



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 4GKA / pdb_00004gka
Title : Crystal structure of purine nucleoside phosphorylase (W16Y, W94Y, W178Y, H257W) mutant from human complexed with phosphate
Authors : Haapalainen, A.M.; Ho, M.C.; Suarez, J.J.; Almo, S.C.; Schramm, V.L.
Deposited on : 2012-08-10
Resolution : 2.20 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:

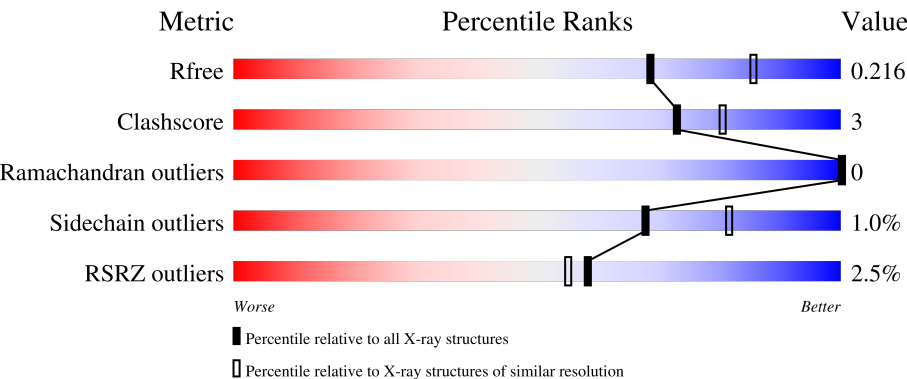
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	324	% 78% 6% 16%
1	B	324	2% 76% 7% 17%
1	C	324	3% 77% • • 18%
1	D	324	% 77% 5% 17%
1	E	324	3% 76% 6% 18%

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Mol	Chain	Length	Quality of chain
1	F	324	3% 76% 6% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13091 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	271	Total	C	N	O	S	0	2	0
			2130	1355	371	388	16			
1	B	269	Total	C	N	O	S	0	2	0
			2121	1349	372	385	15			
1	C	266	Total	C	N	O	S	0	2	0
			2090	1332	365	378	15			
1	D	268	Total	C	N	O	S	0	1	0
			2105	1341	368	381	15			
1	E	267	Total	C	N	O	S	0	2	0
			2103	1339	370	379	15			
1	F	267	Total	C	N	O	S	0	1	0
			2096	1336	367	378	15			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P00491
A	-33	ARG	-	expression tag	UNP P00491
A	-32	GLY	-	expression tag	UNP P00491
A	-31	SER	-	expression tag	UNP P00491
A	-30	HIS	-	expression tag	UNP P00491
A	-29	HIS	-	expression tag	UNP P00491
A	-28	HIS	-	expression tag	UNP P00491
A	-27	HIS	-	expression tag	UNP P00491
A	-26	HIS	-	expression tag	UNP P00491
A	-25	HIS	-	expression tag	UNP P00491
A	-24	GLY	-	expression tag	UNP P00491
A	-23	MET	-	expression tag	UNP P00491
A	-22	ALA	-	expression tag	UNP P00491
A	-21	SER	-	expression tag	UNP P00491
A	-20	MET	-	expression tag	UNP P00491
A	-19	THR	-	expression tag	UNP P00491
A	-18	GLY	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP P00491
A	-16	GLN	-	expression tag	UNP P00491
A	-15	GLN	-	expression tag	UNP P00491
A	-14	MET	-	expression tag	UNP P00491
A	-13	GLY	-	expression tag	UNP P00491
A	-12	ARG	-	expression tag	UNP P00491
A	-11	ASP	-	expression tag	UNP P00491
A	-10	LEU	-	expression tag	UNP P00491
A	-9	TYR	-	expression tag	UNP P00491
A	-8	ASP	-	expression tag	UNP P00491
A	-7	ASP	-	expression tag	UNP P00491
A	-6	ASP	-	expression tag	UNP P00491
A	-5	ASP	-	expression tag	UNP P00491
A	-4	LYS	-	expression tag	UNP P00491
A	-3	ASP	-	expression tag	UNP P00491
A	-2	PRO	-	expression tag	UNP P00491
A	-1	THR	-	expression tag	UNP P00491
A	0	LEU	-	expression tag	UNP P00491
A	16	TYR	TRP	engineered mutation	UNP P00491
A	51	SER	GLY	variant	UNP P00491
A	94	TYR	TRP	engineered mutation	UNP P00491
A	178	TYR	TRP	engineered mutation	UNP P00491
A	257	TRP	HIS	engineered mutation	UNP P00491
B	-34	MET	-	initiating methionine	UNP P00491
B	-33	ARG	-	expression tag	UNP P00491
B	-32	GLY	-	expression tag	UNP P00491
B	-31	SER	-	expression tag	UNP P00491
B	-30	HIS	-	expression tag	UNP P00491
B	-29	HIS	-	expression tag	UNP P00491
B	-28	HIS	-	expression tag	UNP P00491
B	-27	HIS	-	expression tag	UNP P00491
B	-26	HIS	-	expression tag	UNP P00491
B	-25	HIS	-	expression tag	UNP P00491
B	-24	GLY	-	expression tag	UNP P00491
B	-23	MET	-	expression tag	UNP P00491
B	-22	ALA	-	expression tag	UNP P00491
B	-21	SER	-	expression tag	UNP P00491
B	-20	MET	-	expression tag	UNP P00491
B	-19	THR	-	expression tag	UNP P00491
B	-18	GLY	-	expression tag	UNP P00491
B	-17	GLY	-	expression tag	UNP P00491
B	-16	GLN	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	GLN	-	expression tag	UNP P00491
B	-14	MET	-	expression tag	UNP P00491
B	-13	GLY	-	expression tag	UNP P00491
B	-12	ARG	-	expression tag	UNP P00491
B	-11	ASP	-	expression tag	UNP P00491
B	-10	LEU	-	expression tag	UNP P00491
B	-9	TYR	-	expression tag	UNP P00491
B	-8	ASP	-	expression tag	UNP P00491
B	-7	ASP	-	expression tag	UNP P00491
B	-6	ASP	-	expression tag	UNP P00491
B	-5	ASP	-	expression tag	UNP P00491
B	-4	LYS	-	expression tag	UNP P00491
B	-3	ASP	-	expression tag	UNP P00491
B	-2	PRO	-	expression tag	UNP P00491
B	-1	THR	-	expression tag	UNP P00491
B	0	LEU	-	expression tag	UNP P00491
B	16	TYR	TRP	engineered mutation	UNP P00491
B	51	SER	GLY	variant	UNP P00491
B	94	TYR	TRP	engineered mutation	UNP P00491
B	178	TYR	TRP	engineered mutation	UNP P00491
B	257	TRP	HIS	engineered mutation	UNP P00491
C	-34	MET	-	initiating methionine	UNP P00491
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C	-31	SER	-	expression tag	UNP P00491
C	-30	HIS	-	expression tag	UNP P00491
C	-29	HIS	-	expression tag	UNP P00491
C	-28	HIS	-	expression tag	UNP P00491
C	-27	HIS	-	expression tag	UNP P00491
C	-26	HIS	-	expression tag	UNP P00491
C	-25	HIS	-	expression tag	UNP P00491
C	-24	GLY	-	expression tag	UNP P00491
C	-23	MET	-	expression tag	UNP P00491
C	-22	ALA	-	expression tag	UNP P00491
C	-21	SER	-	expression tag	UNP P00491
C	-20	MET	-	expression tag	UNP P00491
C	-19	THR	-	expression tag	UNP P00491
C	-18	GLY	-	expression tag	UNP P00491
C	-17	GLY	-	expression tag	UNP P00491
C	-16	GLN	-	expression tag	UNP P00491
C	-15	GLN	-	expression tag	UNP P00491
C	-14	MET	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	GLY	-	expression tag	UNP P00491
C	-12	ARG	-	expression tag	UNP P00491
C	-11	ASP	-	expression tag	UNP P00491
C	-10	LEU	-	expression tag	UNP P00491
C	-9	TYR	-	expression tag	UNP P00491
C	-8	ASP	-	expression tag	UNP P00491
C	-7	ASP	-	expression tag	UNP P00491
C	-6	ASP	-	expression tag	UNP P00491
C	-5	ASP	-	expression tag	UNP P00491
C	-4	LYS	-	expression tag	UNP P00491
C	-3	ASP	-	expression tag	UNP P00491
C	-2	PRO	-	expression tag	UNP P00491
C	-1	THR	-	expression tag	UNP P00491
C	0	LEU	-	expression tag	UNP P00491
C	16	TYR	TRP	engineered mutation	UNP P00491
C	51	SER	GLY	variant	UNP P00491
C	94	TYR	TRP	engineered mutation	UNP P00491
C	178	TYR	TRP	engineered mutation	UNP P00491
C	257	TRP	HIS	engineered mutation	UNP P00491
D	-34	MET	-	initiating methionine	UNP P00491
D	-33	ARG	-	expression tag	UNP P00491
D	-32	GLY	-	expression tag	UNP P00491
D	-31	SER	-	expression tag	UNP P00491
D	-30	HIS	-	expression tag	UNP P00491
D	-29	HIS	-	expression tag	UNP P00491
D	-28	HIS	-	expression tag	UNP P00491
D	-27	HIS	-	expression tag	UNP P00491
D	-26	HIS	-	expression tag	UNP P00491
D	-25	HIS	-	expression tag	UNP P00491
D	-24	GLY	-	expression tag	UNP P00491
D	-23	MET	-	expression tag	UNP P00491
D	-22	ALA	-	expression tag	UNP P00491
D	-21	SER	-	expression tag	UNP P00491
D	-20	MET	-	expression tag	UNP P00491
D	-19	THR	-	expression tag	UNP P00491
D	-18	GLY	-	expression tag	UNP P00491
D	-17	GLY	-	expression tag	UNP P00491
D	-16	GLN	-	expression tag	UNP P00491
D	-15	GLN	-	expression tag	UNP P00491
D	-14	MET	-	expression tag	UNP P00491
D	-13	GLY	-	expression tag	UNP P00491
D	-12	ARG	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ASP	-	expression tag	UNP P00491
D	-10	LEU	-	expression tag	UNP P00491
D	-9	TYR	-	expression tag	UNP P00491
D	-8	ASP	-	expression tag	UNP P00491
D	-7	ASP	-	expression tag	UNP P00491
D	-6	ASP	-	expression tag	UNP P00491
D	-5	ASP	-	expression tag	UNP P00491
D	-4	LYS	-	expression tag	UNP P00491
D	-3	ASP	-	expression tag	UNP P00491
D	-2	PRO	-	expression tag	UNP P00491
D	-1	THR	-	expression tag	UNP P00491
D	0	LEU	-	expression tag	UNP P00491
D	16	TYR	TRP	engineered mutation	UNP P00491
D	51	SER	GLY	variant	UNP P00491
D	94	TYR	TRP	engineered mutation	UNP P00491
D	178	TYR	TRP	engineered mutation	UNP P00491
D	257	TRP	HIS	engineered mutation	UNP P00491
E	-34	MET	-	initiating methionine	UNP P00491
E	-33	ARG	-	expression tag	UNP P00491
E	-32	GLY	-	expression tag	UNP P00491
E	-31	SER	-	expression tag	UNP P00491
E	-30	HIS	-	expression tag	UNP P00491
E	-29	HIS	-	expression tag	UNP P00491
E	-28	HIS	-	expression tag	UNP P00491
E	-27	HIS	-	expression tag	UNP P00491
E	-26	HIS	-	expression tag	UNP P00491
E	-25	HIS	-	expression tag	UNP P00491
E	-24	GLY	-	expression tag	UNP P00491
E	-23	MET	-	expression tag	UNP P00491
E	-22	ALA	-	expression tag	UNP P00491
E	-21	SER	-	expression tag	UNP P00491
E	-20	MET	-	expression tag	UNP P00491
E	-19	THR	-	expression tag	UNP P00491
E	-18	GLY	-	expression tag	UNP P00491
E	-17	GLY	-	expression tag	UNP P00491
E	-16	GLN	-	expression tag	UNP P00491
E	-15	GLN	-	expression tag	UNP P00491
E	-14	MET	-	expression tag	UNP P00491
E	-13	GLY	-	expression tag	UNP P00491
E	-12	ARG	-	expression tag	UNP P00491
E	-11	ASP	-	expression tag	UNP P00491
E	-10	LEU	-	expression tag	UNP P00491

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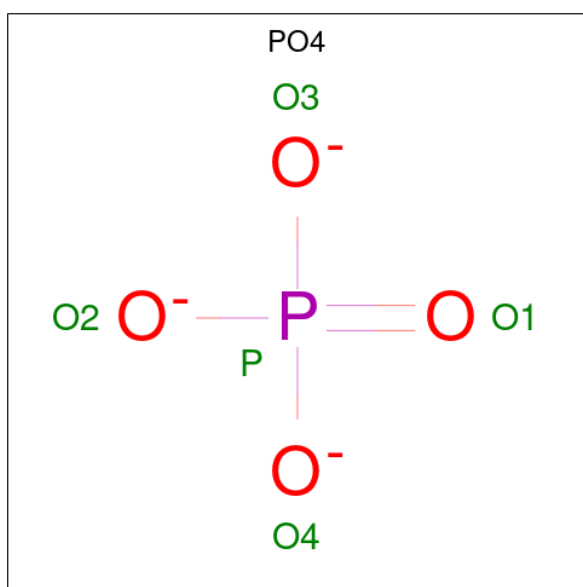
Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	TYR	-	expression tag	UNP P00491
E	-8	ASP	-	expression tag	UNP P00491
E	-7	ASP	-	expression tag	UNP P00491
E	-6	ASP	-	expression tag	UNP P00491
E	-5	ASP	-	expression tag	UNP P00491
E	-4	LYS	-	expression tag	UNP P00491
E	-3	ASP	-	expression tag	UNP P00491
E	-2	PRO	-	expression tag	UNP P00491
E	-1	THR	-	expression tag	UNP P00491
E	0	LEU	-	expression tag	UNP P00491
E	16	TYR	TRP	engineered mutation	UNP P00491
E	51	SER	GLY	variant	UNP P00491
E	94	TYR	TRP	engineered mutation	UNP P00491
E	178	TYR	TRP	engineered mutation	UNP P00491
E	257	TRP	HIS	engineered mutation	UNP P00491
F	-34	MET	-	initiating methionine	UNP P00491
F	-33	ARG	-	expression tag	UNP P00491
F	-32	GLY	-	expression tag	UNP P00491
F	-31	SER	-	expression tag	UNP P00491
F	-30	HIS	-	expression tag	UNP P00491
F	-29	HIS	-	expression tag	UNP P00491
F	-28	HIS	-	expression tag	UNP P00491
F	-27	HIS	-	expression tag	UNP P00491
F	-26	HIS	-	expression tag	UNP P00491
F	-25	HIS	-	expression tag	UNP P00491
F	-24	GLY	-	expression tag	UNP P00491
F	-23	MET	-	expression tag	UNP P00491
F	-22	ALA	-	expression tag	UNP P00491
F	-21	SER	-	expression tag	UNP P00491
F	-20	MET	-	expression tag	UNP P00491
F	-19	THR	-	expression tag	UNP P00491
F	-18	GLY	-	expression tag	UNP P00491
F	-17	GLY	-	expression tag	UNP P00491
F	-16	GLN	-	expression tag	UNP P00491
F	-15	GLN	-	expression tag	UNP P00491
F	-14	MET	-	expression tag	UNP P00491
F	-13	GLY	-	expression tag	UNP P00491
F	-12	ARG	-	expression tag	UNP P00491
F	-11	ASP	-	expression tag	UNP P00491
F	-10	LEU	-	expression tag	UNP P00491
F	-9	TYR	-	expression tag	UNP P00491
F	-8	ASP	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	ASP	-	expression tag	UNP P00491
F	-6	ASP	-	expression tag	UNP P00491
F	-5	ASP	-	expression tag	UNP P00491
F	-4	LYS	-	expression tag	UNP P00491
F	-3	ASP	-	expression tag	UNP P00491
F	-2	PRO	-	expression tag	UNP P00491
F	-1	THR	-	expression tag	UNP P00491
F	0	LEU	-	expression tag	UNP P00491
F	16	TYR	TRP	engineered mutation	UNP P00491
F	51	SER	GLY	variant	UNP P00491
F	94	TYR	TRP	engineered mutation	UNP P00491
F	178	TYR	TRP	engineered mutation	UNP P00491
F	257	TRP	HIS	engineered mutation	UNP P00491

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



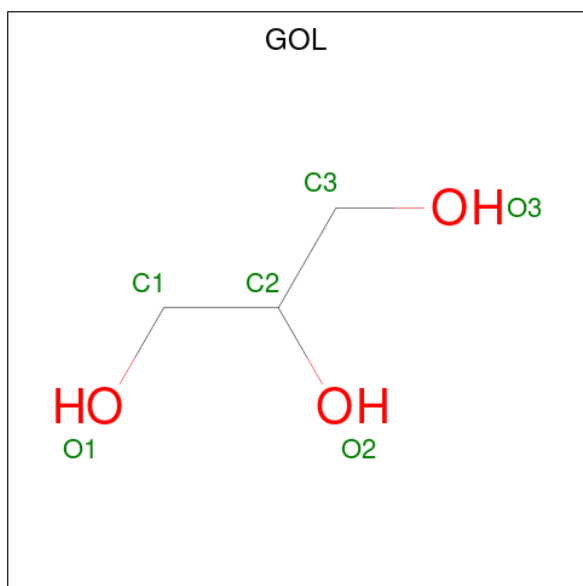
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

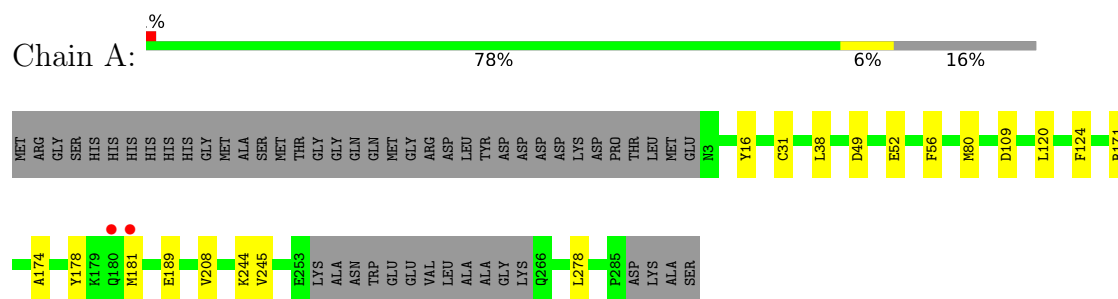
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	45	Total	O	0	0
			45	45		
4	C	100	Total	O	0	0
			100	100		
4	D	46	Total	O	0	0
			46	46		
4	E	38	Total	O	0	0
			38	38		
4	F	119	Total	O	0	0
			119	119		

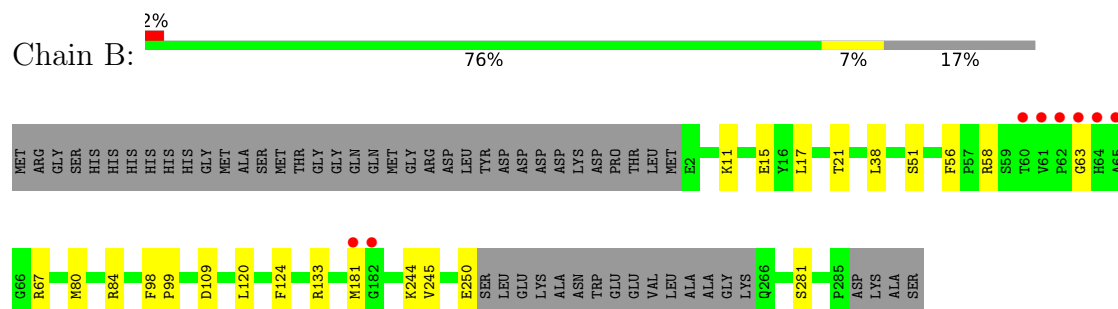
3 Residue-property plots [i](#)

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.

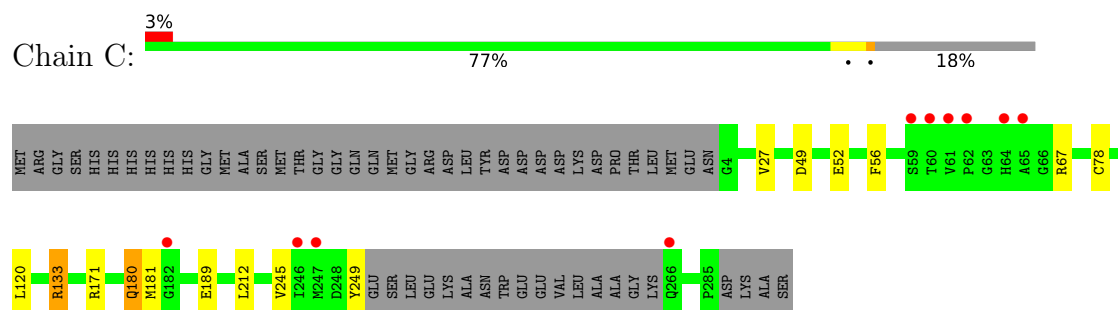
- Molecule 1: Purine nucleoside phosphorylase



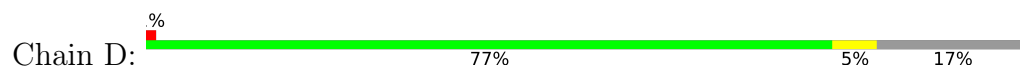
- Molecule 1: Purine nucleoside phosphorylase

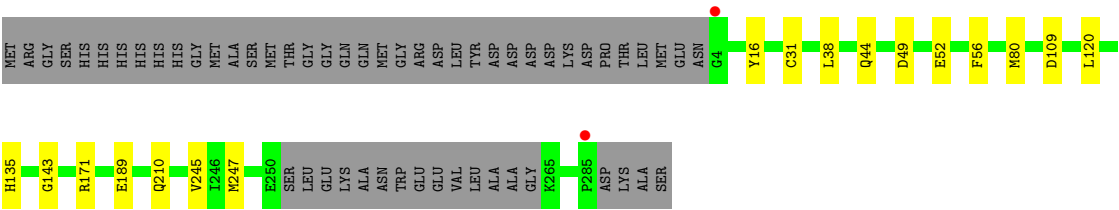


- Molecule 1: Purine nucleoside phosphorylase

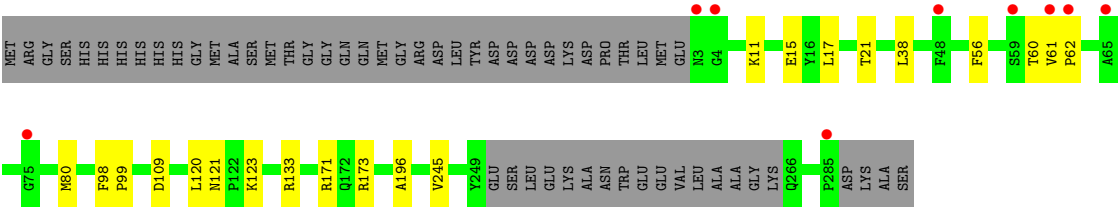
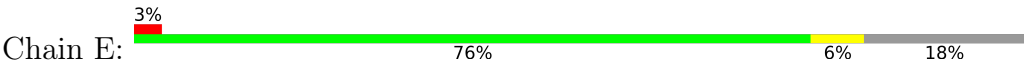


- Molecule 1: Purine nucleoside phosphorylase

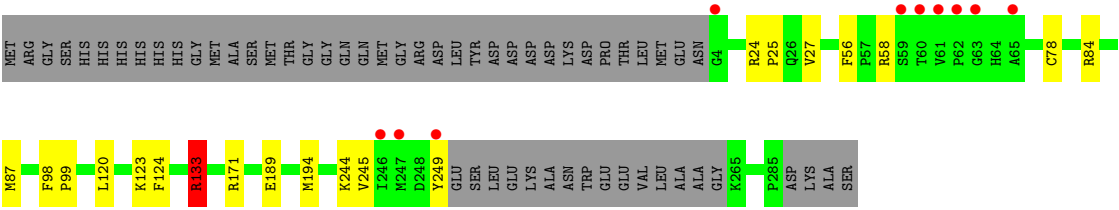
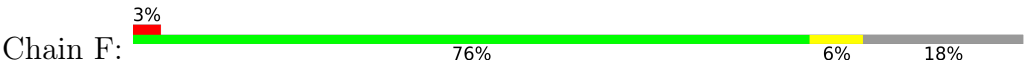




● Molecule 1: Purine nucleoside phosphorylase



● Molecule 1: Purine nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 233.67Å 70.08Å 90.00° 97.33° 90.00°	Depositor
Resolution (Å)	45.29 – 2.20 45.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.29-2.20) 99.6 (45.29-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.188 , 0.232 (Not available) , 0.216	Depositor DCC
R_{free} test set	4320 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13091	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL

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	0.64	0/2183	0.83	0/2951
1	B	0.58	0/2174	0.83	3/2938 (0.1%)
1	C	0.79	0/2143	0.89	1/2897 (0.0%)
1	D	0.62	0/2155	0.81	0/2912
1	E	0.58	0/2156	0.77	0/2914
1	F	0.83	0/2146	0.90	1/2900 (0.0%)
All	All	0.68	0/12957	0.84	5/17512 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	MET	N-CA-C	-6.86	101.48	110.53
1	B	67	ARG	N-CA-C	6.09	118.38	108.76
1	F	133	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	C	67	ARG	N-CA-C	5.18	116.71	108.79
1	B	63	GLY	N-CA-C	-5.12	107.81	113.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2130	0	2115	13	0
1	B	2121	0	2107	13	0
1	C	2090	0	2081	12	0
1	D	2105	0	2095	13	0
1	E	2103	0	2095	19	0
1	F	2096	0	2089	14	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	C	6	0	8	0	0
3	F	6	0	8	2	0
4	A	56	0	0	0	0
4	B	45	0	0	0	0
4	C	100	0	0	0	0
4	D	46	0	0	1	0
4	E	38	0	0	0	0
4	F	119	0	0	1	0
All	All	13091	0	12598	80	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 3.

All (80) 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:F:133:ARG:HG2	1:F:133:ARG:HH21	1.21	1.01
1:C:133:ARG:HG2	1:C:133:ARG:HH21	1.33	0.94
1:E:173[B]:ARG:HH21	1:E:173[B]:ARG:CG	1.82	0.93
1:F:133:ARG:HH21	1:F:133:ARG:CG	1.85	0.87
1:E:173[B]:ARG:HH21	1:E:173[B]:ARG:HG2	1.44	0.82
1:F:24:ARG:HB3	3:F:302:GOL:H31	1.73	0.71
1:C:133:ARG:HH21	1:C:133:ARG:CG	1.99	0.69
1:E:173[B]:ARG:HH21	1:E:173[B]:ARG:HG3	1.62	0.62
1:F:120:LEU:HD23	1:F:245:VAL:HG21	1.81	0.61
1:C:120:LEU:HD23	1:C:245:VAL:HG21	1.83	0.61
1:C:133:ARG:CG	1:C:133:ARG:NH2	2.63	0.60
1:A:178:TYR:O	1:A:181:MET:O	2.21	0.59
1:F:133:ARG:CG	1:F:133:ARG:NH2	2.57	0.57
1:A:31:CYS:SG	1:A:80:MET:HE2	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173[B]:ARG:CG	1:E:173[B]:ARG:NH2	2.53	0.56
1:F:171[A]:ARG:NE	1:F:189:GLU:OE2	2.32	0.56
1:C:171[A]:ARG:NE	1:C:189:GLU:OE2	2.32	0.55
1:C:133:ARG:HG2	1:C:133:ARG:NH2	2.12	0.54
1:E:38:LEU:HG	1:E:80:MET:HE1	1.89	0.53
1:B:38:LEU:HG	1:B:80:MET:HE1	1.89	0.53
1:D:31:CYS:SG	1:D:80:MET:HE2	2.50	0.50
1:E:133:ARG:HH11	1:F:249:TYR:CB	2.24	0.50
1:C:180:GLN:CG	1:C:181:MET:N	2.74	0.50
1:A:171[A]:ARG:NE	1:A:189:GLU:OE2	2.38	0.50
1:E:60:THR:HG22	1:E:60:THR:O	2.12	0.49
1:F:124:PHE:O	1:F:244:LYS:HD3	2.13	0.49
1:B:120:LEU:HD23	1:B:245:VAL:HG21	1.95	0.48
1:B:11:LYS:O	1:B:15:GLU:HG2	2.12	0.48
1:C:27:VAL:O	1:C:78:CYS:HB2	2.14	0.48
1:D:171[A]:ARG:NE	1:D:189:GLU:OE2	2.39	0.48
1:B:38:LEU:CG	1:B:80:MET:HE1	2.45	0.47
1:E:11:LYS:O	1:E:15:GLU:HG2	2.14	0.47
1:E:38:LEU:CG	1:E:80:MET:HE1	2.44	0.47
1:E:173[B]:ARG:HG2	1:E:173[B]:ARG:NH2	2.22	0.47
1:D:38:LEU:HB3	1:D:80:MET:HE1	1.97	0.47
1:E:120:LEU:HD23	1:E:245:VAL:HG21	1.96	0.47
1:B:17:LEU:O	1:B:21:THR:HG22	2.15	0.46
1:C:49:ASP:O	1:C:52:GLU:HG2	2.14	0.46
1:A:120:LEU:HD23	1:A:245:VAL:HG21	1.98	0.46
1:E:61:VAL:HB	1:E:62:PRO:CD	2.46	0.45
1:A:16:TYR:CD2	1:A:16:TYR:C	2.94	0.45
1:A:38:LEU:HG	1:A:80:MET:HE1	1.99	0.45
1:A:38:LEU:HB3	1:A:80:MET:HE1	1.99	0.45
1:B:133:ARG:HH21	1:B:133:ARG:HD2	1.60	0.45
1:E:133:ARG:HH22	1:E:171[A]:ARG:NH2	2.15	0.45
1:F:123:LYS:HE3	4:F:467:HOH:O	2.16	0.45
1:F:87:MET:HE3	1:F:194:MET:HE2	1.98	0.45
1:D:16:TYR:CD2	1:D:16:TYR:C	2.94	0.44
1:F:120:LEU:HD23	1:F:245:VAL:CG2	2.48	0.44
1:D:49:ASP:O	1:D:52:GLU:HG2	2.18	0.44
1:B:51:SER:HB2	1:B:58:ARG:HH11	1.82	0.44
1:B:98:PHE:HB3	1:B:99:PRO:HD3	2.00	0.44
1:D:135:HIS:CD2	1:D:135:HIS:C	2.96	0.44
1:A:38:LEU:CG	1:A:80:MET:HE1	2.48	0.43
1:A:208:VAL:HG13	1:C:212:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD23	1:D:245:VAL:HG21	1.99	0.43
1:F:25:PRO:O	3:F:302:GOL:H32	2.18	0.43
1:E:98:PHE:HB3	1:E:99:PRO:HD3	2.00	0.43
1:D:44:GLN:N	4:D:432:HOH:O	2.51	0.43
1:F:98:PHE:HB3	1:F:99:PRO:HD3	2.00	0.43
1:E:173[B]:ARG:HG3	1:E:173[B]:ARG:NH2	2.26	0.43
1:B:84:ARG:HD2	2:B:301:PO4:O3	2.19	0.43
1:D:109:ASP:OD1	1:D:109:ASP:C	2.62	0.43
1:F:27:VAL:O	1:F:78:CYS:HB2	2.19	0.43
1:A:49:ASP:O	1:A:52:GLU:HG2	2.19	0.42
1:D:143:GLY:HA2	1:E:196:ALA:CB	2.50	0.42
1:A:124:PHE:O	1:A:244:LYS:HD3	2.19	0.42
1:E:109:ASP:OD1	1:E:109:ASP:C	2.63	0.41
1:B:51:SER:HA	1:B:58:ARG:HD3	2.02	0.41
1:B:124:PHE:O	1:B:244:LYS:HD3	2.20	0.41
1:D:38:LEU:HG	1:D:80:MET:HE1	2.02	0.41
1:B:109:ASP:OD1	1:B:109:ASP:C	2.64	0.41
1:D:210:GLN:HB2	1:D:247:MET:HE1	2.03	0.41
1:E:121:ASN:OD1	1:E:123:LYS:HG2	2.20	0.41
1:B:133:ARG:HH11	1:C:249:TYR:CB	2.33	0.41
1:C:133:ARG:HD2	1:C:189:GLU:OE2	2.21	0.41
1:E:17:LEU:O	1:E:21:THR:HG22	2.21	0.41
1:A:174:ALA:HA	1:A:278:LEU:HD21	2.03	0.41
1:D:38:LEU:CG	1:D:80:MET:HE1	2.51	0.41
1:A:109:ASP:OD1	1:A:109:ASP:C	2.64	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	269/324 (83%)	268 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	258/324 (80%)	255 (99%)	3 (1%)	0	100	100
1	C	264/324 (82%)	258 (98%)	6 (2%)	0	100	100
1	D	257/324 (79%)	256 (100%)	1 (0%)	0	100	100
1	E	265/324 (82%)	258 (97%)	7 (3%)	0	100	100
1	F	264/324 (82%)	260 (98%)	4 (2%)	0	100	100
All	All	1577/1944 (81%)	1555 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	229/269 (85%)	228 (100%)	1 (0%)	84	92
1	B	227/269 (84%)	224 (99%)	3 (1%)	61	76
1	C	224/269 (83%)	221 (99%)	3 (1%)	61	76
1	D	225/269 (84%)	224 (100%)	1 (0%)	84	92
1	E	225/269 (84%)	224 (100%)	1 (0%)	84	92
1	F	224/269 (83%)	220 (98%)	4 (2%)	51	68
All	All	1354/1614 (84%)	1341 (99%)	13 (1%)	68	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	PHE
1	B	56	PHE
1	B	250	GLU
1	B	281	SER
1	C	56	PHE
1	C	133	ARG
1	C	180	GLN
1	D	56	PHE

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Mol	Chain	Res	Type
1	E	56	PHE
1	F	56	PHE
1	F	58	ARG
1	F	84	ARG
1	F	133	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	C	64	HIS
1	C	180	GLN
1	D	180	GLN
1	D	210	GLN
1	E	3	ASN
1	E	188	GLN

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 [i](#)

8 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	D	301	-	4,4,4	0.82	0	6,6,6	0.78	0
2	PO4	A	301	-	4,4,4	1.32	0	6,6,6	0.94	0
3	GOL	C	302	-	5,5,5	0.57	0	5,5,5	0.59	0
3	GOL	F	302	-	5,5,5	0.60	0	5,5,5	1.02	0
2	PO4	B	301	-	4,4,4	1.12	0	6,6,6	0.93	0
2	PO4	E	301	-	4,4,4	1.00	0	6,6,6	0.88	0
2	PO4	F	301	-	4,4,4	1.59	0	6,6,6	0.57	0
2	PO4	C	301	-	4,4,4	1.80	1 (25%)	6,6,6	1.42	1 (16%)

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	GOL	C	302	-	-	0/4/4/4	-
3	GOL	F	302	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	PO4	P-O2	-2.09	1.48	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	PO4	O3-P-O1	-2.99	100.37	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	GOL	2	0
2	B	301	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	271/324 (83%)	0.07	2 (0%) 84 82	24, 47, 72, 113	2 (0%)
1	B	269/324 (83%)	0.35	8 (2%) 52 49	25, 53, 87, 135	2 (0%)
1	C	266/324 (82%)	-0.20	10 (3%) 44 41	21, 33, 76, 104	2 (0%)
1	D	268/324 (82%)	0.22	2 (0%) 84 82	25, 51, 76, 100	1 (0%)
1	E	267/324 (82%)	0.45	9 (3%) 48 45	26, 55, 83, 127	2 (0%)
1	F	267/324 (82%)	-0.32	10 (3%) 45 42	19, 31, 60, 115	1 (0%)
All	All	1608/1944 (82%)	0.10	41 (2%) 58 55	19, 44, 79, 135	10 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	ALA	4.2
1	B	61	VAL	3.8
1	D	4	GLY	3.8
1	C	62	PRO	3.7
1	F	246	ILE	3.4
1	C	247	MET	3.3
1	C	59	SER	3.3
1	E	61	VAL	3.1
1	C	246	ILE	3.0
1	F	65	ALA	3.0
1	E	62	PRO	3.0
1	C	182	GLY	2.9
1	E	3	ASN	2.9
1	C	61	VAL	2.8
1	B	60	THR	2.7
1	F	60	THR	2.7
1	F	63	GLY	2.6
1	B	182	GLY	2.6
1	C	64	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	62	PRO	2.4
1	B	63	GLY	2.4
1	F	247	MET	2.4
1	C	60	THR	2.3
1	F	61	VAL	2.3
1	B	181	MET	2.3
1	E	4	GLY	2.2
1	B	64	HIS	2.2
1	A	181	MET	2.2
1	F	62	PRO	2.2
1	C	266	GLN	2.2
1	A	180	GLN	2.1
1	E	59	SER	2.1
1	E	65	ALA	2.1
1	E	48	PHE	2.1
1	E	75	GLY	2.1
1	F	4	GLY	2.1
1	E	285	PRO	2.1
1	F	59	SER	2.0
1	C	65	ALA	2.0
1	D	285	PRO	2.0
1	F	249	TYR	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	GOL	F	302	6/6	0.84	0.15	33,44,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	302	6/6	0.91	0.11	43,52,54,56	0
2	PO4	B	301	5/5	0.94	0.08	46,47,50,53	0
2	PO4	D	301	5/5	0.96	0.06	33,34,37,38	0
2	PO4	E	301	5/5	0.96	0.06	45,46,51,51	0
2	PO4	F	301	5/5	0.98	0.06	35,36,40,41	0
2	PO4	A	301	5/5	0.98	0.04	30,31,33,34	0
2	PO4	C	301	5/5	0.98	0.06	35,35,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.