



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:02 pm GMT

PDB ID : 4PFQ
Title : Crystal structure of hypoxanthine phosphoribosyltransferase from *Brachybac-*
terium faecium DSM 4810, NYSGRC Target 029763.
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth,
S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.;
Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Seidel, R.; Bo-
nanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium
(NYSGRC)
Deposited on : 2014-04-30
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

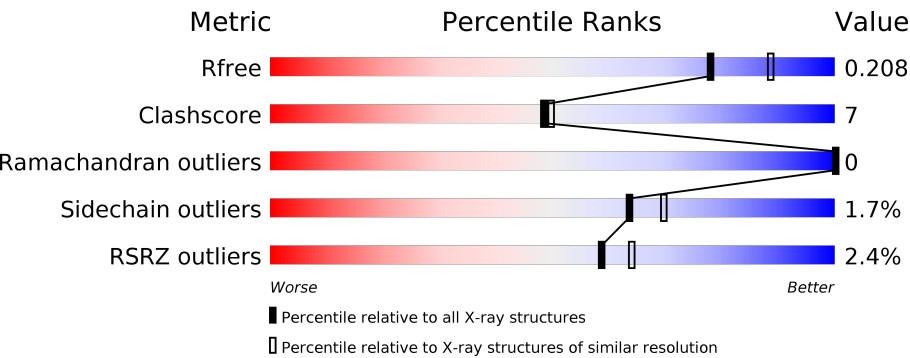
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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 $\leq 5\%$. 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	207	<div><div>%</div><div><div></div><div>77%</div><div>7%</div><div>•</div><div>14%</div></div></div>
1	B	207	<div><div>%</div><div><div></div><div>76%</div><div>9%</div><div></div><div>14%</div></div></div>
1	C	207	<div><div>4%</div><div><div></div><div>79%</div><div>9%</div><div></div><div>11%</div></div></div>
1	D	207	<div><div></div><div><div></div><div>78%</div><div>7%</div><div></div><div>14%</div></div></div>
1	E	207	<div><div>4%</div><div><div></div><div>77%</div><div>12%</div><div></div><div>11%</div></div></div>
1	F	207	<div><div>4%</div><div><div></div><div>76%</div><div>12%</div><div></div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	207	<div><div></div><div>77%</div><div>8%</div><div>14%</div></div>
1	H	207	<div><div>2%</div><div></div><div>79%</div><div>9%</div><div>11%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11835 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 Hypoxanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	Se	0	1	0
			1387	880	238	265	4			
1	B	177	Total	C	N	O	Se	0	0	0
			1379	875	235	265	4			
1	C	184	Total	C	N	O	Se	0	0	0
			1437	909	245	279	4			
1	D	178	Total	C	N	O	Se	0	0	0
			1388	880	236	268	4			
1	E	184	Total	C	N	O	Se	0	0	0
			1437	909	245	279	4			
1	F	184	Total	C	N	O	Se	0	0	0
			1436	909	245	278	4			
1	G	177	Total	C	N	O	Se	0	0	0
			1379	875	235	265	4			
1	H	184	Total	C	N	O	Se	0	0	0
			1437	909	245	279	4			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP C7MC15
A	2	HIS	-	expression tag	UNP C7MC15
A	3	HIS	-	expression tag	UNP C7MC15
A	4	HIS	-	expression tag	UNP C7MC15
A	5	HIS	-	expression tag	UNP C7MC15
A	6	HIS	-	expression tag	UNP C7MC15
A	7	HIS	-	expression tag	UNP C7MC15
A	8	SER	-	expression tag	UNP C7MC15
A	9	SER	-	expression tag	UNP C7MC15
A	10	GLY	-	expression tag	UNP C7MC15
A	11	VAL	-	expression tag	UNP C7MC15
A	12	ASP	-	expression tag	UNP C7MC15
A	13	LEU	-	expression tag	UNP C7MC15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP C7MC15
A	15	THR	-	expression tag	UNP C7MC15
A	16	GLU	-	expression tag	UNP C7MC15
A	17	ASN	-	expression tag	UNP C7MC15
A	18	LEU	-	expression tag	UNP C7MC15
A	19	TYR	-	expression tag	UNP C7MC15
A	20	PHE	-	expression tag	UNP C7MC15
A	21	GLN	-	expression tag	UNP C7MC15
A	22	SER	-	expression tag	UNP C7MC15
A	23	MSE	-	expression tag	UNP C7MC15
A	24	VAL	-	expression tag	UNP C7MC15
B	1	MSE	-	expression tag	UNP C7MC15
B	2	HIS	-	expression tag	UNP C7MC15
B	3	HIS	-	expression tag	UNP C7MC15
B	4	HIS	-	expression tag	UNP C7MC15
B	5	HIS	-	expression tag	UNP C7MC15
B	6	HIS	-	expression tag	UNP C7MC15
B	7	HIS	-	expression tag	UNP C7MC15
B	8	SER	-	expression tag	UNP C7MC15
B	9	SER	-	expression tag	UNP C7MC15
B	10	GLY	-	expression tag	UNP C7MC15
B	11	VAL	-	expression tag	UNP C7MC15
B	12	ASP	-	expression tag	UNP C7MC15
B	13	LEU	-	expression tag	UNP C7MC15
B	14	GLY	-	expression tag	UNP C7MC15
B	15	THR	-	expression tag	UNP C7MC15
B	16	GLU	-	expression tag	UNP C7MC15
B	17	ASN	-	expression tag	UNP C7MC15
B	18	LEU	-	expression tag	UNP C7MC15
B	19	TYR	-	expression tag	UNP C7MC15
B	20	PHE	-	expression tag	UNP C7MC15
B	21	GLN	-	expression tag	UNP C7MC15
B	22	SER	-	expression tag	UNP C7MC15
B	23	MSE	-	expression tag	UNP C7MC15
B	24	VAL	-	expression tag	UNP C7MC15
C	1	MSE	-	expression tag	UNP C7MC15
C	2	HIS	-	expression tag	UNP C7MC15
C	3	HIS	-	expression tag	UNP C7MC15
C	4	HIS	-	expression tag	UNP C7MC15
C	5	HIS	-	expression tag	UNP C7MC15
C	6	HIS	-	expression tag	UNP C7MC15
C	7	HIS	-	expression tag	UNP C7MC15

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	SER	-	expression tag	UNP C7MC15
C	9	SER	-	expression tag	UNP C7MC15
C	10	GLY	-	expression tag	UNP C7MC15
C	11	VAL	-	expression tag	UNP C7MC15
C	12	ASP	-	expression tag	UNP C7MC15
C	13	LEU	-	expression tag	UNP C7MC15
C	14	GLY	-	expression tag	UNP C7MC15
C	15	THR	-	expression tag	UNP C7MC15
C	16	GLU	-	expression tag	UNP C7MC15
C	17	ASN	-	expression tag	UNP C7MC15
C	18	LEU	-	expression tag	UNP C7MC15
C	19	TYR	-	expression tag	UNP C7MC15
C	20	PHE	-	expression tag	UNP C7MC15
C	21	GLN	-	expression tag	UNP C7MC15
C	22	SER	-	expression tag	UNP C7MC15
C	23	MSE	-	expression tag	UNP C7MC15
C	24	VAL	-	expression tag	UNP C7MC15
D	1	MSE	-	expression tag	UNP C7MC15
D	2	HIS	-	expression tag	UNP C7MC15
D	3	HIS	-	expression tag	UNP C7MC15
D	4	HIS	-	expression tag	UNP C7MC15
D	5	HIS	-	expression tag	UNP C7MC15
D	6	HIS	-	expression tag	UNP C7MC15
D	7	HIS	-	expression tag	UNP C7MC15
D	8	SER	-	expression tag	UNP C7MC15
D	9	SER	-	expression tag	UNP C7MC15
D	10	GLY	-	expression tag	UNP C7MC15
D	11	VAL	-	expression tag	UNP C7MC15
D	12	ASP	-	expression tag	UNP C7MC15
D	13	LEU	-	expression tag	UNP C7MC15
D	14	GLY	-	expression tag	UNP C7MC15
D	15	THR	-	expression tag	UNP C7MC15
D	16	GLU	-	expression tag	UNP C7MC15
D	17	ASN	-	expression tag	UNP C7MC15
D	18	LEU	-	expression tag	UNP C7MC15
D	19	TYR	-	expression tag	UNP C7MC15
D	20	PHE	-	expression tag	UNP C7MC15
D	21	GLN	-	expression tag	UNP C7MC15
D	22	SER	-	expression tag	UNP C7MC15
D	23	MSE	-	expression tag	UNP C7MC15
D	24	VAL	-	expression tag	UNP C7MC15
E	1	MSE	-	expression tag	UNP C7MC15

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	HIS	-	expression tag	UNP C7MC15
E	3	HIS	-	expression tag	UNP C7MC15
E	4	HIS	-	expression tag	UNP C7MC15
E	5	HIS	-	expression tag	UNP C7MC15
E	6	HIS	-	expression tag	UNP C7MC15
E	7	HIS	-	expression tag	UNP C7MC15
E	8	SER	-	expression tag	UNP C7MC15
E	9	SER	-	expression tag	UNP C7MC15
E	10	GLY	-	expression tag	UNP C7MC15
E	11	VAL	-	expression tag	UNP C7MC15
E	12	ASP	-	expression tag	UNP C7MC15
E	13	LEU	-	expression tag	UNP C7MC15
E	14	GLY	-	expression tag	UNP C7MC15
E	15	THR	-	expression tag	UNP C7MC15
E	16	GLU	-	expression tag	UNP C7MC15
E	17	ASN	-	expression tag	UNP C7MC15
E	18	LEU	-	expression tag	UNP C7MC15
E	19	TYR	-	expression tag	UNP C7MC15
E	20	PHE	-	expression tag	UNP C7MC15
E	21	GLN	-	expression tag	UNP C7MC15
E	22	SER	-	expression tag	UNP C7MC15
E	23	MSE	-	expression tag	UNP C7MC15
E	24	VAL	-	expression tag	UNP C7MC15
F	1	MSE	-	expression tag	UNP C7MC15
F	2	HIS	-	expression tag	UNP C7MC15
F	3	HIS	-	expression tag	UNP C7MC15
F	4	HIS	-	expression tag	UNP C7MC15
F	5	HIS	-	expression tag	UNP C7MC15
F	6	HIS	-	expression tag	UNP C7MC15
F	7	HIS	-	expression tag	UNP C7MC15
F	8	SER	-	expression tag	UNP C7MC15
F	9	SER	-	expression tag	UNP C7MC15
F	10	GLY	-	expression tag	UNP C7MC15
F	11	VAL	-	expression tag	UNP C7MC15
F	12	ASP	-	expression tag	UNP C7MC15
F	13	LEU	-	expression tag	UNP C7MC15
F	14	GLY	-	expression tag	UNP C7MC15
F	15	THR	-	expression tag	UNP C7MC15
F	16	GLU	-	expression tag	UNP C7MC15
F	17	ASN	-	expression tag	UNP C7MC15
F	18	LEU	-	expression tag	UNP C7MC15
F	19	TYR	-	expression tag	UNP C7MC15

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Chain	Residue	Modelled	Actual	Comment	Reference
F	20	PHE	-	expression tag	UNP C7MC15
F	21	GLN	-	expression tag	UNP C7MC15
F	22	SER	-	expression tag	UNP C7MC15
F	23	MSE	-	expression tag	UNP C7MC15
F	24	VAL	-	expression tag	UNP C7MC15
G	1	MSE	-	expression tag	UNP C7MC15
G	2	HIS	-	expression tag	UNP C7MC15
G	3	HIS	-	expression tag	UNP C7MC15
G	4	HIS	-	expression tag	UNP C7MC15
G	5	HIS	-	expression tag	UNP C7MC15
G	6	HIS	-	expression tag	UNP C7MC15
G	7	HIS	-	expression tag	UNP C7MC15
G	8	SER	-	expression tag	UNP C7MC15
G	9	SER	-	expression tag	UNP C7MC15
G	10	GLY	-	expression tag	UNP C7MC15
G	11	VAL	-	expression tag	UNP C7MC15
G	12	ASP	-	expression tag	UNP C7MC15
G	13	LEU	-	expression tag	UNP C7MC15
G	14	GLY	-	expression tag	UNP C7MC15
G	15	THR	-	expression tag	UNP C7MC15
G	16	GLU	-	expression tag	UNP C7MC15
G	17	ASN	-	expression tag	UNP C7MC15
G	18	LEU	-	expression tag	UNP C7MC15
G	19	TYR	-	expression tag	UNP C7MC15
G	20	PHE	-	expression tag	UNP C7MC15
G	21	GLN	-	expression tag	UNP C7MC15
G	22	SER	-	expression tag	UNP C7MC15
G	23	MSE	-	expression tag	UNP C7MC15
G	24	VAL	-	expression tag	UNP C7MC15
H	1	MSE	-	expression tag	UNP C7MC15
H	2	HIS	-	expression tag	UNP C7MC15
H	3	HIS	-	expression tag	UNP C7MC15
H	4	HIS	-	expression tag	UNP C7MC15
H	5	HIS	-	expression tag	UNP C7MC15
H	6	HIS	-	expression tag	UNP C7MC15
H	7	HIS	-	expression tag	UNP C7MC15
H	8	SER	-	expression tag	UNP C7MC15
H	9	SER	-	expression tag	UNP C7MC15
H	10	GLY	-	expression tag	UNP C7MC15
H	11	VAL	-	expression tag	UNP C7MC15
H	12	ASP	-	expression tag	UNP C7MC15
H	13	LEU	-	expression tag	UNP C7MC15

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Chain	Residue	Modelled	Actual	Comment	Reference
H	14	GLY	-	expression tag	UNP C7MC15
H	15	THR	-	expression tag	UNP C7MC15
H	16	GLU	-	expression tag	UNP C7MC15
H	17	ASN	-	expression tag	UNP C7MC15
H	18	LEU	-	expression tag	UNP C7MC15
H	19	TYR	-	expression tag	UNP C7MC15
H	20	PHE	-	expression tag	UNP C7MC15
H	21	GLN	-	expression tag	UNP C7MC15
H	22	SER	-	expression tag	UNP C7MC15
H	23	MSE	-	expression tag	UNP C7MC15
H	24	VAL	-	expression tag	UNP C7MC15

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total 1 Mg 1	0	0
2	D	2	Total 2 Mg 2	0	0
2	E	2	Total 2 Mg 2	0	0
2	H	2	Total 2 Mg 2	0	0
2	B	2	Total 2 Mg 2	0	0
2	C	1	Total 1 Mg 1	0	0
2	A	1	Total 1 Mg 1	0	0
2	F	1	Total 1 Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	72	Total 72 O 72	0	0
3	B	60	Total 60 O 60	0	0
3	C	63	Total 63 O 63	0	0
3	D	82	Total 82 O 82	0	0

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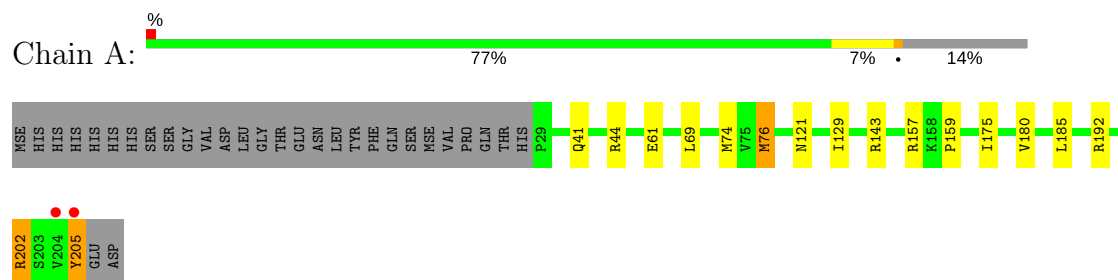
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	64	Total 64	O 64	0	0
3	F	75	Total 75	O 75	0	0
3	G	70	Total 70	O 70	0	0
3	H	57	Total 57	O 57	0	0

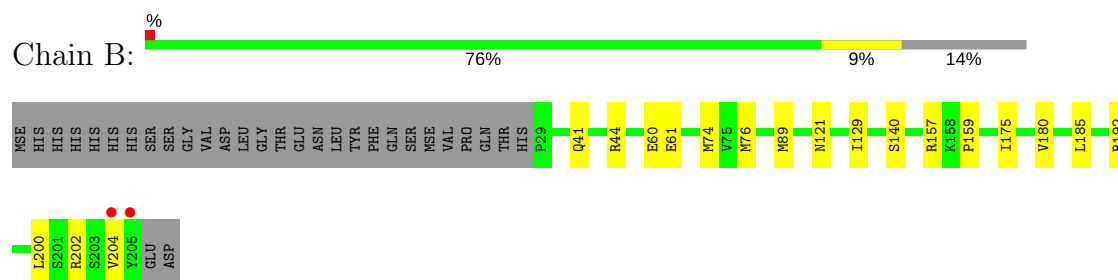
3 Residue-property plots

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

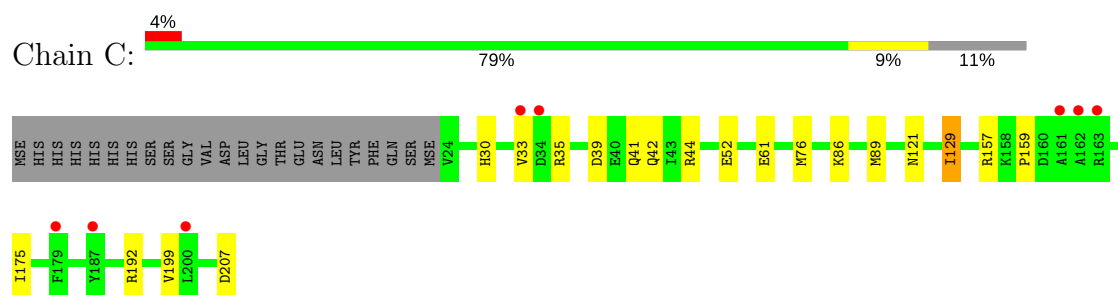
- Molecule 1: Hypoxanthine phosphoribosyltransferase



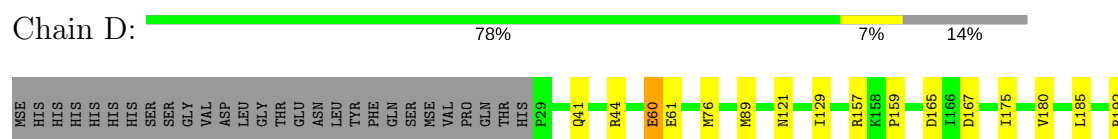
- Molecule 1: Hypoxanthine phosphoribosyltransferase

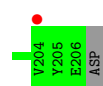


- Molecule 1: Hypoxanthine phosphoribosyltransferase

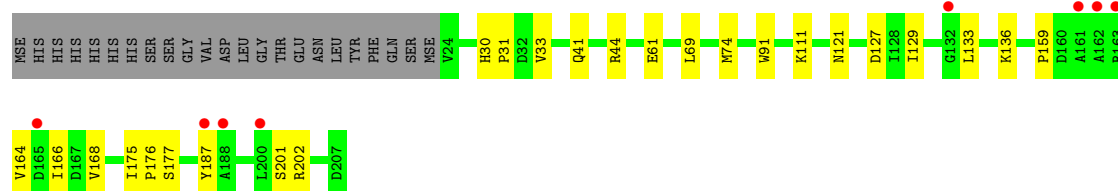
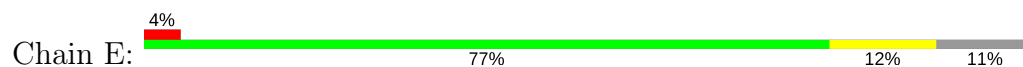


- Molecule 1: Hypoxanthine phosphoribosyltransferase

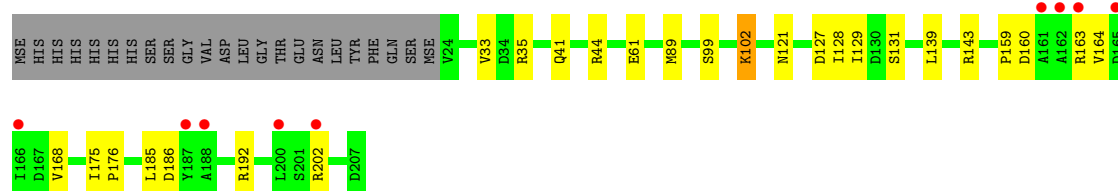
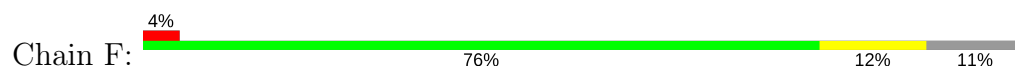




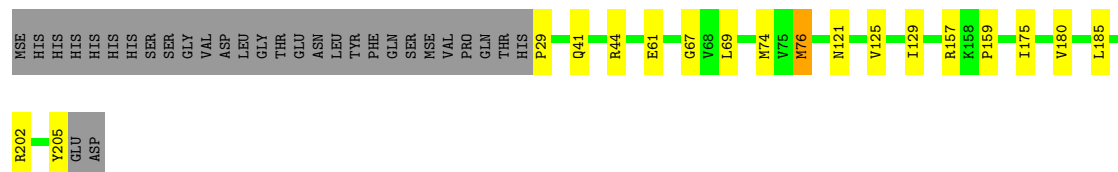
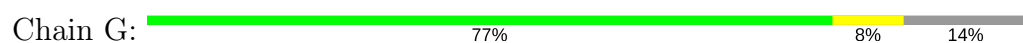
- Molecule 1: Hypoxanthine phosphoribosyltransferase



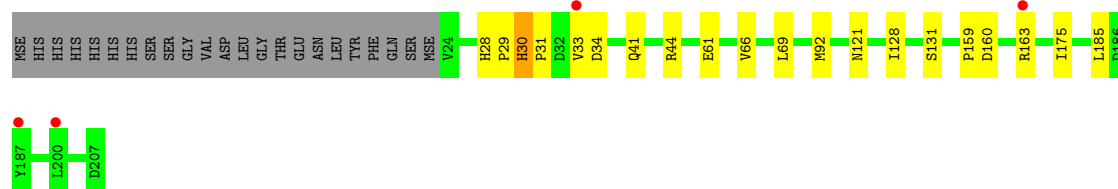
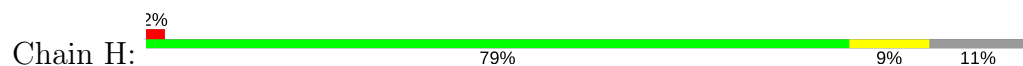
- Molecule 1: Hypoxanthine phosphoribosyltransferase



- Molecule 1: Hypoxanthine phosphoribosyltransferase



- Molecule 1: Hypoxanthine phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.21Å 123.59Å 123.28Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	33.31 – 2.10 33.12 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.8 (33.31-2.10) 93.8 (33.12-2.09)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.173 , 0.213 0.179 , 0.208	Depositor DCC
R_{free} test set	4320 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k 0.004 for -h,l,k 0.437 for h,-k,-l	Xtriage
Reported twinning fraction	0.637 for H, K, L 0.363 for -h,-k,l	Depositor
Outliers	0 of 86140 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11835	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.90	0/1408	0.94	3/1903 (0.2%)
1	B	0.90	0/1397	0.91	0/1889
1	C	0.87	0/1457	0.92	0/1972
1	D	0.92	0/1406	0.95	0/1901
1	E	0.96	0/1457	0.95	1/1972 (0.1%)
1	F	0.97	0/1456	1.01	2/1972 (0.1%)
1	G	0.89	0/1397	0.91	0/1889
1	H	0.92	2/1457 (0.1%)	0.96	2/1972 (0.1%)
All	All	0.92	2/11435 (0.0%)	0.94	8/15470 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	31	PRO	N-CD	5.27	1.55	1.47
1	H	29	PRO	N-CD	5.07	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	127	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	202	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	F	202	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	76	MSE	CA-CB-CG	-5.50	103.95	113.30
1	H	28	HIS	C-N-CD	5.41	139.76	128.40
1	H	30	HIS	C-N-CD	5.33	139.58	128.40
1	A	202	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	E	127	ASP	CB-CG-OD1	5.04	122.83	118.30

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	1387	0	1412	9	0
1	B	1379	0	1399	29	0
1	C	1437	0	1446	33	0
1	D	1388	0	1405	26	0
1	E	1437	0	1446	16	0
1	F	1436	0	1446	49	0
1	G	1379	0	1399	14	0
1	H	1437	0	1446	12	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
3	A	72	0	0	2	0
3	B	60	0	0	1	0
3	C	63	0	0	1	0
3	D	82	0	0	1	0
3	E	64	0	0	2	0
3	F	75	0	0	3	0
3	G	70	0	0	1	0
3	H	57	0	0	1	0
All	All	11835	0	11399	148	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 7.

All (148) 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:131:SER:CB	1:F:163:ARG:HD3	1.78	1.12
1:F:131:SER:HB3	1:F:163:ARG:HD3	1.12	1.08
1:F:131:SER:HB3	1:F:163:ARG:CD	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HB2	1:C:89:MSE:HE2	1.34	1.06
1:B:89:MSE:HE2	1:C:192:ARG:HB2	1.37	1.05
1:G:76:MSE:HE2	1:G:125:VAL:HB	1.36	1.02
1:D:192:ARG:HB2	1:F:89:MSE:HE2	1.43	1.00
1:D:89:MSE:HE2	1:F:192:ARG:HB2	1.42	0.98
1:G:76:MSE:CE	1:G:125:VAL:HB	1.93	0.97
1:B:192:ARG:CB	1:C:89:MSE:HE2	1.96	0.95
1:B:89:MSE:HE2	1:C:192:ARG:CB	1.99	0.91
1:B:192:ARG:CB	1:C:89:MSE:CE	2.50	0.89
1:B:192:ARG:HB3	1:C:89:MSE:CE	2.03	0.89
1:D:192:ARG:CB	1:F:89:MSE:HE2	2.03	0.87
1:D:89:MSE:HE2	1:F:192:ARG:CB	2.06	0.85
1:D:192:ARG:HB3	1:F:89:MSE:CE	2.07	0.85
1:B:200:LEU:HD11	1:B:204:VAL:HG21	1.59	0.83
1:D:192:ARG:CB	1:F:89:MSE:CE	2.56	0.83
1:G:67:GLY:HA3	1:G:76:MSE:HE3	1.60	0.81
1:B:89:MSE:CE	1:C:192:ARG:HB3	2.11	0.81
1:B:89:MSE:CE	1:C:192:ARG:CB	2.57	0.81
1:H:160:ASP:O	1:H:163:ARG:HG2	1.79	0.81
1:D:192:ARG:HD2	1:F:89:MSE:HE3	1.63	0.80
1:D:89:MSE:CE	1:F:192:ARG:CB	2.60	0.80
1:D:89:MSE:CE	1:F:192:ARG:HB3	2.12	0.79
1:B:192:ARG:HD2	1:C:89:MSE:HE3	1.64	0.78
1:F:131:SER:CB	1:F:163:ARG:CD	2.50	0.77
1:B:192:ARG:HB3	1:C:89:MSE:HE1	1.65	0.76
1:D:192:ARG:HB3	1:F:89:MSE:HE1	1.70	0.74
1:C:35:ARG:NH1	1:C:199:VAL:HG21	2.02	0.73
1:C:33:VAL:O	1:C:33:VAL:HG23	1.89	0.72
1:E:166:ILE:HG22	1:E:168:VAL:HG23	1.72	0.71
1:G:29:PRO:N	3:G:546:HOH:O	2.24	0.70
1:B:89:MSE:HE1	1:C:192:ARG:HB3	1.74	0.70
1:B:89:MSE:HE3	1:C:192:ARG:HD2	1.74	0.69
1:B:192:ARG:CD	1:C:89:MSE:HE3	2.22	0.69
1:D:89:MSE:HE1	1:F:192:ARG:HB3	1.73	0.68
1:D:192:ARG:CD	1:F:89:MSE:HE3	2.24	0.68
1:D:89:MSE:HE3	1:F:192:ARG:HD2	1.77	0.67
1:F:35:ARG:HD3	3:F:508:HOH:O	1.96	0.65
1:F:163:ARG:HG3	1:F:164:VAL:HG23	1.78	0.64
1:G:67:GLY:CA	1:G:76:MSE:HE3	2.27	0.64
1:F:131:SER:OG	1:F:163:ARG:HD2	1.98	0.63
1:F:131:SER:OG	1:F:160:ASP:O	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:GLU:CD	1:D:60:GLU:H	2.02	0.62
1:F:131:SER:OG	1:F:160:ASP:HB2	2.00	0.62
1:H:66:VAL:CG1	1:H:92:MSE:HE2	2.30	0.61
1:B:200:LEU:HD11	1:B:204:VAL:CG2	2.29	0.61
1:F:143:ARG:HD3	3:F:549:HOH:O	2.00	0.60
1:B:60:GLU:CD	1:B:60:GLU:H	2.05	0.60
1:F:131:SER:OG	1:F:160:ASP:CB	2.50	0.60
1:C:33:VAL:O	1:C:33:VAL:CG2	2.49	0.59
1:H:33:VAL:HG23	1:H:33:VAL:O	2.03	0.59
1:C:129:ILE:HD11	1:C:157:ARG:HB2	1.84	0.59
1:C:35:ARG:HH11	1:C:199:VAL:HG21	1.67	0.59
1:F:163:ARG:CG	1:F:164:VAL:HG23	2.32	0.58
1:B:192:ARG:HB2	1:C:89:MSE:CE	2.15	0.58
1:A:202:ARG:HA	1:A:205:TYR:HB2	1.87	0.57
1:B:89:MSE:HE3	1:C:192:ARG:CD	2.34	0.57
1:H:131:SER:CB	1:H:163:ARG:HD2	2.36	0.56
1:B:192:ARG:HD2	1:C:89:MSE:CE	2.33	0.56
1:C:39:ASP:OD1	1:C:42:GLN:OE1	2.25	0.55
1:B:89:MSE:CE	1:C:192:ARG:HD2	2.36	0.55
1:E:187:TYR:CZ	1:E:202:ARG:NH2	2.75	0.55
1:F:131:SER:OG	1:F:163:ARG:CD	2.55	0.55
1:D:192:ARG:HD2	1:F:89:MSE:CE	2.34	0.54
1:A:69:LEU:HD11	1:H:69:LEU:HD11	1.89	0.54
1:F:128:ILE:HD11	1:F:185:LEU:HD22	1.88	0.54
1:F:129:ILE:HD13	1:F:168:VAL:HG21	1.89	0.54
1:G:67:GLY:CA	1:G:76:MSE:CE	2.85	0.54
1:D:44:ARG:HD2	3:D:563:HOH:O	2.06	0.54
1:F:131:SER:HG	1:F:163:ARG:HD2	1.74	0.53
1:H:131:SER:HB3	1:H:163:ARG:HD2	1.89	0.53
1:B:140:SER:OG	1:D:165:ASP:OD2	2.23	0.53
1:D:89:MSE:HE3	1:F:192:ARG:CD	2.39	0.53
1:E:129:ILE:HD13	1:E:168:VAL:HG21	1.91	0.53
1:H:61:GLU:HG2	1:H:121:ASN:ND2	2.24	0.53
1:C:39:ASP:OD1	1:C:42:GLN:HG3	2.08	0.52
1:B:61:GLU:HG2	1:B:121:ASN:ND2	2.23	0.52
1:B:192:ARG:CD	1:C:89:MSE:CE	2.88	0.52
1:H:69:LEU:O	3:H:534:HOH:O	2.19	0.52
1:D:89:MSE:CE	1:F:192:ARG:HD2	2.41	0.51
1:F:139:LEU:O	1:F:143:ARG:HG3	2.10	0.51
1:F:131:SER:CA	1:F:163:ARG:HD3	2.40	0.50
1:D:192:ARG:CD	1:F:89:MSE:CE	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:PRO:HA	3:E:502:HOH:O	2.12	0.49
1:C:30:HIS:HB3	3:C:550:HOH:O	2.13	0.49
1:A:61:GLU:HG2	1:A:121:ASN:ND2	2.28	0.48
1:F:131:SER:HG	1:F:163:ARG:CD	2.26	0.48
1:C:61:GLU:HG2	1:C:121:ASN:ND2	2.28	0.48
1:E:33:VAL:O	1:E:33:VAL:HG23	2.14	0.48
1:G:61:GLU:HG2	1:G:121:ASN:ND2	2.29	0.47
1:G:76:MSE:HE1	1:G:125:VAL:HB	1.89	0.47
1:E:61:GLU:HG2	1:E:121:ASN:ND2	2.29	0.47
1:E:69:LEU:HD11	1:G:69:LEU:HD11	1.97	0.47
1:C:129:ILE:HD11	1:C:157:ARG:CB	2.45	0.47
1:F:128:ILE:HD11	1:F:185:LEU:CD2	2.45	0.46
1:B:89:MSE:CE	1:C:192:ARG:CD	2.93	0.46
1:A:143[B]:ARG:NE	3:A:551:HOH:O	2.49	0.46
1:D:61:GLU:HG2	1:D:121:ASN:ND2	2.31	0.46
1:E:166:ILE:HG22	1:E:168:VAL:CG2	2.44	0.46
1:F:131:SER:OG	1:F:160:ASP:CG	2.54	0.46
1:A:41:GLN:OE1	1:A:44:ARG:NH1	2.48	0.46
1:H:66:VAL:HG11	1:H:92:MSE:HE2	1.96	0.46
1:G:180:VAL:HG23	1:G:185:LEU:HD23	1.99	0.45
1:C:129:ILE:HD13	1:C:157:ARG:HA	1.97	0.45
1:B:41:GLN:OE1	1:B:44:ARG:NH1	2.49	0.45
1:F:99:SER:O	1:F:102:LYS:HG3	2.17	0.45
1:F:41:GLN:OE1	1:F:44:ARG:NH1	2.49	0.45
1:E:41:GLN:OE1	1:E:44:ARG:NH1	2.50	0.45
1:F:175:ILE:HB	1:F:176:PRO:HD2	1.99	0.45
1:G:41:GLN:OE1	1:G:44:ARG:NH1	2.49	0.44
1:E:91:TRP:O	1:E:111:LYS:NZ	2.48	0.44
1:G:159:PRO:HD3	1:G:175:ILE:O	2.17	0.44
1:B:140:SER:HB3	3:B:536:HOH:O	2.16	0.44
1:E:177:SER:HB2	3:E:537:HOH:O	2.18	0.44
1:E:136:LYS:HB2	1:E:166:ILE:HD11	2.00	0.44
1:F:131:SER:HG	1:F:160:ASP:C	2.13	0.44
1:F:61:GLU:HG2	1:F:121:ASN:ND2	2.32	0.44
1:F:131:SER:OG	1:F:160:ASP:C	2.54	0.44
1:H:41:GLN:OE1	1:H:44:ARG:NH1	2.49	0.44
1:G:202:ARG:HG2	1:G:205:TYR:OH	2.17	0.43
1:H:159:PRO:HD3	1:H:175:ILE:O	2.18	0.43
1:D:41:GLN:OE1	1:D:44:ARG:NH1	2.50	0.43
1:C:41:GLN:OE1	1:C:44:ARG:NH1	2.49	0.43
1:C:159:PRO:HD3	1:C:175:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HD11	1:B:157:ARG:HD3	2.01	0.42
1:B:159:PRO:HD3	1:B:175:ILE:O	2.20	0.42
1:B:180:VAL:HG23	1:B:185:LEU:HD23	2.01	0.42
1:E:164:VAL:HG12	1:E:166:ILE:HG13	2.02	0.42
1:F:99:SER:HA	1:F:102:LYS:HG2	2.01	0.42
1:A:129:ILE:HD11	1:A:157:ARG:HD3	2.01	0.42
1:D:129:ILE:HD11	1:D:157:ARG:HD3	2.02	0.42
1:F:159:PRO:HD3	1:F:175:ILE:O	2.19	0.41
1:A:192:ARG:HD3	3:A:570:HOH:O	2.20	0.41
1:D:159:PRO:HD3	1:D:175:ILE:O	2.19	0.41
1:G:129:ILE:HD11	1:G:157:ARG:HD3	2.02	0.41
1:E:175:ILE:HB	1:E:176:PRO:HD2	2.03	0.41
1:E:133:LEU:CD1	1:E:133:LEU:N	2.82	0.41
1:F:186:ASP:OD1	3:F:562:HOH:O	2.22	0.41
1:F:131:SER:CB	1:F:163:ARG:HD2	2.41	0.41
1:A:159:PRO:HD3	1:A:175:ILE:O	2.21	0.41
1:A:180:VAL:HG23	1:A:185:LEU:HD23	2.01	0.41
1:D:180:VAL:HG23	1:D:185:LEU:HD23	2.03	0.41
1:H:128:ILE:HD11	1:H:185:LEU:HD22	2.03	0.41
1:C:86:LYS:HB3	1:C:86:LYS:HE2	1.96	0.40
1:E:30:HIS:ND1	1:E:31:PRO:HD2	2.37	0.40
1:D:89:MSE:CE	1:F:192:ARG:CD	2.99	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	176/207 (85%)	173 (98%)	3 (2%)	0	100	100
1	B	175/207 (84%)	172 (98%)	3 (2%)	0	100	100
1	C	182/207 (88%)	177 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	176/207 (85%)	174 (99%)	2 (1%)	0	100	100
1	E	182/207 (88%)	178 (98%)	4 (2%)	0	100	100
1	F	182/207 (88%)	178 (98%)	4 (2%)	0	100	100
1	G	175/207 (84%)	171 (98%)	4 (2%)	0	100	100
1	H	182/207 (88%)	178 (98%)	4 (2%)	0	100	100
All	All	1430/1656 (86%)	1401 (98%)	29 (2%)	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	152/173 (88%)	149 (98%)	3 (2%)	58	63
1	B	151/173 (87%)	148 (98%)	3 (2%)	58	63
1	C	158/173 (91%)	154 (98%)	4 (2%)	50	55
1	D	152/173 (88%)	149 (98%)	3 (2%)	58	63
1	E	158/173 (91%)	156 (99%)	2 (1%)	71	78
1	F	158/173 (91%)	156 (99%)	2 (1%)	71	78
1	G	151/173 (87%)	149 (99%)	2 (1%)	71	78
1	H	158/173 (91%)	156 (99%)	2 (1%)	71	78
All	All	1238/1384 (90%)	1217 (98%)	21 (2%)	63	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	MSE
1	A	76	MSE
1	A	205	TYR
1	B	74	MSE
1	B	76	MSE

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Mol	Chain	Res	Type
1	B	202	ARG
1	C	52	GLU
1	C	76	MSE
1	C	129	ILE
1	C	207	ASP
1	D	60	GLU
1	D	76	MSE
1	D	167	ASP
1	E	74	MSE
1	E	201	SER
1	F	33	VAL
1	F	102	LYS
1	G	74	MSE
1	G	76	MSE
1	H	30	HIS
1	H	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	190	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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	173/207 (83%)	-0.27	2 (1%) 79 82	27, 38, 67, 82	0
1	B	173/207 (83%)	-0.21	2 (1%) 79 82	28, 41, 64, 95	0
1	C	180/207 (86%)	0.07	8 (4%) 34 40	27, 45, 78, 102	0
1	D	174/207 (84%)	-0.28	1 (0%) 89 91	29, 39, 58, 82	0
1	E	180/207 (86%)	0.03	8 (4%) 34 40	27, 41, 74, 109	0
1	F	180/207 (86%)	-0.01	9 (5%) 29 35	28, 38, 73, 93	0
1	G	173/207 (83%)	-0.30	0 100 100	28, 40, 61, 84	0
1	H	180/207 (86%)	-0.02	4 (2%) 62 67	29, 45, 78, 97	0
All	All	1413/1656 (85%)	-0.12	34 (2%) 59 64	27, 40, 69, 109	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	163	ARG	7.0
1	E	162	ALA	7.0
1	C	162	ALA	5.6
1	F	162	ALA	5.6
1	H	33	VAL	4.7
1	B	204	VAL	4.3
1	E	161	ALA	4.1
1	F	165	ASP	3.7
1	F	163	ARG	3.7
1	F	166	ILE	3.7
1	E	165	ASP	3.4
1	E	187	TYR	3.4
1	F	187	TYR	3.2
1	C	187	TYR	3.2
1	C	163	ARG	3.1
1	A	204	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	163	ARG	2.8
1	D	204	VAL	2.7
1	F	202	ARG	2.7
1	F	161	ALA	2.6
1	F	188	ALA	2.6
1	C	200	LEU	2.6
1	C	33	VAL	2.5
1	H	187	TYR	2.4
1	H	200	LEU	2.4
1	C	179	PHE	2.3
1	B	205	TYR	2.3
1	E	200	LEU	2.3
1	C	34	ASP	2.2
1	A	205	TYR	2.2
1	C	161	ALA	2.1
1	F	200	LEU	2.1
1	E	188	ALA	2.1
1	E	132	GLY	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. 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
2	MG	B	401	1/1	0.83	0.14	53,53,53,53	0
2	MG	H	400	1/1	0.86	0.13	51,51,51,51	0
2	MG	G	400	1/1	0.87	0.09	39,39,39,39	0
2	MG	B	400	1/1	0.88	0.10	49,49,49,49	0
2	MG	E	400	1/1	0.91	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	H	401	1/1	0.93	0.12	42,42,42,42	0
2	MG	D	400	1/1	0.93	0.09	35,35,35,35	0
2	MG	D	401	1/1	0.94	0.13	38,38,38,38	0
2	MG	E	401	1/1	0.94	0.14	34,34,34,34	0
2	MG	C	400	1/1	0.94	0.14	52,52,52,52	0
2	MG	A	400	1/1	0.94	0.12	40,40,40,40	0
2	MG	F	400	1/1	0.97	0.07	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.