



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 AM UTC

PDB ID : 3H40 / pdb_00003h40
Title : Binary complex of human DNA polymerase iota with template U/T
Authors : Jain, R.; Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on : 2009-04-17
Resolution : 2.30 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

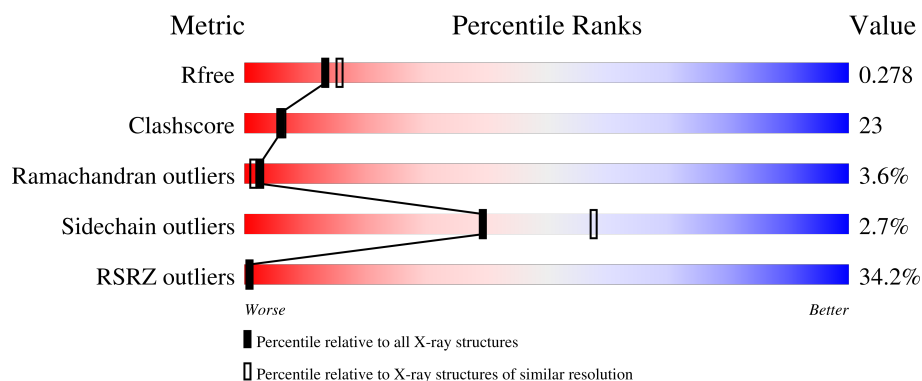
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	389	32% 61% 32% . .
2	P	7	71% 100%
3	T	9	22% 67% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3391 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 DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	3	0
			2808	1765	488	535	20			

- Molecule 2 is a DNA chain called 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total	Br	C	N	O	P	0	1
			201	2	96	31	63	9		0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

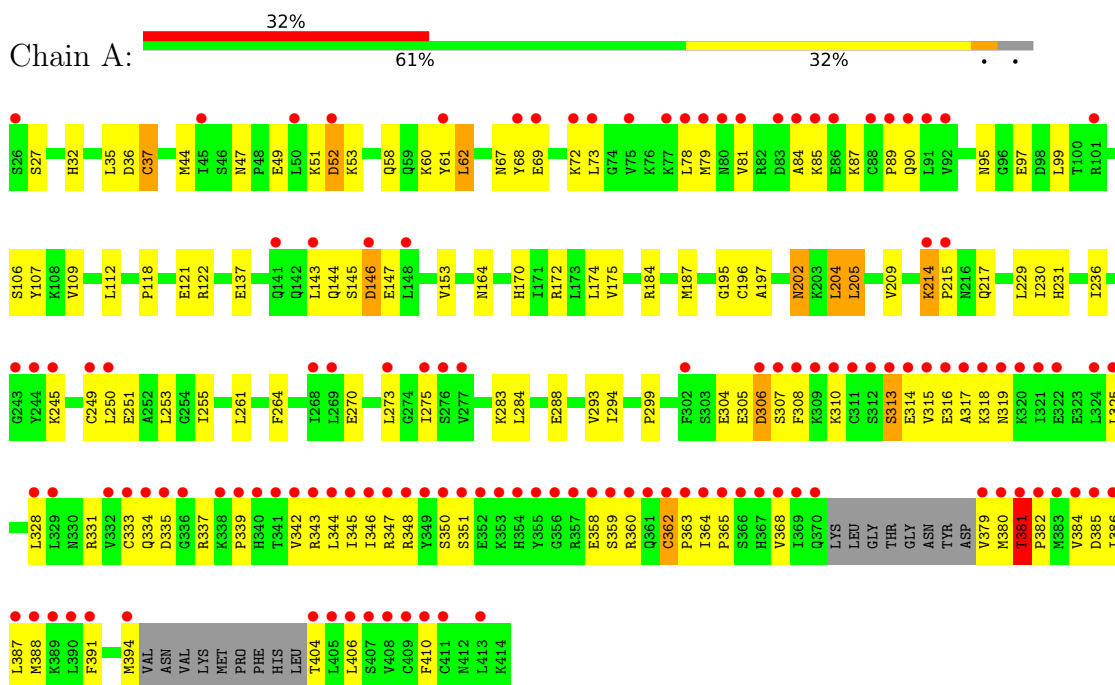
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	P	8	Total	O	0	0
			8	8		
5	T	14	Total	O	0	1
			15	15		

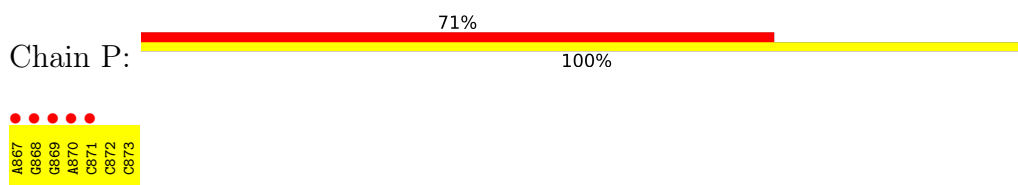
3 Residue-property plots [i](#)

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.

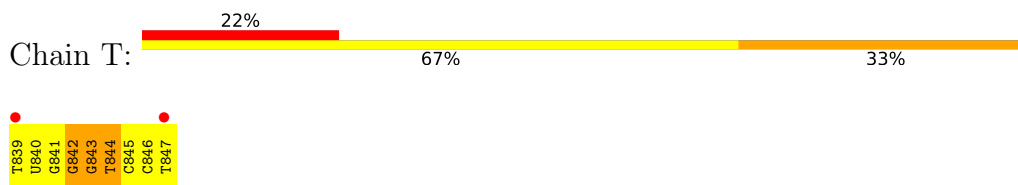
- Molecule 1: DNA polymerase iota



- Molecule 2: 5'-D(*TP*(BRU)P*GP*GP*GP*TP*CP*CP*T)-3'



- Molecule 3: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.24Å 98.24Å 203.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.67 – 2.30 43.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (43.67-2.30) 95.9 (43.67-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.277 0.247 , 0.278	Depositor DCC
R_{free} test set	2013 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3391	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: SO4, BRU, DOC

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	0.40	0/2863	0.92	7/3880 (0.2%)
2	P	0.29	0/136	0.71	0/208
3	T	0.30	0/178	0.94	0/271
All	All	0.39	0/3177	0.91	7/4359 (0.2%)

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
3	T	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LYS	N-CA-C	10.71	127.18	113.25
1	A	293	VAL	N-CA-C	-6.68	100.07	108.89
1	A	87	LYS	N-CA-C	-5.84	106.78	114.31
1	A	175	VAL	N-CA-C	-5.73	104.77	110.62
1	A	319	ASN	N-CA-C	-5.36	106.00	112.54
1	A	118	PRO	N-CA-C	5.34	120.86	113.65
1	A	386	ILE	N-CA-C	-5.00	105.67	110.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	842	DG	Sidechain
3	T	843	DG	Sidechain
3	T	844	DT	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2808	0	2729	112	0
2	P	139	0	79	9	0
3	T	201	0	111	21	0
4	A	5	0	0	0	0
5	A	215	0	0	4	1
5	P	8	0	0	2	0
5	T	15	0	0	0	0
All	All	3391	0	2919	139	1

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 23.

All (139) 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:MET:HE3	1:A:67:ASN:HD22	1.26	0.97
1:A:44:MET:HE2	1:A:51:LYS:HA	1.48	0.94
3:T:841:DG:H2''	3:T:842:DG:H5''	1.49	0.94
3:T:842:DG:H2''	3:T:843:DG:H5''	1.52	0.91
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.53	0.88
1:A:344:LEU:HD21	1:A:387:LEU:HB3	1.55	0.88
3:T:839:DT:H2''	3:T:840[A]:BRU:O5'	1.75	0.85
3:T:842:DG:H2''	3:T:843:DG:C5'	2.05	0.85
1:A:164:ASN:H	1:A:170:HIS:HD2	1.25	0.85
3:T:839:DT:H2''	3:T:840[B]:BRU:O5'	1.76	0.84
1:A:27:SER:HB2	5:A:553:HOH:O	1.81	0.80
1:A:79:MET:HE3	1:A:84:ALA:HA	1.63	0.80
3:T:841:DG:C2'	3:T:842:DG:H5''	2.12	0.80
1:A:347:ARG:HD2	1:A:404:THR:OG1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:867:DA:H1'	2:P:868:DG:H5'	1.66	0.77
1:A:184:ARG:HA	1:A:187:MET:HE3	1.68	0.76
2:P:868:DG:N7	5:P:155:HOH:O	2.18	0.75
1:A:388:MET:O	1:A:391:PHE:HB3	1.88	0.74
1:A:44:MET:CE	1:A:67:ASN:HD22	1.99	0.73
1:A:365:PRO:O	1:A:368:VAL:HG22	1.90	0.72
1:A:331:ARG:HD2	5:A:454:HOH:O	1.90	0.70
1:A:384:VAL:O	1:A:388:MET:HG2	1.94	0.67
1:A:335:ASP:OD2	1:A:337:ARG:HD3	1.95	0.67
1:A:215:PRO:O	1:A:217:GLN:HG3	1.95	0.66
1:A:343:ARG:C	1:A:344:LEU:HD12	2.21	0.66
1:A:385:ASP:HA	1:A:388:MET:HB2	1.79	0.65
1:A:44:MET:HE3	1:A:67:ASN:ND2	2.06	0.64
1:A:342:VAL:HG21	1:A:387:LEU:HD21	1.78	0.64
1:A:51:LYS:O	1:A:53:LYS:N	2.27	0.63
1:A:112:LEU:C	1:A:112:LEU:HD23	2.23	0.63
1:A:214:LYS:HB3	1:A:215:PRO:HD3	1.80	0.63
1:A:381:THR:OG1	1:A:382:PRO:HD3	1.98	0.63
1:A:137:GLU:OE2	1:A:172:ARG:NH2	2.33	0.62
1:A:345:ILE:HG12	1:A:359:SER:HB3	1.82	0.61
1:A:315:VAL:C	1:A:317:ALA:H	2.08	0.61
1:A:379:VAL:O	1:A:382:PRO:HD2	2.00	0.61
1:A:236:ILE:HD12	1:A:250:LEU:CD1	2.30	0.60
3:T:841:DG:H2''	3:T:842:DG:C5'	2.26	0.60
1:A:202:ASN:HD22	1:A:202:ASN:C	2.09	0.60
1:A:164:ASN:H	1:A:170:HIS:CD2	2.15	0.60
1:A:202:ASN:ND2	1:A:205:LEU:H	2.00	0.59
1:A:68:TYR:O	1:A:72:LYS:HG3	2.03	0.59
3:T:847:DT:H6	3:T:847:DT:H5'	1.68	0.59
1:A:325:LEU:HD23	1:A:325:LEU:O	2.01	0.59
1:A:325:LEU:HD22	1:A:380:MET:HG2	1.86	0.58
1:A:51:LYS:C	1:A:53:LYS:H	2.11	0.57
1:A:236:ILE:HD12	1:A:250:LEU:HD12	1.85	0.57
1:A:202:ASN:HD21	1:A:205:LEU:H	1.53	0.57
1:A:106:SER:OG	1:A:122:ARG:NH2	2.39	0.56
1:A:283[A]:LYS:HE3	1:A:288:GLU:HB3	1.87	0.56
1:A:137:GLU:HG3	5:A:549:HOH:O	2.04	0.56
1:A:36:ASP:O	1:A:37:CYS:C	2.47	0.56
1:A:143:LEU:HA	1:A:147:GLU:OE2	2.06	0.55
3:T:841:DG:H1'	3:T:842:DG:H5''	1.88	0.55
2:P:872:DC:H2''	2:P:873:DOC:OP2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:842:DG:H2''	3:T:843:DG:H5'	1.90	0.54
1:A:61:TYR:CE1	1:A:62:LEU:HD12	2.43	0.54
1:A:325:LEU:HD23	1:A:325:LEU:C	2.33	0.54
1:A:107:TYR:OH	1:A:299:PRO:HG3	2.07	0.53
1:A:196:CYS:HA	1:A:217:GLN:O	2.09	0.53
1:A:313:SER:O	1:A:314:GLU:HB2	2.08	0.53
1:A:339:PRO:HG3	1:A:410:PHE:HD2	1.74	0.52
1:A:347:ARG:HG2	1:A:348:ARG:N	2.24	0.52
3:T:839:DT:H2'	3:T:840[A]:BRU:BR	2.65	0.52
1:A:308:PHE:C	1:A:310:LYS:H	2.18	0.51
1:A:344:LEU:HD12	1:A:344:LEU:N	2.25	0.51
1:A:344:LEU:HD11	1:A:387:LEU:CD2	2.34	0.51
1:A:270:GLU:HG3	1:A:275:ILE:HA	1.93	0.51
1:A:62:LEU:HD23	1:A:78:LEU:HA	1.93	0.50
1:A:85:LYS:O	1:A:89:PRO:HG3	2.12	0.50
1:A:385:ASP:HA	1:A:388:MET:CG	2.41	0.50
2:P:871:DC:H2''	2:P:872:DC:OP2	2.11	0.49
1:A:304:GLU:HG3	1:A:328:LEU:HD21	1.94	0.49
1:A:35:LEU:HD11	1:A:109:VAL:HG21	1.94	0.49
1:A:345:ILE:HA	1:A:358:GLU:O	2.13	0.48
1:A:137:GLU:CG	5:A:549:HOH:O	2.60	0.48
1:A:365:PRO:HB2	1:A:368:VAL:HG22	1.94	0.48
1:A:95:ASN:HD21	1:A:97:GLU:CD	2.21	0.48
3:T:841:DG:C1'	3:T:842:DG:H5''	2.43	0.48
3:T:840[B]:BRU:H2'	3:T:840[B]:BRU:O2	2.13	0.48
1:A:99:LEU:HD12	3:T:842:DG:H4'	1.96	0.48
1:A:304:GLU:HG3	1:A:328:LEU:CD2	2.44	0.48
1:A:60:LYS:HE2	1:A:307:SER:O	2.14	0.48
1:A:62:LEU:HD11	3:T:839:DT:O2	2.14	0.47
1:A:358:GLU:C	1:A:394:MET:HE1	2.38	0.47
1:A:344:LEU:O	1:A:359:SER:HA	2.14	0.47
3:T:847:DT:H5'	3:T:847:DT:C6	2.49	0.47
1:A:121:GLU:HB2	1:A:294:ILE:O	2.15	0.47
3:T:843:DG:C8	3:T:844:DT:H72	2.50	0.47
1:A:380:MET:O	1:A:381:THR:C	2.58	0.47
1:A:261:LEU:HD12	1:A:261:LEU:O	2.16	0.46
1:A:385:ASP:HA	1:A:388:MET:CB	2.44	0.46
1:A:365:PRO:HB2	1:A:368:VAL:HG13	1.96	0.46
1:A:196:CYS:SG	1:A:214:LYS:O	2.74	0.46
1:A:251:GLU:C	1:A:253:LEU:N	2.74	0.46
1:A:313:SER:C	1:A:315:VAL:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:842:DG:C2'	3:T:843:DG:H5''	2.36	0.46
2:P:869:DG:H2''	2:P:870:DA:OP2	2.16	0.46
1:A:343:ARG:HG2	1:A:344:LEU:N	2.31	0.46
2:P:868:DG:H2''	2:P:869:DG:OP2	2.15	0.46
1:A:342:VAL:HG22	1:A:343:ARG:N	2.31	0.46
1:A:325:LEU:HD22	1:A:380:MET:HE3	1.97	0.46
1:A:325:LEU:CD2	1:A:380:MET:HG2	2.46	0.46
1:A:381:THR:CB	1:A:382:PRO:HD3	2.46	0.46
1:A:230:ILE:CG2	1:A:231:HIS:N	2.80	0.45
1:A:249:CYS:SG	1:A:273:LEU:HD21	2.57	0.45
1:A:316:GLU:C	1:A:318:LYS:H	2.23	0.45
1:A:112:LEU:HD23	1:A:112:LEU:O	2.17	0.45
1:A:144:GLN:H	1:A:147:GLU:CG	2.29	0.45
1:A:153:VAL:HB	1:A:174:LEU:HD22	1.98	0.45
1:A:347:ARG:HG2	1:A:348:ARG:H	1.82	0.45
1:A:62:LEU:HD11	3:T:839:DT:C2	2.53	0.44
1:A:144:GLN:O	1:A:146:ASP:N	2.49	0.44
1:A:47:ASN:OD1	1:A:49:GLU:HB2	2.18	0.44
1:A:51:LYS:C	1:A:53:LYS:N	2.75	0.44
1:A:79:MET:HE3	1:A:84:ALA:CA	2.43	0.44
1:A:202:ASN:C	1:A:202:ASN:ND2	2.76	0.44
2:P:871:DC:H2''	5:P:129:HOH:O	2.17	0.43
1:A:69:GLU:O	1:A:73:LEU:HD13	2.18	0.43
1:A:51:LYS:O	1:A:52:ASP:CG	2.62	0.43
3:T:845:DC:H2''	3:T:846:DC:OP2	2.18	0.42
1:A:58:GLN:NE2	1:A:81:VAL:HG21	2.35	0.42
1:A:305:GLU:O	1:A:306:ASP:HB2	2.20	0.42
1:A:346:ILE:HG22	1:A:406:LEU:CD2	2.50	0.42
2:P:870:DA:H1'	2:P:871:DC:H5'	2.01	0.42
3:T:846:DC:H2''	3:T:847:DT:H5'	2.02	0.41
1:A:308:PHE:C	1:A:310:LYS:N	2.78	0.41
1:A:184:ARG:HD2	1:A:195:GLY:O	2.21	0.41
1:A:283[A]:LYS:NZ	1:A:288:GLU:OE1	2.46	0.41
1:A:32:HIS:O	1:A:197:ALA:HA	2.20	0.41
1:A:315:VAL:C	1:A:317:ALA:N	2.75	0.41
1:A:360:ARG:HG2	1:A:394:MET:CG	2.51	0.41
1:A:81:VAL:O	1:A:84:ALA:HB3	2.20	0.41
1:A:342:VAL:HG22	1:A:343:ARG:H	1.86	0.41
1:A:255:ILE:HD11	1:A:264:PHE:CG	2.56	0.40
1:A:342:VAL:HB	1:A:364:ILE:HD11	2.02	0.40
1:A:204:LEU:HG	1:A:284:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:CYS:HA	1:A:363:PRO:HD3	1.94	0.40
2:P:872:DC:C2'	2:P:873:DOC:OP2	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:464:HOH:O	5:A:500:HOH:O[5_555]	2.18	0.02

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	369/389 (95%)	321 (87%)	35 (10%)	13 (4%)	3 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	SER
1	A	52	ASP
1	A	146	ASP
1	A	37	CYS
1	A	306	ASP
1	A	313	SER
1	A	381	THR
1	A	90	GLN
1	A	145	SER
1	A	245	LYS
1	A	334	GLN
1	A	333	CYS
1	A	351	SER

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	302/354 (85%)	294 (97%)	8 (3%)	40 59

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	209	VAL
1	A	229	LEU
1	A	362	CYS
1	A	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	95	ASN
1	A	170	HIS
1	A	202	ASN
1	A	235	HIS
1	A	262	GLN
1	A	334	GLN
1	A	361	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](#)

3 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	DOC	P	873	2,3	16,19,20	0.34	0	20,26,29	0.61	0
3	BRU	T	840[A]	3	18,21,22	0.28	0	25,30,33	0.52	0
3	BRU	T	840[B]	3	18,21,22	0.46	0	25,30,33	0.57	0

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	DOC	P	873	2,3	-	0/7/18/19	0/2/2/2
3	BRU	T	840[A]	3	-	4/7/21/22	0/2/2/2
3	BRU	T	840[B]	3	-	5/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840[B]	BRU	C2'-C1'-N1-C2
3	T	840[B]	BRU	O4'-C1'-N1-C6
3	T	840[B]	BRU	C2'-C1'-N1-C6
3	T	840[B]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C6
3	T	840[A]	BRU	O4'-C1'-N1-C6
3	T	840[B]	BRU	O4'-C4'-C5'-O5'
3	T	840[A]	BRU	O4'-C1'-N1-C2
3	T	840[A]	BRU	C2'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	873	DOC	2	0
3	T	840[A]	BRU	2	0
3	T	840[B]	BRU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	SO4	A	1	-	4,4,4	1.06	0	6,6,6	1.39	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	SO4	O4-S-O3	3.07	125.47	108.54

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 ⓘ

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	372/389 (95%)	1.39	125 (33%)  	18, 46, 101, 117	3 (0%)
2	P	6/7 (85%)	2.62	5 (83%)  	49, 60, 64, 66	0
3	T	8/9 (88%)	0.98	2 (25%)  	37, 40, 57, 88	0
All	All	386/405 (95%)	1.40	132 (34%)  	18, 46, 100, 117	3 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	TYR	7.5
1	A	346	ILE	6.9
1	A	308	PHE	6.2
1	A	406	LEU	5.9
1	A	348	ARG	5.8
1	A	345	ILE	5.8
1	A	354	HIS	5.7
1	A	347	ARG	5.6
1	A	321	ILE	5.6
1	A	364	ILE	5.6
1	A	312	SER	5.5
1	A	361	GLN	5.5
1	A	360	ARG	5.3
1	A	390	LEU	5.1
1	A	379	VAL	5.1
1	A	368	VAL	5.0
1	A	317	ALA	5.0
1	A	363	PRO	4.9
1	A	356	GLY	4.9
1	A	359	SER	4.8
1	A	387	LEU	4.7
1	A	342	VAL	4.7
1	A	310	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	4.6
1	A	325	LEU	4.6
1	A	362	CYS	4.6
1	A	311	CYS	4.5
1	A	26	SER	4.5
1	A	357	ARG	4.5
1	A	315	VAL	4.4
1	A	332	VAL	4.4
1	A	351	SER	4.4
1	A	344	LEU	4.4
1	A	80	ASN	4.4
1	A	394	MET	4.4
1	A	355	TYR	4.3
1	A	350	SER	4.3
1	A	391	PHE	4.3
1	A	314	GLU	4.2
1	A	383	MET	4.2
1	A	369	ILE	4.2
1	A	386	ILE	4.1
1	A	408	VAL	4.1
1	A	367	HIS	4.1
1	A	381	THR	4.0
1	A	384	VAL	4.0
1	A	318	LYS	3.9
1	A	343	ARG	3.9
1	A	78	LEU	3.9
1	A	366	SER	3.8
1	A	382	PRO	3.8
1	A	341	THR	3.8
2	P	867	DA	3.8
1	A	404	THR	3.8
1	A	358	GLU	3.7
1	A	389	LYS	3.7
1	A	73	LEU	3.6
1	A	268	ILE	3.6
1	A	380	MET	3.6
1	A	309	LYS	3.6
1	A	75	VAL	3.6
1	A	328	LEU	3.5
1	A	407	SER	3.5
1	A	353	LYS	3.4
1	A	146	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	3.3
1	A	316	GLU	3.3
1	A	269	LEU	3.3
1	A	324	LEU	3.3
1	A	68	TYR	3.2
1	A	277	VAL	3.2
1	A	214	LYS	3.1
1	A	313	SER	3.1
2	P	868	DG	3.1
3	T	839	DT	3.1
1	A	370	GLN	3.1
1	A	320	LYS	3.1
1	A	273	LEU	3.1
1	A	405	LEU	3.1
1	A	352	GLU	3.0
1	A	385	ASP	3.0
1	A	388	MET	2.9
1	A	411	CYS	2.9
1	A	69	GLU	2.8
1	A	413	LEU	2.8
1	A	84	ALA	2.8
1	A	275	ILE	2.8
1	A	334	GLN	2.8
1	A	336	GLY	2.8
1	A	410	PHE	2.8
2	P	869	DG	2.7
1	A	339	PRO	2.7
1	A	365	PRO	2.7
1	A	409	CYS	2.7
1	A	307	SER	2.7
1	A	79	MET	2.7
1	A	52	ASP	2.6
1	A	61	TYR	2.6
1	A	243	GLY	2.6
2	P	870	DA	2.6
1	A	81	VAL	2.6
1	A	89	PRO	2.6
1	A	148	LEU	2.5
1	A	245	LYS	2.5
1	A	340	HIS	2.5
1	A	90	GLN	2.5
1	A	329	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	871	DC	2.4
1	A	333	CYS	2.4
1	A	86	GLU	2.4
1	A	88	CYS	2.4
1	A	249	CYS	2.4
1	A	302	PHE	2.4
1	A	306	ASP	2.4
3	T	847	DT	2.3
1	A	91	LEU	2.3
1	A	322	GLU	2.3
1	A	45	ILE	2.3
1	A	335	ASP	2.2
1	A	85	LYS	2.2
1	A	141	GLN	2.2
1	A	92	VAL	2.2
1	A	50	LEU	2.1
1	A	72	LYS	2.1
1	A	276	SER	2.1
1	A	77	LYS	2.1
1	A	143	LEU	2.1
1	A	338	LYS	2.0
1	A	83	ASP	2.0
1	A	250	LEU	2.0
1	A	101	ARG	2.0
1	A	215	PRO	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	BRU	T	840[A]	20/21	0.82	0.20	62,75,80,80	20
3	BRU	T	840[B]	20/21	0.82	0.20	60,64,78,78	20
2	DOC	P	873	18/19	0.95	0.09	34,38,44,45	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($\text{\AA}^2$)	Q<0.9
4	SO4	A	1	5/5	0.87	0.16	86,87,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.