



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:24 AM UTC

PDB ID : 9ICS / pdb_00009ics
Title : DNA POLYMERASE BETA (E.C.2.7.7.7)/DNA COMPLEX + 2',3'-DIDEOXYCYTIDINE-5'-TRIPHOSPHATE, SOAKED IN THE PRESENCE OF DDCTP AND MNCL2
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-16
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

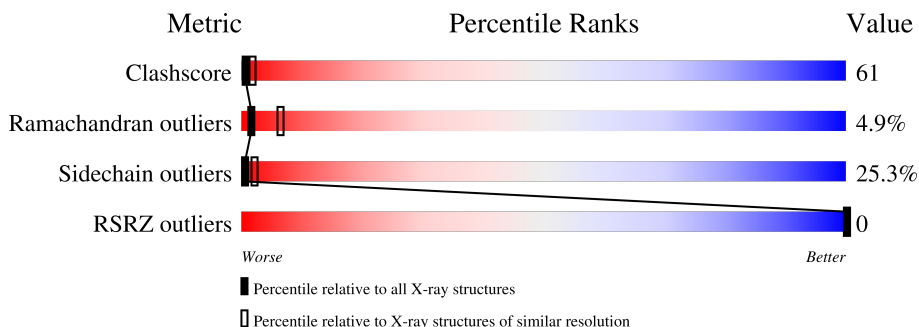
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

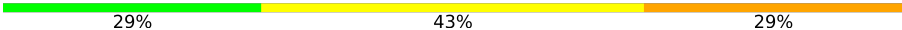
The reported resolution of this entry is 2.90 Å.

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	7	
2	P	6	
3	A	335	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3048 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*CP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	7	Total	C	N	O	P	0	0	0
			122	58	20	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	P	0	0	0
			126	59	25	36	6			

- 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	26	0	0
			2623	1657	458	499	9			

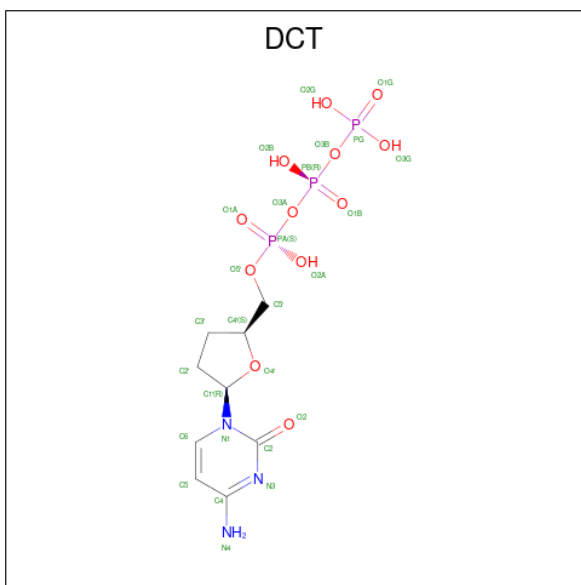
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	13	Total O 13 13	0	0
7	P	23	Total O 23 23	0	0
7	A	110	Total O 110 110	0	0

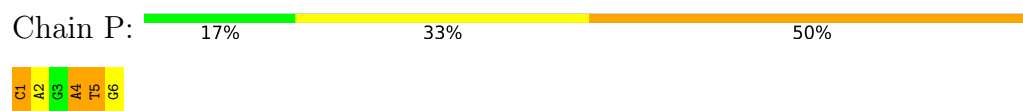
3 Residue-property plots

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.

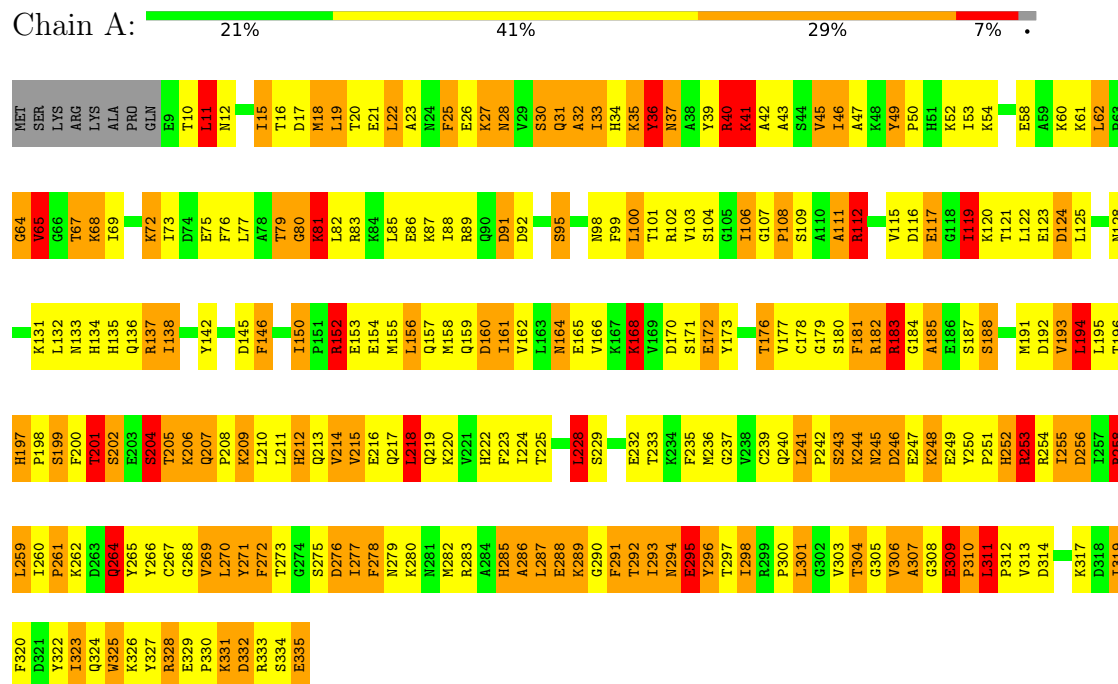
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- Molecule 2: DNA (5'-D(*CP*AP*GP*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	178.87Å 57.67Å 48.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.90) 92.7 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.165 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 160.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3048	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DCT, MN

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	1.02	0/135	2.40	8/207 (3.9%)
2	P	1.23	1/141 (0.7%)	2.10	5/214 (2.3%)
3	A	1.65	15/2672 (0.6%)	2.23	131/3590 (3.6%)
All	All	1.61	16/2948 (0.5%)	2.23	144/4011 (3.6%)

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	1	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	DC	OP3-P	7.12	1.62	1.48
3	A	199	SER	N-CA	-7.08	1.38	1.46
3	A	138	ILE	CA-CB	-6.61	1.46	1.54
3	A	138	ILE	N-CA	-6.46	1.39	1.46
3	A	192	ASP	CA-C	-6.40	1.44	1.52
3	A	137	ARG	CA-C	-6.06	1.45	1.52
3	A	193	VAL	CA-CB	-6.05	1.47	1.54
3	A	91	ASP	CA-C	-5.90	1.44	1.52
3	A	69	ILE	N-CA	-5.81	1.39	1.46
3	A	116	ASP	CA-C	-5.66	1.44	1.52
3	A	256	ASP	CA-C	-5.42	1.46	1.52
3	A	215	VAL	C-N	-5.39	1.27	1.33
3	A	36	TYR	N-CA	-5.26	1.40	1.46
3	A	65	VAL	CA-C	-5.23	1.46	1.52
3	A	271	TYR	CA-CB	-5.19	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	31	GLN	N-CA	-5.10	1.40	1.46

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	49	TYR	CA-C-N	14.45	134.30	119.56
3	A	49	TYR	C-N-CA	14.45	134.30	119.56
1	T	4	DT	C6-N1-C1'	-13.49	99.11	119.35
1	T	4	DT	C2-N1-C1'	13.48	139.57	119.35
2	P	5	DT	C6-N1-C1'	-11.61	101.94	119.35
2	P	5	DT	C2-N1-C1'	11.17	136.10	119.35
1	T	2	DC	C2-N1-C1'	10.74	135.82	119.70
3	A	49	TYR	O-C-N	10.25	130.23	121.31
1	T	2	DC	C6-N1-C1'	-10.19	104.42	119.70
3	A	192	ASP	CA-CB-CG	10.07	122.67	112.60
3	A	291	PHE	N-CA-C	10.02	121.47	108.34
3	A	192	ASP	CB-CA-C	-9.02	95.40	110.19
3	A	28	ASN	N-CA-C	8.75	120.59	111.14
3	A	65	VAL	N-CA-CB	8.69	122.28	111.41
3	A	20	THR	CB-CA-C	8.55	124.31	110.88
3	A	161	ILE	N-CA-C	8.45	118.43	110.74
3	A	296	TYR	CB-CA-C	-8.21	94.34	109.29
3	A	20	THR	N-CA-CB	8.13	121.79	110.01
2	P	4	DA	P-O3'-C3'	8.07	132.30	120.20
3	A	40	ARG	N-CA-C	7.99	119.99	111.28
3	A	192	ASP	N-CA-CB	7.87	122.90	110.55
3	A	296	TYR	N-CA-C	7.68	122.95	113.50
3	A	112	ARG	N-CA-CB	7.45	120.79	109.91
3	A	98	ASN	CA-CB-CG	-7.43	105.17	112.60
3	A	40	ARG	N-CA-CB	7.40	121.00	110.12
3	A	181	PHE	CA-C-N	7.40	131.55	120.31
3	A	181	PHE	C-N-CA	7.40	131.55	120.31
3	A	156	LEU	N-CA-CB	7.34	120.91	110.12
3	A	111	ALA	N-CA-C	-7.31	102.48	111.33
3	A	152	ARG	N-CA-CB	7.31	122.84	110.49
3	A	168	LYS	N-CA-CB	7.27	120.97	110.06
3	A	117	GLU	N-CA-C	-7.13	104.45	113.72
3	A	328	ARG	CB-CA-C	-7.12	98.62	110.29
3	A	116	ASP	CA-CB-CG	-7.03	105.57	112.60
3	A	332	ASP	CA-CB-CG	7.02	119.62	112.60
3	A	323	ILE	CB-CA-C	6.84	122.51	111.29
3	A	204	SER	CA-C-N	-6.79	112.42	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	204	SER	C-N-CA	-6.79	112.42	122.41
3	A	278	PHE	CA-CB-CG	-6.72	107.08	113.80
3	A	194	LEU	N-CA-CB	6.67	121.31	110.43
3	A	41	LYS	N-CA-CB	6.67	120.03	110.16
3	A	64	GLY	N-CA-C	-6.67	106.75	114.69
3	A	209	LYS	O-C-N	6.64	129.16	122.12
3	A	261	PRO	CB-CA-C	-6.63	103.13	111.56
3	A	313	VAL	N-CA-C	6.62	117.44	108.17
3	A	192	ASP	CA-C-N	-6.61	114.57	123.10
3	A	192	ASP	C-N-CA	-6.61	114.57	123.10
3	A	146	PHE	CA-CB-CG	-6.50	107.30	113.80
1	T	6	DT	C6-N1-C1'	-6.50	109.60	119.35
3	A	104	SER	CA-C-N	-6.39	116.52	123.30
3	A	104	SER	C-N-CA	-6.39	116.52	123.30
3	A	241	LEU	CA-C-N	6.38	127.81	119.84
3	A	241	LEU	C-N-CA	6.38	127.81	119.84
3	A	32	ALA	N-CA-C	6.38	120.19	108.58
3	A	21	GLU	CB-CA-C	-6.35	100.64	110.81
3	A	205	THR	N-CA-C	6.33	119.12	107.99
1	T	5	DC	C2-N1-C1'	6.29	129.14	119.70
3	A	142	TYR	CB-CA-C	-6.28	101.02	111.13
3	A	41	LYS	N-CA-C	-6.26	104.53	111.36
3	A	146	PHE	N-CA-C	6.24	118.88	111.71
3	A	241	LEU	O-C-N	6.17	126.55	121.31
2	P	4	DA	C8-N9-C1'	-6.08	117.92	127.05
3	A	309	GLU	CA-C-N	6.05	127.40	119.84
3	A	309	GLU	C-N-CA	6.05	127.40	119.84
3	A	132	LEU	CB-CA-C	-6.02	99.33	109.50
3	A	264	GLN	O-C-N	5.98	128.46	122.30
3	A	313	VAL	CB-CA-C	-5.98	101.93	110.83
3	A	30	SER	CA-C-N	-5.97	112.18	122.14
3	A	30	SER	C-N-CA	-5.97	112.18	122.14
3	A	36	TYR	CB-CA-C	5.94	120.20	110.88
3	A	258	ARG	N-CA-C	5.91	118.75	108.76
3	A	292	THR	CB-CA-C	5.89	121.33	109.38
3	A	201	THR	N-CA-C	5.85	117.74	108.79
3	A	228	LEU	N-CA-C	-5.84	103.63	112.04
3	A	160	ASP	CA-CB-CG	-5.83	106.77	112.60
3	A	112	ARG	N-CA-C	5.81	117.31	110.97
3	A	269	VAL	CB-CA-C	-5.80	104.44	112.04
3	A	214	VAL	N-CA-CB	5.78	119.25	110.58
3	A	81	LYS	N-CA-CB	-5.76	102.14	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	222	HIS	CB-CA-C	-5.75	102.48	111.39
3	A	243	SER	N-CA-C	-5.74	100.63	109.76
3	A	212	HIS	N-CA-C	5.73	117.20	111.07
3	A	106	ILE	CB-CA-C	-5.72	103.07	110.84
3	A	222	HIS	N-CA-C	5.71	119.55	112.58
3	A	194	LEU	CA-C-N	-5.69	113.50	122.73
3	A	194	LEU	C-N-CA	-5.69	113.50	122.73
3	A	295	GLU	CB-CA-C	5.69	120.23	110.79
3	A	181	PHE	O-C-N	5.68	128.14	122.12
3	A	11	LEU	N-CA-CB	5.67	118.64	110.20
3	A	246	ASP	N-CA-C	5.67	122.87	110.80
3	A	159	GLN	CB-CA-C	-5.66	101.39	110.79
3	A	108	PRO	CB-CA-C	-5.65	104.07	113.06
1	T	5	DC	C6-N1-C1'	-5.63	111.26	119.70
3	A	35	LYS	CB-CA-C	-5.57	101.54	110.79
3	A	87	LYS	CB-CA-C	5.56	119.60	110.88
3	A	34	HIS	CA-CB-CG	-5.54	108.26	113.80
3	A	199	SER	N-CA-CB	-5.53	102.61	110.79
3	A	65	VAL	N-CA-C	5.51	115.72	107.51
3	A	128	ASN	CA-CB-CG	-5.50	107.10	112.60
3	A	183	ARG	N-CA-C	5.50	119.62	113.02
3	A	138	ILE	CB-CA-C	-5.37	105.09	111.97
3	A	272	PHE	N-CA-CB	5.36	118.59	110.28
3	A	311	LEU	CB-CA-C	5.34	117.96	109.52
3	A	201	THR	N-CA-CB	-5.34	103.29	111.56
3	A	218	LEU	CB-CA-C	5.32	119.62	110.79
3	A	146	PHE	N-CA-CB	5.31	118.39	110.22
3	A	240	GLN	N-CA-C	5.30	117.01	108.32
3	A	286	ALA	O-C-N	5.30	127.74	122.12
3	A	107	GLY	CA-C-N	5.30	124.48	118.97
3	A	107	GLY	C-N-CA	5.30	124.48	118.97
3	A	123	GLU	CB-CA-C	5.27	119.15	110.88
3	A	92	ASP	CB-CA-C	5.25	120.35	110.63
3	A	232	GLU	CB-CG-CD	-5.24	103.69	112.60
3	A	41	LYS	O-C-N	5.23	128.11	122.15
3	A	17	ASP	N-CA-C	5.23	116.79	111.14
3	A	271	TYR	N-CA-C	5.23	117.65	111.33
3	A	335	GLU	N-CA-CB	5.21	119.36	110.50
3	A	253	ARG	N-CA-C	5.20	117.88	109.40
3	A	329	GLU	N-CA-C	-5.18	102.64	109.84
3	A	334	SER	CB-CA-C	5.16	119.31	110.74
2	P	4	DA	C4-N9-C1'	5.16	134.79	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	123	GLU	N-CA-CB	5.16	117.49	110.01
3	A	197	HIS	CA-C-N	5.15	126.27	119.84
3	A	197	HIS	C-N-CA	5.15	126.27	119.84
3	A	252	HIS	CA-CB-CG	-5.13	108.67	113.80
3	A	160	ASP	CA-C-N	-5.13	114.62	120.88
3	A	160	ASP	C-N-CA	-5.13	114.62	120.88
3	A	241	LEU	C-N-CD	-5.12	103.99	125.00
3	A	16	THR	N-CA-CB	5.12	118.10	110.22
3	A	319	ILE	N-CA-C	5.11	115.22	110.42
3	A	164	ASN	N-CA-CB	5.09	117.85	110.26
3	A	67	THR	CB-CA-C	5.08	119.48	110.85
3	A	225	THR	N-CA-C	5.07	119.60	113.41
3	A	334	SER	N-CA-CB	5.07	118.05	109.78
3	A	201	THR	CA-C-N	5.06	131.20	121.54
3	A	201	THR	C-N-CA	5.06	131.20	121.54
1	T	6	DT	C2-N1-C1'	5.06	126.93	119.35
3	A	285	HIS	CA-C-N	5.05	127.05	120.28
3	A	285	HIS	C-N-CA	5.05	127.05	120.28
3	A	271	TYR	N-CA-CB	-5.04	102.50	110.06
3	A	119	ILE	CA-CB-CG1	-5.03	101.86	110.40
3	A	313	VAL	N-CA-CB	-5.02	104.42	111.25
3	A	137	ARG	CD-NE-CZ	-5.02	117.37	124.40
3	A	124	ASP	N-CA-C	-5.01	105.10	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	246	ASP	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	122	0	69	4	0
2	P	126	0	68	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2623	0	2641	331	1
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	27	0	12	1	0
7	A	110	0	0	18	0
7	P	23	0	0	2	0
7	T	13	0	0	2	0
All	All	3048	0	2790	344	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 61.

All (344) 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:172:GLU:HG2	3:A:198:PRO:HG3	1.30	1.10
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.52	1.05
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.36	1.03
2:P:5:DT:H2''	2:P:6:DG:H5'	1.42	1.02
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.38	1.02
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.47	0.95
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.48	0.94
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.50	0.94
3:A:31:GLN:HG3	3:A:112:ARG:HH22	1.34	0.91
3:A:245:ASN:N	3:A:245:ASN:HD22	1.72	0.88
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.08	0.88
3:A:11:LEU:HD23	3:A:11:LEU:H	1.38	0.87
3:A:157:GLN:HE22	3:A:244:LYS:NZ	1.73	0.87
3:A:157:GLN:HE22	3:A:244:LYS:HZ1	1.22	0.86
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.17	0.85
3:A:197:HIS:ND1	3:A:198:PRO:HD2	1.92	0.84
3:A:282:MET:HE3	3:A:323:ILE:HD11	1.56	0.84
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.60	0.83
2:P:2:DA:C8	2:P:2:DA:H5'	2.13	0.83
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.08	0.83
3:A:18:MET:HE1	3:A:76:PHE:CB	2.10	0.82
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.78	0.82
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.62	0.82
2:P:1:DC:H2''	2:P:2:DA:H5''	1.61	0.81
3:A:108:PRO:O	3:A:112:ARG:HG2	1.81	0.80
3:A:278:PHE:HB2	3:A:333:ARG:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:296:TYR:HB2	3:A:297:THR:HG23	1.63	0.79
3:A:68:LYS:HB2	3:A:68:LYS:NZ	1.96	0.79
3:A:176:THR:HG22	3:A:178:CYS:SG	2.23	0.79
3:A:194:LEU:HD12	3:A:258:ARG:HG2	1.65	0.78
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.64	0.78
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.13	0.78
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.67	0.77
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.15	0.77
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.67	0.77
2:P:1:DC:C2'	2:P:2:DA:H5''	2.14	0.76
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.15	0.76
3:A:58:GLU:O	3:A:61:LYS:HB2	1.87	0.75
3:A:271:TYR:HB2	7:A:592:HOH:O	1.86	0.75
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.32	0.75
3:A:31:GLN:HG3	3:A:112:ARG:NH2	2.02	0.75
3:A:41:LYS:HD3	3:A:42:ALA:N	2.02	0.75
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.68	0.74
3:A:68:LYS:O	3:A:72:LYS:HE3	1.88	0.73
3:A:133:ASN:O	3:A:137:ARG:HG3	1.88	0.73
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.23	0.73
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.33	0.73
2:P:5:DT:H2''	2:P:6:DG:C5'	2.18	0.72
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.52	0.72
3:A:262:LYS:O	3:A:262:LYS:HG3	1.89	0.71
3:A:155:MET:HA	3:A:158:MET:HE3	1.72	0.71
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.25	0.71
3:A:259:LEU:O	3:A:260:ILE:HD13	1.90	0.71
3:A:201:THR:HA	3:A:261:PRO:HB3	1.73	0.70
3:A:40:ARG:HD3	7:A:506:HOH:O	1.90	0.70
3:A:279:ASN:O	3:A:283:ARG:HG3	1.92	0.70
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.22	0.70
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.22	0.69
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.74	0.69
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.27	0.69
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.73	0.69
3:A:253:ARG:HG2	3:A:253:ARG:HH11	1.58	0.69
3:A:292:THR:C	3:A:293:ILE:HD13	2.18	0.68
2:P:5:DT:H2'	2:P:6:DG:C8	2.30	0.67
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.76	0.67
3:A:172:GLU:HG2	3:A:198:PRO:CG	2.18	0.67
3:A:31:GLN:N	7:A:641:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:LYS:HD3	3:A:42:ALA:H	1.58	0.67
3:A:179:GLY:O	3:A:182:ARG:HB3	1.95	0.67
3:A:12:ASN:HD21	3:A:53:ILE:H	1.42	0.66
3:A:75:GLU:O	3:A:79:THR:HG23	1.95	0.66
3:A:150:ILE:HG21	3:A:158:MET:CE	2.24	0.66
3:A:212:HIS:HB3	7:A:541:HOH:O	1.96	0.66
3:A:306:VAL:HG23	3:A:307:ALA:N	2.10	0.66
3:A:259:LEU:C	3:A:260:ILE:HD13	2.21	0.65
1:T:7:DG:N3	7:T:634:HOH:O	2.29	0.65
3:A:26:GLU:HB2	3:A:36:TYR:HB2	1.78	0.65
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.11	0.65
3:A:245:ASN:N	3:A:245:ASN:ND2	2.38	0.65
3:A:162:VAL:O	3:A:166:VAL:HG23	1.97	0.64
3:A:254:ARG:HH11	3:A:255:ILE:H	1.44	0.64
3:A:154:GLU:O	3:A:158:MET:HG3	1.97	0.64
3:A:326:LYS:HG3	3:A:326:LYS:O	1.97	0.64
3:A:229:SER:HB3	7:A:513:HOH:O	1.97	0.64
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.62	0.64
3:A:241:LEU:HB3	3:A:242:PRO:HD2	1.79	0.64
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.13	0.63
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.26	0.63
3:A:79:THR:O	3:A:81:LYS:N	2.32	0.63
3:A:200:PHE:CE2	3:A:261:PRO:HD3	2.34	0.63
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.12	0.63
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.62	0.63
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.12	0.62
3:A:82:LEU:CD2	3:A:85:LEU:HD22	2.29	0.62
3:A:254:ARG:NH1	3:A:255:ILE:H	1.96	0.62
3:A:80:GLY:O	3:A:81:LYS:HG2	2.00	0.62
3:A:295:GLU:CD	3:A:295:GLU:H	2.08	0.62
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.29	0.61
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.82	0.61
3:A:27:LYS:HB3	3:A:36:TYR:CD2	2.35	0.61
3:A:42:ALA:O	3:A:46:ILE:HG23	2.00	0.61
3:A:266:TYR:HA	3:A:269:VAL:HB	1.82	0.61
3:A:213:GLN:HG2	7:A:644:HOH:O	2.01	0.60
3:A:25:PHE:CE2	3:A:88:ILE:HG12	2.37	0.60
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.27	0.60
3:A:133:ASN:HD22	3:A:135:HIS:N	1.99	0.60
3:A:11:LEU:H	3:A:11:LEU:CD2	2.14	0.60
3:A:195:LEU:O	3:A:259:LEU:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:282:MET:HB3	7:A:555:HOH:O	2.01	0.60
3:A:319:ILE:O	3:A:322:TYR:HB2	2.02	0.60
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.35	0.60
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.36	0.60
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.17	0.59
3:A:292:THR:O	3:A:298:ILE:HA	2.02	0.59
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.84	0.59
3:A:285:HIS:CE1	3:A:289:LYS:HG2	2.38	0.59
3:A:82:LEU:HD22	3:A:85:LEU:HD22	1.83	0.59
3:A:157:GLN:O	3:A:161:ILE:HG13	2.02	0.59
3:A:292:THR:O	3:A:293:ILE:HD13	2.03	0.59
3:A:165:GLU:OE1	3:A:168:LYS:NZ	2.30	0.59
3:A:330:PRO:O	3:A:333:ARG:HG3	2.03	0.59
3:A:288:GLU:C	3:A:290:GLY:H	2.11	0.58
3:A:294:ASN:HB2	3:A:295:GLU:OE2	2.04	0.58
3:A:23:ALA:O	3:A:36:TYR:HD2	1.87	0.58
3:A:32:ALA:O	3:A:36:TYR:N	2.31	0.57
3:A:111:ALA:O	3:A:115:VAL:HG23	2.04	0.57
3:A:157:GLN:O	3:A:160:ASP:HB3	2.04	0.57
3:A:331:LYS:HD2	3:A:332:ASP:N	2.19	0.57
3:A:255:ILE:HG12	3:A:256:ASP:N	2.20	0.57
3:A:272:PHE:O	6:A:338:DCT:H4'	2.04	0.57
3:A:68:LYS:HB2	3:A:68:LYS:HZ1	1.67	0.57
3:A:89:ARG:HB2	7:A:645:HOH:O	2.05	0.57
3:A:259:LEU:HD12	3:A:260:ILE:N	2.20	0.57
3:A:251:PRO:HG2	3:A:253:ARG:NH2	2.19	0.56
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.35	0.56
3:A:207:GLN:O	3:A:210:LEU:HB2	2.04	0.56
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.88	0.56
3:A:327:TYR:HE1	3:A:333:ARG:NH2	2.04	0.56
3:A:133:ASN:ND2	3:A:136:GLN:HG3	2.21	0.56
3:A:12:ASN:HB3	3:A:46:ILE:HD11	1.88	0.56
3:A:259:LEU:HD12	3:A:260:ILE:H	1.70	0.56
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.41	0.55
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.41	0.55
3:A:248:LYS:O	3:A:248:LYS:HG2	2.06	0.55
3:A:283:ARG:HB2	7:A:630:HOH:O	2.06	0.55
3:A:133:ASN:HD22	3:A:135:HIS:H	1.52	0.55
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.19	0.55
3:A:155:MET:SD	3:A:158:MET:HE3	2.46	0.55
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:LEU:CD1	3:A:258:ARG:HG2	2.35	0.55
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.88	0.55
3:A:287:LEU:HD22	3:A:291:PHE:O	2.07	0.54
3:A:32:ALA:O	3:A:36:TYR:HB3	2.08	0.54
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.89	0.54
3:A:157:GLN:NE2	3:A:244:LYS:NZ	2.52	0.53
3:A:193:VAL:C	3:A:194:LEU:HD13	2.33	0.53
3:A:200:PHE:HB2	3:A:210:LEU:CD1	2.39	0.53
3:A:28:ASN:HD22	3:A:28:ASN:N	2.07	0.53
3:A:270:LEU:HD12	3:A:333:ARG:NH1	2.23	0.53
3:A:289:LYS:HG3	3:A:323:ILE:O	2.09	0.53
3:A:207:GLN:OE1	3:A:210:LEU:HG	2.08	0.53
3:A:278:PHE:CZ	3:A:328:ARG:HG3	2.43	0.52
3:A:303:VAL:C	3:A:305:GLY:H	2.16	0.52
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.08	0.52
3:A:242:PRO:HG2	7:A:589:HOH:O	2.09	0.52
3:A:43:ALA:O	3:A:47:ALA:HB2	2.08	0.52
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.40	0.52
3:A:317:LYS:HG3	7:A:501:HOH:O	2.09	0.52
3:A:46:ILE:HD12	3:A:46:ILE:O	2.09	0.52
1:T:6:DT:H5"	7:T:547:HOH:O	2.09	0.51
3:A:277:ILE:CG1	3:A:335:GLU:HA	2.40	0.51
3:A:254:ARG:NH1	3:A:255:ILE:N	2.58	0.51
3:A:194:LEU:HD11	3:A:258:ARG:CD	2.38	0.51
3:A:235:PHE:CZ	3:A:237:GLY:HA3	2.45	0.51
3:A:286:ALA:O	3:A:291:PHE:HB2	2.10	0.51
3:A:62:LEU:HB2	3:A:65:VAL:HG13	1.91	0.51
3:A:18:MET:HE3	3:A:76:PHE:CD1	2.45	0.51
3:A:18:MET:CE	3:A:76:PHE:HB2	2.33	0.51
3:A:133:ASN:ND2	3:A:136:GLN:H	2.08	0.51
3:A:18:MET:HE1	3:A:76:PHE:CG	2.47	0.50
3:A:79:THR:C	3:A:81:LYS:H	2.18	0.50
3:A:172:GLU:CG	3:A:198:PRO:HG3	2.21	0.50
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.92	0.50
3:A:150:ILE:O	3:A:187:SER:HA	2.11	0.50
3:A:251:PRO:HG2	3:A:253:ARG:CZ	2.41	0.50
2:P:4:DA:H1'	7:P:595:HOH:O	2.12	0.50
3:A:288:GLU:O	3:A:290:GLY:N	2.44	0.50
3:A:18:MET:HG2	3:A:22:LEU:HD23	1.94	0.50
3:A:201:THR:HG23	3:A:204:SER:HB3	1.94	0.50
3:A:267:CYS:SG	3:A:297:THR:HA	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:O	3:A:185:ALA:HB3	2.12	0.49
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.11	0.49
3:A:49:TYR:CB	3:A:50:PRO:HD2	2.32	0.49
3:A:223:PHE:O	3:A:239:CYS:HB2	2.13	0.49
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.94	0.49
3:A:80:GLY:C	3:A:81:LYS:HG2	2.38	0.49
3:A:193:VAL:O	3:A:194:LEU:HD13	2.12	0.49
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.40	0.49
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.95	0.49
3:A:200:PHE:O	3:A:262:LYS:N	2.36	0.49
3:A:155:MET:CE	3:A:188:SER:HB2	2.43	0.48
3:A:121:THR:O	3:A:124:ASP:HB2	2.13	0.48
3:A:164:ASN:O	3:A:168:LYS:HG2	2.14	0.48
3:A:276:ASP:N	3:A:276:ASP:OD1	2.45	0.48
3:A:331:LYS:CD	3:A:332:ASP:N	2.77	0.48
3:A:119:ILE:HA	3:A:124:ASP:HB3	1.95	0.48
3:A:215:VAL:O	3:A:219:GLN:HG2	2.13	0.48
3:A:296:TYR:CD1	3:A:296:TYR:N	2.81	0.48
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.95	0.47
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.96	0.47
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.79	0.47
3:A:310:PRO:O	3:A:312:PRO:HD3	2.14	0.47
3:A:41:LYS:NZ	3:A:64:GLY:O	2.29	0.47
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.48	0.47
3:A:311:LEU:HA	3:A:312:PRO:HD2	1.80	0.47
3:A:33:ILE:O	3:A:37:ASN:HB2	2.14	0.47
3:A:60:LYS:CA	3:A:65:VAL:HG22	2.34	0.47
3:A:22:LEU:HD21	3:A:82:LEU:CD2	2.45	0.47
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.45	0.47
3:A:283:ARG:O	3:A:286:ALA:HB3	2.15	0.47
3:A:285:HIS:CD2	3:A:325:TRP:CD1	3.03	0.46
3:A:211:LEU:HD12	3:A:211:LEU:O	2.15	0.46
3:A:279:ASN:C	3:A:283:ARG:HG3	2.40	0.46
3:A:99:PHE:O	3:A:102:ARG:HG3	2.14	0.46
3:A:285:HIS:NE2	3:A:323:ILE:O	2.45	0.46
3:A:331:LYS:HD2	3:A:332:ASP:H	1.80	0.46
3:A:11:LEU:CD2	3:A:11:LEU:N	2.77	0.46
3:A:235:PHE:CD1	3:A:235:PHE:C	2.92	0.46
3:A:254:ARG:HH11	3:A:255:ILE:N	2.11	0.46
3:A:184:GLY:O	3:A:185:ALA:O	2.33	0.46
3:A:259:LEU:HD12	3:A:259:LEU:HA	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.64	0.46
3:A:176:THR:HB	3:A:265:TYR:OH	2.16	0.46
3:A:325:TRP:HD1	7:A:583:HOH:O	1.98	0.46
3:A:62:LEU:HB2	3:A:65:VAL:CG1	2.46	0.46
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.36	0.46
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.97	0.45
3:A:133:ASN:HD21	3:A:136:GLN:HG3	1.81	0.45
3:A:37:ASN:HD22	3:A:37:ASN:HA	1.57	0.45
3:A:205:THR:O	3:A:206:LYS:O	2.34	0.45
3:A:133:ASN:HD21	3:A:136:GLN:H	1.64	0.45
3:A:145:ASP:CG	3:A:252:HIS:H	2.24	0.45
3:A:200:PHE:HE2	3:A:261:PRO:HD3	1.80	0.45
3:A:158:MET:O	3:A:161:ILE:N	2.49	0.45
3:A:280:LYS:HA	3:A:283:ARG:HG3	1.98	0.45
3:A:150:ILE:HD13	3:A:253:ARG:HG2	1.98	0.45
3:A:18:MET:CE	3:A:76:PHE:CD1	3.00	0.45
2:P:5:DT:H1'	7:A:565:HOH:O	2.17	0.45
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.79	0.45
3:A:95:SER:HA	7:A:639:HOH:O	2.15	0.45
3:A:180:SER:HB2	3:A:185:ALA:HB3	1.98	0.45
3:A:15:ILE:HD11	3:A:77:LEU:CD1	2.47	0.44
3:A:188:SER:HB3	7:A:659:HOH:O	2.16	0.44
3:A:253:ARG:NH1	7:A:503:HOH:O	2.50	0.44
3:A:85:LEU:O	3:A:89:ARG:HG3	2.16	0.44
3:A:264:GLN:HB3	3:A:296:TYR:O	2.17	0.44
3:A:83:ARG:O	3:A:86:GLU:N	2.49	0.44
3:A:298:ILE:HG21	3:A:322:TYR:CD2	2.52	0.44
2:P:4:DA:H5''	7:P:614:HOH:O	2.18	0.44
3:A:183:ARG:NH1	3:A:275:SER:HA	2.31	0.44
3:A:194:LEU:HD21	3:A:272:PHE:CD2	2.53	0.44
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.26	0.44
3:A:146:PHE:HD1	3:A:146:PHE:HA	1.39	0.44
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.99	0.44
3:A:245:ASN:HD22	3:A:245:ASN:H	1.60	0.44
3:A:18:MET:HG2	3:A:22:LEU:CD2	2.47	0.44
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.40	0.44
3:A:255:ILE:HG23	3:A:255:ILE:O	2.17	0.44
3:A:133:ASN:ND2	3:A:135:HIS:N	2.66	0.44
3:A:245:ASN:ND2	3:A:245:ASN:H	2.12	0.44
3:A:311:LEU:HA	3:A:311:LEU:HD12	1.82	0.44
3:A:45:VAL:HG22	3:A:46:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:VAL:HG22	3:A:193:VAL:HG22	2.00	0.43
3:A:88:ILE:HD13	3:A:88:ILE:HG21	1.82	0.43
3:A:208:PRO:O	3:A:212:HIS:HD2	2.01	0.43
3:A:212:HIS:N	3:A:212:HIS:CD2	2.86	0.43
3:A:275:SER:OG	3:A:277:ILE:HG12	2.18	0.43
3:A:268:GLY:O	3:A:271:TYR:HB3	2.18	0.43
3:A:277:ILE:HG13	3:A:335:GLU:HA	2.00	0.43
3:A:320:PHE:CE1	3:A:325:TRP:HE3	2.37	0.43
3:A:204:SER:O	3:A:204:SER:OG	2.32	0.43
3:A:322:TYR:C	3:A:324:GLN:H	2.24	0.43
3:A:133:ASN:ND2	7:A:512:HOH:O	2.52	0.43
3:A:134:HIS:HD2	7:A:515:HOH:O	2.01	0.43
3:A:195:LEU:O	3:A:260:ILE:N	2.44	0.43
3:A:25:PHE:CD1	3:A:25:PHE:C	2.97	0.42
3:A:31:GLN:CD	3:A:112:ARG:HH12	2.23	0.42
3:A:82:LEU:HD23	3:A:85:LEU:HD22	2.01	0.42
3:A:213:GLN:HE21	3:A:213:GLN:HB2	1.58	0.42
3:A:282:MET:CE	3:A:323:ILE:HD11	2.40	0.42
3:A:27:LYS:HG2	3:A:28:ASN:ND2	2.34	0.42
3:A:100:LEU:N	3:A:100:LEU:CD1	2.79	0.42
3:A:180:SER:OG	3:A:188:SER:HB3	2.19	0.42
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.77	0.42
3:A:288:GLU:C	3:A:290:GLY:N	2.77	0.42
3:A:36:TYR:CD1	3:A:36:TYR:C	2.95	0.42
3:A:99:PHE:CD1	3:A:99:PHE:C	2.98	0.42
3:A:115:VAL:C	3:A:117:GLU:N	2.77	0.42
3:A:120:LYS:N	3:A:124:ASP:OD2	2.41	0.42
3:A:209:LYS:O	3:A:213:GLN:HG3	2.19	0.42
3:A:11:LEU:HD23	3:A:11:LEU:N	2.13	0.42
3:A:19:LEU:HD12	3:A:19:LEU:HA	1.83	0.42
3:A:155:MET:HE3	3:A:188:SER:OG	2.20	0.42
3:A:180:SER:HB2	3:A:185:ALA:CB	2.49	0.42
3:A:177:VAL:HG21	3:A:191:MET:HE2	2.02	0.42
3:A:243:SER:HB3	3:A:249:GLU:HA	2.02	0.42
3:A:288:GLU:OE1	3:A:288:GLU:HA	1.90	0.42
3:A:18:MET:CG	3:A:22:LEU:CD2	2.98	0.42
3:A:135:HIS:C	3:A:135:HIS:CD2	2.98	0.42
3:A:241:LEU:HA	3:A:242:PRO:HD3	1.66	0.42
3:A:320:PHE:CZ	3:A:328:ARG:HB2	2.55	0.42
3:A:206:LYS:O	3:A:207:GLN:HB2	2.19	0.41
3:A:330:PRO:C	3:A:333:ARG:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:ILE:CD1	3:A:298:ILE:CG1	2.97	0.41
3:A:15:ILE:HG12	3:A:73:ILE:HG23	2.02	0.41
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.85	0.41
3:A:254:ARG:HD2	3:A:254:ARG:HA	1.71	0.41
3:A:12:ASN:ND2	3:A:53:ILE:H	2.15	0.41
3:A:85:LEU:HG	3:A:89:ARG:HH21	1.84	0.41
3:A:152:ARG:NH2	3:A:181:PHE:O	2.53	0.41
3:A:156:LEU:HD23	3:A:181:PHE:CE1	2.55	0.41
3:A:197:HIS:CE1	3:A:199:SER:HB3	2.54	0.41
3:A:243:SER:CB	3:A:249:GLU:HA	2.50	0.41
3:A:133:ASN:ND2	3:A:133:ASN:C	2.78	0.41
3:A:165:GLU:HB2	3:A:218:LEU:HD11	2.01	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.81	0.41
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.49	0.41
3:A:216:GLU:O	3:A:220:LYS:N	2.54	0.41
3:A:266:TYR:O	3:A:270:LEU:N	2.39	0.41
2:P:5:DT:P	3:A:109:SER:HB3	2.61	0.41
3:A:196:THR:OG1	3:A:197:HIS:N	2.53	0.41
1:T:6:DT:H2''	1:T:7:DG:C8	2.56	0.41
3:A:12:ASN:CB	3:A:46:ILE:CD1	2.97	0.41
3:A:18:MET:CE	3:A:76:PHE:CG	3.04	0.41
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.09	0.41
1:T:2:DC:H6	1:T:2:DC:H2'	1.63	0.40
3:A:138:ILE:HD13	3:A:138:ILE:HG23	1.76	0.40
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.35	0.40
3:A:308:GLY:O	3:A:309:GLU:HB2	2.20	0.40
3:A:200:PHE:HB2	3:A:210:LEU:HD11	2.03	0.40
3:A:115:VAL:C	3:A:117:GLU:H	2.28	0.40
3:A:301:LEU:HA	3:A:301:LEU:HD12	1.67	0.40
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.40
3:A:196:THR:OG1	3:A:262:LYS:HA	2.22	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)
3:A:83:ARG:NH1	3:A:117:GLU:CB[3_558]	2.11	0.09

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%)	271 (83%)	38 (12%)	16 (5%)	1 6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	289	LYS
3	A	309	GLU
3	A	10	THR
3	A	80	GLY
3	A	246	ASP
3	A	247	GLU
3	A	307	ALA
3	A	204	SER
3	A	304	THR
3	A	310	PRO
3	A	91	ASP
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	215 (75%)	73 (25%)	0 2

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	22	LEU
3	A	25	PHE
3	A	27	LYS
3	A	30	SER
3	A	33	ILE
3	A	36	TYR
3	A	37	ASN
3	A	40	ARG
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	52	LYS
3	A	54	LYS
3	A	62	LEU
3	A	65	VAL
3	A	67	THR
3	A	68	LYS
3	A	72	LYS
3	A	79	THR
3	A	81	LYS
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	112	ARG
3	A	119	ILE
3	A	122	LEU
3	A	131	LYS
3	A	150	ILE
3	A	152	ARG
3	A	153	GLU
3	A	168	LYS

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Mol	Chain	Res	Type
3	A	171	SER
3	A	172	GLU
3	A	176	THR
3	A	182	ARG
3	A	183	ARG
3	A	188	SER
3	A	194	LEU
3	A	201	THR
3	A	202	SER
3	A	204	SER
3	A	214	VAL
3	A	218	LEU
3	A	228	LEU
3	A	233	THR
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	258	ARG
3	A	259	LEU
3	A	264	GLN
3	A	270	LEU
3	A	276	ASP
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
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	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	51	HIS
3	A	90	GLN
3	A	133	ASN
3	A	136	GLN
3	A	157	GLN
3	A	159	GLN
3	A	212	HIS
3	A	213	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	DCT	A	338	4	27,28,28	1.75	4 (14%)	37,43,43	1.93	3 (8%)

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	DCT	A	338	4	-	8/22/31/31	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	338	DCT	PG-O1G	-3.97	1.38	1.50
6	A	338	DCT	PA-O3A	-3.94	1.55	1.59
6	A	338	DCT	C1'-N1	3.90	1.57	1.48
6	A	338	DCT	O4'-C4'	-2.39	1.40	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	338	DCT	C1'-N1-C6	-7.24	107.28	121.53
6	A	338	DCT	C1'-N1-C2	7.08	129.98	117.83
6	A	338	DCT	PA-O5'-C5'	2.06	133.15	121.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

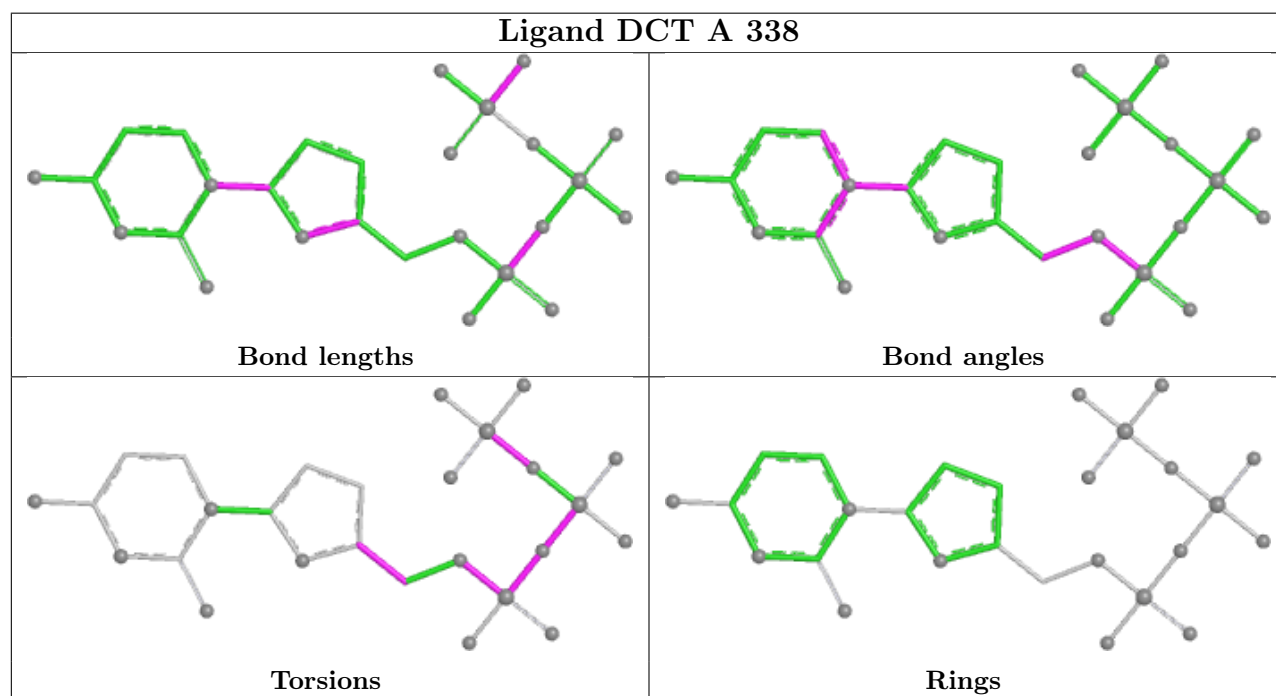
Mol	Chain	Res	Type	Atoms
6	A	338	DCT	C3'-C4'-C5'-O5'
6	A	338	DCT	O4'-C4'-C5'-O5'
6	A	338	DCT	C5'-O5'-PA-O1A
6	A	338	DCT	PB-O3A-PA-O5'
6	A	338	DCT	PB-O3B-PG-O2G
6	A	338	DCT	PB-O3B-PG-O1G
6	A	338	DCT	PA-O3A-PB-O2B
6	A	338	DCT	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	338	DCT	1	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 [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	7/7 (100%)	-1.26	0 100 100	20, 34, 66, 100	0
2	P	6/6 (100%)	-1.56	0 100 100	17, 25, 29, 34	0
3	A	324/335 (96%)	-0.90	0 100 100	7, 38, 89, 100	0
All	All	337/348 (96%)	-0.92	0 100 100	7, 36, 89, 100	0

There are no RSRZ outliers to report.

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](#)

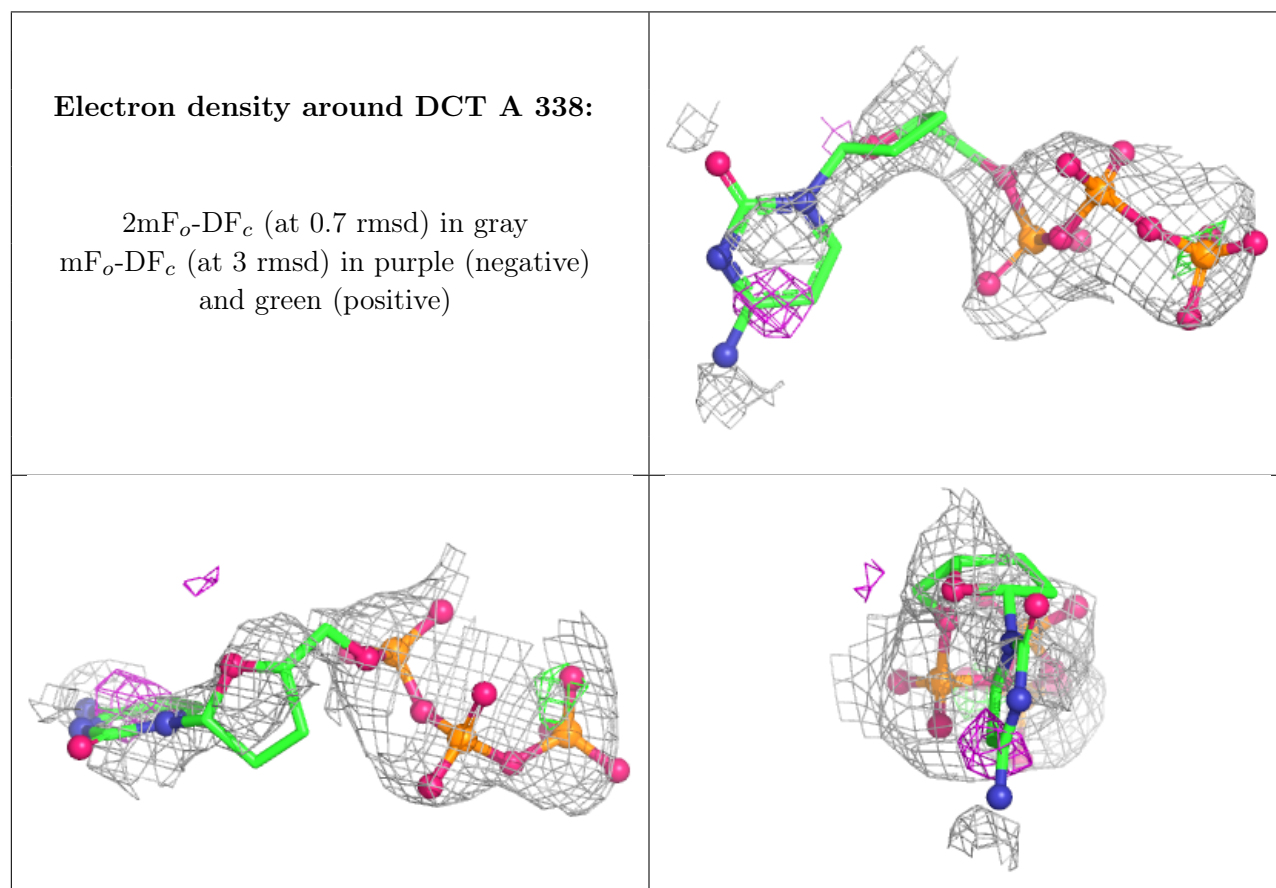
There are no oligosaccharides in this entry.

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
6	DCT	A	338	27/27	0.85	0.15	59,71,81,82	27
4	MN	A	340	1/1	0.93	0.08	30,30,30,30	1
4	MN	A	339	1/1	0.96	0.03	30,30,30,30	1
5	NA	A	341	1/1	0.97	0.04	31,31,31,31	0
5	NA	A	342	1/1	0.98	0.04	40,40,40,40	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 ⓘ

There are no such residues in this entry.