



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:35 PM UTC

PDB ID : 3RTX / pdb_00003rtx
Title : Crystal structure of mammalian capping enzyme (Mce1) and Pol II CTD complex
Authors : Ghosh, A.; Lima, C.D.
Deposited on : 2011-05-04
Resolution : 2.81 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

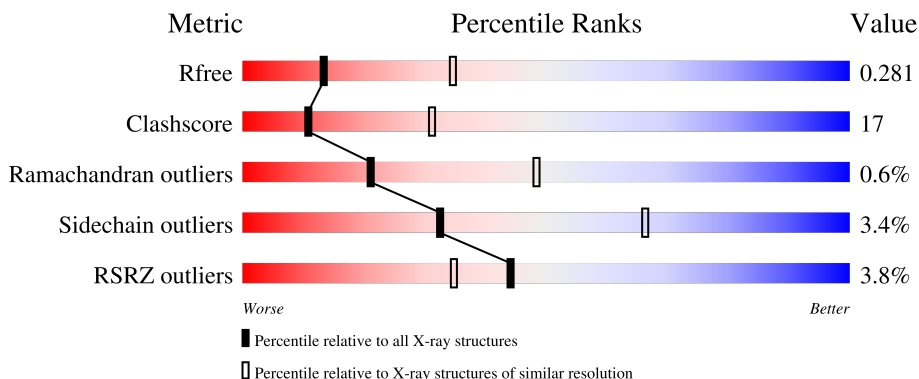
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	343	 2% 49% 26% 24%
1	B	343	 3% 48% 25% 26%
2	C	18	 6% 44% 22% 6% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4388 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 mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2094	1336	360	382	16	0	0	0
1	B	254	2039	1302	351	370	16	0	0	0

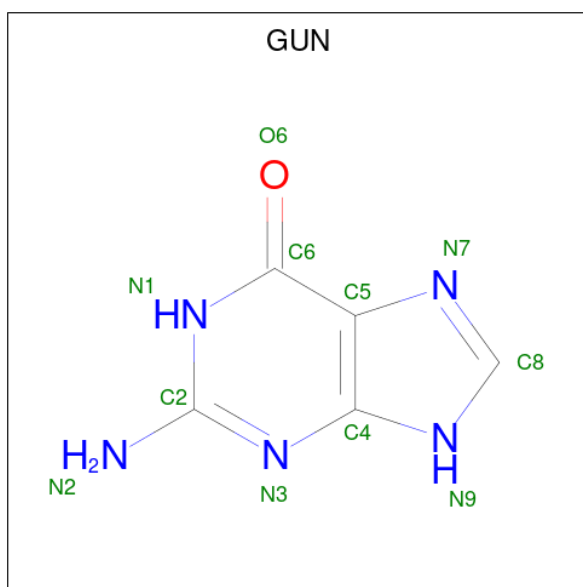
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	SER	-	expression tag	UNP O55236
B	225	SER	-	expression tag	UNP O55236

- Molecule 2 is a protein called RNA Polymerase II C-terminal domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	13	111	60	13	34	4	0	0	0

- Molecule 3 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).

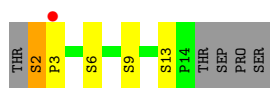


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	5	1		
3	B	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	63	Total	O	0	0
			63	63		

- Molecule 2: RNA Polymerase II C-terminal domain



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.98Å 114.75Å 150.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.81) 98.8 (50.00-2.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.224 , 0.280 0.224 , 0.281	Depositor DCC
R_{free} test set	910 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.671	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4388	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% 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: GUN, SEP

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	0.33	0/2137	0.85	5/2878 (0.2%)
1	B	0.33	0/2081	0.82	2/2800 (0.1%)
2	C	0.26	0/73	0.62	0/94
All	All	0.33	0/4291	0.83	7/5772 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	327	PHE	CA-C-N	6.61	126.53	119.85
1	A	327	PHE	C-N-CA	6.61	126.53	119.85
1	B	327	PHE	CA-C-N	5.99	125.90	119.85
1	B	327	PHE	C-N-CA	5.99	125.90	119.85
1	A	245	THR	N-CA-C	-5.36	107.75	114.56
1	A	238	VAL	N-CA-C	5.14	114.15	106.85
1	A	454	ASP	N-CA-C	-5.07	107.16	113.19

There are no chirality outliers.

There are no planarity outliers.

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	2094	0	2108	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2039	0	2057	71	0
2	C	111	0	78	4	0
3	A	11	0	5	0	0
3	B	11	0	5	0	0
4	A	59	0	0	1	0
4	B	63	0	0	3	0
All	All	4388	0	4253	141	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 17.

All (141) 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:423:LYS:HE2	1:B:428:ASN:HD22	1.31	0.93
1:A:420:ILE:HD11	1:B:414:GLN:HE22	1.46	0.80
1:A:286:GLN:HA	1:B:397:LYS:HD3	1.66	0.77
1:A:305:ASP:HA	1:A:338:SER:HA	1.67	0.75
1:B:358:ARG:HG2	1:B:409:SER:HB3	1.69	0.73
1:A:420:ILE:O	1:A:420:ILE:HG22	1.88	0.72
1:B:397:LYS:NZ	1:B:397:LYS:HB3	2.06	0.70
1:A:390:SER:HB3	1:A:391:PRO:HD3	1.74	0.70
1:A:386:ARG:HH12	2:C:3:PRO:HD2	1.57	0.70
1:B:390:SER:HB2	1:B:391:PRO:HD3	1.72	0.70
1:B:397:LYS:HB3	1:B:397:LYS:HZ2	1.57	0.70
1:A:386:ARG:HH22	2:C:2:SEP:HA	1.57	0.69
1:A:285:GLU:HB3	1:A:565:CYS:SG	2.33	0.68
1:A:247:GLN:OE1	1:A:250:LEU:HB3	1.94	0.67
1:A:395:LYS:HB3	1:A:401:ILE:HD12	1.75	0.67
1:B:422:ARG:NH2	1:B:563:ASP:HB2	2.12	0.65
1:B:416:PHE:HB3	1:B:420:ILE:HD12	1.77	0.65
1:B:392:ARG:O	1:B:396:MET:HG3	1.96	0.65
1:B:315:ARG:HG3	4:B:100:HOH:O	1.97	0.64
1:A:395:LYS:HD3	1:A:401:ILE:HD11	1.80	0.63
1:B:268:PHE:CE2	1:B:270:GLY:HA3	2.33	0.63
1:A:278:LYS:HD3	1:A:551:ASN:HB3	1.80	0.62
1:B:393:HIS:HA	1:B:396:MET:HE2	1.82	0.61
1:A:351:VAL:HG12	1:A:352:ASN:ND2	2.16	0.60
1:A:402:ASP:HB3	1:A:405:GLN:HG2	1.82	0.60
1:A:420:ILE:CD1	1:B:414:GLN:HE22	2.13	0.60
1:A:567:ALA:O	1:B:411:ARG:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:MET:HE3	1:A:543:MET:HA	1.86	0.58
1:B:345:GLU:HG2	1:B:362:TYR:HE2	1.69	0.58
1:B:444:PRO:HG3	1:B:455:ASP:HB3	1.84	0.58
1:B:239:LYS:HA	4:B:34:HOH:O	2.04	0.57
1:B:247:GLN:HG3	1:B:248:PRO:HA	1.85	0.57
1:A:247:GLN:HG3	1:A:248:PRO:HA	1.85	0.57
1:B:314:ASP:OD2	1:B:318:SER:HB2	2.05	0.56
1:A:233:LEU:HD13	1:A:236:ILE:HD11	1.86	0.56
1:A:286:GLN:HA	1:B:397:LYS:CD	2.33	0.56
1:A:286:GLN:HG2	1:B:397:LYS:HD2	1.88	0.56
1:A:453:CYS:C	1:A:455:ASP:H	2.12	0.56
1:B:422:ARG:HH22	1:B:563:ASP:CG	2.14	0.56
1:A:291:VAL:HG22	1:A:292:SER:N	2.20	0.56
1:A:294:LYS:NZ	1:A:460:LYS:HE3	2.21	0.56
1:B:278:LYS:HE3	1:B:557:MET:HE1	1.88	0.55
1:B:330:ARG:HD3	1:B:386:ARG:O	2.07	0.55
1:A:340:THR:HA	1:A:366:LYS:O	2.07	0.55
1:B:559:PHE:O	1:B:563:ASP:HB2	2.06	0.55
1:A:345:GLU:HG2	1:A:362:TYR:HE2	1.72	0.54
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.22	0.54
1:A:313:ILE:HD12	1:A:313:ILE:N	2.23	0.54
1:A:358:ARG:HG2	1:A:409:SER:OG	2.08	0.54
1:A:294:LYS:HZ3	1:A:460:LYS:HE3	1.72	0.53
1:A:423:LYS:HE2	1:B:428:ASN:ND2	2.12	0.53
1:B:376:ASP:OD1	1:B:445:ILE:HB	2.08	0.53
1:A:417:ASP:HB3	1:A:419:ASN:OD1	2.09	0.52
1:B:274:VAL:O	1:B:458:LYS:HG2	2.10	0.52
1:B:333:LEU:HB3	1:B:395:LYS:HE3	1.92	0.52
1:A:274:VAL:HG21	1:A:454:ASP:HA	1.92	0.51
1:B:365:ILE:HD12	1:B:365:ILE:N	2.25	0.51
1:A:418:ILE:C	1:A:420:ILE:H	2.19	0.51
1:B:300:TYR:CE1	1:B:314:ASP:HB3	2.46	0.51
1:B:422:ARG:HH22	1:B:563:ASP:HB2	1.75	0.50
1:B:555:LYS:HB3	1:B:555:LYS:NZ	2.26	0.50
1:B:425:LEU:HD12	1:B:559:PHE:HZ	1.76	0.50
1:A:420:ILE:O	1:A:420:ILE:CG2	2.59	0.50
1:B:247:GLN:OE1	1:B:250:LEU:HB3	2.12	0.50
1:B:253:VAL:HG13	1:B:303:LEU:HD23	1.93	0.50
1:A:445:ILE:HD12	1:A:446:GLY:N	2.27	0.50
1:A:364:ILE:HG23	1:A:364:ILE:O	2.12	0.50
1:A:232:PHE:CD2	1:A:241:VAL:HG11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:CG	1:A:241:VAL:HG11	2.47	0.49
1:B:368:ASN:O	1:B:369:ALA:HB3	2.12	0.49
1:B:315:ARG:HD3	4:B:16:HOH:O	2.11	0.49
1:A:446:GLY:HA3	4:A:88:HOH:O	2.12	0.49
1:A:232:PHE:HZ	1:A:312:MET:HE2	1.78	0.49
1:B:342:LEU:HD23	1:B:364:ILE:HG13	1.95	0.49
1:A:361:ILE:HG22	1:A:384:ILE:HD13	1.95	0.48
1:A:386:ARG:NH1	2:C:3:PRO:HD2	2.25	0.48
1:A:393:HIS:HA	1:A:396:MET:HE3	1.94	0.48
1:B:248:PRO:O	1:B:252:GLU:HG3	2.13	0.48
1:B:386:ARG:HG3	1:B:386:ARG:HH11	1.78	0.48
1:B:556:GLU:O	1:B:560:GLU:HG2	2.14	0.48
1:B:268:PHE:CE1	1:B:301:MET:HG3	2.49	0.48
1:B:263:TRP:CE3	1:B:450:PRO:HB2	2.48	0.48
1:B:293:TRP:HB2	1:B:424:LEU:HD21	1.95	0.48
1:A:453:CYS:C	1:A:455:ASP:N	2.71	0.47
1:A:386:ARG:NH2	2:C:2:SEP:HA	2.29	0.47
1:B:362:TYR:CZ	1:B:413:LYS:HE2	2.51	0.46
1:A:305:ASP:OD1	1:A:338:SER:HB2	2.16	0.46
1:B:441:ILE:HD11	1:B:456:ILE:HG22	1.97	0.46
1:A:346:MET:HE3	1:A:358:ARG:C	2.41	0.46
1:A:466:SER:C	1:A:545:VAL:HG11	2.41	0.46
1:B:554:THR:C	1:B:556:GLU:N	2.73	0.46
1:B:554:THR:C	1:B:556:GLU:H	2.23	0.46
1:A:411:ARG:HG3	1:A:412:PRO:HD2	1.99	0.45
1:B:422:ARG:HH22	1:B:563:ASP:CB	2.29	0.45
1:A:539:TYR:O	1:A:543:MET:HB2	2.17	0.45
1:A:282:ARG:O	1:A:285:GLU:HG2	2.16	0.45
1:A:314:ASP:OD2	1:A:318:SER:HB2	2.17	0.45
1:A:368:ASN:O	1:A:369:ALA:HB3	2.17	0.44
1:A:281:ILE:O	1:A:281:ILE:HG12	2.16	0.44
1:A:445:ILE:HD12	1:A:445:ILE:C	2.41	0.44
1:B:294:LYS:O	1:B:438:ASP:HB2	2.17	0.44
1:B:366:LYS:HG3	1:B:370:GLN:O	2.18	0.44
1:B:425:LEU:C	1:B:427:GLY:H	2.25	0.44
1:B:560:GLU:O	1:B:564:ARG:HG3	2.17	0.44
1:A:425:LEU:HD12	1:A:559:PHE:HZ	1.82	0.44
1:A:397:LYS:NZ	1:A:397:LYS:HB3	2.32	0.43
1:B:459:TRP:CH2	1:B:461:PRO:HG3	2.53	0.43
1:A:441:ILE:O	1:A:441:ILE:HG23	2.18	0.43
1:B:367:PHE:O	1:B:370:GLN:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:CE2	1:B:381:LEU:HD11	2.53	0.43
1:A:463:SER:O	1:A:464:LEU:HB2	2.18	0.43
1:A:345:GLU:HG2	1:A:362:TYR:CE2	2.52	0.43
1:B:228:LEU:HD12	1:B:228:LEU:N	2.34	0.43
1:B:313:ILE:HD12	1:B:313:ILE:N	2.33	0.43
1:A:545:VAL:O	1:A:549:ILE:HG13	2.18	0.43
1:A:347:ILE:HD13	1:A:360:LEU:HD11	2.01	0.43
1:A:376:ASP:OD2	1:A:376:ASP:C	2.61	0.43
1:B:273:PRO:HB3	1:B:456:ILE:HG22	2.01	0.42
1:A:567:ALA:HB2	1:B:396:MET:HE1	2.02	0.42
1:A:365:ILE:N	1:A:365:ILE:HD12	2.34	0.42
1:B:459:TRP:CZ3	1:B:461:PRO:HG3	2.54	0.42
1:A:249:LYS:O	1:A:253:VAL:HG23	2.19	0.42
1:B:225:SER:O	1:B:226:LEU:C	2.61	0.42
1:B:282:ARG:HA	1:B:561:PHE:CZ	2.55	0.42
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.84	0.42
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.84	0.41
1:B:416:PHE:CD1	1:B:416:PHE:N	2.88	0.41
1:A:402:ASP:O	1:A:405:GLN:HG2	2.20	0.41
1:B:420:ILE:O	1:B:420:ILE:HG22	2.21	0.41
1:A:278:LYS:CD	1:A:551:ASN:HB3	2.49	0.41
1:B:305:ASP:HA	1:B:338:SER:HA	2.03	0.41
1:B:367:PHE:O	1:B:368:ASN:C	2.64	0.41
1:A:295:ALA:HB3	1:A:345:GLU:OE1	2.20	0.41
1:A:351:VAL:HG21	1:A:358:ARG:NH2	2.36	0.41
1:A:396:MET:HG2	1:A:401:ILE:HG22	2.01	0.41
1:A:260:PHE:HA	1:A:366:LYS:HE3	2.03	0.41
1:A:307:THR:O	1:A:309:GLU:HG2	2.21	0.40
1:B:549:ILE:HG22	1:B:549:ILE:O	2.21	0.40
1:A:294:LYS:HB3	1:A:439:GLY:C	2.46	0.40
1:A:338:SER:O	1:A:339:ASN:C	2.63	0.40
1:B:346:MET:HE1	1:B:408:PHE:CD1	2.56	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	256/343 (75%)	234 (91%)	20 (8%)	2 (1%)	16	41
1	B	248/343 (72%)	219 (88%)	28 (11%)	1 (0%)	30	58
2	C	8/18 (44%)	6 (75%)	2 (25%)	0	100	100
All	All	512/704 (73%)	459 (90%)	50 (10%)	3 (1%)	21	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLY
1	B	418	ILE
1	A	278	LYS

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	
1	A	234/307 (76%)	227 (97%)	7 (3%)	36	69
1	B	229/307 (75%)	220 (96%)	9 (4%)	28	62
2	C	9/13 (69%)	9 (100%)	0	100	100
All	All	472/627 (75%)	456 (97%)	16 (3%)	32	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	GLU
1	A	317	ASN
1	A	397	LYS
1	A	443	GLN
1	A	447	LYS
1	A	457	LEU

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Mol	Chain	Res	Type
1	A	555	LYS
1	B	237	THR
1	B	247	GLN
1	B	279	GLN
1	B	366	LYS
1	B	397	LYS
1	B	417	ASP
1	B	424	LEU
1	B	443	GLN
1	B	555	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	259	GLN
1	A	308	ASN
1	A	321	HIS
1	A	339	ASN
1	A	352	ASN
1	A	368	ASN
1	A	382	GLN
1	A	443	GLN
1	A	551	ASN
1	B	243	GLN
1	B	254	GLN
1	B	317	ASN
1	B	339	ASN
1	B	352	ASN
1	B	414	GLN
1	B	428	ASN
1	B	443	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](#)

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	SEP	C	2	2	8,9,10	2.24	1 (12%)	7,12,14	5.37	3 (42%)
2	SEP	C	6	2	8,9,10	2.26	1 (12%)	7,12,14	5.34	3 (42%)
2	SEP	C	9	2	8,9,10	2.27	1 (12%)	7,12,14	5.24	3 (42%)
2	SEP	C	13	2	8,9,10	2.22	1 (12%)	7,12,14	5.39	3 (42%)

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	SEP	C	2	2	-	6/6/8/10	-
2	SEP	C	6	2	-	2/6/8/10	-
2	SEP	C	9	2	-	6/6/8/10	-
2	SEP	C	13	2	-	3/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9	SEP	OG-CB	-5.77	1.22	1.44
2	C	6	SEP	OG-CB	-5.77	1.22	1.44
2	C	2	SEP	OG-CB	-5.66	1.23	1.44
2	C	13	SEP	OG-CB	-5.58	1.23	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	SEP	OG-CB-CA	13.70	121.47	108.14
2	C	2	SEP	OG-CB-CA	13.65	121.43	108.14
2	C	6	SEP	OG-CB-CA	13.60	121.38	108.14
2	C	9	SEP	OG-CB-CA	13.31	121.10	108.14
2	C	9	SEP	O3P-P-O1P	2.63	121.07	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	SEP	O3P-P-O1P	2.60	120.97	110.83
2	C	2	SEP	O3P-P-O1P	2.59	120.93	110.83
2	C	13	SEP	O3P-P-O1P	2.59	120.92	110.83
2	C	13	SEP	O2P-P-OG	2.22	112.46	106.67
2	C	2	SEP	O2P-P-OG	2.18	112.36	106.67
2	C	9	SEP	O2P-P-OG	2.08	112.09	106.67
2	C	6	SEP	O2P-P-OG	2.08	112.09	106.67

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	SEP	N-CA-CB-OG
2	C	2	SEP	C-CA-CB-OG
2	C	2	SEP	CB-OG-P-O3P
2	C	9	SEP	N-CA-CB-OG
2	C	9	SEP	C-CA-CB-OG
2	C	9	SEP	CB-OG-P-O2P
2	C	9	SEP	CB-OG-P-O3P
2	C	13	SEP	CB-OG-P-O2P
2	C	13	SEP	CB-OG-P-O3P
2	C	2	SEP	CB-OG-P-O1P
2	C	13	SEP	CB-OG-P-O1P
2	C	6	SEP	CA-CB-OG-P
2	C	9	SEP	CA-CB-OG-P
2	C	6	SEP	N-CA-CB-OG
2	C	2	SEP	CB-OG-P-O2P
2	C	9	SEP	CB-OG-P-O1P
2	C	2	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	GUN	A	1	-	12,12,12	1.41	2 (16%)	15,17,17	2.63	8 (53%)
3	GUN	B	2	-	12,12,12	1.43	3 (25%)	15,17,17	2.58	9 (60%)

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	GUN	A	1	-	-	-	0/2/2/2
3	GUN	B	2	-	-	-	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	GUN	C4-N3	3.09	1.40	1.36
3	B	2	GUN	C4-N3	3.03	1.40	1.36
3	B	2	GUN	C2-N3	2.49	1.39	1.33
3	A	1	GUN	C2-N3	2.45	1.39	1.33
3	B	2	GUN	C5-N7	-2.13	1.34	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	GUN	N9-C4-N3	5.96	133.24	125.99
3	B	2	GUN	N9-C4-N3	5.88	133.15	125.99
3	A	1	GUN	C2-N3-C4	4.33	121.00	113.36
3	B	2	GUN	C2-N3-C4	4.23	120.82	113.36
3	A	1	GUN	N9-C8-N7	-2.85	109.67	112.98
3	A	1	GUN	C5-C6-N1	2.73	120.21	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	GUN	C5-C6-N1	2.73	120.20	113.25
3	B	2	GUN	N9-C8-N7	-2.70	109.84	112.98
3	B	2	GUN	O6-C6-C5	-2.55	119.80	126.53
3	A	1	GUN	O6-C6-C5	-2.50	119.92	126.53
3	A	1	GUN	C8-N7-C5	2.39	107.61	104.38
3	B	2	GUN	C8-N7-C5	2.37	107.58	104.38
3	A	1	GUN	C6-C5-N7	2.29	134.45	130.29
3	B	2	GUN	C6-C5-N7	2.17	134.23	130.29
3	A	1	GUN	N1-C2-N3	-2.06	119.56	123.32
3	B	2	GUN	N1-C2-N3	-2.02	119.62	123.32
3	B	2	GUN	C2-N1-C6	-2.01	121.47	125.11

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 [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	A	262/343 (76%)	0.28	7 (2%) 56 46	27, 52, 106, 122	2 (0%)
1	B	254/343 (74%)	0.31	12 (4%) 36 28	29, 51, 107, 143	0
2	C	9/18 (50%)	1.45	1 (11%) 10 7	64, 89, 107, 111	0
All	All	525/704 (74%)	0.32	20 (3%) 44 35	27, 52, 107, 143	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	5.0
1	B	549	ILE	3.9
1	A	294	LYS	3.9
1	A	541	THR	3.5
1	A	540	ASN	3.5
1	B	567	ALA	3.0
1	B	438	ASP	2.9
2	C	3	PRO	2.8
1	B	546	CYS	2.8
1	B	355	ALA	2.7
1	B	421	SER	2.7
1	A	462	PRO	2.5
1	A	293	TRP	2.4
1	A	403	LYS	2.4
1	A	334	ARG	2.3
1	B	293	TRP	2.3
1	B	294	LYS	2.2
1	B	327	PHE	2.2
1	B	332	ASP	2.1
1	B	425	LEU	2.1

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
2	SEP	C	2	10/11	0.55	0.15	116,122,134,135	0
2	SEP	C	6	10/11	0.60	0.14	85,94,116,117	0
2	SEP	C	13	10/11	0.61	0.13	98,108,120,121	0
2	SEP	C	9	10/11	0.85	0.11	87,89,91,91	0

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
3	GUN	A	1	11/11	0.85	0.19	90,96,98,98	0
3	GUN	B	2	11/11	0.91	0.15	80,89,96,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.