



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:19 PM UTC

PDB ID : 8UDK / pdb_00008udk
Title : Human Mitochondrial DNA Polymerase gamma R853A Ternary Complex
Authors : Park, J.; Herrmann, G.K.; Yin, Y.W.
Deposited on : 2023-09-28
Resolution : 3.43 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

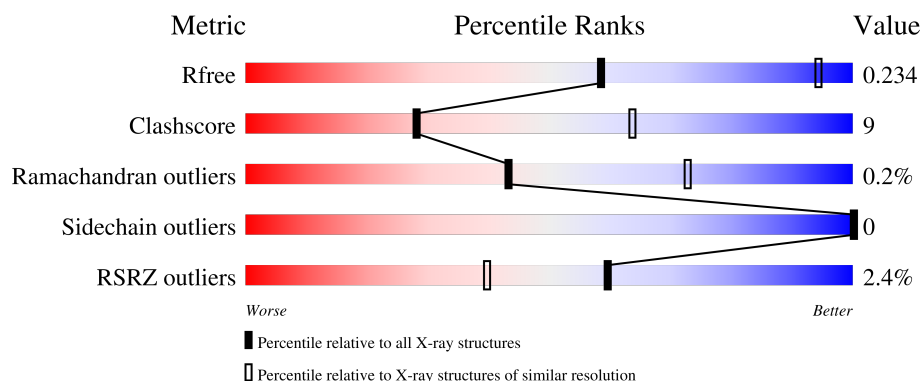
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.43 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.



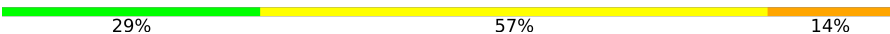
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	1239	
2	B	485	
2	C	485	
3	P	24	
4	T	28	

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Mol	Chain	Length	Quality of chain
5	D	14	 21% 79%
6	E	14	 29% 57% 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15401 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 subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1012	Total	C	N	O	S	0	0	0
			7930	5047	1367	1466	50			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ALA	ASP	engineered mutation	UNP P54098
A	200	ALA	GLU	engineered mutation	UNP P54098
A	853	ALA	ARG	engineered mutation	UNP P54098

- Molecule 2 is a protein called DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	369	Total	C	N	O	S	0	0	0
			2983	1912	524	531	16			
2	C	367	Total	C	N	O	S	0	0	0
			2920	1875	500	529	16			

- Molecule 3 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	22	Total	C	N	O	P	0	0	0
			450	213	90	125	22			

- Molecule 4 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	25	Total	C	N	O	P	0	0	0
			516	245	91	155	25			

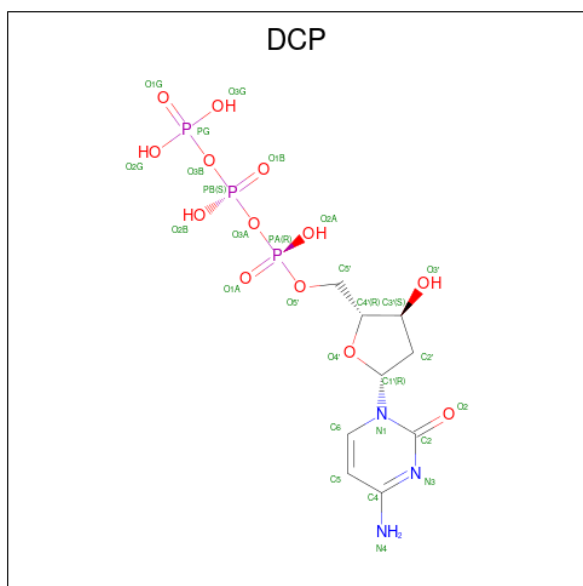
- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*AP*GP*GP*GP*CP*CP*TP*AP*TP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	14	Total	C	N	O	P	0	0	0
			291	138	60	79	14			

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	14	Total	C	N	O	P	0	0	0
			283	137	43	89	14			

- Molecule 7 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

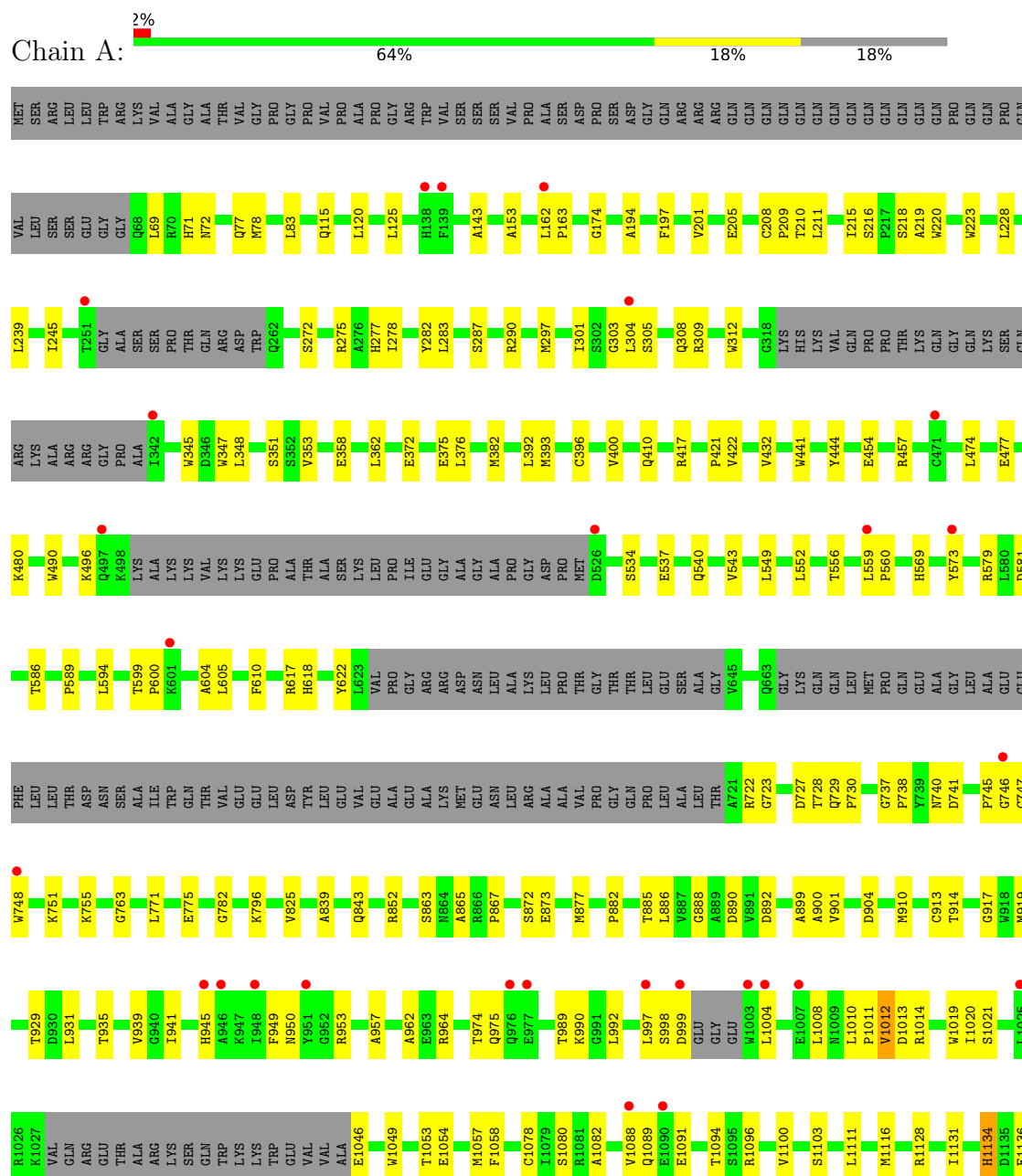


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

3 Residue-property plots

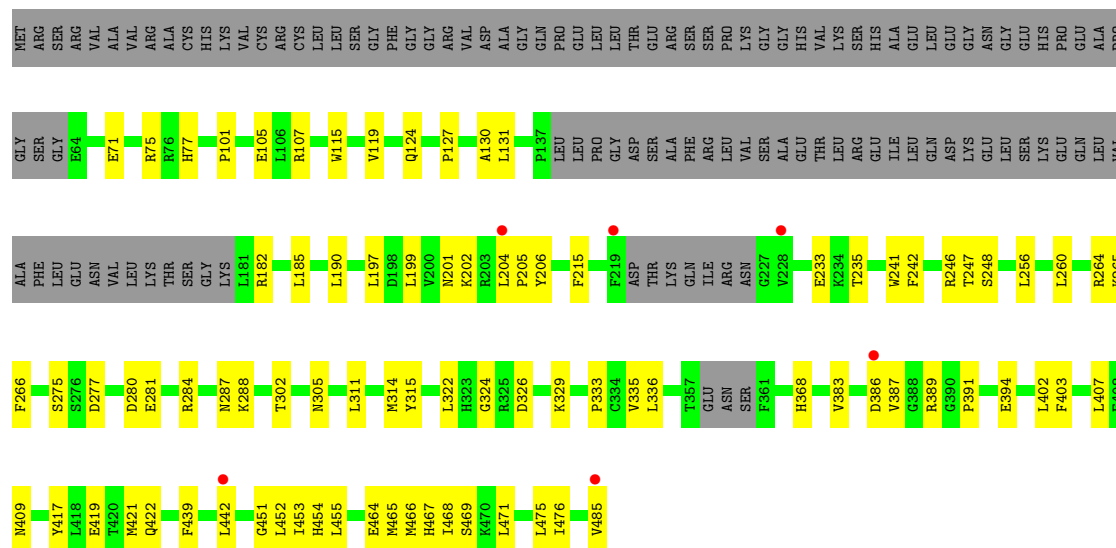
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 subunit gamma-1

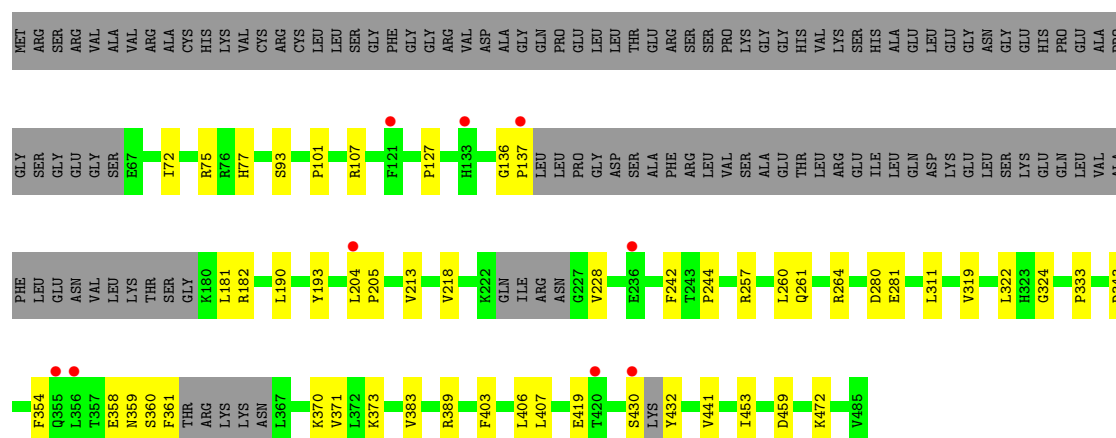




- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial



- Molecule 2: DNA polymerase subunit gamma-2, mitochondrial



- Molecule 3: DNA (24-MER)



- Molecule 4: DNA (28-MER)

Chain T:  50% 39% 11%



- Molecule 5: DNA (5'-D(P*AP*AP*GP*GP*GP*CP*CP*TP*AP*TP*AP*AP*AP*A)-3')

Chain D:  21% 79%



- Molecule 6: DNA (5'-D(P*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*CP*TP*T)-3')

Chain E:  29% 57% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	215.41 Å 215.41 Å 169.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 3.43 48.87 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.87-3.43) 98.2 (48.87-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.40 Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286+SVN	Depositor
R, R_{free}	0.198 , 0.234 0.198 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	119.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15401	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: DCP, 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	0.13	0/8140	0.31	0/11071
2	B	0.11	0/3058	0.30	0/4134
2	C	0.11	0/2993	0.30	0/4055
3	P	0.17	0/486	0.30	0/747
4	T	0.18	0/577	0.38	0/890
5	D	0.17	0/328	0.32	0/504
6	E	0.28	0/314	1.09	4/482 (0.8%)
All	All	0.13	0/15896	0.35	4/21883 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	97	DT	OP2-P-O3'	-12.57	70.28	108.00
6	E	97	DT	OP1-P-O3'	-10.48	76.56	108.00
6	E	98	DT	OP1-P-OP2	8.46	145.38	120.00
6	E	98	DT	O5'-P-OP2	-7.18	86.46	108.00

There are no chirality outliers.

There are no planarity outliers.

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	7930	0	7647	150	0
2	B	2983	0	2967	58	0
2	C	2920	0	2851	35	0
3	P	450	0	245	8	0
4	T	516	0	284	9	0
5	D	291	0	157	9	0
6	E	283	0	162	10	0
7	A	28	0	12	2	0
All	All	15401	0	14325	263	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 9.

All (263) 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:422:VAL:HG11	1:A:1111:LEU:HD12	1.63	0.81
2:C:204:LEU:HD11	2:C:333:PRO:HB3	1.65	0.79
2:C:204:LEU:HD13	2:C:324:GLY:HA3	1.66	0.77
1:A:618:HIS:HB3	1:A:751:LYS:HD2	1.66	0.75
1:A:899:ALA:HB1	1:A:1057:MET:HE3	1.70	0.72
2:B:199:LEU:HD11	2:C:101:PRO:HG3	1.72	0.72
1:A:1010:LEU:HB3	1:A:1012:VAL:HG23	1.73	0.70
1:A:205:GLU:HG3	1:A:382:MET:HE2	1.74	0.70
1:A:953:ARG:HA	1:A:957:ALA:HB3	1.75	0.69
1:A:950:ASN:OD1	1:A:953:ARG:NH2	2.27	0.68
1:A:1111:LEU:HB3	1:A:1160:THR:HG22	1.76	0.67
1:A:1204:THR:HB	1:A:1209:ARG:HG2	1.76	0.67
2:B:204:LEU:HD11	2:B:333:PRO:HB3	1.75	0.67
1:A:852:ARG:NH1	1:A:1103:SER:OG	2.29	0.66
2:C:280:ASP:OD1	2:C:281:GLU:N	2.28	0.66
2:B:204:LEU:HD13	2:B:324:GLY:HA3	1.78	0.65
2:C:260:LEU:HG	2:C:264:ARG:HE	1.61	0.65
1:A:825:VAL:HG13	1:A:882:PRO:HG2	1.78	0.65
1:A:163:PRO:HD3	1:A:218:SER:HA	1.79	0.64
1:A:304:LEU:HB2	1:A:308:GLN:HB3	1.80	0.63
2:B:260:LEU:HD21	2:B:264:ARG:HH21	1.62	0.63
1:A:755:LYS:O	1:A:964:ARG:NH1	2.31	0.63
1:A:914:THR:HG23	1:A:917:GLY:H	1.63	0.63
1:A:723:GLY:HA2	1:A:730:PRO:HG3	1.82	0.62
1:A:496:LYS:HB2	1:A:560:PRO:HG3	1.82	0.62
1:A:579:ARG:NH1	1:A:581:ASP:OD2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:430:SER:O	2:C:432:TYR:N	2.33	0.62
1:A:559:LEU:HB3	1:A:560:PRO:HD2	1.81	0.61
2:B:107:ARG:HD2	2:B:235:THR:HG21	1.81	0.61
1:A:890:ASP:HB3	1:A:1136:GLU:HG2	1.82	0.60
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.84	0.60
2:B:280:ASP:HB3	2:B:284:ARG:H	1.67	0.60
2:B:248:SER:HB3	2:B:305:ASN:HD21	1.66	0.59
1:A:998:SER:HG	1:A:1046:GLU:N	2.00	0.59
2:B:130:ALA:O	2:B:182:ARG:NH2	2.36	0.59
5:D:24:DG:N2	6:E:105:DC:O2	2.35	0.59
6:E:96:DT:H1'	6:E:97:DT:H5'	1.83	0.59
1:A:1089:GLN:OE1	1:A:1089:GLN:N	2.34	0.59
1:A:1091:GLU:O	4:T:3:DA:N6	2.36	0.58
1:A:1150:ALA:HB1	1:A:1183:VAL:HG21	1.85	0.58
2:C:257:ARG:O	2:C:261:GLN:NE2	2.37	0.58
1:A:211:LEU:HB2	1:A:393:MET:HE2	1.85	0.58
1:A:552:LEU:HG	2:B:468:ILE:HD12	1.86	0.58
5:D:20:DA:H2'	5:D:21:DA:C8	2.38	0.57
2:B:260:LEU:HG	2:B:264:ARG:HE	1.67	0.57
1:A:569:HIS:ND1	2:B:464:GLU:OE2	2.29	0.57
1:A:297:MET:HE2	1:A:410:GLN:HB3	1.86	0.57
1:A:283:LEU:O	1:A:1128:ARG:NH1	2.38	0.57
6:E:100:DT:H2''	6:E:101:DA:C8	2.39	0.57
1:A:287:SER:O	1:A:290:ARG:NH1	2.33	0.56
1:A:1131:ILE:HG21	1:A:1189:LEU:HD21	1.86	0.56
1:A:309:ARG:HD3	1:A:353:VAL:HG23	1.87	0.56
1:A:618:HIS:CE1	1:A:738:PRO:HG2	2.40	0.56
2:B:452:LEU:HB3	2:B:465:MET:HG3	1.86	0.56
1:A:900:ALA:HB1	1:A:917:GLY:HA2	1.86	0.55
1:A:417:ARG:HG2	1:A:1078:CYS:HB2	1.88	0.55
1:A:201:VAL:HG12	1:A:209:PRO:HA	1.88	0.55
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.87	0.55
2:B:205:PRO:HA	2:B:242:PHE:O	2.07	0.55
2:C:311:LEU:HG	2:C:322:LEU:HD23	1.89	0.55
1:A:372:GLU:OE1	1:A:375:GLU:N	2.41	0.54
1:A:1203:PRO:HD2	1:A:1209:ARG:HH21	1.72	0.54
1:A:1204:THR:HG22	1:A:1208:ARG:HB2	1.90	0.54
1:A:72:ASN:HB2	1:A:78:MET:HE3	1.89	0.54
1:A:115:GLN:HG2	1:A:929:THR:HG21	1.90	0.54
1:A:549:LEU:HD11	2:B:468:ILE:HG21	1.89	0.54
2:B:383:VAL:HG21	2:B:475:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HH21	1:A:432:VAL:HG23	1.74	0.53
2:B:451:GLY:HA3	2:B:467:HIS:CE1	2.44	0.53
6:E:107:DT:H2''	6:E:108:DT:H5''	1.90	0.53
1:A:1010:LEU:N	1:A:1011:PRO:HA	2.23	0.53
6:E:102:DG:H5''	6:E:102:DG:H8	1.74	0.53
2:C:107:ARG:NH1	2:C:343:ASP:OD1	2.42	0.53
1:A:297:MET:O	1:A:301:ILE:HG12	2.09	0.52
1:A:941:ILE:HD13	1:A:945:HIS:HB2	1.91	0.52
1:A:162:LEU:HD23	1:A:162:LEU:H	1.74	0.52
6:E:97:DT:H1'	6:E:98:DT:OP2	2.09	0.52
1:A:1197:CYS:HB2	1:A:1206:MET:HG2	1.92	0.51
2:B:105:GLU:HG2	2:C:127:PRO:HG3	1.92	0.51
1:A:376:LEU:HD12	1:A:392:LEU:HD11	1.91	0.51
4:T:4:DG:H2'	4:T:5:DG:H8	1.75	0.51
2:C:93:SER:HB3	2:C:218:VAL:HG21	1.92	0.51
2:C:354:PHE:CZ	2:C:370:LYS:HD2	2.46	0.51
1:A:931:LEU:H	1:A:931:LEU:HD23	1.76	0.51
1:A:610:PHE:HB3	1:A:622:TYR:HB2	1.92	0.50
1:A:901:VAL:HG22	1:A:1168:LEU:HD12	1.93	0.50
1:A:999:ASP:HB2	1:A:1004:LEU:HD21	1.92	0.50
1:A:1013:ASP:OD1	1:A:1014:ARG:N	2.44	0.50
2:C:205:PRO:HA	2:C:242:PHE:O	2.12	0.50
1:A:594:LEU:HA	1:A:599:THR:HG21	1.94	0.50
2:C:182:ARG:NH2	2:C:213:VAL:O	2.28	0.50
1:A:208:CYS:HB2	1:A:239:LEU:HD11	1.93	0.50
1:A:1053:THR:HG23	1:A:1054:GLU:HG3	1.93	0.50
1:A:919:MET:HE3	1:A:931:LEU:HA	1.93	0.50
1:A:990:LYS:HD3	1:A:1058:PHE:CG	2.47	0.50
2:B:311:LEU:HG	2:B:322:LEU:HD23	1.94	0.50
1:A:873:GLU:OE2	1:A:1201:SER:OG	2.26	0.49
1:A:83:LEU:HD21	1:A:125:LEU:HD23	1.93	0.49
1:A:741:ASP:N	1:A:741:ASP:OD1	2.46	0.49
6:E:101:DA:H2''	6:E:102:DG:C8	2.48	0.49
4:T:5:DG:H2'	4:T:6:DT:C6	2.48	0.49
1:A:1019:TRP:CE2	1:A:1021:SER:HB3	2.48	0.49
1:A:353:VAL:HG12	1:A:358:GLU:OE1	2.13	0.48
1:A:949:PHE:HE1	1:A:962:ALA:HA	1.78	0.48
1:A:1019:TRP:NE1	1:A:1021:SER:HB3	2.28	0.48
2:B:419:GLU:OE2	2:B:422:GLN:NE2	2.46	0.48
1:A:888:GLY:HA3	1:A:1138:ARG:HH11	1.76	0.48
1:A:215:ILE:HD11	1:A:220:TRP:CH2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:SER:HB2	1:A:537:GLU:HB2	1.95	0.48
2:B:215:PHE:HD1	2:B:233:GLU:HG2	1.78	0.48
1:A:1204:THR:HG22	1:A:1208:ARG:CB	2.43	0.48
1:A:223:TRP:CZ2	1:A:245:ILE:HG22	2.49	0.48
1:A:935:THR:O	1:A:939:VAL:HG12	2.13	0.48
2:B:124:GLN:HB2	2:B:206:TYR:HA	1.95	0.48
1:A:272:SER:HB3	1:A:843:GLN:HA	1.96	0.48
1:A:737:GLY:HA3	1:A:751:LYS:HB2	1.95	0.48
2:B:246:ARG:HG3	2:B:247:THR:HG23	1.96	0.47
2:B:277:ASP:OD1	2:B:287:ASN:ND2	2.47	0.47
5:D:29:DT:H2''	5:D:30:DA:C8	2.49	0.47
1:A:604:ALA:HB3	1:A:782:GLY:HA3	1.96	0.47
6:E:104:DC:H2''	6:E:105:DC:C5	2.49	0.47
2:B:71:GLU:HG3	2:B:75:ARG:HH12	1.80	0.47
1:A:727:ASP:HA	1:A:745:PRO:HA	1.96	0.47
1:A:865:ALA:HA	1:A:872:SER:HB2	1.95	0.47
1:A:216:SER:OG	1:A:219:ALA:HB3	2.15	0.47
1:A:610:PHE:CE2	1:A:748:TRP:HD1	2.33	0.47
2:B:403:PHE:CZ	2:B:407:LEU:HD11	2.50	0.47
2:B:389:ARG:HH12	2:B:421:MET:HE2	1.80	0.46
5:D:30:DA:H2''	5:D:31:DA:N7	2.30	0.46
1:A:999:ASP:HB2	1:A:1004:LEU:HD11	1.96	0.46
1:A:771:LEU:O	1:A:775:GLU:HG2	2.16	0.46
2:B:389:ARG:HH22	2:B:421:MET:HE2	1.79	0.46
3:P:11:DG:H2''	3:P:12:DG:C8	2.50	0.46
1:A:223:TRP:CH2	1:A:245:ILE:HG22	2.51	0.46
2:B:439:PHE:HB3	2:B:455:LEU:HD11	1.97	0.46
2:C:190:LEU:HD22	2:C:311:LEU:HD13	1.98	0.46
1:A:444:TYR:CG	1:A:877:MET:HG3	2.50	0.46
1:A:904:ASP:OD1	1:A:914:THR:HG22	2.16	0.46
4:T:11:DC:H2''	4:T:12:DA:C8	2.51	0.46
1:A:77:GLN:HG2	1:A:120:LEU:HB2	1.97	0.46
1:A:345:TRP:HE3	1:A:348:LEU:HD11	1.80	0.46
1:A:728:THR:OG1	1:A:740:ASN:OD1	2.24	0.46
4:T:11:DC:H2''	4:T:12:DA:H8	1.80	0.46
1:A:282:TYR:HD2	1:A:839:ALA:HB3	1.81	0.45
1:A:1210:TYR:HB2	1:A:1212:ILE:HD13	1.97	0.45
2:C:389:ARG:HH11	2:C:389:ARG:HA	1.81	0.45
6:E:102:DG:H5''	6:E:102:DG:C8	2.50	0.45
2:B:315:TYR:HB2	2:B:322:LEU:HD11	1.98	0.45
2:C:383:VAL:HG11	2:C:406:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TRP:O	1:A:444:TYR:HB3	2.16	0.45
1:A:540:GLN:HA	1:A:543:VAL:HG12	1.98	0.45
1:A:990:LYS:HD2	1:A:1049:TRP:CZ2	2.50	0.45
5:D:26:DC:H2''	5:D:27:DT:O5'	2.16	0.45
2:B:387:VAL:HG13	2:B:417:TYR:HB2	1.99	0.45
1:A:910:MET:HB2	1:A:913:CYS:HB3	1.99	0.45
1:A:1116:MET:HG2	1:A:1156:THR:HG21	1.98	0.45
1:A:396:CYS:O	1:A:400:VAL:HG23	2.17	0.45
1:A:573:TYR:OH	1:A:589:PRO:HD3	2.16	0.45
1:A:1096:ARG:O	1:A:1100:VAL:HG23	2.17	0.45
1:A:312:TRP:NE1	1:A:351:SER:O	2.50	0.45
1:A:1134:HIS:HB2	3:P:24:DOC:H4'	1.99	0.45
2:B:115:TRP:CZ2	2:B:119:VAL:HG11	2.52	0.45
1:A:477:GLU:HB3	1:A:480:LYS:HE2	1.99	0.44
2:C:193:TYR:OH	2:C:333:PRO:HG3	2.17	0.44
1:A:974:THR:O	1:A:975:GLN:C	2.60	0.44
2:B:280:ASP:OD1	2:B:281:GLU:N	2.50	0.44
1:A:796:LYS:HE2	1:A:796:LYS:HB3	1.80	0.44
2:C:354:PHE:HZ	2:C:370:LYS:HD2	1.82	0.44
3:P:14:DC:H2''	3:P:15:DA:C8	2.52	0.44
1:A:885:THR:HG23	1:A:1143:GLU:HG2	2.00	0.44
1:A:351:SER:HB3	1:A:1082:ALA:HB2	2.00	0.44
4:T:10:DG:H2''	4:T:11:DC:C6	2.53	0.44
1:A:556:THR:HG1	2:B:467:HIS:CG	2.35	0.44
1:A:723:GLY:HA2	1:A:730:PRO:CG	2.46	0.44
2:B:265:LYS:HE3	2:B:266:PHE:CZ	2.53	0.44
1:A:763:GLY:HA3	3:P:19:DC:H4'	2.00	0.44
1:A:600:PRO:HB3	1:A:605:LEU:HD12	2.00	0.44
2:C:257:ARG:HG2	2:C:261:GLN:NE2	2.33	0.44
1:A:210:THR:HG22	1:A:228:LEU:HD22	2.00	0.43
1:A:863:SER:HA	3:P:23:DA:H5'	2.00	0.43
2:B:288:LYS:HG2	2:B:302:THR:HG22	1.99	0.43
2:B:368:HIS:O	2:B:368:HIS:ND1	2.49	0.43
2:C:319:VAL:HA	2:C:322:LEU:HD13	2.00	0.43
2:C:358:GLU:HA	2:C:371:VAL:HG12	2.01	0.43
2:C:373:LYS:HE3	2:C:459:ASP:HA	2.00	0.43
2:B:197:LEU:HG	2:B:202:LYS:HG2	2.01	0.43
3:P:7:DC:H2''	3:P:8:DG:C8	2.53	0.43
1:A:1152:ALA:O	1:A:1156:THR:HG23	2.18	0.43
2:B:326:ASP:N	2:B:329:LYS:O	2.44	0.43
1:A:610:PHE:CD2	1:A:622:TYR:HD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:THR:HG21	4:T:3:DA:H2'	2.01	0.43
2:B:314:MET:HB2	2:B:314:MET:HE3	1.84	0.43
3:P:22:DT:H2'	3:P:23:DA:C8	2.54	0.43
5:D:21:DA:H2'	5:D:22:DG:C8	2.53	0.43
1:A:69:LEU:HD21	1:A:71:HIS:CE1	2.54	0.43
2:B:241:TRP:HB3	2:B:336:LEU:HB3	2.01	0.43
2:B:386:ASP:HA	2:B:417:TYR:HB3	2.01	0.43
2:B:453:ILE:HG12	2:B:466:MET:O	2.18	0.43
2:C:136:GLY:HA2	2:C:137:PRO:HD3	1.88	0.43
1:A:939:VAL:HG13	1:A:941:ILE:HG13	2.01	0.43
2:B:201:ASN:ND2	2:C:419:GLU:HG2	2.34	0.43
2:C:181:LEU:HD23	2:C:181:LEU:HA	1.86	0.43
2:C:403:PHE:CZ	2:C:407:LEU:HD11	2.54	0.43
1:A:586:THR:HB	2:B:485:VAL:HG22	2.00	0.43
1:A:556:THR:OG1	2:B:467:HIS:ND1	2.50	0.43
5:D:30:DA:H2''	5:D:31:DA:C8	2.54	0.43
1:A:174:GLY:O	1:A:223:TRP:HA	2.18	0.42
1:A:197:PHE:HZ	1:A:245:ILE:HD11	1.84	0.42
1:A:474:LEU:HD12	1:A:490:TRP:HB3	2.01	0.42
2:B:402:LEU:HD11	2:B:471:LEU:HD23	2.00	0.42
1:A:729:GLN:OE1	1:A:746:GLY:HA2	2.20	0.42
1:A:1008:LEU:O	1:A:1011:PRO:HA	2.19	0.42
4:T:7:DA:C8	4:T:8:DT:H72	2.55	0.42
1:A:556:THR:HG21	2:B:469:SER:OG	2.20	0.42
2:B:131:LEU:C	2:B:182:ARG:HH21	2.27	0.42
2:B:190:LEU:HD21	2:B:335:VAL:HG11	2.01	0.42
2:C:204:LEU:HD23	2:C:244:PRO:HG3	2.02	0.42
1:A:454:GLU:HG2	1:A:457:ARG:HH22	1.84	0.42
2:B:115:TRP:CZ2	2:B:127:PRO:HB3	2.55	0.42
2:B:256:LEU:HD21	2:B:275:SER:OG	2.20	0.42
2:B:391:PRO:HB2	2:B:394:GLU:OE1	2.20	0.42
2:C:472:LYS:HB3	2:C:472:LYS:HE3	1.90	0.42
5:D:32:DA:H2''	5:D:33:DA:N7	2.35	0.42
1:A:729:GLN:H	1:A:747:CYS:HB3	1.84	0.42
2:B:182:ARG:HD3	2:B:185:LEU:HD23	2.01	0.42
6:E:104:DC:H2''	6:E:105:DC:C6	2.55	0.42
1:A:303:GLY:N	1:A:1080:SER:OG	2.51	0.42
1:A:351:SER:C	1:A:362:LEU:HD11	2.45	0.42
2:C:358:GLU:HG2	2:C:359:ASN:O	2.20	0.42
1:A:892:ASP:HA	7:A:4000:DCP:H2'2	2.02	0.41
2:C:77:HIS:HB3	2:C:101:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TRP:CD1	1:A:1088:VAL:HG12	2.55	0.41
2:B:215:PHE:CD1	2:B:233:GLU:HG2	2.55	0.41
1:A:992:LEU:HD12	1:A:992:LEU:H	1.85	0.41
1:A:997:LEU:HA	1:A:1004:LEU:HD22	2.02	0.41
1:A:1192:GLU:OE2	7:A:4000:DCP:H5	2.21	0.41
2:C:360:SER:OG	2:C:361:PHE:N	2.45	0.41
3:P:8:DG:H2"	3:P:9:DA:H8	1.86	0.41
1:A:78:MET:HE1	1:A:1174:PRO:HG3	2.03	0.41
1:A:1057:MET:HE2	1:A:1057:MET:HB2	1.85	0.41
2:B:77:HIS:HB3	2:B:101:PRO:HD2	2.02	0.41
2:C:441:VAL:HG13	2:C:453:ILE:HD12	2.02	0.41
1:A:143:ALA:HB3	1:A:421:PRO:HB2	2.02	0.41
1:A:886:LEU:HD13	1:A:1189:LEU:HD12	2.03	0.41
1:A:989:THR:HA	1:A:1053:THR:HG22	2.03	0.41
1:A:990:LYS:HD2	1:A:1049:TRP:CE2	2.55	0.41
4:T:21:DC:H2"	4:T:22:DG:C8	2.56	0.41
1:A:275:ARG:O	1:A:278:ILE:HG12	2.20	0.41
2:C:72:ILE:HD12	2:C:354:PHE:CE2	2.56	0.41
1:A:305:SER:O	1:A:309:ARG:N	2.52	0.41
1:A:722:ARG:O	1:A:730:PRO:HB3	2.21	0.41
1:A:867:PRO:HA	1:A:1198:LYS:O	2.21	0.41
1:A:1207:GLU:HG2	1:A:1212:ILE:O	2.21	0.41
5:D:20:DA:H8	5:D:20:DA:P	2.44	0.41
1:A:617:ARG:HB3	1:A:618:HIS:CD2	2.56	0.41
1:A:197:PHE:CZ	1:A:245:ILE:HD11	2.56	0.40
1:A:1019:TRP:O	1:A:1020:ILE:HG12	2.22	0.40
2:C:72:ILE:HG12	2:C:75:ARG:NH2	2.36	0.40
1:A:1010:LEU:H	1:A:1011:PRO:HA	1.86	0.40
2:B:204:LEU:HD12	2:B:204:LEU:HA	1.81	0.40
1:A:209:PRO:HD3	1:A:277:HIS:HD2	1.85	0.40
1:A:873:GLU:O	1:A:877:MET:HG2	2.22	0.40
2:B:409:ASN:HB3	2:B:476:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

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	
1	A	996/1239 (80%)	952 (96%)	42 (4%)	2 (0%)	43	73
2	B	361/485 (74%)	356 (99%)	5 (1%)	0	100	100
2	C	357/485 (74%)	351 (98%)	5 (1%)	1 (0%)	36	66
All	All	1714/2209 (78%)	1659 (97%)	52 (3%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1134	HIS
2	C	228	VAL
1	A	1012	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	
1	A	831/1041 (80%)	831 (100%)	0	100	100
2	B	329/426 (77%)	329 (100%)	0	100	100
2	C	318/426 (75%)	318 (100%)	0	100	100
All	All	1478/1893 (78%)	1478 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	146	GLN
1	A	360	HIS
1	A	388	ASN

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Mol	Chain	Res	Type
1	A	394	GLN
1	A	922	GLN
1	A	971	HIS
1	A	1023	GLN
2	B	187	HIS
2	B	305	ASN
2	B	309	HIS
2	C	261	GLN
2	C	409	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	$\# Z > 2$
3	DOC	P	24	3,4	16,19,20	1.39	3 (18%)	20,26,29	1.50	4 (20%)

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	DOC	P	24	3,4	-	0/7/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	24	DOC	O5'-C5'	-2.73	1.36	1.44
3	P	24	DOC	C4-N4	2.36	1.39	1.33
3	P	24	DOC	C2-N1	2.30	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	24	DOC	O4'-C1'-C2'	3.02	109.99	106.41
3	P	24	DOC	N4-C4-N3	-2.56	113.33	117.91
3	P	24	DOC	C5-C4-N3	2.39	125.34	121.32
3	P	24	DOC	C4-N3-C2	-2.24	116.73	120.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	24	DOC	1	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	$\# Z > 2$
7	DCP	A	4000	-	28,29,29	3.00	8 (28%)	41,45,45	2.12	12 (29%)

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
7	DCP	A	4000	-	-	6/22/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4000	DCP	PB-O3A	11.55	1.72	1.59
7	A	4000	DCP	PA-O5'	5.87	1.82	1.59
7	A	4000	DCP	PA-O3A	-5.34	1.53	1.59
7	A	4000	DCP	PB-O3B	-3.64	1.55	1.59
7	A	4000	DCP	O5'-C5'	-2.91	1.33	1.44
7	A	4000	DCP	C2-N3	2.83	1.42	1.36
7	A	4000	DCP	C2-N1	2.28	1.44	1.40
7	A	4000	DCP	C4-N4	2.28	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4000	DCP	O2A-PA-O3A	6.20	124.02	107.27
7	A	4000	DCP	O2B-PB-O3B	6.19	124.00	107.27
7	A	4000	DCP	C1'-N1-C2	4.14	124.94	117.83
7	A	4000	DCP	C1'-N1-C6	-3.60	114.45	121.53
7	A	4000	DCP	O3A-PB-O1B	-3.55	100.03	110.70
7	A	4000	DCP	C4'-O4'-C1'	-3.03	102.30	109.51
7	A	4000	DCP	C5-C4-N3	2.31	125.22	121.32
7	A	4000	DCP	O5'-PA-O1A	-2.24	100.08	108.94
7	A	4000	DCP	O3G-PG-O2G	2.18	115.97	107.80
7	A	4000	DCP	C2'-C1'-N1	2.14	119.17	113.81
7	A	4000	DCP	O4'-C4'-C3'	-2.11	100.83	105.65
7	A	4000	DCP	O2-C2-N3	-2.09	119.03	122.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4000	DCP	C5'-O5'-PA-O1A
7	A	4000	DCP	C5'-O5'-PA-O2A
7	A	4000	DCP	C5'-O5'-PA-O3A
7	A	4000	DCP	C3'-C4'-C5'-O5'

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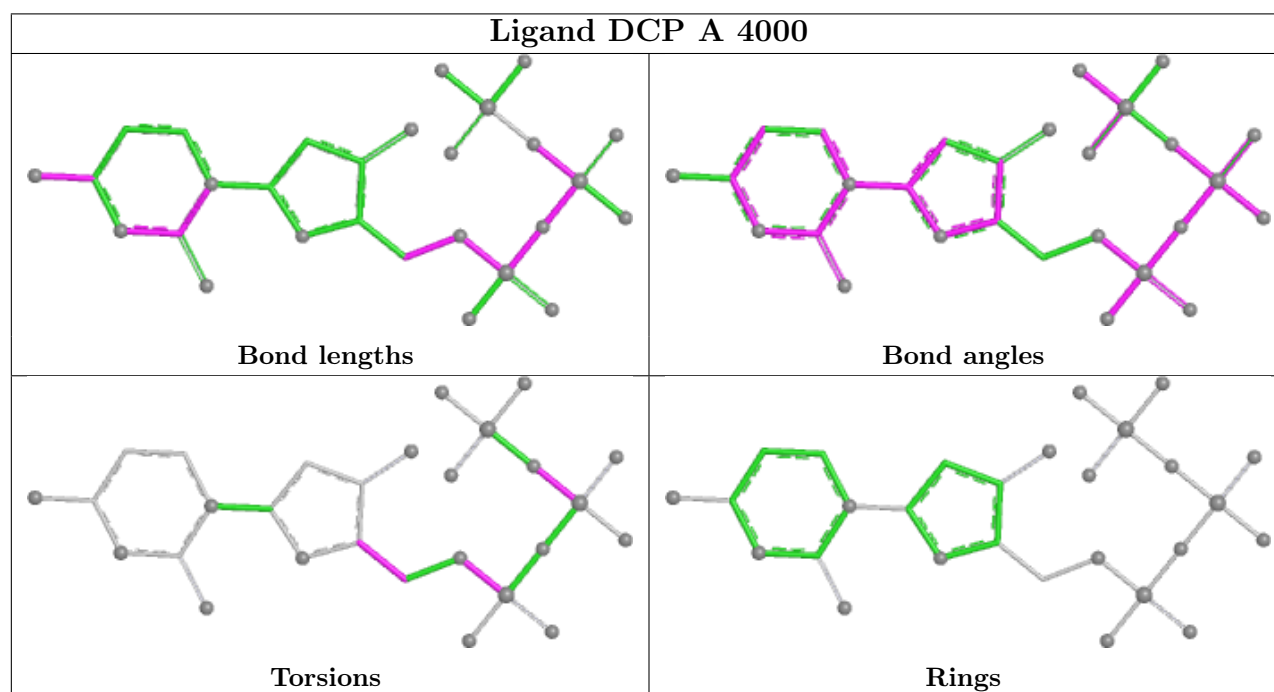
Mol	Chain	Res	Type	Atoms
7	A	4000	DCP	O4'-C4'-C5'-O5'
7	A	4000	DCP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	4000	DCP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1012/1239 (81%)	0.05	29 (2%) 53 35	75, 125, 220, 302	0
2	B	369/485 (76%)	-0.06	6 (1%) 70 50	76, 108, 192, 268	0
2	C	367/485 (75%)	-0.04	9 (2%) 58 39	84, 119, 187, 252	0
3	P	21/24 (87%)	-0.19	0 100 100	146, 181, 252, 269	0
4	T	25/28 (89%)	0.06	0 100 100	134, 202, 270, 306	0
5	D	14/14 (100%)	0.72	0 100 100	231, 258, 307, 364	0
6	E	14/14 (100%)	0.56	0 100 100	192, 231, 304, 305	0
All	All	1822/2289 (79%)	0.02	44 (2%) 59 40	75, 122, 222, 364	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	999	ASP	6.0
1	A	997	LEU	4.1
2	C	204	LEU	3.9
2	C	430	SER	3.7
1	A	559	LEU	3.6
2	B	204	LEU	3.5
2	C	133	HIS	3.5
1	A	951	TYR	3.4
2	B	485	VAL	3.4
1	A	1025	LEU	3.1
1	A	748	TRP	3.0
1	A	1004	LEU	3.0
1	A	976	GLN	2.9
2	B	386	ASP	2.9
2	B	219	PHE	2.9
1	A	573	TYR	2.6
1	A	139	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	138	HIS	2.6
1	A	526	ASP	2.5
2	C	356	LEU	2.5
2	C	420	THR	2.5
1	A	1007	GLU	2.4
2	C	121	PHE	2.4
1	A	945	HIS	2.4
1	A	1090	GLU	2.4
1	A	977	GLU	2.3
1	A	746	GLY	2.3
2	B	442	LEU	2.2
1	A	251	THR	2.2
2	B	228	VAL	2.2
1	A	162	LEU	2.2
1	A	304	LEU	2.2
1	A	946	ALA	2.2
2	C	137	PRO	2.2
1	A	948	ILE	2.2
2	C	355	GLN	2.2
2	C	236	GLU	2.2
1	A	342	ILE	2.1
1	A	497	GLN	2.1
1	A	471	CYS	2.1
1	A	1170	LEU	2.1
1	A	1088	VAL	2.1
1	A	1003	TRP	2.1
1	A	601	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	DOC	P	24	18/19	0.84	0.14	136,142,167,325	0

6.3 Carbohydrates [i](#)

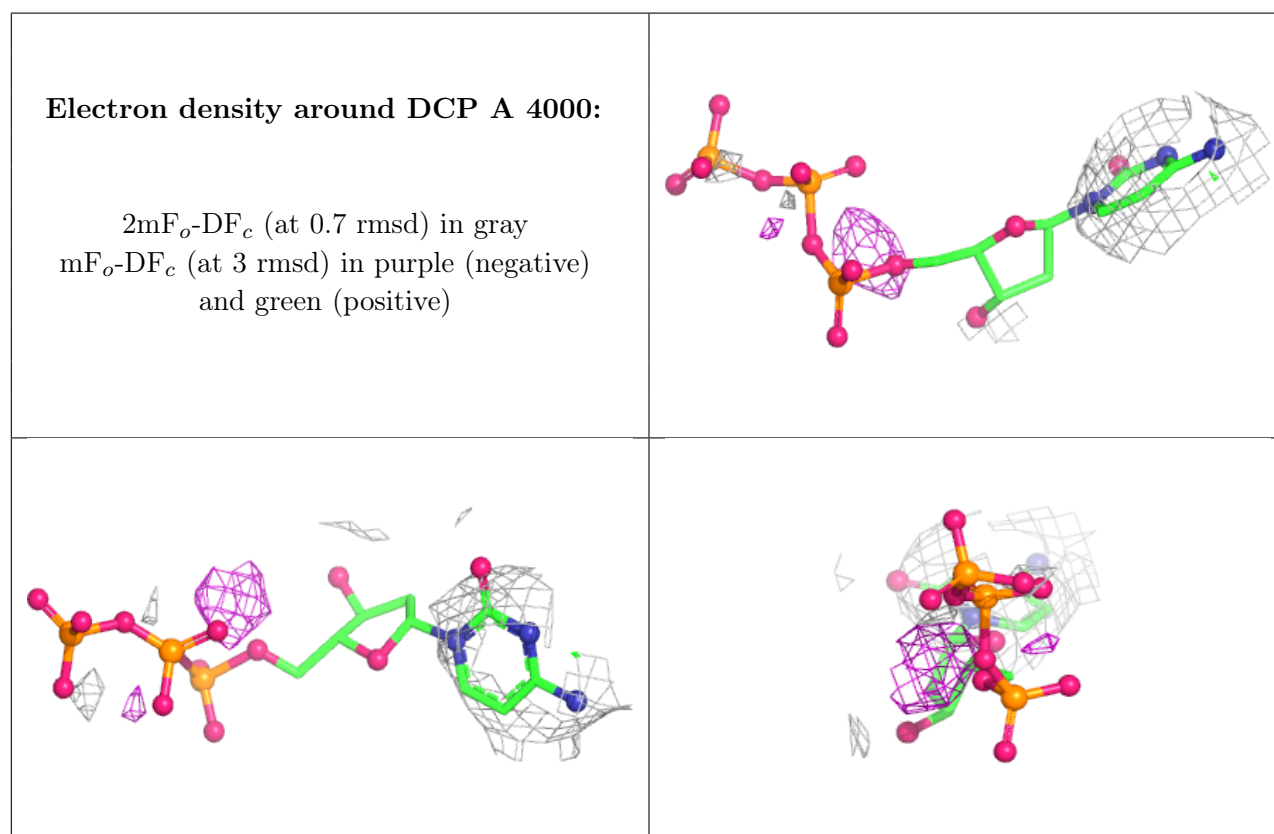
There are no oligosaccharides in this entry.

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
7	DCP	A	4000	28/28	0.43	0.12	145,245,356,376	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.