



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:00 PM GMT

PDB ID : 1OVG  
Title : M64V PNP +MePdr  
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Deposited on : 2003-03-26  
Resolution : 2.20 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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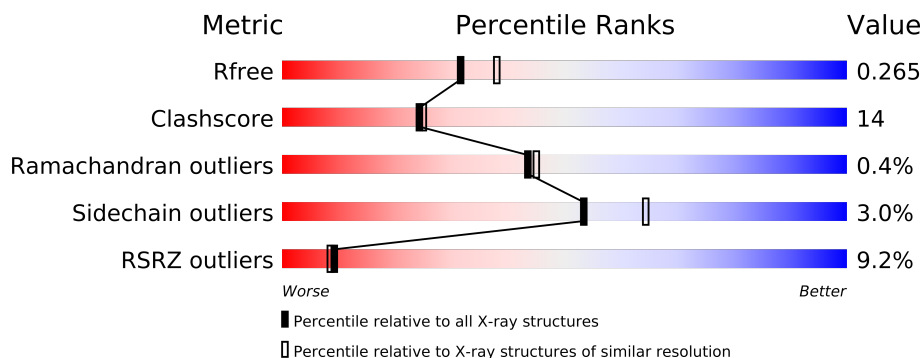
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	238	
1	B	238	
1	C	238	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MDR	C	247	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5671 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.

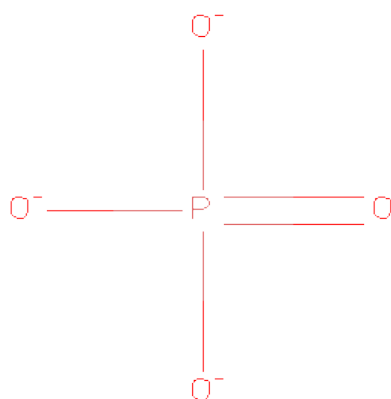
- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			
1	B	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			
1	C	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			

There are 3 discrepancies between the modelled and reference sequences:

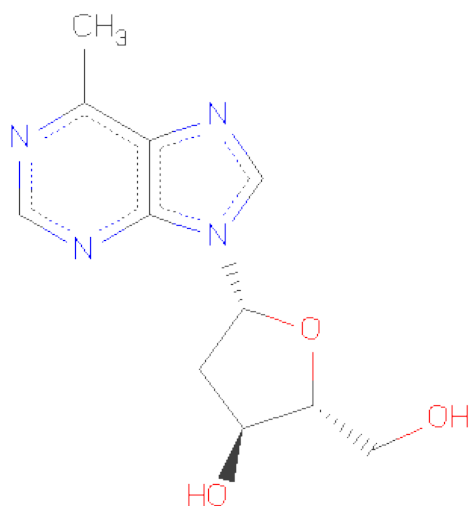
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	VAL	MET	ENGINEERED	UNP P0ABP8
B	64	VAL	MET	ENGINEERED	UNP P0ABP8
C	64	VAL	MET	ENGINEERED	UNP P0ABP8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 9-(2-DEOXY-BETA-D-RIBOFURANOSYL)-6-METHYLPURINE (three-letter code: MDR) (formula: C<sub>11</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	11	4	3		
3	B	1	Total	C	N	O	0	0
			18	11	4	3		
3	C	1	Total	C	N	O	0	0
			18	11	4	3		

- Molecule 4 is water.

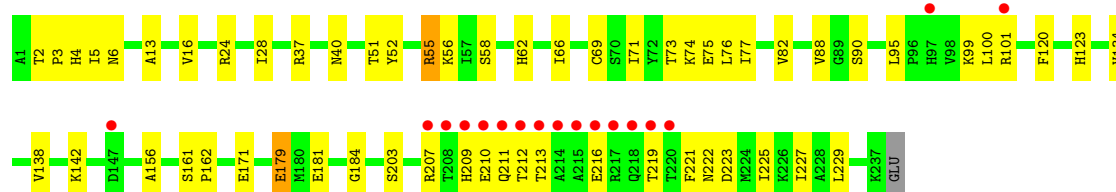
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	82	Total	O	0	0
			82	82		
4	B	73	Total	O	0	0
			73	73		
4	C	71	Total	O	0	0
			71	71		

### 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.

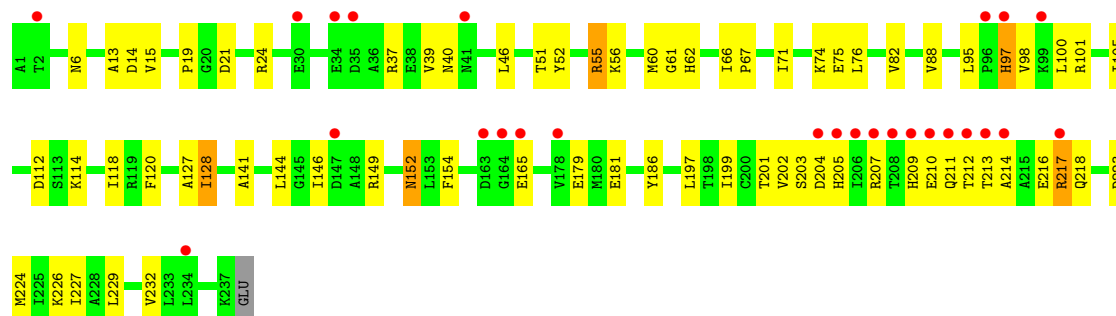
- Molecule 1: Purine nucleoside phosphorylase

Chain A: 



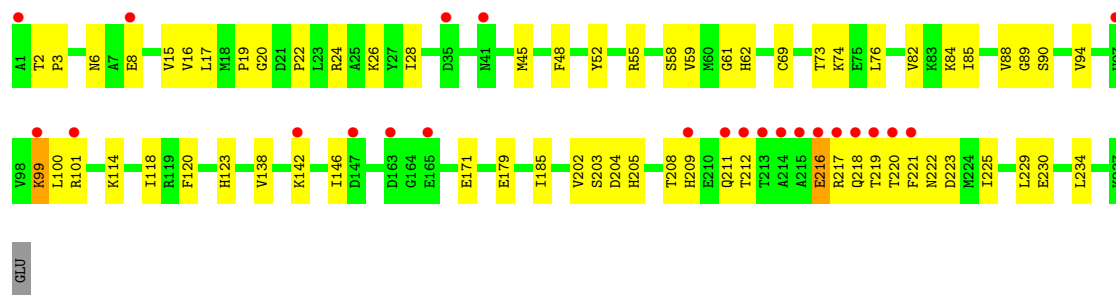
- Molecule 1: Purine nucleoside phosphorylase

Chain B: 



- Molecule 1: Purine nucleoside phosphorylase

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.80Å 120.80Å 240.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.62 – 2.20 20.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.62-2.20) 98.2 (20.62-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.229 , 0.259 0.240 , 0.265	Depositor DCC
$R_{free}$ test set	4646 reflections (8.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 42.4	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	1 of 52277 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: MDR, PO4

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	0.28	0/1821	0.55	0/2457
1	B	0.28	0/1821	0.54	0/2457
1	C	0.28	0/1821	0.55	0/2457
All	All	0.28	0/5463	0.55	0/7371

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	1792	0	1791	44	0
1	B	1792	0	1791	62	0
1	C	1792	0	1791	49	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	18	0	14	1	0
3	B	18	0	14	0	0
3	C	18	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	82	0	0	5	0
4	B	73	0	0	2	0
4	C	71	0	0	3	0
All	All	5671	0	5415	153	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 14.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:LEU:HD12	1:B:227:ILE:HD13	1.55	0.88
1:A:210:GLU:HG2	1:A:211:GLN:H	1.42	0.83
1:C:212:THR:HG22	1:C:217:ARG:HG2	1.59	0.81
1:C:90:SER:HB2	1:C:203:SER:HB2	1.63	0.81
1:C:218:GLN:HG2	1:C:222:ASN:HD21	1.47	0.80
1:B:67:PRO:O	1:B:71:ILE:HD13	1.83	0.77
1:B:229:LEU:O	1:B:232:VAL:HG22	1.86	0.74
1:C:219:THR:HA	1:C:222:ASN:HD22	1.51	0.74
1:C:73:THR:HG21	1:C:185:ILE:HD12	1.67	0.74
1:A:95:LEU:HD23	1:A:171:GLU:HG3	1.71	0.73
1:A:222:ASN:HA	1:A:225:ILE:HD12	1.72	0.72
1:B:223:ASP:O	1:B:227:ILE:HG12	1.89	0.71
1:B:141:ALA:HA	1:B:227:ILE:HD12	1.72	0.71
1:B:6:ASN:H	1:B:40:ASN:ND2	1.89	0.70
1:C:99:LYS:HD2	1:C:99:LYS:H	1.57	0.69
1:C:146:ILE:HD13	1:C:223:ASP:HB3	1.75	0.68
1:A:213:THR:OG1	1:A:216:GLU:HG3	1.94	0.68
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.28	0.68
1:A:13:ALA:HB2	1:A:56:LYS:HG2	1.75	0.68
1:B:213:THR:HA	1:B:217:ARG:HD2	1.75	0.68
1:B:128:ILE:HD13	1:B:128:ILE:H	1.59	0.67
1:A:142:LYS:HE3	1:A:142:LYS:HA	1.78	0.66
1:A:100:LEU:HD22	1:A:210:GLU:HB3	1.78	0.65
1:B:197:LEU:HD21	1:B:199:ILE:HD11	1.77	0.65
1:C:230:GLU:O	1:C:234:LEU:HD13	1.96	0.65
1:A:24:ARG:O	1:A:28:ILE:HG12	1.96	0.65
1:B:114:LYS:O	1:B:118:ILE:HG12	1.97	0.64
1:B:144:LEU:HD12	1:B:227:ILE:CD1	2.26	0.64
1:C:76:LEU:HB3	1:C:82:VAL:HG21	1.79	0.64
1:C:204:ASP:HB3	1:C:211:GLN:HA	1.80	0.64
1:C:138:VAL:O	1:C:142:LYS:HG2	1.99	0.63
1:C:101:ARG:HA	1:C:220:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:HIS:CE1	1:B:207:ARG:HB2	2.34	0.62
1:B:205:HIS:ND1	1:B:207:ARG:HB2	2.15	0.61
1:A:221:PHE:CD1	1:A:225:ILE:HD11	2.35	0.61
1:B:141:ALA:HA	1:B:227:ILE:CD1	2.31	0.60
1:B:213:THR:HG23	1:B:217:ARG:NH1	2.18	0.59
1:C:100:LEU:H	1:C:100:LEU:HD12	1.67	0.58
1:B:214:ALA:H	1:B:217:ARG:HD2	1.67	0.58
1:A:71:ILE:O	1:A:75:GLU:HG3	2.04	0.58
1:B:217:ARG:HD3	1:B:218:GLN:HG3	1.84	0.58
1:A:73:THR:O	1:A:77:ILE:HG12	2.04	0.58
1:B:146:ILE:HD13	1:B:223:ASP:HB3	1.86	0.57
1:B:105:ILE:HG12	1:B:199:ILE:HD12	1.87	0.57
1:A:100:LEU:HD23	1:A:212:THR:HG23	1.86	0.56
1:B:201:THR:HB	4:B:293:HOH:O	2.04	0.56
1:B:21:ASP:HB3	1:B:24:ARG:HB2	1.88	0.56
1:A:101:ARG:HD2	1:A:216:GLU:HB3	1.88	0.55
1:C:114:LYS:O	1:C:118:ILE:HG12	2.06	0.55
1:C:69:CYS:HB2	1:C:185:ILE:HD11	1.87	0.55
1:C:16:VAL:HG22	1:C:58:SER:HB2	1.89	0.54
1:A:134:VAL:O	1:A:138:VAL:HG23	2.07	0.54
1:C:218:GLN:HA	4:C:268:HOH:O	2.08	0.54
1:B:212:THR:OG1	1:B:217:ARG:HB2	2.08	0.54
1:A:100:LEU:O	1:A:101:ARG:HB2	2.08	0.54
1:B:88:VAL:HG23	1:B:88:VAL:O	2.08	0.54
1:C:15:VAL:HG12	1:C:84:LYS:HB2	1.90	0.53
1:C:100:LEU:O	1:C:101:ARG:HB2	2.09	0.53
1:B:71:ILE:O	1:B:75:GLU:HG3	2.09	0.52
1:A:179:GLU:HA	3:A:245:MDR:H2'1	1.91	0.52
1:C:220:THR:HA	1:C:223:ASP:OD2	2.08	0.52
1:A:76:LEU:HB3	1:A:82:VAL:HG21	1.89	0.52
1:C:99:LYS:HD2	1:C:99:LYS:N	2.23	0.52
1:B:14:ASP:OD2	1:B:15:VAL:HG23	2.10	0.52
1:A:74:LYS:HD3	1:A:74:LYS:C	2.31	0.52
1:C:88:VAL:O	1:C:88:VAL:HG23	2.09	0.52
1:B:76:LEU:HB3	1:B:82:VAL:HG21	1.92	0.51
1:A:99:LYS:HE2	1:A:210:GLU:OE1	2.11	0.51
1:B:141:ALA:CA	1:B:227:ILE:HD12	2.41	0.51
1:A:209:HIS:HA	4:A:284:HOH:O	2.11	0.51
1:C:100:LEU:N	1:C:100:LEU:HD12	2.25	0.51
1:A:13:ALA:CB	1:A:56:LYS:HG2	2.42	0.50
1:C:208:THR:O	1:C:209:HIS:HB2	2.12	0.49
1:B:165:GLU:OE1	1:B:165:GLU:N	2.44	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:52:TYR:CD2	1:C:229:LEU:HD13	2.47	0.49
1:C:22:PRO:HG3	1:C:45:MET:SD	2.53	0.49
1:B:212:THR:O	1:B:217:ARG:HG3	2.12	0.49
1:A:156:ALA:HB1	4:A:256:HOH:O	2.11	0.49
1:C:205:HIS:HB3	1:C:208:THR:OG1	2.13	0.49
1:C:101:ARG:CA	1:C:220:THR:HG21	2.42	0.48
1:C:26:LYS:HA	1:C:48:PHE:CE2	2.49	0.48
1:A:219:THR:HA	4:A:249:HOH:O	2.12	0.48
1:B:52:TYR:CD2	1:B:229:LEU:HD13	2.49	0.48
1:B:203:SER:O	1:B:212:THR:HG22	2.13	0.48
1:A:37:ARG:NH2	4:A:280:HOH:O	2.46	0.48
1:A:123:HIS:HD2	1:C:114:LYS:NZ	2.12	0.47
1:C:74:LYS:HD3	1:C:74:LYS:C	2.34	0.47
1:C:20:GLY:HA2	1:C:62:HIS:CE1	2.49	0.47
1:A:6:ASN:H	1:A:40:ASN:ND2	2.13	0.47
1:C:24:ARG:O	1:C:28:ILE:HG13	2.15	0.47
1:B:100:LEU:HD22	1:B:100:LEU:N	2.29	0.47
1:C:19:PRO:O	1:C:61:GLY:HA2	2.15	0.47
1:B:74:LYS:C	1:B:74:LYS:HD3	2.35	0.46
1:A:161:SER:HA	1:A:162:PRO:HD3	1.82	0.46
1:A:219:THR:HG23	4:A:249:HOH:O	2.16	0.46
1:B:112:ASP:OD2	1:B:154:PHE:HZ	1.98	0.46
1:C:73:THR:HG22	1:C:85:ILE:HD13	1.98	0.46
1:B:97:HIS:HD2	1:B:149:ARG:NH2	2.14	0.45
1:C:221:PHE:O	1:C:225:ILE:HG12	2.15	0.45
1:C:100:LEU:CD1	1:C:100:LEU:H	2.29	0.45
1:B:46:LEU:O	1:B:60:MET:HG3	2.16	0.45
1:B:95:LEU:HB2	1:B:98:VAL:HG23	1.99	0.45
1:B:211:GLN:OE1	1:B:211:GLN:N	2.50	0.45
1:C:73:THR:HG21	1:C:185:ILE:CD1	2.43	0.45
1:A:4:HIS:O	1:A:5:ILE:HD13	2.17	0.45
1:B:213:THR:HG23	1:B:217:ARG:CZ	2.47	0.44
1:B:100:LEU:H	1:B:100:LEU:HD22	1.82	0.44
1:A:88:VAL:HG23	1:A:88:VAL:O	2.18	0.44
1:A:223:ASP:O	1:A:227:ILE:HG13	2.18	0.44
1:B:201:THR:HG23	1:B:224:MET:SD	2.58	0.43
1:B:202:VAL:N	4:B:293:HOH:O	2.51	0.43
1:A:210:GLU:HG2	1:A:211:GLN:N	2.21	0.43
1:A:90:SER:HB2	1:A:203:SER:HB3	2.00	0.43
1:B:213:THR:HA	1:B:217:ARG:CD	2.46	0.43
1:B:204:ASP:HA	1:B:210:GLU:O	2.18	0.43
1:A:2:THR:HB	1:A:3:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:ILE:HG23	1:A:184:GLY:HA3	1.99	0.43
1:B:37:ARG:NH2	1:B:39:VAL:HG12	2.34	0.43
1:B:144:LEU:HD22	1:B:226:LYS:HZ1	1.84	0.43
1:A:69:CYS:O	1:A:73:THR:HG23	2.18	0.43
1:B:212:THR:HG23	1:B:212:THR:O	2.19	0.43
1:C:216:GLU:OE1	1:C:216:GLU:N	2.52	0.43
1:A:52:TYR:CD2	1:A:229:LEU:HD13	2.54	0.43
1:B:51:THR:HA	1:B:55:ARG:O	2.18	0.43
1:B:66:ILE:HB	1:B:67:PRO:HD3	2.01	0.42
1:B:101:ARG:NH1	1:B:216:GLU:HB3	2.34	0.42
1:B:6:ASN:H	1:B:40:ASN:HD21	1.63	0.42
1:B:144:LEU:HD13	1:B:226:LYS:HZ2	1.84	0.42
1:B:118:ILE:HD12	1:C:123:HIS:HE1	1.85	0.42
1:C:94:VAL:HG12	1:C:171:GLU:HB2	2.01	0.42
1:B:144:LEU:HD22	1:B:226:LYS:NZ	2.35	0.42
1:B:127:ALA:HB1	1:B:186:TYR:HB2	2.01	0.42
1:B:152:ASN:HA	1:B:152:ASN:HD22	1.60	0.42
1:C:17:LEU:O	1:C:59:VAL:HA	2.19	0.42
1:C:2:THR:HB	1:C:3:PRO:HD2	2.02	0.41
1:B:6:ASN:N	1:B:40:ASN:ND2	2.64	0.41
1:B:100:LEU:O	1:B:101:ARG:HB2	2.20	0.41
1:B:13:ALA:HB2	1:B:56:LYS:HG2	2.03	0.41
1:B:19:PRO:O	1:B:61:GLY:HA2	2.21	0.41
1:C:220:THR:HB	4:C:303:HOH:O	2.21	0.41
1:A:210:GLU:CG	1:A:211:GLN:H	2.23	0.41
1:B:6:ASN:H	1:B:40:ASN:HD22	1.65	0.41
1:C:100:LEU:O	1:C:101:ARG:CB	2.69	0.41
1:C:24:ARG:HA	1:C:24:ARG:HD3	1.96	0.41
1:B:62:HIS:CE1	1:B:181:GLU:HG2	2.56	0.41
1:A:51:THR:HA	1:A:55:ARG:O	2.21	0.41
1:C:2:THR:HB	1:C:3:PRO:CD	2.51	0.41
1:A:16:VAL:HG22	1:A:58:SER:HB2	2.03	0.40
1:A:62:HIS:CE1	1:A:181:GLU:HG2	2.56	0.40
1:C:89:GLY:HA2	4:C:277:HOH:O	2.21	0.40
1:A:100:LEU:HB3	1:A:212:THR:HG21	2.03	0.40
1:C:101:ARG:HD3	1:C:216:GLU:HB3	2.03	0.40
1:A:2:THR:HB	1:A:3:PRO:CD	2.52	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	235/238 (99%)	221 (94%)	13 (6%)	1 (0%)	43	45
1	B	235/238 (99%)	222 (94%)	12 (5%)	1 (0%)	43	45
1	C	235/238 (99%)	219 (93%)	15 (6%)	1 (0%)	43	45
All	All	705/714 (99%)	662 (94%)	40 (6%)	3 (0%)	43	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	B	209	HIS
1	C	202	VAL

### 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	187/189 (99%)	184 (98%)	3 (2%)	75	85
1	B	187/189 (99%)	180 (96%)	7 (4%)	45	54
1	C	187/189 (99%)	180 (96%)	7 (4%)	45	54
All	All	561/567 (99%)	544 (97%)	17 (3%)	53	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	120	PHE
1	A	179	GLU

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Mol	Chain	Res	Type
1	B	55	ARG
1	B	97	HIS
1	B	120	PHE
1	B	128	ILE
1	B	152	ASN
1	B	179	GLU
1	B	217	ARG
1	C	6	ASN
1	C	8	GLU
1	C	55	ARG
1	C	99	LYS
1	C	120	PHE
1	C	179	GLU
1	C	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	116	ASN
1	A	123	HIS
1	B	40	ASN
1	B	152	ASN
1	B	222	ASN
1	C	6	ASN
1	C	116	ASN
1	C	123	HIS
1	C	211	GLN
1	C	222	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MDR	A	245	-	20,20,20	2.41	7 (35%)	29,29,29	1.89	10 (34%)
2	PO4	A	248	-	4,4,4	0.90	0	6,6,6	0.31	0
3	MDR	B	246	-	20,20,20	2.50	6 (30%)	29,29,29	2.06	11 (37%)
2	PO4	B	249	-	4,4,4	0.96	0	6,6,6	0.31	0
3	MDR	C	247	-	20,20,20	2.69	6 (30%)	29,29,29	2.16	11 (37%)
2	PO4	C	250	-	4,4,4	0.93	0	6,6,6	0.31	0

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	MDR	A	245	-	-	0/4/18/18	0/1/3/3
2	PO4	A	248	-	-	0/0/0/0	0/0/0/0
3	MDR	B	246	-	-	0/4/18/18	0/1/3/3
2	PO4	B	249	-	-	0/0/0/0	0/0/0/0
3	MDR	C	247	-	-	0/4/18/18	0/1/3/3
2	PO4	C	250	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	247	MDR	C6-N1	8.80	1.41	1.32
3	B	246	MDR	C6-N1	8.41	1.40	1.32
3	A	245	MDR	C6-N1	8.06	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	247	MDR	C4-N3	4.24	1.42	1.35
3	A	245	MDR	C4-N3	3.98	1.41	1.35
3	B	246	MDR	C4-N3	3.95	1.41	1.35
3	C	247	MDR	C4-N9	3.73	1.43	1.37
3	C	247	MDR	C6-C5	-3.00	1.40	1.43
3	B	246	MDR	C4-N9	2.87	1.41	1.37
3	B	246	MDR	C6-C5	-2.84	1.41	1.43
3	C	247	MDR	C8-N7	-2.70	1.29	1.34
3	A	245	MDR	C6-C5	-2.60	1.41	1.43
3	A	245	MDR	C4-N9	2.55	1.41	1.37
3	B	246	MDR	C8-N7	-2.54	1.29	1.34
3	A	245	MDR	O4'-C1'	2.45	1.48	1.42
3	B	246	MDR	C2-N3	2.36	1.36	1.32
3	C	247	MDR	C2-N3	2.35	1.36	1.32
3	A	245	MDR	C8-N7	-2.29	1.30	1.34
3	A	245	MDR	C2-N3	2.14	1.36	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	245	MDR	N3-C2-N1	-5.42	124.18	128.71
3	C	247	MDR	N3-C2-N1	-5.32	124.26	128.71
3	B	246	MDR	N3-C2-N1	-5.26	124.31	128.71
3	C	247	MDR	C2'-C1'-N9	3.70	123.71	114.08
3	C	247	MDR	C1'-N9-C4	3.66	135.75	126.84
3	C	247	MDR	C8-N9-C4	-3.64	104.12	106.90
3	B	246	MDR	C2'-C1'-N9	3.60	123.44	114.08
3	B	246	MDR	C1'-N9-C4	3.40	135.13	126.84
3	C	247	MDR	C8-N9-C1'	-3.20	120.13	126.15
3	B	246	MDR	C8-N9-C1'	-3.14	120.23	126.15
3	B	246	MDR	C8-N9-C4	-2.97	104.63	106.90
3	B	246	MDR	C6'-C6-N1	2.94	124.39	117.93
3	C	247	MDR	N3-C4-N9	2.94	130.74	125.43
3	C	247	MDR	C6'-C6-N1	2.91	124.33	117.93
3	C	247	MDR	C4-C5-N7	2.88	111.99	109.52
3	A	245	MDR	C2'-C1'-N9	2.85	121.50	114.08
3	A	245	MDR	C8-N9-C4	-2.80	104.76	106.90
3	A	245	MDR	C6'-C6-N1	2.78	124.05	117.93
3	A	245	MDR	C1'-N9-C4	2.78	133.62	126.84
3	B	246	MDR	C4-C5-N7	2.77	111.90	109.52
3	C	247	MDR	C6'-C6-C5	-2.72	115.78	122.39
3	B	246	MDR	C6'-C6-C5	-2.68	115.88	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	246	MDR	N3-C4-N9	2.64	130.20	125.43
3	A	245	MDR	C4-C5-N7	2.52	111.68	109.52
3	A	245	MDR	N3-C4-N9	2.50	129.94	125.43
3	A	245	MDR	C6'-C6-C5	-2.48	116.37	122.39
3	C	247	MDR	C3'-C2'-C1'	2.45	109.00	102.47
3	A	245	MDR	C8-N9-C1'	-2.41	121.61	126.15
3	C	247	MDR	C5-C4-N9	-2.41	103.69	107.16
3	B	246	MDR	C5-C4-N9	-2.33	103.80	107.16
3	B	246	MDR	C3'-C2'-C1'	2.29	108.58	102.47
3	A	245	MDR	C5-C4-N9	-2.11	104.11	107.16

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	237/238 (99%)	0.58	17 (7%) 15 15	14, 21, 59, 100	0
1	B	237/238 (99%)	0.61	26 (10%) 6 6	15, 24, 48, 104	0
1	C	237/238 (99%)	0.52	23 (9%) 8 7	13, 24, 52, 90	0
All	All	711/714 (99%)	0.57	66 (9%) 9 8	13, 23, 52, 104	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	ALA	16.1
1	A	214	ALA	14.2
1	A	219	THR	13.5
1	B	212	THR	13.4
1	B	213	THR	12.9
1	A	213	THR	11.8
1	C	215	ALA	11.7
1	A	212	THR	10.8
1	A	208	THR	10.3
1	C	218	GLN	10.2
1	A	209	HIS	10.1
1	C	214	ALA	9.8
1	B	207	ARG	9.6
1	C	213	THR	9.5
1	B	211	GLN	9.4
1	B	209	HIS	9.3
1	A	211	GLN	7.5
1	A	216	GLU	7.1
1	C	220	THR	6.9
1	A	207	ARG	6.4
1	B	206	ILE	6.3
1	C	216	GLU	6.1
1	B	205	HIS	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLN	5.8
1	B	208	THR	5.7
1	C	219	THR	5.7
1	A	210	GLU	5.4
1	C	212	THR	5.3
1	B	147	ASP	5.2
1	B	210	GLU	5.1
1	B	163	ASP	4.9
1	C	211	GLN	4.8
1	B	97	HIS	4.6
1	C	217	ARG	4.4
1	B	204	ASP	4.4
1	A	220	THR	4.3
1	B	165	GLU	4.3
1	C	221	PHE	3.9
1	A	97	HIS	3.9
1	B	164	GLY	3.8
1	C	209	HIS	3.8
1	C	35	ASP	3.6
1	B	30	GLU	3.2
1	B	214	ALA	3.1
1	A	217	ARG	2.9
1	C	142	LYS	2.9
1	C	165	GLU	2.8
1	C	8	GLU	2.7
1	C	163	ASP	2.6
1	B	34	GLU	2.6
1	B	35	ASP	2.5
1	C	101	ARG	2.5
1	C	41	ASN	2.5
1	B	217	ARG	2.5
1	C	97	HIS	2.3
1	B	99	LYS	2.2
1	B	178	VAL	2.2
1	C	99	LYS	2.2
1	A	101	ARG	2.1
1	B	96	PRO	2.1
1	B	41	ASN	2.1
1	C	1	ALA	2.1
1	B	2	THR	2.1
1	B	234	LEU	2.1
1	C	147	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	147	ASP	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
3	MDR	C	247	18/18	0.22	2.22	28,32,35,37	0
2	PO4	B	249	5/5	0.12	0.02	21,22,23,24	0
3	MDR	B	246	18/18	0.16	0.01	25,28,29,29	0
3	MDR	A	245	18/18	0.11	-0.65	17,20,24,24	0
2	PO4	C	250	5/5	0.08	-1.52	19,20,21,22	0
2	PO4	A	248	5/5	0.09	-1.85	23,24,24,25	0

## 6.5 Other polymers

There are no such residues in this entry.