



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:27 am GMT

PDB ID : 1TDA
Title : STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH₂H₄FOLATE
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Deposited on : 1993-02-15
Resolution : 3.09 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

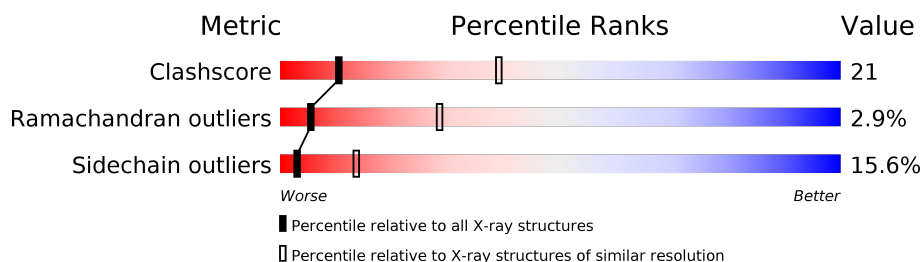
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	

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	317	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2641 atoms, of which 0 are hydrogens and 16 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	315	Total	C	D	N	O	S	0	0	0
			2599	1672	16	437	466	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is water.

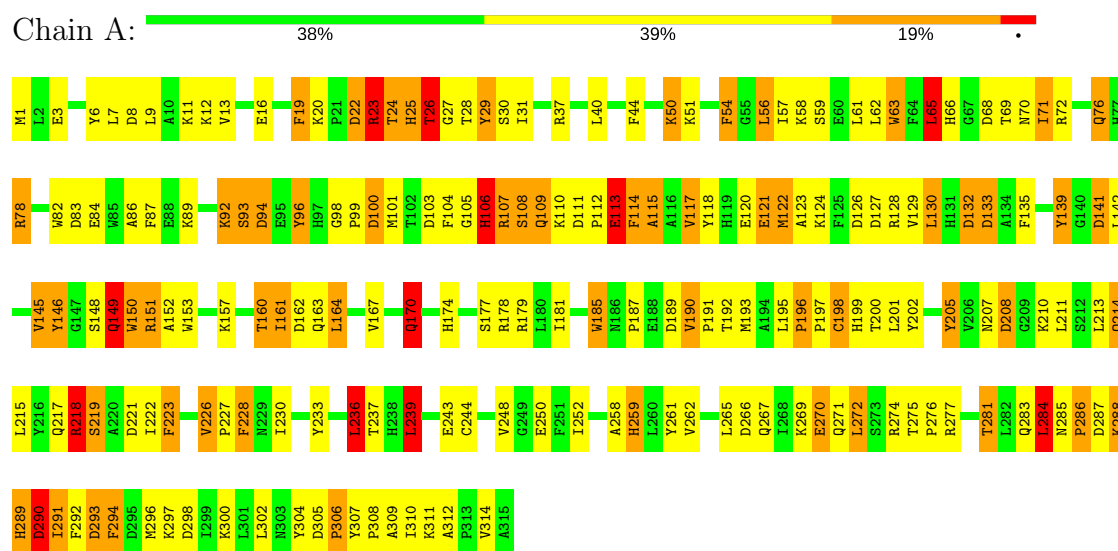
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		

3 Residue-property plots

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.

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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 78.80Å 243.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.09	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.09)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2641	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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	1.77	25/2667 (0.9%)	2.38	154/3624 (4.2%)

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	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	THR	C-N	33.18	1.92	1.33
1	A	114	PHE	C-N	25.76	1.93	1.34
1	A	108	SER	C-N	25.24	1.92	1.34
1	A	219	SER	CA-CB	-9.64	1.38	1.52
1	A	19	PHE	C-N	-8.92	1.13	1.34
1	A	192	THR	CA-CB	7.52	1.72	1.53
1	A	82	TRP	CG-CD2	-6.26	1.33	1.43
1	A	63	TRP	CD2-CE2	-6.08	1.34	1.41
1	A	113	GLU	CG-CD	6.02	1.60	1.51
1	A	196	PRO	N-CD	-5.83	1.39	1.47
1	A	82	TRP	CD2-CE2	-5.76	1.34	1.41
1	A	250	GLU	CD-OE1	-5.69	1.19	1.25
1	A	108	SER	CA-CB	5.59	1.61	1.52
1	A	63	TRP	CG-CD2	-5.52	1.34	1.43
1	A	185	TRP	CD2-CE2	-5.52	1.34	1.41
1	A	78	ARG	NE-CZ	5.42	1.40	1.33
1	A	219	SER	CB-OG	-5.38	1.35	1.42
1	A	150	TRP	NE1-CE2	-5.37	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	HIS	CB-CG	5.30	1.59	1.50
1	A	82	TRP	NE1-CE2	-5.28	1.30	1.37
1	A	66	HIS	CG-ND1	-5.25	1.27	1.38
1	A	187	PRO	CA-CB	-5.24	1.43	1.53
1	A	267	GLN	CA-CB	-5.16	1.42	1.53
1	A	150	TRP	CG-CD2	-5.09	1.34	1.43
1	A	63	TRP	NE1-CE2	-5.03	1.31	1.37

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	THR	O-C-N	-16.03	95.95	123.20
1	A	178	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	A	108	SER	O-C-N	-14.11	100.13	122.70
1	A	108	SER	CA-C-N	13.21	146.26	117.20
1	A	108	SER	C-N-CA	12.71	153.49	121.70
1	A	78	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	37	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	A	139	TYR	CB-CG-CD2	-12.47	113.52	121.00
1	A	292	PHE	CB-CG-CD2	-11.99	112.41	120.80
1	A	114	PHE	O-C-N	-10.36	106.12	122.70
1	A	26	THR	CA-C-N	10.24	136.68	116.20
1	A	151	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	151	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	23	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	261	TYR	CB-CG-CD1	-9.24	115.45	121.00
1	A	114	PHE	C-N-CA	9.00	144.21	121.70
1	A	205	TYR	CB-CG-CD1	-8.84	115.70	121.00
1	A	307	TYR	CB-CG-CD1	-8.46	115.92	121.00
1	A	174	HIS	CA-CB-CG	-8.34	99.42	113.60
1	A	226	VAL	CG1-CB-CG2	-8.28	97.66	110.90
1	A	266	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	A	205	TYR	CB-CG-CD2	7.88	125.73	121.00
1	A	193	MET	CG-SD-CE	7.86	112.77	100.20
1	A	160	THR	CA-CB-CG2	7.74	123.24	112.40
1	A	24	THR	O-C-N	7.72	135.05	122.70
1	A	78	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	223	PHE	CB-CG-CD1	-7.35	115.65	120.80
1	A	84	GLU	CA-CB-CG	-7.34	97.25	113.40
1	A	106	HIS	N-CA-CB	7.33	123.80	110.60
1	A	37	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	44	PHE	CB-CG-CD2	-7.21	115.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	CG-CD-NE	7.19	126.89	111.80
1	A	71	ILE	CG1-CB-CG2	-7.15	95.66	111.40
1	A	153	TRP	CD1-CG-CD2	7.03	111.92	106.30
1	A	178	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	A	274	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	150	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	A	150	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	106	HIS	CB-CA-C	-6.88	96.65	110.40
1	A	29	TYR	CB-CG-CD2	6.83	125.09	121.00
1	A	239	LEU	CA-CB-CG	6.68	130.66	115.30
1	A	262	VAL	CG1-CB-CG2	-6.67	100.22	110.90
1	A	244	CYS	CA-CB-SG	-6.66	102.02	114.00
1	A	122	MET	CG-SD-CE	6.58	110.73	100.20
1	A	54	PHE	CA-C-N	6.54	129.29	116.20
1	A	178	ARG	CB-CG-CD	-6.50	94.69	111.60
1	A	218	ARG	N-CA-C	6.39	128.27	111.00
1	A	201	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	24	THR	CA-C-N	-6.32	103.31	117.20
1	A	177	SER	CA-C-N	-6.32	103.31	117.20
1	A	44	PHE	CB-CG-CD1	6.30	125.21	120.80
1	A	170	GLN	CA-C-N	6.30	131.06	117.20
1	A	179	ARG	CA-CB-CG	6.27	127.19	113.40
1	A	63	TRP	CA-CB-CG	6.25	125.57	113.70
1	A	219	SER	CA-CB-OG	-6.23	94.37	111.20
1	A	150	TRP	CG-CD2-CE3	6.20	139.48	133.90
1	A	82	TRP	CD1-CG-CD2	6.20	111.26	106.30
1	A	270	GLU	CA-CB-CG	6.20	127.03	113.40
1	A	266	ASP	CB-CG-OD1	6.19	123.88	118.30
1	A	8	ASP	N-CA-CB	-6.18	99.47	110.60
1	A	288	LYS	CA-CB-CG	-6.14	99.88	113.40
1	A	121	GLU	N-CA-CB	-6.14	99.55	110.60
1	A	161	ILE	CG1-CB-CG2	-6.14	97.89	111.40
1	A	146	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	109	GLN	CB-CA-C	6.11	122.62	110.40
1	A	210	LYS	CA-C-N	-6.06	103.87	117.20
1	A	290	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	22	ASP	CB-CA-C	-6.05	98.30	110.40
1	A	118	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	A	314	VAL	CA-C-N	-6.00	104.01	117.20
1	A	164	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	259	HIS	CA-C-N	-5.95	104.12	117.20
1	A	117	VAL	CA-CB-CG2	5.94	119.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	TYR	O-C-N	5.92	132.18	122.70
1	A	193	MET	N-CA-CB	-5.92	99.94	110.60
1	A	250	GLU	N-CA-CB	-5.92	99.94	110.60
1	A	185	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	A	208	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	277	ARG	CB-CG-CD	-5.90	96.27	111.60
1	A	109	GLN	N-CA-CB	-5.88	100.02	110.60
1	A	152	ALA	N-CA-CB	-5.85	101.91	110.10
1	A	211	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	A	66	HIS	CA-C-N	5.82	127.83	116.20
1	A	167	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	A	25	HIS	CB-CA-C	5.80	122.00	110.40
1	A	272	LEU	O-C-N	-5.76	113.49	122.70
1	A	153	TRP	CE2-CD2-CG	-5.75	102.70	107.30
1	A	106	HIS	N-CA-C	-5.72	95.54	111.00
1	A	272	LEU	CA-C-N	5.69	129.71	117.20
1	A	202	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	189	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	185	TRP	CD1-CG-CD2	5.62	110.80	106.30
1	A	122	MET	CA-CB-CG	5.61	122.84	113.30
1	A	82	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	A	50	LYS	CA-CB-CG	5.59	125.70	113.40
1	A	29	TYR	CG-CD1-CE1	5.58	125.77	121.30
1	A	149	GLN	CG-CD-NE2	-5.58	103.31	116.70
1	A	284	LEU	CB-CA-C	-5.56	99.64	110.20
1	A	115	ALA	CA-C-N	5.53	129.37	117.20
1	A	294	PHE	CA-C-N	-5.52	105.07	117.20
1	A	133	ASP	CA-C-N	-5.51	105.07	117.20
1	A	305	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	6	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	A	151	ARG	CA-C-N	5.46	129.20	117.20
1	A	141	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	114	PHE	CA-C-N	5.42	129.13	117.20
1	A	62	LEU	O-C-N	-5.42	114.03	122.70
1	A	133	ASP	O-C-N	5.42	131.37	122.70
1	A	193	MET	N-CA-C	5.41	125.61	111.00
1	A	230	ILE	CG1-CB-CG2	-5.41	99.51	111.40
1	A	198	CYS	CA-CB-SG	-5.40	104.28	114.00
1	A	160	THR	CA-CB-OG1	-5.39	97.69	109.00
1	A	218	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	214	GLN	CG-CD-NE2	5.34	129.51	116.70
1	A	290	ASP	CA-CB-CG	5.31	125.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PHE	CA-C-O	-5.31	108.95	120.10
1	A	261	TYR	CB-CG-CD2	5.30	124.18	121.00
1	A	276	PRO	CA-C-N	5.29	128.84	117.20
1	A	100	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	277	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	139	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	214	GLN	OE1-CD-NE2	-5.27	109.79	121.90
1	A	281	THR	CA-CB-CG2	5.25	119.75	112.40
1	A	189	ASP	CA-CB-CG	5.25	124.94	113.40
1	A	100	ASP	N-CA-C	5.24	125.16	111.00
1	A	292	PHE	CG-CD1-CE1	-5.23	115.04	120.80
1	A	96	TYR	CA-CB-CG	-5.21	103.50	113.40
1	A	208	ASP	N-CA-CB	-5.20	101.23	110.60
1	A	56	LEU	CD1-CG-CD2	-5.20	94.91	110.50
1	A	83	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	221	ASP	CA-CB-CG	5.17	124.78	113.40
1	A	152	ALA	O-C-N	-5.15	114.46	122.70
1	A	1	MET	N-CA-CB	5.14	119.85	110.60
1	A	117	VAL	CA-CB-CG1	-5.13	103.21	110.90
1	A	76	GLN	OE1-CD-NE2	-5.12	110.12	121.90
1	A	82	TRP	CA-C-N	-5.12	105.94	117.20
1	A	291	ILE	CA-CB-CG1	5.11	120.71	111.00
1	A	199	HIS	CA-C-N	-5.09	105.99	117.20
1	A	93	SER	O-C-N	5.09	130.84	122.70
1	A	304	TYR	N-CA-C	-5.08	97.28	111.00
1	A	286	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	281	THR	N-CA-CB	-5.07	100.67	110.30
1	A	304	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	A	66	HIS	O-C-N	-5.04	114.62	123.20
1	A	132	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	150	TRP	CB-CG-CD2	-5.03	120.06	126.60
1	A	123	ALA	CB-CA-C	-5.03	102.56	110.10
1	A	300	LYS	CA-C-N	5.03	128.26	117.20
1	A	236	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	A	199	HIS	O-C-N	5.02	130.73	122.70
1	A	65	LEU	CA-C-N	5.01	128.23	117.20
1	A	145	VAL	O-C-N	-5.01	114.69	122.70
1	A	37	ARG	CB-CA-C	-5.00	100.39	110.40
1	A	306	PRO	CA-C-N	-5.00	106.20	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	233	TYR	Sidechain
1	A	239	LEU	Mainchain
1	A	98	GLY	Peptide

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	2599	0	2483	105	0
2	A	5	0	0	0	0
3	A	37	0	0	4	0
All	All	2641	0	2483	105	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 21.

All (105) 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:108:SER:C	1:A:109:GLN:N	1.92	1.23
1:A:26:THR:C	1:A:27:GLY:N	1.92	1.22
1:A:114:PHE:C	1:A:115:ALA:N	1.93	1.21
1:A:114:PHE:O	1:A:117:VAL:HG22	1.59	1.03
1:A:107:ARG:HB3	1:A:114:PHE:CE2	1.97	0.99
1:A:290:ASP:HB2	1:A:293:ASP:HB2	1.58	0.85
1:A:107:ARG:C	1:A:114:PHE:CD2	2.60	0.76
1:A:57:ILE:HD11	1:A:228:PHE:HD1	1.51	0.75
1:A:107:ARG:C	1:A:114:PHE:HD2	1.91	0.74
1:A:71:ILE:HG22	1:A:129:VAL:HG11	1.70	0.73
1:A:92:LYS:HD2	1:A:93:SER:N	2.05	0.71
1:A:108:SER:N	1:A:114:PHE:CE2	2.59	0.71
1:A:108:SER:N	1:A:114:PHE:CD2	2.59	0.70
1:A:214:GLN:HG3	1:A:252:ILE:HB	1.73	0.70
1:A:23:ARG:NH1	1:A:24:THR:HB	2.07	0.69
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.31	0.66
1:A:92:LYS:HD2	1:A:93:SER:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HB3	1:A:309:ALA:HB2	1.79	0.65
1:A:101:MET:HB3	1:A:104:PHE:HD2	1.61	0.65
1:A:126:ASP:O	1:A:130:LEU:HD22	1.96	0.64
1:A:94:ASP:C	1:A:96:TYR:H	2.01	0.64
1:A:103:ASP:HB3	1:A:106:HIS:HD2	1.63	0.63
1:A:23:ARG:HH11	1:A:24:THR:HB	1.64	0.63
1:A:222:ILE:HD11	1:A:258:ALA:HB1	1.80	0.63
1:A:54:PHE:O	1:A:57:ILE:HB	1.99	0.62
1:A:93:SER:OG	1:A:94:ASP:OD2	2.14	0.62
1:A:89:LYS:O	1:A:89:LYS:HG2	2.00	0.61
1:A:13:VAL:HG21	1:A:222:ILE:HG13	1.83	0.60
1:A:223:PHE:HE2	1:A:312:ALA:HB2	1.65	0.60
1:A:239:LEU:HG	1:A:284:LEU:HD11	1.85	0.58
1:A:72:ARG:HG2	1:A:76:GLN:HE21	1.68	0.58
1:A:198:CYS:HA	1:A:218:ARG:HG3	1.86	0.57
1:A:223:PHE:CE2	1:A:312:ALA:HB2	2.39	0.57
1:A:101:MET:HE3	1:A:117:VAL:HG23	1.87	0.55
1:A:105:GLY:O	1:A:106:HIS:ND1	2.39	0.55
1:A:57:ILE:HD11	1:A:228:PHE:CD1	2.39	0.55
1:A:146:TYR:HA	1:A:149:GLN:HE21	1.72	0.54
1:A:106:HIS:O	1:A:110:LYS:N	2.34	0.54
1:A:103:ASP:HB3	1:A:106:HIS:CD2	2.41	0.54
1:A:92:LYS:CD	1:A:93:SER:H	2.22	0.53
1:A:26:THR:O	1:A:27:GLY:N	2.40	0.53
1:A:108:SER:N	1:A:114:PHE:HE2	2.05	0.53
1:A:71:ILE:CG2	1:A:129:VAL:HG11	2.36	0.53
1:A:197:PRO:O	1:A:218:ARG:NE	2.41	0.52
1:A:265:LEU:O	1:A:269:LYS:HB2	2.10	0.52
1:A:94:ASP:C	1:A:96:TYR:N	2.62	0.52
1:A:50:LYS:HD2	3:A:323:HOH:O	2.10	0.52
1:A:239:LEU:HG	1:A:284:LEU:CD1	2.41	0.50
1:A:108:SER:N	1:A:114:PHE:HD2	2.03	0.50
1:A:243:GLU:HG3	1:A:289:HIS:O	2.11	0.50
1:A:108:SER:CA	1:A:114:PHE:CD2	2.95	0.50
1:A:213:LEU:HD13	1:A:237:THR:OG1	2.13	0.48
1:A:127:ASP:HA	1:A:130:LEU:HD22	1.95	0.48
1:A:113:GLU:O	1:A:117:VAL:HG13	2.13	0.48
1:A:99:PRO:HD2	1:A:121:GLU:OE2	2.14	0.48
1:A:86:ALA:HB2	1:A:142:LEU:HD21	1.94	0.48
1:A:170:GLN:HA	1:A:170:GLN:HE21	1.78	0.48
1:A:196:PRO:O	1:A:218:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:HA	1:A:114:PHE:CD2	2.50	0.47
1:A:291:ILE:O	1:A:294:PHE:HB2	2.15	0.47
1:A:69:THR:CG2	1:A:148:SER:HB2	2.45	0.46
1:A:70:ASN:HA	1:A:141:ASP:HA	1.97	0.46
1:A:87:PHE:CE2	1:A:122:MET:HA	2.50	0.46
1:A:132:ASP:HB3	1:A:135:PHE:CB	2.46	0.46
1:A:61:LEU:HD11	1:A:236:LEU:HG	1.97	0.45
1:A:89:LYS:O	1:A:92:LYS:CG	2.64	0.45
1:A:101:MET:HB3	1:A:104:PHE:CD2	2.47	0.45
1:A:205:TYR:HE1	1:A:207:ASN:ND2	2.15	0.45
1:A:57:ILE:CD1	1:A:228:PHE:HD1	2.25	0.45
1:A:40:LEU:HD12	1:A:237:THR:HG21	1.99	0.45
1:A:12:LYS:O	1:A:16:GLU:HB2	2.17	0.45
1:A:19:PHE:HD2	1:A:29:TYR:HE1	1.63	0.45
1:A:30:SER:HB3	1:A:259:HIS:HB3	2.00	0.44
1:A:185:TRP:HB3	3:A:342:HOH:O	2.18	0.44
1:A:11:LYS:HD3	3:A:337:HOH:O	2.18	0.44
1:A:151:ARG:O	1:A:162:ASP:HA	2.18	0.43
1:A:198:CYS:O	1:A:217:GLN:HA	2.19	0.43
1:A:107:ARG:CB	1:A:114:PHE:CE2	2.85	0.43
1:A:145:VAL:O	1:A:149:GLN:NE2	2.52	0.43
1:A:285:ASN:HA	1:A:286:PRO:HD3	1.75	0.43
1:A:63:TRP:CH2	1:A:145:VAL:HG11	2.54	0.43
1:A:31:ILE:HG12	1:A:258:ALA:HB3	2.00	0.43
1:A:271:GLN:HB2	1:A:310:ILE:CD1	2.49	0.43
1:A:89:LYS:HE2	1:A:139:TYR:HD1	1.84	0.43
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.53	0.42
1:A:104:PHE:HA	1:A:114:PHE:CE2	2.54	0.42
1:A:19:PHE:CZ	1:A:27:GLY:HA3	2.55	0.42
1:A:50:LYS:HE3	3:A:321:HOH:O	2.19	0.42
1:A:89:LYS:O	1:A:92:LYS:HG2	2.19	0.42
1:A:145:VAL:HG12	1:A:146:TYR:H	1.85	0.42
1:A:20:LYS:HB3	1:A:22:ASP:OD2	2.20	0.42
1:A:7:LEU:HD22	1:A:272:LEU:HD23	2.02	0.42
1:A:226:VAL:N	1:A:227:PRO:HD2	2.35	0.41
1:A:149:GLN:HG2	1:A:149:GLN:H	1.64	0.41
1:A:51:LYS:HG3	1:A:306:PRO:HG2	2.02	0.41
1:A:22:ASP:OD2	1:A:28:THR:OG1	2.36	0.41
1:A:150:TRP:O	1:A:163:GLN:HB3	2.21	0.41
1:A:181:ILE:HD13	1:A:181:ILE:HG21	1.89	0.41
1:A:108:SER:CA	1:A:114:PHE:HD2	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HG2	1:A:289:HIS:N	2.36	0.41
1:A:108:SER:HA	1:A:114:PHE:HD2	1.86	0.40
1:A:132:ASP:HB3	1:A:135:PHE:HB2	2.02	0.40
1:A:65:LEU:O	1:A:151:ARG:NH1	2.54	0.40
1:A:71:ILE:HG22	1:A:129:VAL:CG1	2.45	0.40
1:A:190:VAL:HG12	1:A:191:PRO:HD3	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	313/315 (99%)	264 (84%)	40 (13%)	9 (3%)	5	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	112	PRO
1	A	25	HIS
1	A	94	ASP
1	A	106	HIS
1	A	26	THR
1	A	296	MET
1	A	208	ASP
1	A	190	VAL

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	276/277 (100%)	233 (84%)	43 (16%)	3 13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	9	LEU
1	A	23	ARG
1	A	56	LEU
1	A	58	LYS
1	A	59	SER
1	A	65	LEU
1	A	78	ARG
1	A	92	LYS
1	A	113	GLU
1	A	120	GLU
1	A	124	LYS
1	A	130	LEU
1	A	133	ASP
1	A	149	GLN
1	A	157	LYS
1	A	160	THR
1	A	161	ILE
1	A	164	LEU
1	A	170	GLN
1	A	195	LEU
1	A	200	THR
1	A	215	LEU
1	A	218	ARG
1	A	219	SER
1	A	228	PHE
1	A	236	LEU
1	A	239	LEU
1	A	248	VAL
1	A	270	GLU
1	A	275	THR
1	A	281	THR
1	A	283	GLN
1	A	284	LEU

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Mol	Chain	Res	Type
1	A	287	ASP
1	A	289	HIS
1	A	290	ASP
1	A	293	ASP
1	A	297	LYS
1	A	298	ASP
1	A	302	LEU
1	A	308	PRO
1	A	311	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	106	HIS
1	A	149	GLN
1	A	170	GLN
1	A	214	GLN
1	A	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	317	-	4,4,4	2.29	1 (25%)	6,6,6	2.80	4 (66%)

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	PO4	A	317	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	PO4	P-O1	3.95	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	PO4	O4-P-O1	-2.94	98.47	110.97
2	A	317	PO4	O3-P-O1	-2.74	99.30	110.97
2	A	317	PO4	O2-P-O1	-2.21	101.58	110.97
2	A	317	PO4	O4-P-O2	4.70	125.17	107.90

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 ⓘ

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

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.