



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:56 PM UTC

PDB ID : 4TMS / pdb_00004tms
Title : PLASTIC ADAPTATION TOWARD MUTATIONS IN PROTEINS: STRUCTURAL COMPARISON OF THYMIDYLATE SYNTHASES
Authors : Finer-Moore, J.; Stroud, R.
Deposited on : 1992-01-07
Resolution : 2.35 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

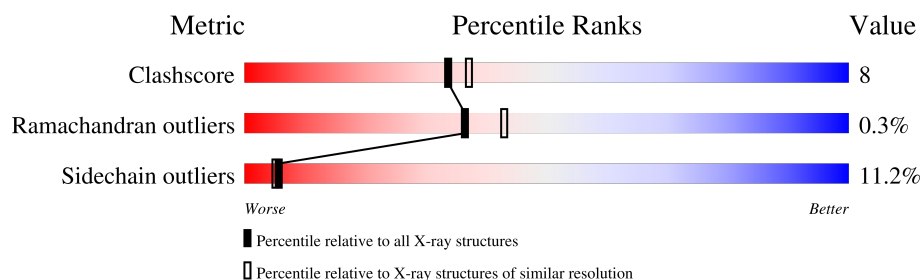
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	316	

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](#)

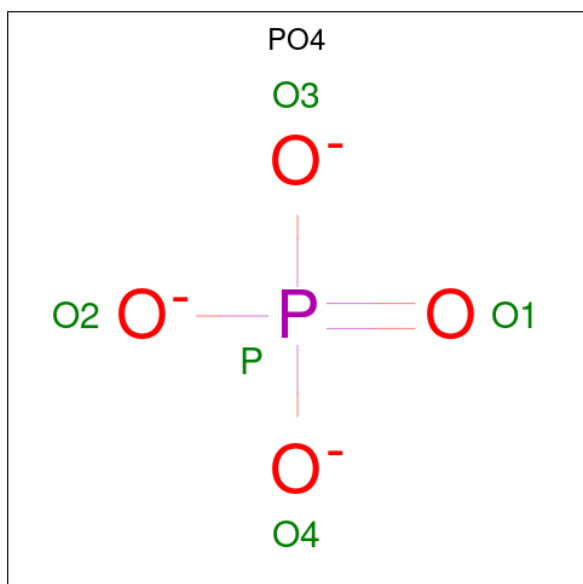
There are 3 unique types of molecules in this entry. The entry contains 2634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	316	Total	C	N	O	S	0	0	0
			2590	1677	438	467	8			

- 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.

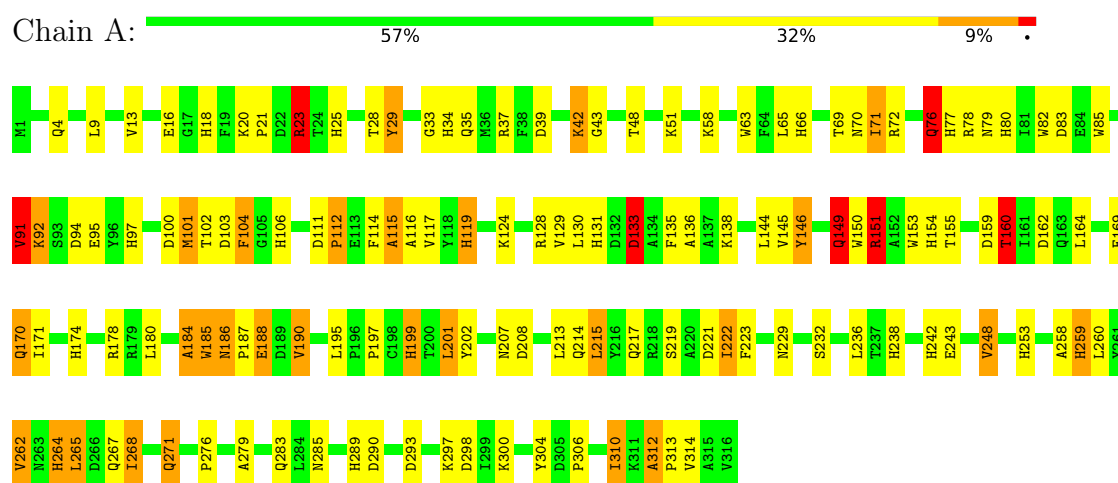
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		

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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.30 Å 78.30 Å 243.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: 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	1.35	29/2674 (1.1%)	2.13	116/3634 (3.2%)

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	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ILE	CA-CB	7.36	1.64	1.54
1	A	199	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	264	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	238	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	34	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	77	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	131	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	66	HIS	CG-ND1	-6.29	1.31	1.38
1	A	129	VAL	CA-CB	6.24	1.62	1.54
1	A	119	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	80	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	242	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	289	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	76	GLN	CA-CB	-5.95	1.43	1.53
1	A	97	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	174	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	154	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	151	ARG	CG-CD	-5.70	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	259	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	34	HIS	CG-ND1	-5.68	1.32	1.38
1	A	106	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	66	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	267	GLN	CD-NE2	-5.38	1.22	1.33
1	A	16	GLU	CA-CB	-5.37	1.45	1.53
1	A	253	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	18	HIS	CD2-NE2	-5.26	1.32	1.37
1	A	82	TRP	CG-CD2	-5.12	1.34	1.43
1	A	133	ASP	CA-CB	-5.03	1.45	1.53

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	NH1-CZ-NH2	-12.70	102.79	119.30
1	A	159	ASP	CA-CB-CG	12.13	124.73	112.60
1	A	77	HIS	CA-CB-CG	-10.83	102.97	113.80
1	A	221	ASP	CA-CB-CG	9.65	122.25	112.60
1	A	178	ARG	NE-CZ-NH2	9.16	127.44	119.20
1	A	37	ARG	NE-CZ-NH2	8.47	126.82	119.20
1	A	23	ARG	NE-CZ-NH1	-8.17	113.33	121.50
1	A	70	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	A	80	HIS	CB-CG-CD2	-7.97	120.84	131.20
1	A	77	HIS	CB-CG-CD2	-7.69	121.20	131.20
1	A	160	THR	N-CA-CB	-7.61	97.52	111.37
1	A	222	ILE	N-CA-C	7.47	118.24	110.62
1	A	248	VAL	N-CA-CB	-7.42	100.32	110.56
1	A	97	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	A	23	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	A	70	ASN	CA-CB-CG	-7.03	105.58	112.60
1	A	151	ARG	CA-CB-CG	-6.82	100.46	114.10
1	A	131	HIS	CB-CG-CD2	-6.78	122.38	131.20
1	A	133	ASP	CA-CB-CG	-6.66	105.94	112.60
1	A	37	ARG	CA-C-O	-6.65	112.62	120.60
1	A	115	ALA	CA-C-O	-6.54	114.13	121.00
1	A	238	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	248	VAL	CB-CA-C	6.53	120.15	111.21
1	A	97	HIS	CB-CG-ND1	6.44	132.35	122.70
1	A	80	HIS	CB-CG-ND1	6.43	132.35	122.70
1	A	154	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	4	GLN	OE1-CD-NE2	-6.26	116.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	154	HIS	CB-CG-ND1	6.17	131.95	122.70
1	A	51	LYS	CA-C-O	-6.14	113.46	120.58
1	A	174	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	312	ALA	CA-C-N	6.12	127.08	119.98
1	A	312	ALA	C-N-CA	6.12	127.08	119.98
1	A	178	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	A	214	GLN	CG-CD-NE2	6.04	125.46	116.40
1	A	146	TYR	CA-C-O	-5.99	114.20	120.55
1	A	232	SER	CB-CA-C	-5.97	100.70	110.85
1	A	70	ASN	CA-C-N	5.95	128.92	120.53
1	A	70	ASN	C-N-CA	5.95	128.92	120.53
1	A	70	ASN	CB-CG-ND2	5.94	125.31	116.40
1	A	129	VAL	O-C-N	-5.91	116.14	121.87
1	A	131	HIS	CB-CG-ND1	5.90	131.55	122.70
1	A	133	ASP	N-CA-C	5.88	118.17	111.11
1	A	39	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	213	LEU	CD1-CG-CD2	-5.87	97.90	110.80
1	A	289	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	A	258	ALA	O-C-N	-5.82	116.69	123.27
1	A	111	ASP	CA-C-O	5.82	124.43	119.66
1	A	298	ASP	N-CA-C	5.82	120.22	113.18
1	A	35	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	A	195	LEU	CA-C-N	5.79	126.34	120.38
1	A	195	LEU	C-N-CA	5.79	126.34	120.38
1	A	160	THR	CB-CA-C	5.78	121.47	109.38
1	A	119	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	100	ASP	N-CA-C	5.74	117.62	111.36
1	A	201	LEU	O-C-N	-5.74	117.21	123.52
1	A	186	ASN	CA-C-N	5.74	126.12	119.47
1	A	186	ASN	C-N-CA	5.74	126.12	119.47
1	A	190	VAL	N-CA-CB	-5.72	103.20	111.21
1	A	314	VAL	N-CA-C	-5.67	102.26	109.80
1	A	150	TRP	CG-CD1-NE1	-5.66	102.84	110.20
1	A	279	ALA	CA-C-O	-5.63	114.56	120.70
1	A	85	TRP	CG-CD2-CE3	5.61	139.51	133.90
1	A	271	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	79	ASN	CA-C-O	5.59	126.47	120.32
1	A	199	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	155	THR	O-C-N	-5.58	116.15	122.68
1	A	184	ALA	N-CA-C	-5.55	105.72	112.88
1	A	29	TYR	N-CA-C	-5.55	100.14	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	TRP	O-C-N	-5.53	116.92	123.22
1	A	71	ILE	CA-CB-CG2	5.51	119.86	110.50
1	A	16	GLU	N-CA-C	5.48	121.19	113.02
1	A	58	LYS	CB-CG-CD	-5.47	98.72	111.30
1	A	170	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	312	ALA	O-C-N	5.46	125.67	121.85
1	A	77	HIS	CB-CG-ND1	5.45	130.87	122.70
1	A	190	VAL	CA-CB-CG2	-5.45	101.14	110.40
1	A	169	GLU	CA-CB-CG	5.44	124.99	114.10
1	A	207	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	160	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	111	ASP	N-CA-C	5.39	116.45	109.72
1	A	229	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	106	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	A	208	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	265	LEU	CD1-CG-CD2	-5.37	98.99	110.80
1	A	25	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	285	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	63	TRP	N-CA-C	-5.33	104.71	111.11
1	A	232	SER	N-CA-CB	5.32	118.03	110.16
1	A	48	THR	N-CA-C	-5.31	106.85	113.38
1	A	202	TYR	CA-CB-CG	5.30	123.44	113.90
1	A	238	HIS	CB-CG-ND1	5.30	130.65	122.70
1	A	34	HIS	CA-CB-CG	-5.29	108.51	113.80
1	A	207	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	219	SER	O-C-N	-5.24	117.45	123.42
1	A	43	GLY	CA-C-O	-5.23	116.65	122.14
1	A	264	HIS	N-CA-C	-5.22	105.64	113.89
1	A	103	ASP	CA-C-N	5.21	131.48	121.54
1	A	103	ASP	C-N-CA	5.21	131.48	121.54
1	A	217	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	85	TRP	CE2-CD2-CG	-5.16	101.00	107.20
1	A	58	LYS	N-CA-C	-5.14	105.57	111.07
1	A	42	LYS	N-CA-C	-5.13	107.02	113.28
1	A	149	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	33	GLY	O-C-N	-5.13	116.03	122.70
1	A	82	TRP	CE2-CD2-CE3	5.12	123.92	118.80
1	A	190	VAL	N-CA-C	5.12	119.93	108.88
1	A	91	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	A	188	GLU	CA-C-O	5.10	125.96	120.70
1	A	293	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	92	LYS	CG-CD-CE	5.08	122.99	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	N-CA-C	5.07	117.70	111.82
1	A	35	GLN	O-C-N	-5.06	117.01	123.24
1	A	103	ASP	CA-C-O	5.05	128.13	122.27
1	A	119	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	310	ILE	N-CA-C	-5.03	100.33	107.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	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	2590	0	2496	39	0
2	A	5	0	0	1	0
3	A	39	0	0	1	0
All	All	2634	0	2496	39	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 8.

All (39) 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:260:LEU:HD21	1:A:268:ILE:HG21	1.80	0.64
1:A:69:THR:HG22	1:A:145:VAL:HG12	1.81	0.62
1:A:151:ARG:HG2	1:A:162:ASP:OD2	2.04	0.57
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.36	0.56
1:A:184:ALA:O	1:A:197:PRO:HG2	2.05	0.56
1:A:185:TRP:CZ2	1:A:190:VAL:HG11	2.41	0.56
1:A:283:GLN:HB3	1:A:300:LYS:HB2	1.88	0.54
1:A:112:PRO:HG2	1:A:114:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HE1	1:A:117:VAL:HG12	1.92	0.52
1:A:223:PHE:CE1	1:A:312:ALA:HB2	2.45	0.50
1:A:171:ILE:HG12	1:A:180:LEU:HD13	1.93	0.49
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.27	0.48
1:A:69:THR:HG22	1:A:145:VAL:CG1	2.44	0.48
1:A:112:PRO:HG2	1:A:114:PHE:CB	2.44	0.48
1:A:102:THR:HA	3:A:340:HOH:O	2.14	0.47
1:A:72:ARG:HH12	1:A:133:ASP:HA	1.79	0.47
1:A:91:VAL:HG11	1:A:104:PHE:HE1	1.80	0.47
1:A:271:GLN:HB2	1:A:310:ILE:CD1	2.44	0.47
1:A:223:PHE:HE1	1:A:312:ALA:HB2	1.79	0.47
1:A:72:ARG:HG2	1:A:76:GLN:HE22	1.80	0.46
1:A:153:TRP:O	1:A:160:THR:HA	2.15	0.46
1:A:264:HIS:NE2	1:A:313:PRO:O	2.45	0.46
1:A:13:VAL:HG21	1:A:222:ILE:HD11	1.99	0.45
1:A:71:ILE:HD13	1:A:71:ILE:HA	1.71	0.44
1:A:20:LYS:HA	1:A:21:PRO:HD2	1.72	0.43
1:A:29:TYR:HE2	1:A:262:VAL:HG22	1.82	0.43
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.54	0.43
1:A:72:ARG:HH11	1:A:136:ALA:HB2	1.84	0.43
1:A:23:ARG:NH1	2:A:317:PO4:O2	2.52	0.42
1:A:149:GLN:HE21	1:A:149:GLN:HB3	1.71	0.42
1:A:116:ALA:HA	1:A:119:HIS:HB2	2.01	0.42
1:A:115:ALA:O	1:A:119:HIS:CD2	2.74	0.41
1:A:264:HIS:CD2	1:A:312:ALA:HB1	2.55	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.94	0.41
1:A:186:ASN:HA	1:A:187:PRO:HD3	1.91	0.41
1:A:199:HIS:HB3	1:A:215:LEU:HD21	2.03	0.41
1:A:146:TYR:HA	1:A:149:GLN:HG2	2.03	0.40
1:A:28:THR:HB	1:A:259:HIS:HB2	2.03	0.40
1:A:304:TYR:CZ	1:A:306:PRO:HB3	2.57	0.40

There are no symmetry-related clashes.

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	314/316 (99%)	293 (93%)	20 (6%)	1 (0%)	36	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO

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	277/278 (100%)	246 (89%)	31 (11%)	6	5

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	23	ARG
1	A	42	LYS
1	A	65	LEU
1	A	76	GLN
1	A	78	ARG
1	A	91	VAL
1	A	92	LYS
1	A	94	ASP
1	A	95	GLU
1	A	101	MET
1	A	104	PHE
1	A	124	LYS
1	A	133	ASP
1	A	138	LYS
1	A	149	GLN
1	A	151	ARG
1	A	160	THR

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	170	GLN
1	A	188	GLU
1	A	201	LEU
1	A	215	LEU
1	A	236	LEU
1	A	243	GLU
1	A	248	VAL
1	A	262	VAL
1	A	265	LEU
1	A	276	PRO
1	A	290	ASP
1	A	297	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	76	GLN
1	A	119	HIS
1	A	131	HIS
1	A	149	GLN

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	317	-	4,4,4	2.52	3 (75%)	6,6,6	2.35	3 (50%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	PO4	P-O1	3.08	1.57	1.50
2	A	317	PO4	P-O2	-2.75	1.46	1.54
2	A	317	PO4	P-O3	-2.19	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	PO4	O4-P-O2	3.56	119.00	107.91
2	A	317	PO4	O2-P-O1	-2.74	101.28	110.95
2	A	317	PO4	O4-P-O1	-2.22	103.08	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	PO4	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

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.