



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2017 – 01:00 PM EDT

PDB ID : 5LHA
Title : Amine transaminase crystal structure from an uncultivated *Pseudomonas* species in the PMP-bound form
Authors : Reddem, E.; Thunnissen, A.M.W.H.
Deposited on : 2016-07-10
Resolution : 1.89 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	:	rb-20029077
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)	:	rb-20029077

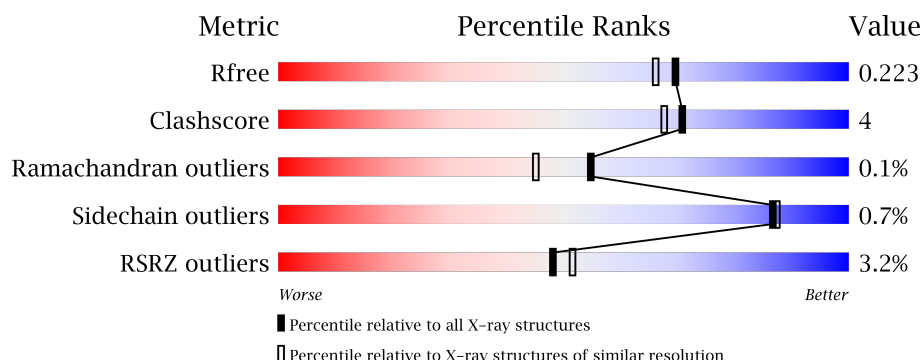
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 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	458	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	B	458	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	C	458	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	D	458	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div></div> </div> <div></div> </div>

2 Entry composition [i](#)

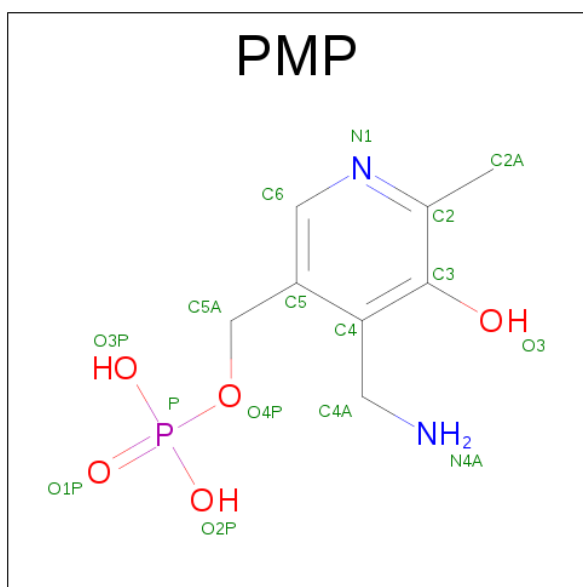
There are 3 unique types of molecules in this entry. The entry contains 14339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OMEGA TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	2	0
			3402	2141	620	621	20			
1	B	446	Total	C	N	O	S	0	0	0
			3377	2127	617	614	19			
1	C	447	Total	C	N	O	S	0	2	0
			3402	2141	620	621	20			
1	D	446	Total	C	N	O	S	0	0	0
			3377	2127	617	614	19			

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

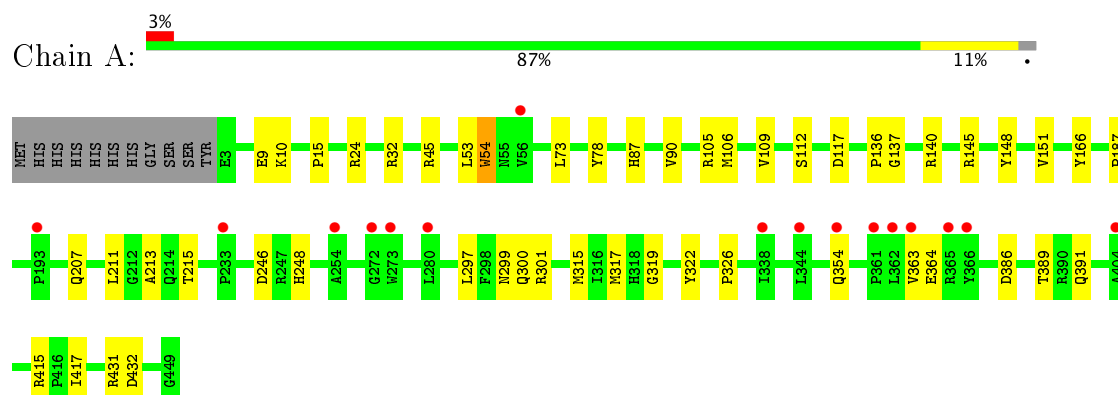
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total	O	0	0
			176	176		
3	B	162	Total	O	0	0
			162	162		
3	C	214	Total	O	0	0
			214	214		
3	D	165	Total	O	0	0
			165	165		

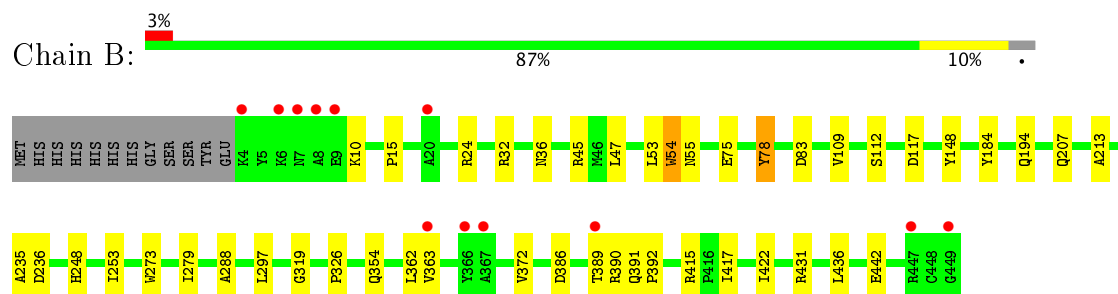
3 Residue-property plots [i](#)

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.

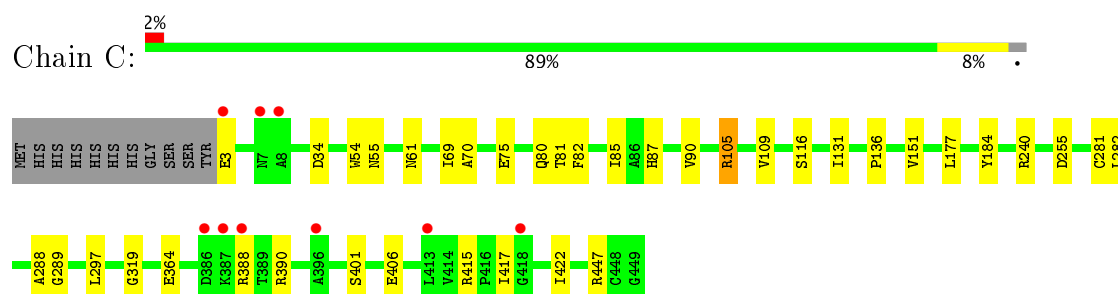
• Molecule 1: OMEGA TRANSAMINASE



• Molecule 1: OMEGA TRANSAMINASE

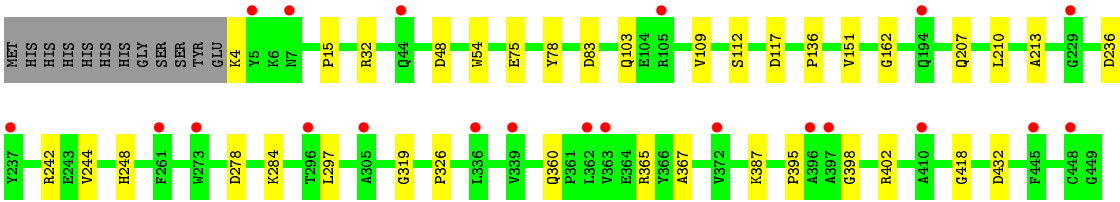


• Molecule 1: OMEGA TRANSAMINASE



• Molecule 1: OMEGA TRANSAMINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.79Å 97.07Å 153.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 1.89 48.53 – 1.89	Depositor EDS
% Data completeness (in resolution range)	87.3 (48.53-1.89) 92.4 (48.53-1.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.172 , 0.225 0.168 , 0.223	Depositor DCC
R_{free} test set	5439 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.416 for k,h,-l	Xtriage
Reported twinning fraction	0.440 for k,h,-l	Depositor
Outliers	0 of 107289 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14339	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.32	0/3475	0.54	0/4715
1	B	0.34	0/3450	0.55	0/4682
1	C	0.32	0/3475	0.55	0/4715
1	D	0.31	0/3450	0.53	0/4682
All	All	0.32	0/13850	0.54	0/18794

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	TYR	Peptide

5.2 Too-close contacts [i](#)

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	3402	0	3378	35	1
1	B	3377	0	3361	31	0
1	C	3402	0	3378	26	0
1	D	3377	0	3361	27	0
2	A	16	0	11	2	0
2	B	16	0	11	2	0
2	C	16	0	11	3	0
2	D	16	0	11	4	0
3	A	176	0	0	5	0
3	B	162	0	0	3	1
3	C	214	0	0	5	1
3	D	165	0	0	9	1
All	All	14339	0	13522	111	3

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 (111) 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:D:360:GLN:NE2	3:D:601:HOH:O	2.08	0.86
1:A:207:GLN:NE2	3:A:601:HOH:O	2.15	0.79
1:C:105:ARG:NH2	3:C:601:HOH:O	2.16	0.77
1:A:145:ARG:NH2	1:B:207:GLN:OE1	2.17	0.74
1:B:362:LEU:HD21	1:B:442:GLU:HG2	1.70	0.73
1:B:45:ARG:NH2	3:B:602:HOH:O	2.22	0.72
1:B:386:ASP:HB3	1:B:389:THR:HG22	1.78	0.64
2:A:501:PMP:O3	2:A:501:PMP:N4A	2.27	0.64
1:C:34:ASP:OD1	1:C:61:ASN:ND2	2.30	0.63
1:A:166:TYR:O	3:A:602:HOH:O	2.16	0.62
1:A:32:ARG:HG2	1:C:75:GLU:HG3	1.79	0.62
1:B:194:GLN:OE1	3:B:601:HOH:O	2.16	0.61
1:A:363:VAL:O	3:A:603:HOH:O	2.16	0.61
1:A:105:ARG:HH12	1:A:301:ARG:H	1.48	0.60
1:A:207:GLN:OE1	3:A:604:HOH:O	2.17	0.60
1:D:4:LYS:N	3:D:618:HOH:O	2.35	0.59
1:D:365:ARG:NH2	3:D:620:HOH:O	2.36	0.59
1:A:315:MET:HB3	1:A:317[A]:MET:HE3	1.84	0.58
2:B:501:PMP:N4A	2:B:501:PMP:O3	2.34	0.57
1:B:389:THR:HG23	1:B:391:GLN:H	1.69	0.57
1:A:389:THR:HG23	1:A:391:GLN:H	1.70	0.56
1:A:386:ASP:HB3	1:A:389:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:O	3:A:605:HOH:O	2.19	0.53
1:A:364:GLU:OE1	1:A:364:GLU:N	2.42	0.53
2:C:501:PMP:N4A	3:C:612:HOH:O	2.34	0.53
1:C:388:ARG:NH2	3:C:606:HOH:O	2.27	0.52
1:C:417:ILE:HD12	1:C:422:ILE:HG13	1.92	0.52
1:B:32:ARG:HG2	1:D:75:GLU:HG3	1.91	0.52
1:D:367:ALA:HA	1:D:387:LYS:HE2	1.92	0.52
1:A:105:ARG:NH1	1:A:301:ARG:H	2.08	0.52
1:D:109:VAL:HG22	1:D:297:LEU:HG	1.92	0.51
1:B:417:ILE:HD12	1:B:422:ILE:HG13	1.93	0.50
1:A:53:LEU:O	1:A:54:TRP:HD1	1.94	0.50
1:D:48:ASP:OD2	3:D:602:HOH:O	2.19	0.50
1:A:78:TYR:HA	1:A:326:PRO:HD2	1.93	0.49
1:C:109:VAL:HG22	1:C:297:LEU:HG	1.94	0.49
1:B:319:GLY:HA3	1:D:15:PRO:HB3	1.94	0.49
1:C:80:GLN:OE1	1:C:82:PHE:HB2	2.12	0.49
1:A:140:ARG:HH11	1:A:211:LEU:HB3	1.78	0.49
1:A:106:MET:HA	1:A:299:ASN:HA	1.95	0.48
1:B:184:TYR:CZ	1:B:390:ARG:HG2	2.49	0.48
1:D:236:ASP:N	1:D:236:ASP:OD1	2.44	0.48
1:C:415:ARG:CZ	1:C:417:ILE:HD11	2.44	0.48
1:D:78:TYR:HA	1:D:326:PRO:HD2	1.95	0.48
1:D:207:GLN:NE2	3:D:605:HOH:O	2.26	0.47
1:C:282:LEU:HD12	1:C:297:LEU:HD13	1.94	0.47
1:A:354:GLN:OE1	1:A:431:ARG:HG2	2.14	0.47
2:C:501:PMP:N4A	2:C:501:PMP:O3	2.48	0.47
1:C:240:ARG:NH1	3:C:610:HOH:O	2.33	0.47
1:D:284:LYS:HE2	2:D:501:PMP:H4A2	1.95	0.47
1:B:148:TYR:HE2	2:B:501:PMP:H4A1	1.80	0.46
1:A:322:TYR:OH	1:C:289:GLY:HA2	2.15	0.46
1:A:415:ARG:CZ	1:A:417:ILE:HD11	2.45	0.46
1:A:87:HIS:O	1:A:90:VAL:HG12	2.16	0.46
1:B:354:GLN:HE22	1:B:431:ARG:HB3	1.81	0.46
1:C:55:ASN:O	1:C:288:ALA:HA	2.17	0.45
1:A:187:PRO:HG3	3:B:676:HOH:O	2.16	0.45
1:B:389:THR:HG23	1:B:391:GLN:HB2	1.98	0.45
1:B:213:ALA:HB1	1:B:248:HIS:HB3	1.99	0.45
1:B:253:ILE:HG12	1:B:279:ILE:HD12	1.99	0.44
1:A:109:VAL:HG22	1:A:297:LEU:HG	1.98	0.44
1:B:78:TYR:HA	1:B:326:PRO:HD2	1.99	0.44
1:C:70:ALA:HB2	3:C:714:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HG12	1:C:136:PRO:HB3	1.98	0.44
1:A:137:GLY:O	1:A:215:THR:HA	2.16	0.44
1:B:363:VAL:HG21	1:B:372:VAL:HG12	1.98	0.44
1:B:319:GLY:H	1:D:151:VAL:HG21	1.82	0.44
2:D:501:PMP:N4A	3:D:616:HOH:O	2.35	0.44
1:C:177:LEU:HD12	1:D:210:LEU:HD21	2.00	0.44
1:A:136:PRO:HD2	1:D:136:PRO:HD2	2.00	0.44
1:B:10:LYS:O	1:B:24:ARG:NH2	2.31	0.44
1:B:112:SER:HB2	1:B:117:ASP:HB3	2.00	0.44
1:B:55:ASN:O	1:B:288:ALA:HA	2.18	0.44
1:A:151:VAL:HG21	1:C:319:GLY:H	1.83	0.44
1:B:15:PRO:HB3	1:D:319:GLY:HA3	1.99	0.44
1:B:415:ARG:CZ	1:B:417:ILE:HD11	2.48	0.43
1:A:105:ARG:HH11	1:A:300:GLN:HB3	1.83	0.43
1:C:116:SER:N	2:C:501:PMP:H5A2	2.34	0.43
1:C:364:GLU:OE1	1:C:364:GLU:N	2.52	0.43
1:A:140:ARG:NH1	1:A:211:LEU:HB3	2.34	0.43
1:C:87:HIS:O	1:C:90:VAL:HG12	2.19	0.43
1:A:112:SER:HB2	1:A:117:ASP:HB3	2.01	0.42
1:A:213:ALA:HB1	1:A:248:HIS:HB3	2.01	0.42
1:D:242:ARG:NH1	1:D:278:ASP:OD2	2.50	0.42
1:B:109:VAL:HG22	1:B:297:LEU:HG	2.02	0.42
1:A:10:LYS:HB3	1:A:24:ARG:HH12	1.84	0.42
1:A:319:GLY:H	1:C:151:VAL:HG21	1.84	0.42
1:B:53:LEU:O	1:B:54:TRP:HD1	2.03	0.42
1:A:148:TYR:HE2	2:A:501:PMP:H4A1	1.85	0.41
1:B:75:GLU:HG3	1:D:32:ARG:HG2	2.01	0.41
1:C:184:TYR:CZ	1:C:390:ARG:HG2	2.55	0.41
1:D:284:LYS:CE	2:D:501:PMP:H4A2	2.50	0.41
1:D:398:GLY:O	1:D:402:ARG:HG3	2.20	0.41
1:A:73:LEU:HD11	1:C:69:ILE:HG21	2.02	0.41
1:B:36:ASN:O	1:B:47:LEU:HD12	2.20	0.41
1:C:255:ASP:HA	1:C:281:CYS:HB2	2.02	0.41
1:B:236:ASP:OD1	1:B:236:ASP:N	2.50	0.41
1:D:103:GLN:HG3	3:D:689:HOH:O	2.18	0.41
1:D:213:ALA:HB1	1:D:248:HIS:HB3	2.02	0.41
1:B:47:LEU:HD22	1:B:436:LEU:HD23	2.02	0.41
1:D:162:GLY:N	3:D:633:HOH:O	2.53	0.41
1:D:4:LYS:HG2	3:D:728:HOH:O	2.20	0.41
1:A:15:PRO:HB3	1:C:319:GLY:HA3	2.02	0.41
1:B:235:ALA:HA	1:B:273:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HG2	1:C:447:ARG:HB3	2.03	0.41
1:D:112:SER:HB2	1:D:117:ASP:HB3	2.03	0.40
2:D:501:PMP:O3	2:D:501:PMP:N4A	2.54	0.40
1:D:244:VAL:O	1:D:248:HIS:ND1	2.51	0.40
1:D:395:PRO:HG3	1:D:418:GLY:HA2	2.04	0.40
1:B:391:GLN:OE1	1:B:392:PRO:HD2	2.21	0.40
1:C:81:THR:HA	1:C:85:ILE:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH1	1:A:246:ASP:OD1[3_454]	2.13	0.07
3:D:714:HOH:O	3:D:733:HOH:O[4_545]	2.16	0.04
3:B:721:HOH:O	3:C:772:HOH:O[2_454]	2.19	0.01

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	447/458 (98%)	422 (94%)	25 (6%)	0	100	100
1	B	444/458 (97%)	421 (95%)	22 (5%)	1 (0%)	51	41
1	C	447/458 (98%)	420 (94%)	27 (6%)	0	100	100
1	D	444/458 (97%)	422 (95%)	21 (5%)	1 (0%)	51	41
All	All	1782/1832 (97%)	1685 (95%)	95 (5%)	2 (0%)	55	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	83	ASP

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Mol	Chain	Res	Type
1	B	83	ASP

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	342/350 (98%)	340 (99%)	2 (1%)	89	90
1	B	339/350 (97%)	338 (100%)	1 (0%)	94	94
1	C	342/350 (98%)	338 (99%)	4 (1%)	75	75
1	D	339/350 (97%)	337 (99%)	2 (1%)	89	90
All	All	1362/1400 (97%)	1353 (99%)	9 (1%)	87	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TRP
1	A	432	ASP
1	B	54	TRP
1	C	3	GLU
1	C	54	TRP
1	C	105	ARG
1	C	401	SER
1	D	54	TRP
1	D	432	ASP

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

Mol	Chain	Res	Type
1	C	314	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	501	-	16,16,16	1.03	2 (12%)	20,23,23	1.23	4 (20%)
2	PMP	B	501	-	16,16,16	0.97	2 (12%)	20,23,23	1.06	2 (10%)
2	PMP	C	501	-	16,16,16	0.93	1 (6%)	20,23,23	1.15	2 (10%)
2	PMP	D	501	-	16,16,16	1.03	2 (12%)	20,23,23	1.11	2 (10%)

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	501	-	-	0/8/8/8	0/1/1/1
2	PMP	B	501	-	-	0/8/8/8	0/1/1/1
2	PMP	C	501	-	-	0/8/8/8	0/1/1/1
2	PMP	D	501	-	-	0/8/8/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PMP	C3-C2	-2.16	1.39	1.40
2	D	501	PMP	C3-C2	-2.16	1.39	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PMP	C3-C2	-2.15	1.39	1.40
2	B	501	PMP	C2-N1	2.12	1.38	1.33
2	D	501	PMP	C2-N1	2.32	1.38	1.33
2	C	501	PMP	C2-N1	2.38	1.38	1.33
2	A	501	PMP	C2-N1	2.47	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PMP	C5-C6-N1	-2.66	119.37	123.87
2	D	501	PMP	C5-C6-N1	-2.41	119.79	123.87
2	C	501	PMP	C5-C6-N1	-2.33	119.92	123.87
2	A	501	PMP	C5-C6-N1	-2.27	120.03	123.87
2	A	501	PMP	C3-C2-N1	-2.09	118.01	120.75
2	A	501	PMP	C2A-C2-C3	-2.09	118.47	120.96
2	B	501	PMP	O3P-P-O4P	2.07	112.24	106.73
2	A	501	PMP	O3P-P-O4P	2.18	112.55	106.73
2	D	501	PMP	C6-C5-C4	2.29	119.83	118.13
2	C	501	PMP	C6-C5-C4	2.34	119.87	118.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PMP	2	0
2	B	501	PMP	2	0
2	C	501	PMP	3	0
2	D	501	PMP	4	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	447/458 (97%)	0.45	16 (3%) 43 47	18, 30, 48, 92	0
1	B	446/458 (97%)	0.19	12 (2%) 55 59	14, 24, 47, 122	0
1	C	447/458 (97%)	0.06	9 (2%) 65 69	12, 22, 40, 102	0
1	D	446/458 (97%)	0.56	21 (4%) 32 36	19, 32, 55, 99	0
All	All	1786/1832 (97%)	0.32	58 (3%) 48 51	12, 28, 50, 122	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	396	ALA	5.0
1	B	389	THR	4.7
1	B	8	ALA	4.3
1	D	372	VAL	3.9
1	B	367	ALA	3.8
1	A	354	GLN	3.7
1	D	396	ALA	3.7
1	B	9	GLU	3.6
1	D	363	VAL	3.6
1	B	7	ASN	3.5
1	A	344	LEU	3.4
1	D	445	PHE	3.3
1	D	261	PHE	3.3
1	A	365	ARG	3.2
1	D	7	ASN	3.1
1	D	339	VAL	3.1
1	A	338	ILE	3.1
1	D	229	GLY	2.9
1	C	7	ASN	2.9
1	A	272	GLY	2.9
1	D	105	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	8	ALA	2.8
1	B	6	LYS	2.7
1	D	305	ALA	2.7
1	D	336	LEU	2.7
1	C	388	ARG	2.7
1	D	5	TYR	2.6
1	A	273	TRP	2.6
1	C	3	GLU	2.5
1	C	418	GLY	2.4
1	D	410	ALA	2.4
1	A	361	PRO	2.4
1	D	448	CYS	2.4
1	A	366	TYR	2.3
1	B	366	TYR	2.3
1	D	44	GLN	2.3
1	B	449	GLY	2.3
1	D	273	TRP	2.3
1	D	194	GLN	2.3
1	A	280	LEU	2.3
1	A	233	PRO	2.2
1	B	4	LYS	2.2
1	D	237	TYR	2.2
1	A	254	ALA	2.2
1	B	20	ALA	2.2
1	C	387	LYS	2.2
1	C	386	ASP	2.2
1	D	296	THR	2.2
1	A	56	VAL	2.2
1	A	193	PRO	2.2
1	A	363	VAL	2.2
1	A	362	LEU	2.1
1	A	404	ALA	2.1
1	D	362	LEU	2.1
1	D	397	ALA	2.1
1	B	447	ARG	2.1
1	C	413	LEU	2.1
1	B	363	VAL	2.0

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

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(\AA^2)	Q<0.9
2	PMP	B	501	16/16	0.93	0.13	1.12	25,28,33,35	0
2	PMP	D	501	16/16	0.94	0.12	0.73	17,21,23,24	0
2	PMP	A	501	16/16	0.94	0.12	0.40	16,22,27,29	0
2	PMP	C	501	16/16	0.95	0.10	-0.26	23,26,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.