



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 1NH3 / pdb_00001nh3
Title : Human Topoisomerase I Ara-C Complex
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Deposited on : 2002-12-18
Resolution : 3.10 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

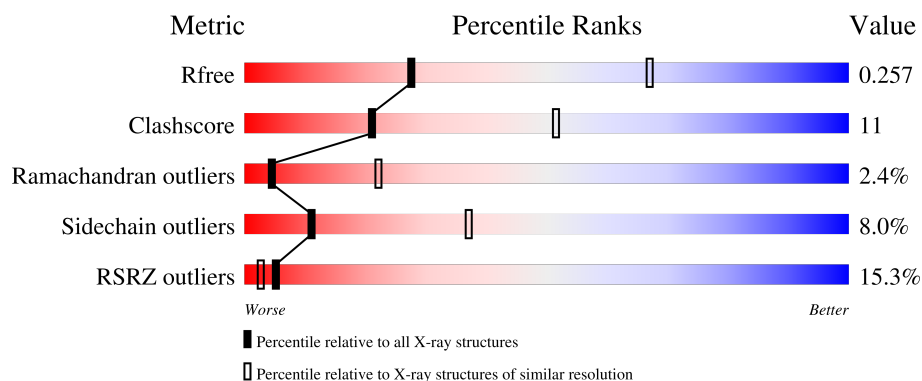
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	B	10	8% 30% 50% 10% 10%
2	C	12	8% 25% 42% 25% 8%
3	D	22	5% 18% 50% 27% 5%
4	A	563	13% 67% 14% .. 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4394 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 DNA chain called 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*UP*(UBB))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			201	97	42	53	9			

- Molecule 2 is a DNA chain called 5'-D(*(GNG)P*GP*AP*AP*AP*AP*AP*UP*UP*UP*UP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			242	116	45	70	11			

- Molecule 3 is DNA/RNA hybrid called 5'-D(*AP*AP*AP*AP*AP*TP*UP*UP*UP*UP*CP*(CAR)P*AP*AP*GP*UP*CP*UP*UP*UP*UP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			435	208	71	135	21			

- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	471	Total	C	N	O	P	0	0	0
			3483	2227	612	625	1 18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	MET	-	initiating methionine	UNP P11387
A	723	PTR	TYR	modified residue	UNP P11387

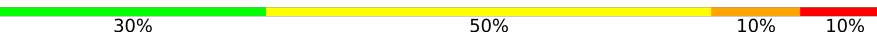
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	O 2	0	0
5	C	5	Total 5	O 5	0	0
5	D	5	Total 5	O 5	0	0
5	A	21	Total 21	O 21	0	0

3 Residue-property plots [i](#)

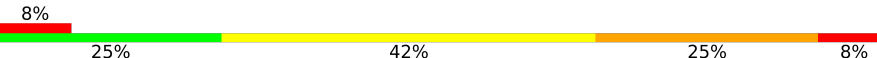
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

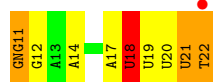
- Molecule 1: 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*UP*(UBB))-3'

Chain B: 



- Molecule 2: 5'-D(*(GNG)P*GP*AP*AP*AP*AP*AP*UP*UP*UP*UP*T))-3'

Chain C: 



- Molecule 3: 5'-D(*AP*AP*AP*AP*AP*TP*UP*UP*UP*UP*CP*(CAR)P*AP*AP*GP*UP*CP*UP*UP*UP*UP*T))-3'

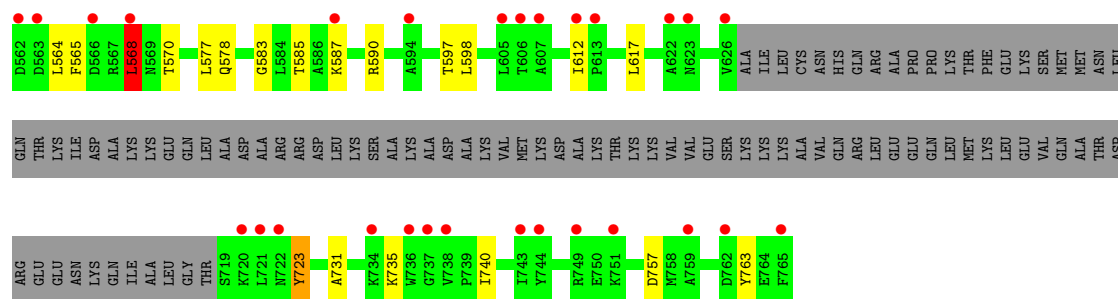
Chain D: 



- Molecule 4: DNA topoisomerase I

Chain A: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	72.97 Å 72.97 Å 186.29 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.29 – 3.10 44.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	74.6 (44.29-3.10) 84.0 (44.29-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.311 0.255 , 0.257	Depositor DCC
R_{free} test set	857 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	1.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 102.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.062 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNG, PTR, CAR, UBB

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	B	0.57	1/207 (0.5%)	0.82	0/317
2	C	0.83	2/250 (0.8%)	0.83	1/382 (0.3%)
3	D	0.94	7/463 (1.5%)	0.76	0/706
4	A	0.70	0/3558	1.53	36/4798 (0.8%)
All	All	0.73	10/4478 (0.2%)	1.40	37/6203 (0.6%)

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	1
2	C	0	1
3	D	0	1
4	A	0	3
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	109	DU	O3'-P	6.34	1.62	1.56
2	C	21	DU	O3'-P	5.71	1.61	1.56
3	D	110	DU	O3'-P	5.66	1.61	1.56
3	D	116	DU	O3'-P	5.58	1.61	1.56
3	D	106	DT	O3'-P	5.58	1.61	1.56
3	D	120	DU	O3'-P	5.52	1.61	1.56
2	C	18	DU	O3'-P	5.42	1.61	1.56
1	B	8	DC	O3'-P	5.28	1.61	1.56
3	D	115	DG	O3'-P	5.22	1.61	1.56
3	D	121	DU	O3'-P	5.02	1.61	1.56

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	556	GLU	O-C-N	-35.15	83.24	122.96
4	A	557	ASN	N-CA-CB	-28.08	65.56	110.21
4	A	555	MET	CA-C-N	22.37	158.52	121.39
4	A	555	MET	C-N-CA	22.37	158.52	121.39
4	A	555	MET	O-C-N	-17.78	98.94	122.59
4	A	556	GLU	CA-C-O	-14.15	105.20	121.47
4	A	556	GLU	CA-C-N	11.70	137.98	122.42
4	A	556	GLU	C-N-CA	11.70	137.98	122.42
4	A	555	MET	CA-C-O	-10.22	105.89	120.51
4	A	557	ASN	N-CA-C	-8.89	94.09	108.41
4	A	351	ALA	N-CA-C	6.91	118.89	111.36
4	A	303	THR	N-CA-C	6.84	119.61	111.33
4	A	496	GLY	N-CA-C	-6.65	106.57	114.48
4	A	320	SER	N-CA-C	6.62	118.87	110.33
4	A	364	ARG	N-CA-C	6.44	119.25	110.55
4	A	504	CYS	N-CA-C	6.44	118.09	111.14
4	A	568	LEU	N-CA-C	6.42	118.15	108.46
4	A	412	TRP	N-CA-C	6.19	120.01	110.42
4	A	597	THR	N-CA-C	-6.01	104.36	111.03
4	A	396	PRO	CA-C-N	5.98	127.32	119.84
4	A	396	PRO	C-N-CA	5.98	127.32	119.84
4	A	237	ASN	N-CA-C	5.94	119.79	112.54
4	A	489	ALA	N-CA-C	5.93	118.98	111.69
4	A	556	GLU	N-CA-C	-5.84	101.83	110.48
2	C	22	DT	C2'-C3'-O3'	-5.84	102.75	111.50
4	A	236	GLU	N-CA-C	5.76	118.30	111.33
4	A	476	ALA	N-CA-C	5.75	118.01	111.11
4	A	441	TRP	N-CA-C	-5.62	105.07	111.14
4	A	735	LYS	N-CA-C	-5.53	105.27	112.23
4	A	307	GLN	N-CA-C	-5.44	105.38	112.23
4	A	469	GLU	N-CA-C	5.43	118.42	109.72
4	A	392	VAL	N-CA-C	5.40	114.05	109.02
4	A	617	LEU	N-CA-C	-5.30	106.32	112.89
4	A	329	GLU	N-CA-C	-5.27	105.99	112.90
4	A	249	LEU	N-CA-C	5.19	117.86	109.40
4	A	757	ASP	N-CA-C	5.16	119.44	113.20
4	A	260	PHE	N-CA-C	-5.05	106.62	112.89

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	555	MET	Mainchain
4	A	556	GLU	Peptide,Mainchain
1	B	8	DC	Sidechain
2	C	18	DU	Sidechain
3	D	115	DG	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	B	201	0	109	10	0
2	C	242	0	131	17	0
3	D	435	0	237	36	0
4	A	3483	0	3181	38	0
5	A	21	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	2	0
All	All	4394	0	3658	87	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 11.

All (87) 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)
3:D:110:DU:H2'	3:D:111:DC:H5''	1.22	1.18
2:C:17:DA:H2''	2:C:18:DU:H5''	1.30	1.11
3:D:110:DU:H2'	3:D:111:DC:C5'	1.93	0.97
3:D:101:DA:H2''	3:D:102:DA:OP2	1.69	0.93
3:D:110:DU:C2'	3:D:111:DC:H5''	2.04	0.86
2:C:17:DA:C2'	2:C:18:DU:H5''	2.06	0.85
3:D:118:DU:H4'	5:D:23:HOH:O	1.75	0.85
3:D:111:DC:H2''	3:D:112:CAR:O5'	1.83	0.78
3:D:102:DA:H2''	3:D:103:DA:C8	2.19	0.77
1:B:8:DC:H5''	4:A:439:LYS:NZ	2.09	0.67
4:A:488:ARG:NH1	4:A:590:ARG:HH12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:578:GLN:HE22	4:A:583:GLY:H	1.42	0.66
3:D:120:DU:H5'	5:D:31:HOH:O	1.95	0.65
2:C:22:DT:O2	3:D:101:DA:C2	2.50	0.65
1:B:10:UBB:C2'	4:A:723:PTR:O3P	2.45	0.63
3:D:102:DA:H2''	3:D:103:DA:H8	1.64	0.62
4:A:491:ASN:HD22	4:A:491:ASN:N	1.96	0.62
3:D:119:DU:H2'	3:D:120:DU:C5'	2.31	0.61
1:B:6:DG:H2''	4:A:426:TYR:OH	2.02	0.59
4:A:491:ASN:HD22	4:A:491:ASN:H	1.51	0.59
3:D:118:DU:H2'	3:D:119:DU:C6	2.33	0.59
3:D:119:DU:H2'	3:D:120:DU:H5''	1.84	0.59
2:C:17:DA:H2''	2:C:18:DU:C5'	2.18	0.58
3:D:109:DU:H2'	3:D:110:DU:H6	1.85	0.58
4:A:278:PHE:O	4:A:282:TRP:HB2	2.04	0.58
3:D:115:DG:H8	3:D:115:DG:C5'	2.18	0.56
2:C:21:DU:H2''	2:C:22:DT:C7	2.36	0.56
2:C:20:DU:H2'	2:C:21:DU:OP2	2.05	0.56
1:B:8:DC:H2''	1:B:9:DU:OP2	2.05	0.55
1:B:8:DC:H5''	4:A:439:LYS:HZ1	1.71	0.54
4:A:384:ILE:HD13	4:A:414:VAL:HG22	1.91	0.53
4:A:424:ILE:HD12	4:A:424:ILE:H	1.74	0.52
4:A:555:MET:O	4:A:556:GLU:O	2.27	0.52
3:D:105:DA:H1'	3:D:106:DT:H5''	1.92	0.52
1:B:6:DG:H2'	4:A:424:ILE:HD13	1.93	0.50
4:A:723:PTR:HE1	4:A:723:PTR:O1P	2.11	0.50
4:A:491:ASN:N	4:A:491:ASN:ND2	2.58	0.50
4:A:488:ARG:NH1	4:A:590:ARG:NH1	2.60	0.49
3:D:113:DA:H2''	3:D:114:DA:O5'	2.14	0.48
3:D:118:DU:C2'	3:D:119:DU:C6	2.93	0.47
3:D:119:DU:H2'	3:D:120:DU:H5'	1.96	0.47
1:B:8:DC:H5''	4:A:439:LYS:HZ3	1.78	0.47
2:C:21:DU:H2'	2:C:22:DT:O5'	2.14	0.46
4:A:473:ARG:O	4:A:477:VAL:HG23	2.16	0.46
4:A:467:SER:OG	4:A:468:LYS:N	2.48	0.46
3:D:112:CAR:O2'	3:D:113:DA:C8	2.68	0.45
3:D:117:DC:H2''	3:D:118:DU:OP2	2.16	0.45
2:C:11:GNG:H2'2	2:C:12:DG:C8	2.52	0.45
3:D:115:DG:C5'	3:D:115:DG:C8	3.00	0.45
4:A:556:GLU:O	4:A:557:ASN:C	2.57	0.45
2:C:21:DU:H2''	2:C:22:DT:H72	1.98	0.44
4:A:442:GLN:HE22	4:A:449:ARG:NH2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:DC:H4'	4:A:439:LYS:HE2	1.99	0.44
2:C:21:DU:OP2	2:C:21:DU:H6	2.17	0.44
3:D:115:DG:H2''	3:D:116:DU:H5'	1.99	0.43
3:D:115:DG:H8	3:D:115:DG:H5'	1.82	0.43
2:C:22:DT:O2	3:D:101:DA:H2	1.99	0.43
4:A:302:PHE:HA	4:A:305:MET:HE3	1.99	0.43
2:C:14:DA:H61	3:D:109:DU:H3	1.67	0.43
2:C:19:DU:H2'	2:C:20:DU:H6	1.99	0.43
3:D:114:DA:C2	3:D:115:DG:C4	3.07	0.43
3:D:115:DG:H2''	3:D:116:DU:C5'	2.48	0.43
3:D:119:DU:H2'	3:D:120:DU:H6	2.00	0.43
4:A:565:PHE:HB3	4:A:568:LEU:HB3	2.01	0.43
2:C:21:DU:H3'	5:C:23:HOH:O	2.19	0.43
3:D:110:DU:H2'	3:D:111:DC:H5'	1.93	0.42
2:C:12:DG:N2	3:D:112:CAR:O2	2.52	0.42
2:C:22:DT:O2	3:D:101:DA:N1	2.52	0.42
4:A:320:SER:C	4:A:322:GLU:H	2.27	0.42
3:D:101:DA:C2	3:D:102:DA:C6	3.08	0.42
3:D:113:DA:H3'	4:A:361:PHE:CZ	2.54	0.42
4:A:408:ASN:H	4:A:408:ASN:HD22	1.66	0.42
1:B:6:DG:C6	1:B:7:DA:C6	3.08	0.42
2:C:19:DU:H2'	2:C:20:DU:C6	2.50	0.42
3:D:117:DC:H3'	4:A:585:THR:HG21	2.03	0.41
4:A:408:ASN:H	4:A:408:ASN:ND2	2.19	0.41
3:D:119:DU:C2'	3:D:120:DU:H5''	2.51	0.41
4:A:731:ALA:HB2	4:A:763:TYR:HB3	2.03	0.41
1:B:4:DA:H2''	1:B:5:DA:H8	1.86	0.41
4:A:367:HIS:HA	4:A:368:PRO:HD2	1.99	0.41
4:A:266:HIS:C	4:A:268:TYR:H	2.29	0.40
4:A:403:GLU:HG2	4:A:404:VAL:H	1.87	0.40
4:A:509:VAL:HG13	4:A:555:MET:HB3	2.02	0.40
4:A:558:LYS:NZ	4:A:564:LEU:O	2.54	0.40
4:A:467:SER:HB3	4:A:473:ARG:HG3	2.02	0.40
4:A:477:VAL:O	4:A:480:TYR:HB3	2.21	0.40
4:A:541:VAL:HA	4:A:542:PRO:HD3	1.77	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	
4	A	466/563 (83%)	402 (86%)	53 (11%)	11 (2%)	4	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	612	ILE
4	A	397	PRO
4	A	470	MET
4	A	240	PHE
4	A	345	ASN
4	A	555	MET
4	A	230	PRO
4	A	344	ASP
4	A	451	LYS
4	A	365	GLY
4	A	490	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	325/506 (64%)	299 (92%)	26 (8%)	11	37

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	221	GLU
4	A	230	PRO
4	A	238	VAL
4	A	266	HIS
4	A	282	TRP
4	A	343	MET
4	A	387	SER
4	A	391	LYS
4	A	397	PRO
4	A	417	THR
4	A	424	ILE
4	A	431	PRO
4	A	442	GLN
4	A	456	LYS
4	A	469	GLU
4	A	491	ASN
4	A	502	VAL
4	A	539	ASN
4	A	553	LEU
4	A	555	MET
4	A	568	LEU
4	A	570	THR
4	A	577	LEU
4	A	587	LYS
4	A	598	LEU
4	A	740	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	385	ASN
4	A	408	ASN
4	A	442	GLN
4	A	491	ASN
4	A	552	GLN
4	A	578	GLN
4	A	601	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	GNG	C	11	3,2	21,21,21	0.81	1 (4%)	25,31,31	1.07	2 (8%)
4	PTR	A	723	4,1	15,16,17	1.21	2 (13%)	17,22,24	0.89	0
1	UBB	B	10	4,3,1	16,19,20	0.38	0	20,26,29	0.73	1 (5%)
3	CAR	D	112	3,2	18,21,22	0.59	0	25,30,33	0.81	1 (4%)

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	GNG	C	11	3,2	-	0/6/18/18	0/3/3/3
4	PTR	A	723	4,1	-	1/10/11/13	0/1/1/1
1	UBB	B	10	4,3,1	-	1/7/18/19	0/2/2/2
3	CAR	D	112	3,2	-	3/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	723	PTR	CE2-CD2	2.08	1.42	1.38
2	C	11	GNG	C2-N1	2.05	1.38	1.33
4	A	723	PTR	CE1-CD1	2.03	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	GNG	C5-C4-N9	-3.10	104.81	106.25
1	B	10	UBB	C2'-C1'-N1	2.59	117.31	112.40
3	D	112	CAR	C2'-C1'-N1	2.37	119.84	113.25
2	C	11	GNG	N2-C2-N1	-2.04	115.69	119.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	723	PTR	O-C-CA-CB
3	D	112	CAR	C4'-C5'-O5'-P
3	D	112	CAR	O4'-C4'-C5'-O5'
3	D	112	CAR	C3'-C4'-C5'-O5'
1	B	10	UBB	O4'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	GNG	1	0
4	A	723	PTR	2	0
1	B	10	UBB	1	0
3	D	112	CAR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	B	8/10 (80%)	0.19	0 100 100	17, 37, 64, 71	0
2	C	7/12 (58%)	0.70	1 (14%) 6 3	36, 45, 73, 91	0
3	D	12/22 (54%)	0.71	1 (8%) 17 9	24, 54, 88, 122	0
4	A	470/563 (83%)	0.99	74 (15%) 5 2	9, 68, 138, 199	0
All	All	497/607 (81%)	0.97	76 (15%) 5 3	9, 66, 138, 199	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	721	LEU	6.2
4	A	293	ILE	5.8
4	A	765	PHE	4.9
4	A	373	LEU	4.8
4	A	365	GLY	4.3
4	A	303	THR	4.3
4	A	244	GLY	4.2
4	A	743	ILE	4.2
4	A	289	GLU	4.2
3	D	101	DA	4.1
4	A	737	GLY	4.0
4	A	286	MET	4.0
4	A	449	ARG	4.0
4	A	607	ALA	4.0
4	A	261	ALA	3.9
4	A	343	MET	3.8
4	A	759	ALA	3.7
4	A	203	TRP	3.7
4	A	749	ARG	3.6
4	A	566	ASP	3.6
4	A	255	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	A	353	PHE	3.5
4	A	605	LEU	3.5
4	A	738	VAL	3.4
4	A	448	ARG	3.3
4	A	421	GLN	3.3
4	A	204	LYS	3.2
4	A	736	TRP	3.2
4	A	562	ASP	3.2
4	A	314	GLU	3.2
2	C	22	DT	3.1
4	A	279	PHE	3.1
4	A	284	LYS	3.1
4	A	292	ASN	3.0
4	A	306	SER	2.9
4	A	418	GLU	2.9
4	A	720	LYS	2.9
4	A	563	ASP	2.8
4	A	528	ASP	2.8
4	A	419	ASN	2.8
4	A	744	TYR	2.8
4	A	287	THR	2.8
4	A	762	ASP	2.8
4	A	240	PHE	2.7
4	A	587	LYS	2.6
4	A	622	ALA	2.6
4	A	296	ASN	2.6
4	A	722	ASN	2.5
4	A	493	LYS	2.5
4	A	243	ASP	2.4
4	A	313	THR	2.4
4	A	464	ASP	2.4
4	A	626	VAL	2.4
4	A	751	LYS	2.4
4	A	568	LEU	2.4
4	A	290	GLU	2.4
4	A	252	LYS	2.3
4	A	241	TYR	2.3
4	A	340	PHE	2.3
4	A	308	TYR	2.3
4	A	613	PRO	2.3
4	A	316	ARG	2.3
4	A	606	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	A	305	MET	2.2
4	A	612	ILE	2.2
4	A	408	ASN	2.2
4	A	594	ALA	2.2
4	A	323	GLU	2.1
4	A	269	THR	2.1
4	A	389	ASP	2.1
4	A	417	THR	2.1
4	A	277	ASN	2.0
4	A	345	ASN	2.0
4	A	623	ASN	2.0
4	A	519	ASP	2.0
4	A	734	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	CAR	D	112	20/21	0.86	0.13	25,46,55,55	0
4	PTR	A	723	16/17	0.89	0.23	105,106,108,108	0
2	GNG	C	11	19/19	0.92	0.11	26,38,70,74	0
1	UBB	B	10	18/19	0.96	0.09	14,23,34,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.