



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:15 PM UTC

PDB ID : 4D9B / pdb_00004d9b
Title : Pyridoxamine 5' phosphate (PMP) bound form of Salmonella typhimurium D-Cysteine desulphydrase obtained after co-crystallization with D-cycloserine
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2012-01-11
Resolution : 1.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

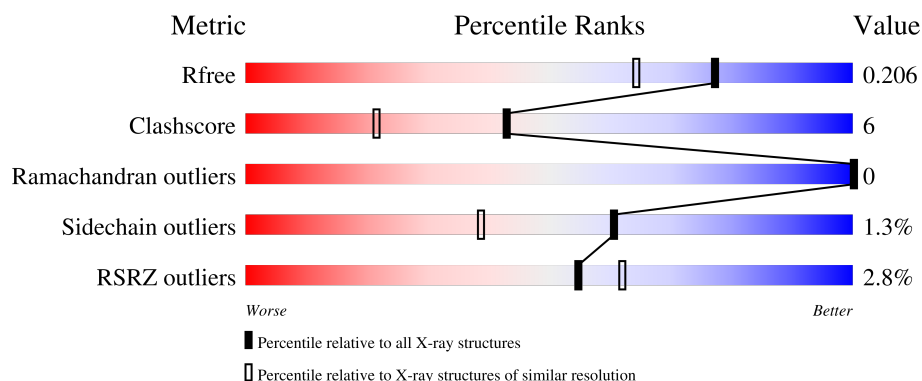
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	% 81% 14% . .
1	B	342	3% 82% 13% . .
1	C	342	5% 77% 16% . 6%
1	D	342	% 79% 16% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10773 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 D-cysteine desulfhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	6	0
			2472	1578	417	468	9			
1	B	328	Total	C	N	O	S	0	1	0
			2427	1549	411	458	9			
1	C	322	Total	C	N	O	S	0	4	0
			2411	1538	407	456	10			
1	D	328	Total	C	N	O	S	3	4	0
			2461	1573	416	463	9			

There are 56 discrepancies between the modelled and reference sequences:

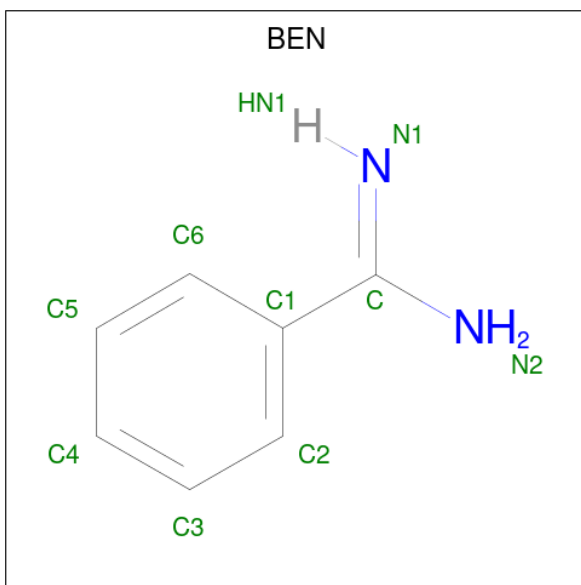
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8ZNT7
A	-12	ARG	-	expression tag	UNP Q8ZNT7
A	-11	GLY	-	expression tag	UNP Q8ZNT7
A	-10	SER	-	expression tag	UNP Q8ZNT7
A	-9	HIS	-	expression tag	UNP Q8ZNT7
A	-8	HIS	-	expression tag	UNP Q8ZNT7
A	-7	HIS	-	expression tag	UNP Q8ZNT7
A	-6	HIS	-	expression tag	UNP Q8ZNT7
A	-5	HIS	-	expression tag	UNP Q8ZNT7
A	-4	HIS	-	expression tag	UNP Q8ZNT7
A	-3	GLY	-	expression tag	UNP Q8ZNT7
A	-2	MET	-	expression tag	UNP Q8ZNT7
A	-1	ALA	-	expression tag	UNP Q8ZNT7
A	0	SER	-	expression tag	UNP Q8ZNT7
B	-13	MET	-	expression tag	UNP Q8ZNT7
B	-12	ARG	-	expression tag	UNP Q8ZNT7
B	-11	GLY	-	expression tag	UNP Q8ZNT7
B	-10	SER	-	expression tag	UNP Q8ZNT7
B	-9	HIS	-	expression tag	UNP Q8ZNT7
B	-8	HIS	-	expression tag	UNP Q8ZNT7
B	-7	HIS	-	expression tag	UNP Q8ZNT7

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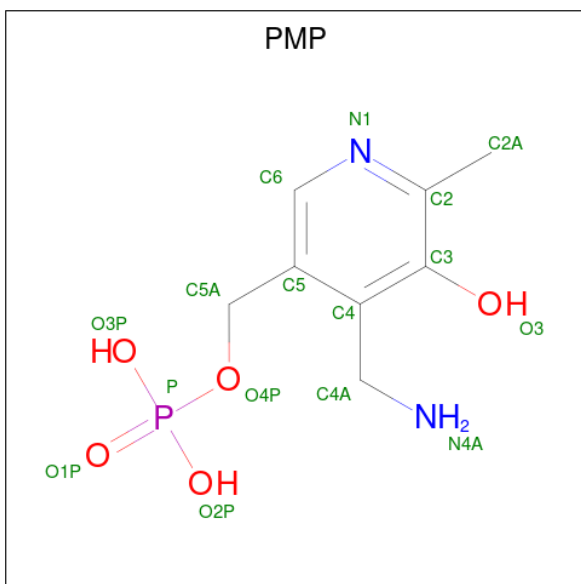
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q8ZNT7
B	-5	HIS	-	expression tag	UNP Q8ZNT7
B	-4	HIS	-	expression tag	UNP Q8ZNT7
B	-3	GLY	-	expression tag	UNP Q8ZNT7
B	-2	MET	-	expression tag	UNP Q8ZNT7
B	-1	ALA	-	expression tag	UNP Q8ZNT7
B	0	SER	-	expression tag	UNP Q8ZNT7
C	-13	MET	-	expression tag	UNP Q8ZNT7
C	-12	ARG	-	expression tag	UNP Q8ZNT7
C	-11	GLY	-	expression tag	UNP Q8ZNT7
C	-10	SER	-	expression tag	UNP Q8ZNT7
C	-9	HIS	-	expression tag	UNP Q8ZNT7
C	-8	HIS	-	expression tag	UNP Q8ZNT7
C	-7	HIS	-	expression tag	UNP Q8ZNT7
C	-6	HIS	-	expression tag	UNP Q8ZNT7
C	-5	HIS	-	expression tag	UNP Q8ZNT7
C	-4	HIS	-	expression tag	UNP Q8ZNT7
C	-3	GLY	-	expression tag	UNP Q8ZNT7
C	-2	MET	-	expression tag	UNP Q8ZNT7
C	-1	ALA	-	expression tag	UNP Q8ZNT7
C	0	SER	-	expression tag	UNP Q8ZNT7
D	-13	MET	-	expression tag	UNP Q8ZNT7
D	-12	ARG	-	expression tag	UNP Q8ZNT7
D	-11	GLY	-	expression tag	UNP Q8ZNT7
D	-10	SER	-	expression tag	UNP Q8ZNT7
D	-9	HIS	-	expression tag	UNP Q8ZNT7
D	-8	HIS	-	expression tag	UNP Q8ZNT7
D	-7	HIS	-	expression tag	UNP Q8ZNT7
D	-6	HIS	-	expression tag	UNP Q8ZNT7
D	-5	HIS	-	expression tag	UNP Q8ZNT7
D	-4	HIS	-	expression tag	UNP Q8ZNT7
D	-3	GLY	-	expression tag	UNP Q8ZNT7
D	-2	MET	-	expression tag	UNP Q8ZNT7
D	-1	ALA	-	expression tag	UNP Q8ZNT7
D	0	SER	-	expression tag	UNP Q8ZNT7

- Molecule 2 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



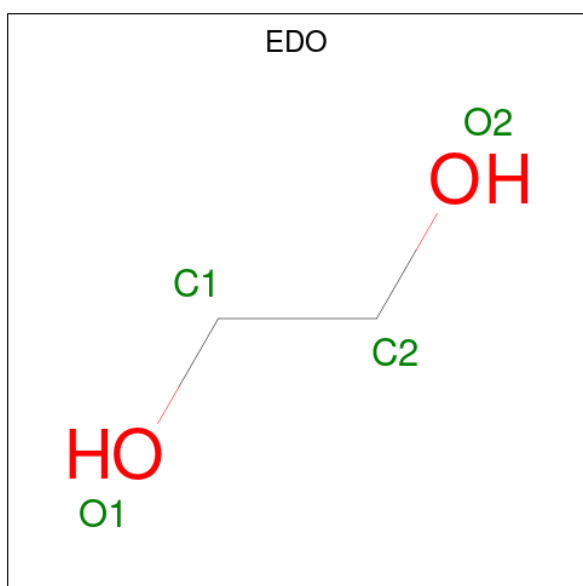
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			9	7	2		
2	C	1	Total	C	N	0	0
			9	7	2		
2	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



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

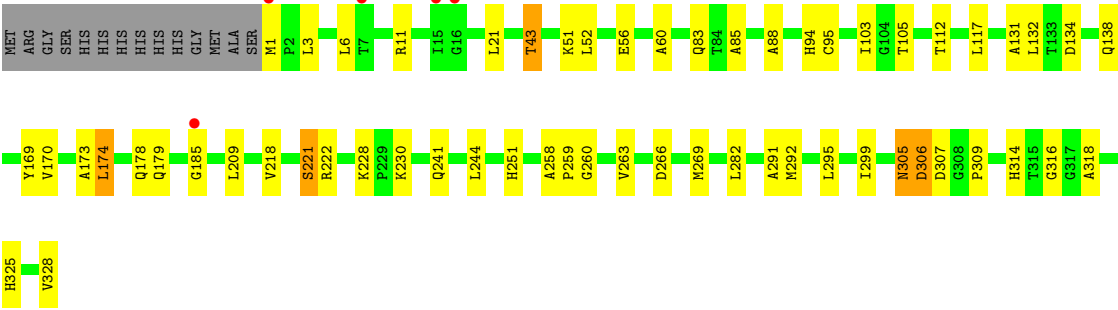
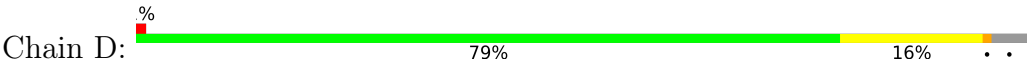
- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	256	Total 256	O 256	0	0
5	B	191	Total 191	O 191	0	0
5	C	192	Total 192	O 192	0	0
5	D	248	Total 248	O 248	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.32Å 164.93Å 68.31Å 90.00° 118.97° 90.00°	Depositor
Resolution (Å)	39.91 – 1.67 39.91 – 1.67	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.91-1.67) 97.5 (39.91-1.67)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.171 , 0.206 0.172 , 0.206	Depositor DCC
R_{free} test set	7377 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.023 for -h-l,-k,l 0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10773	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, EDO, BEN

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	1.58	16/2539 (0.6%)	1.31	13/3461 (0.4%)
1	B	1.56	15/2477 (0.6%)	1.31	9/3379 (0.3%)
1	C	1.57	20/2465 (0.8%)	1.34	10/3358 (0.3%)
1	D	1.58	11/2517 (0.4%)	1.35	13/3429 (0.4%)
All	All	1.57	62/9998 (0.6%)	1.33	45/13627 (0.3%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	ILE	C-O	-9.72	1.13	1.24
1	D	318	ALA	C-O	-7.35	1.17	1.24
1	D	43	THR	CA-C	7.03	1.60	1.53
1	A	318	ALA	CA-CB	6.85	1.64	1.54
1	C	198	THR	CA-CB	6.74	1.63	1.53
1	C	294	GLY	N-CA	6.72	1.54	1.45
1	A	85	ALA	CA-CB	-6.59	1.43	1.53
1	A	113	ASN	N-CA	6.57	1.54	1.45
1	D	131	ALA	CA-CB	6.57	1.64	1.53
1	C	190	VAL	N-CA	-6.42	1.38	1.46
1	A	108[A]	GLU	C-O	-6.41	1.16	1.24
1	A	108[B]	GLU	C-O	-6.41	1.16	1.24
1	B	107	ALA	N-CA	6.40	1.53	1.46
1	D	88	ALA	N-CA	6.21	1.53	1.46
1	C	37	ILE	CA-CB	6.18	1.63	1.54
1	C	72	THR	C-O	6.18	1.31	1.23
1	A	49	GLY	N-CA	6.12	1.53	1.45
1	B	33	ARG	C-O	-6.12	1.16	1.23
1	C	213	VAL	CA-CB	6.07	1.62	1.54
1	A	49	GLY	C-O	6.02	1.29	1.23
1	D	258	ALA	CA-C	-6.00	1.46	1.53
1	A	158	VAL	C-O	5.99	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	ARG	C-O	-5.93	1.16	1.23
1	B	72	THR	C-O	-5.89	1.16	1.23
1	A	162	SER	C-O	5.82	1.31	1.23
1	B	236	GLN	N-CA	5.78	1.53	1.46
1	C	290	LYS	N-CA	5.73	1.53	1.46
1	C	88	ALA	N-CA	5.70	1.53	1.46
1	C	134	ASP	C-O	5.63	1.30	1.24
1	B	74	GLY	C-O	-5.61	1.16	1.23
1	A	28	SER	N-CA	5.53	1.53	1.46
1	B	73	ALA	C-O	-5.50	1.17	1.23
1	D	260	GLY	N-CA	5.50	1.51	1.45
1	A	89	ALA	CA-CB	-5.48	1.44	1.53
1	A	84	THR	C-O	5.47	1.30	1.24
1	B	200	ALA	N-CA	5.42	1.52	1.46
1	C	192	ALA	CA-CB	5.39	1.62	1.53
1	C	248	ALA	C-O	5.38	1.30	1.23
1	C	55	LEU	C-O	-5.38	1.17	1.24
1	D	60	ALA	N-CA	5.38	1.52	1.46
1	D	85	ALA	C-O	5.34	1.30	1.24
1	D	241	GLN	N-CA	5.32	1.52	1.46
1	B	26	ARG	C-O	-5.28	1.18	1.24
1	A	165	GLY	N-CA	5.28	1.52	1.45
1	C	126	ILE	CA-CB	5.25	1.60	1.54
1	C	103	ILE	N-CA	5.25	1.51	1.46
1	C	238	ILE	CA-CB	5.22	1.60	1.54
1	A	191	VAL	C-O	5.21	1.29	1.23
1	C	69	THR	CA-C	5.18	1.58	1.52
1	C	68	ASP	C-O	-5.17	1.17	1.24
1	B	131	ALA	CA-CB	5.16	1.62	1.53
1	D	269	MET	C-O	-5.13	1.18	1.24
1	B	43	THR	C-O	-5.12	1.18	1.24
1	C	81	VAL	CA-CB	-5.11	1.48	1.54
1	B	240	GLY	N-CA	5.09	1.52	1.45
1	A	314	HIS	CA-CB	5.06	1.59	1.52
1	C	263	VAL	CA-C	5.06	1.57	1.52
1	A	155	VAL	CA-CB	5.05	1.60	1.54
1	B	271	ALA	C-O	-5.04	1.18	1.24
1	D	221	SER	C-O	5.04	1.29	1.23
1	C	96	VAL	CA-CB	5.03	1.61	1.54
1	B	37	ILE	CA-CB	5.01	1.61	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	MET	CA-C-N	-8.13	110.58	119.19
1	D	1	MET	C-N-CA	-8.13	110.58	119.19
1	D	43	THR	CB-CA-C	6.71	120.13	109.52
1	C	43	THR	CA-C-N	6.29	126.42	119.87
1	C	43	THR	C-N-CA	6.29	126.42	119.87
1	D	170	VAL	N-CA-C	-6.08	104.58	110.72
1	B	169	TYR	CA-CB-CG	-5.96	103.16	113.90
1	B	307	ASP	CB-CA-C	-5.96	100.17	110.72
1	A	4	HIS	N-CA-C	5.86	119.24	111.75
1	B	1	MET	CA-C-N	-5.79	113.79	120.04
1	B	1	MET	C-N-CA	-5.79	113.79	120.04
1	C	306	ASP	N-CA-C	5.70	115.54	108.19
1	D	266	ASP	N-CA-C	5.68	117.47	111.28
1	C	235	GLN	N-CA-C	-5.61	105.16	111.28
1	A	239	ALA	CA-C-N	5.46	126.16	119.99
1	A	239	ALA	C-N-CA	5.46	126.16	119.99
1	C	62	ALA	N-CA-C	-5.41	105.38	111.28
1	C	155	VAL	CA-C-N	-5.38	118.65	123.33
1	C	155	VAL	C-N-CA	-5.38	118.65	123.33
1	B	196	ALA	N-CA-CB	-5.38	108.72	114.10
1	A	44	PRO	CA-C-N	-5.38	116.16	122.93
1	A	44	PRO	C-N-CA	-5.38	116.16	122.93
1	C	293	ALA	N-CA-C	-5.36	105.44	111.28
1	B	222	ARG	N-CA-C	5.30	117.24	109.24
1	D	307	ASP	CB-CA-C	-5.24	100.15	110.11
1	A	183	VAL	CB-CA-C	-5.21	106.49	111.44
1	A	64	ARG	N-CA-C	-5.21	105.78	111.82
1	A	169	TYR	CA-CB-CG	-5.19	104.56	113.90
1	D	173	ALA	N-CA-C	5.18	117.60	111.33
1	D	299	ILE	CA-C-O	-5.17	115.37	120.85
1	A	43	THR	CA-C-N	5.12	126.05	120.83
1	A	43	THR	C-N-CA	5.12	126.05	120.83
1	A	45	ILE	N-CA-C	5.08	115.62	108.36
1	D	228	LYS	O-C-N	5.07	125.48	120.71
1	B	263	VAL	CA-C-O	5.05	124.46	119.62
1	B	266	ASP	N-CA-C	5.04	116.77	111.28
1	D	169	TYR	CA-CB-CG	-5.03	104.84	113.90
1	B	145	ARG	N-CA-CB	5.03	117.46	109.82
1	A	317	GLY	N-CA-C	5.03	121.45	114.92
1	D	179	GLN	N-CA-C	5.02	117.65	111.82
1	D	292	MET	N-CA-C	-5.02	106.00	111.82
1	C	239	ALA	CA-C-N	5.02	125.51	119.94
1	C	239	ALA	C-N-CA	5.02	125.51	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	ASP	O-C-N	5.02	128.79	122.92
1	A	170	VAL	N-CA-C	-5.01	105.66	110.72

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	2472	0	2486	32	0
1	B	2427	0	2436	22	0
1	C	2411	0	2428	31	0
1	D	2461	0	2482	44	0
2	A	9	0	7	0	0
2	C	9	0	7	1	0
2	D	9	0	7	0	0
3	A	16	0	10	0	0
3	B	16	0	10	1	0
3	C	16	0	10	0	0
3	D	16	0	10	0	0
4	A	8	0	12	0	0
4	B	8	0	12	4	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	256	0	0	7	0
5	B	191	0	0	4	0
5	C	192	0	0	6	0
5	D	248	0	0	7	0
All	All	10773	0	9929	123	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 6.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD23	1:B:244:LEU:HD11	1.31	1.12
1:D:105:THR:OG1	1:D:328[A]:VAL:HG12	1.54	1.06
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.64	0.96
1:B:152:ARG:HH11	1:B:152:ARG:HB3	1.34	0.93
1:D:178:GLN:HG3	5:D:748:HOH:O	1.73	0.89
1:C:167[B]:MET:HE1	1:C:242:LEU:HD11	1.55	0.87
1:A:145:ARG:HH12	1:C:328[A]:VAL:HG21	1.40	0.85
1:B:3:LEU:CD2	1:B:244:LEU:HD11	2.06	0.84
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.44	0.83
1:C:325:HIS:HD2	5:C:622:HOH:O	1.65	0.78
1:D:251:HIS:HE1	5:D:691:HOH:O	1.74	0.70
1:A:325:HIS:HD2	5:A:689:HOH:O	1.74	0.69
1:D:305:ASN:ND2	5:D:732:HOH:O	2.26	0.69
1:C:251:HIS:HE1	5:C:686:HOH:O	1.75	0.69
1:D:305:ASN:OD1	1:D:306:ASP:N	2.26	0.69
1:B:314:HIS:CD2	1:B:316:GLY:H	2.11	0.68
4:B:403:EDO:H22	5:B:684:HOH:O	1.93	0.67
1:A:251:HIS:HE1	5:A:694:HOH:O	1.76	0.67
1:A:208[A]:HIS:HD2	5:A:754:HOH:O	1.77	0.67
1:D:185:GLY:O	1:D:309:PRO:HD2	1.96	0.66
1:B:314:HIS:HD2	1:B:316:GLY:H	1.41	0.66
1:A:314:HIS:HD2	1:A:316:GLY:H	1.44	0.66
1:C:300:SER:CB	5:C:676:HOH:O	2.42	0.66
1:D:117:LEU:C	1:D:117:LEU:HD23	2.21	0.65
1:B:208:HIS:HE1	1:B:245:THR:O	1.79	0.65
1:B:325:HIS:HD2	5:B:639:HOH:O	1.79	0.65
1:B:152:ARG:HB3	1:B:152:ARG:NH1	2.11	0.64
1:A:145:ARG:NH1	1:C:328[A]:VAL:HG11	2.13	0.64
1:C:105:THR:HG1	1:C:328[A]:VAL:HG12	1.61	0.63
1:C:300:SER:HB2	5:C:676:HOH:O	1.98	0.62
1:D:222:ARG:NH2	1:D:230[B]:LYS:HE2	2.15	0.61
1:B:134:ASP:H	1:B:138:GLN:NE2	1.99	0.60
1:C:66:GLY:O	1:C:152:ARG:HD3	2.02	0.60
1:B:52:LEU:HG	1:B:83:GLN:HE21	1.67	0.59
1:D:134:ASP:H	1:D:138:GLN:NE2	1.99	0.58
1:A:145:ARG:NH1	1:C:328[A]:VAL:HG21	2.15	0.58
1:A:314:HIS:CD2	1:A:316:GLY:H	2.21	0.58
1:D:305:ASN:CG	5:D:732:HOH:O	2.45	0.58
1:C:314:HIS:HD2	1:C:316:GLY:H	1.50	0.57
1:D:314:HIS:HD2	1:D:316:GLY:H	1.53	0.57
1:D:134:ASP:H	1:D:138:GLN:HE21	1.53	0.56
1:D:11:ARG:NH1	1:D:56:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLN:CG	5:D:748:HOH:O	2.41	0.56
1:A:117:LEU:HD12	5:A:736:HOH:O	2.06	0.56
4:B:403:EDO:H12	1:D:94:HIS:CD2	2.41	0.55
1:D:174:LEU:HD13	1:D:209:LEU:HD11	1.88	0.55
1:A:149:GLN:HE22	1:C:328[A]:VAL:HG22	1.72	0.55
1:D:103:ILE:CD1	1:D:328[B]:VAL:HG21	2.38	0.54
1:C:147:GLU:HG2	1:C:153:PRO:HD2	1.90	0.53
5:A:652:HOH:O	1:C:327:HIS:HD2	1.91	0.53
1:A:302:LYS:HE3	5:A:755:HOH:O	2.08	0.53
1:D:103:ILE:HD11	1:D:328[B]:VAL:HG21	1.91	0.52
1:C:216:ILE:HD13	1:C:304:PHE:CE1	2.45	0.52
1:D:52:LEU:HG	1:D:83:GLN:HE21	1.74	0.52
1:C:300:SER:OG	2:C:401:BEN:H6	2.10	0.52
1:D:314:HIS:CD2	1:D:316:GLY:H	2.28	0.52
1:B:26:ARG:HD3	1:B:278:LEU:O	2.09	0.52
1:D:132:LEU:HA	1:D:138:GLN:HE22	1.75	0.51
1:C:52:LEU:HG	1:C:83:GLN:HE21	1.75	0.51
1:C:105:THR:OG1	1:C:328[A]:VAL:CG1	2.47	0.51
1:A:325:HIS:HE1	1:B:112:THR:OG1	1.93	0.51
1:C:325:HIS:HE1	1:D:112:THR:OG1	1.94	0.51
1:B:282:LEU:O	1:B:314:HIS:HE1	1.93	0.50
1:A:134:ASP:H	1:A:138:GLN:HE21	1.58	0.50
1:D:51:LYS:H	1:D:83:GLN:HE22	1.58	0.50
1:D:221:SER:C	1:D:222:ARG:HG3	2.36	0.50
1:A:145:ARG:HG2	1:A:145:ARG:NH1	2.20	0.50
1:C:7:THR:HG23	1:C:167[B]:MET:HE2	1.93	0.50
1:B:295:LEU:C	1:B:295:LEU:HD23	2.36	0.49
1:A:52:LEU:HG	1:A:83:GLN:HE21	1.78	0.49
4:B:403:EDO:H12	1:D:94:HIS:CG	2.47	0.49
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.96	0.49
1:C:314:HIS:CD2	1:C:316:GLY:H	2.29	0.49
1:A:50:ASN:H	1:A:50:ASN:HD22	1.60	0.48
4:B:403:EDO:H21	5:B:598:HOH:O	2.12	0.48
1:A:134:ASP:H	1:A:138:GLN:NE2	2.12	0.48
1:D:43:THR:OG1	1:D:52:LEU:HD12	2.14	0.48
1:D:282:LEU:O	1:D:314:HIS:HE1	1.97	0.48
1:B:134:ASP:H	1:B:138:GLN:HE21	1.61	0.48
1:D:251:HIS:HD2	5:D:690:HOH:O	1.97	0.48
1:D:21:LEU:HD23	1:D:21:LEU:C	2.39	0.47
1:A:51:LYS:H	1:A:83:GLN:HE22	1.61	0.47
1:A:112:THR:OG1	1:B:325:HIS:HE1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:VAL:HG13	1:C:125:GLN:HG2	1.95	0.46
1:D:259:PRO:HG2	1:D:263:VAL:HG11	1.98	0.46
1:B:152:ARG:HH11	1:B:152:ARG:CB	2.18	0.46
1:B:5:HIS:HB2	5:B:676:HOH:O	2.15	0.46
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.80	0.46
1:C:272:VAL:HG22	1:C:283:LEU:HB2	1.98	0.45
1:D:105:THR:HG1	1:D:328[A]:VAL:HG12	1.75	0.45
1:D:174:LEU:O	1:D:178:GLN:HG3	2.17	0.45
1:A:282:LEU:O	1:A:314:HIS:HE1	2.00	0.45
1:A:50:ASN:HD22	1:A:50:ASN:N	2.15	0.45
1:D:295:LEU:C	1:D:295:LEU:HD23	2.41	0.44
1:C:155:VAL:O	5:C:664:HOH:O	2.21	0.44
1:C:43:THR:OG1	1:C:52:LEU:HD12	2.18	0.44
1:C:142:LEU:O	1:C:146:ILE:HG12	2.18	0.44
3:B:401:PMP:O3	3:B:401:PMP:N4A	2.51	0.44
1:D:305:ASN:OD1	1:D:305:ASN:C	2.61	0.44
1:D:105:THR:CB	1:D:328[A]:VAL:HG12	2.45	0.43
1:A:325:HIS:CD2	1:A:326:PRO:HA	2.53	0.43
1:C:295:LEU:HD23	1:C:295:LEU:C	2.43	0.43
1:B:189:VAL:HG23	1:B:213:VAL:HG11	2.01	0.42
1:D:105:THR:HB	1:D:328[B]:VAL:HG22	2.00	0.42
1:A:302:LYS:CE	5:A:755:HOH:O	2.67	0.42
1:B:144:THR:O	1:B:145:ARG:C	2.62	0.42
1:A:94:HIS:HD2	5:C:512:HOH:O	2.01	0.42
1:B:39:ARG:O	1:B:42:VAL:HG22	2.20	0.42
1:A:94:HIS:HE1	1:A:125:GLN:NE2	2.18	0.42
1:A:145:ARG:HH12	1:C:328[A]:VAL:CG2	2.22	0.42
1:D:94:HIS:CD2	1:D:95:CYS:H	2.38	0.42
1:D:230[B]:LYS:HB3	1:D:230[B]:LYS:HE3	1.90	0.42
1:D:305:ASN:CG	1:D:306:ASP:N	2.78	0.42
1:D:51:LYS:HD3	1:D:51:LYS:HA	1.88	0.41
1:A:218:VAL:HG11	1:A:291:ALA:HA	2.01	0.41
1:D:218:VAL:HG11	1:D:291:ALA:HA	2.03	0.41
1:B:2:PRO:O	1:B:244:LEU:HD21	2.20	0.41
1:D:94:HIS:HD2	5:D:538:HOH:O	2.02	0.41
1:C:26:ARG:HD3	1:C:278:LEU:O	2.21	0.40
1:D:3:LEU:HD23	1:D:244:LEU:HD11	2.02	0.40
1:A:33:ARG:HD3	1:A:308:GLY:O	2.22	0.40
1:A:15:ILE:CD1	1:A:53:ARG:HG2	2.52	0.40
1:A:217:GLY:O	1:A:252:LEU:HA	2.22	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	332/342 (97%)	321 (97%)	11 (3%)	0	100	100
1	B	327/342 (96%)	314 (96%)	13 (4%)	0	100	100
1	C	323/342 (94%)	311 (96%)	12 (4%)	0	100	100
1	D	329/342 (96%)	320 (97%)	9 (3%)	0	100	100
All	All	1311/1368 (96%)	1266 (97%)	45 (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	257/267 (96%)	255 (99%)	2 (1%)	73	59
1	B	250/267 (94%)	244 (98%)	6 (2%)	43	17
1	C	250/267 (94%)	248 (99%)	2 (1%)	73	59
1	D	254/267 (95%)	251 (99%)	3 (1%)	63	43
All	All	1011/1068 (95%)	998 (99%)	13 (1%)	61	39

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	145	ARG

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Mol	Chain	Res	Type
1	B	7	THR
1	B	33	ARG
1	B	152	ARG
1	B	184	VAL
1	B	216	ILE
1	B	305	ASN
1	C	171	GLU
1	C	230	LYS
1	D	6	LEU
1	D	174	LEU
1	D	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	5	HIS
1	A	50	ASN
1	A	80	HIS
1	A	83	GLN
1	A	94	HIS
1	A	138	GLN
1	A	140	GLN
1	A	149	GLN
1	A	251	HIS
1	A	314	HIS
1	A	325	HIS
1	B	80	HIS
1	B	83	GLN
1	B	138	GLN
1	B	208	HIS
1	B	301	GLN
1	B	305	ASN
1	B	314	HIS
1	B	325	HIS
1	C	80	HIS
1	C	83	GLN
1	C	138	GLN
1	C	251	HIS
1	C	314	HIS
1	C	325	HIS
1	C	327	HIS

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Mol	Chain	Res	Type
1	D	5	HIS
1	D	80	HIS
1	D	83	GLN
1	D	94	HIS
1	D	138	GLN
1	D	140	GLN
1	D	149	GLN
1	D	208	HIS
1	D	251	HIS
1	D	301	GLN
1	D	314	HIS
1	D	325	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	PMP	B	401	-	16,16,16	2.15	5 (31%)	22,23,23	2.64	10 (45%)
4	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PMP	D	402	-	16,16,16	1.13	1 (6%)	22,23,23	1.20	2 (9%)
4	EDO	A	403	-	3,3,3	0.60	0	2,2,2	0.14	0
4	EDO	C	403	-	3,3,3	0.74	0	2,2,2	0.91	0
2	BEN	A	401	-	9,9,9	2.60	4 (44%)	7,11,11	2.07	3 (42%)
4	EDO	A	404	-	3,3,3	0.82	0	2,2,2	1.09	0
4	EDO	B	403	-	3,3,3	0.24	0	2,2,2	0.28	0
3	PMP	A	402	-	16,16,16	0.97	1 (6%)	22,23,23	2.15	5 (22%)
4	EDO	D	403	-	3,3,3	1.17	0	2,2,2	0.95	0
2	BEN	C	401	-	9,9,9	1.20	1 (11%)	7,11,11	2.40	2 (28%)
2	BEN	D	401	-	9,9,9	2.20	3 (33%)	7,11,11	2.92	5 (71%)
3	PMP	C	402	-	16,16,16	2.06	4 (25%)	22,23,23	2.91	9 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	B	401	-	-	1/8/8/8	0/1/1/1
4	EDO	B	402	-	-	0/1/1/1	-
3	PMP	D	402	-	-	1/8/8/8	0/1/1/1
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
2	BEN	A	401	-	-	0/4/4/4	0/1/1/1
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
3	PMP	A	402	-	-	2/8/8/8	0/1/1/1
4	EDO	D	403	-	-	0/1/1/1	-
2	BEN	C	401	-	-	0/4/4/4	0/1/1/1
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1
3	PMP	C	402	-	-	1/8/8/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PMP	C3-C4	5.86	1.48	1.40
3	B	401	PMP	C3-C2	-4.71	1.36	1.41
2	D	401	BEN	C3-C2	4.62	1.46	1.38
2	A	401	BEN	C6-C1	4.40	1.46	1.39
2	A	401	BEN	C3-C2	3.66	1.45	1.38
3	B	401	PMP	C3-C4	3.63	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	BEN	C4-C3	3.54	1.46	1.38
3	B	401	PMP	C6-N1	3.39	1.41	1.34
3	C	402	PMP	C6-N1	3.27	1.41	1.34
2	A	401	BEN	C5-C6	2.62	1.43	1.38
3	B	401	PMP	O3-C3	-2.53	1.31	1.36
2	D	401	BEN	C4-C3	2.52	1.43	1.38
3	C	402	PMP	C2-N1	2.49	1.38	1.33
2	C	401	BEN	C1-C	-2.37	1.42	1.47
2	D	401	BEN	C1-C	-2.35	1.42	1.47
3	B	401	PMP	P-O4P	2.29	1.67	1.60
3	A	402	PMP	O3-C3	-2.29	1.31	1.36
3	C	402	PMP	P-O3P	-2.14	1.46	1.54
3	D	402	PMP	P-O2P	-2.10	1.47	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PMP	C6-C5-C4	8.94	124.82	118.06
3	B	401	PMP	C6-C5-C4	7.32	123.60	118.06
3	A	402	PMP	C6-C5-C4	6.99	123.35	118.06
2	C	401	BEN	C1-C-N2	5.52	126.39	118.01
3	B	401	PMP	O3-C3-C2	4.84	127.61	117.58
3	C	402	PMP	C5-C6-N1	-4.59	116.36	123.83
2	D	401	BEN	C5-C6-C1	-4.50	115.94	120.36
3	C	402	PMP	C5A-C5-C6	-4.49	112.04	119.36
3	C	402	PMP	O3-C3-C2	4.25	126.39	117.58
2	D	401	BEN	C4-C5-C6	4.22	125.45	120.24
3	B	401	PMP	C5-C6-N1	-3.90	117.48	123.83
3	A	402	PMP	C3-C4-C5	-3.73	115.34	118.73
3	A	402	PMP	C5-C6-N1	-3.71	117.79	123.83
3	B	401	PMP	C3-C2-N1	3.60	125.50	120.96
2	A	401	BEN	C5-C6-C1	-3.36	117.06	120.36
3	B	401	PMP	O4P-C5A-C5	-2.91	103.91	109.36
3	C	402	PMP	C4-C3-C2	-2.85	115.60	119.91
2	D	401	BEN	C6-C1-C2	2.81	122.14	118.57
3	D	402	PMP	C4A-C4-C3	2.68	124.76	120.22
2	D	401	BEN	C4-C3-C2	-2.43	117.24	120.24
3	C	402	PMP	O3P-P-O2P	2.42	116.88	107.80
3	B	401	PMP	O3P-P-O2P	2.38	116.73	107.80
2	D	401	BEN	C1-C-N2	2.34	121.57	118.01
2	A	401	BEN	C4-C5-C6	2.33	123.11	120.24
3	C	402	PMP	C3-C2-N1	2.32	123.89	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PMP	C4A-C4-C3	2.29	124.11	120.22
3	A	402	PMP	C5A-C5-C6	-2.29	115.63	119.36
3	B	401	PMP	O2P-P-O4P	2.25	112.55	106.67
3	D	402	PMP	C4A-C4-C5	-2.25	115.75	120.27
3	B	401	PMP	C4-C3-C2	-2.22	116.56	119.91
3	A	402	PMP	C6-N1-C2	2.19	123.17	119.20
2	A	401	BEN	C4-C3-C2	-2.10	117.65	120.24
2	C	401	BEN	C5-C6-C1	2.07	122.40	120.36
3	B	401	PMP	C2A-C2-N1	-2.06	113.76	117.64
3	C	402	PMP	C2A-C2-N1	-2.04	113.81	117.64
3	B	401	PMP	C3-C4-C5	-2.02	116.90	118.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PMP	C3-C4-C4A-N4A
3	B	401	PMP	C3-C4-C4A-N4A
3	C	402	PMP	C3-C4-C4A-N4A
3	D	402	PMP	C3-C4-C4A-N4A
3	A	402	PMP	C5-C4-C4A-N4A
4	A	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	PMP	1	0
4	B	403	EDO	4	0
2	C	401	BEN	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, 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	328/342 (95%)	-0.35	5 (1%) 72 80	11, 16, 33, 44	6 (1%)
1	B	328/342 (95%)	0.01	10 (3%) 52 59	13, 20, 42, 52	1 (0%)
1	C	322/342 (94%)	0.33	17 (5%) 32 40	9, 23, 40, 52	4 (1%)
1	D	328/342 (95%)	-0.35	5 (1%) 72 80	10, 16, 34, 42	5 (1%)
All	All	1306/1368 (95%)	-0.09	37 (2%) 55 62	9, 19, 38, 52	16 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.0
1	C	148	ALA	3.9
1	A	1	MET	3.9
1	B	148	ALA	3.6
1	D	15	ILE	3.5
1	B	181	GLU	3.4
1	B	184	VAL	3.3
1	B	305	ASN	3.2
1	C	8	ARG	3.2
1	C	141	THR	2.9
1	C	213	VAL	2.9
1	C	184	VAL	2.8
1	D	7	THR	2.8
1	C	211	PRO	2.8
1	B	2	PRO	2.7
1	C	142	LEU	2.7
1	B	245	THR	2.7
1	C	212	ASP	2.6
1	C	133	THR	2.5
1	C	7	THR	2.5
1	C	143	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	2.5
1	D	16	GLY	2.4
1	C	149	GLN	2.4
1	C	150	GLY	2.3
1	A	307	ASP	2.3
1	D	1	MET	2.3
1	C	183	VAL	2.3
1	A	4	HIS	2.2
1	C	246	ALA	2.2
1	A	7	THR	2.2
1	B	149	GLN	2.2
1	C	94[A]	HIS	2.2
1	A	183	VAL	2.1
1	C	208	HIS	2.1
1	D	185	GLY	2.1
1	B	307	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	D	403	4/4	0.84	0.13	23,27,32,32	0
4	EDO	A	403	4/4	0.87	0.12	36,37,40,41	0
4	EDO	B	403	4/4	0.89	0.17	24,30,30,33	0
4	EDO	C	403	4/4	0.91	0.10	28,28,30,30	0
4	EDO	B	402	4/4	0.91	0.10	29,33,35,35	0
2	BEN	C	401	9/9	0.93	0.08	27,31,34,36	0
4	EDO	A	404	4/4	0.94	0.10	25,28,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BEN	A	401	9/9	0.95	0.06	14,15,17,18	0
2	BEN	D	401	9/9	0.97	0.05	13,14,16,17	0
3	PMP	C	402	16/16	0.97	0.06	14,18,22,23	0
3	PMP	B	401	16/16	0.99	0.04	11,15,20,22	0
3	PMP	A	402	16/16	0.99	0.04	11,13,17,22	0
3	PMP	D	402	16/16	0.99	0.03	11,13,16,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.