:A:54:THR:HG22	2.18	0.44
1:B:281:ARG:NH1	1:B:285:GLU:OE1	2.51	0.43
1:A:328:GLN:C	1:A:330:LEU:H	2.22	0.43
1:A:241:PRO:O	1:A:245:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ILE:C	1:A:120:PRO:O	2.56	0.43
1:A:173:MET:HE1	1:B:172:SER:HB2	2.00	0.43
1:A:18:SER:O	1:A:22:GLY:N	2.46	0.43
1:B:176:LYS:HG2	5:B:1553:HOH:O	2.18	0.43
1:A:359:ILE:CD1	1:A:363:LEU:HG	2.44	0.43
1:B:223:ALA:C	1:B:225:PRO:HD3	2.39	0.43
1:A:345:ILE:HG13	1:A:348:PRO:CD	2.48	0.43
1:B:230:LEU:HD22	1:B:240:PHE:CD2	2.53	0.43
1:A:45:ARG:HD3	1:A:53:LEU:CB	2.39	0.43
1:A:266:ILE:CG1	1:A:267:THR:N	2.79	0.43
1:B:192:GLU:OE2	1:B:192:GLU:HA	2.18	0.43
1:A:16:LEU:HB2	1:A:17:PRO:HD3	2.00	0.43
1:B:76:GLY:N	1:B:82:LYS:HD3	2.34	0.43
1:B:72:VAL:HG13	1:B:151:PHE:CE1	2.53	0.43
1:B:152:PHE:CD1	1:B:152:PHE:N	2.85	0.43
1:B:87:ASN:HB3	1:B:92:ILE:O	2.19	0.42
1:A:396:ASP:HB3	5:A:531:HOH:O	2.19	0.42
1:A:35:SER:OG	1:A:38:ILE:HG12	2.19	0.42
1:B:40:ASN:O	1:B:44:LEU:HB2	2.19	0.42
1:B:138:ASP:CG	1:B:139:THR:H	2.22	0.42
1:A:391:LYS:HE3	5:A:527:HOH:O	2.19	0.42
1:B:101:LYS:H	1:B:101:LYS:HG2	1.59	0.42
1:B:108:THR:O	1:B:108:THR:HG22	2.18	0.42
1:A:119:ILE:CG2	5:A:502:HOH:O	2.68	0.42
1:A:70:LEU:HD23	1:A:259:PHE:CD1	2.54	0.42
1:A:234:ASN:ND2	1:A:237:HIS:ND1	2.66	0.42
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.90	0.42
1:A:275:ARG:HB2	1:A:399:THR:HG21	2.00	0.42
1:B:139:THR:O	1:B:143:LYS:HG2	2.20	0.42
1:B:298:LEU:O	1:B:298:LEU:HG	2.19	0.42
1:B:215:ASN:O	1:B:219:GLU:HG2	2.19	0.42
1:A:135:PHE:CD1	1:A:143:LYS:HG3	2.54	0.42
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.34	0.42
1:A:307:GLU:O	1:A:311:LYS:HG3	2.20	0.42
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.57	0.42
1:A:51:ILE:C	1:A:54:THR:HG22	2.40	0.42
1:A:175:LYS:HD3	1:A:175:LYS:C	2.39	0.42
1:B:293:ASN:ND2	1:B:293:ASN:C	2.73	0.42
1:A:119:ILE:HG23	5:A:502:HOH:O	2.18	0.42
1:A:33:ILE:HG12	1:A:33:ILE:O	2.20	0.42
1:A:183:THR:HA	1:A:230:LEU:O	2.19	0.41
1:B:186:ASP:OD1	3:B:1500:GNP:N1	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:GLY:HA2	5:B:1560:HOH:O	2.19	0.41
1:B:140:TYR:O	1:B:144:MET:HG2	2.20	0.41
1:B:47:ARG:NH1	1:B:47:ARG:HG3	2.31	0.41
1:A:267:THR:CG2	1:A:268:ASP:H	2.33	0.41
1:B:152:PHE:CG	1:B:171:ILE:HD13	2.55	0.41
1:A:331:ALA:HA	1:A:336:ILE:HG22	2.02	0.41
1:B:73:ALA:HB2	1:B:149:TYR:CD1	2.56	0.41
1:A:275:ARG:HD3	1:A:279:LYS:HD2	2.02	0.41
1:B:298:LEU:CD1	1:B:301:LEU:HB2	2.50	0.41
1:A:49:GLY:O	1:A:51:ILE:HD12	2.21	0.41
1:A:185:VAL:HG11	1:A:229:LEU:HB3	2.02	0.41
1:B:230:LEU:C	1:B:230:LEU:HD12	2.41	0.41
1:A:33:ILE:HG12	1:A:65:ILE:HD13	2.02	0.41
4:B:1000:MPD:H12	5:B:1562:HOH:O	2.21	0.41
1:B:222:ILE:HG22	1:B:225:PRO:HG3	2.03	0.41
1:B:158:THR:OG1	1:B:159:ARG:N	2.50	0.40
1:A:286:GLY:HA2	1:A:388:PHE:CE1	2.56	0.40
1:B:298:LEU:HD11	1:B:301:LEU:CD2	2.46	0.40
1:B:387:ILE:O	1:B:391:LYS:HG3	2.22	0.40
1:B:243:LEU:O	1:B:247:LEU:HG	2.21	0.40
1:B:82:LYS:HA	1:B:155:ILE:HD12	2.04	0.40
1:B:366:TYR:CD1	1:B:393:TYR:CE2	3.10	0.40
1:A:295:ILE:HG12	1:A:383:PHE:CZ	2.56	0.40
1:B:139:THR:HA	1:B:142:GLU:HB2	2.03	0.40
1:A:211:LEU:CA	1:A:214:VAL:HG12	2.49	0.40
1:B:108:THR:HG23	1:B:128:PRO:CB	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	345 (88%)	31 (8%)	15 (4%)	5	10
1	B	388/422 (92%)	343 (88%)	33 (8%)	12 (3%)	7	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	779/844 (92%)	688 (88%)	64 (8%)	27 (4%)	6	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	203	GLU
1	A	235	VAL
1	A	302	LEU
1	B	107	VAL
1	B	223	ALA
1	A	96	GLU
1	A	105	VAL
1	A	158	THR
1	B	234	ASN
1	A	103	GLY
1	A	204	LYS
1	B	96	GLU
1	A	301	LEU
1	A	350	VAL
1	B	77	GLU
1	B	108	THR
1	B	238	TYR
1	B	302	LEU
1	A	290	ASP
1	A	120	PRO
1	B	94	ASN
1	B	204	LYS
1	B	290	ASP
1	A	253	ILE
1	B	359	ILE
1	A	137	PRO

### 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	359/386 (93%)	344 (96%)	15 (4%)	40	73
1	B	358/386 (93%)	342 (96%)	16 (4%)	38	70
All	All	717/772 (93%)	686 (96%)	31 (4%)	40	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	VAL
1	A	109	MET
1	A	118	ASN
1	A	135	PHE
1	A	159	ARG
1	A	175	LYS
1	A	234	ASN
1	A	240	PHE
1	A	302	LEU
1	A	330	LEU
1	A	359	ILE
1	A	360	GLN
1	A	368	GLN
1	A	383	PHE
1	A	390	LEU
1	B	101	LYS
1	B	108	THR
1	B	109	MET
1	B	224	GLU
1	B	234	ASN
1	B	235	VAL
1	B	240	PHE
1	B	245	ASP
1	B	269	SER
1	B	275	ARG
1	B	293	ASN
1	B	303	ASP
1	B	339	ASP
1	B	359	ILE
1	B	368	GLN
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	215	ASN
1	A	220	ASN
1	A	234	ASN
1	A	258	ASN
1	A	276	GLN
1	A	280	GLN
1	A	293	ASN
1	A	328	GLN
1	A	381	ASN
1	B	50	ASN
1	B	94	ASN
1	B	118	ASN
1	B	134	ASN
1	B	163	ASN
1	B	191	ASN
1	B	207	GLN
1	B	212	ASN
1	B	215	ASN
1	B	258	ASN
1	B	293	ASN
1	B	368	GLN
1	B	374	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 1 is 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
3	GNP	A	500	-	34,34,34	4.85	21 (61%)	50,54,54	16.29	26 (52%)
4	MPD	B	1000	-	7,7,7	0.54	0	10,10,10	0.37	0
3	GNP	B	1500	2	34,34,34	4.86	20 (58%)	50,54,54	16.63	26 (52%)

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	GNP	A	500	-	-	0/18/38/38	0/1/3/3
4	MPD	B	1000	-	-	0/5/5/5	0/0/0/0
3	GNP	B	1500	2	-	0/18/38/38	0/1/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1500	GNP	PB-N3B	15.59	1.77	1.64
3	A	500	GNP	PB-N3B	15.03	1.77	1.64
3	A	500	GNP	PG-O1G	10.93	1.59	1.46
3	B	1500	GNP	PG-O1G	10.73	1.59	1.46
3	A	500	GNP	C2-N1	9.13	1.51	1.36
3	B	1500	GNP	C2-N1	8.95	1.51	1.36
3	A	500	GNP	C8-N9	8.40	1.49	1.36
3	B	1500	GNP	C8-N9	8.28	1.48	1.36
3	B	1500	GNP	PB-O2B	-7.46	1.33	1.55
3	A	500	GNP	PB-O2B	-7.38	1.33	1.55
3	B	1500	GNP	PA-O3A	6.24	1.71	1.59
3	A	500	GNP	PA-O3A	6.12	1.71	1.59
3	B	1500	GNP	O6-C6	5.97	1.36	1.24
3	B	1500	GNP	C2-N3	-5.81	1.26	1.33
3	A	500	GNP	O6-C6	5.76	1.35	1.24
3	A	500	GNP	C2-N3	-5.68	1.26	1.33
3	A	500	GNP	O3'-C3'	4.74	1.54	1.43
3	B	1500	GNP	O3'-C3'	4.64	1.54	1.43
3	A	500	GNP	O4'-C1'	4.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1500	GNP	O4'-C1'	4.36	1.48	1.41
3	B	1500	GNP	PG-O2G	-3.82	1.44	1.55
3	A	500	GNP	PG-O2G	-3.81	1.44	1.55
3	A	500	GNP	C2'-C1'	3.34	1.58	1.53
3	B	1500	GNP	C2-N2	-3.01	1.27	1.32
3	B	1500	GNP	C2'-C1'	2.84	1.57	1.53
3	A	500	GNP	C2-N2	-2.82	1.28	1.32
3	A	500	GNP	C5-C4	2.69	1.46	1.40
3	A	500	GNP	PB-O1B	2.58	1.49	1.46
3	B	1500	GNP	C5-C4	2.58	1.46	1.40
3	B	1500	GNP	PB-O3A	-2.55	1.55	1.59
3	B	1500	GNP	O2'-C2'	2.53	1.49	1.43
3	A	500	GNP	O4'-C4'	2.51	1.50	1.45
3	A	500	GNP	O2'-C2'	2.50	1.49	1.43
3	B	1500	GNP	C8-N7	2.45	1.39	1.34
3	B	1500	GNP	PB-O1B	2.42	1.49	1.46
3	A	500	GNP	PG-N3B	-2.37	1.62	1.64
3	A	500	GNP	PB-O3A	-2.34	1.55	1.59
3	A	500	GNP	C8-N7	2.28	1.39	1.34
3	B	1500	GNP	O4'-C4'	2.22	1.50	1.45
3	B	1500	GNP	C5'-C4'	-2.07	1.44	1.51
3	A	500	GNP	C2'-C3'	2.02	1.59	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1500	GNP	C6-C5-N7	113.90	149.48	134.14
3	A	500	GNP	C6-C5-N7	111.43	149.14	134.14
3	B	1500	GNP	C8-N9-C4	15.97	119.09	106.90
3	A	500	GNP	C8-N9-C4	15.83	118.99	106.90
3	B	1500	GNP	C4-C5-N7	-9.22	101.62	109.52
3	A	500	GNP	C4-C5-N7	-8.93	101.87	109.52
3	B	1500	GNP	N7-C8-N9	-8.38	90.66	114.36
3	A	500	GNP	N7-C8-N9	-8.29	90.91	114.36
3	A	500	GNP	PB-N3B-PG	-7.51	117.44	130.07
3	B	1500	GNP	C8-N7-C5	6.93	125.06	103.58
3	A	500	GNP	C4'-O4'-C1'	6.92	117.26	109.75
3	B	1500	GNP	PB-N3B-PG	-6.91	118.44	130.07
3	A	500	GNP	C8-N7-C5	6.84	124.78	103.58
3	B	1500	GNP	C4'-O4'-C1'	6.80	117.14	109.75
3	A	500	GNP	N2-C2-N3	6.61	129.25	120.30
3	B	1500	GNP	N2-C2-N3	6.49	129.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1500	GNP	C2-N3-C4	6.42	124.11	115.09
3	A	500	GNP	C2-N3-C4	6.32	123.97	115.09
3	B	1500	GNP	O3'-C3'-C4'	-4.76	97.05	111.08
3	A	500	GNP	O3'-C3'-C4'	-4.75	97.07	111.08
3	B	1500	GNP	N2-C2-N1	-4.67	112.72	117.86
3	A	500	GNP	N2-C2-N1	-4.64	112.75	117.86
3	A	500	GNP	O1G-PG-N3B	-4.57	104.92	111.83
3	B	1500	GNP	O1G-PG-N3B	-4.26	105.39	111.83
3	A	500	GNP	C8-N9-C1'	-4.22	118.07	126.38
3	B	1500	GNP	C8-N9-C1'	-4.16	118.19	126.38
3	B	1500	GNP	C2'-C3'-C4'	4.09	110.81	102.65
3	A	500	GNP	C5-C6-N1	4.02	127.16	115.39
3	B	1500	GNP	C5-C6-N1	4.00	127.09	115.39
3	A	500	GNP	C2'-C3'-C4'	3.95	110.52	102.65
3	B	1500	GNP	O2G-PG-N3B	3.74	116.75	106.61
3	A	500	GNP	O2G-PG-N3B	3.65	116.51	106.61
3	B	1500	GNP	O3G-PG-O1G	-3.38	104.91	113.60
3	A	500	GNP	O3G-PG-O1G	-3.38	104.92	113.60
3	A	500	GNP	O2G-PG-O1G	-2.84	106.30	113.60
3	B	1500	GNP	O3'-C3'-C2'	-2.76	102.84	111.83
3	B	1500	GNP	N3-C4-N9	2.75	130.94	126.91
3	A	500	GNP	O3'-C3'-C2'	-2.75	102.89	111.83
3	A	500	GNP	N3-C4-N9	2.75	130.94	126.91
3	A	500	GNP	N1-C2-N3	-2.70	117.99	121.78
3	B	1500	GNP	O2G-PG-O1G	-2.65	106.80	113.60
3	B	1500	GNP	O3A-PB-N3B	2.60	113.81	106.59
3	A	500	GNP	C5-C4-N9	-2.57	103.45	107.16
3	B	1500	GNP	N1-C2-N3	-2.56	118.19	121.78
3	B	1500	GNP	C5-C4-N9	-2.49	103.57	107.16
3	A	500	GNP	O4'-C4'-C3'	-2.47	100.16	105.17
3	A	500	GNP	O3A-PB-N3B	2.42	113.31	106.59
3	B	1500	GNP	O4'-C4'-C3'	-2.36	100.38	105.17
3	B	1500	GNP	C1'-N9-C4	-2.26	122.72	126.64
3	A	500	GNP	O3G-PG-O2G	2.22	114.02	107.66
3	A	500	GNP	C1'-N9-C4	-2.14	122.94	126.64
3	B	1500	GNP	O3G-PG-O2G	2.07	113.60	107.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	395/422 (93%)	0.07	21 (5%) 25 28	25, 55, 98, 109	0
1	B	392/422 (92%)	-0.01	14 (3%) 41 46	27, 52, 93, 103	0
All	All	787/844 (93%)	0.03	35 (4%) 31 37	25, 53, 96, 109	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	6.5
1	B	108	THR	5.7
1	A	414	GLY	5.2
1	B	105	VAL	4.4
1	A	107	VAL	4.3
1	B	192	GLU	4.0
1	A	194	ASP	3.9
1	B	104	VAL	3.7
1	A	193	ALA	3.6
1	A	101	LYS	3.6
1	A	237	HIS	3.3
1	A	192	GLU	3.2
1	A	105	VAL	3.1
1	B	300	PHE	3.1
1	A	134	ASN	3.0
1	A	300	PHE	2.9
1	B	134	ASN	2.9
1	B	135	PHE	2.8
1	A	415	ARG	2.7
1	A	413	LEU	2.6
1	B	413	LEU	2.6
1	A	50	ASN	2.6
1	A	332	ARG	2.5
1	A	202	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	191	ASN	2.4
1	B	101	LYS	2.3
1	A	329	ARG	2.3
1	B	14	ASN	2.3
1	B	107	VAL	2.3
1	B	138	ASP	2.2
1	A	108	THR	2.2
1	A	211	LEU	2.1
1	A	190	THR	2.1
1	B	356	GLU	2.1
1	B	372	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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
4	MPD	B	1000	8/8	0.31	8.45	66,68,72,73	0
3	GNP	A	500	32/32	0.31	0.82	109,109,114,115	32
3	GNP	B	1500	32/32	0.22	-0.04	68,71,72,74	32
2	MG	B	1501	1/1	0.34	-0.07	55,55,55,55	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.