



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 PM UTC

PDB ID : 9AAT / pdb_00009aat
Title : X-RAY STRUCTURE REFINEMENT AND COMPARISON OF THREE
FORMS OF MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
Authors : Mcphalen, C.A.; Vincent, M.G.; Jansonius, J.N.
Deposited on : 1991-12-02
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

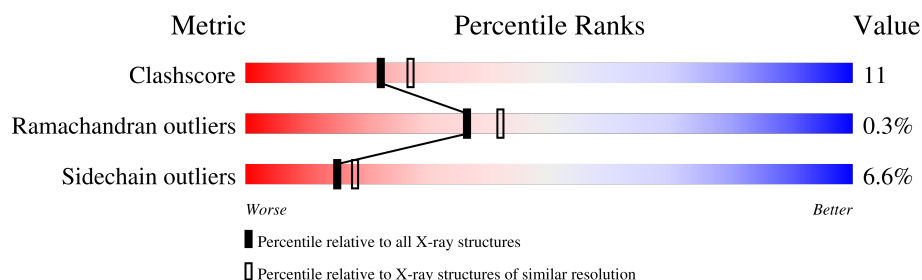
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6974 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.

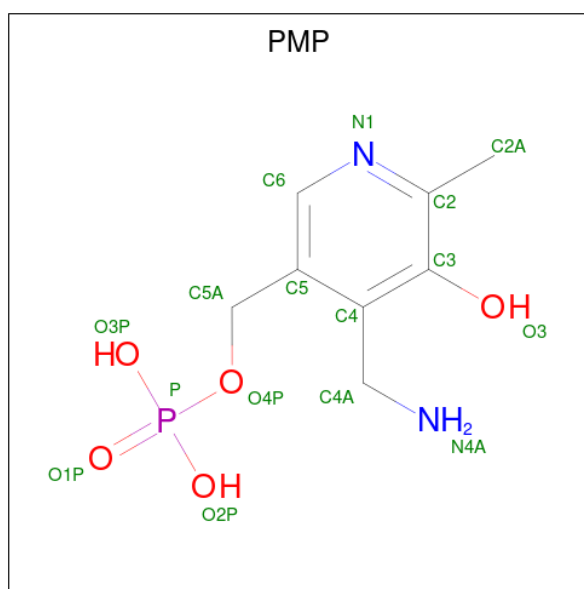
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3161	2004	558	581	18			
1	B	401	Total	C	N	O	S	0	0	0
			3161	2004	558	581	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508
B	47	PRO	SER	conflict	UNP P00508

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



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

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

- Molecule 3 is water.

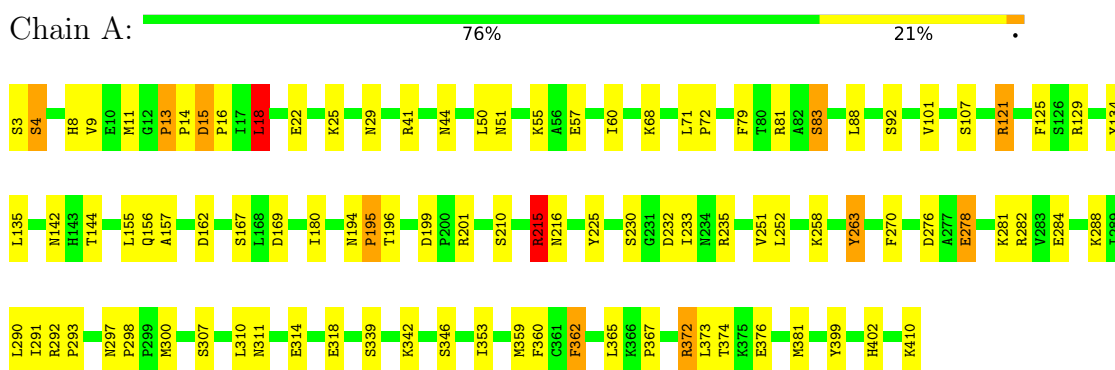
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	311	Total	O	0	0
			311	311		
3	B	309	Total	O	0	0
			309	309		

3 Residue-property plots

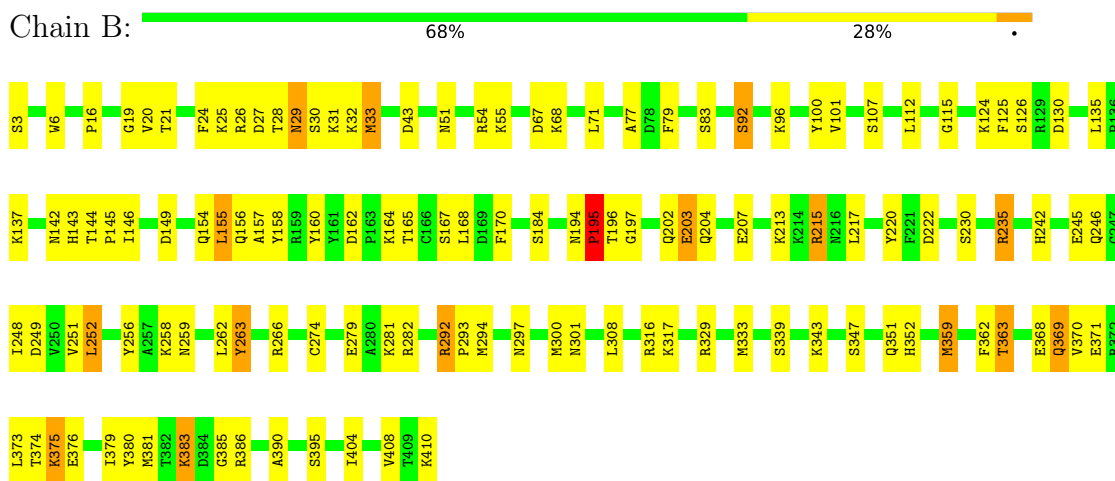
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.67Å 58.66Å 75.79Å 85.20° 109.30° 115.70°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.131 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6974	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.83	0/3231	1.69	35/4360 (0.8%)
1	B	0.83	0/3231	1.65	37/4360 (0.8%)
All	All	0.83	0/6462	1.67	72/8720 (0.8%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	CB-CG-CD	8.21	126.55	112.60
1	B	215	ARG	CD-NE-CZ	-7.51	113.89	124.40
1	B	300	MET	N-CA-C	7.40	121.55	112.23
1	A	297	ASN	CB-CA-C	7.36	119.92	109.92
1	A	298	PRO	N-CA-C	7.26	119.56	110.70
1	B	33	MET	CB-CA-C	7.02	123.25	109.35
1	A	232	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	300	MET	N-CA-C	6.87	120.89	112.23
1	B	71	LEU	N-CA-C	-6.84	101.19	110.36
1	B	266	ARG	N-CA-C	6.80	118.87	110.91
1	A	215	ARG	CD-NE-CZ	-6.80	114.88	124.40
1	B	196	THR	N-CA-C	6.80	120.80	112.23
1	B	6	TRP	N-CA-C	6.73	121.56	112.88
1	A	8	HIS	CA-CB-CG	-6.69	107.11	113.80
1	A	13	PRO	O-C-N	6.64	124.27	121.15
1	A	270	PHE	CA-C-O	-6.42	113.42	120.36
1	A	251	VAL	CB-CA-C	6.35	120.61	110.82
1	B	376	GLU	N-CA-C	6.27	121.21	113.50
1	B	375	LYS	N-CA-C	6.12	117.62	111.07
1	B	297	ASN	CB-CA-C	6.06	119.07	109.55
1	A	252	LEU	N-CA-CB	-6.01	100.33	111.52
1	A	199	ASP	O-C-N	5.91	127.30	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	B	197	GLY	N-CA-C	-5.77	107.70	115.21
1	A	225	TYR	CA-C-O	-5.69	115.28	121.20
1	B	251	VAL	CB-CA-C	5.69	119.80	110.69
1	A	72	PRO	N-CA-C	-5.66	102.57	111.34
1	B	252	LEU	N-CA-CB	-5.63	101.05	111.52
1	A	71	LEU	N-CA-C	-5.57	102.89	110.36
1	A	251	VAL	N-CA-C	-5.56	100.29	108.85
1	B	316	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	18	LEU	N-CA-C	-5.54	105.16	111.14
1	B	195	PRO	N-CA-C	5.50	126.40	112.10
1	A	196	THR	N-CA-C	5.47	120.07	112.90
1	A	125	PHE	N-CA-C	5.44	118.13	111.82
1	A	233	ILE	N-CA-C	5.44	116.17	110.62
1	A	210	SER	O-C-N	5.44	128.35	122.15
1	B	115	GLY	CA-C-N	5.42	127.54	120.28
1	B	115	GLY	C-N-CA	5.42	127.54	120.28
1	B	363	THR	CA-CB-OG1	-5.41	101.48	109.60
1	B	215	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	B	101	VAL	N-CA-CB	5.39	120.31	111.58
1	B	143	HIS	N-CA-CB	5.38	118.13	110.06
1	B	126	SER	N-CA-CB	-5.37	102.56	111.57
1	A	374	THR	O-C-N	5.35	127.81	122.03
1	B	130	ASP	CA-CB-CG	5.33	117.92	112.60
1	B	301	ASN	N-CA-C	5.32	117.52	111.02
1	B	251	VAL	CA-C-O	-5.25	115.19	121.28
1	A	225	TYR	N-CA-CB	-5.24	104.31	111.65
1	B	251	VAL	N-CA-C	-5.24	100.32	108.86
1	B	404	ILE	O-C-N	5.23	126.94	121.87
1	A	346	SER	N-CA-CB	5.22	117.63	109.85
1	B	184	SER	CA-C-O	-5.22	115.79	121.89
1	A	216	ASN	N-CA-CB	-5.18	104.03	111.70
1	A	44	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	362	PHE	N-CA-C	-5.18	100.07	108.41
1	B	248	ILE	N-CA-CB	-5.17	105.17	111.21
1	A	15	ASP	CB-CA-C	5.14	117.74	109.41
1	A	291	ILE	N-CA-C	5.14	115.91	110.72
1	A	201	ARG	N-CA-C	-5.13	103.15	110.59
1	B	213	LYS	CA-C-N	5.12	127.13	120.28
1	B	213	LYS	C-N-CA	5.12	127.13	120.28
1	A	29	ASN	CB-CA-C	5.10	117.91	110.26
1	B	92	SER	N-CA-C	-5.10	102.74	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ALA	N-CA-C	5.09	116.83	111.28
1	B	125	PHE	N-CA-C	5.09	117.57	111.71
1	A	144	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	245	GLU	CA-CB-CG	5.08	124.25	114.10
1	B	410	LYS	N-CA-CB	5.05	119.09	110.50
1	A	180	ILE	O-C-N	5.04	127.37	121.57
1	B	54	ARG	N-CA-CB	5.04	117.52	110.12
1	A	60	ILE	O-C-N	5.03	126.84	121.91

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	3161	0	3154	51	0
1	B	3161	0	3154	90	0
2	A	16	0	11	3	0
2	B	16	0	11	5	0
3	A	311	0	0	10	0
3	B	309	0	0	13	0
All	All	6974	0	6330	134	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 11.

All (134) 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:207:GLU:HG2	3:B:711:HOH:O	1.33	1.26
1:B:164:LYS:HG3	1:B:165:THR:HG23	1.27	1.16
1:B:29:ASN:HD21	1:B:31:LYS:HB2	1.06	1.13
1:B:29:ASN:ND2	1:B:31:LYS:HB2	1.71	1.06
1:A:57:GLU:OE1	3:A:665:HOH:O	1.79	0.99
1:B:29:ASN:ND2	1:B:31:LYS:H	1.62	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HD22	1:B:31:LYS:H	0.94	0.94
1:B:258:LYS:NZ	2:B:411:PMP:HNA2	1.64	0.94
1:A:129:ARG:HA	1:A:129:ARG:HE	1.34	0.93
1:A:372:ARG:HD3	1:A:376:GLU:OE2	1.68	0.91
1:A:258:LYS:NZ	2:A:411:PMP:HNA2	1.76	0.84
1:B:164:LYS:CG	1:B:165:THR:HG23	2.07	0.84
1:B:258:LYS:HZ3	2:B:411:PMP:HNA2	1.24	0.84
1:B:29:ASN:HD21	1:B:31:LYS:CB	1.88	0.84
1:B:29:ASN:HD22	1:B:31:LYS:N	1.75	0.84
1:B:347:SER:HB3	3:B:649:HOH:O	1.76	0.84
1:B:167:SER:HB2	3:B:592:HOH:O	1.78	0.82
1:B:359:MET:HE2	1:B:390:ALA:HB2	1.59	0.82
1:B:164:LYS:HG3	1:B:165:THR:CG2	2.10	0.77
1:A:276:ASP:OD1	1:A:278:GLU:HB3	1.86	0.75
1:A:129:ARG:HE	1:A:129:ARG:CA	2.01	0.74
1:A:258:LYS:HZ3	2:A:411:PMP:HNA2	1.36	0.73
1:B:29:ASN:ND2	1:B:31:LYS:CB	2.49	0.71
1:B:359:MET:CE	1:B:390:ALA:HB2	2.20	0.71
1:B:370:VAL:HG22	1:B:381:MET:HE2	1.73	0.70
1:A:167:SER:HB2	3:A:579:HOH:O	1.93	0.67
1:B:26:ARG:O	1:B:26:ARG:HG3	1.96	0.66
1:B:29:ASN:ND2	1:B:31:LYS:N	2.38	0.66
1:B:162:ASP:OD1	1:B:164:LYS:HG2	1.96	0.66
1:B:3:SER:O	3:B:690:HOH:O	2.13	0.65
1:A:3:SER:HB2	1:B:249:ASP:OD2	1.97	0.65
1:B:137:LYS:HG3	1:B:158:TYR:O	1.97	0.65
1:B:258:LYS:HZ2	2:B:411:PMP:HNA2	1.44	0.65
1:A:57:GLU:HG2	3:A:577:HOH:O	1.96	0.64
1:A:57:GLU:OE2	3:A:577:HOH:O	2.15	0.64
3:A:716:HOH:O	1:B:294:MET:HE3	1.98	0.64
1:B:369:GLN:HB3	1:B:408:VAL:CG1	2.28	0.64
1:B:374:THR:HG23	1:B:380:TYR:CD1	2.31	0.64
1:B:317:LYS:HG3	3:B:605:HOH:O	1.99	0.61
1:B:386:ARG:NH1	3:B:514:HOH:O	2.32	0.61
1:A:318:GLU:OE1	3:A:548:HOH:O	2.17	0.60
1:A:372:ARG:CD	1:A:376:GLU:OE2	2.48	0.60
1:B:79:PHE:O	1:B:83:SER:HB2	2.01	0.59
1:A:263:TYR:HB2	1:B:68:LYS:O	2.02	0.58
1:B:203:GLU:CD	1:B:203:GLU:H	2.11	0.58
1:A:129:ARG:HA	1:A:129:ARG:NE	2.12	0.58
1:A:81:ARG:NH1	3:A:675:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:O	1:B:263:TYR:HB2	2.04	0.57
1:A:79:PHE:O	1:A:83:SER:HB2	2.05	0.56
1:A:342:LYS:HG3	3:A:630:HOH:O	2.04	0.56
1:A:4:SER:HA	3:B:692:HOH:O	2.06	0.56
1:B:230:SER:CB	1:B:235:ARG:HE	2.19	0.56
1:B:135:LEU:O	1:B:157:ALA:HA	2.07	0.55
1:B:137:LYS:HG2	1:B:157:ALA:HB1	1.88	0.55
1:B:347:SER:CB	3:B:649:HOH:O	2.45	0.54
1:B:33:MET:HG2	1:B:379:ILE:HG12	1.90	0.54
1:B:92:SER:O	1:B:96:LYS:HG2	2.08	0.53
1:A:230:SER:HB2	1:A:235:ARG:HH11	1.73	0.53
1:B:374:THR:CG2	1:B:380:TYR:CE1	2.92	0.52
1:A:135:LEU:O	1:A:157:ALA:HA	2.10	0.52
1:B:21:THR:O	1:B:24:PHE:HB3	2.10	0.52
1:A:51:ASN:O	1:A:55:LYS:HG3	2.11	0.51
1:A:258:LYS:HZ2	2:A:411:PMP:HNA2	1.55	0.51
1:A:3:SER:OG	1:A:4:SER:N	2.44	0.51
1:B:215:ARG:HB2	1:B:217:LEU:HG	1.92	0.51
1:A:373:LEU:CD1	1:A:381:MET:HE3	2.41	0.51
1:B:154:GLN:NE2	3:B:543:HOH:O	2.41	0.50
1:A:307:SER:O	1:A:311:ASN:HB2	2.12	0.49
1:B:235:ARG:CG	1:B:235:ARG:HH11	2.25	0.49
1:A:22:GLU:HA	1:A:25:LYS:HE3	1.93	0.49
1:B:170:PHE:CE1	1:B:204:GLN:HB3	2.48	0.49
1:B:374:THR:HG23	1:B:380:TYR:CE1	2.46	0.49
1:A:9:VAL:O	1:B:282:ARG:NH1	2.44	0.49
1:B:352:HIS:HE1	1:B:363:THR:O	1.95	0.49
1:B:29:ASN:HD22	1:B:29:ASN:C	2.21	0.48
1:A:292:ARG:HD3	3:A:664:HOH:O	2.12	0.48
1:A:88:LEU:O	1:A:92:SER:HB2	2.14	0.48
1:A:373:LEU:HD13	1:A:381:MET:HE3	1.96	0.47
1:B:279:GLU:OE2	3:B:500:HOH:O	2.20	0.47
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.97	0.47
1:A:278:GLU:OE1	1:A:282:ARG:NH2	2.42	0.47
1:A:3:SER:CB	1:B:249:ASP:OD2	2.62	0.47
1:A:359:MET:HE2	1:A:360:PHE:CZ	2.50	0.47
1:B:262:LEU:O	1:B:263:TYR:C	2.57	0.47
1:A:134:TYR:CD2	1:A:156:GLN:HB2	2.49	0.47
1:B:160:TYR:O	1:B:168:LEU:HD12	2.14	0.47
1:B:207:GLU:CG	3:B:711:HOH:O	2.17	0.47
1:A:15:ASP:HA	1:A:16:PRO:HD3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:MET:CE	1:B:385:GLY:HA2	2.45	0.46
1:B:230:SER:HB2	1:B:235:ARG:HE	1.80	0.46
1:B:235:ARG:CG	1:B:235:ARG:NH1	2.78	0.46
1:B:222:ASP:OD2	2:B:411:PMP:N1	2.49	0.46
1:A:399:TYR:O	1:A:402:HIS:HB3	2.16	0.45
1:A:11:MET:HE2	1:A:11:MET:HB2	1.85	0.45
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.80	0.45
1:B:162:ASP:CG	1:B:164:LYS:HG2	2.41	0.45
1:A:9:VAL:O	1:B:282:ARG:HD2	2.17	0.45
1:A:194:ASN:HA	1:A:195:PRO:HA	1.75	0.45
1:B:27:ASP:HB3	1:B:32:LYS:HD2	1.99	0.45
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.40	0.45
1:A:50:LEU:N	1:A:50:LEU:HD12	2.32	0.44
1:B:194:ASN:HA	1:B:195:PRO:HA	1.82	0.44
1:A:367:PRO:HD3	3:A:451:HOH:O	2.16	0.44
1:B:29:ASN:ND2	1:B:31:LYS:CA	2.80	0.44
1:B:51:ASN:O	1:B:55:LYS:HG3	2.17	0.44
1:B:142:ASN:O	1:B:146:ILE:HG13	2.18	0.44
1:B:112:LEU:HA	1:B:220:TYR:OH	2.17	0.44
1:B:145:PRO:O	1:B:149:ASP:HB2	2.18	0.44
1:A:162:ASP:HB2	1:A:169:ASP:HB2	2.00	0.44
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.83	0.43
1:A:284:GLU:O	1:A:288:LYS:HG3	2.19	0.43
1:B:144:THR:HB	1:B:145:PRO:HD3	2.00	0.43
1:B:329:ARG:O	1:B:333:MET:HG2	2.17	0.43
1:B:256:TYR:HA	1:B:259:ASN:OD1	2.19	0.43
1:B:274:CYS:HB3	1:B:279:GLU:HG2	2.00	0.42
1:B:374:THR:CG2	1:B:380:TYR:CD1	3.01	0.42
1:B:155:LEU:C	1:B:156:GLN:HG2	2.45	0.42
1:A:41:ARG:HA	1:A:41:ARG:HD3	1.85	0.42
1:A:293:PRO:CG	1:B:145:PRO:HB2	2.49	0.42
1:B:100:TYR:CD1	1:B:100:TYR:C	2.98	0.42
1:B:292:ARG:N	1:B:293:PRO:CD	2.82	0.42
1:B:258:LYS:NZ	2:B:411:PMP:N4A	2.48	0.42
1:B:370:VAL:CG2	1:B:381:MET:HE2	2.43	0.41
1:B:371:GLU:HG3	1:B:383:LYS:HE2	2.01	0.41
1:B:203:GLU:CD	1:B:203:GLU:N	2.78	0.41
1:B:242:HIS:O	1:B:246:GLN:HG2	2.20	0.41
1:B:67:ASP:HB3	3:B:695:HOH:O	2.20	0.41
1:A:25:LYS:HE3	1:A:25:LYS:HB2	1.92	0.41
1:A:13:PRO:HA	1:A:14:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:HE2	1:B:165:THR:CG2	2.50	0.41
1:B:142:ASN:O	1:B:145:PRO:HD2	2.21	0.40
1:B:16:PRO:O	1:B:19:GLY:N	2.54	0.40
1:B:124:LYS:NZ	3:B:679:HOH:O	2.43	0.40
1:B:29:ASN:HD22	1:B:30:SER:N	2.19	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	399/401 (100%)	387 (97%)	11 (3%)	1 (0%)	36	42
1	B	399/401 (100%)	384 (96%)	14 (4%)	1 (0%)	36	42
All	All	798/802 (100%)	771 (97%)	25 (3%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	263	TYR

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	335/335 (100%)	315 (94%)	20 (6%)	17	21
1	B	335/335 (100%)	311 (93%)	24 (7%)	13	15
All	All	670/670 (100%)	626 (93%)	44 (7%)	15	18

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	18	LEU
1	A	83	SER
1	A	101	VAL
1	A	107	SER
1	A	121	ARG
1	A	142	ASN
1	A	155	LEU
1	A	195	PRO
1	A	215	ARG
1	A	281	LYS
1	A	290	LEU
1	A	310	LEU
1	A	314	GLU
1	A	339	SER
1	A	353	ILE
1	A	362	PHE
1	A	365	LEU
1	A	372	ARG
1	A	410	LYS
1	B	20	VAL
1	B	25	LYS
1	B	28	THR
1	B	29	ASN
1	B	43	ASP
1	B	107	SER
1	B	155	LEU
1	B	195	PRO
1	B	202	GLN
1	B	203	GLU
1	B	235	ARG
1	B	252	LEU
1	B	281	LYS
1	B	292	ARG
1	B	339	SER

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Mol	Chain	Res	Type
1	B	343	LYS
1	B	351	GLN
1	B	359	MET
1	B	362	PHE
1	B	368	GLU
1	B	369	GLN
1	B	375	LYS
1	B	383	LYS
1	B	395	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	117	ASN
1	A	142	ASN
1	A	154	GLN
1	A	202	GLN
1	A	297	ASN
1	A	349	ASN
1	A	351	GLN
1	B	29	ASN
1	B	154	GLN
1	B	216	ASN
1	B	336	GLN
1	B	340	ASN
1	B	348	HIS
1	B	351	GLN
1	B	352	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	411	-	16,16,16	1.01	0	22,23,23	2.10	6 (27%)
2	PMP	B	411	-	16,16,16	1.07	1 (6%)	22,23,23	2.08	6 (27%)

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	411	-	-	4/8/8/8	0/1/1/1
2	PMP	B	411	-	-	5/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PMP	P-O3P	-2.04	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PMP	C5-C6-N1	-4.98	115.72	123.83
2	B	411	PMP	C5-C6-N1	-4.75	116.10	123.83
2	A	411	PMP	C3-C2-N1	-4.67	115.07	120.96
2	B	411	PMP	C3-C2-N1	-4.17	115.70	120.96
2	B	411	PMP	C6-N1-C2	4.16	126.75	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	PMP	C6-N1-C2	3.82	126.12	119.20
2	B	411	PMP	C6-C5-C4	3.25	120.52	118.06
2	A	411	PMP	C2A-C2-N1	2.89	123.08	117.64
2	A	411	PMP	C6-C5-C4	2.81	120.19	118.06
2	B	411	PMP	C2A-C2-N1	2.65	122.63	117.64
2	A	411	PMP	C5A-C5-C4	-2.50	117.41	122.67
2	B	411	PMP	C4A-C4-C3	-2.07	116.72	120.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	PMP	C5A-O4P-P-O1P
2	A	411	PMP	C5A-O4P-P-O2P
2	A	411	PMP	C5A-O4P-P-O3P
2	B	411	PMP	C6-C5-C5A-O4P
2	B	411	PMP	C5A-O4P-P-O1P
2	B	411	PMP	C5A-O4P-P-O2P
2	B	411	PMP	C5A-O4P-P-O3P
2	A	411	PMP	C6-C5-C5A-O4P
2	B	411	PMP	C4-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PMP	3	0
2	B	411	PMP	5	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.