



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 PM UTC

PDB ID : 1GRC / pdb_00001grc
Title : CRYSTAL STRUCTURE OF GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE FROM ESCHERICHIA COLI AT 3.0 ANGSTROMS RESOLUTION: A TARGET ENZYME FOR CHEMOTHERAPY
Authors : Chen, P.; Wilson, I.A.
Deposited on : 1992-07-21
Resolution : 3.00 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

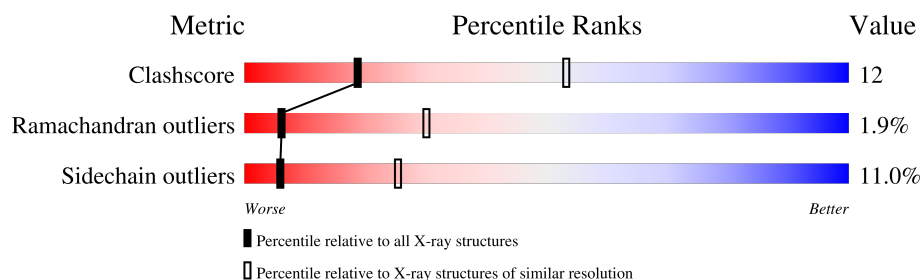
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	212	
1	B	212	

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	301	-	X	-	-
2	PO4	B	301	-	X	-	-

2 Entry composition [i](#)

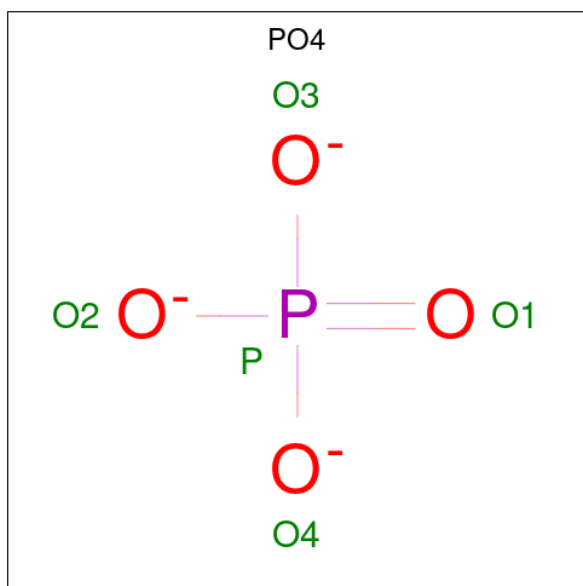
There are 2 unique types of molecules in this entry. The entry contains 2963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	1
			1487	943	262	277	5			
1	B	192	Total	C	N	O	S	0	0	1
			1466	932	258	271	5			

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



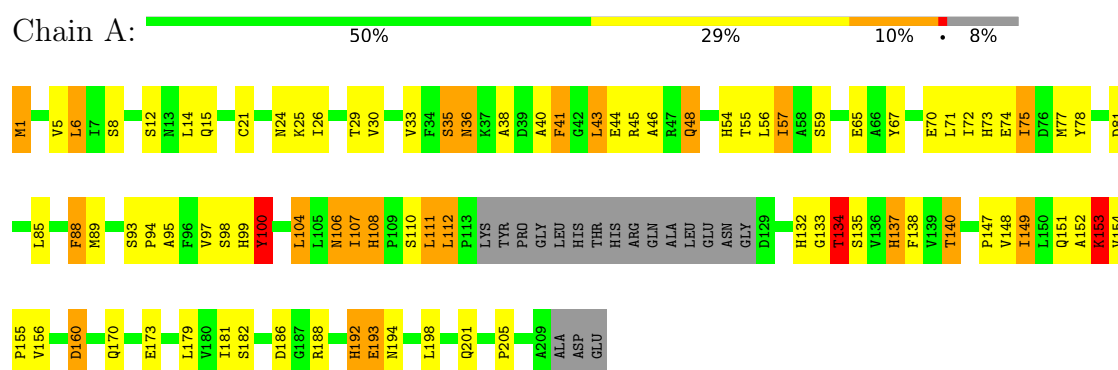
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

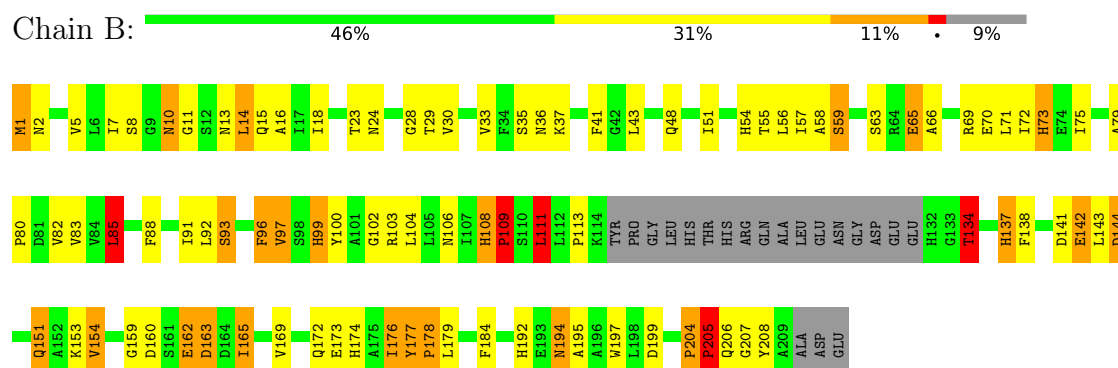
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.50Å 98.20Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2963	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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	1.30	11/1518 (0.7%)	2.06	51/2062 (2.5%)
1	B	1.32	10/1497 (0.7%)	2.17	61/2035 (3.0%)
All	All	1.31	21/3015 (0.7%)	2.11	112/4097 (2.7%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIS	CD2-NE2	-7.31	1.29	1.37
1	A	112	LEU	C-N	-7.17	1.23	1.34
1	B	113	PRO	C-N	-7.05	1.23	1.33
1	A	99	HIS	CD2-NE2	-7.02	1.30	1.37
1	B	99	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	137	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	108	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	54	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	192	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	43	LEU	CA-CB	-6.08	1.44	1.53
1	B	174	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	137	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	192	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	132	HIS	CD2-NE2	-5.68	1.31	1.37
1	B	57	ILE	CA-CB	-5.59	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	HIS	CG-ND1	-5.52	1.32	1.38
1	B	205	PRO	CA-CB	-5.43	1.46	1.53
1	A	108	HIS	CG-ND1	-5.24	1.32	1.38
1	A	54	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	134	THR	CA-CB	-5.01	1.45	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LYS	N-CA-C	-11.06	98.22	112.93
1	B	24	ASN	N-CA-C	9.38	124.30	112.86
1	B	54	HIS	CB-CG-CD2	-9.33	119.07	131.20
1	A	140	THR	N-CA-CB	-9.22	98.81	110.98
1	A	38	ALA	N-CA-C	9.20	123.60	112.38
1	B	208	TYR	N-CA-C	-9.08	96.57	110.10
1	B	108	HIS	CA-CB-CG	-9.05	104.75	113.80
1	A	54	HIS	CB-CG-CD2	-8.78	119.79	131.20
1	B	194	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	A	160	ASP	CA-CB-CG	8.75	121.35	112.60
1	B	165	ILE	N-CA-C	-8.68	102.26	110.42
1	B	151	GLN	OE1-CD-NE2	-8.60	114.00	122.60
1	B	184	PHE	CA-CB-CG	-8.33	105.47	113.80
1	A	153	LYS	CA-C-N	8.11	131.45	123.02
1	A	153	LYS	C-N-CA	8.11	131.45	123.02
1	A	149	ILE	N-CA-C	-7.76	105.13	111.81
1	A	57	ILE	N-CA-CB	-7.74	100.22	111.52
1	A	192	HIS	CB-CG-CD2	-7.72	121.17	131.20
1	B	204	PRO	N-CA-C	7.66	120.04	110.70
1	B	2	ASN	OD1-CG-ND2	-7.39	115.20	122.60
1	A	48	GLN	OE1-CD-NE2	-7.35	115.25	122.60
1	A	54	HIS	CB-CG-ND1	7.32	133.68	122.70
1	B	91	ILE	N-CA-CB	-7.28	104.04	111.90
1	B	23	THR	N-CA-CB	-7.23	98.27	110.49
1	B	93	SER	CA-C-N	6.92	126.43	119.24
1	B	93	SER	C-N-CA	6.92	126.43	119.24
1	B	108	HIS	CA-C-N	6.89	128.45	119.84
1	B	108	HIS	C-N-CA	6.89	128.45	119.84
1	A	26	ILE	N-CA-C	-6.89	98.66	108.58
1	B	104	LEU	N-CA-C	-6.81	97.17	108.34
1	A	57	ILE	CB-CA-C	6.79	120.23	110.33
1	A	33	VAL	N-CA-C	-6.74	99.04	108.27
1	B	54	HIS	CB-CG-ND1	6.74	132.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	CB-CG-ND2	-6.71	106.33	116.40
1	A	6	LEU	O-C-N	-6.71	114.71	123.16
1	B	108	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	B	176	ILE	N-CA-C	6.66	116.79	110.53
1	B	160	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	21	CYS	N-CA-C	-6.47	104.15	111.14
1	B	14	LEU	O-C-N	6.44	128.73	122.03
1	B	103	ARG	CG-CD-NE	-6.40	97.93	112.00
1	B	109	PRO	N-CA-C	6.39	125.63	112.47
1	B	5	VAL	O-C-N	-6.34	116.41	123.26
1	A	132	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	B	65	GLU	O-C-N	6.32	128.81	122.12
1	B	144	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	159	GLY	N-CA-C	-6.22	106.52	113.79
1	B	163	ASP	CA-C-O	-6.19	113.86	120.42
1	A	35	SER	N-CA-C	-6.19	99.93	109.52
1	B	205	PRO	N-CA-C	6.17	125.18	112.47
1	B	79	ALA	CA-C-N	6.09	126.30	119.90
1	B	79	ALA	C-N-CA	6.09	126.30	119.90
1	A	99	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	B	106	ASN	CB-CG-ND2	6.01	125.42	116.40
1	A	106	ASN	CB-CG-ND2	6.01	125.41	116.40
1	B	111	LEU	N-CA-C	-5.98	101.43	110.28
1	A	201	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	2	ASN	N-CA-C	-5.91	98.88	108.52
1	A	88	PHE	N-CA-C	-5.88	98.14	108.20
1	B	134	THR	O-C-N	5.87	129.67	123.03
1	A	104	LEU	O-C-N	-5.85	115.59	122.96
1	B	97	VAL	CB-CA-C	-5.85	104.25	112.14
1	A	156	VAL	N-CA-C	-5.81	99.75	108.12
1	A	140	THR	CB-CA-C	5.75	118.70	109.27
1	B	99	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	108	HIS	CA-C-N	5.71	126.98	119.84
1	A	108	HIS	C-N-CA	5.71	126.98	119.84
1	B	10	ASN	N-CA-C	5.69	119.33	112.38
1	B	59	SER	N-CA-C	5.69	118.42	111.82
1	A	75	ILE	CB-CA-C	-5.66	104.73	111.81
1	A	192	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	100	TYR	O-C-N	5.63	129.28	122.35
1	B	1	MET	CG-SD-CE	5.61	113.23	100.90
1	A	181	ILE	CA-C-O	-5.57	114.94	120.85
1	A	41	PHE	CA-CB-CG	-5.57	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LEU	N-CA-C	-5.55	99.36	108.41
1	A	72	ILE	N-CA-C	-5.55	104.15	111.09
1	A	21	CYS	O-C-N	-5.47	116.18	122.09
1	A	106	ASN	CA-CB-CG	-5.45	107.16	112.60
1	A	73	HIS	N-CA-C	5.39	116.83	111.07
1	A	75	ILE	N-CA-CB	5.37	116.48	110.62
1	B	83	VAL	N-CA-C	-5.36	99.44	107.37
1	B	33	VAL	CA-C-O	-5.35	114.83	120.39
1	B	73	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	B	100	TYR	CA-CB-CG	-5.32	104.32	113.90
1	A	192	HIS	CA-CB-CG	5.31	119.11	113.80
1	B	142	GLU	N-CA-C	-5.29	99.65	108.32
1	A	106	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	104	LEU	N-CA-C	5.27	117.34	109.59
1	A	153	LYS	CA-CB-CG	5.25	124.60	114.10
1	B	102	GLY	O-C-N	5.25	128.40	122.42
1	B	177	TYR	CA-CB-CG	5.25	123.34	113.90
1	B	59	SER	CA-C-O	5.24	126.00	119.97
1	B	96	PHE	N-CA-C	-5.23	105.22	111.03
1	A	46	ALA	N-CA-C	-5.18	105.54	111.14
1	A	89	MET	CA-CB-CG	5.18	124.46	114.10
1	A	193	GLU	CA-CB-CG	5.16	124.42	114.10
1	B	43	LEU	N-CA-C	-5.16	105.57	111.14
1	B	154	VAL	N-CA-CB	-5.14	104.01	111.21
1	B	85	LEU	N-CA-C	5.14	118.59	111.55
1	B	208	TYR	O-C-N	5.13	129.31	122.95
1	B	29	THR	CA-C-N	-5.12	116.08	122.48
1	B	29	THR	C-N-CA	-5.12	116.08	122.48
1	B	143	LEU	O-C-N	5.12	127.41	122.09
1	A	30	VAL	N-CA-CB	-5.11	105.23	111.21
1	B	55	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	135	SER	CA-CB-OG	5.09	121.29	111.10
1	A	95	ALA	N-CA-C	5.08	117.21	111.11
1	B	207	GLY	O-C-N	5.08	128.80	122.95
1	B	141	ASP	N-CA-C	-5.08	99.05	108.24
1	A	73	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	B	199	ASP	CA-CB-CG	-5.00	107.60	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	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	1487	0	1466	33	0
1	B	1466	0	1454	38	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
All	All	2963	0	2920	70	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 12.

All (70) 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:134:THR:HG21	1:A:173:GLU:HG2	1.39	1.04
1:A:137:HIS:HA	1:A:149:ILE:HD12	1.74	0.69
1:B:134:THR:HG21	1:B:173:GLU:HG2	1.77	0.66
1:A:138:PHE:HB2	1:A:147:PRO:HG2	1.78	0.64
1:B:162:GLU:O	1:B:165:ILE:HB	1.98	0.64
1:A:148:VAL:HG11	1:A:151:GLN:HG3	1.80	0.63
1:A:108:HIS:O	1:A:134:THR:HG22	1.98	0.63
1:B:111:LEU:HD21	1:B:153:LYS:HG2	1.82	0.61
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.81	0.60
1:A:106:ASN:ND2	1:A:107:ILE:H	2.01	0.58
1:A:93:SER:O	1:A:97:VAL:HG23	2.02	0.58
1:A:70:GLU:O	1:A:74:GLU:HG3	2.04	0.57
1:B:195:ALA:HB3	1:B:197:TRP:HE1	1.69	0.56
1:A:71:LEU:O	1:A:75:ILE:HG13	2.06	0.56
1:A:15:GLN:OE1	1:A:45:ARG:HD3	2.06	0.55
1:A:77:MET:HE2	1:A:78:TYR:CE1	2.43	0.54
1:B:111:LEU:HB3	1:B:151:GLN:NE2	2.23	0.54
1:B:8:SER:O	1:B:37:LYS:HD2	2.09	0.53
1:B:11:GLY:O	1:B:14:LEU:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD12	1:B:71:LEU:HD12	1.91	0.53
1:B:15:GLN:O	1:B:18:ILE:HB	2.09	0.52
1:B:30:VAL:HB	1:B:51:ILE:HD13	1.92	0.52
1:B:93:SER:O	1:B:97:VAL:HG23	2.10	0.52
1:B:7:ILE:O	1:B:35:SER:HA	2.09	0.51
1:A:35:SER:O	1:A:55:THR:HA	2.11	0.51
1:B:65:GLU:O	1:B:69:ARG:HB2	2.11	0.50
1:A:36:ASN:HA	1:A:56:LEU:O	2.12	0.49
1:B:85:LEU:HG	1:B:88:PHE:HB3	1.94	0.49
1:B:70:GLU:O	1:B:73:HIS:HB3	2.13	0.49
1:B:13:ASN:O	1:B:16:ALA:HB3	2.13	0.48
1:B:176:ILE:O	1:B:179:LEU:HB3	2.13	0.48
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.58	0.48
1:B:162:GLU:HA	1:B:165:ILE:HD12	1.94	0.48
1:A:153:LYS:H	1:A:153:LYS:NZ	2.12	0.48
1:A:192:HIS:O	1:A:193:GLU:HG2	2.13	0.48
1:A:12:SER:O	1:A:15:GLN:HB3	2.13	0.48
1:B:75:ILE:HG22	1:B:80:PRO:HG2	1.96	0.48
1:A:133:GLY:HA3	1:A:152:ALA:O	2.14	0.48
1:A:188:ARG:O	1:A:198:LEU:HA	2.15	0.46
1:B:165:ILE:O	1:B:169:VAL:HG23	2.16	0.46
1:B:63:SER:O	1:B:66:ALA:HB3	2.14	0.46
1:B:197:TRP:CD1	1:B:197:TRP:N	2.83	0.46
1:A:153:LYS:H	1:A:153:LYS:HZ3	1.62	0.46
1:A:77:MET:SD	1:B:70:GLU:OE1	2.74	0.45
1:B:108:HIS:HA	1:B:109:PRO:HD2	1.82	0.45
1:A:1:MET:SD	1:A:81:ASP:HB2	2.57	0.44
1:A:100:TYR:HB2	1:A:104:LEU:HD22	1.99	0.44
1:A:111:LEU:HB3	1:A:151:GLN:OE1	2.17	0.44
1:B:1:MET:HB3	1:B:28:GLY:HA3	1.99	0.44
1:A:5:VAL:HG12	1:A:6:LEU:N	2.32	0.43
1:B:137:HIS:CD2	1:B:138:PHE:O	2.72	0.43
1:A:5:VAL:C	1:A:6:LEU:HD12	2.44	0.43
1:A:6:LEU:N	1:A:6:LEU:HD12	2.34	0.42
1:A:41:PHE:O	1:A:44:GLU:HB3	2.19	0.42
1:A:154:VAL:HA	1:A:155:PRO:HD2	1.90	0.42
1:B:10:ASN:HA	1:B:41:PHE:HB3	2.01	0.42
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.49	0.42
1:B:72:ILE:HG23	1:B:99:HIS:CD2	2.55	0.42
1:A:67:TYR:CD1	1:A:67:TYR:C	2.98	0.42
1:A:8:SER:OG	1:A:88:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG12	1:B:51:ILE:HG21	2.01	0.42
1:B:142:GLU:HG3	1:B:194:ASN:ND2	2.34	0.42
1:B:92:LEU:HD23	1:B:97:VAL:HG22	2.01	0.41
1:B:96:PHE:CD1	1:B:96:PHE:C	2.98	0.41
1:A:40:ALA:O	1:A:43:LEU:HB2	2.21	0.41
1:B:142:GLU:HG3	1:B:194:ASN:CG	2.46	0.41
1:A:138:PHE:CD2	1:A:149:ILE:HD11	2.56	0.41
1:A:106:ASN:ND2	1:A:107:ILE:N	2.68	0.40
1:B:172:GLN:O	1:B:176:ILE:HG12	2.21	0.40
1:B:36:ASN:HD22	1:B:88:PHE:HE1	1.65	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	190/212 (90%)	176 (93%)	11 (6%)	3 (2%)	7	34
1	B	188/212 (89%)	174 (93%)	10 (5%)	4 (2%)	5	27
All	All	378/424 (89%)	350 (93%)	21 (6%)	7 (2%)	6	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	PRO
1	B	205	PRO
1	B	162	GLU
1	A	112	LEU
1	B	58	ALA
1	A	94	PRO
1	A	205	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	155/171 (91%)	134 (86%)	21 (14%)	4	18
1	B	153/171 (90%)	140 (92%)	13 (8%)	10	36
All	All	308/342 (90%)	274 (89%)	34 (11%)	6	25

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	LEU
1	A	24	ASN
1	A	29	THR
1	A	48	GLN
1	A	57	ILE
1	A	59	SER
1	A	65	GLU
1	A	98	SER
1	A	107	ILE
1	A	110	SER
1	A	111	LEU
1	A	134	THR
1	A	140	THR
1	A	153	LYS
1	A	160	ASP
1	A	170	GLN
1	A	179	LEU
1	A	182	SER
1	A	186	ASP
1	A	194	ASN
1	B	48	GLN
1	B	59	SER
1	B	82	VAL
1	B	85	LEU
1	B	111	LEU
1	B	134	THR

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Mol	Chain	Res	Type
1	B	144	ASP
1	B	154	VAL
1	B	163	ASP
1	B	178	PRO
1	B	204	PRO
1	B	205	PRO
1	B	206	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	ASN
1	A	48	GLN
1	A	106	ASN
1	A	108	HIS
1	A	174	HIS
1	A	194	ASN
1	A	206	GLN
1	B	48	GLN
1	B	137	HIS
1	B	194	ASN
1	B	206	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](#)

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	PO4	B	301	-	4,4,4	2.85	2 (50%)	6,6,6	2.14	2 (33%)
2	PO4	A	301	-	4,4,4	3.26	3 (75%)	6,6,6	2.37	3 (50%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PO4	P-O1	4.76	1.61	1.50
2	B	301	PO4	P-O1	4.34	1.60	1.50
2	A	301	PO4	P-O4	3.27	1.64	1.54
2	B	301	PO4	P-O4	2.98	1.63	1.54
2	A	301	PO4	P-O3	-2.74	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	PO4	O3-P-O2	4.40	121.62	107.91
2	A	301	PO4	O3-P-O2	4.01	120.38	107.91
2	A	301	PO4	O4-P-O1	-2.73	101.31	110.95
2	A	301	PO4	O3-P-O1	-2.65	101.58	110.95
2	B	301	PO4	O4-P-O1	-2.49	102.14	110.95

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.