WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 8, 2016 – 05:28 PM EDT

PDB ID	:	5ETJ
Title	:	Crystal structure of purine nucleoside phosphorylase (E258D, L261A) mutant from human complexed with DADMe-ImmG and phosphate
Authors	:	Cameron, S.A.; Suarez, J.; Schramm, V.L.; Almo, S.C.
Deposited on	:	2015-11-17
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

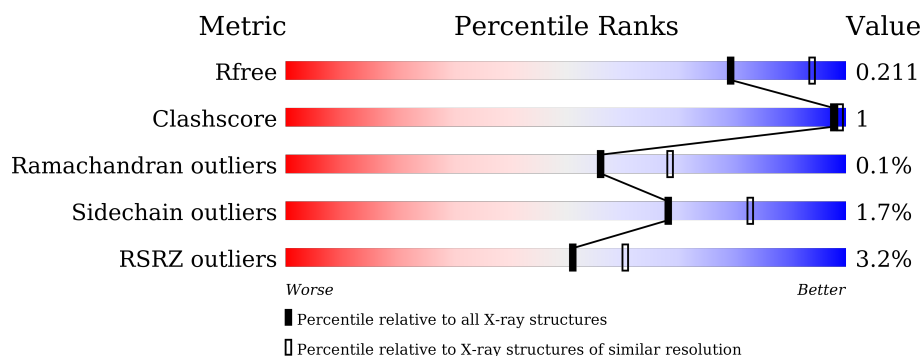|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.30 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	Percentile Ranks	Value
Rfree		0.211
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		1.7%
RSRZ outliers		3.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% ··· 85% ·· · 11%
1	B	324	4% 85% · 11%
1	C	324	% 85% · 11%
1	D	324	2% 82% 6% 11%
1	E	324	2% 87% · 11%
1	F	324	6% 85% · 11%

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	PO4	F	301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13897 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	288	Total	C	N	O	S	0	0	0
			2228	1416	387	409	16			
1	B	287	Total	C	N	O	S	0	0	0
			2220	1410	385	409	16			
1	C	288	Total	C	N	O	S	0	0	0
			2232	1418	387	411	16			
1	D	288	Total	C	N	O	S	0	0	0
			2224	1414	386	408	16			
1	E	288	Total	C	N	O	S	0	0	0
			2230	1417	389	409	15			
1	F	288	Total	C	N	O	S	0	0	0
			2231	1419	389	407	16			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	expression tag	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	51	SER	GLY	conflict	UNP P00491
A	258	ASP	GLU	engineered mutation	UNP P00491
A	261	ALA	LEU	engineered mutation	UNP P00491
B	-34	MET	-	expression tag	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
B	-15	GLN	-	expression tag	UNP P00491
B	-14	MET	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
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	51	SER	GLY	conflict	UNP P00491
B	258	ASP	GLU	engineered mutation	UNP P00491
B	261	ALA	LEU	engineered mutation	UNP P00491
C	-34	MET	-	expression tag	UNP P00491
C	-33	ARG	-	expression tag	UNP P00491
C	-32	GLY	-	expression tag	UNP P00491
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	51	SER	GLY	conflict	UNP P00491
C	258	ASP	GLU	engineered mutation	UNP P00491
C	261	ALA	LEU	engineered mutation	UNP P00491
D	-34	MET	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	51	SER	GLY	conflict	UNP P00491
D	258	ASP	GLU	engineered mutation	UNP P00491
D	261	ALA	LEU	engineered mutation	UNP P00491
E	-34	MET	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	THR	-	expression tag	UNP P00491
E	0	LEU	-	expression tag	UNP P00491
E	51	SER	GLY	conflict	UNP P00491
E	258	ASP	GLU	engineered mutation	UNP P00491
E	261	ALA	LEU	engineered mutation	UNP P00491
F	-34	MET	-	expression tag	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
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	51	SER	GLY	conflict	UNP P00491
F	258	ASP	GLU	engineered mutation	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
F	261	ALA	LEU	engineered mutation	UNP P00491

- Molecule 2 is 2-amino-7-{[(3R,4R)-3-hydroxy-4-(hydroxymethyl)pyrrolidin-1-yl]methyl}-3,5
-dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: IM5) (formula: $C_{12}H_{17}N_5O_3$).
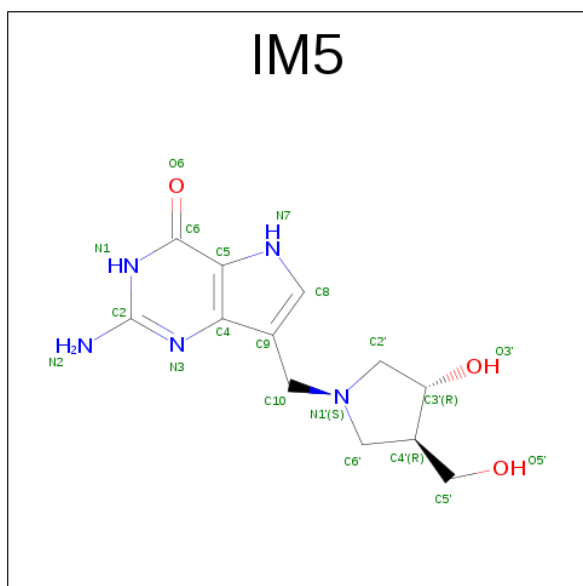
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	12	5	3		
2	B	1	Total	C	N	O	0	0
			20	12	5	3		
2	C	1	Total	C	N	O	0	0
			20	12	5	3		
2	D	1	Total	C	N	O	0	0
			20	12	5	3		
2	E	1	Total	C	N	O	0	0
			20	12	5	3		
2	F	1	Total	C	N	O	0	0
			20	12	5	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P = O O1

P

O⁻

O4
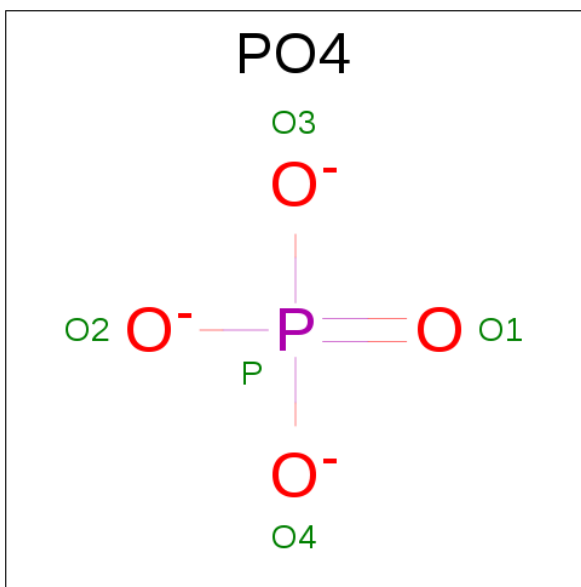
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

W O R L D W I D E
PDB
PROTEIN DATA BANK

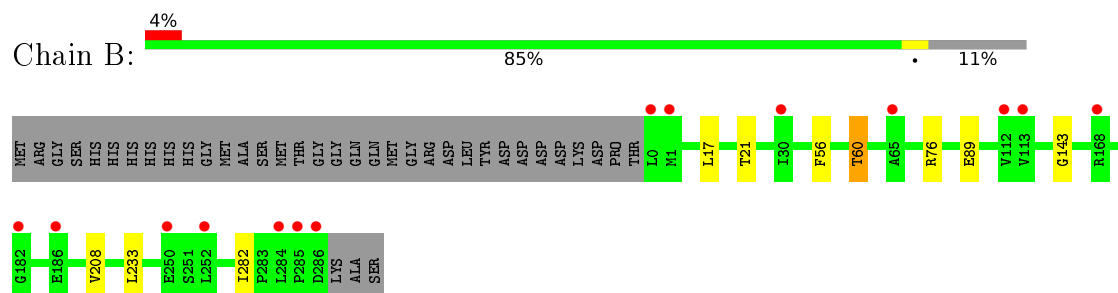| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total 68	O 68	0	0
4	B	45	Total 45	O 45	0	0
4	C	85	Total 85	O 85	0	0
4	D	67	Total 67	O 67	0	0
4	E	41	Total 41	O 41	0	0
4	F	46	Total 46	O 46	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
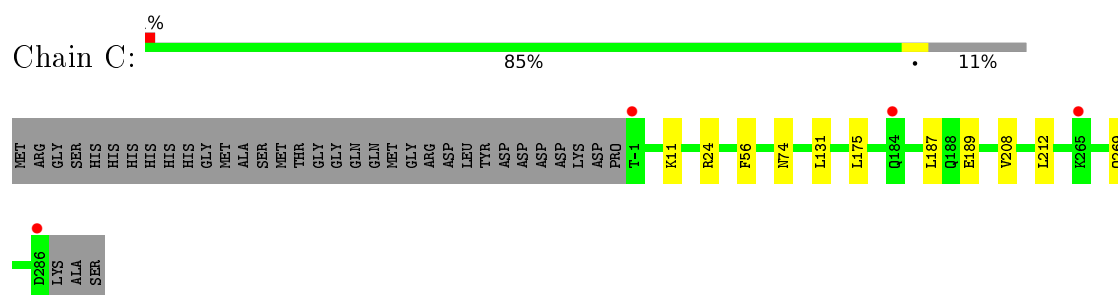
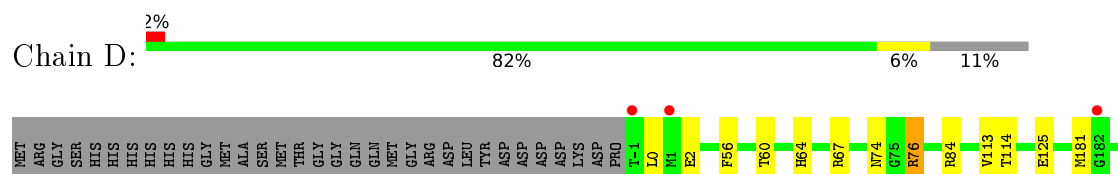- Molecule 1: Purine nucleoside phosphorylase
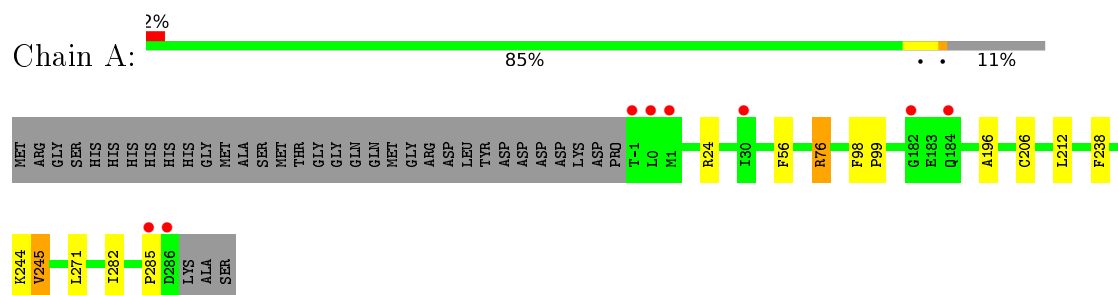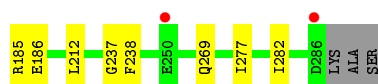

- Molecule 1: Purine nucleoside phosphorylase

- Molecule 1: Purine nucleoside phosphorylase

- Molecule 1: Purine nucleoside phosphorylase

R185 E186 L212 G237 F238 E250 Q269 I277 I282 D286 LYS ALA SER

- Molecule 1: Purine nucleoside phosphorylase

Chain E:

2%

87%   11%

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP ASP LYS ASP PRO T-1 L0 M1 E2 E8 L17 T21 F56 V100 R133 R185 V208 L212 D286 LYS ALA SER
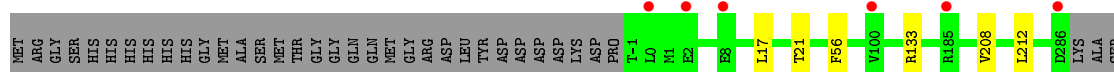
- Molecule 1: Purine nucleoside phosphorylase

Chain F:

6%

85%   11%

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP ASP LYS ASP PRO T-1 L0 M1 A28 I29 I30 L35 D40 A45 F56 T60 V61 P62 G63 H64 A65 L68 V69 F70

V79 F98 P99 T114 R133 R173 G182 E183 Q184 V208 F238 L252 Q269 K270 L271 L284 P285 D286 LYS ALA SER
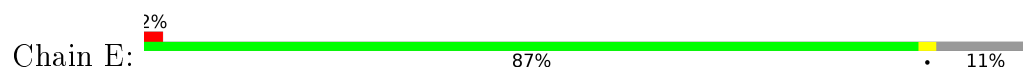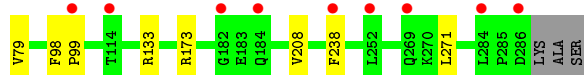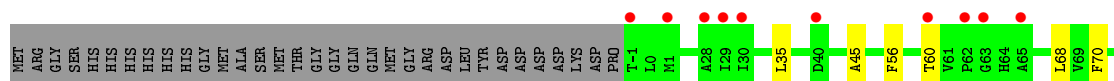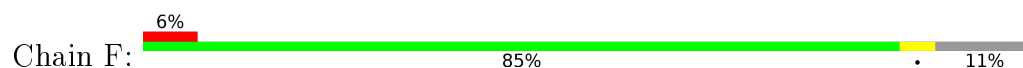
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	268.81Å 58.84Å 173.16Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.30) 99.9 (24.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$<I/\sigma(I)>$ [1]	2.25 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.178 , 0.211 0.184 , 0.211	Depositor DCC
R_{free} test set	5579 reflections (5.26%)	DCC
Wilson B-factor (Å²)	39.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 33.0	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13897	wwPDB-VP
Average B, all atoms (Å²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, IM5

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	0.57	0/2280	0.75	1/3091 (0.0%)
1	B	0.55	0/2272	0.74	0/3081
1	C	0.58	0/2284	0.77	1/3096 (0.0%)
1	D	0.56	0/2276	0.74	0/3086
1	E	0.52	0/2282	0.74	0/3094
1	F	0.55	0/2283	0.74	2/3093 (0.1%)
All	All	0.55	0/13677	0.75	4/18541 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	133	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	C	24	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	173	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	24	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	2228	0	2181	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2220	0	2165	5	0
1	C	2232	0	2185	6	0
1	D	2224	0	2175	7	0
1	E	2230	0	2180	3	0
1	F	2231	0	2188	9	0
2	A	20	0	17	0	0
2	B	20	0	17	0	0
2	C	20	0	17	0	0
2	D	20	0	17	0	0
2	E	20	0	17	0	0
2	F	20	0	17	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	15	0	0	0	0
4	A	68	0	0	0	0
4	B	45	0	0	0	0
4	C	85	0	0	0	0
4	D	67	0	0	0	0
4	E	41	0	0	0	0
4	F	46	0	0	0	0
All	All	13897	0	13176	30	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 1.

All (30) 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:B:60:THR:HB	1:B:89:GLU:OE2	1.99	0.62
1:B:76:ARG:NH2	1:B:282:ILE:O	2.31	0.60
1:A:76:ARG:NH2	1:A:282:ILE:O	2.31	0.59
1:D:76:ARG:NH2	1:D:282:ILE:O	2.37	0.58
1:A:206:CYS:SG	1:A:245:VAL:CG2	2.96	0.54
1:B:17:LEU:O	1:B:21:THR:HG22	2.12	0.50
1:C:175:LEU:HD11	1:C:189:GLU:OE1	2.13	0.49
1:F:68:LEU:HD22	1:F:79:VAL:HG22	1.94	0.48
1:C:269:GLN:HA	1:C:269:GLN:HE21	1.78	0.47
1:E:212:LEU:HD22	1:F:208:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD22	1:C:208:VAL:HG13	1.97	0.47
1:D:60:THR:O	1:D:60:THR:HG22	2.16	0.45
1:F:98:PHE:HB3	1:F:99:PRO:HD3	2.00	0.44
1:D:64:HIS:HD2	1:D:84:ARG:H	1.65	0.44
1:D:114:THR:HG22	1:D:238:PHE:CE2	2.53	0.44
1:F:238:PHE:CE1	1:F:271:LEU:HD22	2.53	0.44
1:F:35:LEU:HD22	1:F:271:LEU:HD13	2.00	0.44
1:D:113:VAL:O	1:D:237:GLY:HA2	2.18	0.43
1:C:74:ASN:HB3	1:D:74:ASN:OD1	2.19	0.43
1:B:208:VAL:HG13	1:C:212:LEU:HD22	2.01	0.43
1:F:68:LEU:HD22	1:F:79:VAL:CG2	2.48	0.43
1:D:212:LEU:HD22	1:E:208:VAL:HG13	1.99	0.43
1:E:17:LEU:O	1:E:21:THR:HG22	2.18	0.42
1:A:98:PHE:HB3	1:A:99:PRO:HD3	2.01	0.42
1:C:131:LEU:HD21	1:C:187:LEU:HD21	2.02	0.42
1:F:45:ALA:HA	1:F:70:PHE:O	2.20	0.42
1:F:271:LEU:HD23	1:F:271:LEU:HA	1.91	0.41
1:A:196:ALA:CB	1:B:143:GLY:HA2	2.50	0.41
1:A:238:PHE:CE1	1:A:271:LEU:HD11	2.57	0.40
1:F:35:LEU:HD22	1:F:271:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/324 (88%)	280 (98%)	5 (2%)	1 (0%)	46	57
1	B	285/324 (88%)	281 (99%)	4 (1%)	0	100	100
1	C	286/324 (88%)	283 (99%)	3 (1%)	0	100	100
1	D	286/324 (88%)	282 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	286/324 (88%)	283 (99%)	3 (1%)	0	100	100
1	F	286/324 (88%)	283 (99%)	3 (1%)	0	100	100
All	All	1715/1944 (88%)	1692 (99%)	22 (1%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	PRO

5.3.2   Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/268 (87%)	230 (98%)	4 (2%)	68	83
1	B	233/268 (87%)	230 (99%)	3 (1%)	76	87
1	C	235/268 (88%)	233 (99%)	2 (1%)	84	93
1	D	233/268 (87%)	222 (95%)	11 (5%)	32	43
1	E	233/268 (87%)	231 (99%)	2 (1%)	84	93
1	F	233/268 (87%)	231 (99%)	2 (1%)	84	93
All	All	1401/1608 (87%)	1377 (98%)	24 (2%)	68	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	PHE
1	A	76	ARG
1	A	244	LYS
1	A	245	VAL
1	B	56	PHE
1	B	60	THR
1	B	233	LEU
1	C	11	LYS
1	C	56	PHE

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Mol	Chain	Res	Type
1	D	0	LEU
1	D	2	GLU
1	D	56	PHE
1	D	67	ARG
1	D	76	ARG
1	D	125	GLU
1	D	181	MET
1	D	185	ARG
1	D	186	GLU
1	D	269	GLN
1	D	277	ILE
1	E	56	PHE
1	E	133	ARG
1	F	56	PHE
1	F	60	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	GLN
1	B	256	ASN
1	C	256	ASN
1	C	269	GLN
1	D	44	GLN
1	D	64	HIS
1	E	180	GLN
1	E	210	GLN
1	E	256	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

18 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	IM5	A	301	-	20,22,22	1.11	1 (5%)	17,32,32	2.72	7 (41%)
3	PO4	A	302	-	4,4,4	1.17	0	6,6,6	0.26	0
3	PO4	A	303	-	4,4,4	0.61	0	6,6,6	0.23	0
2	IM5	B	301	-	20,22,22	0.90	1 (5%)	17,32,32	2.84	6 (35%)
3	PO4	B	302	-	4,4,4	0.75	0	6,6,6	0.26	0
3	PO4	B	303	-	4,4,4	0.63	0	6,6,6	0.27	0
2	IM5	C	301	-	20,22,22	0.89	1 (5%)	17,32,32	2.51	7 (41%)
3	PO4	C	302	-	4,4,4	1.07	0	6,6,6	0.25	0
3	PO4	C	303	-	4,4,4	0.61	0	6,6,6	0.25	0
2	IM5	D	301	-	20,22,22	0.70	1 (5%)	17,32,32	2.81	6 (35%)
3	PO4	D	302	-	4,4,4	1.05	0	6,6,6	0.25	0
3	PO4	D	303	-	4,4,4	0.73	0	6,6,6	0.24	0
2	IM5	E	301	-	20,22,22	1.11	2 (10%)	17,32,32	2.79	7 (41%)
3	PO4	E	302	-	4,4,4	0.98	0	6,6,6	0.27	0
3	PO4	F	301	-	4,4,4	0.43	0	6,6,6	0.26	0
2	IM5	F	302	-	20,22,22	0.98	1 (5%)	17,32,32	2.63	7 (41%)
3	PO4	F	303	-	4,4,4	0.85	0	6,6,6	0.23	0
3	PO4	F	304	-	4,4,4	0.64	0	6,6,6	0.24	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
2	IM5	A	301	-	-	0/5/18/18	0/3/3/3
3	PO4	A	302	-	-	0/0/0/0	0/0/0/0
3	PO4	A	303	-	-	0/0/0/0	0/0/0/0
2	IM5	B	301	-	-	0/5/18/18	0/3/3/3
3	PO4	B	302	-	-	0/0/0/0	0/0/0/0
3	PO4	B	303	-	-	0/0/0/0	0/0/0/0
2	IM5	C	301	-	-	0/5/18/18	0/3/3/3
3	PO4	C	302	-	-	0/0/0/0	0/0/0/0
3	PO4	C	303	-	-	0/0/0/0	0/0/0/0
2	IM5	D	301	-	-	0/5/18/18	0/3/3/3
3	PO4	D	302	-	-	0/0/0/0	0/0/0/0
3	PO4	D	303	-	-	0/0/0/0	0/0/0/0
2	IM5	E	301	-	-	0/5/18/18	0/3/3/3
3	PO4	E	302	-	-	0/0/0/0	0/0/0/0
3	PO4	F	301	-	-	0/0/0/0	0/0/0/0
2	IM5	F	302	-	-	0/5/18/18	0/3/3/3
3	PO4	F	303	-	-	0/0/0/0	0/0/0/0
3	PO4	F	304	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	IM5	C4-N3	-2.19	1.32	1.37
2	D	301	IM5	C6-C5	2.04	1.45	1.41
2	C	301	IM5	C6-C5	2.12	1.45	1.41
2	B	301	IM5	C6-C5	2.78	1.46	1.41
2	A	301	IM5	C6-C5	2.97	1.47	1.41
2	E	301	IM5	C6-C5	3.32	1.48	1.41
2	F	302	IM5	C6-C5	3.55	1.48	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	IM5	C6-C5-C4	-5.72	114.32	120.86
2	B	301	IM5	C6-C5-C4	-5.59	114.47	120.86
2	E	301	IM5	C5-C6-N1	-5.17	116.76	123.52
2	D	301	IM5	C6-C5-C4	-5.16	114.97	120.86
2	F	302	IM5	C6-C5-C4	-4.92	115.24	120.86
2	A	301	IM5	C5-C6-N1	-4.68	117.40	123.52
2	F	302	IM5	C5-C6-N1	-4.68	117.40	123.52
2	E	301	IM5	C6-C5-C4	-4.60	115.61	120.86
2	A	301	IM5	C6-C5-C4	-4.37	115.87	120.86
2	D	301	IM5	C5-C6-N1	-4.35	117.83	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	IM5	N3-C2-N1	-3.99	122.12	127.56
2	A	301	IM5	N3-C2-N1	-3.97	122.16	127.56
2	C	301	IM5	N3-C2-N1	-3.89	122.27	127.56
2	B	301	IM5	C5-C6-N1	-3.88	118.45	123.52
2	B	301	IM5	N3-C2-N1	-3.78	122.42	127.56
2	D	301	IM5	N3-C2-N1	-3.74	122.47	127.56
2	F	302	IM5	N3-C2-N1	-3.22	123.18	127.56
2	A	301	IM5	C3'-C2'-N1'	-3.15	99.29	104.65
2	E	301	IM5	C3'-C2'-N1'	-3.06	99.45	104.65
2	C	301	IM5	C3'-C2'-N1'	-3.01	99.54	104.65
2	D	301	IM5	C3'-C2'-N1'	-2.75	99.98	104.65
2	B	301	IM5	C3'-C2'-N1'	-2.74	99.99	104.65
2	C	301	IM5	C5-C6-N1	-2.46	120.31	123.52
2	F	302	IM5	C3'-C2'-N1'	-2.31	100.72	104.65
2	F	302	IM5	O5'-C5'-C4'	-2.05	106.76	111.38
2	F	302	IM5	C6'-N1'-C2'	2.10	106.27	103.90
2	A	301	IM5	N2-C2-N1	2.41	121.17	117.20
2	E	301	IM5	N2-C2-N1	2.42	121.19	117.20
2	A	301	IM5	C6'-N1'-C2'	2.86	107.12	103.90
2	C	301	IM5	N2-C2-N1	2.86	121.92	117.20
2	C	301	IM5	C6'-N1'-C2'	2.95	107.22	103.90
2	E	301	IM5	C6'-N1'-C2'	2.96	107.23	103.90
2	D	301	IM5	C6'-N1'-C2'	3.57	107.91	103.90
2	C	301	IM5	C6-N1-C2	4.20	120.80	115.88
2	B	301	IM5	C6'-N1'-C2'	4.29	108.73	103.90
2	F	302	IM5	C6-N1-C2	5.90	122.80	115.88
2	A	301	IM5	C6-N1-C2	6.10	123.03	115.88
2	E	301	IM5	C6-N1-C2	6.17	123.11	115.88
2	B	301	IM5	C6-N1-C2	6.31	123.27	115.88
2	D	301	IM5	C6-N1-C2	6.52	123.52	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	288/324 (88%)	-0.18	8 (2%)	56	66	25, 39, 71, 97	0
1	B	287/324 (88%)	0.03	14 (4%)	33	42	26, 43, 75, 101	0
1	C	288/324 (88%)	-0.33	4 (1%)	78	83	23, 35, 59, 84	0
1	D	288/324 (88%)	-0.22	5 (1%)	73	79	25, 37, 65, 98	0
1	E	288/324 (88%)	-0.22	6 (2%)	67	74	27, 45, 69, 105	0
1	F	288/324 (88%)	0.14	19 (6%)	22	29	27, 42, 77, 97	0
All	All	1727/1944 (88%)	-0.13	56 (3%)	51	60	23, 40, 72, 105	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	ASP	6.5
1	E	286	ASP	5.8
1	F	63	GLY	5.7
1	A	286	ASP	5.3
1	D	-1	THR	5.2
1	A	184	GLN	4.8
1	B	182	GLY	4.8
1	F	286	ASP	4.6
1	B	284	LEU	4.2
1	A	-1	THR	4.0
1	C	-1	THR	3.9
1	B	0	LEU	3.9
1	F	-1	THR	3.8
1	C	286	ASP	3.7
1	F	62	PRO	3.7
1	F	182	GLY	3.7
1	A	182	GLY	3.5
1	E	0	LEU	3.2
1	F	99	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	184	GLN	3.0
1	D	286	ASP	3.0
1	B	30	ILE	3.0
1	B	1	MET	2.9
1	F	30	ILE	2.8
1	F	269	GLN	2.8
1	A	285	PRO	2.8
1	B	168	ARG	2.7
1	D	182	GLY	2.7
1	F	40	ASP	2.7
1	F	60	THR	2.6
1	B	252	LEU	2.6
1	C	265	LYS	2.6
1	F	238	PHE	2.6
1	E	100	VAL	2.5
1	E	8	GLU	2.5
1	F	252	LEU	2.5
1	B	113	VAL	2.4
1	F	1	MET	2.4
1	B	250	GLU	2.4
1	E	2	GLU	2.4
1	E	185	ARG	2.3
1	F	65	ALA	2.3
1	B	65	ALA	2.3
1	F	28	ALA	2.3
1	A	0	LEU	2.3
1	D	1	MET	2.3
1	A	1	MET	2.3
1	F	29	ILE	2.3
1	D	250	GLU	2.2
1	A	30	ILE	2.2
1	B	285	PRO	2.2
1	F	114	THR	2.2
1	B	186	GLU	2.2
1	B	112	VAL	2.1
1	F	284	LEU	2.1
1	C	184	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	F	301	5/5	0.96	0.29	2.56	65,68,74,79	0
3	PO4	F	304	5/5	0.97	0.21	1.18	77,81,90,91	0
3	PO4	C	303	5/5	0.96	0.27	1.09	74,81,85,85	0
3	PO4	D	303	5/5	0.96	0.23	0.78	65,70,76,77	0
3	PO4	A	303	5/5	0.95	0.17	0.75	77,79,85,94	0
3	PO4	B	303	5/5	0.96	0.16	0.58	58,59,64,69	0
2	IM5	D	301	20/20	0.97	0.14	0.55	24,27,31,32	0
3	PO4	C	302	5/5	0.99	0.10	-0.21	26,28,31,31	0
2	IM5	F	302	20/20	0.95	0.11	-0.34	35,38,42,45	0
2	IM5	C	301	20/20	0.98	0.09	-0.39	23,25,27,28	0
2	IM5	B	301	20/20	0.97	0.09	-0.54	31,34,36,37	0
3	PO4	D	302	5/5	1.00	0.10	-0.58	31,32,33,34	0
3	PO4	A	302	5/5	0.99	0.10	-0.59	33,34,36,37	0
2	IM5	E	301	20/20	0.98	0.09	-0.62	27,30,34,36	0
3	PO4	E	302	5/5	1.00	0.09	-0.66	31,34,36,38	0
2	IM5	A	301	20/20	0.98	0.08	-0.88	24,28,28,30	0
3	PO4	F	303	5/5	0.99	0.10	-1.13	36,41,42,43	0
3	PO4	B	302	5/5	0.99	0.07	-1.82	38,40,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.