



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:00 PM UTC

PDB ID : 1QMH / pdb_00001qmh
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

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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

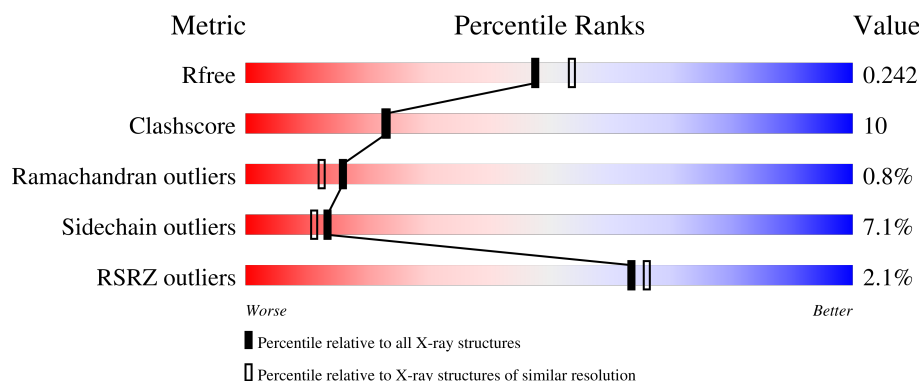
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	
1	B	347	

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:

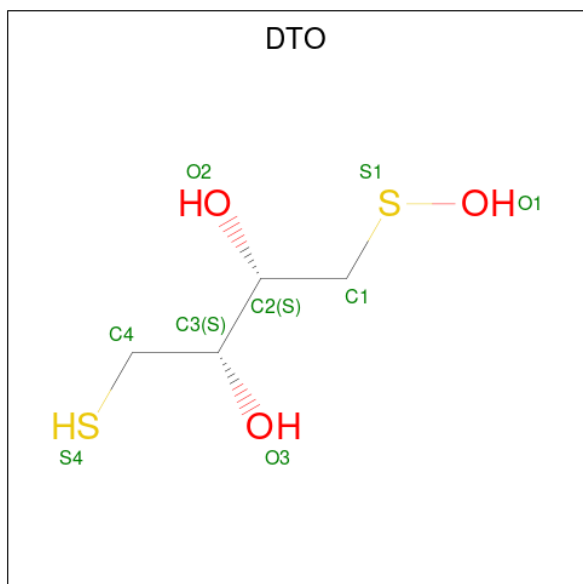
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P46849
A	2	VAL	-	expression tag	UNP P46849
A	340	GLY	-	expression tag	UNP P46849
A	341	SER	-	expression tag	UNP P46849
A	342	HIS	-	expression tag	UNP P46849
A	343	HIS	-	expression tag	UNP P46849
A	344	HIS	-	expression tag	UNP 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 (CCD ID: CIT) (formula: C₆H₈O₇).



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-HYDROXSULFANYL-4-MERCAPTO-BUTANE-2,3-DIOL (CCD ID: 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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.80Å 133.50Å 51.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (10.00-2.10) 87.7 (10.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.09Å)	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 ²)	28.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5430	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.44	12/2526 (0.5%)	2.57	169/3433 (4.9%)
1	B	1.52	15/2531 (0.6%)	2.47	158/3440 (4.6%)
All	All	1.48	27/5057 (0.5%)	2.52	327/6873 (4.8%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	ASP	CA-CB	9.82	1.70	1.53
1	B	291	LEU	N-CA	9.82	1.55	1.46
1	A	193	ARG	CD-NE	-8.74	1.34	1.46
1	B	135	PHE	C-N	7.42	1.43	1.33
1	B	243	SER	N-CA	-7.02	1.37	1.45
1	A	234	GLY	N-CA	6.80	1.51	1.45
1	B	29	ILE	CA-CB	6.41	1.61	1.54
1	A	79	PHE	C-N	-6.16	1.27	1.33
1	B	25	SER	CA-CB	6.00	1.62	1.53
1	A	135	PHE	CA-C	5.93	1.60	1.52
1	B	154	THR	C-O	5.92	1.31	1.24
1	A	253	VAL	CA-C	5.78	1.59	1.52
1	A	175	VAL	CA-C	5.78	1.59	1.52
1	A	156	LEU	CA-C	5.76	1.60	1.52
1	A	240	GLU	N-CA	5.68	1.53	1.46
1	B	84	VAL	CA-CB	5.63	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	LEU	CA-C	-5.43	1.45	1.52
1	B	27	SER	N-CA	5.42	1.52	1.46
1	B	291	LEU	CA-C	-5.37	1.45	1.52
1	A	203	ARG	C-N	5.35	1.41	1.34
1	A	206	ALA	C-N	5.30	1.40	1.33
1	A	259	SER	C-N	-5.13	1.27	1.33
1	B	228	PRO	CA-C	-5.12	1.46	1.52
1	A	170	THR	C-N	-5.11	1.26	1.33
1	B	241	VAL	N-CA	-5.10	1.39	1.46
1	B	290	VAL	N-CA	5.03	1.52	1.46
1	B	121	VAL	C-O	5.00	1.28	1.24

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	CD-NE-CZ	27.36	162.70	124.40
1	A	273	ARG	CD-NE-CZ	25.19	159.67	124.40
1	A	229	ARG	CD-NE-CZ	22.98	156.57	124.40
1	B	137	ARG	CD-NE-CZ	21.90	155.06	124.40
1	B	230	ASP	CA-CB-CG	-16.95	95.65	112.60
1	B	291	LEU	CA-C-O	13.24	131.70	118.73
1	A	96	ALA	N-CA-C	-13.09	96.50	111.03
1	A	226	ASN	OD1-CG-ND2	12.54	135.14	122.60
1	B	137	ARG	NE-CZ-NH1	12.35	133.85	121.50
1	B	291	LEU	O-C-N	-11.69	110.07	120.48
1	A	157	ARG	NE-CZ-NH1	-11.23	110.27	121.50
1	A	164	GLY	N-CA-C	-11.09	97.27	112.13
1	A	137	ARG	CD-NE-CZ	10.84	139.58	124.40
1	A	257	ARG	NE-CZ-NH2	10.28	128.45	119.20
1	A	202	PRO	CA-C-N	10.04	134.13	120.38
1	A	202	PRO	C-N-CA	10.04	134.13	120.38
1	B	43	ARG	CD-NE-CZ	9.79	138.10	124.40
1	B	58	ALA	O-C-N	-9.73	111.81	122.12
1	B	118	ARG	NE-CZ-NH1	9.60	131.10	121.50
1	B	58	ALA	CA-C-O	9.18	130.28	120.55
1	A	157	ARG	CA-CB-CG	9.16	132.42	114.10
1	B	324	ARG	CD-NE-CZ	9.05	137.06	124.40
1	B	80	ARG	CD-NE-CZ	-8.97	111.84	124.40
1	B	154	THR	CA-C-O	8.82	129.88	120.36
1	A	196	VAL	CA-C-N	-8.71	110.71	122.72
1	A	196	VAL	C-N-CA	-8.71	110.71	122.72
1	B	135	PHE	CA-C-O	8.69	129.92	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	CD-NE-CZ	-8.66	112.28	124.40
1	B	118	ARG	NH1-CZ-NH2	-8.62	108.09	119.30
1	A	174	PRO	CA-C-O	-8.57	111.57	121.34
1	A	319	ARG	CA-C-O	-8.56	110.73	120.24
1	A	259	SER	CA-C-N	8.55	131.56	120.44
1	A	259	SER	C-N-CA	8.55	131.56	120.44
1	A	51	GLN	CB-CG-CD	8.54	127.12	112.60
1	A	250	PHE	CA-CB-CG	-8.44	105.36	113.80
1	B	303	VAL	CA-C-O	-8.39	112.38	121.28
1	A	96	ALA	O-C-N	8.38	131.08	122.03
1	B	184	GLY	CA-C-N	8.35	134.05	120.94
1	B	184	GLY	C-N-CA	8.35	134.05	120.94
1	B	164	GLY	N-CA-C	-8.30	100.60	112.55
1	B	268	VAL	O-C-N	-8.29	113.79	121.91
1	A	79	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	215	GLY	CA-C-O	-8.26	111.21	120.30
1	B	88	ASP	N-CA-CB	-8.25	97.61	110.65
1	B	273	ARG	O-C-N	-8.12	113.51	122.12
1	A	82	GLY	N-CA-C	-8.12	103.05	112.79
1	B	273	ARG	CD-NE-CZ	8.09	135.73	124.40
1	A	148	GLY	O-C-N	-8.03	113.06	122.45
1	B	8	LEU	CA-C-O	-7.94	112.12	120.70
1	A	226	ASN	CA-CB-CG	-7.83	104.77	112.60
1	B	150	HIS	CA-CB-CG	-7.81	105.99	113.80
1	B	190	VAL	N-CA-CB	7.69	117.95	111.64
1	A	172	VAL	CA-CB-CG2	7.68	123.45	110.40
1	A	18	GLN	OE1-CD-NE2	-7.65	114.95	122.60
1	A	165	GLY	CA-C-N	-7.58	111.09	120.64
1	A	165	GLY	C-N-CA	-7.58	111.09	120.64
1	A	157	ARG	NH1-CZ-NH2	7.54	129.11	119.30
1	A	149	ILE	CA-C-N	7.52	133.31	122.85
1	A	149	ILE	C-N-CA	7.52	133.31	122.85
1	B	266	GLN	CA-C-O	7.49	128.49	120.55
1	B	99	CYS	O-C-N	-7.49	114.19	122.12
1	B	249	ARG	CD-NE-CZ	-7.43	114.00	124.40
1	A	193	ARG	CG-CD-NE	7.41	128.31	112.00
1	B	193	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	B	96	ALA	N-CA-C	-7.41	103.20	112.90
1	B	246	ILE	CA-C-O	7.39	127.17	120.96
1	A	93	ILE	CA-C-N	7.29	132.57	120.25
1	A	93	ILE	C-N-CA	7.29	132.57	120.25
1	B	273	ARG	CA-C-O	7.28	128.27	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	VAL	CA-C-N	-7.26	112.40	122.93
1	B	84	VAL	C-N-CA	-7.26	112.40	122.93
1	A	313	ASN	N-CA-CB	7.25	120.77	110.12
1	A	293	MET	CA-C-O	-7.24	112.75	120.42
1	A	77	LEU	CA-C-O	-7.21	111.67	120.54
1	A	185	GLU	CB-CG-CD	7.12	124.70	112.60
1	B	328	ILE	CB-CG1-CD1	7.11	128.74	113.80
1	B	137	ARG	NH1-CZ-NH2	-7.09	110.08	119.30
1	A	149	ILE	O-C-N	-7.09	114.87	122.95
1	A	273	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	123	GLY	CA-C-O	-7.07	116.03	120.91
1	A	197	LEU	N-CA-CB	-7.04	98.95	110.43
1	A	122	SER	CA-CB-OG	-7.04	97.02	111.10
1	B	190	VAL	N-CA-C	-7.04	106.06	111.62
1	B	286	ALA	CA-C-N	7.04	129.71	120.28
1	B	286	ALA	C-N-CA	7.04	129.71	120.28
1	A	216	SER	CA-CB-OG	7.04	125.17	111.10
1	A	204	HIS	CA-CB-CG	-7.03	106.77	113.80
1	B	65	ALA	O-C-N	6.98	130.76	122.94
1	B	191	GLN	CA-CB-CG	6.96	128.02	114.10
1	A	222	GLN	OE1-CD-NE2	-6.90	115.70	122.60
1	B	250	PHE	CA-CB-CG	-6.86	106.94	113.80
1	B	189	ILE	CA-C-O	-6.83	114.75	121.58
1	A	134	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	240	GLU	CA-C-N	6.78	132.59	123.10
1	B	240	GLU	C-N-CA	6.78	132.59	123.10
1	A	155	LEU	CA-C-O	-6.78	113.66	120.98
1	B	277	SER	CA-CB-OG	-6.77	97.55	111.10
1	A	233	PRO	CA-C-N	-6.75	112.36	121.27
1	A	233	PRO	C-N-CA	-6.75	112.36	121.27
1	A	195	GLU	CA-C-N	-6.73	114.32	123.14
1	A	195	GLU	C-N-CA	-6.73	114.32	123.14
1	B	40	ARG	CD-NE-CZ	6.71	133.79	124.40
1	B	236	THR	CA-C-N	-6.70	113.82	123.06
1	B	236	THR	C-N-CA	-6.70	113.82	123.06
1	A	266	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	B	269	LYS	N-CA-C	6.66	119.10	111.11
1	B	81	PRO	CB-CA-C	-6.65	102.72	111.23
1	B	34	PHE	CA-C-O	-6.63	114.14	121.23
1	B	114	ASP	CB-CG-OD1	6.61	133.59	118.40
1	B	283	GLU	CB-CG-CD	6.59	123.81	112.60
1	A	98	SER	CA-C-N	6.52	128.92	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	SER	C-N-CA	6.52	128.92	120.44
1	B	158	HIS	CA-CB-CG	-6.50	107.30	113.80
1	A	228	PRO	CA-C-O	6.48	128.68	121.36
1	A	229	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	A	59	ALA	CA-C-N	6.46	129.26	120.54
1	A	59	ALA	C-N-CA	6.46	129.26	120.54
1	B	308	CYS	N-CA-CB	-6.46	100.32	109.94
1	B	268	VAL	CA-C-O	6.44	128.00	121.17
1	A	130	ALA	N-CA-C	6.43	115.71	108.25
1	B	179	ASN	CA-CB-CG	6.41	119.01	112.60
1	B	134	ASP	O-C-N	-6.40	114.00	122.33
1	A	139	VAL	N-CA-CB	-6.40	104.37	111.41
1	B	107	LEU	CA-C-O	6.35	124.50	118.34
1	A	206	ALA	CA-C-N	-6.34	111.78	120.28
1	A	206	ALA	C-N-CA	-6.34	111.78	120.28
1	A	155	LEU	O-C-N	-6.33	114.09	122.57
1	A	133	ALA	CA-C-O	6.31	127.27	120.20
1	B	239	LEU	CD1-CG-CD2	6.29	124.64	110.80
1	B	105	THR	O-C-N	-6.28	114.06	122.23
1	A	49	LEU	CA-C-O	-6.28	114.23	121.82
1	B	209	GLU	CA-C-O	-6.27	114.24	120.70
1	A	141	GLU	OE1-CD-OE2	-6.27	107.86	122.90
1	A	191	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	B	36	ILE	CA-C-O	-6.25	113.62	120.43
1	A	208	ARG	CA-C-O	6.24	127.03	120.42
1	A	137	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	B	287	ASP	CA-C-O	-6.22	113.95	120.55
1	B	263	VAL	CA-C-O	6.21	127.94	121.05
1	A	186	ARG	CB-CA-C	-6.19	101.16	110.88
1	A	205	VAL	CA-C-O	-6.15	114.55	120.95
1	A	239	LEU	CA-C-N	-6.15	114.23	122.72
1	A	239	LEU	C-N-CA	-6.15	114.23	122.72
1	A	263	VAL	O-C-N	-6.15	115.88	121.91
1	B	191	GLN	CA-C-O	-6.11	114.69	121.23
1	A	137	ARG	CG-CD-NE	6.11	125.44	112.00
1	A	331	ASP	CA-CB-CG	6.11	118.70	112.60
1	B	230	ASP	CB-CA-C	-6.11	98.27	110.42
1	A	187	GLY	N-CA-C	-6.10	103.63	112.17
1	B	114	ASP	CB-CG-OD2	-6.09	104.39	118.40
1	A	229	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	B	335	ARG	NH1-CZ-NH2	6.06	127.18	119.30
1	A	160	PHE	CA-CB-CG	6.06	119.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLY	CA-C-O	-6.06	115.11	121.53
1	B	193	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	208	ARG	N-CA-CB	-6.03	101.23	110.16
1	B	51	GLN	CB-CG-CD	6.03	122.85	112.60
1	A	292	PRO	O-C-N	-6.01	115.32	122.24
1	B	338	ILE	CB-CA-C	-6.01	101.67	110.81
1	B	266	GLN	O-C-N	-6.00	115.75	122.12
1	A	32	GLN	CA-C-O	5.97	125.41	119.49
1	B	187	GLY	N-CA-C	-5.97	101.83	112.58
1	B	231	GLN	CA-C-O	-5.97	112.21	119.43
1	B	151	GLN	CA-CB-CG	5.97	126.03	114.10
1	A	258	VAL	CA-C-O	-5.96	113.92	120.72
1	A	131	PRO	CA-C-O	5.96	129.21	120.56
1	A	256	LYS	CA-C-N	-5.96	113.74	122.86
1	A	256	LYS	C-N-CA	-5.96	113.74	122.86
1	A	178	PHE	CA-C-O	-5.94	114.09	120.92
1	A	95	SER	N-CA-CB	-5.93	100.47	110.49
1	A	96	ALA	N-CA-CB	5.92	118.57	109.98
1	A	157	ARG	CG-CD-NE	-5.92	98.97	112.00
1	A	308	CYS	CA-CB-SG	5.92	128.02	114.40
1	B	36	ILE	O-C-N	5.92	129.47	123.07
1	B	112	PHE	CA-CB-CG	-5.92	107.89	113.80
1	A	138	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	B	223	ASN	N-CA-C	5.91	118.84	110.50
1	A	238	SER	CA-C-O	5.91	127.91	121.06
1	A	118	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	164	GLY	CA-C-O	-5.89	115.33	121.28
1	B	217	PHE	CA-C-O	-5.89	114.75	121.40
1	A	136	ILE	CA-CB-CG1	-5.88	100.40	110.40
1	B	186	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	A	32	GLN	O-C-N	-5.87	115.72	121.18
1	B	7	ALA	CA-C-O	-5.87	113.98	120.38
1	B	43	ARG	N-CA-C	5.83	118.06	110.43
1	A	35	THR	CA-C-N	-5.82	114.85	122.94
1	A	35	THR	C-N-CA	-5.82	114.85	122.94
1	A	50	ARG	CB-CG-CD	5.82	124.69	111.30
1	B	338	ILE	CA-C-O	-5.81	114.09	120.72
1	A	193	ARG	CA-C-O	-5.81	114.32	121.06
1	B	331	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	245	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	283	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	257	ARG	NE-CZ-NH1	-5.76	115.74	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	SER	CA-C-N	-5.76	112.87	122.21
1	B	216	SER	C-N-CA	-5.76	112.87	122.21
1	B	336	VAL	CA-C-O	-5.75	113.93	120.66
1	A	112	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	173	SER	O-C-N	-5.74	116.00	121.57
1	B	89	TYR	N-CA-C	5.74	119.07	109.95
1	B	74	SER	CA-C-N	5.72	131.18	122.37
1	B	74	SER	C-N-CA	5.72	131.18	122.37
1	B	93	ILE	CA-C-O	5.72	127.93	120.78
1	A	53	LEU	N-CA-CB	5.71	118.52	110.12
1	B	196	VAL	N-CA-C	-5.71	99.96	108.46
1	B	151	GLN	CG-CD-NE2	5.70	124.94	116.40
1	B	9	ASP	CB-CG-OD2	5.68	131.47	118.40
1	B	172	VAL	CB-CA-C	-5.68	101.60	110.69
1	B	34	PHE	O-C-N	5.68	129.49	123.42
1	B	237	VAL	CA-C-O	-5.65	114.05	120.67
1	A	283	GLU	CB-CA-C	-5.64	101.79	110.81
1	B	228	PRO	O-C-N	-5.64	115.83	122.99
1	A	157	ARG	CB-CA-C	5.60	119.94	109.86
1	B	139	VAL	CA-C-O	5.60	125.46	120.70
1	B	86	GLY	N-CA-C	-5.59	105.10	112.82
1	A	12	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	14	GLU	CB-CG-CD	5.59	122.10	112.60
1	B	138	ARG	CA-CB-CG	-5.59	102.92	114.10
1	B	314	ILE	CA-C-O	-5.57	115.27	121.17
1	B	102	VAL	CA-C-O	5.57	127.23	121.05
1	B	214	ALA	CA-C-N	5.56	127.29	120.22
1	B	214	ALA	C-N-CA	5.56	127.29	120.22
1	A	148	GLY	CA-C-O	5.53	125.42	119.06
1	B	202	PRO	O-C-N	-5.52	115.98	122.99
1	B	130	ALA	CA-C-O	-5.50	115.03	120.26
1	A	181	LEU	CA-C-O	-5.50	114.60	120.92
1	A	338	ILE	CA-C-O	-5.49	111.46	120.80
1	B	330	THR	N-CA-C	5.49	122.50	110.80
1	A	132	PRO	CA-C-O	-5.48	115.09	121.95
1	A	253	VAL	CA-C-N	-5.47	114.52	120.71
1	A	253	VAL	C-N-CA	-5.47	114.52	120.71
1	B	252	VAL	CA-C-N	-5.47	116.01	123.12
1	B	252	VAL	C-N-CA	-5.47	116.01	123.12
1	B	302	THR	O-C-N	5.47	129.94	123.27
1	B	9	ASP	OD1-CG-OD2	-5.46	109.80	122.90
1	B	92	ALA	CA-C-O	-5.45	114.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LEU	CA-C-O	-5.44	114.78	120.55
1	A	227	LEU	N-CA-CB	-5.44	102.16	109.88
1	A	279	ALA	CB-CA-C	5.44	118.46	109.70
1	A	330	THR	CA-C-N	-5.43	114.68	122.67
1	A	330	THR	C-N-CA	-5.43	114.68	122.67
1	B	174	PRO	CA-C-O	-5.43	115.27	121.56
1	A	132	PRO	CB-CA-C	-5.42	104.13	111.12
1	A	209	GLU	CA-C-N	5.40	127.85	120.46
1	A	209	GLU	C-N-CA	5.40	127.85	120.46
1	B	258	VAL	CA-C-O	5.40	125.72	120.27
1	A	313	ASN	CB-CA-C	-5.39	101.84	110.79
1	A	314	ILE	CA-C-O	-5.39	115.34	120.95
1	A	6	ILE	N-CA-CB	-5.39	104.66	110.53
1	B	130	ALA	N-CA-CB	-5.38	105.45	111.10
1	B	29	ILE	CA-C-O	-5.38	115.47	121.17
1	B	213	LEU	CA-C-N	5.38	128.02	120.28
1	B	213	LEU	C-N-CA	5.38	128.02	120.28
1	B	43	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	A	154	THR	OG1-CB-CG2	-5.37	98.56	109.30
1	A	32	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	110	LEU	CA-C-O	5.36	125.97	119.38
1	A	72	LEU	O-C-N	-5.35	117.11	123.11
1	A	137	ARG	NH1-CZ-NH2	-5.35	112.34	119.30
1	B	46	PRO	N-CA-C	5.35	119.70	111.57
1	B	188	ASN	CB-CG-ND2	-5.35	108.37	116.40
1	B	277	SER	O-C-N	-5.34	116.20	123.15
1	B	6	ILE	CB-CG1-CD1	5.34	125.02	113.80
1	B	35	THR	O-C-N	-5.33	116.26	123.19
1	B	88	ASP	CB-CG-OD1	-5.32	106.16	118.40
1	A	226	ASN	CB-CG-OD1	-5.32	110.16	120.80
1	A	324	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	A	24	LEU	N-CA-C	-5.30	105.39	111.07
1	A	184	GLY	N-CA-C	-5.30	100.61	113.18
1	B	157	ARG	CA-C-O	-5.29	115.07	120.99
1	A	24	LEU	N-CA-CB	5.28	117.67	110.01
1	A	278	THR	N-CA-C	-5.28	106.52	113.17
1	A	127	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	96	ALA	CA-C-O	-5.26	115.48	120.90
1	A	72	LEU	CB-CA-C	-5.26	102.40	109.71
1	A	239	LEU	O-C-N	5.26	129.42	123.27
1	B	50	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	106	VAL	N-CA-C	5.25	119.75	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ARG	O-C-N	-5.25	116.08	122.22
1	A	204	HIS	O-C-N	-5.24	116.09	122.22
1	A	164	GLY	O-C-N	5.24	130.41	122.92
1	B	151	GLN	CA-C-O	-5.24	114.98	121.06
1	A	291	LEU	CB-CA-C	-5.23	105.36	113.57
1	A	307	SER	CA-C-N	5.22	127.71	120.29
1	A	307	SER	C-N-CA	5.22	127.71	120.29
1	A	223	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	179	ASN	N-CA-CB	5.21	118.54	110.46
1	B	308	CYS	CA-CB-SG	-5.21	102.41	114.40
1	B	157	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	A	196	VAL	O-C-N	5.18	128.86	123.26
1	A	34	PHE	CA-C-O	5.18	126.77	121.23
1	B	222	GLN	CB-CG-CD	5.17	121.40	112.60
1	A	131	PRO	N-CA-CB	5.16	108.09	103.08
1	B	68	GLU	CA-C-O	-5.16	115.13	120.70
1	B	157	ARG	CG-CD-NE	-5.16	100.65	112.00
1	B	281	VAL	O-C-N	-5.16	117.58	123.10
1	A	201	VAL	CA-C-O	5.15	126.85	119.95
1	A	126	ASP	CA-C-O	-5.15	113.52	120.47
1	B	84	VAL	CA-CB-CG2	-5.15	101.65	110.40
1	B	260	ALA	CA-C-O	5.14	126.72	121.07
1	B	186	ARG	CD-NE-CZ	5.13	131.59	124.40
1	B	328	ILE	CA-CB-CG1	5.13	119.12	110.40
1	B	270	GLU	CB-CA-C	-5.13	102.13	110.85
1	B	15	GLY	O-C-N	-5.12	117.31	122.54
1	B	61	GLU	N-CA-C	5.12	117.60	111.71
1	B	266	GLN	CA-C-N	5.10	127.38	120.44
1	B	266	GLN	C-N-CA	5.10	127.38	120.44
1	A	120	GLU	CA-C-O	5.10	125.94	120.38
1	B	253	VAL	CA-C-O	-5.09	115.09	120.53
1	B	265	ALA	CA-C-O	5.09	125.82	119.97
1	A	244	GLU	N-CA-C	5.08	116.82	111.28
1	A	189	ILE	CA-C-O	-5.08	115.25	121.04
1	A	100	THR	OG1-CB-CG2	-5.08	99.15	109.30
1	A	193	ARG	CA-C-N	-5.07	118.20	121.65
1	A	193	ARG	C-N-CA	-5.07	118.20	121.65
1	B	120	GLU	CB-CA-C	5.07	118.98	109.71
1	A	181	LEU	CB-CA-C	-5.06	101.17	109.53
1	A	147	ILE	CA-CB-CG2	5.06	119.10	110.50
1	A	138	ARG	CA-CB-CG	-5.05	103.99	114.10
1	B	150	HIS	N-CA-C	5.04	117.13	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	GLU	OE1-CD-OE2	5.03	134.98	122.90
1	B	192	MET	N-CA-CB	5.02	119.48	110.80
1	A	186	ARG	N-CA-CB	5.02	117.28	110.01
1	A	322	PRO	CA-C-O	5.02	125.10	118.98
1	B	245	ASN	CB-CG-ND2	5.01	123.92	116.40
1	B	23	ALA	CA-C-O	-5.01	115.11	120.42

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 [i](#)

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	57	0
1	B	2488	0	2523	49	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	104	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 (104) 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:CE	1:A:275:LEU:HD11	2.14	0.77
1:A:192:MET:HE1	1:A:275:LEU:HD11	1.66	0.76
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:5:MET:HE1	1:B:78:LEU:HG	1.69	0.72
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:93:ILE:HD11	1:A:121:VAL:HG23	1.85	0.57
1:A:208:ARG:HH21	1:A:261:GLU:HG3	1.68	0.57
1:B:5:MET:HE1	1:B:78:LEU:CG	2.34	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:B:96:ALA:O	1:B:97:GLY:C	2.48	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:5:MET:HE1	1:A:78:LEU:HD11	1.88	0.54
1:A:257:ARG:HH11	1:A:257:ARG:HG2	1.73	0.54
1:B:198:LEU:HD13	1:B:201:VAL:O	2.09	0.53
1:A:48:LEU:HB3	1:A:53:LEU:HD13	1.91	0.53
1:B:93:ILE:HD13	1:B:93:ILE:N	2.23	0.52
1:A:18:GLN:CD	1:A:313:ASN:HD21	2.17	0.52
1:A:29:ILE:HG12	1:A:112:PHE:CD1	2.46	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:CG	1:A:50:ARG:HH11	2.27	0.48
1:B:213:LEU:HD21	1:B:267:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:100:THR:O	1:A:104:GLN:HG3	2.15	0.47
1:B:48:LEU:HB3	1:B:53:LEU:HD13	1.97	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:18:GLN:CD	1:A:313:ASN:ND2	2.73	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:B:78:LEU:C	1:B:78:LEU:HD23	2.41	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:181:LEU:HB3	1:B:293:MET:HE2	1.99	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:HG2	1:A:257:ARG:NH1	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
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:197:LEU:CD1	1:A:227:LEU:HD22	2.46	0.42
1:A:208:ARG:HH11	1:A:208:ARG:HG2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ARG:HA	1:B:81:PRO:HD2	1.87	0.42
1:B:335:ARG:HH11	1:B:335:ARG:HD3	1.52	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:B:94:GLY:O	1:B:95:SER:C	2.63	0.41
1:A:18:GLN:NE2	1:A:313:ASN:ND2	2.68	0.41
1:B:131:PRO:HG2	1:B:284:TYR:CE2	2.55	0.41
1:B:160:PHE:CG	1:B:234:GLY:HA3	2.55	0.41
1:A:43:ARG:O	1:A:44:ALA:C	2.61	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: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: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: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:249:ARG:HD2	1:B:251:PHE:CZ	2.56	0.40
1:B:308:CYS:O	1:B:309:HIS:C	2.63	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	332/347 (96%)	324 (98%)	6 (2%)	2 (1%)	21	18
1	B	333/347 (96%)	322 (97%)	8 (2%)	3 (1%)	14	10
All	All	665/694 (96%)	646 (97%)	14 (2%)	5 (1%)	16	12

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%)	242 (93%)	19 (7%)	13	10
1	B	261/274 (95%)	243 (93%)	18 (7%)	14	12
All	All	522/548 (95%)	485 (93%)	37 (7%)	13	11

All (37) 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
1	A	162	PRO
1	A	172	VAL
1	A	181	LEU
1	A	210	ILE
1	A	227	LEU
1	A	239	LEU
1	A	255	GLU
1	A	261	GLU
1	A	308	CYS
1	A	323	VAL

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Mol	Chain	Res	Type
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	281	VAL
1	B	305	HIS
1	B	328	ILE
1	B	333	VAL
1	B	338	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	51	GLN
1	A	104	GLN
1	A	150	HIS
1	A	313	ASN
1	B	12	GLN
1	B	18	GLN
1	B	152	GLN
1	B	266	GLN
1	B	288	GLN
1	B	309	HIS

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
2	CIT	A	401	-	12,12,12	1.79	2 (16%)	17,17,17	2.58	8 (47%)
3	DTO	B	402	-	5,8,8	1.59	1 (20%)	3,9,9	0.81	0
2	CIT	B	401	-	12,12,12	1.89	3 (25%)	17,17,17	2.20	6 (35%)

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	CIT	A	401	-	-	0/16/16/16	-
3	DTO	B	402	-	-	5/8/9/9	-
2	CIT	B	401	-	-	4/16/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	CIT	C3-C6	4.69	1.58	1.53
2	A	401	CIT	C3-C6	4.33	1.58	1.53
3	B	402	DTO	C4-C3	2.48	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	CIT	O3-C5	2.26	1.29	1.22
2	A	401	CIT	C4-C5	2.16	1.57	1.50
2	B	401	CIT	O7-C3	2.09	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CIT	O5-C6-C3	-6.01	110.44	122.09
2	A	401	CIT	C4-C3-C2	4.90	121.89	109.31
2	B	401	CIT	O5-C6-C3	-4.07	114.21	122.09
2	B	401	CIT	O7-C3-C6	-3.64	103.80	108.96
2	B	401	CIT	O3-C5-C4	-3.35	113.48	122.95
2	A	401	CIT	O6-C6-C3	3.13	119.14	113.14
2	A	401	CIT	O7-C3-C4	-3.05	102.42	109.38
2	B	401	CIT	O6-C6-C3	2.99	118.88	113.14
2	A	401	CIT	O3-C5-C4	-2.90	114.74	122.95
2	A	401	CIT	O1-C1-C2	-2.85	114.87	122.95
2	B	401	CIT	C4-C3-C2	2.71	116.26	109.31
2	B	401	CIT	O1-C1-C2	-2.70	115.32	122.95
2	A	401	CIT	O7-C3-C2	-2.67	103.29	109.38
2	A	401	CIT	O6-C6-O5	2.05	130.41	123.86

There are no chirality outliers.

All (9) 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	O1-C1-C2-C3
2	B	401	CIT	O2-C1-C2-C3
2	B	401	CIT	C6-C3-C4-C5
2	B	401	CIT	C2-C3-C6-O6

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	334/347 (96%)	-0.28	7 (2%) 63 66	16, 34, 59, 78	0
1	B	335/347 (96%)	-0.33	7 (2%) 63 66	20, 33, 63, 79	0
All	All	669/694 (96%)	-0.30	14 (2%) 63 66	16, 34, 60, 79	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	4.4
1	A	331	ASP	3.5
1	A	95	SER	3.3
1	A	332	GLY	3.3
1	A	130	ALA	3.3
1	B	11	ALA	2.9
1	A	14	GLU	2.8
1	B	94	GLY	2.5
1	B	330	THR	2.4
1	B	96	ALA	2.3
1	A	94	GLY	2.3
1	B	305	HIS	2.1
1	B	257	ARG	2.1
1	B	258	VAL	2.1

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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	CIT	B	401	13/13	0.83	0.10	57,59,61,61	0
3	DTO	B	402	9/9	0.84	0.12	74,78,81,81	0
2	CIT	A	401	13/13	0.85	0.09	60,64,67,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.