



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:06 pm BST

PDB ID : 1QMH  
Title : Crystal structure of RNA 3'-terminal phosphate cyclase, an ubiquitous enzyme with unusual topology  
Authors : Palm, G.J.; Billy, E.; Filipowicz, W.; Wlodawer, A.  
Deposited on : 1999-09-28  
Resolution : 2.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

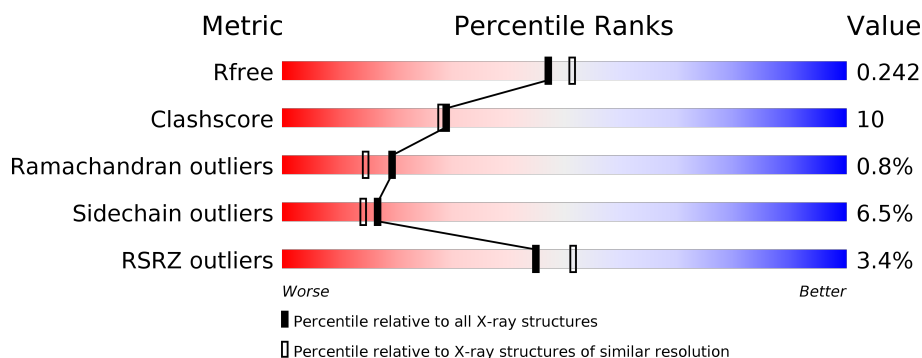
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	347	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>6%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5430 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 RNA 3'-TERMINAL PHOSPHATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2483	1566	445	465	7			
1	B	335	Total	C	N	O	S	0	0	0
			2488	1569	446	466	7			

There are 20 discrepancies between the modelled and reference sequences:

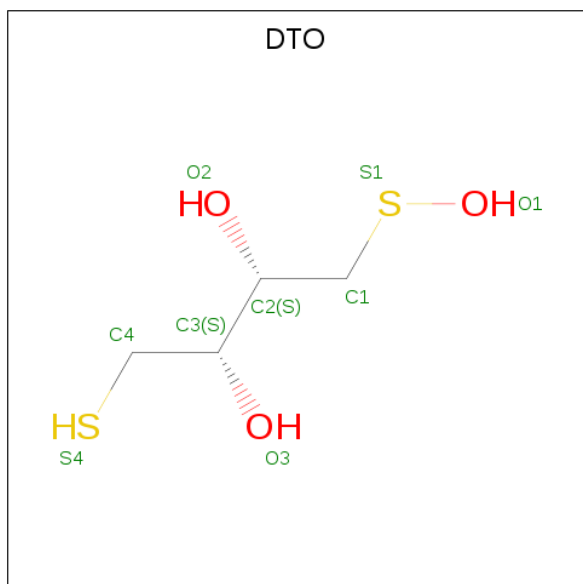
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P46849
A	2	VAL	-	expression tag	UNP P46849
A	340	GLY	-	expression tag	UNP P46849
A	341	SER	-	expression tag	UNP P46849
A	342	HIS	-	expression tag	UNP P46849
A	343	HIS	-	expression tag	UNP P46849
A	344	HIS	-	expression tag	UNP P46849
A	345	HIS	-	expression tag	UNP P46849
A	346	HIS	-	expression tag	UNP P46849
A	347	HIS	-	expression tag	UNP P46849
B	1	MET	-	expression tag	UNP P46849
B	2	VAL	-	expression tag	UNP P46849
B	340	GLY	-	expression tag	UNP P46849
B	341	SER	-	expression tag	UNP P46849
B	342	HIS	-	expression tag	UNP P46849
B	343	HIS	-	expression tag	UNP P46849
B	344	HIS	-	expression tag	UNP P46849
B	345	HIS	-	expression tag	UNP P46849
B	346	HIS	-	expression tag	UNP P46849
B	347	HIS	-	expression tag	UNP P46849

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1-HYDROXYSULFANYL-4-MERCAPTO-BUTANE-2,3-DIOL (three-letter code: DTO) (formula:  $C_4H_{10}O_3S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			9	4	3	2		

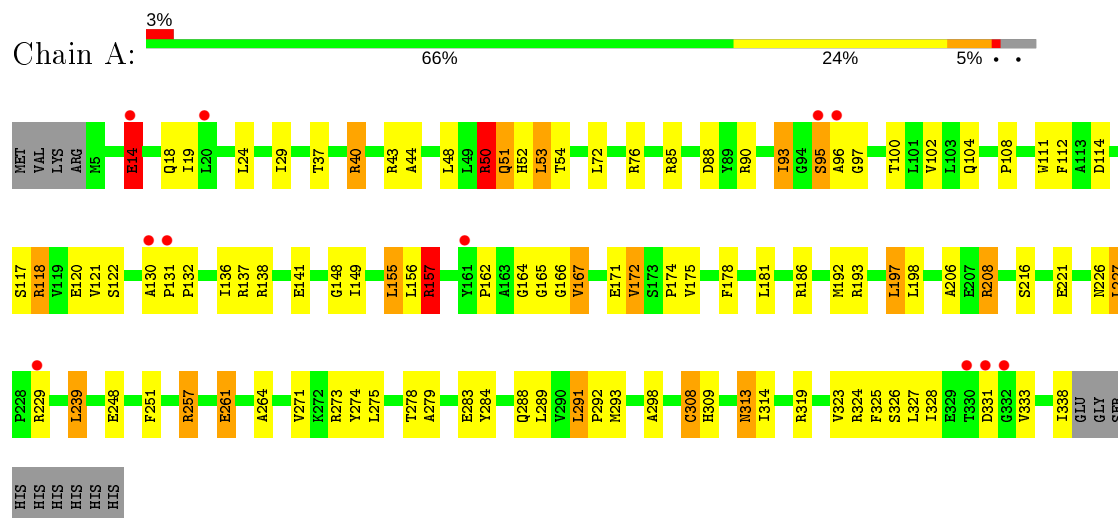
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total 208	O 208	0	0
4	B	216	Total 216	O 216	0	0

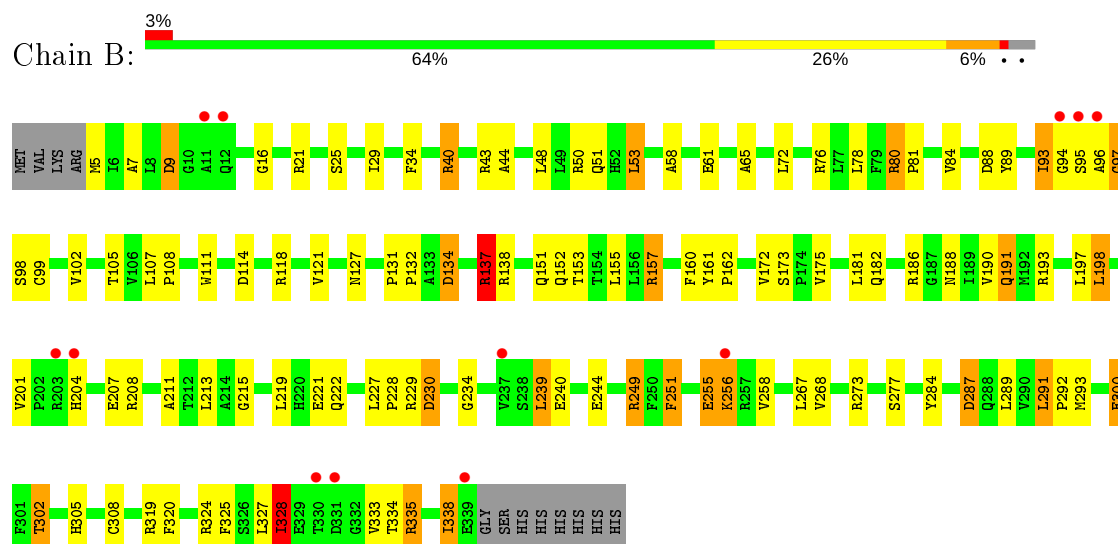
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: RNA 3'-TERMINAL PHOSPHATE CYCLASE



#### • Molecule 1: RNA 3'-TERMINAL PHOSPHATE CYCLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.80 Å   133.50 Å   51.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.10 19.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (10.00-2.10) 88.8 (19.81-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.09 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204   ,   0.276 0.184   ,   0.242	Depositor DCC
$R_{free}$ test set	2434 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTO, CIT

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	1.07	3/2526 (0.1%)	2.15	74/3433 (2.2%)
1	B	1.12	3/2531 (0.1%)	2.19	82/3440 (2.4%)
All	All	1.10	6/5057 (0.1%)	2.17	156/6873 (2.3%)

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	B	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	ASP	CA-CB	7.33	1.70	1.53
1	A	193	ARG	CD-NE	-7.31	1.34	1.46
1	B	25	SER	CA-CB	6.55	1.62	1.52
1	A	122	SER	CB-OG	5.26	1.49	1.42
1	A	166	GLY	CA-C	5.09	1.59	1.51
1	B	277	SER	CA-CB	5.08	1.60	1.52

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	CD-NE-CZ	27.93	162.70	123.60
1	B	137	ARG	NE-CZ-NH1	27.11	133.85	120.30
1	A	273	ARG	CD-NE-CZ	25.77	159.67	123.60
1	A	229	ARG	CD-NE-CZ	23.55	156.57	123.60
1	B	137	ARG	CD-NE-CZ	22.47	155.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	21.59	131.10	120.30
1	A	157	ARG	NE-CZ-NH1	-20.07	110.27	120.30
1	B	114	ASP	CB-CG-OD1	16.99	133.59	118.30
1	A	257	ARG	NE-CZ-NH2	16.30	128.45	120.30
1	B	193	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	B	114	ASP	CB-CG-OD2	-15.45	104.39	118.30
1	A	137	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	B	9	ASP	CB-CG-OD2	14.63	131.47	118.30
1	B	88	ASP	CB-CG-OD1	-13.49	106.16	118.30
1	B	43	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	A	141	GLU	OE1-CD-OE2	-12.87	107.86	123.30
1	A	138	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	B	186	ARG	NE-CZ-NH2	-12.79	113.91	120.30
1	B	230	ASP	CB-CG-OD2	12.73	129.75	118.30
1	A	324	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	B	157	ARG	NE-CZ-NH2	-11.57	114.51	120.30
1	A	137	ARG	CD-NE-CZ	11.41	139.58	123.60
1	B	249	ARG	NE-CZ-NH1	11.33	125.97	120.30
1	A	118	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	B	76	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	273	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	B	43	ARG	CD-NE-CZ	10.36	138.10	123.60
1	B	118	ARG	NH1-CZ-NH2	-10.28	108.09	119.40
1	B	193	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	229	ARG	NE-CZ-NH1	-9.77	115.42	120.30
1	B	300	GLU	OE1-CD-OE2	9.73	134.98	123.30
1	B	324	ARG	CD-NE-CZ	9.62	137.06	123.60
1	B	335	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	A	229	ARG	NE-CZ-NH2	9.44	125.02	120.30
1	A	257	ARG	NE-CZ-NH1	-9.13	115.74	120.30
1	A	157	ARG	NH1-CZ-NH2	8.82	129.11	119.40
1	B	138	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	273	ARG	CD-NE-CZ	8.66	135.73	123.60
1	A	157	ARG	CA-CB-CG	8.65	132.42	113.40
1	B	137	ARG	NH1-CZ-NH2	-8.48	110.08	119.40
1	B	137	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	B	80	ARG	CD-NE-CZ	-8.40	111.84	123.60
1	A	172	VAL	CA-CB-CG2	8.37	123.45	110.90
1	B	186	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	89	TYR	CB-CG-CD1	-8.20	116.08	121.00
1	A	138	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	B	230	ASP	CA-CB-CG	-8.07	95.65	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLU	OE1-CD-OE2	-8.04	113.65	123.30
1	A	331	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	193	ARG	CG-CD-NE	7.86	128.31	111.80
1	A	114	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	308	CYS	CA-CB-SG	7.79	128.02	114.00
1	A	40	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	193	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	B	273	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	251	PHE	CB-CG-CD1	7.37	125.96	120.80
1	B	76	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	40	ARG	CD-NE-CZ	7.28	133.79	123.60
1	B	50	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	B	88	ASP	N-CA-CB	-7.22	97.61	110.60
1	B	9	ASP	OD1-CG-OD2	-7.10	109.80	123.30
1	A	283	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	335	ARG	NH1-CZ-NH2	7.08	127.18	119.40
1	B	230	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	B	240	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	B	249	ARG	CD-NE-CZ	-6.86	114.00	123.60
1	B	208	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	B	58	ALA	O-C-N	-6.81	111.81	122.70
1	B	50	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	B	34	PHE	CB-CG-CD2	6.70	125.49	120.80
1	A	95	SER	N-CA-CB	-6.68	100.47	110.50
1	B	191	GLN	CA-CB-CG	6.65	128.02	113.40
1	B	193	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	291	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	40	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	138	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	155	LEU	CA-C-N	6.55	131.60	117.20
1	A	85	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	137	ARG	CG-CD-NE	6.49	125.44	111.80
1	A	118	ARG	CD-NE-CZ	6.47	132.66	123.60
1	B	308	CYS	CA-CB-SG	-6.44	102.41	114.00
1	A	239	LEU	CA-CB-CG	-6.43	100.50	115.30
1	A	137	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	B	324	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	164	GLY	N-CA-C	-6.33	97.27	113.10
1	A	24	LEU	CB-CG-CD2	6.30	121.70	111.00
1	B	173	SER	N-CA-CB	6.29	119.94	110.50
1	B	84	VAL	CA-CB-CG2	-6.17	101.65	110.90
1	B	239	LEU	CA-CB-CG	-6.16	101.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	CG-CD-NE	-6.11	98.97	111.80
1	B	230	ASP	CB-CA-C	-6.07	98.27	110.40
1	A	96	ALA	N-CA-CB	6.05	118.57	110.10
1	B	21	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	335	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	148	GLY	O-C-N	-6.03	113.06	122.70
1	A	319	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	287	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	65	ALA	CB-CA-C	-5.97	101.14	110.10
1	A	51	GLN	CB-CG-CD	5.97	127.12	111.60
1	A	327	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	80	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	327	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	291	LEU	O-C-N	-5.80	110.07	121.10
1	A	226	ASN	OD1-CG-ND2	5.76	135.14	121.90
1	B	151	GLN	CA-CB-CG	5.74	126.03	113.40
1	B	273	ARG	O-C-N	-5.74	113.51	122.70
1	A	197	LEU	N-CA-CB	-5.72	98.95	110.40
1	A	226	ASN	CB-CG-OD1	-5.72	110.16	121.60
1	B	308	CYS	N-CA-CB	-5.71	100.32	110.60
1	B	186	ARG	CD-NE-CZ	5.70	131.59	123.60
1	A	251	PHE	CG-CD1-CE1	-5.67	114.56	120.80
1	A	313	ASN	N-CA-CB	5.65	120.77	110.60
1	B	89	TYR	CB-CG-CD2	5.63	124.38	121.00
1	B	302	THR	CA-CB-CG2	-5.61	104.55	112.40
1	A	14	GLU	OE1-CD-OE2	-5.59	116.60	123.30
1	A	136	ILE	CA-CB-CG1	-5.58	100.40	111.00
1	A	167	VAL	CG1-CB-CG2	-5.57	101.98	110.90
1	A	279	ALA	CB-CA-C	5.57	118.46	110.10
1	B	221	GLU	OE1-CD-OE2	5.57	129.98	123.30
1	B	268	VAL	O-C-N	-5.57	113.79	122.70
1	B	291	LEU	CA-C-O	5.53	131.70	120.10
1	A	43	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	229	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	B	134	ASP	O-C-N	-5.43	114.00	122.70
1	A	118	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	324	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	105	THR	O-C-N	-5.40	114.06	122.70
1	A	155	LEU	O-C-N	-5.38	114.09	122.70
1	B	320	PHE	CB-CG-CD1	5.37	124.56	120.80
1	A	96	ALA	N-CA-C	-5.37	96.50	111.00
1	A	165	GLY	C-N-CA	-5.34	111.09	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASP	OD1-CG-OD2	5.33	133.42	123.30
1	A	88	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	99	CYS	O-C-N	-5.32	114.19	122.70
1	B	157	ARG	CG-CD-NE	-5.31	100.65	111.80
1	B	328	ILE	CB-CG1-CD1	5.30	128.74	113.90
1	A	122	SER	CA-CB-OG	-5.25	97.02	111.20
1	B	251	PHE	CB-CA-C	-5.23	99.95	110.40
1	A	251	PHE	CD1-CE1-CZ	5.22	126.36	120.10
1	B	215	GLY	CA-C-O	-5.21	111.21	120.60
1	A	208	ARG	N-CA-CB	-5.20	101.23	110.60
1	A	221	GLU	CB-CA-C	-5.19	100.02	110.40
1	B	61	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	216	SER	CA-CB-OG	5.17	125.17	111.20
1	B	172	VAL	CB-CA-C	-5.16	101.60	111.40
1	A	174	PRO	CA-C-N	5.13	128.50	117.20
1	A	141	GLU	CG-CD-OE1	5.13	128.55	118.30
1	A	264	ALA	CB-CA-C	5.11	117.77	110.10
1	A	130	ALA	CB-CA-C	-5.11	102.44	110.10
1	A	319	ARG	CD-NE-CZ	5.07	130.70	123.60
1	B	277	SER	CA-CB-OG	-5.05	97.55	111.20
1	A	90	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	65	ALA	O-C-N	5.04	130.76	122.70
1	A	43	ARG	CD-NE-CZ	5.04	130.65	123.60
1	A	50	ARG	CB-CG-CD	5.03	124.69	111.60
1	B	277	SER	N-CA-CB	-5.01	102.99	110.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	LEU	Mainchain
1	B	211	ALA	Mainchain
1	B	244	GLU	Mainchain
1	B	287	ASP	Mainchain
1	B	29	ILE	Mainchain

## 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	2483	0	2521	55	0
1	B	2488	0	2523	44	0
2	A	13	0	5	3	0
2	B	13	0	5	0	0
3	B	9	0	10	0	0
4	A	208	0	0	2	0
4	B	216	0	0	5	0
All	All	5430	0	5064	97	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 10.

All (97) 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:44:ALA:HA	1:B:44:ALA:HA	1.63	0.80
1:A:197:LEU:HD11	1:A:227:LEU:CD2	2.13	0.78
1:A:192:MET:HE1	1:A:275:LEU:HD11	1.65	0.77
1:A:192:MET:CE	1:A:275:LEU:HD11	2.14	0.77
1:B:7:ALA:O	1:B:319:ARG:NH2	2.19	0.75
1:A:197:LEU:HD11	1:A:227:LEU:HD22	1.70	0.73
1:B:93:ILE:HD12	1:B:102:VAL:HG21	1.72	0.71
1:A:93:ILE:N	1:A:93:ILE:HD13	2.08	0.69
1:B:93:ILE:CD1	1:B:102:VAL:HG21	2.25	0.67
1:A:40:ARG:HH21	2:A:401:CIT:C1	2.08	0.66
1:B:289:LEU:O	1:B:293:MET:HG3	1.98	0.64
1:A:149:ILE:HD11	1:A:178:PHE:HE1	1.64	0.62
1:A:104:GLN:NE2	1:A:284:TYR:OH	2.33	0.62
1:B:111:TRP:HB3	1:B:175:VAL:HG23	1.83	0.60
1:A:93:ILE:CD1	1:A:102:VAL:HG21	2.34	0.58
1:A:289:LEU:O	1:A:293:MET:HG3	2.03	0.58
1:A:208:ARG:HH21	1:A:261:GLU:HG3	1.68	0.57
1:A:93:ILE:HD11	1:A:121:VAL:HG23	1.85	0.57
1:A:197:LEU:HD11	1:A:227:LEU:HD21	1.87	0.56
1:B:228:PRO:HB2	1:B:230:ASP:HB2	1.87	0.56
1:A:208:ARG:HD3	4:A:2121:HOH:O	2.06	0.56
1:A:111:TRP:HB3	1:A:175:VAL:HG23	1.88	0.55
1:B:204:HIS:HA	1:B:207:GLU:OE1	2.08	0.54
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.73	0.54
1:B:198:LEU:HD13	1:B:201:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HB3	1:A:53:LEU:HD13	1.91	0.53
1:B:93:ILE:N	1:B:93:ILE:HD13	2.23	0.52
1:A:29:ILE:HG12	1:A:112:PHE:CD1	2.46	0.51
1:B:96:ALA:O	1:B:97:GLY:C	2.48	0.51
1:A:54:THR:HG21	1:A:93:ILE:HD12	1.92	0.51
1:A:157:ARG:HD2	4:A:2094:HOH:O	2.10	0.51
1:B:94:GLY:HA2	4:B:2088:HOH:O	2.11	0.50
1:A:298:ALA:HA	1:A:338:ILE:HB	1.92	0.49
1:A:37:THR:HG22	1:A:76:ARG:HG3	1.95	0.49
1:A:54:THR:HG21	1:A:93:ILE:HG23	1.95	0.49
1:B:152:GLN:NE2	1:B:153:THR:O	2.46	0.49
1:A:50:ARG:HH11	1:A:50:ARG:CG	2.27	0.48
1:B:213:LEU:HD21	1:B:267:LEU:HD23	1.95	0.48
1:B:325:PHE:CE2	1:B:338:ILE:HG13	2.48	0.48
1:A:291:LEU:HB3	1:A:292:PRO:CD	2.44	0.47
1:A:108:PRO:HA	1:A:111:TRP:CD2	2.49	0.47
1:B:137:ARG:HD3	1:B:152:GLN:HE22	1.80	0.47
1:B:48:LEU:HB3	1:B:53:LEU:HD13	1.97	0.47
1:A:100:THR:O	1:A:104:GLN:HG3	2.15	0.47
1:A:18:GLN:CD	1:A:313:ASN:HD21	2.17	0.47
1:A:198:LEU:HD11	1:A:206:ALA:HB2	1.96	0.47
1:B:94:GLY:HA2	4:B:2121:HOH:O	2.15	0.47
1:B:319:ARG:NH1	4:B:2208:HOH:O	2.43	0.46
1:A:186:ARG:HD3	1:A:274:TYR:CZ	2.51	0.46
1:B:157:ARG:HD2	4:B:2116:HOH:O	2.16	0.46
1:A:328:ILE:HG12	1:B:328:ILE:HG23	1.98	0.46
1:B:255:GLU:HB3	1:B:258:VAL:CG2	2.47	0.45
1:B:53:LEU:CD2	1:B:72:LEU:HD23	2.46	0.45
1:A:19:ILE:HD12	1:A:19:ILE:H	1.81	0.45
1:A:278:THR:OG1	1:A:333:VAL:HG21	2.17	0.45
1:B:291:LEU:N	1:B:292:PRO:HD2	2.32	0.45
1:A:118:ARG:HD2	1:A:171:GLU:OE2	2.17	0.44
1:A:284:TYR:O	1:A:288:GLN:HG2	2.17	0.44
1:B:16:GLY:HA2	1:B:40:ARG:HG2	1.99	0.44
1:B:131:PRO:HA	1:B:132:PRO:HD3	1.76	0.44
1:B:93:ILE:HD11	1:B:121:VAL:HG13	1.99	0.44
1:A:93:ILE:HD11	1:A:102:VAL:HG21	2.00	0.44
1:A:257:ARG:NH1	1:A:257:ARG:HG2	2.33	0.43
1:B:107:LEU:N	1:B:108:PRO:CD	2.81	0.43
1:A:314:ILE:HG23	1:A:325:PHE:CD1	2.54	0.43
1:A:93:ILE:HD11	1:A:121:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:NE2	1:B:300:GLU:OE1	2.48	0.43
1:A:149:ILE:HD11	1:A:178:PHE:CE1	2.49	0.43
1:B:190:VAL:HG12	1:B:191:GLN:HG2	2.01	0.43
1:B:302:THR:HA	1:B:334:THR:O	2.19	0.43
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.83	0.42
1:A:197:LEU:CD1	1:A:227:LEU:HD22	2.46	0.42
1:A:309:HIS:O	1:A:313:ASN:ND2	2.49	0.42
1:B:219:LEU:HD12	1:B:222:GLN:OE1	2.19	0.42
1:A:291:LEU:HB3	1:A:292:PRO:HD3	2.00	0.42
1:B:291:LEU:HB3	1:B:292:PRO:HD3	2.00	0.42
1:A:14:GLU:HG2	1:A:309:HIS:NE2	2.33	0.42
1:B:80:ARG:HA	1:B:81:PRO:HD2	1.87	0.42
1:B:335:ARG:HD3	1:B:335:ARG:HH11	1.52	0.42
1:A:18:GLN:CD	1:A:313:ASN:ND2	2.73	0.42
1:B:108:PRO:HA	1:B:111:TRP:CD2	2.55	0.42
1:B:127:ASN:ND2	1:B:161:TYR:CD2	2.88	0.41
1:A:156:LEU:N	1:A:167:VAL:O	2.51	0.41
1:B:188:ASN:HB3	4:B:2136:HOH:O	2.19	0.41
1:A:18:GLN:NE2	1:A:313:ASN:ND2	2.68	0.41
1:B:160:PHE:CG	1:B:234:GLY:HA3	2.55	0.41
1:B:131:PRO:HG2	1:B:284:TYR:CE2	2.55	0.41
1:A:131:PRO:HA	1:A:132:PRO:HD3	1.65	0.41
1:B:161:TYR:CG	1:B:162:PRO:HA	2.56	0.41
1:A:239:LEU:HD22	1:A:271:VAL:HG21	2.03	0.41
1:A:291:LEU:N	1:A:292:PRO:HD2	2.35	0.41
1:A:51:GLN:NE2	2:A:401:CIT:O4	2.54	0.41
1:A:52:HIS:HE2	2:A:401:CIT:C5	2.33	0.41
1:B:197:LEU:HD11	1:B:227:LEU:HD11	2.03	0.41
1:A:208:ARG:NH2	1:A:261:GLU:HG3	2.33	0.40
1:B:78:LEU:HD23	1:B:78:LEU:C	2.41	0.40
1:B:249:ARG:HD2	1:B:251:PHE:CZ	2.56	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	332/347 (96%)	324 (98%)	6 (2%)	2 (1%)	25	21
1	B	333/347 (96%)	322 (97%)	8 (2%)	3 (1%)	17	12
All	All	665/694 (96%)	646 (97%)	14 (2%)	5 (1%)	19	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	97	GLY
1	B	95	SER
1	B	97	GLY
1	B	256	LYS

### 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	261/274 (95%)	244 (94%)	17 (6%)	17	14
1	B	261/274 (95%)	244 (94%)	17 (6%)	17	14
All	All	522/548 (95%)	488 (94%)	34 (6%)	17	14

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

Mol	Chain	Res	Type
1	A	14	GLU
1	A	50	ARG
1	A	53	LEU
1	A	72	LEU
1	A	93	ILE
1	A	117	SER
1	A	155	LEU
1	A	157	ARG

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Mol	Chain	Res	Type
1	A	162	PRO
1	A	172	VAL
1	A	181	LEU
1	A	227	LEU
1	A	248	GLU
1	A	261	GLU
1	A	308	CYS
1	A	323	VAL
1	A	326	SER
1	B	5	MET
1	B	9	ASP
1	B	51	GLN
1	B	53	LEU
1	B	93	ILE
1	B	98	SER
1	B	134	ASP
1	B	137	ARG
1	B	155	LEU
1	B	181	LEU
1	B	239	LEU
1	B	255	GLU
1	B	256	LYS
1	B	305	HIS
1	B	328	ILE
1	B	333	VAL
1	B	338	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	51	GLN
1	A	104	GLN
1	A	313	ASN
1	B	12	GLN
1	B	18	GLN
1	B	152	GLN
1	B	309	HIS
1	B	313	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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
3	DTO	B	402	-	5,8,8	1.56	1 (20%)	3,9,9	0.87	0
2	CIT	A	401	-	3,12,12	1.36	1 (33%)	3,17,17	2.93	1 (33%)
2	CIT	B	401	-	3,12,12	1.71	1 (33%)	3,17,17	1.85	1 (33%)

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
3	DTO	B	402	-	-	5/8/9/9	-
2	CIT	A	401	-	-	0/6/16/16	-
2	CIT	B	401	-	-	1/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	CIT	O7-C3	2.62	1.47	1.43
3	B	402	DTO	C4-C3	2.48	1.58	1.51
2	A	401	CIT	O7-C3	2.14	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	C4-C3-C2	4.70	121.89	109.33
2	B	401	CIT	C4-C3-C2	2.59	116.26	109.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	DTO	C1-C2-C3-O3
3	B	402	DTO	C1-C2-C3-C4
3	B	402	DTO	O2-C2-C3-O3
3	B	402	DTO	O2-C2-C3-C4
3	B	402	DTO	S1-C1-C2-O2
2	B	401	CIT	C6-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	3	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/347 (96%)	-0.02	11 (3%) 46 53	16, 34, 59, 78	0
1	B	335/347 (96%)	-0.13	12 (3%) 42 49	20, 33, 63, 79	0
All	All	669/694 (96%)	-0.08	23 (3%) 45 51	16, 34, 61, 79	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	5.6
1	A	331	ASP	5.3
1	B	94	GLY	4.0
1	B	331	ASP	4.0
1	A	95	SER	3.9
1	B	11	ALA	3.4
1	A	330	THR	3.2
1	B	339	GLU	3.1
1	B	96	ALA	2.8
1	A	14	GLU	2.6
1	A	20	LEU	2.6
1	B	256	LYS	2.6
1	B	95	SER	2.5
1	A	161	TYR	2.5
1	A	332	GLY	2.4
1	B	237	VAL	2.4
1	B	330	THR	2.3
1	A	130	ALA	2.2
1	A	229	ARG	2.2
1	A	131	PRO	2.2
1	B	12	GLN	2.0
1	B	204	HIS	2.0
1	B	203	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DTO	B	402	9/9	0.78	0.21	74,78,81,81	0
2	CIT	A	401	13/13	0.85	0.17	60,64,67,69	0
2	CIT	B	401	13/13	0.92	0.18	57,59,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.