



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:46 PM EDT

PDB ID : 5C51 / pdb_00005c51
Title : Probing the Structural and Molecular Basis of Nucleotide Selectivity by Human Mitochondrial DNA Polymerase gamma
Authors : Sohl, C.D.; Szymanski, M.R.; Mislak, A.C.; Shumate, C.K.; Amiralaie, S.; Schinazi, R.F.; Anderson, K.S.; Whitney, Y.Y.
Deposited on : 2015-06-19
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

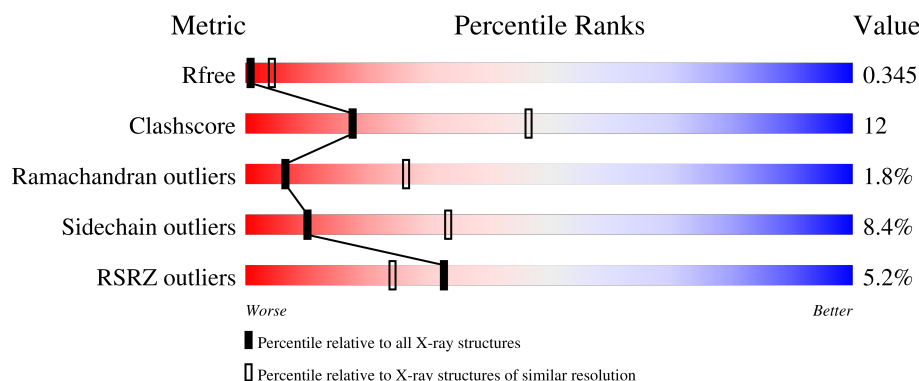
1 Overall quality at a glance

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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	1205	
2	B	485	
2	C	485	
3	P	22	

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Mol	Chain	Length	Quality of chain
4	T	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DOC	P	24	-	-	X	-
6	1RY	A	4003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14620 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	983	Total	C	N	O	S	0	0	0
			7802	4966	1374	1413	49			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	?	-	GLN	deletion	UNP P54098
A	948	ARG	ILE	conflict	UNP P54098

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2943	1885	520	522	16			
2	C	358	Total	C	N	O	S	0	0	0
			2888	1852	506	514	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	22	Total	C	N	O	P	0	0	0
			451	214	92	124	21			

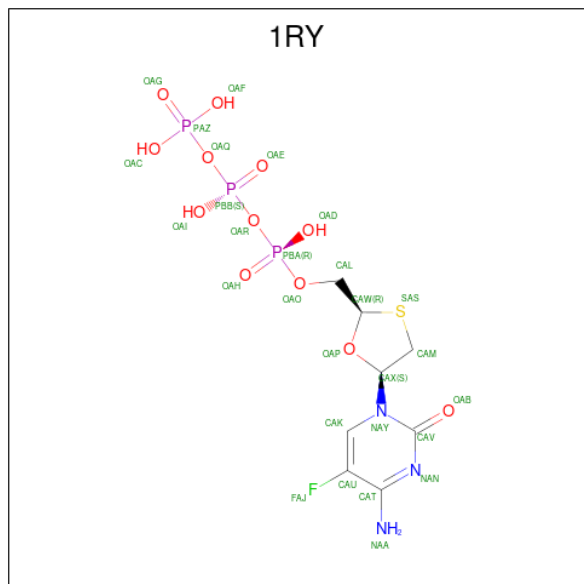
- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	25	Total	C	N	O	P	0	0	0
			506	241	87	154	24			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

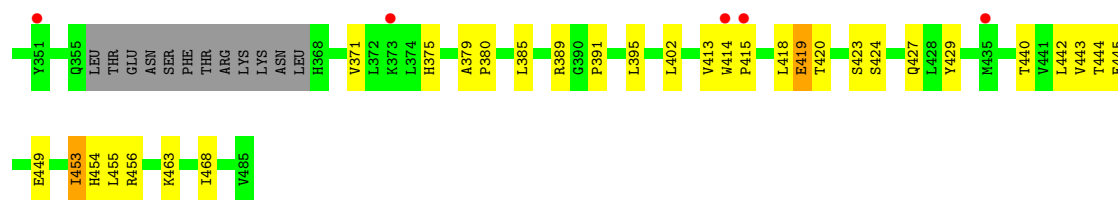
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is [[(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: 1RY) (formula: C₈H₁₃FN₃O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	P	S	
			28	8	1	3	12	3	1	

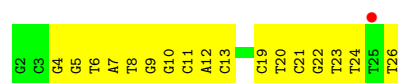




- Molecule 3: DNA (5'-D(*(AD)P*AP*AP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3')



- Molecule 4: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	215.05Å 215.05Å 161.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 3.43 47.02 – 3.43	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.02-3.43) 84.7 (47.02-3.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.315 , 0.345 0.342 , 0.345	Depositor DCC
R_{free} test set	2000 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	134.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	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	0.89	EDS
Total number of atoms	14620	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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, MG, 1RY

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	0.30	0/8002	0.75	14/10855 (0.1%)
2	B	0.26	0/3016	0.70	0/4074
2	C	0.27	0/2961	0.73	4/4002 (0.1%)
3	P	0.14	0/488	0.25	0/752
4	T	0.11	0/565	0.55	0/870
All	All	0.27	0/15032	0.72	18/20553 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	PRO	CA-N-CD	-9.04	99.35	112.00
1	A	1069	ILE	CA-C-N	8.23	130.13	119.84
1	A	1069	ILE	C-N-CA	8.23	130.13	119.84
2	C	96	HIS	C-N-CD	-7.00	105.19	120.60
1	A	752	LEU	CA-C-N	6.81	143.34	127.00
1	A	752	LEU	C-N-CA	6.81	143.34	127.00
1	A	752	LEU	C-N-CD	-6.60	106.07	120.60
1	A	1054	GLU	CB-CA-C	-5.77	109.38	117.23
2	C	96	HIS	CA-C-N	5.70	140.67	127.00
2	C	96	HIS	C-N-CA	5.70	140.67	127.00
1	A	856	GLU	CA-C-N	5.50	125.33	119.28
1	A	856	GLU	C-N-CA	5.50	125.33	119.28
1	A	127	LEU	CA-C-N	5.49	123.67	119.66
1	A	127	LEU	C-N-CA	5.49	123.67	119.66
1	A	1199	THR	CA-C-N	-5.11	114.78	120.45
1	A	1199	THR	C-N-CA	-5.11	114.78	120.45
1	A	165	LYS	CA-C-N	5.05	123.34	119.66
1	A	165	LYS	C-N-CA	5.05	123.34	119.66

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	7802	0	7694	212	1
2	B	2943	0	2939	65	0
2	C	2888	0	2862	66	1
3	P	451	0	245	30	0
4	T	506	0	279	36	0
5	A	2	0	0	0	0
6	A	28	0	11	15	0
All	All	14620	0	14030	351	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 12.

All (351) 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)
6:A:4003:1RY:CAX	6:A:4003:1RY:OAP	1.63	1.38
1:A:948:ARG:NE	6:A:4003:1RY:NAA	1.86	1.23
1:A:948:ARG:NH2	3:P:24:DOC:N4	1.88	1.21
1:A:948:ARG:NH2	3:P:24:DOC:HN42	1.42	1.18
2:C:135:PRO:HD2	2:C:136:GLY:H	1.13	1.12
3:P:20:DC:O2	4:T:10:DG:N2	1.86	1.08
1:A:948:ARG:CZ	6:A:4003:1RY:NAA	2.21	1.04
1:A:948:ARG:NH2	6:A:4003:1RY:NAA	2.12	0.97
1:A:948:ARG:NH2	6:A:4003:1RY:H12	1.67	0.92
1:A:948:ARG:NE	6:A:4003:1RY:H13	1.64	0.91
2:C:419:GLU:H	2:C:420:THR:HA	1.35	0.91
3:P:20:DC:C2	4:T:10:DG:N2	2.39	0.91
1:A:948:ARG:NE	6:A:4003:1RY:H12	1.63	0.89
2:C:135:PRO:HD2	2:C:136:GLY:N	1.88	0.87
1:A:850:ILE:HG22	4:T:6:DT:H4'	1.58	0.86
1:A:948:ARG:HH22	3:P:24:DOC:HN42	0.86	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:DG:N2	4:T:19:DC:O2	2.09	0.85
1:A:948:ARG:HE	6:A:4003:1RY:H12	1.15	0.84
1:A:948:ARG:HH21	6:A:4003:1RY:H12	1.22	0.83
1:A:948:ARG:CZ	6:A:4003:1RY:H12	1.84	0.82
2:C:135:PRO:CD	2:C:136:GLY:H	1.94	0.80
3:P:10:DG:N2	4:T:20:DT:O2	2.17	0.78
1:A:963:GLU:HG3	1:A:981:LYS:HZ3	1.48	0.78
2:C:442:LEU:HB3	2:C:454:HIS:HB2	1.70	0.74
1:A:211:LEU:HD22	1:A:393:MET:HE2	1.70	0.74
2:C:67:GLU:HG3	2:C:88:ARG:NH2	2.03	0.73
2:B:77:HIS:HE1	2:B:431:LYS:HG3	1.54	0.72
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.72	0.72
2:C:443:VAL:HG22	2:C:453:ILE:HD11	1.71	0.71
1:A:487:ASP:OD2	1:A:601:LYS:NZ	2.23	0.70
1:A:561:LYS:HE2	4:T:22:DG:OP2	1.92	0.70
1:A:243:ASP:HB3	1:A:279:ARG:HE	1.57	0.68
1:A:1108:TYR:OH	1:A:1161:ARG:NH1	2.27	0.68
3:P:18:DG:C2	4:T:12:DA:C2	2.81	0.67
3:P:21:DG:N2	4:T:8:DT:H3	1.92	0.67
1:A:1068:ASP:HA	1:A:1085:PRO:HG2	1.75	0.67
3:P:10:DG:N1	4:T:19:DC:N3	2.35	0.66
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.78	0.66
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.77	0.65
2:B:197:LEU:HD22	2:B:202:LYS:HA	1.78	0.65
1:A:79:LEU:H	1:A:83:LEU:HG	1.62	0.65
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.79	0.64
1:A:856:GLU:OE1	1:A:859:TRP:N	2.28	0.64
1:A:1161:ARG:HE	1:A:1177:VAL:HG22	1.63	0.64
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.78	0.64
1:A:1057:MET:SD	1:A:1057:MET:N	2.71	0.64
2:C:134:LYS:HG2	2:C:135:PRO:CD	2.27	0.63
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.72	0.63
2:C:134:LYS:HG2	2:C:135:PRO:HD2	1.80	0.63
1:A:1069:ILE:O	1:A:1071:ARG:N	2.33	0.62
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.81	0.62
1:A:208:CYS:SG	1:A:227:ARG:NH2	2.73	0.62
1:A:899:ALA:HB1	1:A:1057:MET:HE3	1.81	0.61
2:C:135:PRO:CD	2:C:136:GLY:N	2.56	0.61
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.81	0.61
1:A:1135:ASP:HB2	6:A:4003:1RY:H5	1.83	0.61
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:THR:H	1:A:939:VAL:HA	1.66	0.60
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.84	0.60
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.73	0.60
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.83	0.60
1:A:849:THR:HG22	1:A:850:ILE:HD13	1.81	0.60
1:A:134:ASN:ND2	1:A:1166:TYR:OH	2.34	0.60
1:A:533:CYS:SG	1:A:534:SER:N	2.70	0.59
1:A:502:LYS:HB3	1:A:503:VAL:HB	1.83	0.59
1:A:861:THR:HG21	4:T:8:DT:H1'	1.84	0.59
2:C:429:TYR:HE1	2:C:463:LYS:HZ3	1.49	0.59
1:A:978:ALA:HA	1:A:981:LYS:HD2	1.84	0.59
1:A:232:ARG:NH2	2:C:468:ILE:HG21	2.17	0.59
3:P:10:DG:C2	4:T:20:DT:O2	2.56	0.59
1:A:744:ILE:HG23	1:A:745:PRO:HD3	1.84	0.58
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.37	0.58
1:A:239:LEU:O	1:A:279:ARG:NH1	2.37	0.58
1:A:800:PHE:HB2	1:A:869:ARG:HE	1.68	0.58
4:T:9:DG:H2'	4:T:10:DG:C8	2.39	0.58
1:A:1142:ARG:NH1	1:A:1144:GLU:OE1	2.34	0.57
3:P:21:DG:H22	4:T:8:DT:H3	1.50	0.57
1:A:911:HIS:NE2	1:A:1172:ASP:O	2.36	0.57
1:A:1098:ASN:ND2	4:T:5:DG:H1'	2.20	0.57
3:P:4:DA:N3	4:T:26:DT:C1'	2.62	0.56
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.88	0.56
2:C:419:GLU:N	2:C:420:THR:HA	2.07	0.56
2:B:83:LYS:HG2	2:B:85:GLN:H	1.70	0.56
1:A:556:THR:OG1	2:B:450:ASN:O	2.13	0.56
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.87	0.56
1:A:488:LEU:HD13	1:A:488:LEU:H	1.70	0.56
2:B:363:ARG:HD3	2:B:364:LYS:H	1.70	0.56
1:A:831:TYR:H	1:A:832:ASP:HA	1.70	0.56
3:P:21:DG:N2	4:T:8:DT:C2	2.73	0.56
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.88	0.56
2:B:132:HIS:CD2	2:C:213:VAL:HG11	2.40	0.56
1:A:299:MET:HG2	1:A:848:GLY:HA2	1.87	0.56
2:C:184:ASN:OD1	2:C:185:LEU:N	2.39	0.55
3:P:21:DG:N2	4:T:8:DT:N3	2.52	0.55
1:A:567:PRO:HD2	2:B:464:GLU:OE1	2.07	0.55
2:B:428:LEU:HD13	2:B:428:LEU:H	1.71	0.55
2:C:107:ARG:HB2	2:C:346:MET:HE2	1.87	0.55
1:A:353:VAL:HG13	1:A:355:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:N	1:A:743:ASP:OD1	2.40	0.55
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.89	0.54
1:A:94:MET:HG3	1:A:1170:LEU:HD11	1.88	0.54
1:A:752:LEU:HB2	1:A:753:PRO:HA	1.88	0.54
1:A:869:ARG:HB2	1:A:872:SER:HB2	1.90	0.54
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.24	0.54
1:A:372:GLU:HG3	1:A:375:GLU:H	1.72	0.54
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.90	0.54
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.43	0.54
1:A:761:ASN:OD1	1:A:761:ASN:N	2.42	0.53
2:B:185:LEU:H	2:B:185:LEU:HD23	1.74	0.53
1:A:921:LEU:HD22	1:A:1174:PRO:HG2	1.91	0.53
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.24	0.53
2:B:219:PHE:HA	2:B:229:LYS:N	2.24	0.53
1:A:296:SER:HB2	1:A:847:ALA:HB3	1.91	0.53
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.90	0.53
2:B:365:LYS:H	2:B:365:LYS:HD2	1.72	0.53
2:B:77:HIS:CE1	2:B:431:LYS:HG3	2.41	0.52
1:A:472:GLN:OE1	2:B:369:ARG:HD3	2.09	0.52
1:A:484:TRP:CZ3	2:B:364:LYS:NZ	2.76	0.52
1:A:606:THR:HB	1:A:612:LEU:HD13	1.90	0.52
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.74	0.52
1:A:948:ARG:CZ	6:A:4003:1RY:H13	2.07	0.52
1:A:107:LEU:O	1:A:112:LEU:N	2.42	0.52
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.92	0.52
2:B:404:ASN:HA	2:B:407:LEU:HG	1.91	0.52
2:C:219:PHE:HD1	2:C:229:LYS:HG2	1.74	0.52
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.92	0.52
2:C:444:THR:OG1	2:C:445:GLU:N	2.43	0.52
1:A:468:ASN:HB3	2:B:459:ASP:O	2.10	0.52
1:A:803:ASN:HA	4:T:10:DG:H4'	1.90	0.52
2:B:129:ASP:HB2	2:C:104:VAL:HG22	1.92	0.52
1:A:887:VAL:HG22	1:A:1185:ILE:HG23	1.91	0.52
3:P:4:DA:C6	4:T:26:DT:N3	2.72	0.52
2:B:213:VAL:HG11	2:C:132:HIS:CE1	2.46	0.51
1:A:597:ARG:NH1	4:T:13:DC:H4'	2.26	0.51
1:A:851:THR:O	1:A:851:THR:OG1	2.29	0.51
2:B:215:PHE:HE1	2:C:132:HIS:HB2	1.75	0.51
1:A:484:TRP:HZ3	2:B:364:LYS:HZ1	1.57	0.51
1:A:93:GLU:HA	1:A:94:MET:HB2	1.92	0.51
1:A:1115:ALA:HB3	1:A:1156:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ASN:O	2:C:77:HIS:NE2	2.44	0.51
1:A:457:ARG:NH1	2:B:265:LYS:HA	2.25	0.50
1:A:1098:ASN:CG	4:T:5:DG:H2''	2.36	0.50
2:B:457:SER:OG	2:B:460:THR:O	2.28	0.50
1:A:750:PHE:HD1	1:A:751:LYS:HG2	1.75	0.50
1:A:1183:VAL:HB	1:A:1214:GLN:HB3	1.93	0.50
3:P:14:DC:H2'	3:P:15:DA:C8	2.46	0.50
1:A:1096:ARG:HA	1:A:1099:TRP:HB3	1.93	0.50
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.46	0.50
1:A:384:ASP:OD1	1:A:384:ASP:N	2.36	0.50
2:B:241:TRP:HB3	2:B:336:LEU:HB3	1.93	0.50
1:A:1074:VAL:HB	1:A:1167:LYS:HB3	1.94	0.50
2:C:205:PRO:HB3	2:C:243:THR:HA	1.94	0.49
1:A:566:LEU:HD13	1:A:566:LEU:H	1.77	0.49
2:B:209:ALA:HB2	2:B:239:LEU:HD13	1.95	0.49
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.77	0.49
1:A:136:ASP:HA	1:A:1163:MET:HE1	1.94	0.48
1:A:866:ARG:HE	1:A:869:ARG:HD2	1.78	0.48
1:A:856:GLU:H	1:A:860:LEU:HD12	1.78	0.48
1:A:178:TYR:O	1:A:219:ALA:HB1	2.14	0.48
1:A:818:ARG:H	1:A:818:ARG:HE	1.61	0.48
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.95	0.48
1:A:1154:GLN:HG3	1:A:1218:LEU:HD21	1.95	0.48
2:B:215:PHE:CE1	2:C:132:HIS:HB2	2.49	0.48
3:P:23:DA:H2'	3:P:24:DOC:H6	1.96	0.48
2:C:67:GLU:HG3	2:C:88:ARG:HH22	1.76	0.48
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	1.94	0.48
2:B:104:VAL:HG23	2:B:107:ARG:HH21	1.79	0.47
2:B:372:LEU:HD13	2:B:436:SER:HB2	1.96	0.47
3:P:20:DC:O2	4:T:10:DG:C2	2.61	0.47
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.95	0.47
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.61	0.47
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.95	0.47
2:B:82:SER:OG	2:C:195:ASN:OD1	2.20	0.47
2:C:262:TRP:HA	2:C:265:LYS:HE2	1.97	0.47
1:A:135:LEU:HD23	1:A:135:LEU:H	1.78	0.47
1:A:175:TRP:CD2	1:A:223:TRP:HB2	2.50	0.47
1:A:579:ARG:HH12	3:P:11:DG:H5''	1.80	0.47
1:A:782:GLY:HA2	1:A:784:GLY:HA2	1.97	0.47
1:A:817:PRO:HB2	1:A:818:ARG:HH21	1.79	0.47
6:A:4003:1RY:OAP	6:A:4003:1RY:CAK	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:HD12	2:B:394:GLU:HG2	1.97	0.47
2:C:241:TRP:HD1	2:C:336:LEU:HD22	1.79	0.47
2:C:389:ARG:HD3	2:C:395:LEU:HD11	1.97	0.47
1:A:642:SER:HA	1:A:643:ALA:HA	1.59	0.47
3:P:8:DG:H1	4:T:21:DC:H42	1.63	0.47
1:A:1060:LYS:HE2	1:A:1064:ILE:HD11	1.96	0.47
1:A:484:TRP:HZ3	2:B:364:LYS:NZ	2.10	0.46
1:A:617:ARG:HB2	1:A:763:GLY:HA3	1.97	0.46
1:A:977:GLU:HB3	1:A:981:LYS:NZ	2.30	0.46
2:C:252:LEU:HD22	2:C:305:ASN:HB2	1.98	0.46
1:A:586:THR:OG1	1:A:590:SER:OG	2.27	0.46
1:A:869:ARG:NH1	3:P:22:DT:OP1	2.48	0.46
2:B:75:ARG:NH1	2:B:84:GLN:OE1	2.49	0.46
2:B:441:VAL:HG23	2:B:453:ILE:HG13	1.97	0.46
1:A:91:GLY:HA2	1:A:92:GLY:HA3	1.60	0.46
1:A:593:SER:O	1:A:599:THR:OG1	2.21	0.46
1:A:953:ARG:HG3	1:A:957:ALA:HB2	1.97	0.46
1:A:275:ARG:NH2	1:A:433:SER:O	2.42	0.46
1:A:475:SER:HA	1:A:476:GLY:HA2	1.50	0.46
2:B:323:HIS:HB3	2:B:330:ASN:HB2	1.97	0.46
2:B:213:VAL:HA	2:B:235:THR:HA	1.97	0.46
1:A:268:GLY:HA2	1:A:403:THR:HG21	1.97	0.46
1:A:611:PRO:HG3	1:A:652:ILE:HD13	1.98	0.46
2:C:134:LYS:CG	2:C:135:PRO:CD	2.92	0.46
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.97	0.46
1:A:435:LEU:HG	1:A:842:PRO:HG3	1.98	0.45
1:A:804:ALA:O	1:A:808:ILE:HG12	2.16	0.45
1:A:272:SER:HB3	1:A:843:GLN:HA	1.98	0.45
1:A:556:THR:HA	1:A:559:LEU:HD13	1.98	0.45
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.51	0.45
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.52	0.45
1:A:505:LYS:HD3	1:A:505:LYS:HA	1.81	0.45
4:T:4:DG:H2'	4:T:5:DG:H8	1.82	0.45
1:A:206:GLY:HA3	1:A:207:THR:HA	1.79	0.45
1:A:267:VAL:HG12	1:A:292:LEU:HB3	1.98	0.45
1:A:942:SER:HA	1:A:943:ARG:HA	1.59	0.45
1:A:1200:PRO:O	1:A:1202:ASN:N	2.46	0.45
1:A:616:GLU:HB2	1:A:617:ARG:HD3	1.99	0.45
1:A:887:VAL:HG13	1:A:1185:ILE:HG12	1.99	0.45
2:B:79:LEU:HG	2:B:102:LEU:HB2	1.98	0.45
2:C:201:ASN:O	2:C:201:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:THR:HG21	1:A:1103:SER:HB2	1.99	0.45
1:A:849:THR:O	4:T:7:DA:O5'	2.35	0.44
1:A:864:ASN:HB3	1:A:1191:LYS:HD3	1.98	0.44
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.98	0.44
2:C:303:LEU:HD22	2:C:338:VAL:HG22	1.99	0.44
1:A:799:SER:HA	1:A:802:ARG:HH12	1.82	0.44
1:A:298:HIS:HB2	1:A:410:GLN:HE22	1.83	0.44
2:C:67:GLU:N	2:C:88:ARG:HH21	2.14	0.44
2:C:444:THR:OG1	2:C:445:GLU:OE2	2.36	0.44
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.71	0.44
1:A:948:ARG:NH2	3:P:24:DOC:HN41	2.02	0.44
2:B:252:LEU:HD13	2:B:336:LEU:HD11	1.99	0.44
3:P:3:DA:C6	4:T:26:DT:O4	2.70	0.44
2:B:133:HIS:ND1	2:C:233:GLU:OE2	2.48	0.44
1:A:888:GLY:HA3	1:A:1138:ARG:HD2	1.99	0.44
1:A:894:GLN:HG3	1:A:895:GLU:N	2.32	0.44
1:A:243:ASP:OD1	1:A:243:ASP:N	2.44	0.44
1:A:800:PHE:HB2	1:A:869:ARG:HH21	1.82	0.44
2:B:421:MET:HA	2:B:422:GLN:HB3	1.99	0.44
1:A:110:HIS:HB3	1:A:111:GLY:HA2	1.99	0.43
1:A:569:HIS:HA	2:B:462:MET:HG2	2.00	0.43
1:A:1183:VAL:N	1:A:1214:GLN:O	2.50	0.43
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.60	0.43
2:C:414:TRP:HA	2:C:415:PRO:HD3	1.85	0.43
1:A:622:TYR:HB2	1:A:770:PHE:HE2	1.83	0.43
1:A:765:PRO:HA	1:A:766:PHE:HA	1.58	0.43
1:A:828:HIS:O	1:A:830:ASP:N	2.43	0.43
1:A:1134:HIS:HD2	3:P:24:DOC:H1'	1.82	0.43
2:C:244:PRO:HA	2:C:245:PRO:HD3	1.82	0.43
1:A:483:PRO:HG2	1:A:484:TRP:CE3	2.52	0.43
1:A:849:THR:HA	1:A:850:ILE:HA	1.80	0.43
2:C:389:ARG:HB3	2:C:395:LEU:HD11	2.00	0.43
1:A:231:GLU:HA	2:C:449:GLU:O	2.19	0.43
1:A:831:TYR:N	1:A:832:ASP:HA	2.29	0.43
1:A:1032:THR:O	1:A:1034:ARG:NH2	2.51	0.43
6:A:4003:1RY:H8	3:P:24:DOC:H2'	2.00	0.43
2:C:440:THR:OG1	2:C:456:ARG:HB3	2.19	0.43
1:A:149:PRO:HB3	1:A:262:GLN:N	2.34	0.43
1:A:272:SER:OG	1:A:844:VAL:O	2.29	0.43
1:A:299:MET:SD	1:A:849:THR:HG23	2.59	0.43
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:MET:HG3	1:A:849:THR:HG23	2.01	0.42
2:C:315:TYR:N	2:C:316:PRO:HD3	2.34	0.42
2:C:319:VAL:HA	2:C:322:LEU:HD13	2.01	0.42
4:T:11:DC:H6	4:T:11:DC:H2'	1.64	0.42
1:A:1026:ARG:HD2	1:A:1026:ARG:O	2.19	0.42
1:A:976:GLN:O	1:A:980:GLU:HG2	2.19	0.42
2:C:293:PHE:H	2:C:294:PRO:HA	1.83	0.42
3:P:21:DG:H1	4:T:8:DT:H3	1.67	0.42
4:T:23:DT:H2''	4:T:24:DT:C6	2.54	0.42
1:A:463:LEU:HB3	1:A:592:LEU:HD12	2.00	0.42
1:A:618:HIS:CD2	1:A:619:GLY:H	2.37	0.42
1:A:850:ILE:HA	1:A:850:ILE:HD12	1.93	0.42
1:A:973:LEU:HD21	1:A:976:GLN:HG3	2.02	0.42
1:A:1090:GLU:O	1:A:1091:GLU:HG2	2.19	0.42
1:A:1108:TYR:HH	1:A:1161:ARG:HH11	1.63	0.42
2:B:407:LEU:HD13	2:C:120:VAL:HG12	2.01	0.42
2:C:239:LEU:HB3	2:C:338:VAL:HB	2.00	0.42
2:C:264:ARG:HG3	2:C:270:PRO:HB3	2.00	0.42
2:C:293:PHE:HB3	2:C:295:TRP:H	1.84	0.42
1:A:262:GLN:HA	1:A:263:GLU:HA	1.53	0.42
3:P:8:DG:H1	4:T:21:DC:N4	2.18	0.42
1:A:79:LEU:HD13	1:A:80:SER:H	1.85	0.42
1:A:612:LEU:HD12	1:A:612:LEU:HA	1.76	0.42
2:B:439:PHE:HB3	2:B:455:LEU:HD11	2.02	0.42
1:A:599:THR:N	1:A:600:PRO:HD2	2.35	0.42
1:A:891:VAL:HG13	1:A:1161:ARG:HH12	1.84	0.42
2:C:83:LYS:HE2	2:C:83:LYS:HB3	1.95	0.42
1:A:1124:ALA:O	1:A:1148:ARG:NH2	2.45	0.42
1:A:232:ARG:HH21	2:C:468:ILE:HG21	1.84	0.42
1:A:834:GLU:HG3	2:B:328:ARG:HH21	1.85	0.42
1:A:880:ALA:HA	1:A:881:PRO:HD3	1.94	0.42
6:A:4003:1RY:CAT	4:T:4:DG:H1	2.31	0.42
1:A:247:LEU:HD13	1:A:247:LEU:H	1.84	0.41
1:A:499:LYS:H	1:A:499:LYS:HG3	1.62	0.41
1:A:1047:ARG:H	1:A:1047:ARG:HG3	1.62	0.41
1:A:1054:GLU:HB3	1:A:1055:SER:H	1.46	0.41
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.60	0.41
1:A:176:THR:OG1	1:A:222:SER:OG	2.32	0.41
1:A:1075:LEU:HD23	1:A:1075:LEU:H	1.86	0.41
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.81	0.41
2:B:382:LYS:H	2:B:412:SER:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:LEU:HA	2:B:441:VAL:HG13	2.01	0.41
1:A:828:HIS:CG	1:A:829:PRO:HD2	2.55	0.41
2:B:259:ARG:HH22	2:B:262:TRP:CG	2.38	0.41
2:C:205:PRO:HB3	2:C:244:PRO:HD3	2.02	0.41
1:A:570:PRO:HB2	1:A:572:TRP:CD1	2.55	0.41
1:A:790:ARG:HA	1:A:790:ARG:HD2	1.90	0.41
2:B:363:ARG:C	2:B:364:LYS:HG3	2.46	0.41
2:B:365:LYS:HG2	2:B:367:LEU:H	1.86	0.41
2:B:393:LEU:HA	2:B:394:GLU:HA	1.66	0.41
2:C:418:LEU:N	2:C:419:GLU:HA	2.34	0.41
1:A:1193:VAL:HG21	1:A:1213:PRO:HG3	2.02	0.41
2:B:444:THR:OG1	2:B:445:GLU:N	2.54	0.41
2:C:375:HIS:O	2:C:379:ALA:N	2.49	0.41
1:A:133:ASP:N	1:A:133:ASP:OD2	2.53	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.96	0.41
1:A:209:PRO:HG3	1:A:277:HIS:CD2	2.56	0.41
2:B:133:HIS:HE1	2:C:233:GLU:HG3	1.86	0.41
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.86	0.41
1:A:162:LEU:HD22	1:A:163:PRO:HD2	2.01	0.41
1:A:480:LYS:HD3	1:A:646:VAL:HG11	2.03	0.41
1:A:773:LYS:HD2	1:A:773:LYS:HA	1.89	0.41
2:B:420:THR:HG23	2:B:421:MET:HG2	2.03	0.41
2:B:446:THR:O	2:B:450:ASN:ND2	2.53	0.41
1:A:850:ILE:HD12	1:A:851:THR:HA	2.03	0.41
1:A:1079:ILE:HG12	1:A:1099:TRP:CE3	2.56	0.41
1:A:1194:THR:HG22	1:A:1210:TYR:HE1	1.85	0.41
2:B:418:LEU:HD22	2:C:204:LEU:HD12	2.02	0.41
2:B:454:HIS:ND1	2:B:463:LYS:HE3	2.36	0.41
2:B:467:HIS:HB3	2:B:470:LYS:HB2	2.03	0.41
4:T:4:DG:H2'	4:T:5:DG:C8	2.56	0.41
1:A:1098:ASN:OD1	4:T:5:DG:H2''	2.21	0.41
2:C:67:GLU:HG3	2:C:88:ARG:HH21	1.82	0.41
3:P:4:DA:N3	4:T:26:DT:H1'	2.36	0.41
1:A:87:ILE:HD13	1:A:127:LEU:HD22	2.02	0.40
1:A:245:ILE:HG13	1:A:289:MET:HE3	2.02	0.40
1:A:1202:ASN:HA	1:A:1203:PRO:HD2	1.96	0.40
3:P:4:DA:C2	4:T:26:DT:O4'	2.74	0.40
1:A:1072:THR:O	1:A:1072:THR:OG1	2.36	0.40
2:C:215:PHE:CD2	2:C:233:GLU:HG2	2.56	0.40
1:A:165:LYS:HA	1:A:166:PRO:HD3	1.93	0.40
1:A:873:GLU:O	1:A:877:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:GLN:HG3	1:A:895:GLU:H	1.87	0.40
2:B:318:ASN:HB2	2:B:321:LYS:NZ	2.36	0.40
4:T:5:DG:H2'	4:T:6:DT:H6	1.86	0.40
1:A:426:GLY:O	1:A:430:MET:HB2	2.21	0.40
1:A:1133:ILE:O	1:A:1135:ASP:N	2.55	0.40
2:C:316:PRO:HA	2:C:317:GLY:HA2	1.59	0.40
2:C:455:LEU:HD23	2:C:455:LEU:HA	1.94	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:A:136:ASP:OD2	2:C:318:ASN:ND2[5_545]	2.19	0.01

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	969/1205 (80%)	837 (86%)	111 (12%)	21 (2%)	5	23
2	B	355/485 (73%)	326 (92%)	27 (8%)	2 (1%)	21	49
2	C	350/485 (72%)	324 (93%)	19 (5%)	7 (2%)	6	24
All	All	1674/2175 (77%)	1487 (89%)	157 (9%)	30 (2%)	6	26

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	LEU
1	A	1070	PRO
2	C	97	PRO
1	A	749	PHE
1	A	767	ALA

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Mol	Chain	Res	Type
1	A	1134	HIS
1	A	1177	VAL
2	C	423	SER
1	A	1073	PRO
1	A	1080	SER
1	A	1091	GLU
2	C	98	GLY
2	C	316	PRO
2	C	391	PRO
1	A	95	PRO
1	A	642	SER
1	A	743	ASP
1	A	927	ARG
1	A	1207	GLU
2	C	319	VAL
2	C	380	PRO
1	A	610	PHE
1	A	618	HIS
1	A	765	PRO
1	A	1074	VAL
1	A	560	PRO
2	B	317	GLY
2	B	451	GLY
1	A	1043	VAL
1	A	829	PRO

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	823/1017 (81%)	749 (91%)	74 (9%)	9	30
2	B	325/426 (76%)	301 (93%)	24 (7%)	13	37
2	C	317/426 (74%)	292 (92%)	25 (8%)	11	35
All	All	1465/1869 (78%)	1342 (92%)	123 (8%)	10	33

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	101	ARG
1	A	118	VAL
1	A	130	LEU
1	A	195	LEU
1	A	201	VAL
1	A	227	ARG
1	A	236	THR
1	A	245	ILE
1	A	247	LEU
1	A	292	LEU
1	A	304	LEU
1	A	311	LEU
1	A	316	LYS
1	A	376	LEU
1	A	384	ASP
1	A	411	LEU
1	A	424	LEU
1	A	473	LEU
1	A	488	LEU
1	A	496	LYS
1	A	499	LYS
1	A	558	LEU
1	A	565	HIS
1	A	566	LEU
1	A	613	HIS
1	A	617	ARG
1	A	639	THR
1	A	640	LEU
1	A	655	LEU
1	A	661	LEU
1	A	743	ASP
1	A	744	ILE
1	A	751	LYS
1	A	756	ASP
1	A	761	ASN
1	A	762	VAL
1	A	768	LYS
1	A	774	MET
1	A	779	LEU
1	A	813	VAL
1	A	816	LEU

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Mol	Chain	Res	Type
1	A	818	ARG
1	A	841	LEU
1	A	851	THR
1	A	921	LEU
1	A	941	ILE
1	A	964	ARG
1	A	973	LEU
1	A	977	GLU
1	A	992	LEU
1	A	1026	ARG
1	A	1027	LYS
1	A	1038	TRP
1	A	1043	VAL
1	A	1047	ARG
1	A	1057	MET
1	A	1060	LYS
1	A	1069	ILE
1	A	1074	VAL
1	A	1081	ARG
1	A	1099	TRP
1	A	1118	TRP
1	A	1120	PHE
1	A	1133	ILE
1	A	1137	VAL
1	A	1140	LEU
1	A	1141	VAL
1	A	1151	LEU
1	A	1191	LYS
1	A	1197	CYS
1	A	1198	LYS
1	A	1210	TYR
1	A	1218	LEU
2	B	69	LEU
2	B	186	LEU
2	B	197	LEU
2	B	213	VAL
2	B	218	VAL
2	B	231	ILE
2	B	240	VAL
2	B	263	TRP
2	B	332	VAL
2	B	338	VAL

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Mol	Chain	Res	Type
2	B	364	LYS
2	B	365	LYS
2	B	368	HIS
2	B	372	LEU
2	B	394	GLU
2	B	396	ARG
2	B	406	LEU
2	B	413	VAL
2	B	428	LEU
2	B	441	VAL
2	B	453	ILE
2	B	460	THR
2	B	461	THR
2	B	467	HIS
2	C	83	LYS
2	C	86	LEU
2	C	115	TRP
2	C	122	ARG
2	C	186	LEU
2	C	197	LEU
2	C	201	ASN
2	C	204	LEU
2	C	218	VAL
2	C	251	TRP
2	C	256	LEU
2	C	258	HIS
2	C	262	TRP
2	C	281	GLU
2	C	282	GLU
2	C	295	TRP
2	C	300	ILE
2	C	319	VAL
2	C	331	VAL
2	C	371	VAL
2	C	385	LEU
2	C	402	LEU
2	C	413	VAL
2	C	419	GLU
2	C	453	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	106	HIS
1	A	264	GLN
1	A	388	ASN
1	A	803	ASN
1	A	970	ASN
1	A	1134	HIS
1	A	1214	GLN
2	B	195	ASN
2	B	305	ASN
2	B	368	HIS
2	C	210	GLN
2	C	330	ASN
2	C	409	ASN
2	C	427	GLN

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	4,3	16,19,20	0.45	0	20,26,29	0.45	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
3	DOC	P	24	4,3	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	24	DOC	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
6	1RY	A	4003	5	28,29,29	3.58	9 (32%)	40,45,45	1.68	6 (15%)

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
6	1RY	A	4003	5	-	5/22/31/31	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4003	1RY	OAP-CAX	9.64	1.63	1.42
6	A	4003	1RY	CAX-NAY	-8.07	1.27	1.48
6	A	4003	1RY	CAW-SAS	-8.00	1.56	1.81
6	A	4003	1RY	CAM-SAS	-6.05	1.64	1.81
6	A	4003	1RY	CAK-CAU	5.31	1.40	1.33
6	A	4003	1RY	CAV-NAY	-4.06	1.31	1.40
6	A	4003	1RY	CAT-NAA	3.84	1.43	1.34
6	A	4003	1RY	CAL-CAW	2.99	1.60	1.51
6	A	4003	1RY	CAK-NAY	-2.16	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4003	1RY	CAM-SAS-CAW	6.86	105.46	88.41
6	A	4003	1RY	FAJ-CAU-CAT	3.22	120.14	118.09
6	A	4003	1RY	CAW-OAP-CAX	-3.15	106.18	112.68
6	A	4003	1RY	OAB-CAV-NAN	-2.53	118.34	122.33
6	A	4003	1RY	CAU-CAT-NAN	-2.37	118.05	119.59
6	A	4003	1RY	NAY-CAV-NAN	2.11	122.46	118.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4003	1RY	OAO-CAL-CAW-OAP
6	A	4003	1RY	OAO-CAL-CAW-SAS
6	A	4003	1RY	PBA-OAR-PBB-OAE
6	A	4003	1RY	PBA-OAR-PBB-OAI
6	A	4003	1RY	PBB-OAR-PBA-OAD

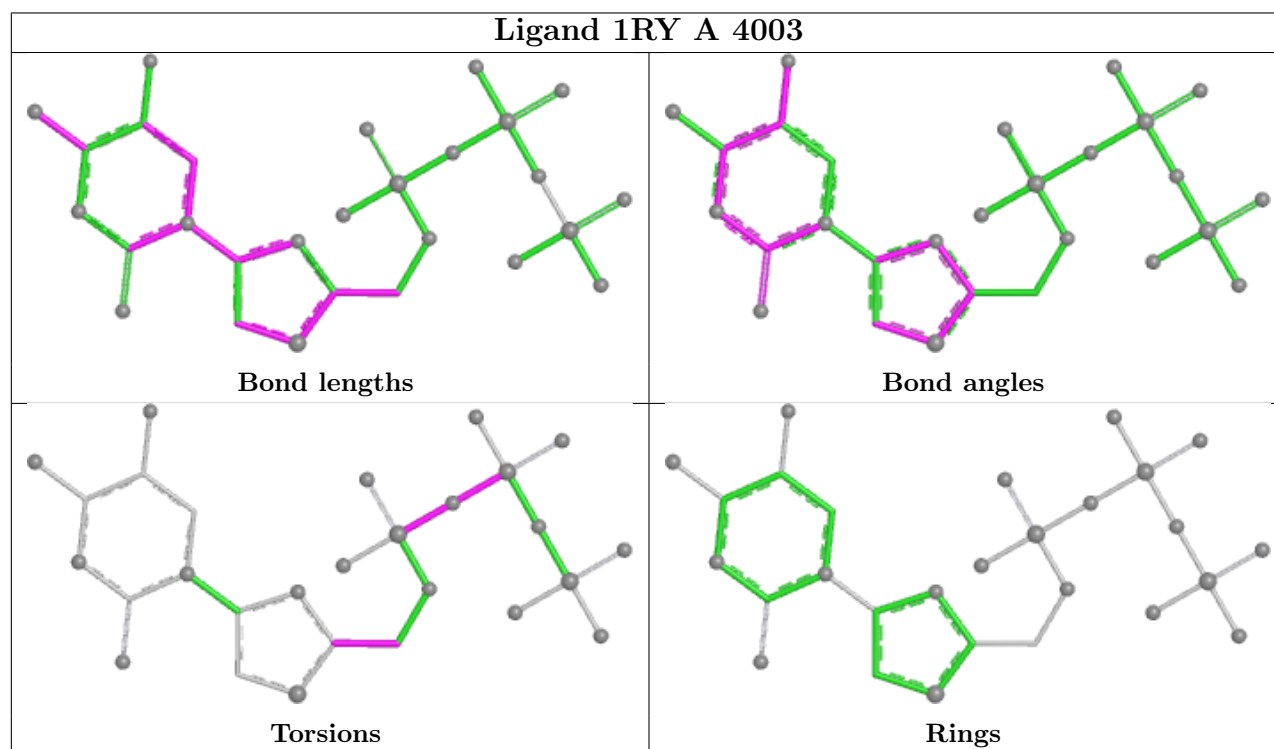
There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4003	1RY	15	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 [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	983/1205 (81%)	0.46	67 (6%) 23 19	38, 67, 106, 401	0
2	B	363/485 (74%)	0.27	9 (2%) 58 43	42, 59, 96, 263	0
2	C	358/485 (73%)	0.26	13 (3%) 46 33	41, 65, 97, 154	0
3	P	21/22 (95%)	0.29	1 (4%) 35 26	101, 105, 106, 111	0
4	T	25/25 (100%)	0.13	1 (4%) 42 30	65, 82, 104, 115	0
All	All	1750/2222 (78%)	0.37	91 (5%) 33 24	38, 66, 105, 401	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	912	GLY	5.8
1	A	850	ILE	5.1
1	A	764	SER	4.8
1	A	619	GLY	4.7
1	A	893	SER	4.7
1	A	746	GLY	4.5
2	C	228	VAL	4.1
1	A	214	ALA	4.1
1	A	604	ALA	4.1
1	A	738	PRO	4.1
1	A	747	CYS	3.9
1	A	1131	ILE	3.9
2	C	414	TRP	3.8
2	C	121	PHE	3.7
1	A	230	GLU	3.7
2	C	435	MET	3.7
2	B	414	TRP	3.5
1	A	894	GLN	3.5
1	A	1070	PRO	3.3
2	B	468	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	611	PRO	3.1
1	A	509	THR	3.1
1	A	599	THR	3.0
1	A	948	ARG	3.0
1	A	865	ALA	3.0
1	A	510	ALA	3.0
1	A	573	TYR	2.9
1	A	610	PHE	2.9
1	A	784	GLY	2.9
1	A	94	MET	2.9
1	A	1099	TRP	2.9
1	A	622	TYR	2.9
2	B	81	GLY	2.9
1	A	1072	THR	2.8
1	A	623	LEU	2.8
1	A	1130	CYS	2.7
1	A	593	SER	2.7
2	C	415	PRO	2.7
1	A	431	GLY	2.7
1	A	909	GLY	2.6
1	A	441	TRP	2.6
2	C	373	LYS	2.6
2	C	219	PHE	2.6
1	A	871	GLY	2.5
1	A	1199	THR	2.5
1	A	229	VAL	2.5
1	A	910	MET	2.5
1	A	389	PHE	2.5
1	A	575	LYS	2.5
1	A	969	PHE	2.5
2	C	124	GLN	2.5
1	A	105	GLU	2.5
1	A	846	THR	2.4
1	A	753	PRO	2.4
2	C	80	SER	2.4
1	A	530	LEU	2.4
2	C	289	LEU	2.4
1	A	744	ILE	2.4
1	A	291	PHE	2.4
1	A	213	VAL	2.4
1	A	1079	ILE	2.3
1	A	228	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	366	ASN	2.3
2	C	236	GLU	2.3
1	A	316	LYS	2.3
4	T	25	DT	2.3
2	B	419	GLU	2.2
2	B	448	LEU	2.2
2	B	403	PHE	2.2
1	A	239	LEU	2.2
1	A	1075	LEU	2.2
1	A	1096	ARG	2.1
1	A	904	ASP	2.1
1	A	849	THR	2.1
2	C	351	TYR	2.1
3	P	4	DA	2.1
1	A	108	GLN	2.1
2	B	422	GLN	2.1
1	A	286	GLY	2.1
1	A	240	SER	2.1
1	A	1133	ILE	2.1
1	A	786	ALA	2.1
1	A	139	PHE	2.1
1	A	352	SER	2.1
1	A	227	ARG	2.1
1	A	760	CYS	2.1
1	A	1179	PHE	2.1
1	A	1208	ARG	2.0
2	B	208	LEU	2.0
2	C	126	PHE	2.0
1	A	1078	CYS	2.0

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

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
3	DOC	P	24	18/19	0.62	0.15	99,102,106,106	0

6.3 Carbohydrates [i](#)

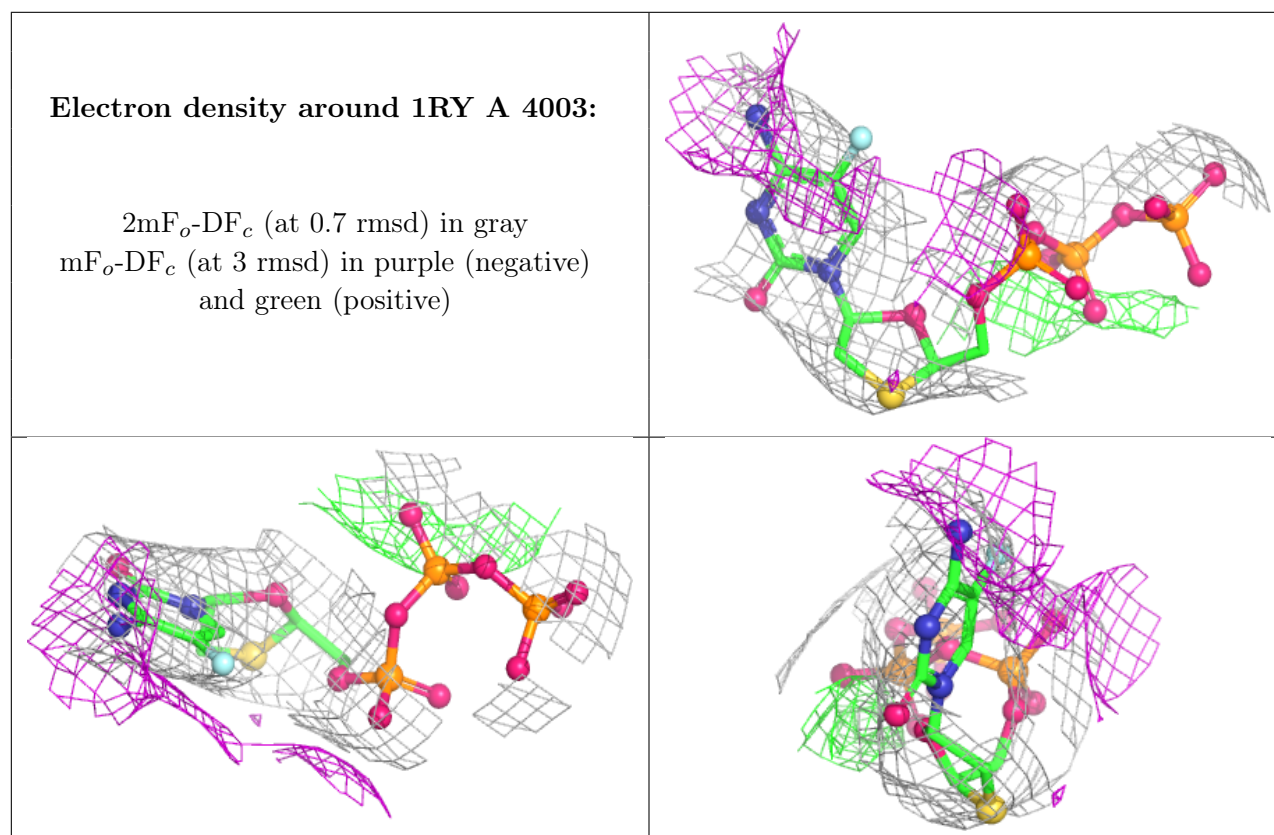
There are no oligosaccharides in this entry.

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
5	MG	A	4001	1/1	0.85	0.12	88,88,88,88	0
6	1RY	A	4003	28/28	0.86	0.11	63,66,78,79	0
5	MG	A	4002	1/1	0.98	0.06	87,87,87,87	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.