



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:44 am GMT

PDB ID : 2F8J
Title : Crystal structure of Histidinol-phosphate aminotransferase (EC 2.6.1.9) (Imidazole acetol-phosphate transferase) (tm1040) from *Thermotoga maritima* at 2.40 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-12-02
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

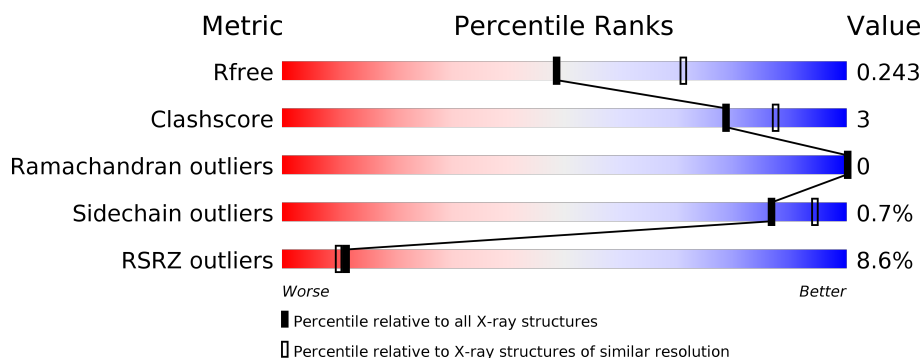
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	347	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>••</div> </div>
1	B	347	<div> <div>6%</div> <div>88%</div> <div>7%</div> <div>•</div> </div>
1	C	347	<div> <div>7%</div> <div>89%</div> <div>7%</div> <div>••</div> </div>
1	D	347	<div> <div>16%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	501	-	-	-	X
3	EDO	B	504	-	-	-	X
3	EDO	B	505	-	-	-	X
3	EDO	C	503	-	-	-	X
3	EDO	D	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11003 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 Histidinol-phosphate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2685	1741	451	484	9			
1	B	333	Total	C	N	O	S	0	0	0
			2636	1709	443	475	9			
1	C	335	Total	C	N	O	S	0	3	0
			2695	1750	449	485	11			
1	D	333	Total	C	N	O	S	0	0	0
			2532	1641	411	472	8			

There are 48 discrepancies between the modelled and reference sequences:

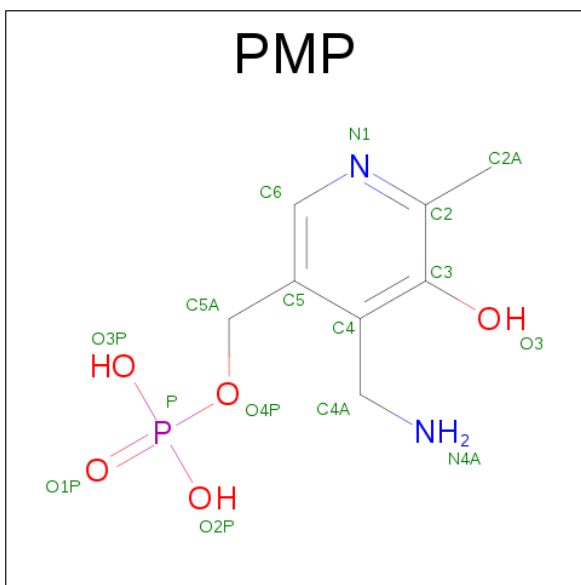
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9X0D0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0D0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9X0D0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0D0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0D0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0D0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
B	-11	MET	-	LEADER SEQUENCE	UNP Q9X0D0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0D0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9X0D0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0D0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0D0
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0D0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0D0

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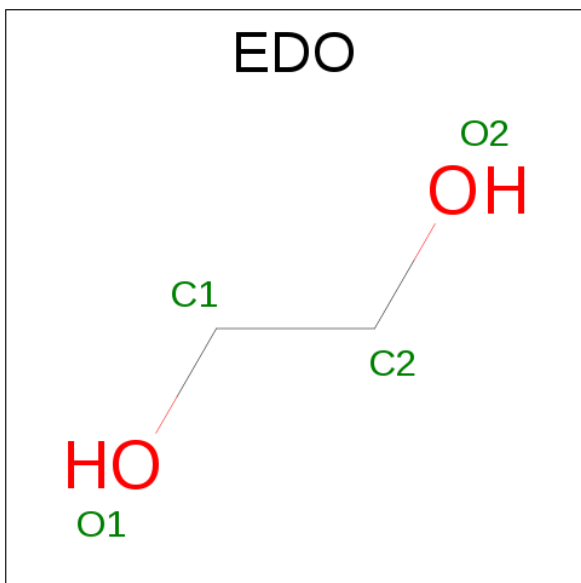
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9X0D0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0D0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9X0D0
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0D0
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0D0
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
C	0	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-11	MET	-	LEADER SEQUENCE	UNP Q9X0D0
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9X0D0
D	-9	SER	-	LEADER SEQUENCE	UNP Q9X0D0
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9X0D0
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9X0D0
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9X0D0
D	0	HIS	-	LEADER SEQUENCE	UNP Q9X0D0

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

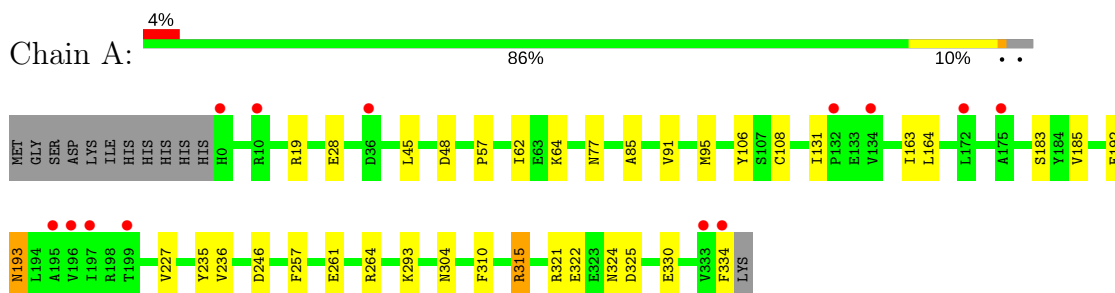
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	B	110	Total O 110 110	0	0
4	C	98	Total O 98 98	0	0
4	D	31	Total O 31 31	0	0

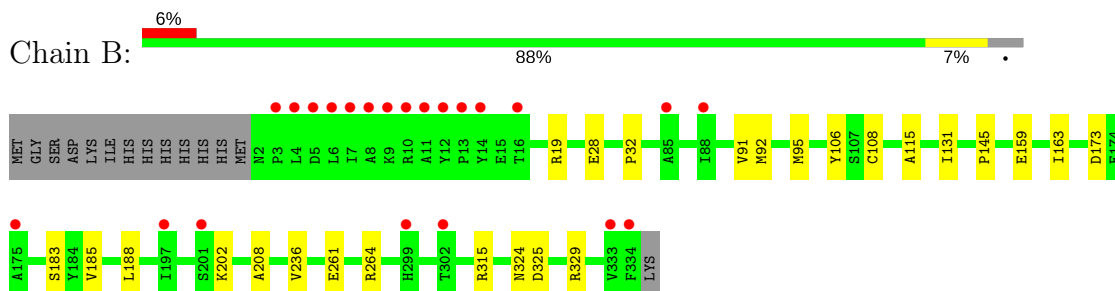
3 Residue-property plots [i](#)

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.

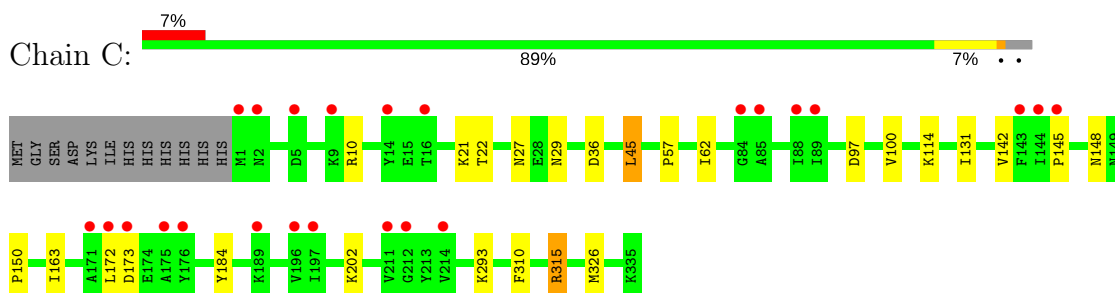
- Molecule 1: Histidinol-phosphate aminotransferase



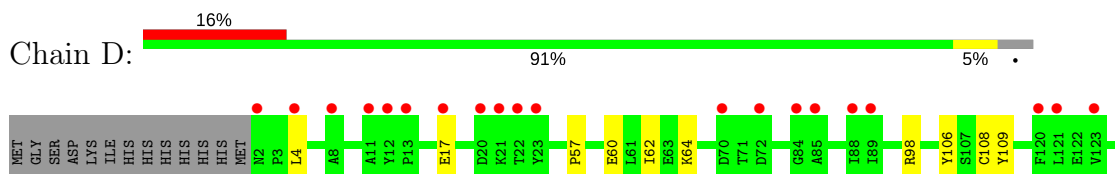
- Molecule 1: Histidinol-phosphate aminotransferase

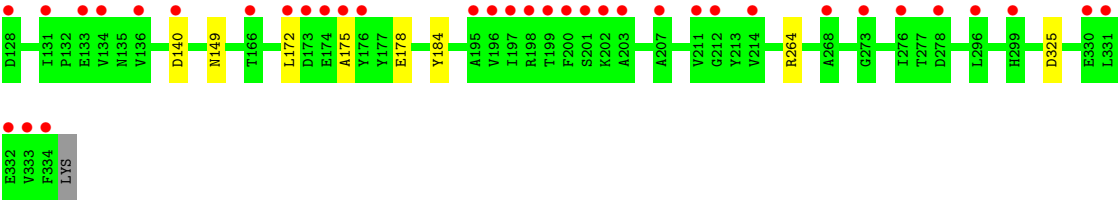


- Molecule 1: Histidinol-phosphate aminotransferase



- Molecule 1: Histidinol-phosphate aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.16Å 187.45Å 54.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.40 29.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.60-2.40) 91.5 (29.79-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.238 0.189 , 0.243	Depositor DCC
R_{free} test set	2736 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11003	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PMP, EDO

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	0.55	0/2745	0.67	2/3715 (0.1%)
1	B	0.56	0/2695	0.65	0/3645
1	C	0.54	0/2761	0.68	3/3730 (0.1%)
1	D	0.44	0/2591	0.57	0/3515
All	All	0.53	0/10792	0.64	5/14605 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	45	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	315	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	315	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	193	ASN	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	GLU	Peptide

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	2685	0	2601	24	0
1	B	2636	0	2533	23	0
1	C	2695	0	2625	16	0
1	D	2532	0	2307	10	0
2	A	16	0	11	1	0
2	B	16	0	10	3	0
2	C	16	0	10	1	0
2	D	16	0	10	2	0
3	A	12	0	18	0	0
3	B	20	0	30	0	0
3	C	12	0	18	0	0
3	D	8	0	12	2	0
4	A	100	0	0	1	0
4	B	110	0	0	2	0
4	C	98	0	0	1	0
4	D	31	0	0	0	0
All	All	11003	0	10185	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (69) 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:131:ILE:HG21	1:C:163:ILE:HD11	1.69	0.74
1:C:10:ARG:NH1	1:C:114:LYS:O	2.25	0.69
1:B:131:ILE:HG21	1:B:163:ILE:HD11	1.82	0.61
1:A:261:GLU:OE2	1:A:321:ARG:HD3	2.01	0.60
1:D:149:ASN:ND2	2:D:500:PMP:O3	2.35	0.59
1:A:45:LEU:HD11	1:A:236:VAL:HG22	1.85	0.58
1:B:183:SER:OG	1:B:185:VAL:HG23	2.03	0.58
1:A:261:GLU:HG3	1:A:324:ASN:ND2	2.19	0.57
1:C:315:ARG:HD2	4:C:520:HOH:O	2.04	0.56
1:C:172:LEU:CD2	1:C:184:TYR:HB2	2.36	0.56
1:C:202:LYS:NZ	2:C:500:PMP:H4A2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLU:H	3:D:502:EDO:H22	1.72	0.54
1:A:57:PRO:HG3	1:A:62:ILE:HD11	1.88	0.54
1:D:172:LEU:CD2	1:D:184:TYR:HB2	2.37	0.54
1:B:159:GLU:O	1:B:163:ILE:HD12	2.08	0.54
1:A:261:GLU:CG	1:A:324:ASN:ND2	2.70	0.53
1:A:236:VAL:HG11	1:B:236:VAL:HG11	1.89	0.53
1:A:235:TYR:HB2	1:B:208:ALA:HB1	1.90	0.52
1:C:100:VAL:HB	1:C:142:VAL:HG22	1.92	0.52
1:C:131:ILE:HG21	1:C:163:ILE:CD1	2.37	0.51
1:D:57:PRO:HG3	1:D:62:ILE:HD11	1.91	0.51
1:A:315:ARG:HD2	4:A:506:HOH:O	2.09	0.51
1:A:164:LEU:O	1:A:193:ASN:ND2	2.43	0.50
1:B:261:GLU:HG2	1:B:324:ASN:ND2	2.26	0.50
1:B:261:GLU:CG	1:B:324:ASN:ND2	2.76	0.49
1:D:106:TYR:CE2	1:D:108:CYS:HB2	2.46	0.49
1:D:175:ALA:O	3:D:502:EDO:O2	2.25	0.49
1:A:293:LYS:NZ	1:A:310:PHE:O	2.38	0.49
1:B:202:LYS:NZ	2:B:500:PMP:C4A	2.76	0.49
1:C:293:LYS:NZ	1:C:310:PHE:O	2.43	0.48
1:C:57:PRO:HG3	1:C:62:ILE:HD11	1.96	0.48
1:A:106:TYR:CE2	1:A:108:CYS:HB2	2.50	0.47
1:A:257:PHE:O	1:A:261:GLU:HB2	2.14	0.47
1:A:57:PRO:CG	1:A:62:ILE:HD11	2.45	0.47
1:A:183:SER:OG	1:A:185:VAL:HG23	2.15	0.46
1:B:19:ARG:NH2	1:B:28:GLU:OE2	2.48	0.46
1:B:202:LYS:HZ1	2:B:500:PMP:C4A	2.30	0.45
1:C:22:THR:HG21	1:C:326:MET:HE1	1.96	0.45
1:B:92:MET:HG2	1:B:95:MET:HE3	1.99	0.45
1:B:261:GLU:CG	1:B:324:ASN:HD22	2.30	0.45
1:A:85:ALA:HB3	2:A:500:PMP:H5A2	1.99	0.45
1:A:91:VAL:O	1:A:95:MET:HG3	2.17	0.44
1:A:330:GLU:O	1:A:334:PHE:HB2	2.17	0.44
1:D:106:TYR:HB3	1:D:109:TYR:CE2	2.52	0.44
1:C:145:PRO:HB2	1:C:148:ASN:HA	1.98	0.44
1:A:48:ASP:HA	1:B:32:PRO:HB3	1.99	0.44
1:B:315:ARG:HD2	4:B:514:HOH:O	2.17	0.43
1:C:29:ASN:HB2	1:C:202:LYS:O	2.19	0.43
1:A:131:ILE:HG21	1:A:163:ILE:HD11	2.01	0.43
1:A:77:ASN:ND2	1:C:97:ASP:OD2	2.51	0.43
1:A:64:LYS:NZ	1:A:246:ASP:OD1	2.50	0.43
1:B:329:ARG:NH2	4:B:520:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HB3	1:D:140:ASP:OD1	2.19	0.42
1:B:91:VAL:O	1:B:95:MET:HG3	2.18	0.42
1:C:145:PRO:HA	1:C:173:ASP:HB3	2.02	0.42
1:C:27:ASN:O	1:C:202:LYS:HD2	2.19	0.42
2:D:500:PMP:O3	2:D:500:PMP:N4A	2.51	0.42
1:C:150:PRO:HB3	1:C:310:PHE:CZ	2.53	0.42
1:B:106:TYR:CE2	1:B:108:CYS:HB2	2.55	0.42
1:B:185:VAL:HG13	1:B:188:LEU:HD12	2.02	0.42
1:A:227:VAL:HA	1:B:115:ALA:HB1	2.02	0.42
1:B:202:LYS:HZ1	2:B:500:PMP:H4A2	1.85	0.42
1:D:60:GLU:HG2	1:D:64:LYS:HE2	2.01	0.41
1:A:19[A]:ARG:NH2	1:A:28:GLU:OE2	2.53	0.41
1:B:264:ARG:NH2	1:B:325:ASP:OD1	2.54	0.41
1:B:131:ILE:HD13	1:B:163:ILE:HD11	2.02	0.41
1:A:264:ARG:NH2	1:A:325:ASP:OD1	2.55	0.40
1:D:264:ARG:NH2	1:D:325:ASP:OD1	2.54	0.40
1:B:145:PRO:HA	1:B:173:ASP:HB3	2.04	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	334/347 (96%)	327 (98%)	7 (2%)	0	100	100
1	B	331/347 (95%)	321 (97%)	10 (3%)	0	100	100
1	C	336/347 (97%)	328 (98%)	8 (2%)	0	100	100
1	D	331/347 (95%)	322 (97%)	9 (3%)	0	100	100
All	All	1332/1388 (96%)	1298 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	272/312 (87%)	270 (99%)	2 (1%)	87	94
1	B	264/312 (85%)	264 (100%)	0	100	100
1	C	273/312 (88%)	270 (99%)	3 (1%)	78	90
1	D	238/312 (76%)	236 (99%)	2 (1%)	85	93
All	All	1047/1248 (84%)	1040 (99%)	7 (1%)	87	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	322	GLU
1	C	21	LYS
1	C	36	ASP
1	C	45	LEU
1	D	4	LEU
1	D	17	GLU

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

Mol	Chain	Res	Type
1	A	77	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](#)

17 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	PMP	A	500	-	16,16,16	1.38	3 (18%)	20,23,23	1.95	5 (25%)
3	EDO	A	501	-	3,3,3	0.59	0	2,2,2	0.20	0
3	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.55	0
3	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.38	0
2	PMP	B	500	-	16,16,16	1.31	1 (6%)	20,23,23	1.83	5 (25%)
3	EDO	B	501	-	3,3,3	0.59	0	2,2,2	0.38	0
3	EDO	B	502	-	3,3,3	0.57	0	2,2,2	0.20	0
3	EDO	B	503	-	3,3,3	0.54	0	2,2,2	0.19	0
3	EDO	B	504	-	3,3,3	0.51	0	2,2,2	0.13	0
3	EDO	B	505	-	3,3,3	0.43	0	2,2,2	0.38	0
2	PMP	C	500	-	16,16,16	1.44	2 (12%)	20,23,23	1.85	7 (35%)
3	EDO	C	501	-	3,3,3	0.63	0	2,2,2	0.11	0
3	EDO	C	502	-	3,3,3	0.48	0	2,2,2	0.29	0
3	EDO	C	503	-	3,3,3	0.42	0	2,2,2	0.25	0
2	PMP	D	500	-	16,16,16	1.41	2 (12%)	20,23,23	1.77	6 (30%)
3	EDO	D	501	-	3,3,3	0.64	0	2,2,2	0.01	0
3	EDO	D	502	-	3,3,3	0.62	0	2,2,2	0.17	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	PMP	A	500	-	-	0/8/8/8	0/1/1/1
3	EDO	A	501	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	502	-	-	0/1/1/1	0/0/0/0
3	EDO	A	503	-	-	0/1/1/1	0/0/0/0
2	PMP	B	500	-	-	0/8/8/8	0/1/1/1
3	EDO	B	501	-	-	0/1/1/1	0/0/0/0
3	EDO	B	502	-	-	0/1/1/1	0/0/0/0
3	EDO	B	503	-	-	0/1/1/1	0/0/0/0
3	EDO	B	504	-	-	0/1/1/1	0/0/0/0
3	EDO	B	505	-	-	0/1/1/1	0/0/0/0
2	PMP	C	500	-	-	0/8/8/8	0/1/1/1
3	EDO	C	501	-	-	0/1/1/1	0/0/0/0
3	EDO	C	502	-	-	0/1/1/1	0/0/0/0
3	EDO	C	503	-	-	0/1/1/1	0/0/0/0
2	PMP	D	500	-	-	0/8/8/8	0/1/1/1
3	EDO	D	501	-	-	0/1/1/1	0/0/0/0
3	EDO	D	502	-	-	0/1/1/1	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PMP	O4P-C5A	-2.03	1.37	1.44
2	C	500	PMP	C2A-C2	2.05	1.54	1.50
2	D	500	PMP	C2A-C2	2.29	1.54	1.50
2	A	500	PMP	C2A-C2	2.55	1.55	1.50
2	B	500	PMP	P-O1P	2.82	1.60	1.50
2	A	500	PMP	P-O1P	2.91	1.60	1.50
2	D	500	PMP	P-O1P	2.97	1.60	1.50
2	C	500	PMP	P-O1P	2.98	1.60	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PMP	O2P-P-O1P	-3.14	98.21	110.50
2	C	500	PMP	O2P-P-O1P	-2.77	99.65	110.50
2	C	500	PMP	C3-C4-C5	-2.57	116.18	118.71
2	A	500	PMP	C5-C6-N1	-2.46	119.71	123.87
2	D	500	PMP	O2P-P-O1P	-2.45	100.92	110.50
2	B	500	PMP	C2A-C2-C3	-2.37	118.14	120.96
2	A	500	PMP	O2P-P-O4P	-2.20	100.87	106.73
2	D	500	PMP	C5A-C5-C6	-2.08	115.75	119.33
2	C	500	PMP	O2P-P-O4P	-2.05	101.27	106.73
2	D	500	PMP	C3-C4-C5	-2.03	116.70	118.71
2	C	500	PMP	C4A-C4-C3	2.06	123.54	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PMP	C2A-C2-N1	2.24	122.37	117.89
2	C	500	PMP	C6-C5-C4	2.39	119.91	118.13
2	B	500	PMP	O3P-P-O4P	2.76	114.07	106.73
2	D	500	PMP	C6-C5-C4	2.87	120.26	118.13
2	A	500	PMP	O3P-P-O4P	3.11	115.00	106.73
2	D	500	PMP	O3P-P-O4P	3.47	115.97	106.73
2	C	500	PMP	O3P-P-O4P	3.48	115.98	106.73
2	C	500	PMP	O4P-C5A-C5	3.54	116.44	109.32
2	D	500	PMP	O4P-C5A-C5	3.65	116.67	109.32
2	A	500	PMP	C6-C5-C4	3.88	121.02	118.13
2	B	500	PMP	O4P-C5A-C5	4.13	117.62	109.32
2	A	500	PMP	O4P-C5A-C5	4.26	117.89	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PMP	1	0
2	B	500	PMP	3	0
2	C	500	PMP	1	0
2	D	500	PMP	2	0
3	D	502	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	335/347 (96%)	-0.06	13 (3%)	40 39	48, 57, 70, 93	0
1	B	333/347 (95%)	0.06	22 (6%)	19 17	48, 57, 72, 84	0
1	C	335/347 (96%)	0.04	24 (7%)	16 15	49, 57, 71, 85	0
1	D	333/347 (95%)	0.63	56 (16%)	2 1	48, 57, 70, 87	0
All	All	1336/1388 (96%)	0.17	115 (8%)	11 10	48, 57, 71, 93	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	273	GLY	5.8
1	D	334	PHE	5.4
1	D	333	VAL	4.7
1	C	197	ILE	4.7
1	D	136	VAL	4.5
1	D	20	ASP	4.5
1	D	175	ALA	4.4
1	D	12	TYR	4.3
1	D	199	THR	4.3
1	B	8	ALA	4.2
1	D	201	SER	4.2
1	A	334	PHE	4.2
1	B	12	TYR	4.1
1	B	9	LYS	4.0
1	B	5	ASP	4.0
1	D	197	ILE	3.9
1	B	13	PRO	3.8
1	D	72	ASP	3.8
1	B	4	LEU	3.8
1	C	175	ALA	3.8
1	A	175	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	14	TYR	3.7
1	B	334	PHE	3.7
1	A	0	HIS	3.7
1	B	333	VAL	3.6
1	C	171	ALA	3.6
1	B	6	LEU	3.6
1	A	197	ILE	3.6
1	C	172	LEU	3.6
1	C	1	MET	3.6
1	B	16	THR	3.5
1	D	84	GLY	3.4
1	D	166	THR	3.4
1	D	296	LEU	3.3
1	D	134	VAL	3.2
1	D	331	LEU	3.2
1	D	17	GLU	3.2
1	D	202	LYS	3.2
1	D	11	ALA	3.1
1	D	4	LEU	3.1
1	D	268	ALA	3.1
1	B	7	ILE	3.1
1	C	145	PRO	3.1
1	B	10	ARG	3.1
1	D	299	HIS	3.1
1	A	172	LEU	3.1
1	C	14	TYR	3.0
1	C	88	ILE	3.0
1	B	11	ALA	2.9
1	D	173	ASP	2.9
1	B	175	ALA	2.9
1	D	2	ASN	2.8
1	C	214	VAL	2.8
1	D	13	PRO	2.8
1	D	276	ILE	2.8
1	D	176	TYR	2.8
1	A	134	VAL	2.8
1	C	173	ASP	2.8
1	C	84	GLY	2.7
1	D	121	LEU	2.7
1	B	302	THR	2.7
1	D	195	ALA	2.7
1	D	203	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	128	ASP	2.6
1	D	198	ARG	2.6
1	A	196	VAL	2.6
1	D	22	THR	2.6
1	D	207	ALA	2.6
1	D	70	ASP	2.6
1	A	333	VAL	2.6
1	C	85	ALA	2.5
1	D	21	LYS	2.5
1	D	172	LEU	2.5
1	B	201	SER	2.5
1	D	200	PHE	2.5
1	A	199	THR	2.5
1	C	89	ILE	2.4
1	D	133	GLU	2.4
1	D	85	ALA	2.4
1	C	5	ASP	2.4
1	C	16	THR	2.4
1	C	211	VAL	2.3
1	D	88	ILE	2.3
1	D	8	ALA	2.3
1	D	89	ILE	2.3
1	D	212	GLY	2.3
1	D	131	ILE	2.3
1	D	123	VAL	2.3
1	C	176	TYR	2.3
1	B	3	PRO	2.2
1	D	330	GLU	2.2
1	D	140	ASP	2.2
1	D	174	GLU	2.2
1	A	10	ARG	2.2
1	D	214	VAL	2.2
1	A	195	ALA	2.2
1	B	85	ALA	2.2
1	C	144	ILE	2.2
1	A	36	ASP	2.2
1	D	196	VAL	2.2
1	B	88	ILE	2.2
1	D	23	TYR	2.1
1	D	278	ASP	2.1
1	C	196	VAL	2.1
1	B	299	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	211	VAL	2.1
1	C	2	ASN	2.1
1	D	120	PHE	2.0
1	B	197	ILE	2.0
1	A	132	PRO	2.0
1	D	332	GLU	2.0
1	C	9	LYS	2.0
1	C	189	LYS	2.0
1	C	212	GLY	2.0
1	C	143	PHE	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	EDO	B	504	4/4	0.90	0.36	10.73	68,72,73,73	0
3	EDO	B	505	4/4	0.95	0.26	4.24	47,49,52,53	0
3	EDO	B	501	4/4	0.88	0.16	4.23	48,60,65,72	0
3	EDO	C	503	4/4	0.96	0.26	2.56	47,50,52,54	0
3	EDO	D	502	4/4	0.89	0.41	1.02	58,67,68,74	0
3	EDO	D	501	4/4	0.94	0.15	-0.29	61,68,69,70	0
3	EDO	B	503	4/4	0.93	0.15	-0.52	75,76,78,79	0
2	PMP	D	500	16/16	0.89	0.22	-0.83	69,90,92,92	0
2	PMP	A	500	16/16	0.93	0.18	-0.84	46,71,79,79	0
2	PMP	B	500	16/16	0.95	0.16	-1.28	40,68,76,86	0
2	PMP	C	500	16/16	0.93	0.17	-1.69	55,69,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	C	502	4/4	0.95	0.08	-2.78	73,75,75,75	0
3	EDO	A	503	4/4	0.88	0.21	-	72,76,76,80	0
3	EDO	A	502	4/4	0.85	0.45	-	65,71,74,77	0
3	EDO	A	501	4/4	0.74	0.26	-	78,78,79,83	0
3	EDO	B	502	4/4	0.86	0.30	-	76,78,80,81	0
3	EDO	C	501	4/4	0.89	0.23	-	63,66,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.