



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 AM UTC

PDB ID : 1TIS / pdb_00001tis
Title : CRYSTAL STRUCTURE OF THYMIDYLATE SYNTHASE FROM T4 PHAGE
Authors : Finer-Moore, J.; Stroud, R.
Deposited on : 1994-01-24
Resolution : 2.70 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

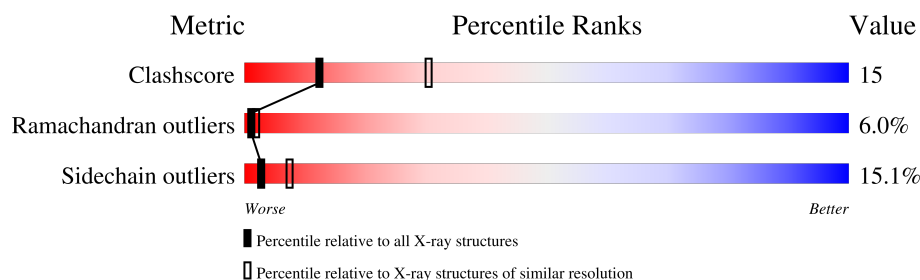
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	286	

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
2	PO4	A	287	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2362 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 THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	1	0
			2337	1512	398	416	11			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

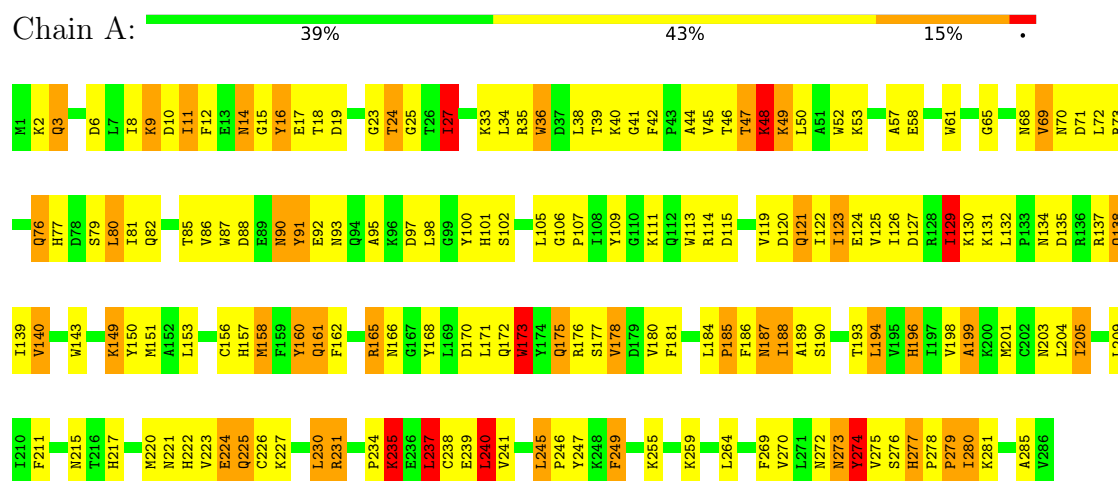
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		

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: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.02Å 68.02Å 140.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2362	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: PO4

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	1.14	12/2402 (0.5%)	2.21	114/3252 (3.5%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	77	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	140	VAL	CA-CB	6.94	1.63	1.54
1	A	217	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	277	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	222[A]	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	222[B]	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	188	ILE	CA-CB	5.80	1.60	1.54
1	A	157	HIS	CG-ND1	-5.79	1.31	1.38
1	A	196	HIS	CG-ND1	-5.61	1.32	1.38
1	A	157	HIS	CD2-NE2	-5.49	1.31	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	PHE	CA-CB-CG	13.52	127.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	VAL	N-CA-C	11.57	124.90	108.36
1	A	14	ASN	OD1-CG-ND2	-9.14	113.46	122.60
1	A	82	GLN	OE1-CD-NE2	-8.45	114.15	122.60
1	A	285	ALA	N-CA-C	8.29	121.78	109.59
1	A	87	TRP	CG-CD2-CE3	8.09	141.99	133.90
1	A	157	HIS	CA-CB-CG	7.96	121.76	113.80
1	A	166	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	121	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	A	217	HIS	CB-CG-CD2	-7.79	121.08	131.20
1	A	166	ASN	N-CA-C	-7.77	91.43	107.67
1	A	24	THR	N-CA-C	-7.62	94.58	110.80
1	A	221	ASN	N-CA-C	7.57	121.20	110.68
1	A	272	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	A	16	TYR	N-CA-C	7.54	122.11	108.17
1	A	278	PRO	N-CA-C	7.40	119.73	110.70
1	A	27	ILE	N-CA-C	-7.31	97.93	108.17
1	A	48	LYS	N-CA-C	-7.31	95.23	110.80
1	A	217	HIS	CA-CB-CG	7.25	121.05	113.80
1	A	186	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	18	THR	N-CA-CB	-6.99	99.53	111.69
1	A	217	HIS	CB-CG-ND1	6.96	133.15	122.70
1	A	129	ILE	CB-CA-C	-6.94	102.77	112.14
1	A	52	TRP	CE2-CD2-CE3	6.93	125.73	118.80
1	A	274	TYR	CA-CB-CG	6.90	126.33	113.90
1	A	226	CYS	N-CA-C	-6.75	103.85	111.14
1	A	23	GLY	O-C-N	6.71	131.42	122.70
1	A	12	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	160	TYR	CA-CB-CG	6.64	125.86	113.90
1	A	82	GLN	CG-CD-NE2	6.59	126.29	116.40
1	A	239	GLU	N-CA-C	-6.58	101.67	110.55
1	A	72	LEU	N-CA-C	-6.55	104.14	111.28
1	A	77	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	A	101	HIS	O-C-N	6.45	130.75	123.27
1	A	205	ILE	N-CA-C	-6.44	101.26	107.76
1	A	139	ILE	CA-C-O	-6.40	113.43	120.72
1	A	127	ASP	CA-C-O	-6.37	114.14	120.70
1	A	231	ARG	N-CA-C	6.32	124.27	110.80
1	A	193	THR	N-CA-C	-6.27	104.37	111.14
1	A	106	GLY	O-C-N	-6.22	115.55	121.77
1	A	18	THR	N-CA-C	6.21	118.62	109.24
1	A	166	ASN	CB-CG-ND2	6.17	125.65	116.40
1	A	193	THR	CA-C-O	-6.10	114.42	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASN	N-CA-C	6.06	119.14	111.69
1	A	274	TYR	N-CA-CB	-6.05	100.00	109.87
1	A	135	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	270	VAL	N-CA-CB	-6.02	99.66	112.00
1	A	11	ILE	N-CA-C	-6.00	104.67	110.72
1	A	156	CYS	N-CA-C	-5.99	104.13	112.45
1	A	140	VAL	CA-C-O	5.96	126.15	120.31
1	A	87	TRP	CB-CG-CD1	-5.96	117.96	126.90
1	A	237	LEU	O-C-N	5.91	129.89	123.10
1	A	91	TYR	N-CA-C	-5.91	103.62	111.24
1	A	138	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	81	ILE	CB-CA-C	-5.89	101.63	111.29
1	A	49	LYS	N-CA-C	-5.78	99.39	108.63
1	A	269	PHE	N-CA-C	-5.76	99.02	108.76
1	A	203	ASN	CA-C-O	5.73	129.25	122.14
1	A	93	ASN	CA-C-O	-5.73	112.31	120.51
1	A	101	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	149	LYS	CA-CB-CG	-5.68	102.73	114.10
1	A	123	ILE	CA-C-O	-5.63	115.19	121.05
1	A	196	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	134	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	131	LYS	N-CA-CB	-5.54	101.12	110.49
1	A	18	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	90	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	119	VAL	CB-CA-C	-5.48	103.99	111.33
1	A	188	ILE	N-CA-C	-5.48	104.53	110.23
1	A	203	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	189	ALA	CA-C-O	-5.47	115.25	121.00
1	A	273	ASN	CA-C-O	5.45	128.31	120.51
1	A	139	ILE	O-C-N	-5.44	117.59	123.14
1	A	187	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	121	GLN	CA-CB-CG	5.38	124.86	114.10
1	A	158	MET	CG-SD-CE	-5.37	89.08	100.90
1	A	240	LEU	N-CA-C	5.37	116.89	109.54
1	A	97	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	123	ILE	CA-CB-CG1	-5.36	101.30	110.40
1	A	58	GLU	N-CA-C	-5.35	105.36	111.14
1	A	69	VAL	CB-CA-C	-5.34	105.13	111.97
1	A	14	ASN	CB-CG-ND2	5.32	124.38	116.40
1	A	138	GLN	O-C-N	5.30	129.23	122.65
1	A	143	TRP	CG-CD2-CE3	5.30	139.20	133.90
1	A	137	ARG	O-C-N	-5.28	115.56	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	TRP	CE2-CD2-CE3	5.28	124.08	118.80
1	A	18	THR	CA-CB-CG2	5.27	119.46	110.50
1	A	277	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	161	GLN	CA-CB-CG	5.23	124.55	114.10
1	A	6	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	61	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	A	16	TYR	CA-C-O	5.19	127.73	121.66
1	A	17	GLU	N-CA-C	-5.18	98.25	107.98
1	A	274	TYR	CB-CA-C	5.17	118.77	110.29
1	A	36	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	87	TRP	CE2-CD2-CG	-5.15	101.03	107.20
1	A	166	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	199	ALA	CA-C-O	-5.12	114.08	119.97
1	A	139	ILE	N-CA-C	5.11	115.94	108.53
1	A	10	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	34	LEU	CA-C-O	-5.10	115.79	121.51
1	A	151	MET	CA-CB-CG	5.10	124.31	114.10
1	A	44	ALA	N-CA-C	5.07	116.74	108.63
1	A	149	LYS	CA-C-O	-5.07	114.52	120.20
1	A	170	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	235	LYS	CA-CB-CG	5.06	124.21	114.10
1	A	131	LYS	CA-CB-CG	5.05	124.19	114.10
1	A	272	ASN	CB-CG-ND2	5.04	123.97	116.40
1	A	88	ASP	N-CA-C	5.04	117.16	111.02
1	A	47	THR	O-C-N	5.03	129.27	122.59
1	A	178	VAL	CA-CB-CG1	-5.03	101.86	110.40
1	A	277	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	36	TRP	CD1-CG-CD2	5.02	114.33	106.30
1	A	76	GLN	CA-CB-CG	5.01	124.12	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	TYR	Sidechain

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	2337	0	2334	72	0
2	A	5	0	0	0	0
3	A	20	0	0	0	0
All	All	2362	0	2334	72	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 15.

All (72) 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:238:CYS:HG	1:A:274:TYR:HD1	1.25	0.84
1:A:9:LYS:NZ	1:A:230:LEU:HB2	1.94	0.83
1:A:33:LYS:HA	1:A:211:PHE:O	1.87	0.74
1:A:57:ALA:CB	1:A:76:GLN:HG2	2.23	0.68
1:A:114:ARG:HH11	1:A:122:ILE:HB	1.57	0.68
1:A:196:HIS:CE1	1:A:240:LEU:HD12	2.31	0.64
1:A:91:TYR:HB2	1:A:105:LEU:HD21	1.80	0.63
1:A:158:MET:HE1	1:A:176:ARG:HB2	1.81	0.63
1:A:126:ILE:O	1:A:130:LYS:HG2	2.00	0.61
1:A:49:LYS:H	1:A:279:PRO:HB3	1.69	0.57
1:A:168:TYR:HA	1:A:205:ILE:O	2.05	0.56
1:A:158:MET:CE	1:A:176:ARG:HB2	2.35	0.56
1:A:165:ARG:HB2	1:A:168:TYR:HB2	1.87	0.56
1:A:25:GLY:HA3	1:A:220:MET:SD	2.45	0.56
1:A:238:CYS:SG	1:A:274:TYR:HD1	2.28	0.56
1:A:9:LYS:HZ3	1:A:230:LEU:HB2	1.70	0.56
1:A:38:LEU:HD11	1:A:209:LEU:HB2	1.87	0.55
1:A:42:PHE:HB2	1:A:240:LEU:HD13	1.88	0.55
1:A:98:LEU:HD12	1:A:100:TYR:CE2	2.44	0.53
1:A:246:PRO:O	1:A:249:PHE:HB2	2.10	0.52
1:A:111:LYS:HD2	1:A:115:ASP:HB3	1.92	0.52
1:A:173:TRP:CH2	1:A:187:ASN:HB3	2.45	0.51
1:A:129:ILE:HD13	1:A:138:GLN:OE1	2.11	0.51
1:A:199:ALA:HB1	1:A:204:LEU:O	2.11	0.50
1:A:11:ILE:HG22	1:A:27:ILE:HG22	1.93	0.50
1:A:14:ASN:OD1	1:A:16:TYR:N	2.45	0.50
1:A:8:ILE:HA	1:A:11:ILE:HD12	1.92	0.49
1:A:173:TRP:CD1	1:A:173:TRP:H	2.29	0.49
1:A:126:ILE:HG21	1:A:201:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD23	1:A:172:GLN:N	2.28	0.48
1:A:65:GLY:CA	1:A:114:ARG:HG3	2.43	0.47
1:A:107:PRO:HD2	1:A:150:TYR:O	2.13	0.47
1:A:113:TRP:O	1:A:121:GLN:HG2	2.15	0.47
1:A:91:TYR:HA	1:A:95:ALA:HB3	1.97	0.47
1:A:11:ILE:O	1:A:14:ASN:HB3	2.15	0.47
1:A:125:VAL:O	1:A:129:ILE:HG12	2.15	0.46
1:A:259:LYS:HB2	1:A:259:LYS:HE3	1.76	0.46
1:A:280:ILE:HG22	1:A:281:LYS:H	1.81	0.46
1:A:173:TRP:HZ3	1:A:175:GLN:NE2	2.13	0.45
1:A:184:LEU:HB3	1:A:185:PRO:HD3	1.99	0.45
1:A:276:SER:O	1:A:277:HIS:ND1	2.49	0.45
1:A:69:VAL:HG22	1:A:105:LEU:HD11	2.00	0.44
1:A:245:LEU:HD12	1:A:249:PHE:CE2	2.53	0.44
1:A:48:LYS:O	1:A:50:LEU:N	2.50	0.44
1:A:9:LYS:HZ1	1:A:230:LEU:HB2	1.79	0.44
1:A:224:GLU:HG3	1:A:227:LYS:HD2	2.00	0.44
1:A:158:MET:HB3	1:A:158:MET:HE2	1.74	0.43
1:A:126:ILE:HD13	1:A:201:MET:SD	2.59	0.43
1:A:38:LEU:HD23	1:A:196:HIS:CE1	2.53	0.43
1:A:41:GLY:HA3	1:A:237:LEU:HD13	2.00	0.43
1:A:180:VAL:HG13	1:A:184:LEU:HD23	2.00	0.43
1:A:194:LEU:O	1:A:198:VAL:HG23	2.19	0.43
1:A:2:LYS:HG3	1:A:3:GLN:N	2.33	0.43
1:A:14:ASN:CG	1:A:15:GLY:N	2.76	0.43
1:A:73:ARG:HB3	1:A:79:SER:O	2.18	0.43
1:A:42:PHE:HB2	1:A:240:LEU:HB3	2.01	0.43
1:A:235:LYS:HE2	1:A:235:LYS:H	1.84	0.42
1:A:114:ARG:O	1:A:120:ASP:HA	2.19	0.42
1:A:173:TRP:CD1	1:A:173:TRP:N	2.87	0.42
1:A:68:ASN:HB3	1:A:71:ASP:OD2	2.20	0.42
1:A:184:LEU:O	1:A:188:ILE:HG13	2.20	0.42
1:A:126:ILE:HG21	1:A:201:MET:CE	2.50	0.42
1:A:70:ASN:HB3	1:A:80:LEU:HG	2.02	0.41
1:A:162:PHE:CE1	1:A:171:LEU:HD12	2.55	0.41
1:A:160:TYR:HA	1:A:172:GLN:O	2.19	0.41
1:A:176:ARG:HH11	1:A:176:ARG:HD3	1.62	0.41
1:A:25:GLY:C	1:A:220:MET:SD	3.04	0.41
1:A:149:LYS:HD3	1:A:149:LYS:HA	1.61	0.41
1:A:223:VAL:HG12	1:A:227:LYS:HG3	2.01	0.41
1:A:38:LEU:HD23	1:A:196:HIS:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:HE3	1:A:209:LEU:O	2.05	0.40
1:A:114:ARG:NH1	1:A:120:ASP:OD1	2.55	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	285/286 (100%)	230 (81%)	38 (13%)	17 (6%)	1 2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ARG
1	A	225	GLN
1	A	90	ASN
1	A	92	GLU
1	A	102	SER
1	A	231	ARG
1	A	249	PHE
1	A	24	THR
1	A	109	TYR
1	A	273	ASN
1	A	279	PRO
1	A	48	LYS
1	A	46	THR
1	A	47	THR
1	A	247	TYR
1	A	275	VAL
1	A	280	ILE

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	253/253 (100%)	215 (85%)	38 (15%)	3 7

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	LYS
1	A	19	ASP
1	A	27	ILE
1	A	35	ARG
1	A	39	THR
1	A	40	LYS
1	A	45	VAL
1	A	53	LYS
1	A	80	LEU
1	A	85	THR
1	A	86	VAL
1	A	123	ILE
1	A	124	GLU
1	A	129	ILE
1	A	132	LEU
1	A	140	VAL
1	A	153	LEU
1	A	161	GLN
1	A	173	TRP
1	A	175	GLN
1	A	177	SER
1	A	178	VAL
1	A	185	PRO
1	A	190	SER
1	A	194	LEU
1	A	215	ASN
1	A	224	GLU
1	A	225	GLN
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	234	PRO
1	A	235	LYS
1	A	237	LEU
1	A	240	LEU
1	A	245	LEU
1	A	255	LYS
1	A	264	LEU
1	A	274	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	172	GLN
1	A	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PO4	A	287	-	4,4,4	2.93	2 (50%)	6,6,6	2.36	5 (83%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	287	PO4	P-O1	4.66	1.61	1.50
2	A	287	PO4	P-O4	-2.39	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	287	PO4	O4-P-O1	-3.05	100.17	110.95
2	A	287	PO4	O4-P-O3	2.75	116.48	107.91
2	A	287	PO4	O3-P-O1	-2.31	102.77	110.95
2	A	287	PO4	O4-P-O2	2.17	114.67	107.91
2	A	287	PO4	O3-P-O2	2.06	114.33	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.