



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:06 PM UTC

PDB ID : 2FLN / pdb_00002fln
Title : binary complex of catalytic core of human DNA polymerase iota with DNA (template A)
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Deposited on : 2006-01-06
Resolution : 2.50 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

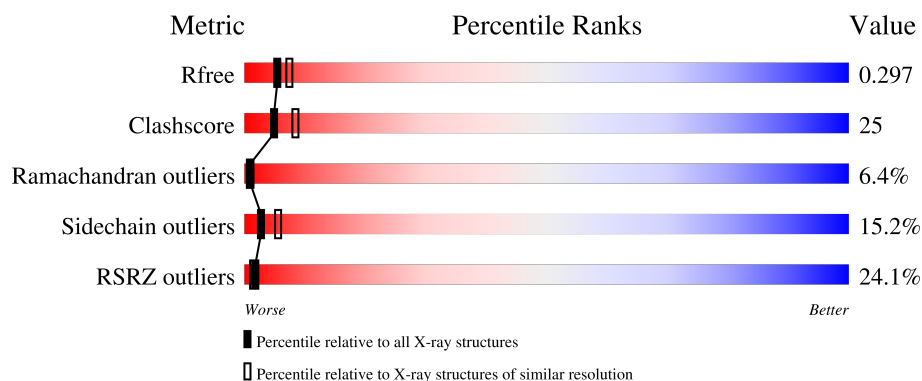
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	T	11	9% 9% 36% 36% 18%
2	P	7	14% 14% 86%
3	A	420	21% 41% 29% 14% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3219 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 DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	9	Total	C	N	O	P	0	0	0
			182	88	32	54	8			

- Molecule 2 is a DNA chain called DNA primer strand.

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 protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	366	Total	C	N	O	S	0	0	0
			2797	1760	489	527	21			

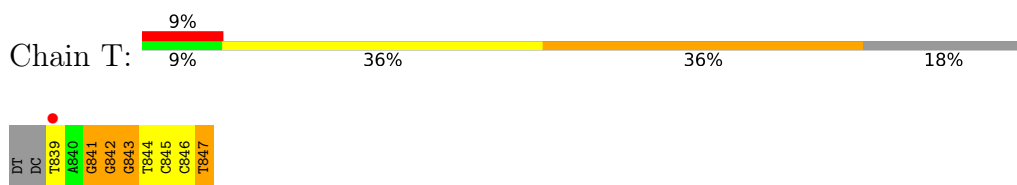
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	T	3	Total	O	0	0
			3	3		
4	P	3	Total	O	0	0
			3	3		
4	A	95	Total	O	0	0
			95	95		

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.

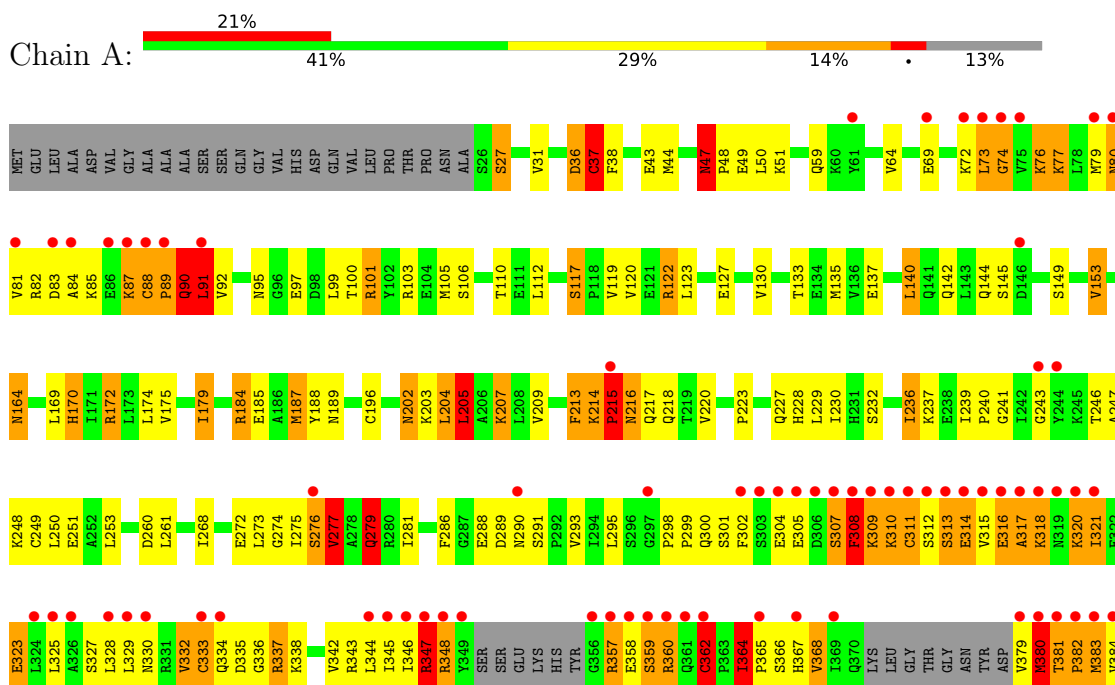
- Molecule 1: DNA template strand

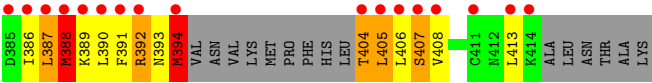


- Molecule 2: DNA primer strand



- Molecule 3: DNA polymerase iota





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.11Å 98.11Å 202.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.22 – 2.50 39.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.22-2.50) 95.6 (39.22-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.78 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.279 (Not available) , 0.297	Depositor DCC
R_{free} test set	2065 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3219	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: 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	T	1.55	1/203 (0.5%)	2.73	22/312 (7.1%)
2	P	1.32	0/136	2.79	15/208 (7.2%)
3	A	1.98	57/2835 (2.0%)	1.70	58/3835 (1.5%)
All	All	1.93	58/3174 (1.8%)	1.86	95/4355 (2.2%)

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	A	0	2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	382	PRO	N-CD	16.32	1.70	1.47
3	A	214	LYS	CA-C	-11.61	1.39	1.52
3	A	47	ASN	CA-C	9.65	1.65	1.52
3	A	187	MET	SD-CE	-9.48	1.55	1.79
3	A	179	ILE	CG1-CD1	-8.57	1.18	1.51
3	A	348	ARG	CA-C	7.83	1.61	1.52
3	A	103	ARG	CZ-NH2	7.74	1.43	1.33
3	A	299	PRO	CA-CB	7.73	1.64	1.53
3	A	213	PHE	C-O	-7.35	1.15	1.24
3	A	317	ALA	C-O	7.22	1.33	1.24
3	A	122	ARG	CD-NE	-6.99	1.36	1.46
3	A	338	LYS	CA-CB	6.83	1.63	1.53
3	A	381	THR	C-N	6.82	1.42	1.34
3	A	277	VAL	CA-CB	6.79	1.63	1.54
3	A	105	MET	CG-SD	6.74	1.97	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	291	SER	CA-C	6.71	1.60	1.53
3	A	300	GLN	CA-C	-6.66	1.43	1.52
3	A	37	CYS	N-CA	-6.65	1.37	1.46
3	A	103	ARG	CZ-NH1	6.57	1.42	1.32
3	A	119	VAL	CA-CB	6.45	1.61	1.53
3	A	140	LEU	C-O	-6.37	1.16	1.24
3	A	105	MET	SD-CE	6.34	1.95	1.79
3	A	36	ASP	CA-C	6.14	1.60	1.52
3	A	293	VAL	N-CA	-6.10	1.39	1.46
3	A	207	LYS	CE-NZ	-6.06	1.31	1.49
3	A	153	VAL	N-CA	-5.97	1.39	1.46
3	A	321	ILE	CB-CG1	5.97	1.65	1.53
3	A	301	SER	CA-C	5.86	1.59	1.52
3	A	276	SER	C-O	-5.84	1.16	1.24
3	A	188	TYR	C-O	-5.78	1.17	1.24
3	A	169	LEU	N-CA	-5.78	1.39	1.46
3	A	288	GLU	CD-OE2	5.78	1.36	1.25
3	A	321	ILE	CA-CB	5.75	1.61	1.54
3	A	295	LEU	C-O	-5.72	1.16	1.24
3	A	220	VAL	C-O	5.72	1.29	1.24
1	T	843	DG	O4'-C1'	-5.64	1.30	1.41
3	A	205	LEU	CA-C	5.62	1.60	1.52
3	A	164	ASN	CA-C	-5.60	1.46	1.52
3	A	110	THR	C-O	-5.58	1.17	1.24
3	A	117	SER	C-O	-5.55	1.16	1.24
3	A	347	ARG	CA-C	5.55	1.59	1.52
3	A	362	CYS	CA-C	5.51	1.59	1.52
3	A	133	THR	C-O	5.49	1.30	1.24
3	A	103	ARG	NE-CZ	5.48	1.39	1.33
3	A	310	LYS	CA-CB	5.47	1.62	1.53
3	A	184	ARG	CD-NE	-5.46	1.38	1.46
3	A	230	ILE	CA-CB	5.42	1.61	1.54
3	A	31	VAL	CA-CB	5.39	1.62	1.54
3	A	170	HIS	C-O	5.37	1.30	1.24
3	A	381	THR	C-O	5.36	1.29	1.24
3	A	239	ILE	C-O	-5.33	1.17	1.24
3	A	286	PHE	C-O	5.27	1.31	1.23
3	A	260	ASP	C-O	-5.24	1.17	1.24
3	A	207	LYS	CA-CB	5.17	1.61	1.53
3	A	279	GLN	CA-C	5.14	1.59	1.52
3	A	394	MET	CG-SD	5.07	1.93	1.80
3	A	289	ASP	CG-OD1	5.04	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	209	VAL	C-O	-5.04	1.18	1.24

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	839	DT	O5'-C5'-C4'	13.61	131.22	110.80
1	T	847	DT	C4'-C3'-O3'	12.04	128.05	110.00
1	T	842	DG	C4'-C3'-O3'	10.23	125.34	110.00
2	P	872	DC	C4'-C3'-O3'	9.49	124.23	110.00
3	A	215	PRO	N-CD-CG	-9.14	89.48	103.20
2	P	871	DC	C4'-C3'-O3'	9.03	123.54	110.00
3	A	215	PRO	CA-C-N	-8.71	109.19	123.04
3	A	215	PRO	C-N-CA	-8.71	109.19	123.04
2	P	869	DG	P-O3'-C3'	-8.61	107.28	120.20
2	P	867	DA	O5'-C5'-C4'	8.60	123.70	110.80
3	A	388	MET	N-CA-C	8.45	121.25	111.11
3	A	299	PRO	CB-CA-C	-8.35	100.02	110.95
2	P	870	DA	C5'-C4'-O4'	-8.32	96.92	109.40
1	T	847	DT	C4-C5-C6	-8.25	106.82	119.20
3	A	407	SER	N-CA-C	7.87	121.19	108.76
3	A	364	ILE	N-CA-C	7.84	114.69	107.56
1	T	839	DT	C5'-C4'-C3'	7.79	126.59	114.90
1	T	844	DT	C4-C5-C6	-7.70	107.66	119.20
3	A	298	PRO	CA-C-N	7.65	127.61	120.03
3	A	298	PRO	C-N-CA	7.65	127.61	120.03
2	P	867	DA	P-O3'-C3'	7.34	131.22	120.20
3	A	27	SER	N-CA-C	7.34	121.15	110.28
2	P	872	DC	C5'-C4'-O4'	-7.20	98.60	109.40
3	A	88	CYS	N-CA-C	7.13	125.56	109.81
3	A	77	LYS	N-CA-C	-7.11	99.64	110.30
3	A	214	LYS	O-C-N	7.09	125.98	120.38
1	T	844	DT	N3-C4-C5	7.09	125.44	114.80
3	A	293	VAL	N-CA-C	-6.98	98.22	108.54
3	A	274	GLY	N-CA-C	-6.89	104.00	112.68
3	A	74	GLY	N-CA-C	6.70	129.05	113.18
2	P	868	DG	O3'-P-O5'	-6.69	93.96	104.00
1	T	842	DG	C5'-C4'-O4'	-6.69	99.37	109.40
3	A	279	GLN	CB-CA-C	6.60	122.39	109.72
3	A	348	ARG	N-CA-C	6.59	120.35	108.69
1	T	843	DG	C3'-C2'-C1'	6.54	111.41	101.60
1	T	844	DT	C5'-C4'-C3'	-6.53	105.11	114.90
1	T	839	DT	C5'-C4'-O4'	6.51	119.17	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	175	VAL	N-CA-C	-6.50	103.99	110.62
3	A	241	GLY	N-CA-C	-6.50	106.63	113.58
3	A	172	ARG	CG-CD-NE	-6.49	97.72	112.00
2	P	868	DG	P-O5'-C5'	6.33	129.50	120.00
2	P	871	DC	O5'-C5'-C4'	-6.26	101.41	110.80
3	A	179	ILE	N-CA-C	-6.22	104.45	110.42
3	A	179	ILE	N-CA-CB	6.22	117.83	110.55
3	A	122	ARG	CG-CD-NE	-6.22	98.32	112.00
1	T	845	DC	OP1-P-O3'	-6.17	89.48	108.00
3	A	85	LYS	N-CA-C	-6.16	104.48	111.07
3	A	214	LYS	N-CA-CB	6.15	117.68	110.42
3	A	204	LEU	CB-CA-C	-6.14	100.99	110.81
3	A	179	ILE	CA-CB-CG1	6.12	120.81	110.40
3	A	279	GLN	N-CA-C	-5.93	106.04	113.28
2	P	867	DA	C5'-C4'-C3'	5.86	123.69	114.90
3	A	386	ILE	N-CA-C	-5.85	104.80	110.42
3	A	260	ASP	N-CA-C	-5.84	104.99	111.36
2	P	870	DA	C4'-C3'-O3'	5.83	118.74	110.00
1	T	846	DC	O3'-P-O5'	-5.82	95.27	104.00
3	A	243	GLY	N-CA-C	5.81	120.91	112.60
1	T	843	DG	O5'-C5'-C4'	5.76	119.44	110.80
1	T	844	DT	N3-C4-O4	-5.75	113.98	122.60
3	A	246	THR	OG1-CB-CG2	-5.74	97.83	109.30
3	A	100	THR	N-CA-C	5.72	117.98	111.11
3	A	38	PHE	N-CA-C	5.72	118.00	111.02
3	A	69	GLU	N-CA-C	-5.70	104.06	111.02
1	T	839	DT	C2-N1-C1'	5.69	127.89	119.35
3	A	268	ILE	N-CA-C	-5.68	103.99	111.09
3	A	218	GLN	N-CA-C	5.64	117.75	109.24
3	A	236	ILE	CB-CG1-CD1	-5.64	101.96	113.80
3	A	302	PHE	N-CA-C	-5.64	98.71	108.69
3	A	232	SER	N-CA-C	-5.61	105.69	112.54
2	P	870	DA	O4'-C1'-N9	5.58	116.77	108.40
1	T	843	DG	C4'-C3'-O3'	5.55	118.33	110.00
3	A	103	ARG	NE-CZ-NH1	-5.52	115.98	121.50
3	A	347	ARG	N-CA-C	5.52	117.36	109.14
2	P	870	DA	O4'-C4'-C3'	5.51	113.66	105.40
3	A	336	GLY	N-CA-C	-5.49	100.16	113.18
1	T	841	DG	O3'-P-O5'	5.49	112.23	104.00
3	A	203	LYS	N-CA-C	5.44	117.29	111.36
3	A	172	ARG	NE-CZ-NH1	-5.43	116.07	121.50
3	A	240	PRO	CA-C-N	-5.37	117.61	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	240	PRO	C-N-CA	-5.37	117.61	123.30
3	A	87	LYS	N-CA-C	-5.30	106.77	113.18
1	T	842	DG	P-O5'-C5'	5.29	127.94	120.00
3	A	223	PRO	N-CD-CG	5.29	111.13	103.20
1	T	847	DT	C6-N1-C1'	5.22	127.18	119.35
3	A	380	MET	CA-C-N	5.21	128.68	120.97
3	A	380	MET	C-N-CA	5.21	128.68	120.97
3	A	382	PRO	CA-C-N	5.19	129.44	121.19
3	A	382	PRO	C-N-CA	5.19	129.44	121.19
3	A	216	ASN	N-CA-C	-5.17	97.83	108.53
1	T	847	DT	N3-C4-C5	5.13	122.49	114.80
2	P	869	DG	O3'-P-O5'	5.08	111.63	104.00
3	A	300	GLN	N-CA-C	-5.03	107.20	113.38
1	T	843	DG	C2'-C3'-O3'	-5.02	103.97	111.50
3	A	320	LYS	N-CA-C	-5.01	105.95	111.71
3	A	321	ILE	CB-CA-C	5.01	118.58	112.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	309	LYS	Peptide

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	T	182	0	104	10	1
2	P	139	0	79	4	1
3	A	2797	0	2781	142	0
4	A	95	0	0	4	0
4	P	3	0	0	0	0
4	T	3	0	0	0	0
All	All	3219	0	2964	154	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 25.

All (154) 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:A:382:PRO:CD	3:A:382:PRO:N	1.70	1.45
3:A:87:LYS:O	3:A:88:CYS:SG	1.98	1.21
3:A:392:ARG:O	3:A:394:MET:N	1.83	1.10
3:A:347:ARG:HD3	3:A:405:LEU:CB	1.80	1.10
3:A:320:LYS:O	3:A:323:GLU:HB2	1.51	1.08
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.31	1.06
3:A:347:ARG:HG2	3:A:404:THR:HG23	1.35	1.03
3:A:79:MET:HE3	3:A:84:ALA:HB2	1.43	1.00
3:A:347:ARG:CG	3:A:404:THR:HG23	1.93	0.97
3:A:89:PRO:O	3:A:91:LEU:N	1.98	0.97
3:A:47:ASN:C	3:A:47:ASN:HD22	1.76	0.92
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.52	0.92
3:A:347:ARG:CD	3:A:405:LEU:CB	2.50	0.89
3:A:379:VAL:O	3:A:382:PRO:HD2	1.72	0.89
3:A:247:ALA:O	3:A:251:GLU:HG3	1.74	0.88
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.56	0.86
3:A:44:MET:HE3	3:A:51:LYS:HA	1.59	0.85
3:A:135:MET:HE2	3:A:179:ILE:HD12	1.58	0.84
3:A:82:ARG:C	3:A:84:ALA:H	1.82	0.82
3:A:79:MET:HE3	3:A:84:ALA:CB	2.09	0.82
1:T:841:DG:H2''	1:T:842:DG:H5''	1.61	0.81
3:A:82:ARG:O	3:A:84:ALA:N	2.14	0.79
3:A:392:ARG:C	3:A:394:MET:H	1.89	0.77
3:A:364:ILE:HG12	3:A:383:MET:HE1	1.66	0.76
3:A:120:VAL:HG22	3:A:130:VAL:HG22	1.68	0.75
1:T:842:DG:C2'	1:T:843:DG:H5'	2.16	0.75
3:A:249:CYS:SG	3:A:273:LEU:HD21	2.27	0.75
3:A:308:PHE:HB2	3:A:311:CYS:HB2	1.68	0.74
2:P:872:DC:H2''	2:P:873:DOC:H5''	1.70	0.74
3:A:47:ASN:C	3:A:47:ASN:ND2	2.46	0.72
1:T:842:DG:H2'	1:T:843:DG:H5'	1.70	0.71
3:A:47:ASN:HD21	3:A:49:GLU:HB2	1.53	0.71
3:A:388:MET:O	3:A:391:PHE:HB3	1.93	0.69
3:A:202:ASN:HD22	3:A:202:ASN:C	1.99	0.69
3:A:47:ASN:ND2	3:A:47:ASN:O	2.16	0.69
3:A:82:ARG:C	3:A:84:ALA:N	2.46	0.69
3:A:164:ASN:H	3:A:170:HIS:HD2	1.42	0.68
3:A:308:PHE:O	3:A:308:PHE:HD1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:CYS:SG	3:A:214:LYS:O	2.53	0.65
3:A:344:LEU:O	3:A:359:SER:HA	1.96	0.65
3:A:137:GLU:HG2	3:A:172:ARG:NH1	2.12	0.65
3:A:335:ASP:OD2	3:A:337:ARG:HB2	1.98	0.64
3:A:236:ILE:CD1	3:A:250:LEU:HD13	2.25	0.64
3:A:172:ARG:HD3	4:A:981:HOH:O	1.97	0.63
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.99	0.63
3:A:36:ASP:OD1	3:A:215:PRO:O	2.17	0.62
3:A:389:LYS:HA	3:A:392:ARG:HD2	1.81	0.62
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.65	0.62
3:A:236:ILE:HD12	3:A:250:LEU:CD1	2.27	0.62
3:A:347:ARG:HG3	3:A:404:THR:HG23	1.79	0.62
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.30	0.61
3:A:253:LEU:HD12	3:A:253:LEU:N	2.15	0.61
3:A:36:ASP:O	3:A:37:CYS:C	2.43	0.60
3:A:380:MET:HE2	3:A:384:VAL:HG23	1.83	0.60
3:A:325:LEU:HD11	3:A:387:LEU:HD12	1.84	0.60
3:A:112:LEU:C	3:A:112:LEU:HD23	2.26	0.60
3:A:333:CYS:O	3:A:335:ASP:N	2.35	0.60
3:A:325:LEU:HB3	3:A:380:MET:HE3	1.84	0.59
3:A:327:SER:O	3:A:328:LEU:C	2.45	0.59
3:A:318:LYS:O	3:A:321:ILE:HB	2.03	0.59
3:A:405:LEU:O	3:A:406:LEU:HD23	2.04	0.58
3:A:318:LYS:O	3:A:318:LYS:HG2	2.00	0.57
3:A:117:SER:OG	4:A:907:HOH:O	2.17	0.57
1:T:842:DG:H2''	1:T:843:DG:C5'	2.34	0.57
3:A:202:ASN:ND2	3:A:205:LEU:H	2.02	0.57
1:T:842:DG:C2'	1:T:843:DG:C5'	2.82	0.56
3:A:379:VAL:C	3:A:382:PRO:HD2	2.30	0.56
1:T:841:DG:OP2	3:A:307:SER:HB2	2.06	0.55
3:A:275:ILE:HG13	3:A:279:GLN:NE2	2.22	0.55
3:A:345:ILE:HA	3:A:358:GLU:O	2.06	0.55
3:A:87:LYS:C	3:A:88:CYS:SG	2.85	0.54
3:A:308:PHE:O	3:A:308:PHE:CD1	2.60	0.54
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.40	0.54
3:A:275:ILE:HG23	3:A:276:SER:N	2.23	0.54
2:P:872:DC:H2''	2:P:873:DOC:C5'	2.36	0.53
3:A:308:PHE:HB2	3:A:311:CYS:CB	2.39	0.53
1:T:842:DG:H2''	1:T:843:DG:H5''	1.91	0.52
3:A:348:ARG:NH1	3:A:358:GLU:OE1	2.42	0.52
3:A:89:PRO:O	3:A:90:GLN:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:320:LYS:HA	3:A:323:GLU:HG3	1.92	0.52
3:A:343:ARG:HG2	3:A:344:LEU:N	2.24	0.52
3:A:89:PRO:C	3:A:91:LEU:N	2.66	0.52
3:A:304:GLU:HG3	3:A:328:LEU:CG	2.35	0.52
3:A:392:ARG:C	3:A:394:MET:N	2.56	0.51
3:A:184:ARG:HA	3:A:187:MET:HE3	1.92	0.51
3:A:90:GLN:O	3:A:91:LEU:C	2.54	0.50
3:A:342:VAL:HG21	3:A:387:LEU:HD21	1.94	0.50
3:A:80:ASN:C	3:A:82:ARG:H	2.19	0.50
3:A:275:ILE:CG1	3:A:279:GLN:NE2	2.75	0.49
3:A:80:ASN:O	3:A:84:ALA:HB3	2.12	0.49
3:A:202:ASN:HD21	3:A:205:LEU:H	1.59	0.49
3:A:76:LYS:HG2	3:A:77:LYS:N	2.27	0.49
3:A:76:LYS:HG2	3:A:77:LYS:H	1.76	0.49
3:A:325:LEU:HB3	3:A:380:MET:CE	2.42	0.49
3:A:261:LEU:HD12	3:A:261:LEU:O	2.12	0.48
3:A:290:ASN:ND2	4:A:900:HOH:O	2.33	0.48
3:A:388:MET:HE3	3:A:388:MET:HA	1.95	0.48
3:A:321:ILE:HD12	3:A:391:PHE:CD1	2.48	0.48
3:A:202:ASN:C	3:A:202:ASN:ND2	2.66	0.48
3:A:72:LYS:C	3:A:74:GLY:H	2.22	0.48
3:A:321:ILE:O	3:A:325:LEU:HD13	2.14	0.47
3:A:316:GLU:O	3:A:318:LYS:N	2.48	0.47
3:A:312:SER:C	3:A:314:GLU:H	2.23	0.47
3:A:365:PRO:O	3:A:368:VAL:HG13	2.15	0.46
2:P:869:DG:H2''	2:P:870:DA:OP2	2.14	0.46
3:A:185:GLU:OE1	3:A:189:ASN:ND2	2.48	0.46
3:A:112:LEU:HD23	3:A:112:LEU:O	2.15	0.46
3:A:214:LYS:N	3:A:215:PRO:CD	2.78	0.46
3:A:80:ASN:C	3:A:82:ARG:N	2.74	0.46
3:A:346:ILE:O	3:A:357:ARG:HA	2.14	0.46
3:A:360:ARG:HG2	3:A:394:MET:CG	2.45	0.46
3:A:320:LYS:C	3:A:323:GLU:HB2	2.35	0.45
1:T:841:DG:H2''	1:T:842:DG:C5'	2.41	0.45
3:A:127:GLU:OE1	3:A:207:LYS:HE3	2.16	0.45
1:T:842:DG:H2''	1:T:843:DG:H5'	1.95	0.45
3:A:275:ILE:HG13	3:A:279:GLN:HE21	1.81	0.44
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.99	0.44
3:A:275:ILE:CG2	3:A:276:SER:N	2.81	0.44
1:T:842:DG:H4'	3:A:99:LEU:HD12	2.00	0.44
3:A:196:CYS:HA	3:A:217:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:248:LYS:HD3	3:A:248:LYS:HA	1.72	0.44
3:A:227:GLN:O	3:A:228:HIS:C	2.59	0.43
3:A:153:VAL:HG23	3:A:174:LEU:HD22	2.00	0.43
3:A:347:ARG:HD2	3:A:405:LEU:CB	2.43	0.43
3:A:79:MET:CE	3:A:84:ALA:CB	2.90	0.43
3:A:275:ILE:CG1	3:A:279:GLN:HE22	2.31	0.43
3:A:364:ILE:O	3:A:364:ILE:HG22	2.17	0.43
3:A:404:THR:O	3:A:405:LEU:CB	2.66	0.43
3:A:59:GLN:OE1	3:A:64:VAL:HG11	2.19	0.43
3:A:325:LEU:HD11	3:A:387:LEU:HD11	2.01	0.43
3:A:277:VAL:O	3:A:281:ILE:HG23	2.19	0.42
3:A:332:VAL:HG12	3:A:333:CYS:N	2.35	0.42
3:A:344:LEU:HD21	3:A:387:LEU:HD13	2.01	0.42
3:A:346:ILE:HG22	3:A:406:LEU:CD2	2.49	0.42
3:A:273:LEU:O	3:A:277:VAL:HB	2.20	0.42
3:A:360:ARG:HD3	3:A:360:ARG:HA	1.92	0.42
3:A:367:HIS:CD2	3:A:368:VAL:HG12	2.55	0.42
3:A:406:LEU:HD23	3:A:406:LEU:HA	1.85	0.42
3:A:95:ASN:HD21	3:A:97:GLU:CD	2.28	0.42
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.91	0.41
3:A:164:ASN:H	3:A:170:HIS:CD2	2.29	0.41
3:A:172:ARG:CD	4:A:981:HOH:O	2.65	0.41
3:A:106:SER:OG	3:A:122:ARG:NH2	2.45	0.41
3:A:50:LEU:CD2	3:A:92:VAL:HG11	2.50	0.41
3:A:237:LYS:O	3:A:237:LYS:HD3	2.20	0.41
3:A:318:LYS:HG3	3:A:388:MET:CE	2.51	0.41
3:A:362:CYS:HB3	3:A:390:LEU:HD21	2.02	0.41
3:A:214:LYS:HE3	3:A:214:LYS:HB3	1.81	0.41
3:A:236:ILE:HG21	3:A:236:ILE:HD13	1.51	0.41
3:A:342:VAL:HB	3:A:364:ILE:HD11	2.03	0.41
3:A:88:CYS:O	3:A:89:PRO:O	2.39	0.40
3:A:90:GLN:O	3:A:91:LEU:O	2.39	0.40
2:P:871:DC:H2''	2:P:872:DC:H5'	2.03	0.40
3:A:164:ASN:N	3:A:170:HIS:HD2	2.15	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)
1:T:847:DT:O3'	2:P:867:DA:O5'[10_665]	1.82	0.38

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	358/420 (85%)	303 (85%)	32 (9%)	23 (6%)	1 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	83	ASP
3	A	89	PRO
3	A	90	GLN
3	A	91	LEU
3	A	145	SER
3	A	308	PHE
3	A	315	VAL
3	A	317	ALA
3	A	333	CYS
3	A	334	GLN
3	A	366	SER
3	A	393	ASN
3	A	215	PRO
3	A	337	ARG
3	A	405	LEU
3	A	313	SER
3	A	323	GLU
3	A	73	LEU
3	A	310	LYS
3	A	37	CYS
3	A	316	GLU
3	A	81	VAL
3	A	277	VAL

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
3	A	309/376 (82%)	262 (85%)	47 (15%)	3 5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	SER
3	A	47	ASN
3	A	48	PRO
3	A	73	LEU
3	A	76	LYS
3	A	80	ASN
3	A	90	GLN
3	A	91	LEU
3	A	101	ARG
3	A	123	LEU
3	A	142	GLN
3	A	144	GLN
3	A	149	SER
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	216	ASN
3	A	229	LEU
3	A	272	GLU
3	A	279	GLN
3	A	307	SER
3	A	308	PHE
3	A	309	LYS
3	A	311	CYS
3	A	313	SER
3	A	314	GLU
3	A	318	LYS
3	A	329	LEU
3	A	330	ASN
3	A	332	VAL

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Mol	Chain	Res	Type
3	A	347	ARG
3	A	357	ARG
3	A	359	SER
3	A	360	ARG
3	A	362	CYS
3	A	364	ILE
3	A	368	VAL
3	A	380	MET
3	A	381	THR
3	A	383	MET
3	A	387	LEU
3	A	388	MET
3	A	392	ARG
3	A	394	MET
3	A	404	THR
3	A	408	VAL
3	A	413	LEU

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

Mol	Chain	Res	Type
3	A	47	ASN
3	A	58	GLN
3	A	128	ASN
3	A	170	HIS
3	A	189	ASN
3	A	202	ASN
3	A	262	GLN
3	A	279	GLN
3	A	393	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
2	DOC	P	873	1,2	16,19,20	1.44	2 (12%)	20,26,29	1.72	5 (25%)

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	1,2	-	1/7/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	O4'-C1'	-3.23	1.35	1.42
2	P	873	DOC	O4'-C4'	2.12	1.48	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C3'-C2'-C1'	3.34	106.72	102.87
2	P	873	DOC	O4'-C4'-C5'	3.21	115.12	109.34
2	P	873	DOC	C5-C6-N1	-2.83	117.23	121.84
2	P	873	DOC	O4'-C4'-C3'	2.69	109.24	104.81
2	P	873	DOC	C2'-C1'-N1	-2.58	107.51	112.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	873	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	873	DOC	2	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	T	9/11 (81%)	0.98	1 (11%) 10 8	29, 33, 46, 74	0
2	P	6/7 (85%)	1.05	1 (16%) 4 3	39, 49, 50, 55	0
3	A	366/420 (87%)	0.90	90 (24%) 2 1	7, 39, 90, 100	0
All	All	381/438 (86%)	0.90	92 (24%) 2 1	7, 39, 90, 100	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	349	TYR	10.3
3	A	381	THR	5.5
3	A	346	ILE	5.2
3	A	321	ILE	5.1
3	A	317	ALA	5.0
3	A	309	LYS	5.0
3	A	394	MET	4.9
3	A	243	GLY	4.9
3	A	314	GLU	4.6
3	A	315	VAL	4.5
3	A	330	ASN	4.4
3	A	386	ILE	4.4
3	A	244	TYR	4.4
3	A	360	ARG	4.3
3	A	313	SER	4.3
3	A	305	GLU	4.3
3	A	391	PHE	4.2
3	A	347	ARG	4.2
3	A	356	GLY	4.0
3	A	312	SER	4.0
3	A	73	LEU	4.0
3	A	345	ILE	4.0
3	A	329	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	379	VAL	4.0
3	A	348	ARG	4.0
3	A	406	LEU	3.9
3	A	316	GLU	3.9
3	A	83	ASP	3.7
3	A	304	GLU	3.7
3	A	392	ARG	3.7
3	A	308	PHE	3.7
3	A	334	GLN	3.6
3	A	361	GLN	3.6
3	A	385	ASP	3.6
3	A	359	SER	3.4
3	A	384	VAL	3.4
3	A	390	LEU	3.4
3	A	407	SER	3.4
3	A	388	MET	3.3
3	A	357	ARG	3.3
3	A	276	SER	3.2
3	A	405	LEU	3.2
3	A	325	LEU	3.2
3	A	307	SER	3.1
3	A	328	LEU	3.1
3	A	369	ILE	3.1
3	A	404	THR	3.0
3	A	413	LEU	2.9
3	A	387	LEU	2.9
3	A	389	LYS	2.9
3	A	74	GLY	2.8
3	A	319	ASN	2.8
3	A	81	VAL	2.8
3	A	84	ALA	2.8
1	T	839	DT	2.8
3	A	318	LYS	2.7
3	A	72	LYS	2.7
3	A	306	ASP	2.7
3	A	89	PRO	2.7
3	A	80	ASN	2.7
3	A	88	CYS	2.6
3	A	367	HIS	2.6
3	A	414	LYS	2.6
3	A	382	PRO	2.6
3	A	380	MET	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	362	CYS	2.5
3	A	61	TYR	2.5
3	A	303	SER	2.4
2	P	867	DA	2.4
3	A	79	MET	2.4
3	A	383	MET	2.3
3	A	333	CYS	2.3
3	A	146	ASP	2.3
3	A	75	VAL	2.3
3	A	324	LEU	2.2
3	A	344	LEU	2.2
3	A	358	GLU	2.2
3	A	215	PRO	2.2
3	A	290	ASN	2.1
3	A	297	GLY	2.1
3	A	87	LYS	2.1
3	A	365	PRO	2.1
3	A	69	GLU	2.1
3	A	320	LYS	2.1
3	A	302	PHE	2.0
3	A	408	VAL	2.0
3	A	326	ALA	2.0
3	A	311	CYS	2.0
3	A	411	CYS	2.0
3	A	86	GLU	2.0
3	A	91	LEU	2.0
3	A	310	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
2	DOC	P	873	18/19	0.90	0.11	23,31,38,39	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.