



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 9D4S / pdb_00009d4s
Title : Structure of G2L4 RT in complex with 15 nucleotide snapback substrate
Authors : Guo, M.; Zhang, Y.
Deposited on : 2024-08-12
Resolution : 2.77 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

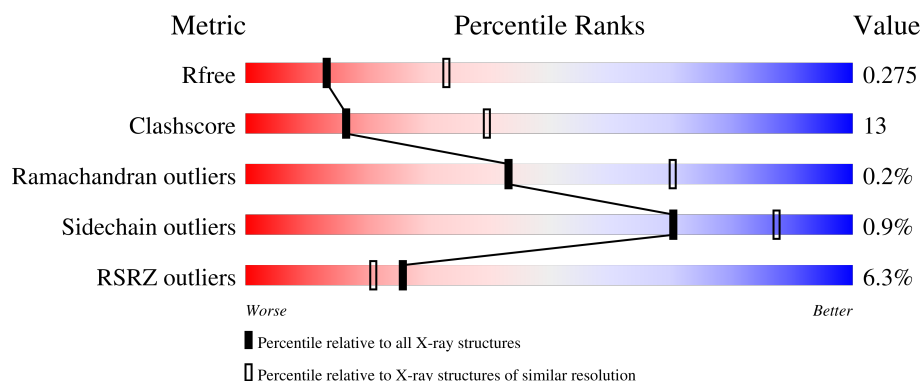
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	408	<div> <div>11%</div> <div>73% 26% .</div> </div>
1	B	408	<div> <div>11%</div> <div>66% 32% .</div> </div>
2	C	18	<div> <div>11%</div> <div>33% 33% 6% 28%</div> </div>
2	P	18	<div> <div></div> <div>39% 28% 6% 28%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7014 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 Group II intron-like 4 reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3210	2032	581	587	10			
1	B	407	Total	C	N	O	S	0	0	0
			3203	2027	580	586	10			

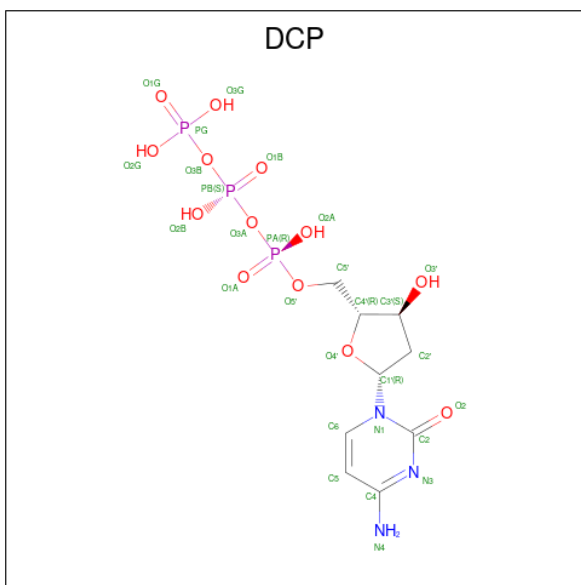
- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			268	127	53	75	13			
2	P	13	Total	C	N	O	P	0	0	0
			268	127	53	75	13			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

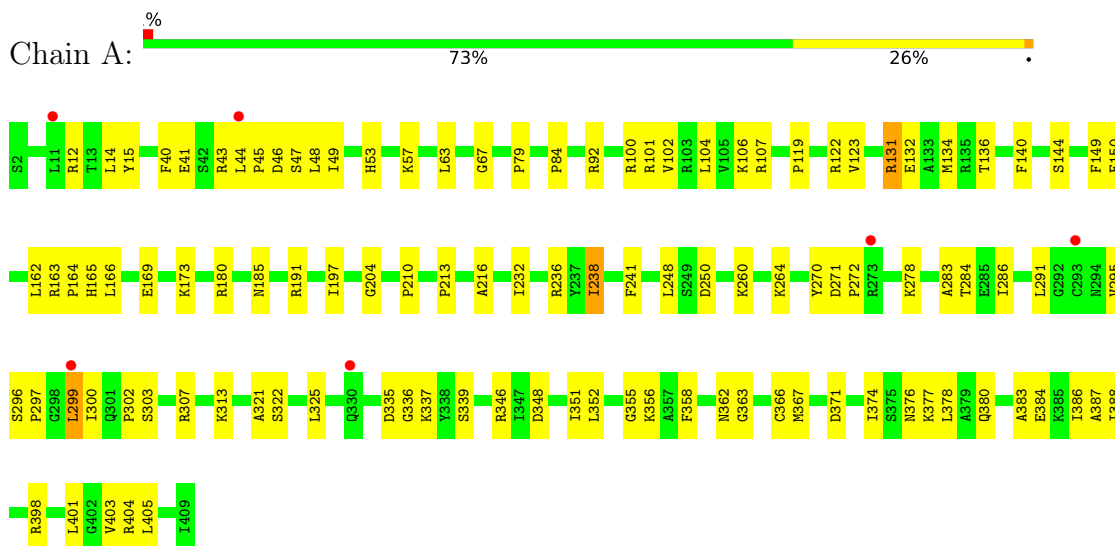
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	C	2	Total O 2 2	0	0
5	B	2	Total O 2 2	0	0

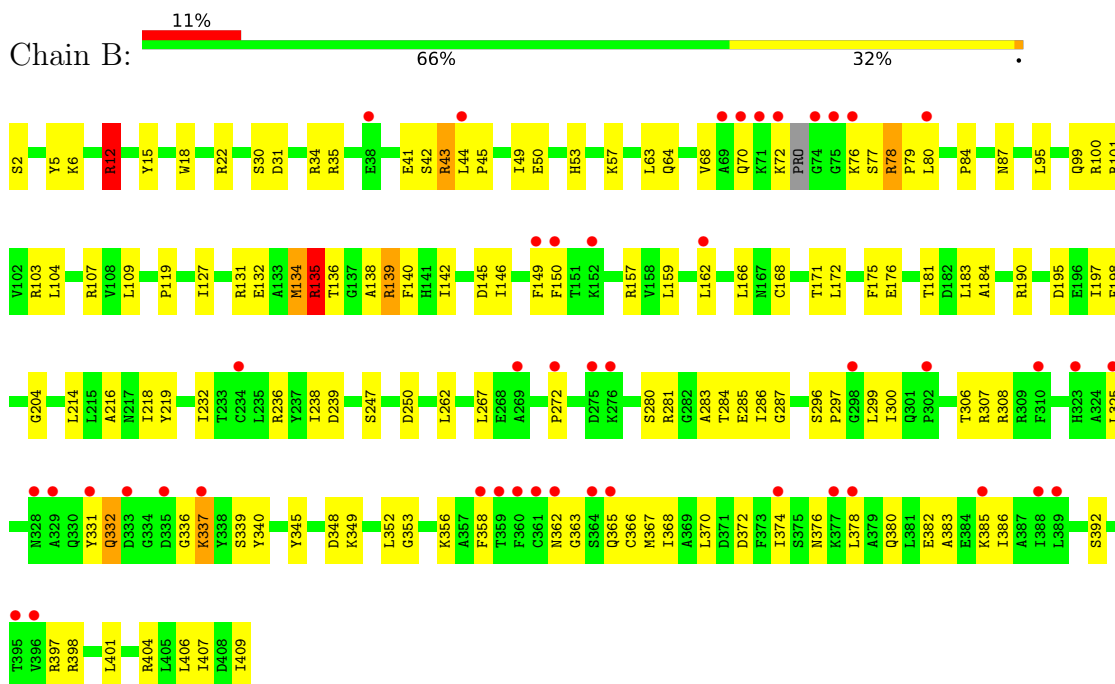
3 Residue-property plots [i](#)

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.

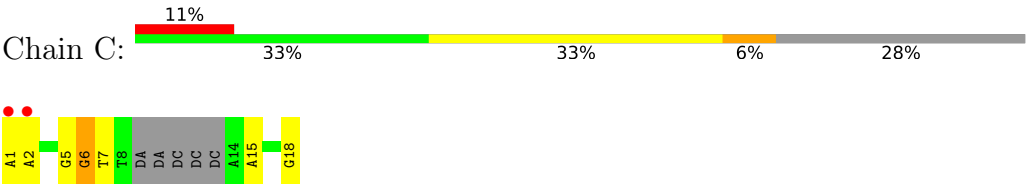
- Molecule 1: Group II intron-like 4 reverse transcriptase



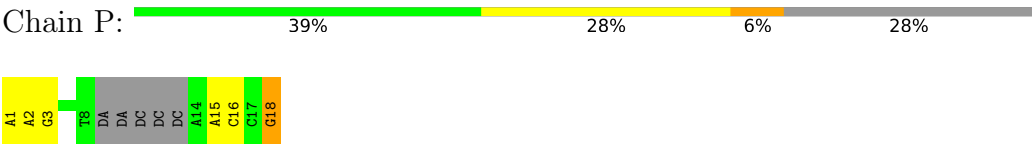
- Molecule 1: Group II intron-like 4 reverse transcriptase



● Molecule 2: DNA



● Molecule 2: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.40Å 99.19Å 157.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.77 47.30 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.30-2.77) 97.6 (47.30-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.235 , 0.277 0.236 , 0.275	Depositor DCC
R_{free} test set	1963 reflections (7.31%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7014	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: MN, DDG, DCP

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	0.71	1/3262 (0.0%)	1.09	2/4397 (0.0%)
1	B	0.67	0/3253	1.04	10/4382 (0.2%)
2	C	0.59	0/276	0.96	1/421 (0.2%)
2	P	0.42	0/276	0.69	0/421
All	All	0.68	1/7067 (0.0%)	1.05	13/9621 (0.1%)

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
1	A	0	9
1	B	0	11
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	LEU	CB-CG	-5.46	1.42	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ARG	CG-CD-NE	7.29	128.04	112.00
1	B	135	ARG	CA-CB-CG	6.20	126.51	114.10
1	B	337	LYS	N-CA-C	-6.11	104.70	111.36
1	B	336	GLY	N-CA-C	-5.99	107.43	115.21
2	C	6	DG	C4'-C3'-O3'	5.52	118.28	110.00
1	B	135	ARG	CD-NE-CZ	-5.49	116.71	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ARG	CB-CG-CD	-5.49	98.67	111.30
1	A	204	GLY	CA-C-O	-5.31	118.56	122.23
1	A	43	ARG	CB-CA-C	-5.30	102.71	111.36
1	B	356	LYS	CA-CB-CG	5.28	124.65	114.10
1	B	12	ARG	CB-CG-CD	5.26	123.40	111.30
1	B	139	ARG	CD-NE-CZ	5.10	131.54	124.40
1	B	134	MET	CG-SD-CE	-5.01	89.89	100.90

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	101	ARG	Sidechain
1	A	107	ARG	Sidechain
1	A	122	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	180	ARG	Sidechain
1	A	191	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	346	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	107	ARG	Sidechain
1	B	12	ARG	Sidechain
1	B	135	ARG	Sidechain
1	B	139	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	308	ARG	Sidechain
1	B	34	ARG	Sidechain
1	B	43	ARG	Sidechain
1	B	78	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3210	0	3296	82	0
1	B	3203	0	3288	103	0
2	C	268	0	147	6	0
2	P	268	0	147	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	12	2	0
4	B	28	0	12	3	0
5	A	3	0	0	1	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
All	All	7014	0	6902	179	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 13.

All (179) 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)
4:B:502:DCP:H5	2:P:3:DG:H1	1.26	0.99
1:A:12:ARG:HA	1:B:45:PRO:HG2	1.57	0.86
1:A:299:LEU:HD12	1:A:362:ASN:OD1	1.75	0.84
1:A:53:HIS:NE2	1:A:57:LYS:NZ	2.27	0.83
1:A:366:CYS:SG	5:A:603:HOH:O	2.37	0.82
1:B:70:GLN:HB3	1:B:78:ARG:HB3	1.61	0.82
1:B:132:GLU:HA	1:B:135:ARG:HH21	1.45	0.81
2:P:1:DA:N6	2:P:2:DA:N7	2.32	0.78
1:A:271:ASP:OD1	1:A:272:PRO:HD2	1.83	0.77
1:B:63:LEU:HB2	1:B:84:PRO:HG2	1.70	0.73
1:A:53:HIS:CE1	1:A:57:LYS:HE3	2.24	0.72
1:A:321:ALA:O	1:A:325:LEU:HG	1.89	0.72
4:B:502:DCP:H5	2:P:3:DG:N1	2.05	0.71
1:A:384:GLU:O	1:A:388:ILE:HG13	1.91	0.70
1:A:15:TYR:CZ	1:B:44:LEU:HD23	2.28	0.68
1:B:127:ILE:CG2	1:B:300:ILE:HD11	2.24	0.68
1:A:299:LEU:HD11	1:A:363:GLY:HA3	1.76	0.67
1:A:378:LEU:HD21	1:B:401:LEU:HD12	1.76	0.67
1:B:45:PRO:O	1:B:49:ILE:HG13	1.96	0.65
1:A:45:PRO:HG2	1:B:12:ARG:HA	1.78	0.65
4:B:502:DCP:C5	2:P:3:DG:H1	2.07	0.65
1:A:53:HIS:CE1	1:A:57:LYS:CE	2.81	0.64
1:A:352:LEU:HD11	1:A:356:LYS:HE3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:HD13	1:B:385:LYS:HB3	1.78	0.64
1:B:131:ARG:HG3	1:B:135:ARG:HH22	1.62	0.64
1:B:232:ILE:HD11	1:B:250:ASP:HB3	1.80	0.63
1:B:127:ILE:HG21	1:B:300:ILE:HD11	1.81	0.63
1:A:53:HIS:NE2	1:A:57:LYS:CE	2.62	0.62
1:A:271:ASP:OD1	1:A:272:PRO:CD	2.48	0.62
1:B:181:THR:CG2	1:B:183:LEU:HD21	2.30	0.62
1:B:283:ALA:O	1:B:286:ILE:HG22	2.00	0.61
1:A:79:PRO:HB3	1:A:197:ILE:HG22	1.83	0.61
1:B:41:GLU:OE1	1:B:44:LEU:HD22	1.99	0.61
1:A:322:SER:HA	1:A:325:LEU:HD12	1.81	0.60
1:B:2:SER:O	1:B:6:LYS:HG3	1.99	0.60
1:B:79:PRO:HG3	1:B:197:ILE:HD12	1.84	0.60
1:B:157:ARG:HD3	1:B:219:TYR:CE1	2.37	0.60
1:A:376:ASN:O	1:A:380:GLN:HG3	2.03	0.59
1:A:144:SER:HB3	1:A:241:PHE:CZ	2.40	0.57
1:A:131:ARG:HA	1:A:134:MET:HE2	1.85	0.57
1:A:299:LEU:HD11	1:A:363:GLY:CA	2.34	0.57
1:B:84:PRO:HD2	1:B:87:ASN:ND2	2.20	0.56
1:A:299:LEU:O	1:A:300:ILE:HD13	2.05	0.56
1:B:12:ARG:HH22	1:B:100:ARG:HH12	1.52	0.56
1:B:262:LEU:HB3	1:B:267:LEU:HB2	1.87	0.56
2:P:1:DA:H61	2:P:2:DA:H62	1.52	0.56
1:A:44:LEU:HD23	1:B:15:TYR:CZ	2.42	0.55
1:A:295:VAL:HA	1:A:300:ILE:HD12	1.88	0.55
1:A:53:HIS:NE2	1:A:57:LYS:HD2	2.22	0.54
2:C:6:DG:H4'	2:C:7:DT:OP1	2.06	0.54
1:A:119:PRO:HA	2:C:7:DT:OP1	2.08	0.54
1:B:132:GLU:CA	1:B:135:ARG:HH21	2.18	0.53
1:B:134:MET:CE	1:B:297:PRO:HG3	2.37	0.53
1:B:307:ARG:NH2	1:B:366:CYS:SG	2.81	0.53
1:B:131:ARG:HG3	1:B:135:ARG:NH2	2.23	0.53
1:B:41:GLU:O	1:B:44:LEU:HB2	2.09	0.53
1:A:14:LEU:HB3	1:A:48:LEU:HD22	1.91	0.53
1:A:404:ARG:NH2	1:B:348:ASP:OD2	2.33	0.53
1:A:44:LEU:O	1:A:45:PRO:C	2.51	0.53
1:B:68:VAL:HG23	1:B:80:LEU:HB2	1.91	0.53
1:B:15:TYR:HE1	1:B:44:LEU:HD21	1.74	0.53
1:A:63:LEU:HB2	1:A:84:PRO:HG2	1.91	0.52
1:B:272:PRO:HB2	1:B:281:ARG:HB2	1.91	0.52
1:B:331:TYR:CD1	1:B:332:GLN:OE1	2.63	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH2	1:A:405:LEU:HA	2.24	0.52
1:B:134:MET:HE2	1:B:297:PRO:HG3	1.91	0.52
1:B:166:LEU:HD23	1:B:172:LEU:HD12	1.92	0.51
1:A:386:ILE:HG13	1:A:387:ALA:N	2.25	0.51
1:B:181:THR:CG2	1:B:183:LEU:CD2	2.89	0.51
1:A:313:LYS:NZ	2:C:15:DA:OP1	2.44	0.50
1:A:371:ASP:OD2	1:B:407:ILE:HG23	2.10	0.50
1:B:149:PHE:CE2	1:B:216:ALA:HB1	2.47	0.50
1:A:40:PHE:CE1	1:A:47:SER:HB3	2.46	0.49
1:A:131:ARG:HD2	1:A:300:ILE:HD11	1.92	0.49
1:B:134:MET:HE1	1:B:297:PRO:CD	2.42	0.49
2:P:15:DA:H2'	2:P:16:DC:C6	2.46	0.49
1:B:331:TYR:CE1	1:B:332:GLN:OE1	2.65	0.49
1:B:376:ASN:O	1:B:380:GLN:HG3	2.11	0.49
1:A:348:ASP:OD2	1:B:404:ARG:NH2	2.36	0.49
1:A:102:VAL:O	1:A:106:LYS:HG3	2.11	0.49
1:A:140:PHE:CD1	1:A:248:LEU:HG	2.47	0.49
1:B:142:ILE:CG1	1:B:281:ARG:HG3	2.42	0.49
1:B:146:ILE:HD13	1:B:267:LEU:HD13	1.93	0.49
1:A:403:VAL:HG21	1:B:378:LEU:HD13	1.95	0.48
1:A:163:ARG:N	1:A:164:PRO:HD2	2.28	0.48
1:B:368:ILE:O	1:B:372:ASP:N	2.45	0.48
1:B:370:LEU:O	1:B:374:ILE:HG13	2.14	0.47
1:B:159:LEU:HD11	1:B:176:GLU:HG2	1.97	0.47
1:B:392:SER:HB2	1:B:397:ARG:HE	1.78	0.47
1:A:404:ARG:NH1	1:B:352:LEU:HD13	2.30	0.47
1:B:363:GLY:O	1:B:367:MET:N	2.36	0.47
1:B:44:LEU:O	1:B:45:PRO:C	2.55	0.47
1:B:190:ARG:HA	1:B:195:ASP:OD1	2.15	0.47
1:B:214:LEU:O	1:B:218:ILE:HG13	2.15	0.47
1:A:53:HIS:CD2	1:A:57:LYS:HD2	2.50	0.46
1:A:149:PHE:CE2	1:A:216:ALA:HB1	2.49	0.46
1:A:336:GLY:O	1:A:339:SER:OG	2.28	0.46
1:A:383:ALA:O	1:A:386:ILE:HG12	2.16	0.46
1:B:12:ARG:HH22	1:B:100:ARG:NH1	2.12	0.46
1:B:365:GLN:H	1:B:365:GLN:CD	2.23	0.46
1:A:46:ASP:HA	1:A:49:ILE:HD12	1.98	0.46
1:B:197:ILE:HG13	1:B:198:PHE:CD1	2.51	0.46
1:B:64:GLN:HB3	1:B:184:ALA:HB2	1.96	0.46
1:A:302:PRO:HG3	1:A:358:PHE:CG	2.51	0.46
1:B:72:LYS:HD3	1:B:76:LYS:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PHE:CD1	1:B:283:ALA:HA	2.51	0.46
1:A:383:ALA:HA	1:A:386:ILE:HG12	1.98	0.45
1:B:382:GLU:O	1:B:386:ILE:HG23	2.16	0.45
1:A:132:GLU:O	1:A:136:THR:HG23	2.17	0.45
1:A:355:GLY:HA3	1:B:409:ILE:HD12	1.99	0.45
1:B:134:MET:O	1:B:135:ARG:CB	2.63	0.45
1:A:303:SER:O	1:A:307:ARG:HG3	2.17	0.45
1:A:169:GLU:HG2	1:A:173:LYS:HE2	1.99	0.45
1:B:382:GLU:O	1:B:385:LYS:HG3	2.16	0.45
1:B:339:SER:O	1:B:340:TYR:C	2.60	0.44
1:B:383:ALA:HA	1:B:386:ILE:HG12	2.00	0.44
1:B:134:MET:N	1:B:138:ALA:HB3	2.32	0.44
1:B:145:ASP:HB2	1:B:239:ASP:OD2	2.18	0.44
1:B:306:THR:HG21	1:B:358:PHE:CZ	2.53	0.44
1:A:401:LEU:HD12	1:B:378:LEU:HD21	2.00	0.44
1:A:67:GLY:O	1:A:185:ASN:ND2	2.51	0.44
1:A:398:ARG:HD2	1:B:378:LEU:HD22	2.00	0.44
2:C:1:DA:H2	2:C:2:DA:C5	2.36	0.44
1:A:302:PRO:O	1:A:307:ARG:NH1	2.51	0.43
1:B:272:PRO:HB3	1:B:280:SER:C	2.43	0.43
1:B:404:ARG:HE	1:B:404:ARG:HB2	1.30	0.43
1:A:367:MET:HG3	1:B:406:LEU:HB3	2.00	0.43
1:A:41:GLU:O	1:A:44:LEU:HB2	2.18	0.43
1:A:150:PHE:CG	4:A:502:DCP:H2'2	2.53	0.43
1:A:335:ASP:OD1	1:A:337:LYS:HG3	2.18	0.43
1:B:43:ARG:NH2	1:B:50:GLU:OE2	2.44	0.43
1:B:18:TRP:CZ2	1:B:22:ARG:HB3	2.54	0.43
1:B:345:TYR:O	1:B:349:LYS:HG2	2.19	0.43
1:A:210:PRO:O	1:A:213:PRO:HD2	2.19	0.43
1:A:232:ILE:HD11	1:A:250:ASP:HB3	2.00	0.43
1:A:104:LEU:HD22	1:A:165:HIS:ND1	2.34	0.43
1:B:42:SER:C	1:B:43:ARG:HG3	2.44	0.43
1:A:12:ARG:CA	1:B:45:PRO:HG2	2.40	0.42
1:A:284:THR:O	1:A:297:PRO:HD3	2.18	0.42
1:B:5:TYR:HD1	1:B:171:THR:HG22	1.84	0.42
1:A:377:LYS:HA	1:A:377:LYS:HD2	1.92	0.42
1:B:134:MET:HE3	1:B:284:THR:HB	2.01	0.42
1:A:210:PRO:HA	2:C:5:DG:H5'	2.01	0.42
1:B:31:ASP:OD1	1:B:35:ARG:HG2	2.20	0.42
1:A:162:LEU:HG	1:A:166:LEU:HG	2.01	0.42
1:A:92:ARG:HD2	1:A:92:ARG:HA	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG13	1:A:291:LEU:HD12	2.02	0.42
1:A:260:LYS:O	1:A:264:LYS:HG3	2.20	0.42
1:B:95:LEU:O	1:B:99:GLN:HG3	2.20	0.42
1:B:285:GLU:C	1:B:287:GLY:H	2.28	0.42
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.88	0.42
1:A:296:SER:HB3	1:A:299:LEU:O	2.20	0.42
1:B:383:ALA:O	1:B:386:ILE:HG12	2.20	0.42
1:B:353:GLY:C	2:P:15:DA:H4'	2.45	0.41
2:P:18:DDG:OP2	2:P:18:DDG:H8	2.20	0.41
1:B:132:GLU:O	1:B:136:THR:HG23	2.21	0.41
1:A:150:PHE:CD2	4:A:502:DCP:H2'2	2.55	0.41
1:A:351:ILE:HD13	1:A:374:ILE:HD13	2.01	0.41
1:A:398:ARG:HH21	1:A:405:LEU:HA	1.85	0.41
2:C:6:DG:H3'	2:C:6:DG:C8	2.55	0.41
1:B:162:LEU:CD2	1:B:175:PHE:CE1	3.03	0.41
1:B:162:LEU:HD22	1:B:175:PHE:CZ	2.56	0.41
1:B:296:SER:HB3	1:B:299:LEU:O	2.20	0.41
1:A:53:HIS:NE2	1:A:57:LYS:CD	2.83	0.41
1:B:76:LYS:O	1:B:77:SER:C	2.63	0.41
1:B:57:LYS:HB2	1:B:57:LYS:HE2	1.81	0.41
1:B:142:ILE:HG13	1:B:281:ARG:HG3	2.03	0.41
1:B:150:PHE:O	1:B:204:GLY:HA2	2.21	0.41
1:B:168:CYS:SG	1:B:171:THR:HG23	2.61	0.41
1:B:181:THR:HG21	1:B:183:LEU:HD21	2.02	0.41
1:A:270:TYR:CE2	1:A:278:LYS:HD3	2.56	0.41
1:A:371:ASP:OD1	1:B:398:ARG:NH2	2.52	0.41
1:B:30:SER:HB2	2:P:2:DA:H5''	2.02	0.41
1:B:53:HIS:CE1	1:B:57:LYS:HD3	2.56	0.40
1:B:109:LEU:HD22	1:B:119:PRO:HD2	2.03	0.40
1:A:283:ALA:O	1:A:286:ILE:HG23	2.20	0.40
1:B:283:ALA:C	1:B:285:GLU:H	2.29	0.40
1:B:283:ALA:C	1:B:285:GLU:N	2.79	0.40
1:B:70:GLN:HB2	1:B:80:LEU:HG	2.03	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	406/408 (100%)	399 (98%)	6 (2%)	1 (0%)	43	70
1	B	403/408 (99%)	392 (97%)	10 (2%)	1 (0%)	43	70
All	All	809/816 (99%)	791 (98%)	16 (2%)	2 (0%)	43	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ILE
1	B	238	ILE

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	341/341 (100%)	340 (100%)	1 (0%)	86	94
1	B	340/341 (100%)	335 (98%)	5 (2%)	57	81
All	All	681/682 (100%)	675 (99%)	6 (1%)	70	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	ILE
1	B	104	LEU
1	B	247	SER
1	B	332	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	337	LYS
1	B	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	294	ASN
1	B	294	ASN
1	B	330	GLN
1	B	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DDG	P	18	2	20,23,24	3.78	13 (65%)	27,33,36	2.50	15 (55%)
2	DDG	C	18	2	20,23,24	3.69	12 (60%)	27,33,36	2.27	10 (37%)

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	DDG	P	18	2	-	2/7/18/19	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DDG	C	18	2	-	2/7/18/19	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	18	DDG	C2'-C1'	-9.12	1.31	1.52
2	C	18	DDG	C2'-C1'	-9.11	1.31	1.52
2	C	18	DDG	C4-N3	6.77	1.49	1.34
2	P	18	DDG	C4-N3	6.19	1.48	1.34
2	P	18	DDG	O4'-C4'	6.10	1.56	1.44
2	C	18	DDG	O4'-C4'	5.49	1.55	1.44
2	C	18	DDG	C3'-C4'	-4.84	1.27	1.52
2	P	18	DDG	C3'-C4'	-4.79	1.28	1.52
2	C	18	DDG	C2-N3	4.56	1.44	1.33
2	P	18	DDG	O4'-C1'	4.44	1.52	1.42
2	P	18	DDG	C2-N2	4.26	1.44	1.34
2	P	18	DDG	C2-N3	4.14	1.43	1.33
2	C	18	DDG	C2-N2	3.58	1.42	1.34
2	C	18	DDG	O4'-C1'	3.34	1.49	1.42
2	C	18	DDG	C4-N9	-3.18	1.30	1.38
2	P	18	DDG	C2-N1	2.78	1.44	1.37
2	P	18	DDG	C2'-C3'	2.76	1.61	1.54
2	C	18	DDG	C5-C6	2.62	1.54	1.44
2	C	18	DDG	C2-N1	2.61	1.44	1.37
2	P	18	DDG	C5-N7	-2.59	1.33	1.39
2	P	18	DDG	C1'-N9	2.45	1.54	1.48
2	P	18	DDG	C4-N9	-2.44	1.31	1.38
2	C	18	DDG	C5-N7	-2.40	1.34	1.39
2	C	18	DDG	C6-N1	2.34	1.43	1.38
2	P	18	DDG	C5-C6	2.30	1.53	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	18	DDG	C4'-O4'-C1'	-6.38	103.79	109.81
2	P	18	DDG	C5-C4-N3	-5.00	120.44	128.39
2	P	18	DDG	C2-N3-C4	4.97	120.87	112.30
2	C	18	DDG	C5-C4-N3	-3.61	122.64	128.39
2	C	18	DDG	C2-N3-C4	3.59	118.48	112.30
2	P	18	DDG	C4'-O4'-C1'	-3.51	106.50	109.81
2	P	18	DDG	C3'-C2'-C1'	3.32	106.70	102.87
2	C	18	DDG	C1'-N9-C4	-3.27	116.68	125.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	18	DDG	N9-C8-N7	-3.19	107.48	113.40
2	P	18	DDG	N9-C8-N7	-3.02	107.80	113.40
2	P	18	DDG	C2-N1-C6	-3.01	119.65	125.11
2	P	18	DDG	C1'-N9-C8	2.87	134.34	127.91
2	P	18	DDG	N2-C2-N1	2.72	122.51	116.76
2	P	18	DDG	C1'-N9-C4	-2.70	118.21	125.50
2	P	18	DDG	C5-C6-N1	2.63	119.94	113.25
2	P	18	DDG	O6-C6-C5	-2.59	119.70	126.53
2	C	18	DDG	C1'-N9-C8	2.58	133.69	127.91
2	C	18	DDG	O6-C6-C5	-2.45	120.07	126.53
2	P	18	DDG	O4'-C1'-N9	2.36	112.06	107.86
2	C	18	DDG	N9-C4-N3	2.20	130.34	125.95
2	P	18	DDG	N9-C4-N3	2.13	130.22	125.95
2	C	18	DDG	C2'-C1'-N9	-2.08	108.46	112.40
2	P	18	DDG	N1-C2-N3	-2.06	119.55	123.32
2	P	18	DDG	C5-C4-N9	2.06	109.33	105.66
2	C	18	DDG	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	18	DDG	O4'-C4'-C5'-O5'
2	P	18	DDG	O4'-C4'-C5'-O5'
2	C	18	DDG	C3'-C4'-C5'-O5'
2	P	18	DDG	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	18	DDG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
4	DCP	A	502	3	28,29,29	0.66	1 (3%)	41,45,45	0.55	0
4	DCP	B	502	3	28,29,29	0.62	0	41,45,45	0.92	3 (7%)

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
4	DCP	A	502	3	-	4/22/34/34	0/2/2/2
4	DCP	B	502	3	-	8/22/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	DCP	PB-O3B	-2.76	1.56	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	DCP	C1'-N1-C2	3.03	123.03	117.83
4	B	502	DCP	O4'-C1'-N1	2.22	111.80	107.86
4	B	502	DCP	C1'-N1-C6	-2.11	117.38	121.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	DCP	O4'-C1'-N1-C2
4	B	502	DCP	O4'-C1'-N1-C6
4	B	502	DCP	O4'-C4'-C5'-O5'
4	A	502	DCP	PA-O3A-PB-O1B
4	A	502	DCP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

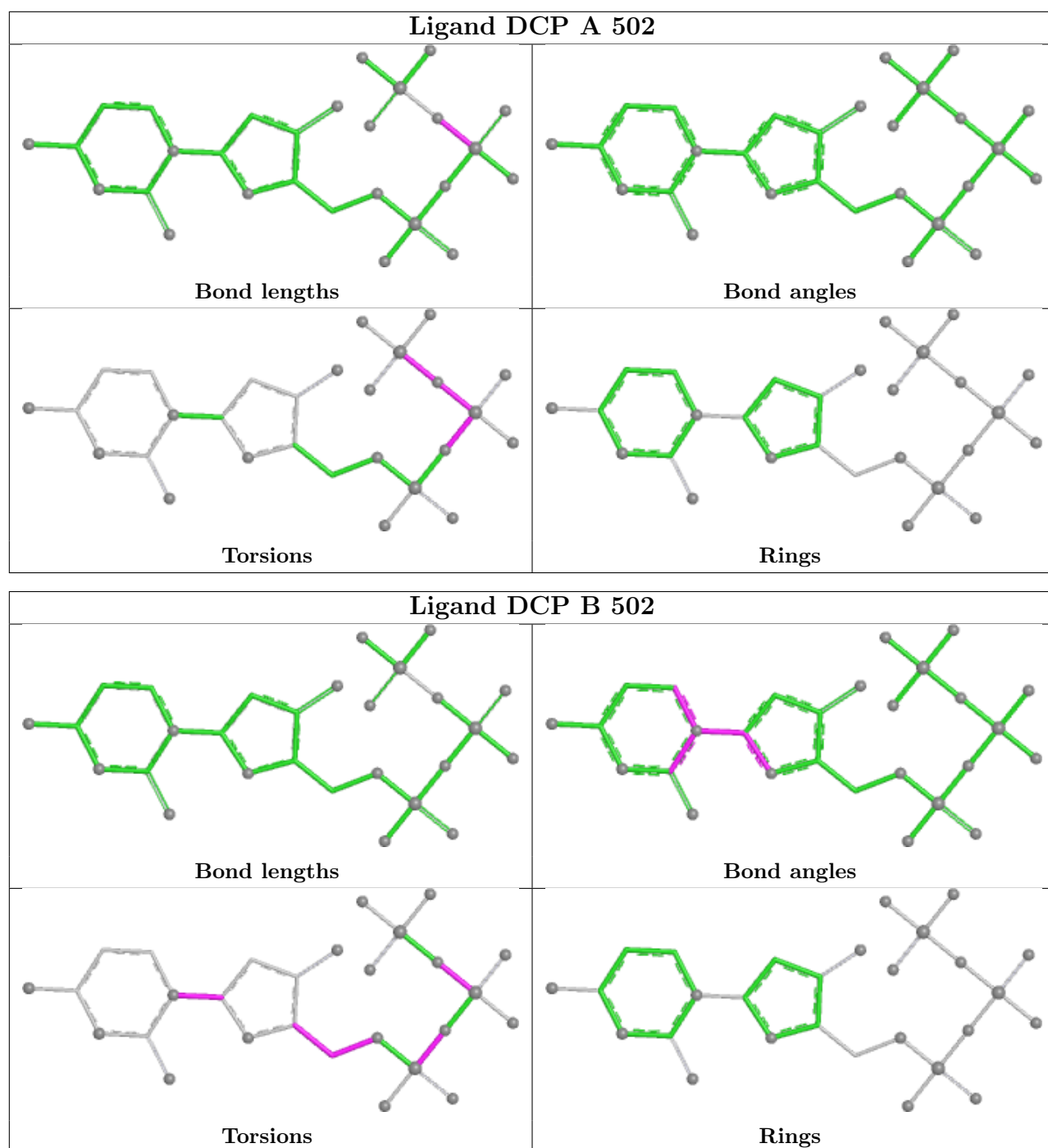
Mol	Chain	Res	Type	Atoms
4	B	502	DCP	PB-O3A-PA-O1A
4	B	502	DCP	C3'-C4'-C5'-O5'
4	A	502	DCP	PG-O3B-PB-O2B
4	B	502	DCP	C4'-C5'-O5'-PA
4	A	502	DCP	PA-O3A-PB-O2B
4	B	502	DCP	PB-O3A-PA-O2A
4	B	502	DCP	PG-O3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	DCP	2	0
4	B	502	DCP	3	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	408/408 (100%)	0.38	6 (1%) 72 65	38, 53, 75, 92	0
1	B	407/408 (99%)	0.83	45 (11%) 10 8	47, 67, 96, 112	0
2	C	12/18 (66%)	0.37	2 (16%) 4 3	42, 51, 83, 97	0
2	P	12/18 (66%)	0.22	0 100 100	52, 66, 96, 107	0
All	All	839/852 (98%)	0.59	53 (6%) 26 21	38, 61, 89, 112	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	CYS	4.7
1	B	272	PRO	4.3
1	B	75	GLY	4.2
1	B	152	LYS	4.2
1	B	395	THR	4.1
1	B	76	LYS	4.1
1	B	275	ASP	4.0
1	B	360	PHE	4.0
1	B	162	LEU	3.8
1	B	329	ALA	3.8
1	A	44	LEU	3.7
1	B	71	LYS	3.6
1	B	70	GLN	3.5
1	B	359	THR	3.5
1	A	299	LEU	3.5
1	B	362	ASN	3.4
1	B	276	LYS	3.4
1	B	44	LEU	3.4
1	B	80	LEU	3.4
1	B	331	TYR	3.3
1	B	69	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	3.3
1	B	335	ASP	3.2
1	B	72	LYS	3.1
1	B	325	LEU	3.1
1	B	365	GLN	2.9
1	B	388	ILE	2.9
1	B	149	PHE	2.9
1	B	38	GLU	2.9
1	B	328	ASN	2.7
1	B	269	ALA	2.7
1	B	234	CYS	2.6
1	B	389	LEU	2.6
1	B	298	GLY	2.5
1	B	310	PHE	2.4
1	B	377	LYS	2.4
2	C	1	DA	2.4
1	B	364	SER	2.4
1	A	293	CYS	2.3
1	A	273	ARG	2.2
2	C	2	DA	2.2
1	B	333	ASP	2.2
1	B	385	LYS	2.2
1	B	150	PHE	2.2
1	B	378	LEU	2.2
1	A	330	GLN	2.2
1	A	11	LEU	2.1
1	B	337	LYS	2.1
1	B	396	VAL	2.1
1	B	358	PHE	2.1
1	B	374	ILE	2.1
1	B	302	PRO	2.0
1	B	323	HIS	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	DDG	P	18	21/22	0.93	0.10	49,56,66,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DDG	C	18	21/22	0.96	0.08	36,44,50,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

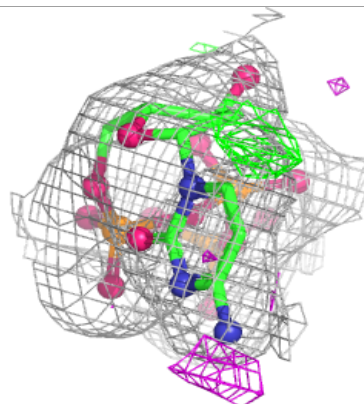
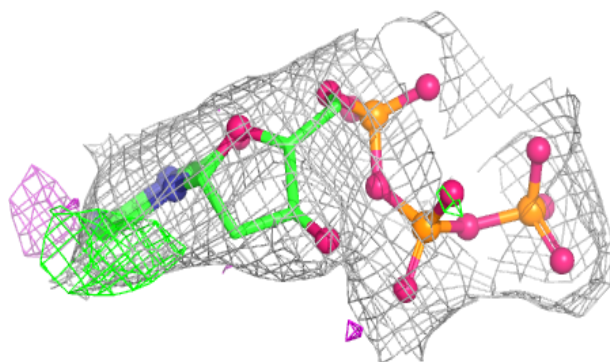
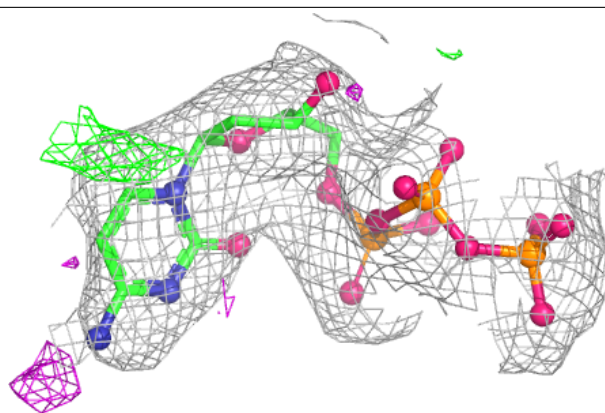
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DCP	B	502	28/28	0.91	0.09	43,54,67,75	0
4	DCP	A	502	28/28	0.97	0.06	36,42,47,48	0
3	MN	B	501	1/1	0.98	0.04	68,68,68,68	0
3	MN	A	501	1/1	0.99	0.02	43,43,43,43	0

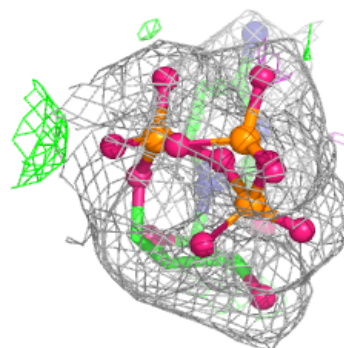
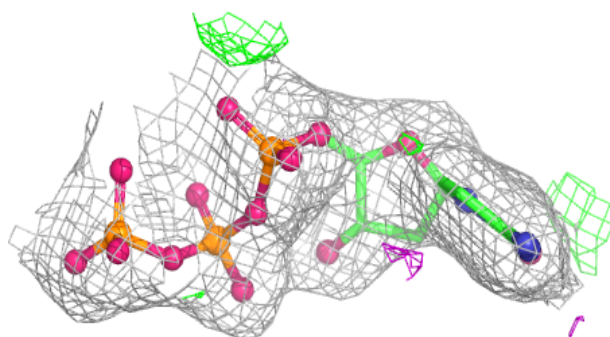
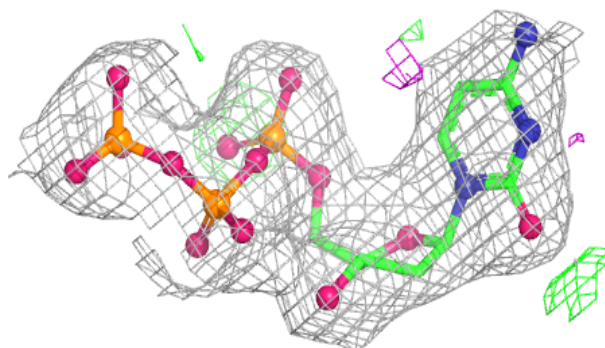
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCP B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

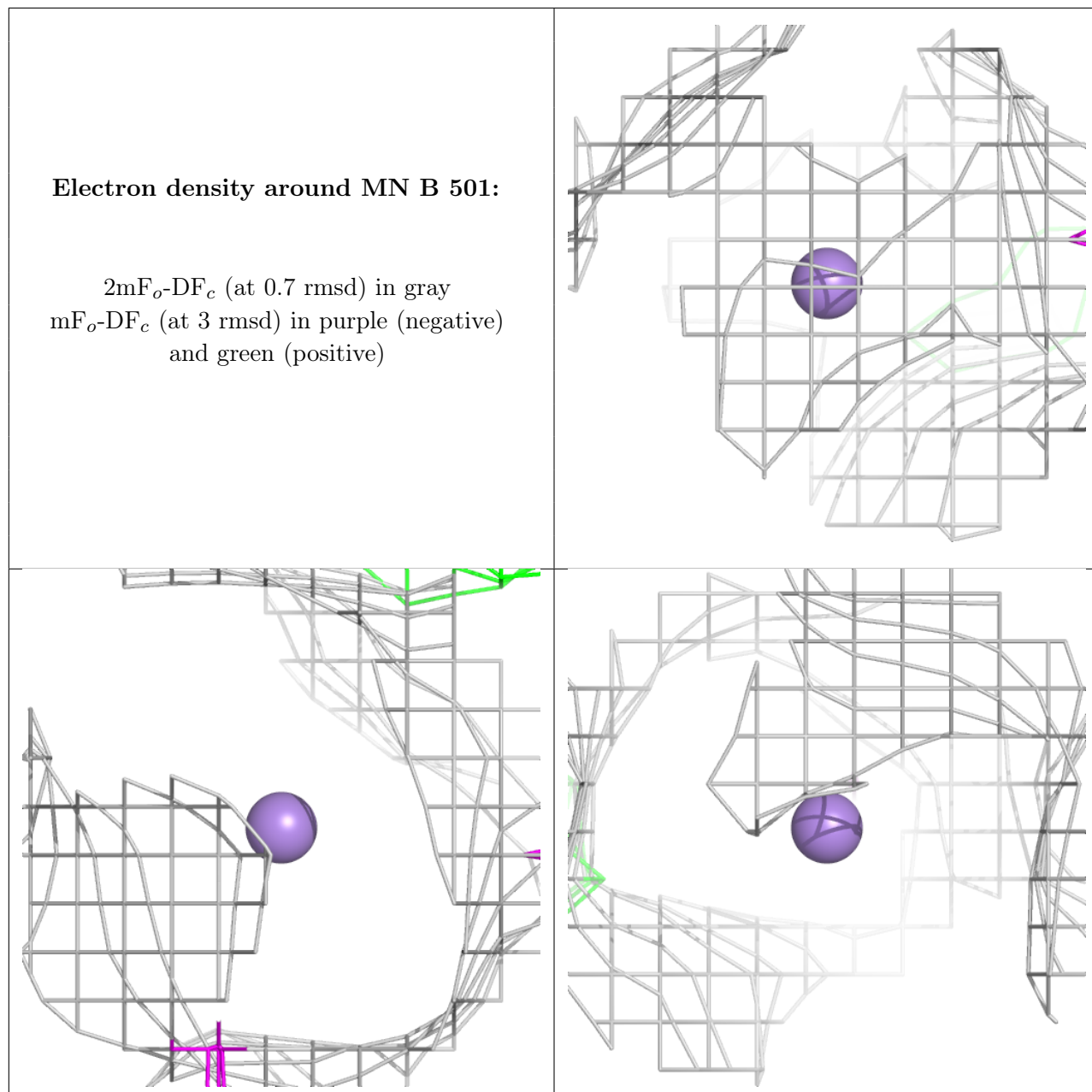
**Electron density around DCP A 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



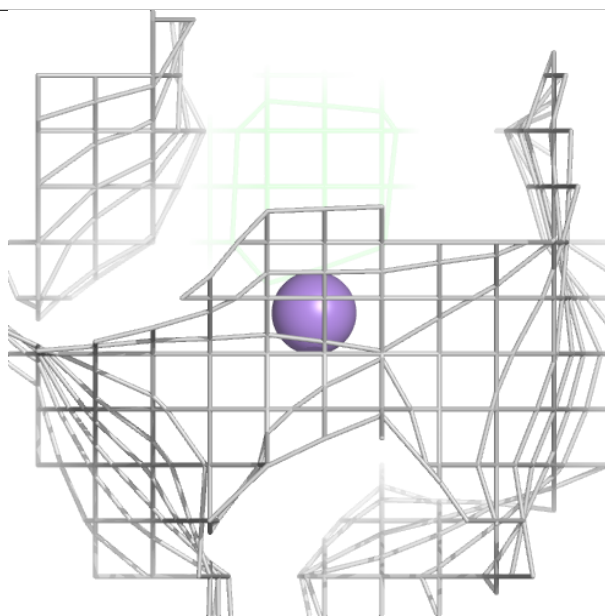
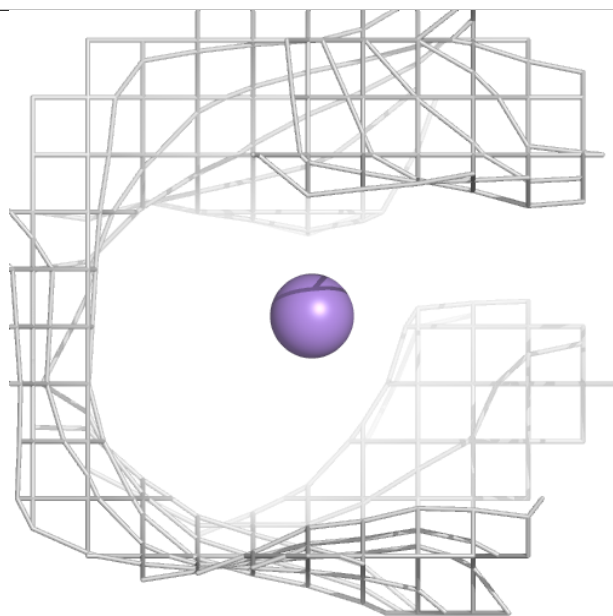
Electron density around MN B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.