



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:10 PM UTC

PDB ID : 8ICS / pdb_00008ics
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF DCTP (1 MILLIMOLAR) AND MNCL2 (5 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-15
Resolution : 2.90 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

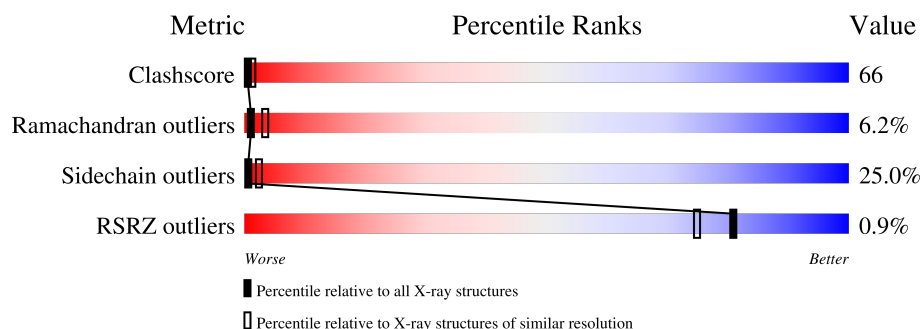
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	8	12% 12% 88%
2	P	7	14% 43% 57%
3	A	335	23% 36% 31% 8% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3063 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	8	Total	C	N	O	P	1	0	0
			145	69	27	42	7			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			144	69	24	44	7			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	327	Total	C	N	O	S	18	0	0
			2623	1657	458	499	9			

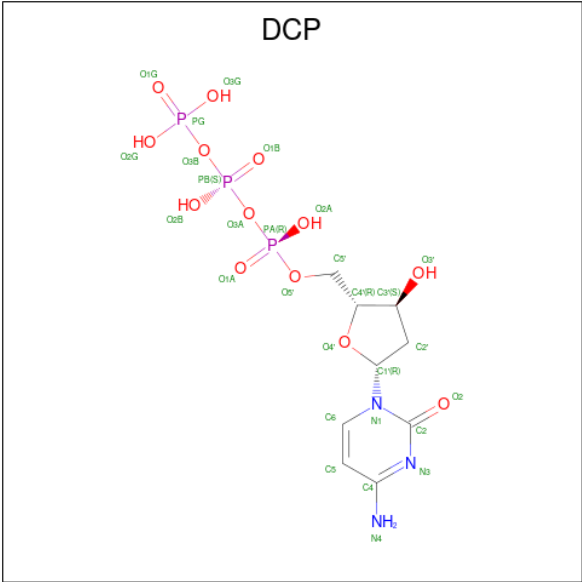
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			15	1	11	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	13	Total	O	0	0
			13	13		
7	P	17	Total	O	0	0
			17	17		
7	A	102	Total	O	0	0
			102	102		

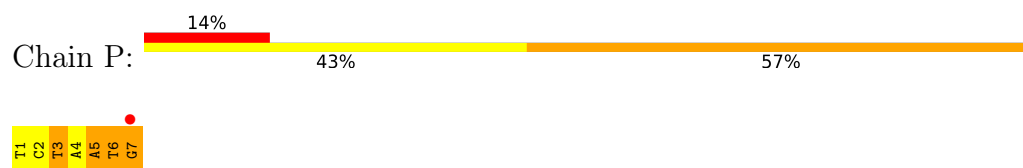
3 Residue-property plots

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.

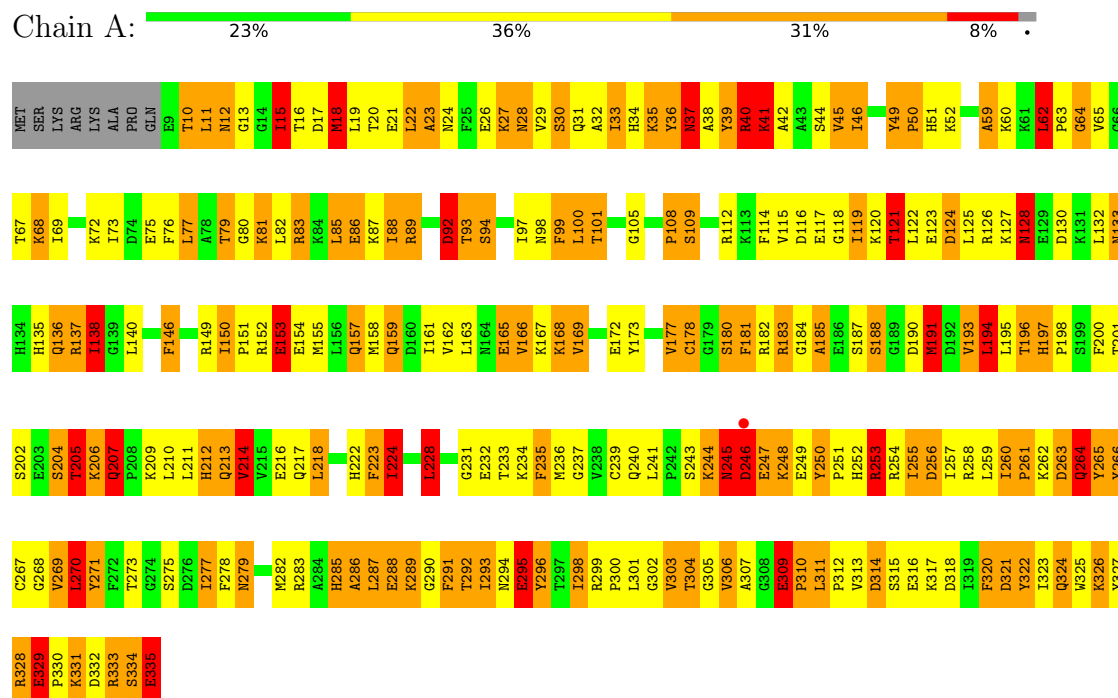
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- Molecule 2: DNA (5'-D(*TP*CP*TP*AP*AP*TP*G)-3')



- Molecule 3: PROTEIN (DNA POLYMERASE BETA (E.C.2.7.7.7))



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.79Å 57.62Å 48.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-2.90) 87.3 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.167 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 184.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3063	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, MN, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T	1.22	0/162	2.86	15/249 (6.0%)
2	P	1.45	2/160 (1.2%)	4.46	19/243 (7.8%)
3	A	1.70	34/2672 (1.3%)	2.22	129/3590 (3.6%)
All	All	1.67	36/2994 (1.2%)	2.45	163/4082 (4.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	4	0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	138	ILE	CA-CB	-7.67	1.44	1.54
3	A	15	ILE	CA-C	-7.64	1.43	1.52
3	A	196	THR	CA-C	-7.17	1.43	1.52
3	A	35	LYS	CA-C	-6.88	1.43	1.52
2	P	1	DT	OP3-P	6.81	1.62	1.48
3	A	269	VAL	CA-CB	-6.41	1.46	1.54
3	A	263	ASP	CG-OD2	6.38	1.37	1.25
3	A	59	ALA	CA-C	-6.20	1.45	1.52
3	A	212	HIS	CA-C	-6.19	1.44	1.52
3	A	328	ARG	CA-C	-6.16	1.45	1.52
3	A	213	GLN	CA-C	-6.12	1.45	1.52
3	A	247	GLU	N-CA	-6.07	1.38	1.46
3	A	247	GLU	CA-C	-5.93	1.44	1.52
3	A	269	VAL	N-CA	-5.92	1.39	1.46
3	A	16	THR	C-N	-5.87	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	245	ASN	C-N	-5.78	1.25	1.33
3	A	167	LYS	CA-C	-5.69	1.45	1.52
3	A	321	ASP	CG-OD2	5.53	1.35	1.25
3	A	214	VAL	CA-C	-5.53	1.45	1.52
3	A	224	ILE	CA-CB	-5.43	1.47	1.54
3	A	140	LEU	CA-C	-5.39	1.46	1.52
3	A	266	TYR	CA-CB	-5.39	1.44	1.53
3	A	246	ASP	CG-OD1	5.39	1.35	1.25
3	A	246	ASP	CA-C	5.37	1.59	1.52
3	A	36	TYR	C-N	-5.21	1.26	1.33
3	A	140	LEU	C-N	-5.21	1.27	1.33
3	A	23	ALA	N-CA	-5.20	1.40	1.46
3	A	69	ILE	CA-CB	-5.18	1.47	1.54
3	A	329	GLU	CD-OE2	5.16	1.35	1.25
2	P	2	DC	C1'-N1	5.16	1.65	1.49
3	A	30	SER	C-N	-5.14	1.26	1.33
3	A	109	SER	N-CA	-5.11	1.40	1.46
3	A	39	TYR	N-CA	-5.11	1.40	1.46
3	A	181	PHE	CA-C	-5.09	1.46	1.52
3	A	196	THR	C-N	-5.07	1.27	1.33
3	A	130	ASP	CG-OD2	5.07	1.34	1.25

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C6-N1-C1'	-26.99	78.86	119.35
2	P	1	DT	C2-N1-C1'	26.71	159.41	119.35
2	P	3	DT	C6-N1-C1'	-22.33	85.86	119.35
2	P	3	DT	C2-N1-C1'	21.42	151.48	119.35
2	P	6	DT	C6-N1-C1'	-20.70	88.30	119.35
2	P	6	DT	C2-N1-C1'	20.45	150.02	119.35
1	T	4	DT	C6-N1-C1'	-19.68	89.83	119.35
1	T	4	DT	C2-N1-C1'	18.66	147.34	119.35
2	P	7	DG	C4-N9-C1'	-14.79	104.81	127.00
2	P	7	DG	C8-N9-C1'	14.79	149.18	127.00
1	T	5	DA	C8-N9-C1'	10.78	143.22	127.05
1	T	5	DA	C4-N9-C1'	-10.77	110.89	127.05
3	A	28	ASN	CA-CB-CG	-10.23	102.37	112.60
3	A	49	TYR	CA-C-N	9.90	132.21	119.84
3	A	49	TYR	C-N-CA	9.90	132.21	119.84
3	A	222	HIS	CA-CB-CG	-9.66	104.14	113.80
3	A	318	ASP	CA-CB-CG	-9.46	103.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	157	GLN	N-CA-CB	9.41	124.09	110.16
3	A	181	PHE	CA-CB-CG	-9.36	104.44	113.80
1	T	6	DG	C8-N9-C1'	9.01	140.52	127.00
2	P	5	DA	C4-N9-C1'	8.97	140.51	127.05
2	P	3	DT	O4'-C1'-N1	8.96	121.84	108.40
1	T	6	DG	C4-N9-C1'	-8.74	113.89	127.00
3	A	303	VAL	N-CA-C	8.74	120.58	110.62
1	T	2	DA	C8-N9-C1'	8.70	140.09	127.05
3	A	266	TYR	CA-CB-CG	-8.38	98.82	113.90
1	T	2	DA	C4-N9-C1'	-8.32	114.56	127.05
2	P	3	DT	N1-C1'-C2'	8.24	125.87	113.50
3	A	59	ALA	O-C-N	8.09	130.40	122.07
3	A	116	ASP	CA-CB-CG	-7.80	104.80	112.60
3	A	92	ASP	N-CA-CB	7.67	121.13	110.01
3	A	35	LYS	N-CA-C	-7.58	103.01	111.28
3	A	334	SER	N-CA-C	7.52	120.13	111.11
3	A	51	HIS	CA-CB-CG	7.44	121.24	113.80
3	A	309	GLU	CA-C-N	7.44	129.13	119.84
3	A	309	GLU	C-N-CA	7.44	129.13	119.84
3	A	286	ALA	CA-C-N	7.35	130.72	120.29
3	A	286	ALA	C-N-CA	7.35	130.72	120.29
3	A	214	VAL	O-C-N	7.33	128.98	121.87
3	A	64	GLY	CA-C-N	-7.28	113.39	122.93
3	A	64	GLY	C-N-CA	-7.28	113.39	122.93
3	A	288	GLU	N-CA-C	-7.28	102.52	111.40
3	A	194	LEU	CA-C-N	-7.26	110.97	122.73
3	A	194	LEU	C-N-CA	-7.26	110.97	122.73
2	P	3	DT	C4'-C3'-O3'	-7.19	99.21	110.00
2	P	2	DC	C2-N1-C1'	7.17	130.45	119.70
3	A	333	ARG	N-CA-C	-7.09	104.99	112.93
2	P	5	DA	C8-N9-C1'	-7.08	116.44	127.05
1	T	3	DT	P-O5'-C5'	7.04	130.56	120.00
3	A	264	GLN	N-CA-CB	7.03	122.23	111.06
2	P	7	DG	O5'-C5'-C4'	7.02	121.33	110.80
3	A	50	PRO	CB-CA-C	-7.02	99.98	111.56
3	A	86	GLU	N-CA-CB	6.90	120.26	110.12
3	A	146	PHE	CA-CB-CG	-6.86	106.94	113.80
3	A	292	THR	N-CA-CB	6.85	122.14	110.57
3	A	291	PHE	CA-CB-CG	-6.83	106.97	113.80
3	A	83	ARG	N-CA-CB	6.82	120.19	109.82
3	A	252	HIS	CA-CB-CG	-6.81	106.99	113.80
3	A	40	ARG	N-CA-C	6.57	118.52	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	P-O3'-C3'	6.56	130.03	120.20
3	A	15	ILE	N-CA-CB	6.52	121.98	111.23
3	A	33	ILE	N-CA-CB	-6.48	100.53	111.23
1	T	6	DG	N9-C1'-C2'	-6.36	103.96	113.50
3	A	168	LYS	N-CA-CB	6.33	120.14	110.14
3	A	223	PHE	N-CA-C	-6.29	103.70	112.45
2	P	6	DT	P-O5'-C5'	-6.29	110.57	120.00
3	A	250	TYR	N-CA-C	6.27	118.97	110.31
3	A	243	SER	CB-CA-C	6.26	120.19	110.67
3	A	264	GLN	CB-CA-C	6.24	118.72	109.29
3	A	64	GLY	N-CA-C	-6.22	107.28	114.69
1	T	4	DT	N1-C1'-C2'	6.22	122.83	113.50
3	A	62	LEU	CA-C-O	6.22	127.84	120.88
3	A	36	TYR	CA-CB-CG	-6.21	102.72	113.90
3	A	92	ASP	CB-CA-C	6.20	120.61	110.88
3	A	98	ASN	CA-CB-CG	-6.18	106.42	112.60
3	A	256	ASP	CA-CB-CG	6.13	118.73	112.60
3	A	314	ASP	N-CA-CB	6.13	119.87	110.61
1	T	5	DA	C5'-C4'-C3'	6.13	124.09	114.90
3	A	228	LEU	N-CA-C	-6.12	103.93	111.40
3	A	17	ASP	CB-CA-C	6.12	120.94	110.79
3	A	68	LYS	CB-CA-C	6.11	120.48	110.88
3	A	271	TYR	N-CA-CB	-6.11	100.53	109.82
3	A	150	ILE	N-CA-CB	6.08	118.71	111.23
3	A	68	LYS	N-CA-C	6.06	117.56	111.07
3	A	285	HIS	N-CA-C	6.06	117.89	111.28
3	A	68	LYS	N-CA-CB	6.05	118.78	110.01
3	A	178	CYS	CA-C-O	-6.05	114.18	120.89
3	A	12	ASN	CB-CA-C	6.03	120.48	109.99
3	A	49	TYR	O-C-N	6.00	128.22	121.32
3	A	108	PRO	O-C-N	5.99	129.41	122.23
3	A	177	VAL	CB-CA-C	5.98	118.07	111.08
3	A	41	LYS	N-CA-C	-5.97	104.86	111.36
3	A	257	ILE	CA-CB-CG2	-5.96	100.37	110.50
3	A	313	VAL	N-CA-C	5.96	116.45	108.11
3	A	334	SER	N-CA-CB	5.94	118.79	109.94
2	P	2	DC	C6-N1-C1'	-5.91	110.84	119.70
3	A	99	PHE	CA-CB-CG	-5.89	107.91	113.80
3	A	253	ARG	N-CA-C	5.86	119.03	109.59
3	A	146	PHE	N-CA-C	5.84	118.42	111.71
3	A	270	LEU	O-C-N	5.84	128.10	122.03
3	A	271	TYR	CA-CB-CG	-5.79	103.48	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	137	ARG	CD-NE-CZ	-5.79	116.30	124.40
3	A	92	ASP	N-CA-C	5.73	117.20	111.07
3	A	114	PHE	CA-CB-CG	-5.72	108.08	113.80
3	A	124	ASP	CB-CA-C	-5.70	101.33	110.79
3	A	118	GLY	CA-C-N	-5.70	115.46	122.93
3	A	118	GLY	C-N-CA	-5.70	115.46	122.93
3	A	18	MET	CA-C-N	5.69	127.90	120.28
3	A	18	MET	C-N-CA	5.69	127.90	120.28
3	A	267	CYS	N-CA-C	-5.68	105.01	111.14
3	A	231	GLY	CA-C-N	-5.63	113.66	122.73
3	A	231	GLY	C-N-CA	-5.63	113.66	122.73
3	A	146	PHE	N-CA-CB	5.59	118.84	110.22
3	A	334	SER	CB-CA-C	5.57	119.72	110.81
3	A	295	GLU	CB-CG-CD	5.55	122.03	112.60
3	A	303	VAL	CB-CA-C	5.53	119.29	112.04
3	A	128	ASN	CA-CB-CG	-5.52	107.08	112.60
3	A	261	PRO	CB-CA-C	-5.51	104.54	111.71
1	T	7	DA	C4-N9-C1'	-5.49	118.82	127.05
3	A	24	ASN	CA-CB-CG	-5.47	107.13	112.60
3	A	271	TYR	N-CA-C	5.41	117.62	111.02
3	A	253	ARG	NE-CZ-NH1	5.40	126.90	121.50
3	A	159	GLN	CA-C-O	5.39	126.45	120.63
3	A	207	GLN	CA-C-N	5.37	125.19	119.28
3	A	207	GLN	C-N-CA	5.37	125.19	119.28
1	T	6	DG	O3'-P-O5'	-5.36	95.97	104.00
3	A	36	TYR	CA-C-O	5.35	126.44	120.82
3	A	309	GLU	CB-CA-C	5.35	120.72	110.17
3	A	235	PHE	CA-C-O	-5.35	114.39	120.32
3	A	286	ALA	O-C-N	5.34	128.47	122.22
3	A	335	GLU	N-CA-CB	5.33	119.56	110.50
3	A	17	ASP	N-CA-C	5.32	117.08	111.28
3	A	320	PHE	N-CA-C	-5.32	105.37	111.07
3	A	153	GLU	O-C-N	5.31	127.75	122.12
3	A	37	ASN	N-CA-C	-5.28	106.10	112.54
3	A	246	ASP	N-CA-CB	5.27	119.40	110.49
3	A	20	THR	N-CA-CB	5.27	117.96	110.16
3	A	256	ASP	N-CA-CB	5.25	119.02	110.77
3	A	108	PRO	N-CA-CB	5.25	109.10	103.33
3	A	181	PHE	O-C-N	5.21	127.44	122.07
3	A	105	GLY	N-CA-C	-5.19	107.83	114.37
3	A	191	MET	N-CA-C	5.19	117.19	109.25
3	A	212	HIS	CA-CB-CG	-5.19	108.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	324	GLN	N-CA-C	5.19	118.55	111.39
3	A	68	LYS	CA-CB-CG	-5.18	103.73	114.10
1	T	1	DC	P-O3'-C3'	5.17	127.95	120.20
3	A	177	VAL	N-CA-C	-5.17	100.89	108.54
3	A	214	VAL	N-CA-CB	5.16	117.56	110.54
3	A	126	ARG	O-C-N	5.16	127.66	122.09
3	A	87	LYS	CA-C-N	5.15	127.52	120.46
3	A	87	LYS	C-N-CA	5.15	127.52	120.46
3	A	121	THR	N-CA-C	5.12	117.66	110.14
3	A	193	VAL	N-CA-CB	-5.11	105.23	111.21
3	A	326	LYS	CD-CE-NZ	5.11	128.26	111.90
3	A	260	ILE	CB-CA-C	-5.09	102.09	111.36
3	A	153	GLU	N-CA-CB	5.08	117.59	110.12
3	A	296	TYR	CB-CA-C	-5.08	100.53	109.07
3	A	197	HIS	O-C-N	5.07	124.95	121.71
3	A	165	GLU	O-C-N	5.06	127.56	122.09
3	A	249	GLU	CB-CA-C	5.05	118.13	109.80
3	A	159	GLN	CB-CA-C	-5.04	102.12	110.68
3	A	88	ILE	CB-CA-C	-5.01	105.38	112.14
2	P	2	DC	C4'-C3'-O3'	-5.00	102.50	110.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	92	ASP	CA
3	A	264	GLN	CA
3	A	309	GLU	CA
3	A	334	SER	CA

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	T	145	0	80	8	0
2	P	144	0	80	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2623	0	2641	357	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	15	0	0	0	0
7	A	102	0	0	19	0
7	P	17	0	0	3	0
7	T	13	0	0	1	0
All	All	3063	0	2801	371	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 66.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.31	1.08
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.32	1.06
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.32	0.93
3:A:245:ASN:H	3:A:245:ASN:ND2	1.66	0.92
3:A:245:ASN:HD22	3:A:245:ASN:N	1.67	0.91
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.15	0.90
3:A:320:PHE:CE2	3:A:328:ARG:HG3	2.08	0.89
1:T:6:DG:H2"	1:T:7:DA:C8	2.08	0.88
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.53	0.88
3:A:245:ASN:H	3:A:245:ASN:HD22	0.88	0.86
3:A:259:LEU:HD12	3:A:260:ILE:H	1.40	0.86
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.73	0.85
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.06	0.85
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.58	0.84
3:A:41:LYS:HD3	3:A:42:ALA:N	1.93	0.83
3:A:33:ILE:HG23	3:A:34:HIS:H	1.44	0.81
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.64	0.80
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.64	0.79
3:A:330:PRO:HA	3:A:333:ARG:CG	2.12	0.79
3:A:180:SER:CB	3:A:183:ARG:HH21	1.95	0.79
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.65	0.79
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.62	0.78
3:A:264:GLN:NE2	3:A:296:TYR:HB3	1.99	0.78
3:A:271:TYR:HB2	7:A:592:HOH:O	1.82	0.77
3:A:177:VAL:HG22	3:A:193:VAL:HG22	1.65	0.77
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.66	0.76
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.83	0.76
3:A:279:ASN:O	3:A:283:ARG:HG3	1.86	0.76
3:A:108:PRO:O	3:A:112:ARG:HG3	1.85	0.75
3:A:268:GLY:O	3:A:271:TYR:HB3	1.86	0.75
3:A:152:ARG:HA	3:A:155:MET:HB2	1.69	0.75
3:A:286:ALA:HB2	3:A:293:ILE:HD11	1.68	0.75
3:A:259:LEU:HD12	3:A:260:ILE:N	2.01	0.74
3:A:180:SER:HB3	3:A:183:ARG:NH2	2.02	0.74
3:A:68:LYS:O	3:A:72:LYS:HE2	1.87	0.74
3:A:201:THR:HA	3:A:261:PRO:HB3	1.70	0.74
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.03	0.73
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.70	0.73
3:A:323:ILE:O	3:A:324:GLN:HG2	1.88	0.73
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.70	0.73
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.23	0.73
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.19	0.72
3:A:180:SER:HB2	3:A:185:ALA:CB	2.18	0.72
3:A:180:SER:HB2	3:A:185:ALA:HB2	1.69	0.72
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.20	0.71
3:A:155:MET:HA	3:A:158:MET:HE3	1.72	0.71
3:A:270:LEU:HD13	3:A:316:GLU:OE2	1.90	0.71
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.20	0.71
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.20	0.71
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.72	0.70
3:A:212:HIS:HB3	7:A:541:HOH:O	1.90	0.70
3:A:302:GLY:H	3:A:307:ALA:HB3	1.56	0.70
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.17	0.70
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.27	0.70
3:A:12:ASN:HA	7:A:553:HOH:O	1.92	0.70
3:A:62:LEU:HD12	3:A:63:PRO:HD2	1.74	0.69
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.73	0.69
3:A:11:LEU:HD23	3:A:11:LEU:H	1.58	0.68
3:A:41:LYS:HD3	3:A:42:ALA:H	1.55	0.68
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.30	0.67
1:T:6:DG:N7	7:T:652:HOH:O	2.27	0.67
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.76	0.67
3:A:163:LEU:HD23	3:A:163:LEU:N	2.07	0.67
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.60	0.67
3:A:207:GLN:O	3:A:210:LEU:HB2	1.94	0.67
3:A:306:VAL:HG23	3:A:307:ALA:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:292:THR:O	3:A:298:ILE:HA	1.95	0.66
3:A:244:LYS:C	3:A:246:ASP:H	2.04	0.66
3:A:33:ILE:HG23	3:A:34:HIS:N	2.08	0.66
3:A:41:LYS:O	3:A:45:VAL:HG13	1.95	0.66
3:A:128:ASN:ND2	3:A:128:ASN:N	2.44	0.65
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.76	0.65
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.77	0.65
3:A:31:GLN:N	7:A:641:HOH:O	2.28	0.65
3:A:18:MET:O	3:A:21:GLU:HB2	1.97	0.65
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.10	0.65
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.26	0.65
3:A:28:ASN:ND2	3:A:108:PRO:HG3	2.11	0.65
3:A:59:ALA:O	3:A:62:LEU:HB2	1.97	0.64
3:A:194:LEU:CD1	3:A:258:ARG:HG3	2.28	0.64
3:A:180:SER:HA	3:A:183:ARG:HE	1.60	0.64
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.10	0.64
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.79	0.64
3:A:127:LYS:HB2	3:A:128:ASN:HD21	1.64	0.63
3:A:152:ARG:NE	3:A:184:GLY:O	2.31	0.63
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.33	0.63
3:A:293:ILE:HD13	3:A:298:ILE:CG1	2.18	0.63
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.35	0.62
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.48	0.62
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.80	0.62
3:A:59:ALA:O	3:A:65:VAL:HG21	1.99	0.62
3:A:195:LEU:O	3:A:260:ILE:N	2.30	0.62
3:A:124:ASP:O	3:A:128:ASN:ND2	2.32	0.62
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.14	0.61
3:A:188:SER:HB3	7:A:522:HOH:O	2.00	0.61
3:A:195:LEU:O	3:A:259:LEU:HD12	1.99	0.61
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.33	0.61
3:A:35:LYS:O	3:A:38:ALA:HB3	2.01	0.61
3:A:260:ILE:HG22	3:A:261:PRO:N	2.14	0.61
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.81	0.61
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.83	0.61
3:A:248:LYS:O	3:A:248:LYS:HG2	2.00	0.60
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.81	0.60
3:A:288:GLU:C	3:A:290:GLY:H	2.10	0.60
3:A:11:LEU:H	3:A:11:LEU:CD2	2.14	0.60
3:A:155:MET:CE	3:A:188:SER:HB2	2.32	0.60
3:A:286:ALA:O	3:A:291:PHE:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.81	0.59
3:A:333:ARG:HH11	3:A:333:ARG:HG3	1.67	0.59
3:A:31:GLN:HB2	3:A:112:ARG:NH1	2.17	0.59
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.85	0.59
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.33	0.59
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.37	0.59
3:A:133:ASN:HD22	3:A:135:HIS:H	1.50	0.58
3:A:277:ILE:HD11	3:A:334:SER:O	2.03	0.58
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.16	0.58
3:A:159:GLN:O	3:A:163:LEU:HG	2.02	0.58
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.32	0.58
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.68	0.58
3:A:303:VAL:C	3:A:305:GLY:H	2.10	0.58
3:A:295:GLU:CD	3:A:295:GLU:H	2.11	0.58
3:A:89:ARG:HD3	3:A:89:ARG:C	2.28	0.58
3:A:180:SER:HA	3:A:183:ARG:HB2	1.84	0.58
3:A:207:GLN:HB3	3:A:210:LEU:HD12	1.86	0.57
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.86	0.57
3:A:306:VAL:HG22	7:A:650:HOH:O	2.03	0.57
3:A:282:MET:HG2	7:A:555:HOH:O	2.03	0.57
3:A:191:MET:HG2	3:A:255:ILE:CG1	2.21	0.57
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.35	0.57
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.35	0.57
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.86	0.57
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.87	0.57
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.39	0.56
3:A:79:THR:O	3:A:81:LYS:N	2.38	0.56
3:A:200:PHE:HE2	3:A:261:PRO:HD3	1.69	0.56
3:A:316:GLU:O	3:A:320:PHE:HD1	1.89	0.56
3:A:18:MET:HE3	3:A:76:PHE:CB	2.34	0.56
3:A:133:ASN:O	3:A:137:ARG:HG3	2.05	0.56
3:A:270:LEU:HD12	3:A:270:LEU:O	2.06	0.56
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.86	0.56
3:A:165:GLU:O	3:A:168:LYS:HG2	2.05	0.56
3:A:200:PHE:O	3:A:262:LYS:N	2.37	0.56
3:A:59:ALA:C	3:A:65:VAL:HG21	2.30	0.56
3:A:120:LYS:N	3:A:124:ASP:OD2	2.33	0.56
1:T:5:DA:H2''	1:T:6:DG:O5'	2.06	0.55
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.06	0.55
3:A:172:GLU:HG3	3:A:198:PRO:CG	2.37	0.55
3:A:240:GLN:NE2	3:A:250:TYR:O	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HD12	3:A:270:LEU:C	2.30	0.55
3:A:150:ILE:O	3:A:187:SER:HA	2.06	0.55
3:A:237:GLY:O	3:A:254:ARG:NH1	2.39	0.55
3:A:302:GLY:N	3:A:307:ALA:HB3	2.21	0.55
3:A:133:ASN:HD22	3:A:135:HIS:N	2.04	0.55
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.34	0.55
3:A:200:PHE:O	3:A:261:PRO:HA	2.07	0.55
3:A:59:ALA:O	3:A:62:LEU:N	2.34	0.54
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.89	0.54
3:A:262:LYS:O	3:A:262:LYS:HG3	2.07	0.54
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.88	0.54
3:A:183:ARG:HH11	3:A:275:SER:HA	1.73	0.54
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.37	0.54
3:A:162:VAL:O	3:A:166:VAL:HG23	2.07	0.54
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.36	0.54
3:A:234:LYS:HD3	7:A:617:HOH:O	2.08	0.54
3:A:155:MET:HE3	3:A:188:SER:OG	2.08	0.54
3:A:93:THR:HG22	3:A:94:SER:N	2.21	0.53
3:A:149:ARG:NH2	3:A:188:SER:HA	2.23	0.53
3:A:286:ALA:O	3:A:291:PHE:HB2	2.08	0.53
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.50	0.53
3:A:121:THR:HG23	3:A:124:ASP:CG	2.34	0.53
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.43	0.53
3:A:196:THR:HB	3:A:265:TYR:CD1	2.43	0.53
2:P:5:DA:H2''	2:P:6:DT:H5'	1.91	0.53
3:A:194:LEU:HD12	3:A:258:ARG:HG3	1.91	0.53
3:A:183:ARG:NH1	3:A:275:SER:HA	2.24	0.53
3:A:302:GLY:H	3:A:307:ALA:CB	2.22	0.53
3:A:326:LYS:O	3:A:328:ARG:HG2	2.08	0.53
3:A:333:ARG:HG3	3:A:333:ARG:NH1	2.23	0.53
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.49	0.52
3:A:18:MET:HG3	3:A:82:LEU:HD22	1.90	0.52
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.89	0.52
3:A:119:ILE:HG23	3:A:124:ASP:CB	2.38	0.52
3:A:150:ILE:HG22	3:A:155:MET:HG2	1.90	0.52
2:P:5:DA:P	3:A:109:SER:HB3	2.50	0.52
3:A:135:HIS:HB2	7:A:596:HOH:O	2.09	0.52
3:A:180:SER:CA	3:A:183:ARG:HH21	2.22	0.52
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.91	0.52
3:A:196:THR:HB	3:A:265:TYR:HD1	1.74	0.52
3:A:155:MET:HE3	3:A:188:SER:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:11:LEU:HD23	3:A:11:LEU:N	2.21	0.51
3:A:18:MET:CE	3:A:76:PHE:HB2	2.38	0.51
3:A:119:ILE:HG22	3:A:124:ASP:HB2	1.91	0.51
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.74	0.51
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.46	0.51
2:P:4:DA:H5"	7:A:614:HOH:O	2.11	0.51
3:A:155:MET:HA	3:A:158:MET:CE	2.39	0.51
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.45	0.50
3:A:205:THR:HG23	3:A:205:THR:O	2.12	0.50
3:A:133:ASN:ND2	3:A:135:HIS:H	2.09	0.50
3:A:165:GLU:HA	3:A:168:LYS:CG	2.41	0.50
3:A:323:ILE:C	3:A:324:GLN:HG2	2.36	0.50
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.93	0.50
3:A:119:ILE:CG2	3:A:124:ASP:HB2	2.42	0.50
3:A:253:ARG:HH11	3:A:253:ARG:HG3	1.76	0.50
3:A:320:PHE:HE2	3:A:328:ARG:HG3	1.71	0.50
3:A:194:LEU:N	3:A:194:LEU:HD13	2.16	0.49
2:P:3:DT:H4'	7:P:569:HOH:O	2.12	0.49
3:A:21:GLU:OE1	3:A:85:LEU:HD11	2.12	0.49
3:A:277:ILE:HD13	3:A:277:ILE:H	1.76	0.49
3:A:133:ASN:HD22	3:A:133:ASN:C	2.21	0.49
3:A:182:ARG:NH2	3:A:316:GLU:OE1	2.29	0.49
3:A:31:GLN:HB2	3:A:112:ARG:HH12	1.78	0.49
3:A:212:HIS:N	3:A:212:HIS:CD2	2.79	0.49
2:P:3:DT:H1'	7:P:511:HOH:O	2.12	0.49
3:A:253:ARG:NH1	7:A:620:HOH:O	2.41	0.49
3:A:330:PRO:C	3:A:333:ARG:HG2	2.38	0.48
3:A:213:GLN:O	3:A:216:GLU:HB3	2.13	0.48
3:A:253:ARG:NH2	7:A:620:HOH:O	2.33	0.48
3:A:331:LYS:HG2	3:A:332:ASP:N	2.20	0.48
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.42	0.48
3:A:265:TYR:CD2	3:A:269:VAL:HG21	2.49	0.48
3:A:265:TYR:CE2	3:A:269:VAL:HG21	2.48	0.48
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.48	0.48
3:A:194:LEU:HD11	3:A:258:ARG:HG3	1.95	0.48
3:A:155:MET:HE3	3:A:188:SER:HB2	1.95	0.48
3:A:235:PHE:CD1	3:A:235:PHE:C	2.90	0.48
3:A:327:TYR:HD1	3:A:328:ARG:N	2.10	0.48
3:A:184:GLY:O	3:A:185:ALA:O	2.32	0.48
3:A:150:ILE:CG1	3:A:253:ARG:HG2	2.43	0.48
3:A:218:LEU:N	3:A:218:LEU:CD1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:PRO:O	3:A:333:ARG:HG2	2.13	0.48
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.49	0.48
3:A:88:ILE:HG22	3:A:89:ARG:N	2.29	0.47
3:A:327:TYR:CD1	3:A:328:ARG:N	2.82	0.47
3:A:177:VAL:CG1	3:A:191:MET:HE2	2.43	0.47
3:A:200:PHE:CE2	3:A:261:PRO:CD	2.97	0.47
3:A:321:ASP:O	3:A:324:GLN:N	2.45	0.47
3:A:328:ARG:O	3:A:333:ARG:NE	2.38	0.47
3:A:97:ILE:O	3:A:101:THR:HB	2.14	0.47
3:A:181:PHE:HA	7:A:530:HOH:O	2.14	0.47
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.49	0.47
3:A:83:ARG:O	3:A:86:GLU:N	2.46	0.47
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.45	0.47
3:A:195:LEU:HA	3:A:195:LEU:HD12	1.55	0.47
3:A:182:ARG:HH11	3:A:273:THR:CB	2.27	0.47
3:A:278:PHE:HZ	3:A:320:PHE:CZ	2.33	0.47
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.97	0.47
3:A:18:MET:CE	3:A:82:LEU:HD13	2.38	0.47
3:A:330:PRO:O	3:A:333:ARG:N	2.45	0.47
3:A:150:ILE:HD11	3:A:253:ARG:HG2	1.97	0.47
3:A:228:LEU:HD12	3:A:228:LEU:HA	1.75	0.47
3:A:259:LEU:O	3:A:260:ILE:HD13	2.15	0.47
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.45	0.46
3:A:200:PHE:HB2	7:A:625:HOH:O	2.16	0.46
3:A:264:GLN:HE22	3:A:296:TYR:HB3	1.79	0.46
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.96	0.46
3:A:92:ASP:HB3	7:A:647:HOH:O	2.15	0.46
3:A:99:PHE:CD1	3:A:99:PHE:C	2.93	0.46
3:A:288:GLU:O	3:A:290:GLY:N	2.48	0.46
3:A:133:ASN:H	3:A:136:GLN:HE21	1.64	0.46
3:A:190:ASP:N	3:A:190:ASP:OD1	2.47	0.46
3:A:309:GLU:N	3:A:309:GLU:OE1	2.48	0.46
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.70	0.46
1:T:2:DA:H2"	1:T:3:DT:OP2	2.16	0.46
3:A:182:ARG:NH1	3:A:273:THR:CB	2.79	0.46
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.96	0.46
3:A:196:THR:CG2	3:A:265:TYR:CD1	2.99	0.46
3:A:255:ILE:HG12	3:A:256:ASP:N	2.31	0.46
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.98	0.46
3:A:191:MET:HB2	3:A:191:MET:HE3	1.44	0.46
3:A:311:LEU:HA	3:A:312:PRO:HD2	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:LYS:CA	3:A:65:VAL:HG23	2.43	0.45
3:A:260:ILE:CG2	3:A:261:PRO:N	2.79	0.45
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.97	0.45
3:A:197:HIS:CD2	3:A:198:PRO:CD	2.98	0.45
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.50	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.49	0.45
3:A:317:LYS:HE3	3:A:321:ASP:OD1	2.16	0.45
3:A:151:PRO:HG2	3:A:154:GLU:CD	2.42	0.45
3:A:254:ARG:NH1	3:A:255:ILE:H	2.13	0.45
3:A:266:TYR:O	3:A:270:LEU:HB2	2.17	0.45
3:A:133:ASN:ND2	3:A:133:ASN:C	2.75	0.45
3:A:138:ILE:HG23	3:A:138:ILE:HD13	1.57	0.45
3:A:22:LEU:HD13	3:A:22:LEU:HA	1.47	0.45
3:A:182:ARG:HB3	3:A:273:THR:HG23	1.99	0.45
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.32	0.45
3:A:333:ARG:NH1	7:A:584:HOH:O	2.49	0.45
3:A:254:ARG:NH1	3:A:255:ILE:N	2.65	0.44
2:P:6:DT:H6	2:P:6:DT:H2'	0.91	0.44
3:A:196:THR:OG1	3:A:197:HIS:N	2.49	0.44
3:A:275:SER:O	3:A:278:PHE:N	2.50	0.44
3:A:40:ARG:O	3:A:44:SER:N	2.50	0.44
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.05	0.44
3:A:197:HIS:O	3:A:262:LYS:HB2	2.18	0.44
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.99	0.44
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.32	0.44
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.38	0.44
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.98	0.44
3:A:181:PHE:N	7:A:522:HOH:O	2.45	0.44
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.50	0.44
3:A:311:LEU:HB3	3:A:322:TYR:HE2	1.80	0.44
1:T:1:DC:H6	1:T:1:DC:H2'	1.55	0.44
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.45	0.44
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.47	0.44
3:A:315:SER:OG	3:A:316:GLU:N	2.50	0.44
3:A:326:LYS:O	3:A:326:LYS:HG3	2.17	0.44
3:A:183:ARG:HH11	3:A:275:SER:CA	2.31	0.44
3:A:322:TYR:C	3:A:324:GLN:H	2.25	0.44
3:A:165:GLU:O	3:A:168:LYS:N	2.51	0.43
2:P:5:DA:OP2	3:A:109:SER:HB3	2.18	0.43
3:A:121:THR:OG1	3:A:123:GLU:N	2.51	0.43
3:A:198:PRO:C	3:A:200:PHE:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:GLY:N	3:A:307:ALA:CB	2.80	0.43
3:A:33:ILE:CG2	3:A:34:HIS:H	2.22	0.43
2:P:4:DA:H5'	7:P:569:HOH:O	2.19	0.43
3:A:11:LEU:CD2	3:A:11:LEU:N	2.79	0.43
3:A:223:PHE:O	3:A:239:CYS:HA	2.18	0.43
3:A:12:ASN:HA	3:A:12:ASN:HD22	1.62	0.43
3:A:278:PHE:HB2	3:A:333:ARG:O	2.18	0.43
3:A:298:ILE:HG23	3:A:298:ILE:O	2.18	0.43
3:A:279:ASN:HD22	3:A:279:ASN:HA	1.41	0.43
3:A:119:ILE:CG2	3:A:124:ASP:CB	2.97	0.43
3:A:232:GLU:C	3:A:233:THR:HG23	2.44	0.43
3:A:75:GLU:O	3:A:79:THR:HG23	2.19	0.42
3:A:79:THR:C	3:A:81:LYS:H	2.27	0.42
3:A:165:GLU:OE2	3:A:168:LYS:HD3	2.19	0.42
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.54	0.42
3:A:266:TYR:O	3:A:270:LEU:N	2.50	0.42
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.68	0.42
3:A:329:GLU:O	3:A:333:ARG:HG2	2.19	0.42
3:A:60:LYS:C	3:A:62:LEU:N	2.76	0.42
3:A:251:PRO:HG2	3:A:253:ARG:CZ	2.49	0.42
3:A:100:LEU:HD13	3:A:100:LEU:HA	1.73	0.42
3:A:209:LYS:HA	3:A:209:LYS:HD3	1.40	0.42
3:A:332:ASP:C	3:A:334:SER:H	2.27	0.42
3:A:128:ASN:N	3:A:128:ASN:HD22	2.15	0.42
3:A:22:LEU:HD21	3:A:82:LEU:HD21	2.02	0.42
3:A:62:LEU:HA	3:A:63:PRO:HD2	1.58	0.42
3:A:18:MET:HG2	3:A:22:LEU:CD2	2.50	0.42
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.37	0.41
3:A:76:PHE:CD1	3:A:76:PHE:C	2.98	0.41
3:A:277:ILE:CG1	3:A:335:GLU:CB	2.98	0.41
3:A:260:ILE:CG2	3:A:261:PRO:CD	2.98	0.41
1:T:4:DT:H2''	1:T:5:DA:O5'	2.20	0.41
3:A:34:HIS:O	3:A:38:ALA:N	2.54	0.41
3:A:204:SER:O	3:A:206:LYS:N	2.54	0.41
3:A:232:GLU:O	3:A:233:THR:HG23	2.20	0.41
3:A:293:ILE:HA	7:A:593:HOH:O	2.19	0.41
3:A:133:ASN:ND2	3:A:135:HIS:N	2.66	0.41
3:A:166:VAL:CG1	3:A:173:TYR:CB	2.99	0.41
3:A:245:ASN:ND2	3:A:245:ASN:N	2.38	0.41
3:A:166:VAL:O	3:A:169:VAL:HG13	2.21	0.41
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2:DA:C2	2:P:7:DG:N2	2.88	0.41
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.44	0.41
3:A:244:LYS:C	3:A:246:ASP:N	2.75	0.41
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.35	0.41
3:A:327:TYR:CD1	3:A:327:TYR:C	2.99	0.41
1:T:1:DC:H2"	1:T:2:DA:OP2	2.21	0.40
3:A:214:VAL:HG23	3:A:218:LEU:HD22	2.03	0.40
3:A:253:ARG:CG	3:A:253:ARG:NH1	2.80	0.40
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.74	0.40
3:A:288:GLU:C	3:A:290:GLY:N	2.78	0.40
3:A:146:PHE:HB2	7:A:514:HOH:O	2.21	0.40
3:A:299:ARG:HG2	3:A:310:PRO:HD3	2.02	0.40
3:A:115:VAL:C	3:A:117:GLU:H	2.30	0.40
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.85	0.40
3:A:211:LEU:HD12	3:A:211:LEU:O	2.22	0.40
3:A:312:PRO:O	3:A:322:TYR:OH	2.31	0.40
3:A:315:SER:C	3:A:317:LYS:H	2.27	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
3	A	325/335 (97%)	267 (82%)	38 (12%)	20 (6%)	1 3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	204	SER
3	A	205	THR
3	A	206	LYS

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Mol	Chain	Res	Type
3	A	244	LYS
3	A	289	LYS
3	A	304	THR
3	A	10	THR
3	A	80	GLY
3	A	202	SER
3	A	247	GLU
3	A	265	TYR
3	A	295	GLU
3	A	322	TYR
3	A	13	GLY
3	A	246	ASP
3	A	310	PRO
3	A	309	GLU
3	A	166	VAL
3	A	207	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	216 (75%)	72 (25%)	0 2

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	37	ASN
3	A	40	ARG

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Mol	Chain	Res	Type
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	62	LEU
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	85	LEU
3	A	89	ARG
3	A	92	ASP
3	A	93	THR
3	A	94	SER
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	138	ILE
3	A	153	GLU
3	A	157	GLN
3	A	161	ILE
3	A	169	VAL
3	A	180	SER
3	A	183	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	205	THR
3	A	214	VAL
3	A	218	LEU
3	A	224	ILE
3	A	228	LEU
3	A	236	MET
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE

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Mol	Chain	Res	Type
3	A	263	ASP
3	A	264	GLN
3	A	270	LEU
3	A	277	ILE
3	A	279	ASN
3	A	287	LEU
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	301	LEU
3	A	304	THR
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	37	ASN
3	A	98	ASN
3	A	128	ASN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	213	GLN
3	A	217	GLN
3	A	219	GLN
3	A	245	ASN
3	A	252	HIS
3	A	264	GLN
3	A	279	ASN
3	A	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 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	DCP	A	338	4	12,13,29	1.37	1 (8%)	17,21,45	1.03	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
6	DCP	A	338	4	-	6/15/15/34	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DCP	PB-O3A	3.61	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

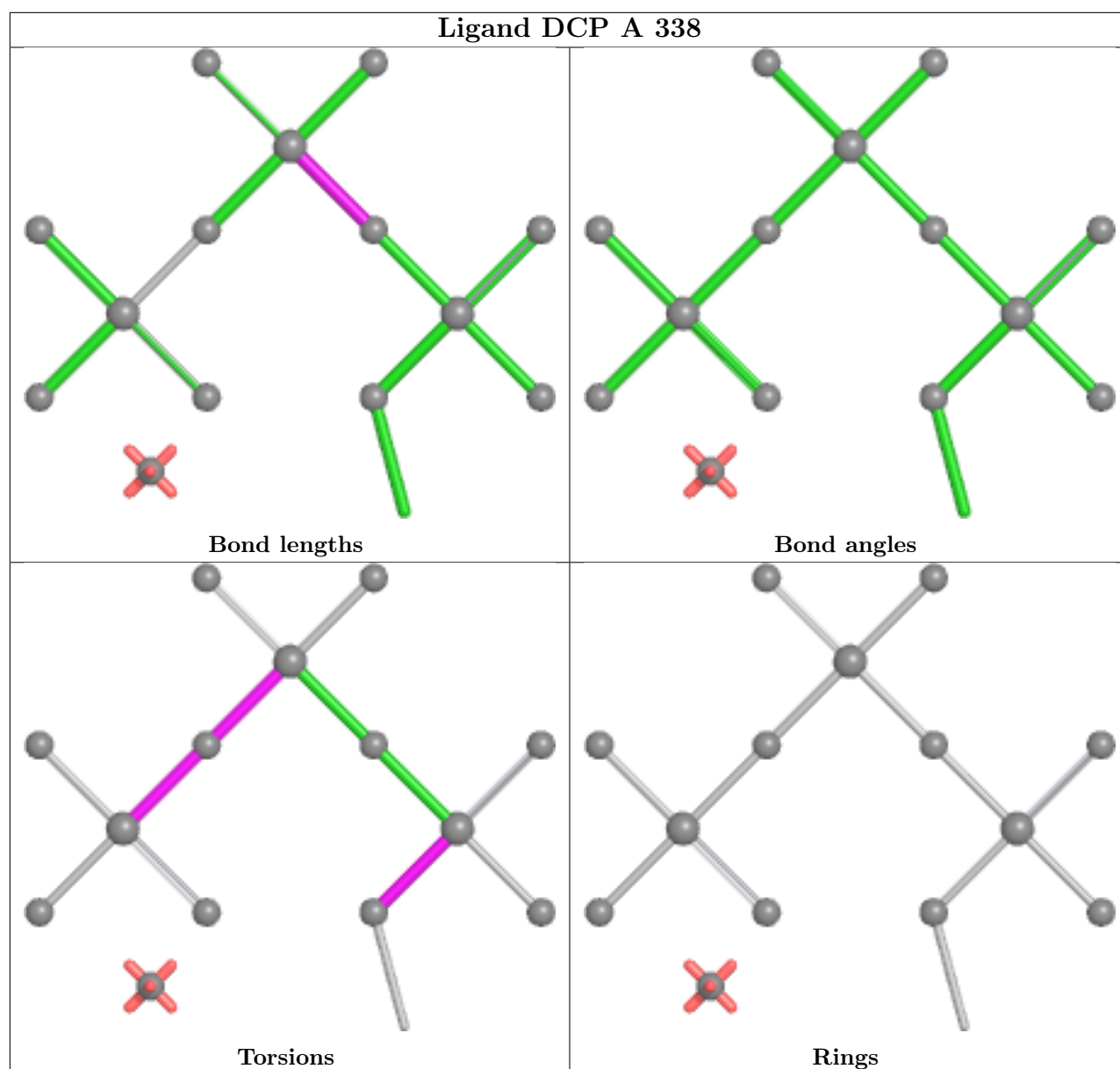
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	338	DCP	C5'-O5'-PA-O2A
6	A	338	DCP	PB-O3B-PG-O2G
6	A	338	DCP	C5'-O5'-PA-O1A
6	A	338	DCP	PB-O3B-PG-O1G
6	A	338	DCP	PG-O3B-PB-O2B
6	A	338	DCP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	8/8 (100%)	-0.25	1 (12%) 8 7	20, 46, 94, 97	0
2	P	7/7 (100%)	-0.72	1 (14%) 6 5	22, 28, 36, 99	0
3	A	325/335 (97%)	-0.84	1 (0%) 90 87	3, 34, 85, 100	0
All	All	340/350 (97%)	-0.82	3 (0%) 81 75	3, 34, 86, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1	DC	3.8
3	A	246	ASP	3.0
2	P	7	DG	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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.

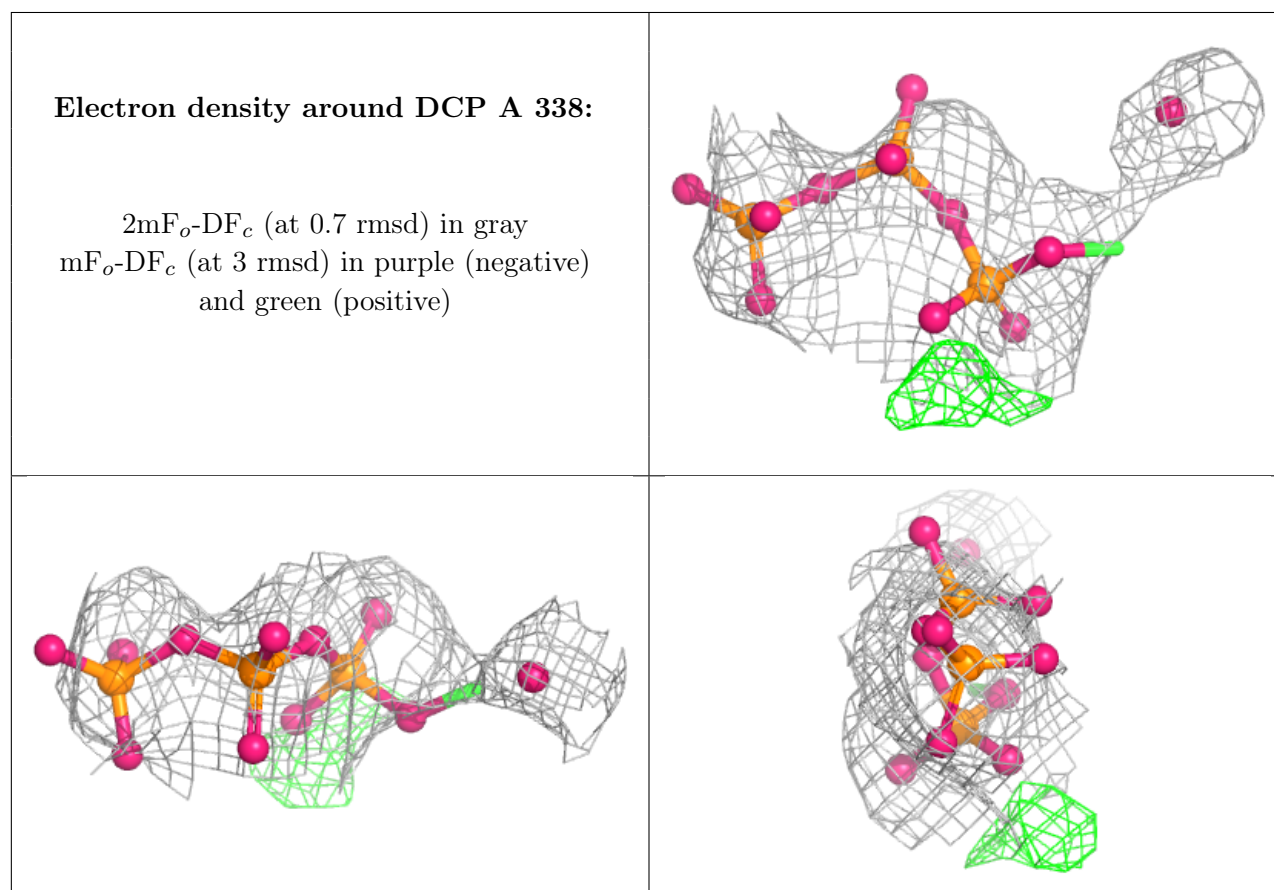
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MN	A	339	1/1	0.82	0.05	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	A	342	1/1	0.88	0.17	63,63,63,63	0
6	DCP	A	338	15/28	0.91	0.13	41,69,88,100	15
4	MN	A	340	1/1	0.93	0.04	30,30,30,30	1
5	NA	A	341	1/1	0.98	0.04	22,22,22,22	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.