Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 11:53 AM EDT

PDB ID	:	4M1E
Title	:	Crystal structure of purine nucleoside phosphorylase I from Planctomyces limnophilus DSM 3776, NYSGRC Target 029364.
Authors	:	Malashkevich, V.N.; Bonanno, J.B.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-08-02
Resolution	:	1.90 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 (i) 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 (1)) were used in the production of this report:

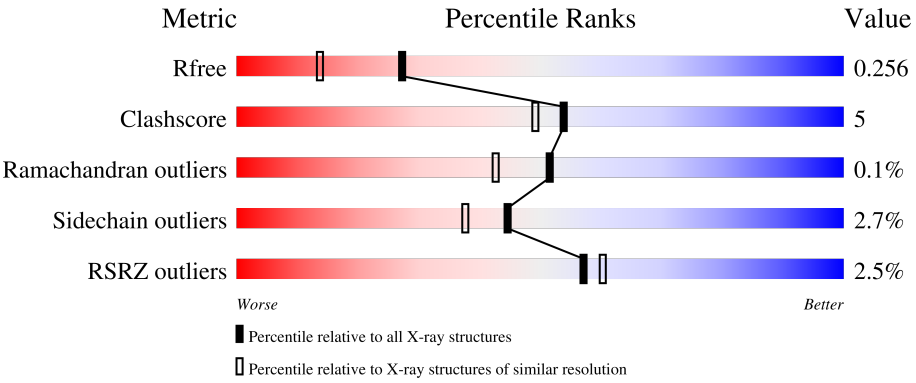
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	297	4% 82% 9% 8%
1	B	297	% 83% 8% 8%
1	C	297	% 81% 10% 8%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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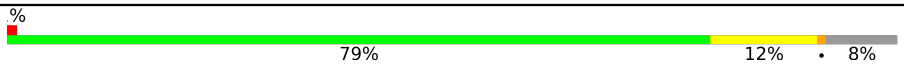
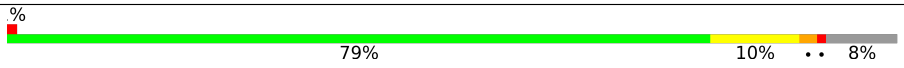
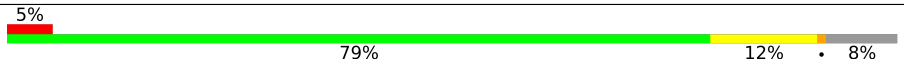
Mol	Chain	Length	Quality of chain
1	D	297	
1	E	297	
1	F	297	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13263 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	272	Total	C	N	O	S	Se	0	0	0
			2068	1316	359	379	4	10			
1	B	273	Total	C	N	O	S	Se	0	1	0
			2082	1324	363	381	4	10			
1	C	273	Total	C	N	O	S	Se	0	0	0
			2074	1319	360	381	4	10			
1	E	273	Total	C	N	O	S	Se	0	2	0
			2091	1330	364	382	4	11			
1	D	273	Total	C	N	O	S	Se	0	0	0
			2074	1319	360	381	4	10			
1	F	272	Total	C	N	O	S	Se	0	0	0
			2068	1316	359	379	4	10			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP D5SMY7
A	-20	HIS	-	expression tag	UNP D5SMY7
A	-19	HIS	-	expression tag	UNP D5SMY7
A	-18	HIS	-	expression tag	UNP D5SMY7
A	-17	HIS	-	expression tag	UNP D5SMY7
A	-16	HIS	-	expression tag	UNP D5SMY7
A	-15	HIS	-	expression tag	UNP D5SMY7
A	-14	SER	-	expression tag	UNP D5SMY7
A	-13	SER	-	expression tag	UNP D5SMY7
A	-12	GLY	-	expression tag	UNP D5SMY7
A	-11	VAL	-	expression tag	UNP D5SMY7
A	-10	ASP	-	expression tag	UNP D5SMY7
A	-9	LEU	-	expression tag	UNP D5SMY7
A	-8	GLY	-	expression tag	UNP D5SMY7
A	-7	THR	-	expression tag	UNP D5SMY7
A	-6	GLU	-	expression tag	UNP D5SMY7
A	-5	ASN	-	expression tag	UNP D5SMY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP D5SMY7
A	-3	TYR	-	expression tag	UNP D5SMY7
A	-2	PHE	-	expression tag	UNP D5SMY7
A	-1	GLN	-	expression tag	UNP D5SMY7
A	0	SER	-	expression tag	UNP D5SMY7
B	-21	MSE	-	expression tag	UNP D5SMY7
B	-20	HIS	-	expression tag	UNP D5SMY7
B	-19	HIS	-	expression tag	UNP D5SMY7
B	-18	HIS	-	expression tag	UNP D5SMY7
B	-17	HIS	-	expression tag	UNP D5SMY7
B	-16	HIS	-	expression tag	UNP D5SMY7
B	-15	HIS	-	expression tag	UNP D5SMY7
B	-14	SER	-	expression tag	UNP D5SMY7
B	-13	SER	-	expression tag	UNP D5SMY7
B	-12	GLY	-	expression tag	UNP D5SMY7
B	-11	VAL	-	expression tag	UNP D5SMY7
B	-10	ASP	-	expression tag	UNP D5SMY7
B	-9	LEU	-	expression tag	UNP D5SMY7
B	-8	GLY	-	expression tag	UNP D5SMY7
B	-7	THR	-	expression tag	UNP D5SMY7
B	-6	GLU	-	expression tag	UNP D5SMY7
B	-5	ASN	-	expression tag	UNP D5SMY7
B	-4	LEU	-	expression tag	UNP D5SMY7
B	-3	TYR	-	expression tag	UNP D5SMY7
B	-2	PHE	-	expression tag	UNP D5SMY7
B	-1	GLN	-	expression tag	UNP D5SMY7
B	0	SER	-	expression tag	UNP D5SMY7
C	-21	MSE	-	expression tag	UNP D5SMY7
C	-20	HIS	-	expression tag	UNP D5SMY7
C	-19	HIS	-	expression tag	UNP D5SMY7
C	-18	HIS	-	expression tag	UNP D5SMY7
C	-17	HIS	-	expression tag	UNP D5SMY7
C	-16	HIS	-	expression tag	UNP D5SMY7
C	-15	HIS	-	expression tag	UNP D5SMY7
C	-14	SER	-	expression tag	UNP D5SMY7
C	-13	SER	-	expression tag	UNP D5SMY7
C	-12	GLY	-	expression tag	UNP D5SMY7
C	-11	VAL	-	expression tag	UNP D5SMY7
C	-10	ASP	-	expression tag	UNP D5SMY7
C	-9	LEU	-	expression tag	UNP D5SMY7
C	-8	GLY	-	expression tag	UNP D5SMY7
C	-7	THR	-	expression tag	UNP D5SMY7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLU	-	expression tag	UNP D5SMY7
C	-5	ASN	-	expression tag	UNP D5SMY7
C	-4	LEU	-	expression tag	UNP D5SMY7
C	-3	TYR	-	expression tag	UNP D5SMY7
C	-2	PHE	-	expression tag	UNP D5SMY7
C	-1	GLN	-	expression tag	UNP D5SMY7
C	0	SER	-	expression tag	UNP D5SMY7
E	-21	MSE	-	expression tag	UNP D5SMY7
E	-20	HIS	-	expression tag	UNP D5SMY7
E	-19	HIS	-	expression tag	UNP D5SMY7
E	-18	HIS	-	expression tag	UNP D5SMY7
E	-17	HIS	-	expression tag	UNP D5SMY7
E	-16	HIS	-	expression tag	UNP D5SMY7
E	-15	HIS	-	expression tag	UNP D5SMY7
E	-14	SER	-	expression tag	UNP D5SMY7
E	-13	SER	-	expression tag	UNP D5SMY7
E	-12	GLY	-	expression tag	UNP D5SMY7
E	-11	VAL	-	expression tag	UNP D5SMY7
E	-10	ASP	-	expression tag	UNP D5SMY7
E	-9	LEU	-	expression tag	UNP D5SMY7
E	-8	GLY	-	expression tag	UNP D5SMY7
E	-7	THR	-	expression tag	UNP D5SMY7
E	-6	GLU	-	expression tag	UNP D5SMY7
E	-5	ASN	-	expression tag	UNP D5SMY7
E	-4	LEU	-	expression tag	UNP D5SMY7
E	-3	TYR	-	expression tag	UNP D5SMY7
E	-2	PHE	-	expression tag	UNP D5SMY7
E	-1	GLN	-	expression tag	UNP D5SMY7
E	0	SER	-	expression tag	UNP D5SMY7
D	-21	MSE	-	expression tag	UNP D5SMY7
D	-20	HIS	-	expression tag	UNP D5SMY7
D	-19	HIS	-	expression tag	UNP D5SMY7
D	-18	HIS	-	expression tag	UNP D5SMY7
D	-17	HIS	-	expression tag	UNP D5SMY7
D	-16	HIS	-	expression tag	UNP D5SMY7
D	-15	HIS	-	expression tag	UNP D5SMY7
D	-14	SER	-	expression tag	UNP D5SMY7
D	-13	SER	-	expression tag	UNP D5SMY7
D	-12	GLY	-	expression tag	UNP D5SMY7
D	-11	VAL	-	expression tag	UNP D5SMY7
D	-10	ASP	-	expression tag	UNP D5SMY7
D	-9	LEU	-	expression tag	UNP D5SMY7

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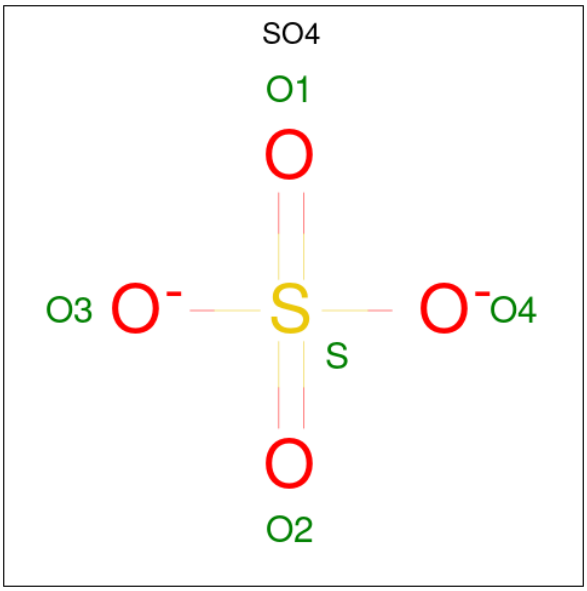
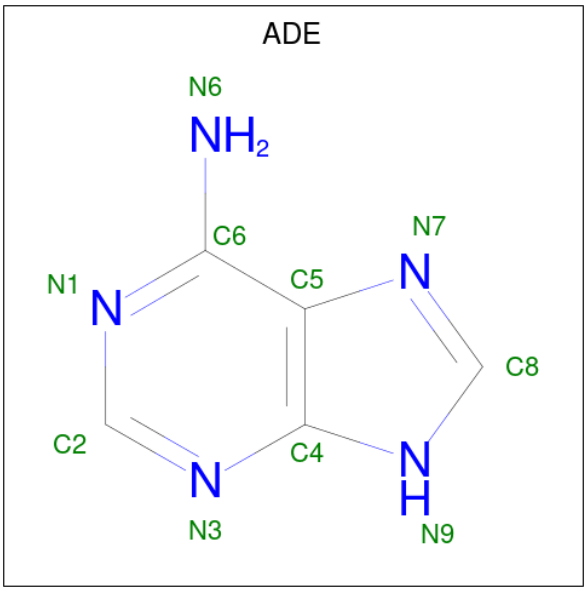
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP D5SMY7
D	-7	THR	-	expression tag	UNP D5SMY7
D	-6	GLU	-	expression tag	UNP D5SMY7
D	-5	ASN	-	expression tag	UNP D5SMY7
D	-4	LEU	-	expression tag	UNP D5SMY7
D	-3	TYR	-	expression tag	UNP D5SMY7
D	-2	PHE	-	expression tag	UNP D5SMY7
D	-1	GLN	-	expression tag	UNP D5SMY7
D	0	SER	-	expression tag	UNP D5SMY7
F	-21	MSE	-	expression tag	UNP D5SMY7
F	-20	HIS	-	expression tag	UNP D5SMY7
F	-19	HIS	-	expression tag	UNP D5SMY7
F	-18	HIS	-	expression tag	UNP D5SMY7
F	-17	HIS	-	expression tag	UNP D5SMY7
F	-16	HIS	-	expression tag	UNP D5SMY7
F	-15	HIS	-	expression tag	UNP D5SMY7
F	-14	SER	-	expression tag	UNP D5SMY7
F	-13	SER	-	expression tag	UNP D5SMY7
F	-12	GLY	-	expression tag	UNP D5SMY7
F	-11	VAL	-	expression tag	UNP D5SMY7
F	-10	ASP	-	expression tag	UNP D5SMY7
F	-9	LEU	-	expression tag	UNP D5SMY7
F	-8	GLY	-	expression tag	UNP D5SMY7
F	-7	THR	-	expression tag	UNP D5SMY7
F	-6	GLU	-	expression tag	UNP D5SMY7
F	-5	ASN	-	expression tag	UNP D5SMY7
F	-4	LEU	-	expression tag	UNP D5SMY7
F	-3	TYR	-	expression tag	UNP D5SMY7
F	-2	PHE	-	expression tag	UNP D5SMY7
F	-1	GLN	-	expression tag	UNP D5SMY7
F	0	SER	-	expression tag	UNP D5SMY7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



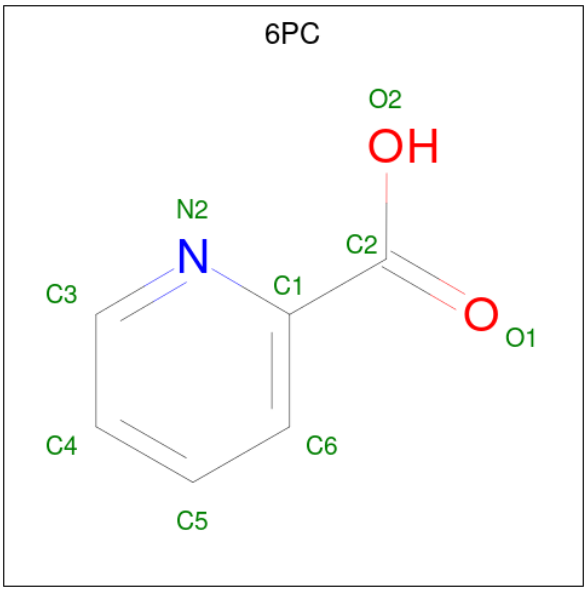
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 5 5	0	0
3	B	1	Total C N 10 5 5	0	0
3	C	1	Total C N 10 5 5	0	0
3	E	1	Total C N 10 5 5	0	0
3	D	1	Total C N 10 5 5	0	0
3	F	1	Total C N 10 5 5	0	0

- Molecule 4 is PYRIDINE-2-CARBOXYLIC ACID (three-letter code: 6PC) (formula: $C_6H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 6 1 2	0	0
4	B	1	Total C N O 9 6 1 2	0	0
4	C	1	Total C N O 9 6 1 2	0	0
4	E	1	Total C N O 9 6 1 2	0	0
4	D	1	Total C N O 9 6 1 2	0	0
4	F	1	Total C N O 9 6 1 2	0	0

- Molecule 5 is water.

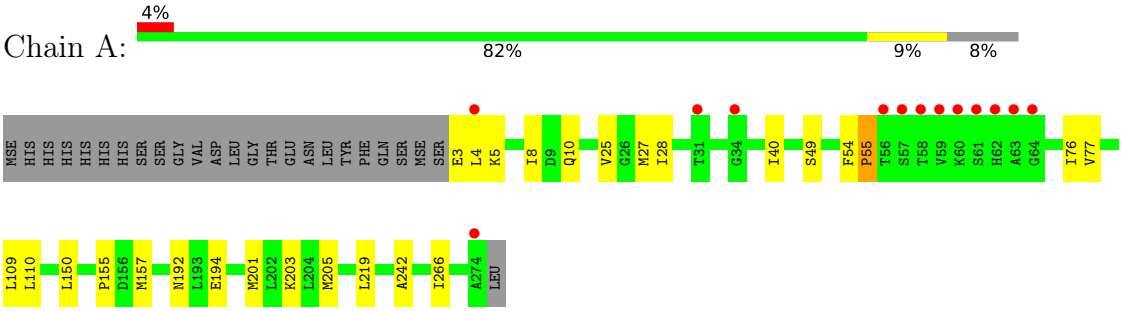
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0
5	B	113	Total O 113 113	0	0
5	C	119	Total O 119 119	0	0
5	E	104	Total O 104 104	0	0
5	D	120	Total O 120 120	0	0
5	F	104	Total O 104 104	0	0

3 Residue-property plots

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.

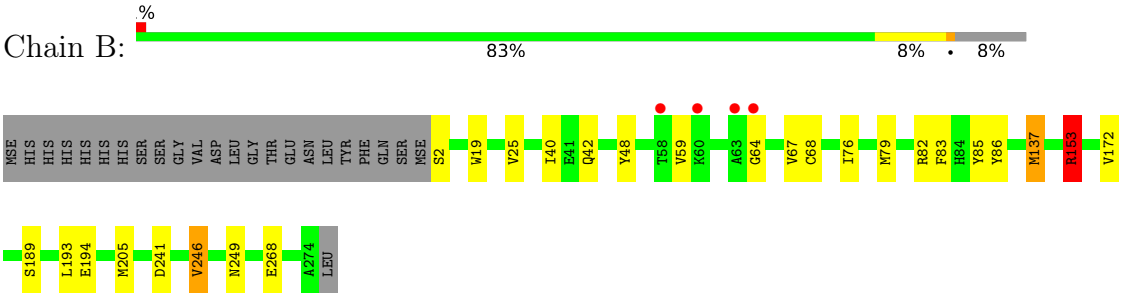
• Molecule 1: Purine nucleoside phosphorylase

Chain A:



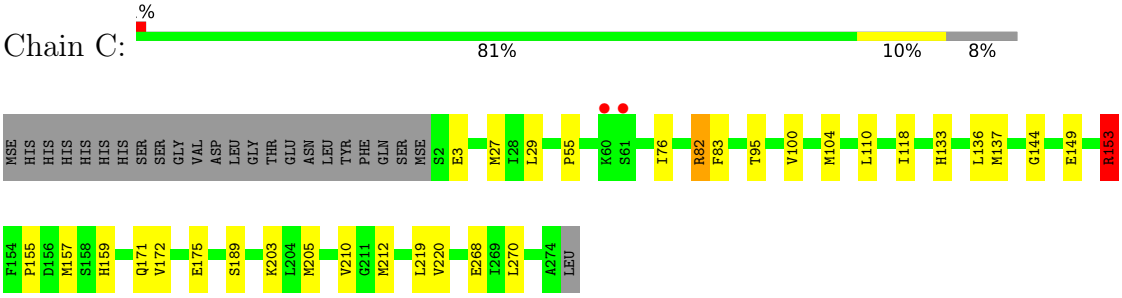
• Molecule 1: Purine nucleoside phosphorylase

Chain B:



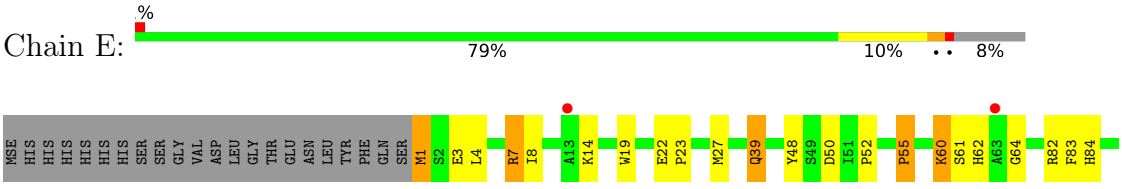
• Molecule 1: Purine nucleoside phosphorylase

Chain C:

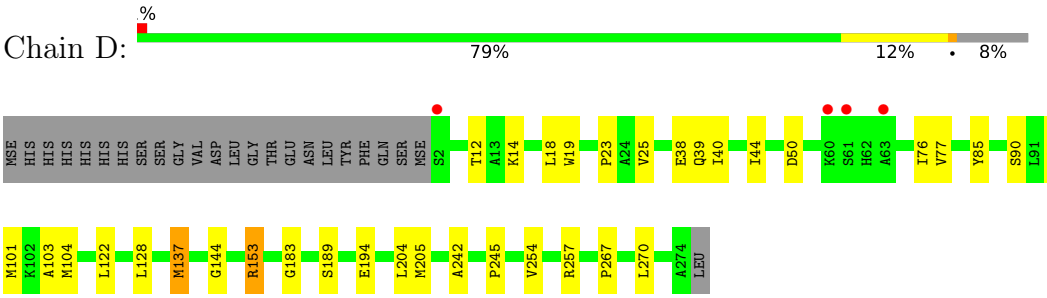


• Molecule 1: Purine nucleoside phosphorylase

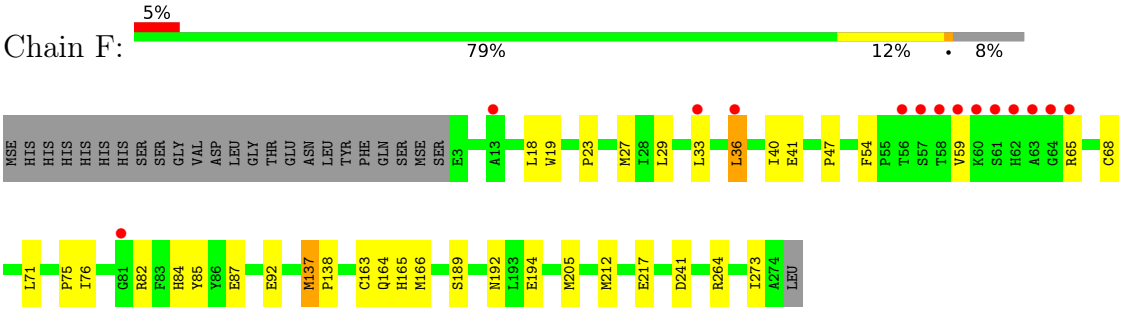
Chain E:



• Molecule 1: Purine nucleoside phosphorylase



• Molecule 1: Purine nucleoside phosphorylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.95Å 81.06Å 91.62Å 103.42° 105.36° 112.73°	Depositor
Resolution (Å)	20.00 – 1.90 31.42 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-1.90) 96.4 (31.42-1.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.258 0.213 , 0.256	Depositor DCC
R_{free} test set	7463 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-h-k-l 0.146 for -k,-h,-l 0.018 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13263	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, 6PC, SO4

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	0.50	0/2099	0.67	0/2836
1	B	0.50	0/2116	0.70	1/2858 (0.0%)
1	C	0.52	0/2105	0.70	1/2844 (0.0%)
1	D	0.51	0/2105	0.68	1/2844 (0.0%)
1	E	0.52	1/2128 (0.0%)	0.70	2/2873 (0.1%)
1	F	0.51	0/2099	0.69	0/2836
All	All	0.51	1/12652 (0.0%)	0.69	5/17091 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	55	PRO	N-CD	5.53	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	153	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	E	153	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	153	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	E	166	MSE	CB-CA-C	5.45	121.31	110.40
1	D	137	MSE	CA-CB-CG	-5.03	104.75	113.30

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	2068	0	2116	16	0
1	B	2082	0	2134	22	0
1	C	2074	0	2121	29	0
1	D	2074	0	2121	26	0
1	E	2091	0	2149	25	0
1	F	2068	0	2116	25	0
2	A	5	0	0	0	0
2	B	5	0	0	0	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	A	10	0	4	1	0
3	B	10	0	4	1	0
3	C	10	0	4	1	0
3	D	10	0	4	1	0
3	E	10	0	4	1	0
3	F	10	0	4	2	0
4	A	9	0	4	0	0
4	B	9	0	4	0	0
4	C	9	0	4	0	0
4	D	9	0	4	1	0
4	E	9	0	4	0	0
4	F	9	0	4	0	0
5	A	102	0	0	1	0
5	B	113	0	0	1	0
5	C	119	0	0	3	0
5	D	120	0	0	0	0
5	E	104	0	0	1	0
5	F	104	0	0	6	0
All	All	13263	0	12805	135	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 5.

All (135) 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:136:LEU:HD11	1:C:205:MSE:HE1	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:MSE:HE2	1:F:29:LEU:HD21	1.50	0.93
1:D:137:MSE:HE3	1:D:189:SER:HA	1.50	0.91
1:B:137:MSE:HE3	1:B:189:SER:HA	1.69	0.73
1:E:55:PRO:HD2	1:E:83:PHE:CE2	2.22	0.73
1:E:3:GLU:O	1:E:7:ARG:HG3	1.91	0.70
1:B:40:ILE:HG12	1:B:76:ILE:HD11	1.73	0.69
1:D:40:ILE:HG12	1:D:76:ILE:HD11	1.74	0.67
1:B:25:VAL:HB	1:B:76:ILE:HG22	1.77	0.67
1:F:27:MSE:CE	1:F:29:LEU:HD21	2.25	0.64
1:B:153:ARG:O	1:B:153:ARG:HD3	1.98	0.63
1:E:60:LYS:O	1:E:61:SER:HB3	1.95	0.63
1:D:18:LEU:HB3	1:D:44:ILE:HD13	1.82	0.62
1:C:136:LEU:HD11	1:C:205:MSE:CE	2.21	0.62
1:E:166:MSE:HG3	1:E:182:LYS:HE2	1.82	0.62
1:A:5:LYS:HG3	1:A:150:LEU:HD21	1.82	0.61
1:C:27:MSE:HE2	1:C:29:LEU:HD21	1.82	0.60
1:D:85:TYR:HB3	1:D:137:MSE:HE1	1.82	0.59
1:C:157:MSE:HE2	1:C:219:LEU:HD23	1.84	0.58
1:A:27:MSE:HE3	1:A:110:LEU:HD22	1.86	0.57
1:F:40:ILE:HG12	1:F:76:ILE:HD11	1.87	0.57
1:F:33:LEU:HA	5:F:578:HOH:O	2.05	0.56
1:F:137:MSE:HG3	1:F:138:PRO:HD2	1.88	0.56
1:F:264:ARG:NH2	5:F:565:HOH:O	2.38	0.56
1:D:25:VAL:HB	1:D:76:ILE:HG22	1.87	0.55
1:A:201:MSE:SE	1:C:205:MSE:HE3	2.58	0.54
1:F:137:MSE:HE3	1:F:189:SER:HA	1.89	0.54
1:A:5:LYS:HA	1:A:8:ILE:HD12	1.90	0.53
1:A:25:VAL:HB	1:A:76:ILE:HG22	1.91	0.53
1:D:254:VAL:HA	1:D:257:ARG:HD3	1.91	0.52
1:A:192:ASN:HA	1:C:155:PRO:HD2	1.92	0.52
1:C:157:MSE:HE2	1:C:219:LEU:CD2	2.39	0.52
1:D:90:SER:OG	1:D:92:GLU:HG2	2.09	0.52
1:B:42:GLN:HG2	1:B:67:VAL:HG13	1.92	0.51
1:B:241:ASP:HB2	1:F:241:ASP:HB2	1.92	0.51
1:B:85:TYR:CB	1:B:137:MSE:HE2	2.40	0.51
1:A:205:MSE:HE2	1:B:205:MSE:HE3	1.93	0.51
1:E:163:CYS:HA	1:E:166:MSE:HE2	1.92	0.51
1:F:84:HIS:HB2	1:F:87:GLU:HG3	1.92	0.51
1:A:157:MSE:HE2	1:A:219:LEU:HD23	1.92	0.51
1:B:153:ARG:O	1:B:153:ARG:CD	2.59	0.50
1:D:92:GLU:HG2	1:D:93:GLN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLY:O	1:D:153:ARG:NH2	2.32	0.50
1:A:27:MSE:HE1	1:A:266:ILE:HD13	1.93	0.50
1:E:27:MSE:HE3	1:E:110:LEU:HD22	1.93	0.50
1:E:1:MSE:HG3	1:E:4:LEU:HD12	1.94	0.50
1:D:128:LEU:HD11	1:D:183:GLY:HA3	1.93	0.50
1:E:14:LYS:HD3	1:E:52:PRO:HD3	1.93	0.49
1:B:85:TYR:HB3	1:B:137:MSE:HE2	1.95	0.49
1:C:27:MSE:HE3	1:C:110:LEU:HD22	1.95	0.49
1:A:242:ALA:HB2	1:D:242:ALA:HB2	1.95	0.49
1:E:84:HIS:HB2	1:E:87:GLU:HG3	1.95	0.49
1:C:157:MSE:CE	1:C:219:LEU:HD23	2.43	0.48
1:D:245:PRO:HD3	5:F:597:HOH:O	2.12	0.48
1:C:27:MSE:HE2	1:C:29:LEU:CD2	2.43	0.48
1:D:19:TRP:CZ3	1:D:23:PRO:HD3	2.49	0.48
1:E:153:ARG:O	1:E:153:ARG:HD3	2.14	0.48
1:A:194:GLU:OE1	3:A:401:ADE:N1	2.46	0.48
1:F:33:LEU:HB3	1:F:36:LEU:HD11	1.95	0.48
1:F:217:GLU:CD	5:F:509:HOH:O	2.52	0.48
1:C:171:GLN:O	1:C:175:GLU:HG2	2.14	0.47
1:B:40:ILE:HG12	1:B:76:ILE:CD1	2.42	0.47
1:C:27:MSE:HG3	1:C:76:ILE:HD11	1.97	0.47
1:E:212:MSE:HE3	3:E:401:ADE:C2	2.50	0.47
1:C:55:PRO:HD2	1:C:83:PHE:CE2	2.50	0.46
1:B:48:TYR:CE2	1:B:64:GLY:HA2	2.50	0.46
1:C:95:THR:CB	1:C:220:VAL:HG21	2.45	0.46
1:E:48:TYR:CE2	1:E:64:GLY:HA2	2.51	0.46
1:C:144:GLY:O	1:C:153:ARG:NH2	2.42	0.46
1:B:246:VAL:HG23	5:B:523:HOH:O	2.15	0.45
1:F:164:GLN:HG2	5:F:526:HOH:O	2.15	0.45
1:D:153:ARG:HD3	1:D:153:ARG:HA	1.69	0.45
1:E:19:TRP:CZ3	1:E:23:PRO:HD3	2.52	0.45
1:B:194:GLU:OE1	3:B:401:ADE:N1	2.49	0.45
1:C:203:LYS:NZ	5:C:588:HOH:O	2.21	0.45
1:E:153:ARG:O	1:E:153:ARG:CD	2.65	0.45
1:D:77:VAL:HG13	1:D:101:MSE:HE2	1.99	0.45
1:C:82:ARG:CG	1:C:83:PHE:N	2.79	0.45
1:E:144:GLY:O	1:E:153:ARG:NH2	2.40	0.45
1:E:4:LEU:HD23	1:E:8:ILE:HD11	1.98	0.45
1:C:203:LYS:CE	5:C:588:HOH:O	2.63	0.45
1:B:40:ILE:CG1	1:B:76:ILE:HD11	2.47	0.44
1:E:155:PRO:HD2	1:F:192:ASN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:MSE:HE2	1:C:189:SER:HA	1.98	0.44
1:E:22:GLU:HG2	5:E:544:HOH:O	2.17	0.44
1:C:95:THR:HB	1:C:220:VAL:HG21	2.00	0.44
1:D:153:ARG:O	1:D:153:ARG:CD	2.65	0.44
1:E:39:GLN:HE21	1:E:39:GLN:HB2	1.57	0.44
1:D:85:TYR:CB	1:D:137:MSE:HE1	2.48	0.44
1:D:122:LEU:CD2	4:D:301:6PC:H5	2.47	0.44
1:A:28:ILE:HG13	1:A:109:LEU:HD11	1.99	0.44
1:C:27:MSE:CE	1:C:29:LEU:HD21	2.47	0.44
1:B:19:TRP:CD2	1:B:68:CYS:HB3	2.53	0.43
1:D:39:GLN:HG2	1:D:267:PRO:HG3	2.00	0.43
1:D:194:GLU:OE1	3:D:303:ADE:N1	2.52	0.43
1:F:92:GLU:HB3	5:F:567:HOH:O	2.16	0.43
1:D:18:LEU:HD23	1:D:44:ILE:HD11	2.00	0.43
1:F:163:CYS:HA	1:F:166:MSE:HE3	2.00	0.43
1:E:1:MSE:O	1:E:4:LEU:HB2	2.19	0.43
1:D:100:VAL:O	1:D:104:MSE:HG3	2.19	0.43
1:F:23:PRO:HA	1:F:75:PRO:HB2	2.01	0.43
1:B:79:MSE:HE2	1:B:82:ARG:HA	2.00	0.42
1:C:212:MSE:HE3	3:C:401:ADE:C2	2.54	0.42
1:A:3:GLU:HG3	1:A:4:LEU:H	1.84	0.42
1:F:85:TYR:CB	1:F:137:MSE:HE2	2.49	0.42
1:E:62:HIS:CE1	1:E:84:HIS:HE1	2.38	0.42
1:C:100:VAL:O	1:C:104:MSE:HG3	2.20	0.42
1:C:172:VAL:HG11	1:C:268:GLU:HB3	2.02	0.42
1:C:159:HIS:CD2	5:C:587:HOH:O	2.73	0.41
1:F:165:HIS:CE1	1:F:273:ILE:HB	2.55	0.41
1:F:212:MSE:HE3	3:F:401:ADE:C2	2.56	0.41
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.87	0.41
1:F:47:PRO:HA	1:F:65:ARG:HA	2.02	0.41
1:A:203:LYS:NZ	5:A:558:HOH:O	2.38	0.41
1:F:71:LEU:HB2	1:F:76:ILE:HD13	2.02	0.41
1:B:153:ARG:HD3	1:B:153:ARG:C	2.32	0.41
1:A:40:ILE:HG12	1:A:76:ILE:HD11	2.02	0.41
1:B:59:VAL:HG21	1:B:86:TYR:OH	2.21	0.41
1:B:153:ARG:HD3	1:B:153:ARG:HA	1.82	0.41
1:B:172:VAL:HG11	1:B:268:GLU:HB3	2.03	0.41
1:E:153:ARG:HD3	1:E:153:ARG:HA	1.72	0.41
1:E:157:MSE:HE2	1:E:219:LEU:CD2	2.51	0.41
1:D:205:MSE:HE3	1:F:205:MSE:HE2	2.03	0.41
1:B:82:ARG:HG3	1:B:83:PHE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:MSE:CE	1:D:205:MSE:HE2	2.51	0.40
1:F:29:LEU:HD22	1:F:36:LEU:HD12	2.03	0.40
1:F:194:GLU:OE1	3:F:401:ADE:N1	2.54	0.40
1:D:14:LYS:O	1:D:18:LEU:HD12	2.22	0.40
1:C:118:ILE:HD11	1:C:210:VAL:HB	2.03	0.40
1:E:194:GLU:HB2	1:E:199:TYR:CE1	2.56	0.40
1:F:19:TRP:CD2	1:F:68:CYS:HB3	2.56	0.40
1:A:54:PHE:HA	1:A:55:PRO:HD3	1.77	0.40
1:C:55:PRO:HB2	1:C:83:PHE:CD1	2.56	0.40
1:C:153:ARG:O	1:C:153:ARG:CD	2.69	0.40
1:D:12:THR:HG21	1:D:103:ALA:HB3	2.03	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	270/297 (91%)	260 (96%)	9 (3%)	1 (0%)	34 24
1	B	272/297 (92%)	262 (96%)	10 (4%)	0	100 100
1	C	271/297 (91%)	265 (98%)	6 (2%)	0	100 100
1	D	271/297 (91%)	266 (98%)	5 (2%)	0	100 100
1	E	273/297 (92%)	265 (97%)	8 (3%)	0	100 100
1	F	270/297 (91%)	259 (96%)	11 (4%)	0	100 100
All	All	1627/1782 (91%)	1577 (97%)	49 (3%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	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	224/235 (95%)	220 (98%)	4 (2%)	59	55
1	B	226/235 (96%)	220 (97%)	6 (3%)	44	38
1	C	225/235 (96%)	220 (98%)	5 (2%)	52	47
1	D	225/235 (96%)	220 (98%)	5 (2%)	52	47
1	E	228/235 (97%)	218 (96%)	10 (4%)	28	19
1	F	224/235 (95%)	217 (97%)	7 (3%)	40	32
All	All	1352/1410 (96%)	1315 (97%)	37 (3%)	44	38

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	49	SER
1	A	77	VAL
1	A	155	PRO
1	B	2	SER
1	B	137	MSE
1	B	153	ARG
1	B	193	LEU
1	B	246	VAL
1	B	249	ASN
1	C	3	GLU
1	C	82	ARG
1	C	133	HIS
1	C	149	GLU
1	C	153	ARG
1	E	1	MSE
1	E	7	ARG
1	E	39	GLN
1	E	50	ASP
1	E	60	LYS
1	E	82	ARG
1	E	153	ARG

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Mol	Chain	Res	Type
1	E	166	MSE
1	E	167	GLU
1	E	246	VAL
1	D	38	GLU
1	D	50	ASP
1	D	153	ARG
1	D	204	LEU
1	D	270	LEU
1	F	18	LEU
1	F	36	LEU
1	F	41	GLU
1	F	54	PHE
1	F	59	VAL
1	F	82	ARG
1	F	137	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	E	39	GLN
1	F	17	GLN
1	F	53	HIS
1	F	62	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides 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	SO4	C	400	-	4,4,4	0.25	0	6,6,6	0.38	0
4	6PC	F	402	-	9,9,9	0.83	1 (11%)	11,11,11	1.60	2 (18%)
3	ADE	F	401	-	9,11,11	1.23	1 (11%)	7,15,15	2.61	4 (57%)
2	SO4	A	400	-	4,4,4	0.15	0	6,6,6	0.32	0
3	ADE	A	401	-	9,11,11	1.52	2 (22%)	7,15,15	1.91	3 (42%)
2	SO4	D	302	-	4,4,4	0.41	0	6,6,6	0.44	0
2	SO4	E	400	-	4,4,4	0.27	0	6,6,6	0.28	0
4	6PC	B	402	-	9,9,9	0.92	1 (11%)	11,11,11	1.16	1 (9%)
2	SO4	B	400	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	F	400	-	4,4,4	0.22	0	6,6,6	0.24	0
3	ADE	B	401	-	9,11,11	1.28	2 (22%)	7,15,15	2.23	3 (42%)
4	6PC	E	402	-	9,9,9	0.99	0	11,11,11	1.25	2 (18%)
4	6PC	C	402	-	9,9,9	0.88	0	11,11,11	1.23	1 (9%)
4	6PC	A	402	-	9,9,9	0.93	0	11,11,11	1.39	2 (18%)
4	6PC	D	301	-	9,9,9	0.89	0	11,11,11	1.42	2 (18%)
3	ADE	E	401	-	9,11,11	1.18	1 (11%)	7,15,15	2.05	3 (42%)
3	ADE	C	401	-	9,11,11	1.30	2 (22%)	7,15,15	2.43	4 (57%)
3	ADE	D	303	-	9,11,11	1.44	1 (11%)	7,15,15	2.13	4 (57%)

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
4	6PC	F	402	-	-	0/4/4/4	0/1/1/1
3	ADE	F	401	-	-	-	0/2/2/2
3	ADE	A	401	-	-	-	0/2/2/2
4	6PC	B	402	-	-	4/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6PC	E	402	-	-	4/4/4/4	0/1/1/1
3	ADE	B	401	-	-	-	0/2/2/2
4	6PC	C	402	-	-	4/4/4/4	0/1/1/1
4	6PC	A	402	-	-	4/4/4/4	0/1/1/1
4	6PC	D	301	-	-	4/4/4/4	0/1/1/1
3	ADE	E	401	-	-	-	0/2/2/2
3	ADE	C	401	-	-	-	0/2/2/2
3	ADE	D	303	-	-	-	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	303	ADE	C5-C4	3.01	1.48	1.40
3	A	401	ADE	C5-C4	2.82	1.48	1.40
3	F	401	ADE	C5-C4	2.42	1.47	1.40
3	E	401	ADE	C5-C4	2.40	1.47	1.40
3	B	401	ADE	C5-C4	2.31	1.47	1.40
3	A	401	ADE	C2-N3	2.31	1.35	1.32
4	B	402	6PC	O2-C2	-2.27	1.23	1.30
3	B	401	ADE	C2-N3	2.22	1.35	1.32
3	C	401	ADE	C5-C4	2.06	1.46	1.40
4	F	402	6PC	O2-C2	-2.03	1.24	1.30
3	C	401	ADE	C2-N3	2.03	1.35	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	401	ADE	N3-C2-N1	-4.24	122.05	128.68
3	B	401	ADE	N3-C2-N1	-4.16	122.17	128.68
3	C	401	ADE	N3-C2-N1	-3.81	122.72	128.68
4	F	402	6PC	C3-N2-C1	3.78	121.84	116.93
3	E	401	ADE	N3-C2-N1	-3.42	123.34	128.68
4	A	402	6PC	C3-N2-C1	3.37	121.30	116.93
4	D	301	6PC	C3-N2-C1	3.26	121.16	116.93
3	F	401	ADE	C2-N3-C4	3.13	120.77	113.45
3	D	303	ADE	N3-C2-N1	-3.12	123.80	128.68
3	C	401	ADE	C2-N3-C4	3.04	120.57	113.45
4	C	402	6PC	C3-N2-C1	3.02	120.84	116.93
3	B	401	ADE	C2-N3-C4	2.98	120.43	113.45
3	F	401	ADE	C2-N1-C6	2.96	123.82	118.75
3	D	303	ADE	C2-N3-C4	2.81	120.02	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	6PC	C3-N2-C1	2.76	120.50	116.93
3	C	401	ADE	C4-C5-N7	-2.66	106.63	109.40
4	E	402	6PC	C3-N2-C1	2.62	120.33	116.93
4	D	301	6PC	C4-C3-N2	-2.50	119.34	123.43
3	E	401	ADE	C2-N3-C4	2.46	119.22	113.45
3	C	401	ADE	C2-N1-C6	2.43	122.91	118.75
3	D	303	ADE	C2-N1-C6	2.41	122.88	118.75
3	E	401	ADE	C2-N1-C6	2.38	122.83	118.75
4	E	402	6PC	C4-C3-N2	-2.37	119.56	123.43
3	F	401	ADE	C4-C5-N7	-2.35	106.95	109.40
3	B	401	ADE	C2-N1-C6	2.35	122.77	118.75
4	F	402	6PC	C4-C3-N2	-2.31	119.66	123.43
3	A	401	ADE	C4-C5-N7	-2.25	107.05	109.40
3	A	401	ADE	N3-C2-N1	-2.21	125.23	128.68
3	D	303	ADE	C4-C5-N7	-2.09	107.23	109.40
3	A	401	ADE	C2-N3-C4	2.07	118.29	113.45
4	A	402	6PC	C4-C3-N2	-2.01	120.14	123.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	6PC	C6-C1-C2-O1
4	A	402	6PC	C6-C1-C2-O2
4	A	402	6PC	N2-C1-C2-O1
4	A	402	6PC	N2-C1-C2-O2
4	D	301	6PC	C6-C1-C2-O1
4	D	301	6PC	C6-C1-C2-O2
4	D	301	6PC	N2-C1-C2-O1
4	D	301	6PC	N2-C1-C2-O2
4	C	402	6PC	N2-C1-C2-O2
4	E	402	6PC	N2-C1-C2-O2
4	E	402	6PC	N2-C1-C2-O1
4	C	402	6PC	C6-C1-C2-O2
4	C	402	6PC	N2-C1-C2-O1
4	E	402	6PC	C6-C1-C2-O2
4	C	402	6PC	C6-C1-C2-O1
4	E	402	6PC	C6-C1-C2-O1
4	B	402	6PC	N2-C1-C2-O2
4	B	402	6PC	C6-C1-C2-O2
4	B	402	6PC	N2-C1-C2-O1
4	B	402	6PC	C6-C1-C2-O1

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	ADE	2	0
3	A	401	ADE	1	0
3	B	401	ADE	1	0
4	D	301	6PC	1	0
3	E	401	ADE	1	0
3	C	401	ADE	1	0
3	D	303	ADE	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, 95^{th} 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	262/297 (88%)	0.04	13 (4%)	28	32	16, 32, 64, 88	0
1	B	263/297 (88%)	-0.15	4 (1%)	73	76	15, 30, 55, 66	0
1	C	263/297 (88%)	-0.08	2 (0%)	86	87	15, 29, 57, 67	0
1	D	263/297 (88%)	-0.17	4 (1%)	73	76	15, 29, 51, 71	0
1	E	262/297 (88%)	-0.10	2 (0%)	86	87	16, 30, 56, 76	0
1	F	262/297 (88%)	0.11	14 (5%)	26	29	15, 30, 64, 128	0
All	All	1575/1782 (88%)	-0.06	39 (2%)	57	60	15, 30, 58, 128	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	60	LYS	10.3
1	F	63	ALA	9.1
1	F	58	THR	8.3
1	F	62	HIS	8.0
1	F	59	VAL	7.6
1	F	57	SER	6.9
1	A	58	THR	5.4
1	A	57	SER	5.1
1	D	2	SER	5.0
1	F	61	SER	4.9
1	A	59	VAL	4.5
1	A	34	GLY	3.9
1	A	61	SER	3.5
1	A	63	ALA	3.3
1	F	56	THR	3.3
1	A	56	THR	3.2
1	D	61	SER	3.1
1	B	58	THR	2.9
1	A	60	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	13	ALA	2.9
1	A	64	GLY	2.7
1	F	13	ALA	2.7
1	F	65	ARG	2.7
1	B	63	ALA	2.7
1	A	62	HIS	2.6
1	B	60	LYS	2.5
1	F	36	LEU	2.5
1	D	63	ALA	2.5
1	F	64	GLY	2.4
1	C	61	SER	2.3
1	A	274	ALA	2.2
1	A	31	THR	2.2
1	B	64	GLY	2.2
1	A	4	LEU	2.1
1	C	60	LYS	2.1
1	F	81	GLY	2.1
1	E	63	ALA	2.1
1	D	60	LYS	2.0
1	F	33	LEU	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 monosaccharides 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, 95^{th} 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
4	6PC	A	402	9/9	0.91	0.10	34,38,39,41	0
3	ADE	E	401	10/10	0.94	0.12	24,24,25,26	0
4	6PC	E	402	9/9	0.94	0.13	31,34,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	6PC	D	301	9/9	0.95	0.10	28,29,32,33	0
4	6PC	F	402	9/9	0.95	0.10	30,35,37,39	0
4	6PC	C	402	9/9	0.96	0.10	27,32,39,39	0
3	ADE	B	401	10/10	0.96	0.09	25,27,29,29	0
3	ADE	A	401	10/10	0.97	0.08	22,25,25,25	0
4	6PC	B	402	9/9	0.97	0.12	30,33,37,38	0
3	ADE	D	303	10/10	0.97	0.09	23,24,25,25	0
3	ADE	C	401	10/10	0.98	0.07	23,23,25,25	0
2	SO4	F	400	5/5	0.98	0.10	40,42,45,49	0
2	SO4	A	400	5/5	0.98	0.10	35,37,41,42	0
3	ADE	F	401	10/10	0.98	0.07	22,23,25,26	0
2	SO4	C	400	5/5	0.98	0.11	33,34,39,41	0
2	SO4	E	400	5/5	0.99	0.09	34,34,37,37	0
2	SO4	D	302	5/5	0.99	0.10	29,30,33,34	0
2	SO4	B	400	5/5	0.99	0.08	33,33,36,38	0

6.5 Other polymers (i)

There are no such residues in this entry.