



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:29 PM UTC

PDB ID : 1OU4 / pdb_00001ou4
Title : Native PNP +Talo
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Deposited on : 2003-03-24
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

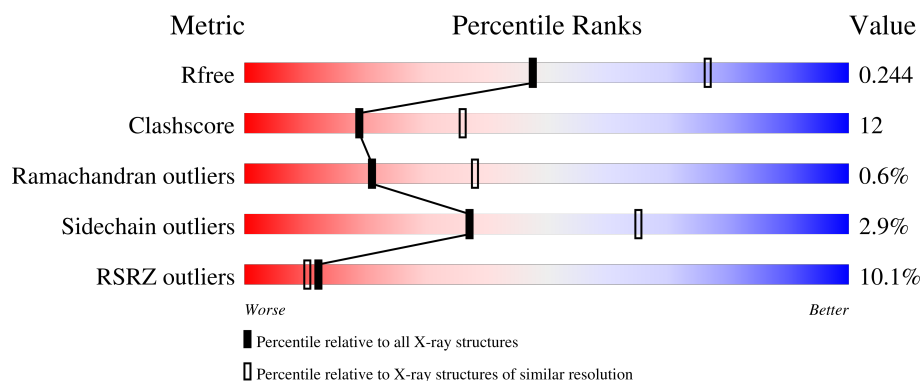
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	238	9% 74% 23% .
1	B	238	11% 72% 25% .
1	C	238	11% 79% 19% .

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
3	6MP	A	244	-	X	-	-
3	6MP	B	245	-	X	-	-
3	6MP	C	246	-	X	-	-

2 Entry composition [i](#)

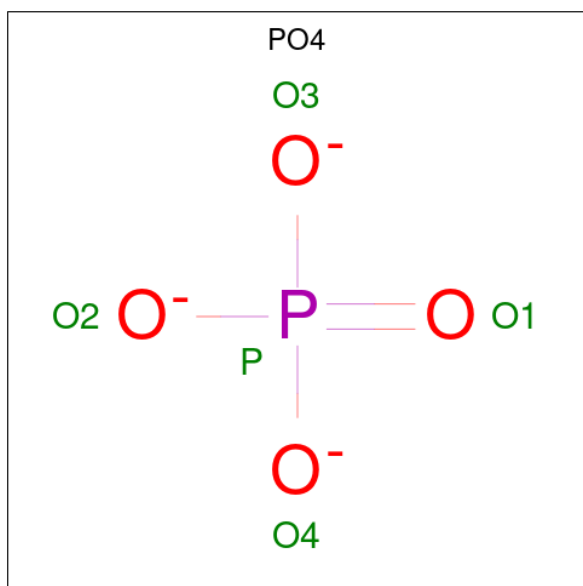
There are 4 unique types of molecules in this entry. The entry contains 5591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine nucleoside phosphorylase.

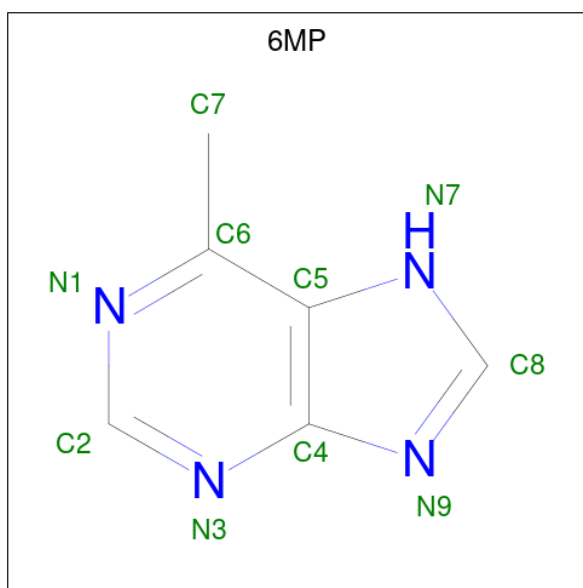
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	B	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	C	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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 6-METHYLPURINE (CCD ID: 6MP) (formula: $C_6H_6N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	6	4		
3	B	1	Total	C	N	0	0
			10	6	4		
3	C	1	Total	C	N	0	0
			10	6	4		

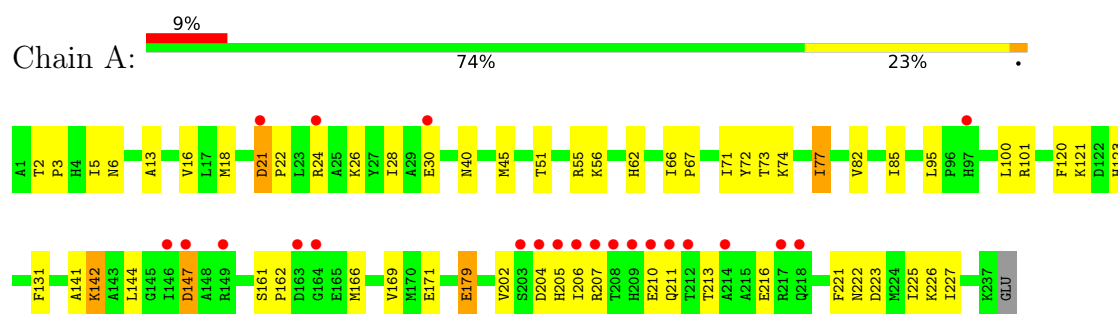
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	70	Total	O	0	0
			70	70		
4	C	51	Total	O	0	0
			51	51		

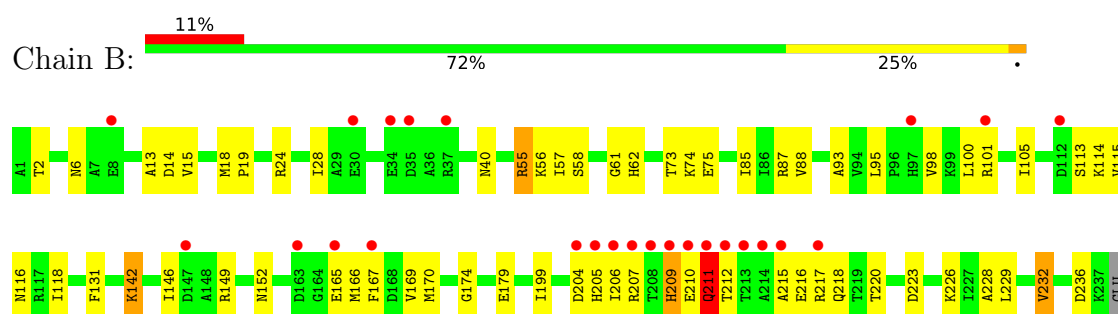
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

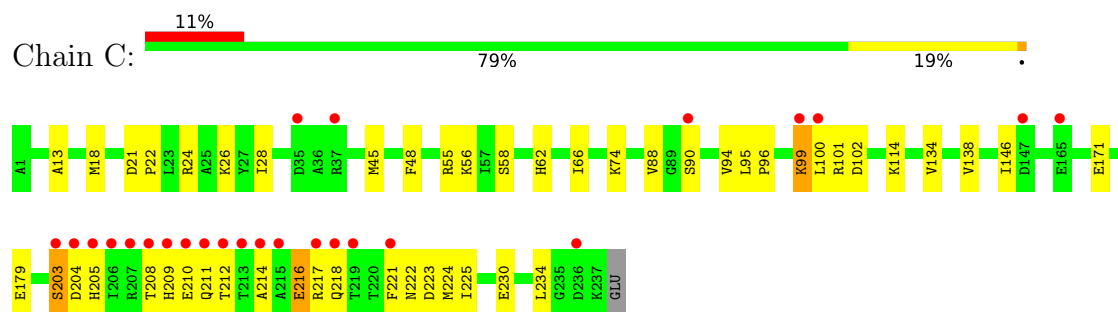
• Molecule 1: Purine nucleoside phosphorylase



• Molecule 1: Purine nucleoside phosphorylase



• Molecule 1: Purine nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.61Å 121.61Å 243.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.32 – 2.50 24.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.32-2.50) 99.8 (24.32-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.83 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.244 0.215 , 0.244	Depositor DCC
R_{free} test set	3592 reflections (9.57%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 6MP, 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	0.40	0/1822	0.91	5/2457 (0.2%)
1	B	0.40	0/1822	0.91	3/2457 (0.1%)
1	C	0.38	1/1822 (0.1%)	0.89	2/2457 (0.1%)
All	All	0.39	1/5466 (0.0%)	0.90	10/7371 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	ILE	CA-CB	5.31	1.56	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ASP	CA-C-N	5.69	125.54	119.28
1	C	21	ASP	C-N-CA	5.69	125.54	119.28
1	A	21	ASP	CA-C-N	5.66	125.51	119.28
1	A	21	ASP	C-N-CA	5.66	125.51	119.28
1	A	16	VAL	N-CA-C	5.40	115.90	108.12
1	B	131	PHE	N-CA-C	5.23	116.66	111.07
1	A	77	ILE	N-CA-C	5.22	115.44	110.53
1	B	174	GLY	N-CA-C	5.09	122.93	115.08
1	A	131	PHE	N-CA-C	5.05	116.47	111.07
1	B	215	ALA	N-CA-C	-5.04	106.97	113.01

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	1793	0	1791	43	0
1	B	1793	0	1791	46	0
1	C	1793	0	1791	41	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	10	0	6	1	0
3	B	10	0	6	0	0
3	C	10	0	6	0	0
4	A	46	0	0	0	0
4	B	70	0	0	0	0
4	C	51	0	0	0	0
All	All	5591	0	5391	128	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 12.

All (128) 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:C:99:LYS:HD2	1:C:99:LYS:H	1.33	0.93
1:C:88:VAL:HB	1:C:224:MET:HE3	1.67	0.76
1:A:221:PHE:CE1	1:A:225:ILE:HD11	2.21	0.76
1:A:210:GLU:HG2	1:A:211:GLN:H	1.51	0.75
1:A:142:LYS:HE3	1:A:142:LYS:HA	1.68	0.75
1:C:218:GLN:HG2	1:C:222:ASN:HD21	1.53	0.74
1:B:211:GLN:NE2	1:B:211:GLN:H	1.87	0.71
1:C:146:ILE:HD13	1:C:223:ASP:HB3	1.74	0.69
1:A:144:LEU:HD12	1:A:227:ILE:HD13	1.75	0.68
1:A:24:ARG:O	1:A:28:ILE:HG12	1.95	0.67
1:A:100:LEU:HD12	1:A:202:VAL:HG12	1.77	0.67
1:B:211:GLN:H	1:B:211:GLN:HE21	1.42	0.66
1:C:99:LYS:HD2	1:C:99:LYS:N	2.10	0.66
1:C:99:LYS:HB3	1:C:99:LYS:NZ	2.10	0.66
1:B:93:ALA:HB3	1:B:205:HIS:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PHE:HA	1:B:170:MET:HE3	1.77	0.65
1:A:141:ALA:HA	1:A:227:ILE:HD12	1.80	0.64
1:A:223:ASP:O	1:A:227:ILE:HG12	1.97	0.64
1:A:21:ASP:HB3	1:A:24:ARG:HD3	1.81	0.63
1:A:22:PRO:HG3	1:A:45:MET:SD	2.38	0.63
1:C:230:GLU:O	1:C:234:LEU:HD13	1.99	0.62
1:A:13:ALA:HB2	1:A:56:LYS:HG2	1.81	0.61
1:C:94:VAL:HG12	1:C:171:GLU:HB2	1.83	0.61
1:B:55:ARG:HD2	1:B:236:ASP:OD2	2.01	0.60
1:B:24:ARG:O	1:B:28:ILE:HG12	2.02	0.60
1:B:167:PHE:HE2	1:B:206:ILE:HD13	1.66	0.59
1:C:212:THR:HB	1:C:217:ARG:HG2	1.84	0.58
1:A:18:MET:HE2	1:A:62:HIS:HB3	1.85	0.58
1:B:205:HIS:ND1	1:B:207:ARG:HB2	2.19	0.58
1:B:142:LYS:HB2	1:B:142:LYS:NZ	2.19	0.58
1:A:100:LEU:O	1:A:101:ARG:HB2	2.04	0.58
1:B:95:LEU:HB2	1:B:98:VAL:HG23	1.84	0.58
1:A:82:VAL:HG11	1:A:85:ILE:HD11	1.85	0.57
1:B:73:THR:HG22	1:B:85:ILE:HD13	1.86	0.57
1:B:166:MET:HE3	1:B:169:VAL:HB	1.86	0.57
1:A:73:THR:O	1:A:77:ILE:HG12	2.05	0.56
1:C:204:ASP:HB3	1:C:211:GLN:HA	1.86	0.56
1:B:167:PHE:CE2	1:B:206:ILE:HD13	2.41	0.56
1:C:22:PRO:HG3	1:C:45:MET:SD	2.45	0.56
1:C:94:VAL:CG1	1:C:171:GLU:HB2	2.36	0.55
1:C:218:GLN:HG2	1:C:222:ASN:ND2	2.20	0.55
1:B:226:LYS:NZ	1:B:226:LYS:HB3	2.22	0.55
1:B:74:LYS:HD3	1:B:74:LYS:C	2.32	0.55
1:C:90:SER:HB2	1:C:203:SER:OG	2.07	0.54
1:A:74:LYS:C	1:A:74:LYS:HD3	2.33	0.53
1:B:217:ARG:HG3	1:B:218:GLN:N	2.24	0.53
1:A:221:PHE:CD1	1:A:225:ILE:HD11	2.43	0.53
1:A:222:ASN:O	1:A:226:LYS:HG3	2.09	0.52
1:C:204:ASP:HA	1:C:210:GLU:O	2.10	0.52
1:B:226:LYS:HB3	1:B:226:LYS:HZ3	1.75	0.52
1:A:21:ASP:H	1:A:24:ARG:NH1	2.08	0.51
1:C:100:LEU:HD12	1:C:100:LEU:H	1.73	0.51
1:A:221:PHE:O	1:A:225:ILE:HG13	2.11	0.51
1:C:100:LEU:HD12	1:C:100:LEU:N	2.25	0.51
1:C:74:LYS:HD3	1:C:74:LYS:C	2.37	0.50
1:C:99:LYS:HG2	1:C:102:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:HB2	1:C:56:LYS:HG2	1.93	0.49
1:A:213:THR:OG1	1:A:216:GLU:HG3	2.12	0.49
1:B:114:LYS:O	1:B:118:ILE:HG12	2.13	0.49
1:A:26:LYS:O	1:A:30:GLU:HG2	2.13	0.48
1:A:123:HIS:HD2	1:C:114:LYS:NZ	2.11	0.48
1:A:204:ASP:OD2	1:A:205:HIS:N	2.46	0.47
1:C:24:ARG:O	1:C:28:ILE:HG13	2.14	0.47
1:C:216:GLU:OE1	1:C:216:GLU:N	2.47	0.47
1:B:14:ASP:OD2	1:B:15:VAL:HG23	2.14	0.47
1:A:66:ILE:HB	1:A:67:PRO:HD3	1.96	0.47
1:C:134:VAL:O	1:C:138:VAL:HG23	2.15	0.47
1:A:67:PRO:O	1:A:71:ILE:HG12	2.15	0.46
1:A:210:GLU:HG2	1:A:211:GLN:N	2.25	0.46
1:B:88:VAL:HG23	1:B:88:VAL:O	2.15	0.46
1:A:6:ASN:H	1:A:40:ASN:ND2	2.13	0.46
1:C:210:GLU:O	1:C:210:GLU:HG3	2.15	0.46
1:B:212:THR:OG1	1:B:217:ARG:HD3	2.14	0.46
1:A:21:ASP:HA	1:A:22:PRO:HD3	1.82	0.46
1:A:82:VAL:HG11	1:A:85:ILE:CD1	2.45	0.46
1:B:229:LEU:O	1:B:232:VAL:HG22	2.15	0.46
1:B:100:LEU:N	1:B:100:LEU:HD22	2.30	0.46
1:B:205:HIS:CE1	1:B:207:ARG:HB2	2.51	0.46
1:B:6:ASN:H	1:B:40:ASN:ND2	2.14	0.46
1:B:211:GLN:NE2	1:B:211:GLN:N	2.60	0.46
1:B:95:LEU:HB2	1:B:98:VAL:CG2	2.46	0.45
1:A:161:SER:HA	1:A:162:PRO:HD3	1.82	0.45
1:B:146:ILE:HD13	1:B:223:ASP:HB3	1.99	0.45
1:B:101:ARG:HD2	1:B:220:THR:OG1	2.16	0.45
1:C:205:HIS:HB3	1:C:208:THR:OG1	2.17	0.44
1:C:99:LYS:HB3	1:C:99:LYS:HZ2	1.79	0.44
1:A:166:MET:HE3	1:A:169:VAL:HB	1.98	0.44
1:B:101:ARG:HD2	1:B:220:THR:HG1	1.82	0.44
1:B:204:ASP:HA	1:B:210:GLU:O	2.18	0.44
1:B:98:VAL:HA	1:B:149:ARG:NH1	2.33	0.44
1:B:205:HIS:O	1:B:209:HIS:HA	2.17	0.44
1:C:18:MET:HE2	1:C:62:HIS:HB3	2.00	0.44
1:A:5:ILE:HA	1:A:40:ASN:ND2	2.33	0.44
1:C:221:PHE:O	1:C:225:ILE:HG12	2.17	0.43
1:A:5:ILE:HD11	1:A:72:TYR:HD1	1.83	0.43
1:C:100:LEU:O	1:C:101:ARG:HB2	2.18	0.43
1:C:214:ALA:HB3	1:C:216:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASP:HB3	1:C:211:GLN:HG3	2.00	0.43
1:B:114:LYS:HD2	1:B:118:ILE:HD11	2.00	0.43
1:A:141:ALA:HA	1:A:227:ILE:CD1	2.46	0.43
1:B:18:MET:HE2	1:B:62:HIS:HB3	2.01	0.43
1:B:228:ALA:O	1:B:232:VAL:HG13	2.19	0.43
1:C:211:GLN:N	1:C:211:GLN:CD	2.77	0.43
1:A:179:GLU:HA	3:A:244:6MP:N9	2.34	0.42
1:C:88:VAL:HG23	1:C:88:VAL:O	2.19	0.42
1:A:28:ILE:CD1	1:A:225:ILE:HD13	2.49	0.42
1:B:87:ARG:HH21	1:B:87:ARG:HG3	1.85	0.42
1:C:48:PHE:O	1:C:58:SER:HA	2.19	0.42
1:B:2:THR:OG1	1:B:75:GLU:OE1	2.37	0.42
1:C:95:LEU:HA	1:C:96:PRO:HD3	1.93	0.42
1:A:51:THR:HA	1:A:55:ARG:O	2.20	0.41
1:A:123:HIS:HD2	1:C:114:LYS:HZ1	1.68	0.41
1:A:147:ASP:OD2	1:A:147:ASP:N	2.39	0.41
1:A:205:HIS:O	1:A:207:ARG:N	2.51	0.41
1:B:105:ILE:HG12	1:B:199:ILE:HD12	2.02	0.41
1:A:2:THR:HB	1:A:3:PRO:HD2	2.01	0.41
1:B:101:ARG:NH1	1:B:216:GLU:HB3	2.36	0.41
1:B:114:LYS:CD	1:B:118:ILE:HD11	2.50	0.41
1:B:115:VAL:HG23	1:B:116:ASN:N	2.36	0.41
1:C:26:LYS:HA	1:C:48:PHE:CE2	2.55	0.41
1:C:208:THR:O	1:C:209:HIS:HB2	2.21	0.41
1:A:95:LEU:HD23	1:A:171:GLU:HG3	2.02	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:B:57:ILE:HG22	1:B:58:SER:N	2.36	0.41
1:C:214:ALA:HB3	1:C:216:GLU:CD	2.46	0.40
1:B:113:SER:OG	1:B:115:VAL:HG13	2.20	0.40
1:C:99:LYS:HB3	1:C:99:LYS:HZ3	1.86	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%)	220 (94%)	14 (6%)	1 (0%)	30	49
1	B	235/238 (99%)	221 (94%)	12 (5%)	2 (1%)	14	27
1	C	235/238 (99%)	216 (92%)	18 (8%)	1 (0%)	30	49
All	All	705/714 (99%)	657 (93%)	44 (6%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	GLN
1	B	209	HIS
1	C	203	SER
1	A	206	ILE

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%)	182 (97%)	5 (3%)	39	67
1	B	187/189 (99%)	180 (96%)	7 (4%)	30	57
1	C	187/189 (99%)	183 (98%)	4 (2%)	47	74
All	All	561/567 (99%)	545 (97%)	16 (3%)	37	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	121	LYS
1	A	142	LYS
1	A	147	ASP
1	A	179	GLU
1	B	55	ARG

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	152	ASN
1	B	165	GLU
1	B	179	GLU
1	B	211	GLN
1	B	232	VAL
1	C	55	ARG
1	C	99	LYS
1	C	179	GLU
1	C	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	123	HIS
1	A	209	HIS
1	A	222	ASN
1	B	152	ASN
1	B	211	GLN
1	B	218	GLN
1	B	222	ASN
1	C	6	ASN
1	C	40	ASN
1	C	116	ASN
1	C	222	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 oligosaccharides 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
2	PO4	A	247	-	4,4,4	1.76	0	6,6,6	0.46	0
3	6MP	B	245	-	10,11,11	3.81	8 (80%)	10,15,15	3.86	7 (70%)
3	6MP	A	244	-	10,11,11	3.91	8 (80%)	10,15,15	3.91	7 (70%)
2	PO4	B	248	-	4,4,4	1.88	3 (75%)	6,6,6	0.46	0
3	6MP	C	246	-	10,11,11	3.89	8 (80%)	10,15,15	3.97	7 (70%)
2	PO4	C	249	-	4,4,4	1.80	2 (50%)	6,6,6	0.47	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	6MP	C	246	-	-	-	0/2/2/2
3	6MP	B	245	-	-	-	0/2/2/2
3	6MP	A	244	-	-	-	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246	6MP	C4-N9	8.88	1.45	1.38
3	A	244	6MP	C4-N9	8.87	1.45	1.38
3	B	245	6MP	C4-N9	8.47	1.44	1.38
3	C	246	6MP	C6-N1	4.63	1.42	1.33
3	B	245	6MP	C6-N1	4.56	1.42	1.33
3	A	244	6MP	C6-N1	4.55	1.41	1.33
3	A	244	6MP	C4-N3	3.73	1.43	1.35
3	C	246	6MP	C4-N3	3.72	1.43	1.35
3	B	245	6MP	C4-N3	3.56	1.43	1.35
3	A	244	6MP	C8-N9	3.12	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246	6MP	C8-N9	3.08	1.38	1.32
3	B	245	6MP	C8-N9	3.08	1.38	1.32
3	B	245	6MP	C2-N3	3.05	1.39	1.33
3	A	244	6MP	C7-C6	2.97	1.55	1.50
3	C	246	6MP	C2-N3	2.96	1.39	1.33
3	B	245	6MP	C7-C6	2.96	1.55	1.50
3	A	244	6MP	C2-N3	2.87	1.39	1.33
3	C	246	6MP	C7-C6	2.73	1.54	1.50
3	A	244	6MP	C2-N1	2.60	1.38	1.33
3	B	245	6MP	C2-N1	2.58	1.38	1.33
3	C	246	6MP	C2-N1	2.46	1.38	1.33
2	B	248	PO4	P-O4	-2.17	1.48	1.54
2	B	248	PO4	P-O3	-2.14	1.48	1.54
2	B	248	PO4	P-O2	-2.09	1.48	1.54
3	B	245	6MP	C5-C4	2.07	1.43	1.40
3	C	246	6MP	C5-C4	2.06	1.43	1.40
2	C	249	PO4	P-O2	-2.05	1.48	1.54
3	A	244	6MP	C5-C4	2.03	1.43	1.40
2	C	249	PO4	P-O4	-2.02	1.48	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	246	6MP	C4-C5-N7	8.89	111.25	105.28
3	A	244	6MP	C4-C5-N7	8.70	111.12	105.28
3	B	245	6MP	C4-C5-N7	8.58	111.04	105.28
3	C	246	6MP	C5-C4-N9	-6.36	105.40	110.46
3	A	244	6MP	C5-C4-N9	-6.30	105.45	110.46
3	B	245	6MP	C5-C4-N9	-6.13	105.58	110.46
3	C	246	6MP	C5-N7-C8	-3.71	103.16	106.27
3	A	244	6MP	C5-N7-C8	-3.66	103.20	106.27
3	B	245	6MP	C5-N7-C8	-3.59	103.27	106.27
3	B	245	6MP	N7-C8-N9	2.62	117.87	113.87
3	A	244	6MP	N7-C8-N9	2.61	117.85	113.87
3	C	246	6MP	N7-C8-N9	2.60	117.83	113.87
3	B	245	6MP	C4-N9-C8	-2.51	102.24	103.84
3	C	246	6MP	C4-N9-C8	-2.33	102.36	103.84
3	B	245	6MP	N1-C2-N3	-2.33	125.06	128.58
3	A	244	6MP	N1-C2-N3	-2.32	125.06	128.58
3	C	246	6MP	N1-C2-N3	-2.32	125.08	128.58
3	A	244	6MP	C4-N9-C8	-2.29	102.38	103.84
3	C	246	6MP	N3-C4-N9	2.16	129.35	125.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	244	6MP	N3-C4-N9	2.14	129.32	125.78
3	B	245	6MP	N3-C4-N9	2.08	129.22	125.78

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
3	A	244	6MP	1	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, 95th 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 ²)	Q<0.9
1	A	237/238 (99%)	0.38	22 (9%) 14 12	18, 32, 70, 113	0
1	B	237/238 (99%)	0.35	25 (10%) 11 10	16, 29, 63, 126	0
1	C	237/238 (99%)	0.46	25 (10%) 11 10	18, 34, 72, 111	0
All	All	711/714 (99%)	0.40	72 (10%) 12 10	16, 31, 71, 126	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	THR	10.0
1	B	214	ALA	9.7
1	B	213	THR	8.3
1	C	212	THR	8.0
1	B	211	GLN	6.3
1	B	206	ILE	5.9
1	A	206	ILE	5.5
1	C	213	THR	5.5
1	B	210	GLU	4.9
1	C	215	ALA	4.8
1	C	211	GLN	4.6
1	A	208	THR	4.6
1	A	210	GLU	4.5
1	A	209	HIS	4.4
1	C	214	ALA	4.4
1	A	207	ARG	4.3
1	B	205	HIS	4.2
1	A	212	THR	4.0
1	B	208	THR	3.9
1	B	163	ASP	3.8
1	B	209	HIS	3.7
1	B	207	ARG	3.6
1	A	217	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	37	ARG	3.5
1	B	97	HIS	3.4
1	B	34	GLU	3.3
1	B	204	ASP	3.2
1	C	210	GLU	3.2
1	C	219	THR	3.2
1	A	97	HIS	3.1
1	C	218	GLN	3.0
1	B	37	ARG	3.0
1	B	101	ARG	3.0
1	C	221	PHE	3.0
1	A	21	ASP	2.9
1	B	147	ASP	2.9
1	C	217	ARG	2.9
1	A	204	ASP	2.7
1	C	147	ASP	2.7
1	B	215	ALA	2.7
1	A	211	GLN	2.7
1	A	163	ASP	2.7
1	C	208	THR	2.6
1	B	112	ASP	2.5
1	C	205	HIS	2.5
1	C	203	SER	2.5
1	A	24	ARG	2.5
1	C	209	HIS	2.5
1	A	149	ARG	2.5
1	C	207	ARG	2.4
1	B	165	GLU	2.4
1	C	90	SER	2.4
1	A	164	GLY	2.4
1	A	147	ASP	2.4
1	A	205	HIS	2.4
1	C	204	ASP	2.3
1	A	30	GLU	2.3
1	A	218	GLN	2.3
1	C	206	ILE	2.3
1	A	214	ALA	2.3
1	A	146	ILE	2.2
1	B	217	ARG	2.2
1	C	99	LYS	2.2
1	C	35	ASP	2.2
1	B	30	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	165	GLU	2.1
1	B	8	GLU	2.1
1	B	35	ASP	2.1
1	B	167	PHE	2.1
1	C	100	LEU	2.1
1	C	236	ASP	2.0
1	A	203	SER	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
3	6MP	B	245	10/10	0.80	0.20	63,64,66,66	0
3	6MP	A	244	10/10	0.82	0.19	70,71,71,71	0
3	6MP	C	246	10/10	0.85	0.20	64,65,65,66	0
2	PO4	A	247	5/5	0.90	0.20	57,59,59,60	0
2	PO4	C	249	5/5	0.94	0.10	39,40,40,41	0
2	PO4	B	248	5/5	0.98	0.08	28,28,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.