



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:56 AM UTC

PDB ID : 4E3Q / pdb_00004e3q
Title : PMP-bound form of Aminotransferase crystal structure from *Vibrio fluvialis*
Authors : Midelfort, K.S.; Kumar, R.; Han, S.; Karmilowicz, M.J.; McConnell, K.; Gehlhaar, D.K.; Mistry, A.; Chang, J.S.; Anderson, M.; Vilalobos, A.; Minshull, J.; Govindarajan, S.; Wong, J.W.
Deposited on : 2012-03-10
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

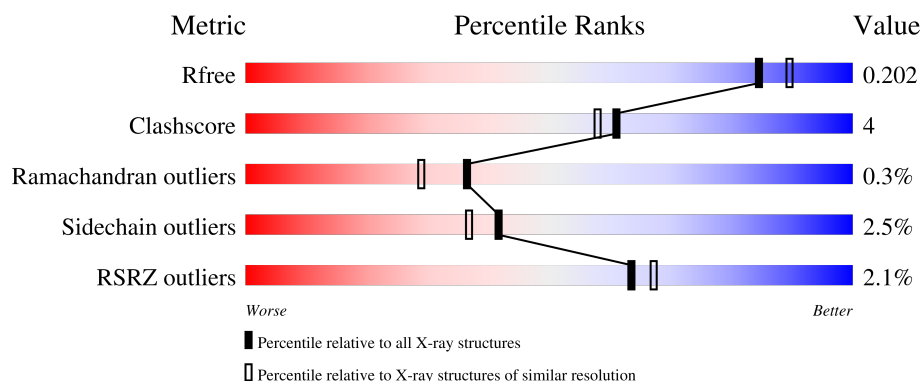
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	473	2% 84% 10% • •
1	B	473	% 85% 10% • 5%
1	C	473	3% 85% 9% • 5%
1	D	473	2% 84% 10% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15466 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 Pyruvate transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	Se	0	0	0
			3522	2252	599	651	7	13			
1	B	450	Total	C	N	O	S	Se	0	0	0
			3505	2242	595	648	7	13			
1	C	451	Total	C	N	O	S	Se	0	0	0
			3517	2249	598	650	7	13			
1	D	452	Total	C	N	O	S	Se	0	0	0
			3522	2252	599	651	7	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP F2XBU9
A	-18	GLY	-	expression tag	UNP F2XBU9
A	-17	SER	-	expression tag	UNP F2XBU9
A	-16	SER	-	expression tag	UNP F2XBU9
A	-15	HIS	-	expression tag	UNP F2XBU9
A	-14	HIS	-	expression tag	UNP F2XBU9
A	-13	HIS	-	expression tag	UNP F2XBU9
A	-12	HIS	-	expression tag	UNP F2XBU9
A	-11	HIS	-	expression tag	UNP F2XBU9
A	-10	HIS	-	expression tag	UNP F2XBU9
A	-9	SER	-	expression tag	UNP F2XBU9
A	-8	SER	-	expression tag	UNP F2XBU9
A	-7	GLY	-	expression tag	UNP F2XBU9
A	-6	LEU	-	expression tag	UNP F2XBU9
A	-5	VAL	-	expression tag	UNP F2XBU9
A	-4	PRO	-	expression tag	UNP F2XBU9
A	-3	ARG	-	expression tag	UNP F2XBU9
A	-2	GLY	-	expression tag	UNP F2XBU9
A	-1	SER	-	expression tag	UNP F2XBU9
A	0	HIS	-	expression tag	UNP F2XBU9
B	-19	MSE	-	expression tag	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP F2XBU9
B	-17	SER	-	expression tag	UNP F2XBU9
B	-16	SER	-	expression tag	UNP F2XBU9
B	-15	HIS	-	expression tag	UNP F2XBU9
B	-14	HIS	-	expression tag	UNP F2XBU9
B	-13	HIS	-	expression tag	UNP F2XBU9
B	-12	HIS	-	expression tag	UNP F2XBU9
B	-11	HIS	-	expression tag	UNP F2XBU9
B	-10	HIS	-	expression tag	UNP F2XBU9
B	-9	SER	-	expression tag	UNP F2XBU9
B	-8	SER	-	expression tag	UNP F2XBU9
B	-7	GLY	-	expression tag	UNP F2XBU9
B	-6	LEU	-	expression tag	UNP F2XBU9
B	-5	VAL	-	expression tag	UNP F2XBU9
B	-4	PRO	-	expression tag	UNP F2XBU9
B	-3	ARG	-	expression tag	UNP F2XBU9
B	-2	GLY	-	expression tag	UNP F2XBU9
B	-1	SER	-	expression tag	UNP F2XBU9
B	0	HIS	-	expression tag	UNP F2XBU9
C	-19	MSE	-	expression tag	UNP F2XBU9
C	-18	GLY	-	expression tag	UNP F2XBU9
C	-17	SER	-	expression tag	UNP F2XBU9
C	-16	SER	-	expression tag	UNP F2XBU9
C	-15	HIS	-	expression tag	UNP F2XBU9
C	-14	HIS	-	expression tag	UNP F2XBU9
C	-13	HIS	-	expression tag	UNP F2XBU9
C	-12	HIS	-	expression tag	UNP F2XBU9
C	-11	HIS	-	expression tag	UNP F2XBU9
C	-10	HIS	-	expression tag	UNP F2XBU9
C	-9	SER	-	expression tag	UNP F2XBU9
C	-8	SER	-	expression tag	UNP F2XBU9
C	-7	GLY	-	expression tag	UNP F2XBU9
C	-6	LEU	-	expression tag	UNP F2XBU9
C	-5	VAL	-	expression tag	UNP F2XBU9
C	-4	PRO	-	expression tag	UNP F2XBU9
C	-3	ARG	-	expression tag	UNP F2XBU9
C	-2	GLY	-	expression tag	UNP F2XBU9
C	-1	SER	-	expression tag	UNP F2XBU9
C	0	HIS	-	expression tag	UNP F2XBU9
D	-19	MSE	-	expression tag	UNP F2XBU9
D	-18	GLY	-	expression tag	UNP F2XBU9
D	-17	SER	-	expression tag	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP F2XBU9
D	-15	HIS	-	expression tag	UNP F2XBU9
D	-14	HIS	-	expression tag	UNP F2XBU9
D	-13	HIS	-	expression tag	UNP F2XBU9
D	-12	HIS	-	expression tag	UNP F2XBU9
D	-11	HIS	-	expression tag	UNP F2XBU9
D	-10	HIS	-	expression tag	UNP F2XBU9
D	-9	SER	-	expression tag	UNP F2XBU9
D	-8	SER	-	expression tag	UNP F2XBU9
D	-7	GLY	-	expression tag	UNP F2XBU9
D	-6	LEU	-	expression tag	UNP F2XBU9
D	-5	VAL	-	expression tag	UNP F2XBU9
D	-4	PRO	-	expression tag	UNP F2XBU9
D	-3	ARG	-	expression tag	UNP F2XBU9
D	-2	GLY	-	expression tag	UNP F2XBU9
D	-1	SER	-	expression tag	UNP F2XBU9
D	0	HIS	-	expression tag	UNP F2XBU9

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

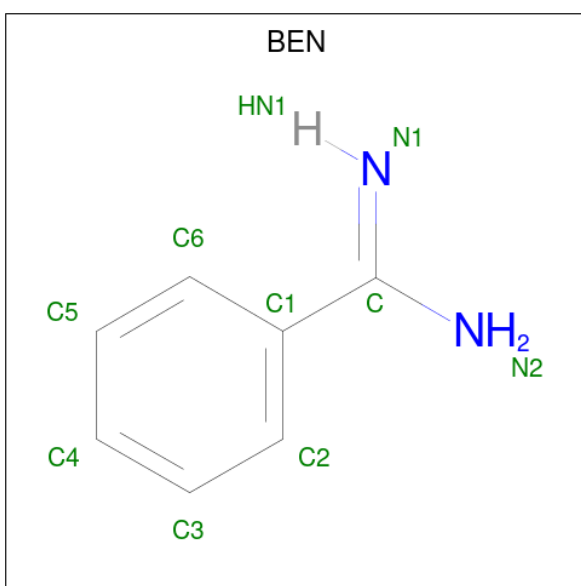
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



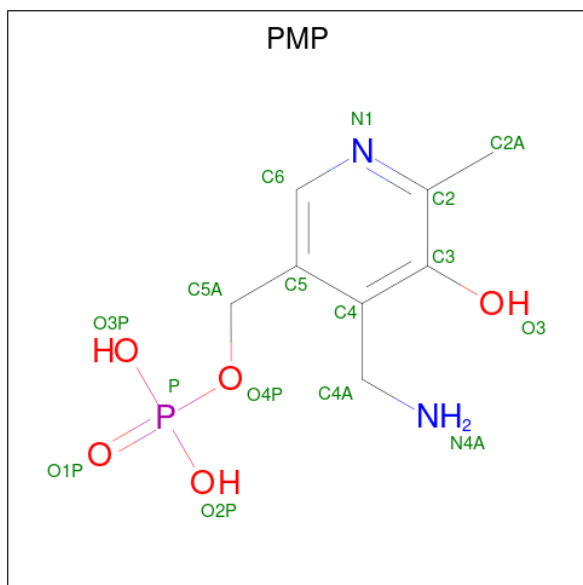
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	A	1	Total	C	N	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 5 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



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

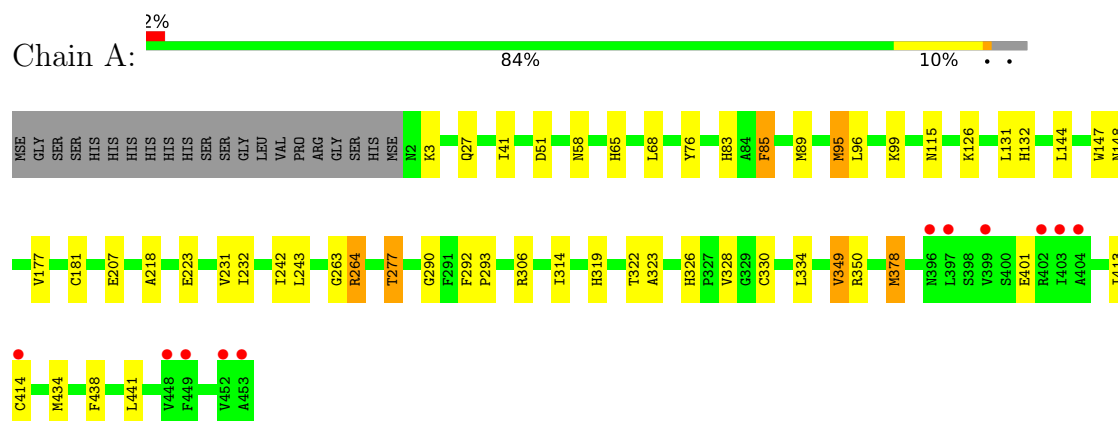
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total	O	0	0
			306	306		
6	B	339	Total	O	0	0
			339	339		
6	C	328	Total	O	0	0
			328	328		
6	D	322	Total	O	0	0
			322	322		

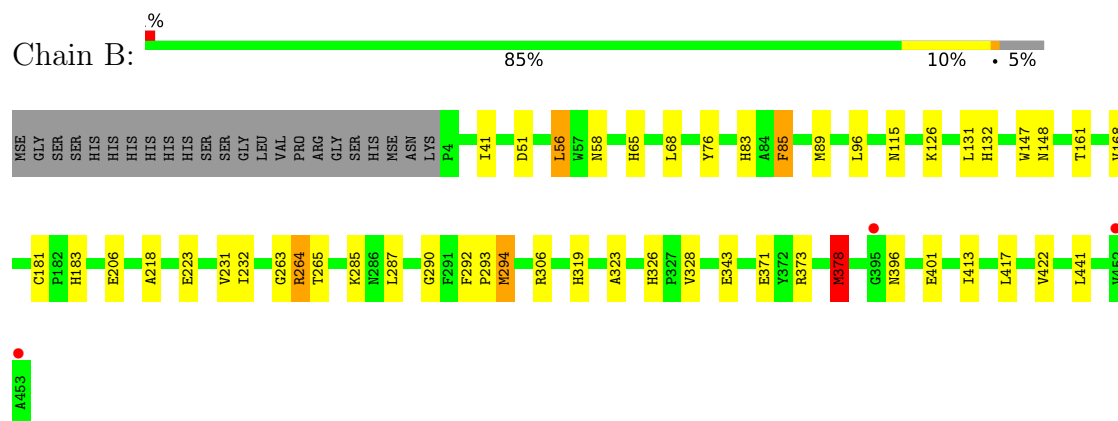
3 Residue-property plots

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

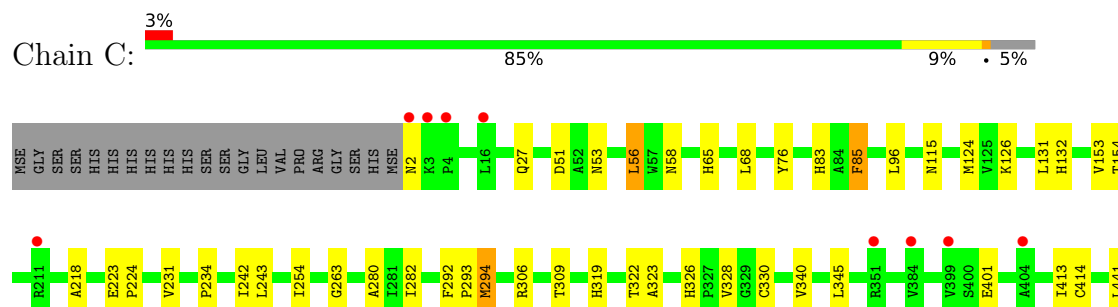
• Molecule 1: Pyruvate transaminase

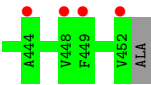


• Molecule 1: Pyruvate transaminase

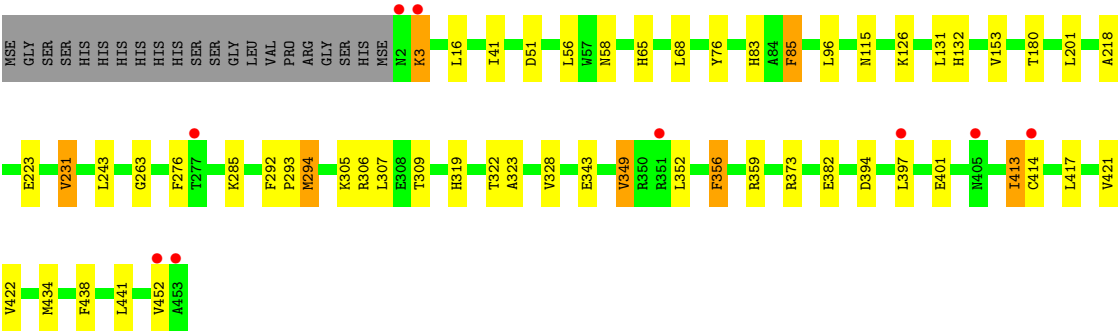
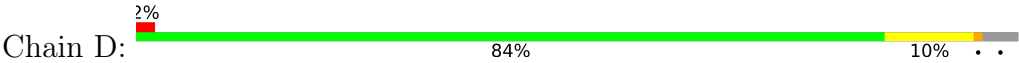


• Molecule 1: Pyruvate transaminase





● Molecule 1: Pyruvate transaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.07Å 162.18Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 1.90 49.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.79-1.90) 98.8 (49.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.9.5	Depositor
R, R_{free}	0.174 , 0.210 (Not available) , 0.202	Depositor DCC
R_{free} test set	7258 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15466	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4223e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BEN, SO4, NA, PMP

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	0.81	0/3600	1.20	12/4860 (0.2%)
1	B	0.86	1/3583 (0.0%)	1.14	8/4837 (0.2%)
1	C	0.83	0/3595	1.20	7/4853 (0.1%)
1	D	0.83	0/3600	1.19	8/4860 (0.2%)
All	All	0.83	1/14378 (0.0%)	1.18	35/19410 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	MSE	SE-CE	-10.09	1.65	1.95

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	GLY	N-CA-C	12.07	129.05	114.69
1	B	263	GLY	N-CA-C	11.46	127.19	113.79
1	A	263	GLY	N-CA-C	11.40	128.26	114.69
1	D	263	GLY	N-CA-C	9.49	127.26	114.92
1	C	85	PHE	CA-CB-CG	8.12	121.92	113.80
1	D	85	PHE	CA-CB-CG	7.92	121.72	113.80
1	A	349	VAL	N-CA-CB	7.50	119.32	110.55
1	D	223	GLU	N-CA-C	-7.08	100.73	109.65
1	B	85	PHE	CA-CB-CG	6.90	120.70	113.80
1	A	277	THR	CB-CA-C	6.82	117.74	110.17
1	A	148	ASN	CA-CB-CG	6.70	119.30	112.60
1	D	349	VAL	N-CA-CB	6.32	119.14	110.54
1	A	223	GLU	N-CA-C	-6.28	101.74	109.65
1	D	58	ASN	N-CA-C	6.20	121.03	112.90
1	A	85	PHE	CA-CB-CG	5.99	119.79	113.80
1	A	232	ILE	N-CA-C	5.79	113.88	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	MSE	CB-CA-C	-5.75	101.94	110.62
1	A	242	ILE	N-CA-C	5.68	117.19	111.00
1	C	58	ASN	N-CA-C	5.64	120.28	112.90
1	A	378	MSE	CB-CA-C	-5.60	102.16	110.62
1	A	58	ASN	N-CA-C	5.57	120.20	112.90
1	B	264	ARG	N-CA-C	5.46	117.99	111.71
1	B	223	GLU	N-CA-C	-5.43	102.81	109.65
1	D	356	PHE	CA-CB-CG	5.38	119.19	113.80
1	B	58	ASN	N-CA-C	5.37	119.94	112.90
1	C	242	ILE	N-CA-C	5.22	116.69	111.00
1	C	154	THR	N-CA-C	-5.19	104.02	110.41
1	D	413	ILE	N-CA-CB	5.19	116.92	111.00
1	C	153	VAL	N-CA-C	5.14	118.09	113.10
1	C	223	GLU	N-CA-C	-5.14	103.17	109.65
1	A	264	ARG	N-CA-C	5.13	117.61	111.71
1	D	153	VAL	N-CA-C	5.12	118.07	113.10
1	B	148	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	89	MSE	N-CA-CB	-5.11	103.11	111.24
1	B	89	MSE	N-CA-CB	-5.08	103.16	111.24

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	3522	0	3447	31	0
1	B	3505	0	3429	34	0
1	C	3517	0	3442	33	0
1	D	3522	0	3447	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	14	0	0
4	B	9	0	7	0	0
5	A	16	0	10	0	0
5	B	16	0	10	0	0
5	C	16	0	10	0	0
5	D	16	0	10	1	0
6	A	306	0	0	2	0
6	B	339	0	0	2	0
6	C	328	0	0	2	0
6	D	322	0	0	0	0
All	All	15466	0	13826	118	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 4.

All (118) 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:A:83:HIS:HD2	1:A:85:PHE:H	1.17	0.93
1:C:83:HIS:HD2	1:C:85:PHE:H	1.24	0.85
1:C:65:HIS:HD2	1:C:68:LEU:H	1.25	0.83
1:B:83:HIS:HD2	1:B:85:PHE:H	1.23	0.82
1:A:65:HIS:HD2	1:A:68:LEU:H	1.30	0.80
1:B:65:HIS:HD2	1:B:68:LEU:H	1.27	0.79
1:C:124:MSE:HE1	1:C:280:ALA:HB1	1.64	0.78
1:D:65:HIS:HD2	1:D:68:LEU:H	1.35	0.73
1:D:414:CYS:SG	1:D:421:VAL:HG13	2.31	0.70
1:B:126:LYS:NZ	1:B:319:HIS:HD2	1.90	0.69
1:D:83:HIS:HD2	1:D:85:PHE:H	1.41	0.69
1:B:265:THR:HG22	1:B:378:MSE:HE1	1.77	0.67
1:A:264:ARG:CD	1:A:378:MSE:HG3	2.25	0.66
1:C:126:LYS:NZ	1:C:319:HIS:HD2	1.93	0.66
1:A:126:LYS:NZ	1:A:319:HIS:HD2	1.94	0.64
1:B:264:ARG:HG2	1:B:378:MSE:HE2	1.80	0.63
1:A:115:ASN:HD21	1:A:323:ALA:HB3	1.67	0.60
1:B:265:THR:CG2	1:B:378:MSE:HE1	2.30	0.59
1:D:394:ASP:HB2	1:D:397:LEU:HD23	1.84	0.59
1:C:56:LEU:HD23	1:D:322:THR:HA	1.86	0.58
1:D:231:VAL:O	1:D:373:ARG:HD2	2.04	0.57
1:D:373:ARG:NH2	1:D:382:GLU:OE1	2.35	0.56
1:D:126:LYS:NZ	1:D:319:HIS:HD2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:CYS:SG	1:D:421:VAL:CG1	2.95	0.54
1:D:352:LEU:HB3	1:D:434:MSE:HE1	1.88	0.54
1:B:126:LYS:HZ3	1:B:319:HIS:HD2	1.55	0.54
1:B:115:ASN:HD21	1:B:323:ALA:HB3	1.73	0.53
1:C:254:ILE:HD12	1:C:280:ALA:HB3	1.90	0.53
1:A:434:MSE:HE3	1:A:438:PHE:HE2	1.72	0.53
1:C:124:MSE:HE1	1:C:280:ALA:CB	2.35	0.53
1:C:326:HIS:HD2	1:C:328:VAL:H	1.57	0.52
1:C:294:MSE:HE2	6:C:623:HOH:O	2.08	0.52
1:C:124:MSE:CE	1:C:280:ALA:HB1	2.38	0.51
1:C:124:MSE:HE2	1:C:282:ILE:HD11	1.92	0.51
1:B:76:TYR:CE2	1:B:328:VAL:HG11	2.45	0.51
1:D:131:LEU:HD11	1:D:306:ARG:HB3	1.93	0.50
1:C:124:MSE:CE	1:C:280:ALA:CB	2.89	0.50
1:C:126:LYS:HZ2	1:C:319:HIS:HD2	1.58	0.50
1:D:115:ASN:HD21	1:D:323:ALA:HB3	1.76	0.50
1:A:83:HIS:CD2	1:A:85:PHE:H	2.10	0.50
1:A:51:ASP:HA	1:A:413:ILE:HB	1.93	0.50
1:D:76:TYR:CE2	1:D:328:VAL:HG11	2.47	0.50
1:B:326:HIS:HD2	1:B:328:VAL:H	1.59	0.50
1:A:126:LYS:HZ2	1:A:319:HIS:HD2	1.60	0.50
1:A:264:ARG:HD3	1:A:378:MSE:HG3	1.91	0.49
1:A:76:TYR:CE2	1:A:328:VAL:HG11	2.47	0.49
1:A:132:HIS:HD2	6:A:762:HOH:O	1.95	0.49
1:A:290:GLY:O	1:B:326:HIS:HE1	1.95	0.49
1:B:264:ARG:CG	1:B:378:MSE:HE2	2.41	0.49
1:B:161:THR:O	6:B:929:HOH:O	2.20	0.49
1:C:131:LEU:HD11	1:C:306:ARG:HB3	1.95	0.49
1:D:132:HIS:HE1	1:D:218:ALA:O	1.96	0.48
1:C:76:TYR:CE2	1:C:328:VAL:HG11	2.49	0.48
1:A:147:TRP:O	1:A:181:CYS:HB2	2.14	0.48
1:A:326:HIS:HD2	1:A:328:VAL:H	1.62	0.48
1:C:293:PRO:HD3	1:D:292:PHE:CZ	2.47	0.48
1:A:131:LEU:HD11	1:A:306:ARG:HB3	1.96	0.48
1:C:126:LYS:HZ3	1:C:319:HIS:HD2	1.61	0.48
1:D:243:LEU:HD22	1:D:276:PHE:HB2	1.94	0.47
1:A:126:LYS:HZ3	1:A:319:HIS:HD2	1.62	0.47
1:C:292:PHE:CZ	1:D:293:PRO:HD3	2.49	0.47
1:B:287:LEU:HD21	1:B:294:MSE:HE2	1.97	0.47
1:A:314:ILE:HD13	1:B:168:VAL:HG11	1.97	0.47
1:A:95:MSE:HG3	1:A:334:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:MSE:HE3	1:A:438:PHE:CE2	2.49	0.46
1:B:132:HIS:HE1	1:B:218:ALA:O	1.99	0.46
1:A:132:HIS:HE1	1:A:218:ALA:O	1.99	0.46
1:B:126:LYS:HZ2	1:B:319:HIS:HD2	1.61	0.46
1:C:322:THR:HA	1:D:56:LEU:HD23	1.98	0.46
1:C:51:ASP:HA	1:C:413:ILE:HB	1.96	0.46
1:B:126:LYS:NZ	1:B:319:HIS:CD2	2.78	0.46
1:C:115:ASN:HD21	1:C:323:ALA:HB3	1.80	0.45
1:D:305:LYS:O	1:D:309:THR:HG23	2.17	0.45
1:C:132:HIS:HE1	1:C:218:ALA:O	1.99	0.45
1:A:326:HIS:HE1	1:B:290:GLY:O	2.00	0.45
1:C:326:HIS:CD2	1:C:328:VAL:H	2.33	0.44
1:C:132:HIS:HD2	6:C:770:HOH:O	1.99	0.44
1:D:359:ARG:HG2	1:D:438:PHE:CG	2.52	0.44
1:A:350:ARG:NH2	6:A:898:HOH:O	2.51	0.44
1:B:183:HIS:HB2	1:B:232:ILE:HG21	2.00	0.44
1:C:83:HIS:CD2	1:C:85:PHE:H	2.16	0.44
1:D:417:LEU:HD12	1:D:422:VAL:HG21	2.00	0.44
1:B:131:LEU:HD11	1:B:306:ARG:HB3	1.99	0.43
1:D:294:MSE:HE2	1:D:294:MSE:HB3	1.78	0.43
1:A:144:LEU:HD23	1:A:177:VAL:HB	2.01	0.43
1:A:65:HIS:CD2	1:A:68:LEU:H	2.21	0.43
1:C:65:HIS:CD2	1:C:68:LEU:H	2.17	0.43
1:D:51:ASP:HA	1:D:413:ILE:HB	2.00	0.43
1:C:126:LYS:NZ	1:C:319:HIS:CD2	2.81	0.43
1:A:293:PRO:HD3	1:B:292:PHE:CZ	2.53	0.42
1:D:65:HIS:HE1	1:D:343:GLU:OE2	2.02	0.42
1:B:294:MSE:HE2	1:B:294:MSE:HB3	1.81	0.42
1:B:378:MSE:HE3	1:B:378:MSE:HB2	1.64	0.42
1:D:65:HIS:CD2	1:D:68:LEU:H	2.25	0.42
1:D:126:LYS:HZ2	1:D:319:HIS:HD2	1.68	0.42
1:C:96:LEU:HD22	1:C:330:CYS:HA	2.00	0.42
1:B:417:LEU:HD12	1:B:422:VAL:HG21	2.00	0.42
1:B:132:HIS:HD2	6:B:647:HOH:O	2.02	0.42
1:D:356:PHE:CD1	1:D:434:MSE:HE2	2.55	0.42
1:C:124:MSE:HE2	1:C:282:ILE:CD1	2.50	0.41
1:C:126:LYS:HZ2	1:C:319:HIS:CD2	2.38	0.41
1:D:96:LEU:HD21	1:D:294:MSE:HE1	2.02	0.41
1:C:340:VAL:HA	1:C:345:LEU:HB2	2.02	0.41
1:A:292:PHE:CZ	1:B:293:PRO:HD3	2.55	0.41
1:B:96:LEU:HD21	1:B:294:MSE:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:LYS:HE2	5:D:502:PMP:H4A2	2.02	0.41
1:A:322:THR:HA	1:B:56:LEU:HD23	2.03	0.41
1:C:53:ASN:HD21	1:C:414:CYS:C	2.27	0.41
1:A:126:LYS:NZ	1:A:319:HIS:CD2	2.82	0.41
1:C:224:PRO:O	1:C:234:PRO:HD3	2.20	0.41
1:A:96:LEU:HD22	1:A:330:CYS:HA	2.02	0.41
1:B:51:ASP:HA	1:B:413:ILE:HB	2.01	0.41
1:B:65:HIS:HE1	1:B:343:GLU:OE2	2.04	0.41
1:B:147:TRP:O	1:B:181:CYS:HB2	2.21	0.41
1:A:264:ARG:HG2	1:A:378:MSE:HG3	2.04	0.40
1:B:287:LEU:HD21	1:B:294:MSE:CE	2.51	0.40
1:B:371:GLU:OE1	1:B:373:ARG:HD3	2.21	0.40
1:D:180:THR:HB	1:D:201:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/473 (95%)	431 (96%)	18 (4%)	1 (0%)	43	36
1	B	448/473 (95%)	433 (97%)	13 (3%)	2 (0%)	30	22
1	C	449/473 (95%)	430 (96%)	18 (4%)	1 (0%)	43	36
1	D	450/473 (95%)	430 (96%)	18 (4%)	2 (0%)	30	22
All	All	1797/1892 (95%)	1724 (96%)	67 (4%)	6 (0%)	36	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	B	285	LYS

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Mol	Chain	Res	Type
1	A	231	VAL
1	B	231	VAL
1	C	231	VAL
1	D	231	VAL

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	368/371 (99%)	356 (97%)	12 (3%)	33	26
1	B	366/371 (99%)	358 (98%)	8 (2%)	45	42
1	C	368/371 (99%)	360 (98%)	8 (2%)	45	42
1	D	368/371 (99%)	359 (98%)	9 (2%)	43	38
All	All	1470/1484 (99%)	1433 (98%)	37 (2%)	42	37

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

Mol	Chain	Res	Type
1	A	3	LYS
1	A	27	GLN
1	A	41	ILE
1	A	95	MSE
1	A	99	LYS
1	A	207	GLU
1	A	243	LEU
1	A	277	THR
1	A	349	VAL
1	A	401	GLU
1	A	414	CYS
1	A	441	LEU
1	B	41	ILE
1	B	56	LEU
1	B	206	GLU
1	B	294	MSE
1	B	378	MSE

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Mol	Chain	Res	Type
1	B	396	ASN
1	B	401	GLU
1	B	441	LEU
1	C	2	ASN
1	C	27	GLN
1	C	56	LEU
1	C	243	LEU
1	C	294	MSE
1	C	309	THR
1	C	401	GLU
1	C	441	LEU
1	D	3	LYS
1	D	16	LEU
1	D	41	ILE
1	D	294	MSE
1	D	307	LEU
1	D	349	VAL
1	D	401	GLU
1	D	441	LEU
1	D	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	45	ASN
1	A	53	ASN
1	A	65	HIS
1	A	83	HIS
1	A	92	GLN
1	A	115	ASN
1	A	121	ASN
1	A	132	HIS
1	A	148	ASN
1	A	319	HIS
1	A	326	HIS
1	A	342	ASN
1	B	53	ASN
1	B	65	HIS
1	B	83	HIS
1	B	92	GLN
1	B	115	ASN

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Mol	Chain	Res	Type
1	B	121	ASN
1	B	132	HIS
1	B	319	HIS
1	B	326	HIS
1	C	45	ASN
1	C	53	ASN
1	C	65	HIS
1	C	83	HIS
1	C	92	GLN
1	C	115	ASN
1	C	121	ASN
1	C	132	HIS
1	C	267	ASN
1	C	319	HIS
1	C	326	HIS
1	C	342	ASN
1	C	368	ASN
1	D	2	ASN
1	D	53	ASN
1	D	65	HIS
1	D	83	HIS
1	D	92	GLN
1	D	115	ASN
1	D	121	ASN
1	D	132	HIS
1	D	319	HIS
1	D	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	SO4	A	502	-	4,4,4	0.36	0	6,6,6	0.29	0
4	BEN	A	503	-	9,9,9	2.09	4 (44%)	7,11,11	1.46	1 (14%)
4	BEN	B	502	-	9,9,9	1.98	4 (44%)	7,11,11	0.63	0
4	BEN	A	504	-	9,9,9	1.85	3 (33%)	7,11,11	0.82	0
5	PMP	A	505	-	16,16,16	1.57	3 (18%)	22,23,23	1.33	4 (18%)
5	PMP	B	503	-	16,16,16	1.44	1 (6%)	22,23,23	1.75	6 (27%)
5	PMP	C	503	-	16,16,16	1.78	6 (37%)	22,23,23	1.58	7 (31%)
5	PMP	D	502	-	16,16,16	1.56	2 (12%)	22,23,23	1.31	3 (13%)
3	SO4	C	502	-	4,4,4	0.49	0	6,6,6	0.25	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
4	BEN	A	503	-	-	4/4/4/4	0/1/1/1
4	BEN	B	502	-	-	4/4/4/4	0/1/1/1
4	BEN	A	504	-	-	4/4/4/4	0/1/1/1
5	PMP	A	505	-	-	2/8/8/8	0/1/1/1
5	PMP	B	503	-	-	2/8/8/8	0/1/1/1
5	PMP	C	503	-	-	2/8/8/8	0/1/1/1
5	PMP	D	502	-	-	2/8/8/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	PMP	C3-C4	4.33	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	PMP	C3-C4	4.21	1.46	1.40
5	C	503	PMP	C6-N1	3.38	1.41	1.34
4	B	502	BEN	C6-C1	3.27	1.44	1.39
4	B	502	BEN	C2-C1	3.19	1.44	1.39
5	A	505	PMP	C3-C4	3.05	1.44	1.40
4	A	503	BEN	C6-C1	2.98	1.43	1.39
5	C	503	PMP	O3-C3	-2.94	1.30	1.36
4	A	503	BEN	C-N2	2.92	1.41	1.33
5	A	505	PMP	C2A-C2	2.92	1.55	1.50
4	A	503	BEN	C2-C1	2.92	1.43	1.39
5	C	503	PMP	C2A-C2	2.75	1.54	1.50
4	A	504	BEN	C6-C1	2.74	1.43	1.39
5	C	503	PMP	P-O4P	2.69	1.68	1.60
5	C	503	PMP	C3-C4	2.60	1.43	1.40
5	D	502	PMP	C6-N1	2.49	1.39	1.34
5	A	505	PMP	C5-C4	2.44	1.43	1.40
4	A	504	BEN	C1-C	2.41	1.51	1.47
4	A	503	BEN	C5-C4	2.16	1.43	1.38
5	C	503	PMP	C6-C5	2.16	1.42	1.37
4	A	504	BEN	C2-C1	2.08	1.42	1.39
4	B	502	BEN	C-N2	2.02	1.39	1.33
4	B	502	BEN	C5-C4	2.01	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	BEN	C1-C-N2	3.39	123.16	118.01
5	B	503	PMP	C6-C5-C4	3.07	120.38	118.06
5	B	503	PMP	O4P-C5A-C5	-3.03	103.67	109.36
5	B	503	PMP	C6-N1-C2	2.96	124.57	119.20
5	B	503	PMP	C5-C6-N1	-2.92	119.09	123.83
5	B	503	PMP	C4A-C4-C3	2.82	125.00	120.22
5	C	503	PMP	C6-C5-C4	2.71	120.11	118.06
5	C	503	PMP	C2A-C2-N1	2.54	122.43	117.64
5	A	505	PMP	C4A-C4-C3	2.49	124.44	120.22
5	D	502	PMP	C6-C5-C4	2.42	119.89	118.06
5	A	505	PMP	C6-N1-C2	2.42	123.58	119.20
5	C	503	PMP	C3-C4-C5	-2.38	116.58	118.73
5	C	503	PMP	O4P-C5A-C5	-2.38	104.90	109.36
5	D	502	PMP	C3-C4-C5	-2.32	116.62	118.73
5	C	503	PMP	C5-C6-N1	-2.32	120.06	123.83
5	C	503	PMP	C3-C2-N1	-2.27	118.09	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	PMP	C5-C6-N1	-2.25	120.16	123.83
5	B	503	PMP	C2A-C2-N1	2.22	121.82	117.64
5	A	505	PMP	C3-C2-N1	-2.12	118.28	120.96
5	C	503	PMP	C4-C3-C2	2.12	123.11	119.91
5	A	505	PMP	O4P-C5A-C5	-2.05	105.51	109.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	PMP	C3-C4-C4A-N4A
5	A	505	PMP	C5-C4-C4A-N4A
5	B	503	PMP	C3-C4-C4A-N4A
5	B	503	PMP	C5-C4-C4A-N4A
5	C	503	PMP	C3-C4-C4A-N4A
5	C	503	PMP	C5-C4-C4A-N4A
5	D	502	PMP	C3-C4-C4A-N4A
5	D	502	PMP	C5-C4-C4A-N4A
4	A	503	BEN	N2-C-C1-C2
4	A	503	BEN	N2-C-C1-C6
4	A	504	BEN	N2-C-C1-C2
4	A	504	BEN	N2-C-C1-C6
4	B	502	BEN	N2-C-C1-C2
4	B	502	BEN	N2-C-C1-C6
4	A	503	BEN	N1-C-C1-C2
4	A	503	BEN	N1-C-C1-C6
4	A	504	BEN	N1-C-C1-C2
4	A	504	BEN	N1-C-C1-C6
4	B	502	BEN	N1-C-C1-C2
4	B	502	BEN	N1-C-C1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	PMP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	439/473 (92%)	-0.02	11 (2%) 58 62	21, 29, 55, 106	0
1	B	437/473 (92%)	-0.13	3 (0%) 84 86	20, 29, 48, 86	0
1	C	438/473 (92%)	0.13	13 (2%) 52 56	22, 33, 58, 81	0
1	D	439/473 (92%)	-0.00	9 (2%) 63 67	22, 30, 51, 88	0
All	All	1753/1892 (92%)	-0.01	36 (2%) 63 67	20, 30, 54, 106	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	ALA	6.0
1	C	452	VAL	5.6
1	A	453	ALA	4.6
1	C	404	ALA	4.1
1	D	453	ALA	3.6
1	B	452	VAL	3.3
1	C	351	ARG	3.2
1	A	414	CYS	3.2
1	A	404	ALA	3.1
1	D	414	CYS	3.1
1	D	2	ASN	3.1
1	D	452	VAL	3.0
1	A	399	VAL	2.9
1	A	449	PHE	2.9
1	A	452	VAL	2.8
1	C	444	ALA	2.8
1	C	399	VAL	2.7
1	C	16	LEU	2.7
1	A	448	VAL	2.7
1	C	211	ARG	2.4
1	D	351	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	448	VAL	2.4
1	A	396	ASN	2.4
1	C	4	PRO	2.3
1	C	2	ASN	2.3
1	A	397	LEU	2.3
1	D	277	THR	2.3
1	D	3	LYS	2.2
1	A	403	ILE	2.1
1	B	395	GLY	2.1
1	D	397	LEU	2.1
1	C	449	PHE	2.1
1	D	405	ASN	2.0
1	A	402	ARG	2.0
1	C	3	LYS	2.0
1	C	384	VAL	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
3	SO4	A	502	5/5	0.81	0.15	79,83,84,85	0
4	BEN	A	504	9/9	0.85	0.12	39,40,41,43	0
4	BEN	A	503	9/9	0.88	0.11	37,38,39,42	0
4	BEN	B	502	9/9	0.88	0.10	32,33,34,36	0
3	SO4	C	502	5/5	0.90	0.10	75,80,81,81	0
2	NA	D	501	1/1	0.96	0.05	35,35,35,35	0
2	NA	C	501	1/1	0.96	0.07	35,35,35,35	0
2	NA	B	501	1/1	0.97	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PMP	C	503	16/16	0.97	0.07	22,25,28,32	0
5	PMP	A	505	16/16	0.98	0.06	20,23,27,28	0
5	PMP	B	503	16/16	0.98	0.05	21,23,27,31	0
2	NA	A	501	1/1	0.98	0.05	33,33,33,33	0
5	PMP	D	502	16/16	0.98	0.05	22,25,28,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.