



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:00 AM UTC

PDB ID : 8ICZ / pdb_00008icz
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF OF DATP (1 MILLIMOLAR), MNCL2 (5 MILLIMOLAR), AND LITHIUM SULFATE (75 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-01-04
Resolution : 3.10 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

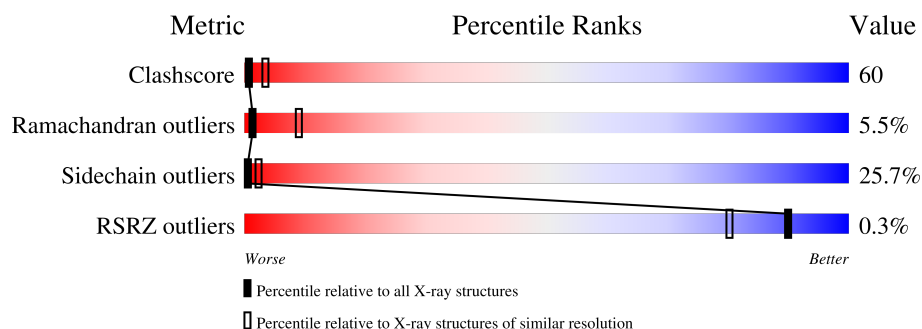
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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% 38% 50%
2	P	7	43% 57%
3	A	335	17% 45% 29% 7% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3060 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	0	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- 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		

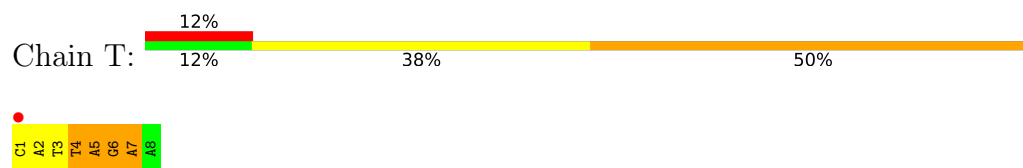
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	15	Total	O	0	0
			15	15		
6	P	16	Total	O	0	0
			16	16		
6	A	110	Total	O	0	0
			110	110		

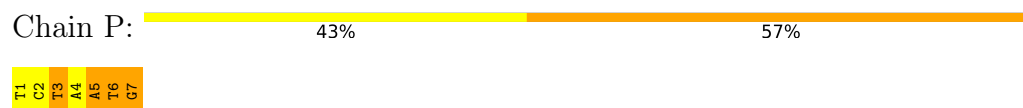
3 Residue-property plots [i](#)

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.

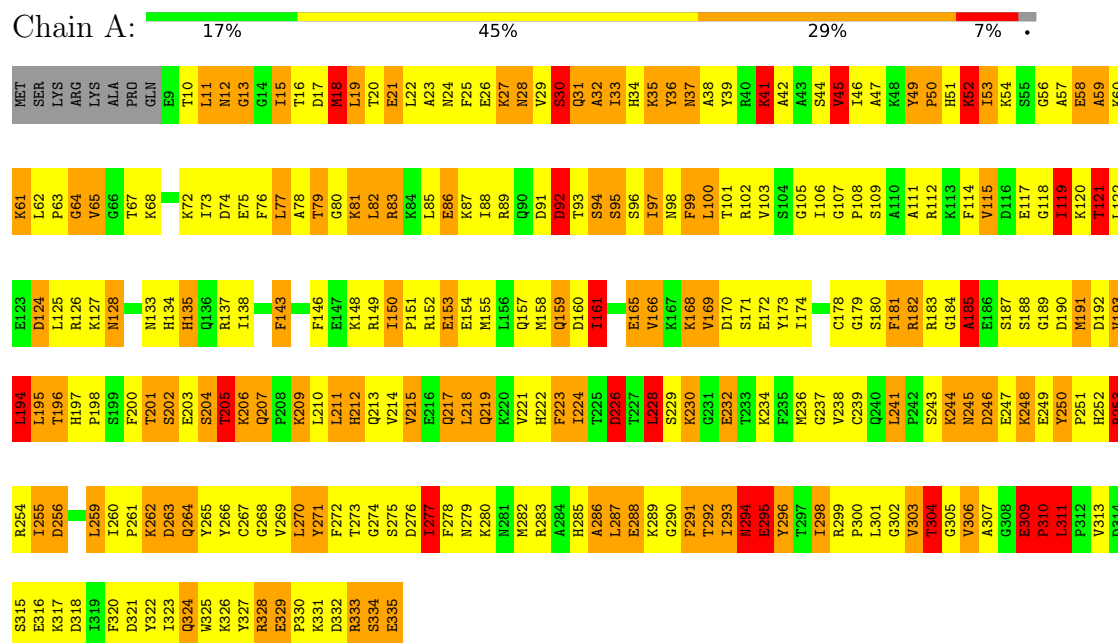
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- 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	178.58Å 57.74Å 48.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.10) 94.1 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.70Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.155 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 264.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3060	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: SO4, 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	1.11	0/162	3.00	12/249 (4.8%)
2	P	1.39	1/160 (0.6%)	4.30	17/243 (7.0%)
3	A	1.52	11/2672 (0.4%)	2.20	125/3590 (3.5%)
All	All	1.50	12/2994 (0.4%)	2.43	154/4082 (3.8%)

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	3	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1	DT	OP3-P	7.04	1.62	1.48
3	A	194	LEU	C-N	-6.87	1.24	1.33
3	A	15	ILE	CA-C	-6.66	1.44	1.52
3	A	30	SER	C-N	-6.59	1.25	1.33
3	A	58	GLU	N-CA	-5.92	1.39	1.46
3	A	63	PRO	N-CA	-5.84	1.40	1.47
3	A	124	ASP	CA-C	-5.57	1.45	1.52
3	A	36	TYR	N-CA	-5.57	1.39	1.46
3	A	35	LYS	C-N	-5.38	1.27	1.33
3	A	246	ASP	CG-OD1	5.03	1.34	1.25
3	A	193	VAL	CA-CB	-5.02	1.48	1.54
3	A	28	ASN	CA-C	-5.00	1.46	1.52

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	DT	C2-N1-C1'	27.31	160.32	119.35
2	P	1	DT	C6-N1-C1'	-27.15	78.62	119.35
2	P	3	DT	C6-N1-C1'	-25.40	81.25	119.35
2	P	3	DT	C2-N1-C1'	25.38	157.42	119.35
1	T	4	DT	C6-N1-C1'	-20.18	89.08	119.35
1	T	4	DT	C2-N1-C1'	18.71	147.42	119.35
2	P	6	DT	C6-N1-C1'	-17.50	93.11	119.35
2	P	6	DT	C2-N1-C1'	17.01	144.86	119.35
3	A	28	ASN	CA-CB-CG	-16.73	95.87	112.60
1	T	6	DG	C8-N9-C1'	15.38	150.07	127.00
1	T	6	DG	C4-N9-C1'	-15.20	104.21	127.00
3	A	49	TYR	CA-C-N	15.14	136.93	120.12
3	A	49	TYR	C-N-CA	15.14	136.93	120.12
1	T	2	DA	C4-N9-C1'	-10.16	111.81	127.05
3	A	49	TYR	O-C-N	9.67	129.73	121.31
1	T	2	DA	C8-N9-C1'	9.45	141.22	127.05
3	A	181	PHE	CA-CB-CG	-8.92	104.88	113.80
2	P	3	DT	N1-C1'-C2'	8.80	126.70	113.50
3	A	291	PHE	CA-CB-CG	-8.51	105.29	113.80
3	A	333	ARG	N-CA-C	-8.41	103.52	112.93
2	P	3	DT	O4'-C1'-N1	8.33	120.90	108.40
3	A	15	ILE	N-CA-CB	8.20	119.61	110.51
3	A	223	PHE	N-CA-C	-8.15	102.93	113.12
3	A	232	GLU	N-CA-C	7.79	122.47	112.34
3	A	157	GLN	N-CA-CB	7.78	121.56	110.12
3	A	99	PHE	CA-CB-CG	-7.76	106.04	113.80
3	A	168	LYS	N-CA-CB	7.71	121.45	110.12
3	A	252	HIS	CA-CB-CG	-7.51	106.29	113.80
3	A	34	HIS	CA-CB-CG	-7.43	106.37	113.80
3	A	45	VAL	N-CA-C	7.32	118.11	110.72
3	A	288	GLU	N-CA-C	-7.25	103.31	111.14
3	A	18	MET	CA-C-N	7.25	129.99	120.28
3	A	18	MET	C-N-CA	7.25	129.99	120.28
3	A	92	ASP	N-CA-CB	7.15	120.74	110.16
2	P	5	DA	P-O5'-C5'	-6.97	109.54	120.00
3	A	68	LYS	N-CA-CB	6.91	120.27	110.12
3	A	313	VAL	N-CA-C	6.90	117.77	108.11
3	A	190	ASP	CA-C-N	-6.87	112.97	122.93
3	A	190	ASP	C-N-CA	-6.87	112.97	122.93
3	A	159	GLN	CB-CA-C	-6.87	99.82	110.81
3	A	31	GLN	N-CA-C	-6.86	99.37	109.11
1	T	5	DA	C4-N9-C1'	-6.83	116.80	127.05
3	A	68	LYS	N-CA-C	6.77	118.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	105	GLY	N-CA-C	-6.75	106.44	114.48
3	A	195	LEU	N-CA-C	6.72	120.41	109.59
3	A	219	GLN	CB-CA-C	-6.62	99.60	110.85
3	A	33	ILE	N-CA-CB	-6.61	100.32	111.23
2	P	7	DG	O5'-C5'-C4'	6.58	120.68	110.80
3	A	117	GLU	N-CA-C	-6.52	105.24	113.72
1	T	1	DC	P-O3'-C3'	6.49	129.94	120.20
3	A	271	TYR	CA-CB-CG	-6.49	102.23	113.90
3	A	135	HIS	O-C-N	6.47	129.00	122.08
3	A	256	ASP	CA-CB-CG	6.43	119.03	112.60
3	A	241	LEU	CA-C-O	6.39	125.45	119.76
3	A	329	GLU	N-CA-C	-6.37	101.55	109.64
3	A	309	GLU	CA-C-N	6.36	127.80	119.84
3	A	309	GLU	C-N-CA	6.36	127.80	119.84
3	A	121	THR	N-CA-C	6.34	119.75	110.17
3	A	194	LEU	CA-C-N	-6.22	113.91	122.93
3	A	194	LEU	C-N-CA	-6.22	113.91	122.93
3	A	296	TYR	N-CA-C	6.20	122.31	114.31
3	A	266	TYR	CA-CB-CG	-6.17	102.79	113.90
3	A	97	ILE	CB-CA-C	-6.16	102.28	112.26
2	P	2	DC	C2-N1-C1'	6.16	128.93	119.70
3	A	50	PRO	CB-CA-C	-6.12	100.75	111.21
3	A	303	VAL	CB-CA-C	6.09	121.27	111.29
3	A	212	HIS	CA-CB-CG	-6.06	107.74	113.80
3	A	310	PRO	N-CA-C	6.05	124.92	112.47
3	A	215	VAL	O-C-N	6.04	127.83	121.91
3	A	87	LYS	CA-C-N	6.01	128.69	120.46
3	A	87	LYS	C-N-CA	6.01	128.69	120.46
3	A	146	PHE	CA-CB-CG	-5.98	107.82	113.80
2	P	5	DA	C4-N9-C1'	5.96	135.99	127.05
3	A	205	THR	N-CA-CB	5.90	120.46	110.49
3	A	224	ILE	CA-CB-CG1	-5.89	100.38	110.40
1	T	1	DC	C6-N1-C1'	-5.87	110.89	119.70
3	A	303	VAL	N-CA-C	5.87	121.54	109.34
3	A	24	ASN	CA-CB-CG	-5.86	106.74	112.60
3	A	205	THR	N-CA-C	5.86	123.28	110.80
3	A	277	ILE	N-CA-CB	5.84	118.04	110.57
3	A	196	THR	N-CA-CB	5.82	121.38	111.66
3	A	267	CYS	N-CA-C	-5.81	104.31	111.40
3	A	185	ALA	CA-C-N	5.81	128.86	120.38
3	A	185	ALA	C-N-CA	5.81	128.86	120.38
3	A	246	ASP	N-CA-C	5.79	123.13	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	DT	C5'-C4'-O4'	5.79	118.08	109.40
1	T	6	DG	C4'-C3'-O3'	-5.78	101.33	110.00
3	A	41	LYS	N-CA-CB	5.77	118.60	110.12
3	A	53	ILE	N-CA-CB	5.77	117.22	110.82
2	P	5	DA	O5'-C5'-C4'	5.77	119.45	110.80
3	A	118	GLY	CA-C-N	-5.77	115.16	122.43
3	A	118	GLY	C-N-CA	-5.77	115.16	122.43
3	A	30	SER	CA-C-N	-5.70	115.16	122.79
3	A	30	SER	C-N-CA	-5.70	115.16	122.79
3	A	250	TYR	N-CA-C	5.68	118.12	110.29
3	A	32	ALA	N-CA-C	5.67	122.89	110.80
3	A	64	GLY	CA-C-N	-5.66	115.40	122.48
3	A	64	GLY	C-N-CA	-5.66	115.40	122.48
3	A	86	GLU	N-CA-CB	5.66	118.50	110.13
3	A	253	ARG	N-CA-C	5.65	118.11	108.90
3	A	102	ARG	CA-CB-CG	-5.63	102.83	114.10
3	A	226	ASP	N-CA-CB	5.63	121.06	111.66
1	T	7	DA	P-O3'-C3'	-5.61	111.78	120.20
3	A	334	SER	N-CA-C	5.59	118.09	111.33
3	A	17	ASP	N-CA-C	5.58	117.44	111.36
3	A	12	ASN	CB-CA-C	5.54	120.09	110.72
3	A	270	LEU	O-C-N	5.52	127.76	122.07
3	A	20	THR	N-CA-CB	5.51	118.41	110.20
3	A	119	ILE	N-CA-CB	5.50	118.07	111.31
3	A	192	ASP	CB-CA-C	-5.49	101.18	110.19
1	T	1	DC	C2-N1-C1'	5.47	127.90	119.70
3	A	52	LYS	N-CA-CB	5.46	118.77	109.87
3	A	161	ILE	N-CA-CB	5.43	117.52	110.57
3	A	102	ARG	CD-NE-CZ	-5.43	116.80	124.40
3	A	228	LEU	N-CA-C	-5.41	105.81	112.90
2	P	3	DT	C4'-C3'-O3'	-5.41	101.89	110.00
3	A	150	ILE	CA-C-N	-5.40	114.42	120.14
3	A	150	ILE	C-N-CA	-5.40	114.42	120.14
3	A	334	SER	CB-CA-C	5.39	119.84	110.68
3	A	318	ASP	CA-CB-CG	-5.38	107.22	112.60
3	A	263	ASP	CA-CB-CG	5.35	117.95	112.60
3	A	143	PHE	CA-CB-CG	-5.34	108.46	113.80
3	A	311	LEU	CA-C-N	5.33	126.16	120.13
3	A	311	LEU	C-N-CA	5.33	126.16	120.13
3	A	215	VAL	N-CA-C	-5.29	105.34	110.42
3	A	82	LEU	CB-CA-C	5.28	119.26	109.70
3	A	271	TYR	N-CA-CB	-5.24	101.85	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	181	PHE	CA-C-N	5.24	129.47	120.72
3	A	181	PHE	C-N-CA	5.24	129.47	120.72
3	A	18	MET	O-C-N	5.23	127.45	122.07
3	A	11	LEU	N-CA-C	-5.18	106.22	112.54
3	A	295	GLU	CB-CG-CD	5.18	121.40	112.60
3	A	115	VAL	N-CA-CB	-5.18	104.49	110.55
3	A	294	ASN	CA-CB-CG	5.17	117.77	112.60
3	A	57	ALA	N-CA-CB	-5.16	101.37	109.78
3	A	207	GLN	CA-C-N	5.12	124.74	119.05
3	A	207	GLN	C-N-CA	5.12	124.74	119.05
2	P	4	DA	C8-N9-C1'	-5.12	119.37	127.05
3	A	27	LYS	N-CA-CB	-5.11	101.86	110.49
2	P	5	DA	C8-N9-C1'	-5.10	119.40	127.05
3	A	292	THR	CB-CA-C	5.09	117.47	110.34
3	A	286	ALA	CA-C-N	5.09	127.52	120.29
3	A	286	ALA	C-N-CA	5.09	127.52	120.29
3	A	21	GLU	CA-C-N	5.08	127.05	120.44
3	A	21	GLU	C-N-CA	5.08	127.05	120.44
3	A	272	PHE	CA-CB-CG	-5.08	108.72	113.80
3	A	98	ASN	CB-CA-C	5.05	120.37	110.67
3	A	215	VAL	CB-CA-C	5.04	118.42	111.97
3	A	134	HIS	N-CA-C	5.01	117.13	111.02
3	A	13	GLY	CA-C-N	5.01	125.50	119.94
3	A	13	GLY	C-N-CA	5.01	125.50	119.94
3	A	59	ALA	O-C-N	5.00	127.22	122.07
3	A	120	LYS	CA-CB-CG	-5.00	104.10	114.10
3	A	304	THR	N-CA-CB	-5.00	102.04	110.49

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	205	THR	CA
3	A	246	ASP	CA
3	A	303	VAL	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	9	0
2	P	144	0	81	13	0
3	A	2623	0	2641	317	0
4	A	5	0	0	1	0
5	A	2	0	0	0	0
6	A	110	0	0	13	0
6	P	16	0	0	0	0
6	T	15	0	0	5	0
All	All	3060	0	2802	336	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 60.

All (336) 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:180:SER:HB3	3:A:183:ARG:HH21	1.08	1.10
3:A:330:PRO:HA	3:A:333:ARG:HG2	1.36	1.07
3:A:72:LYS:HG2	3:A:82:LEU:HD11	1.36	1.03
3:A:155:MET:HA	3:A:158:MET:HE3	1.40	1.03
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.42	1.00
3:A:155:MET:HE2	3:A:188:SER:HB2	1.43	0.98
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.47	0.96
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.48	0.95
3:A:245:ASN:H	3:A:245:ASN:HD22	0.94	0.93
2:P:5:DA:H2''	2:P:6:DT:H5''	1.49	0.93
3:A:217:GLN:HE21	3:A:217:GLN:HA	1.32	0.92
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.49	0.91
3:A:330:PRO:HA	3:A:333:ARG:CG	2.01	0.90
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.07	0.90
3:A:41:LYS:HE2	3:A:64:GLY:HA3	1.55	0.88
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.72	0.87
3:A:180:SER:HB3	3:A:183:ARG:NH2	1.89	0.86
3:A:27:LYS:HB2	3:A:36:TYR:CD1	2.10	0.86
3:A:245:ASN:H	3:A:245:ASN:ND2	1.74	0.85
3:A:15:ILE:HD13	3:A:73:ILE:HG23	1.59	0.84
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.08	0.83
3:A:82:LEU:HD23	3:A:85:LEU:HB2	1.59	0.83
3:A:29:VAL:HG21	3:A:94:SER:HB2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.10	0.81
3:A:180:SER:HA	3:A:183:ARG:HE	1.46	0.81
2:P:5:DA:H2''	2:P:6:DT:C5'	2.11	0.80
3:A:271:TYR:HB2	6:A:592:HOH:O	1.81	0.79
3:A:285:HIS:HD2	3:A:323:ILE:HD12	1.48	0.79
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.13	0.78
3:A:302:GLY:H	3:A:307:ALA:HB3	1.47	0.78
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.29	0.78
3:A:18:MET:CE	3:A:82:LEU:HD13	2.14	0.77
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.14	0.77
3:A:277:ILE:HG12	3:A:335:GLU:HA	1.67	0.77
3:A:18:MET:HE3	3:A:76:PHE:HB2	1.67	0.77
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.66	0.77
3:A:60:LYS:HA	3:A:65:VAL:HG23	1.66	0.76
3:A:191:MET:HG3	3:A:255:ILE:HG13	1.65	0.76
3:A:33:ILE:O	3:A:37:ASN:HB2	1.87	0.75
3:A:49:TYR:CE2	3:A:51:HIS:HB2	2.21	0.75
3:A:323:ILE:O	3:A:324:GLN:HG2	1.87	0.75
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.02	0.74
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.17	0.74
3:A:212:HIS:HB3	6:A:541:HOH:O	1.87	0.74
3:A:245:ASN:HD22	3:A:245:ASN:N	1.73	0.74
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.70	0.73
3:A:91:ASP:O	3:A:95:SER:HB2	1.88	0.73
3:A:172:GLU:HB3	3:A:197:HIS:NE2	2.04	0.73
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.71	0.72
3:A:172:GLU:HG3	3:A:198:PRO:HG2	1.70	0.72
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.70	0.72
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.55	0.72
3:A:182:ARG:HH11	3:A:273:THR:HG21	1.55	0.71
2:P:6:DT:H2''	2:P:7:DG:H5''	1.71	0.71
3:A:254:ARG:NH1	3:A:255:ILE:H	1.88	0.71
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.20	0.71
3:A:302:GLY:N	3:A:307:ALA:HB3	2.04	0.70
3:A:179:GLY:O	3:A:182:ARG:HB3	1.92	0.70
3:A:327:TYR:HD1	3:A:328:ARG:N	1.88	0.70
3:A:83:ARG:HA	3:A:86:GLU:HG2	1.73	0.70
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.28	0.69
3:A:108:PRO:O	3:A:112:ARG:HG3	1.92	0.69
3:A:155:MET:HA	3:A:158:MET:CE	2.21	0.69
3:A:237:GLY:O	3:A:254:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:270:LEU:HA	3:A:316:GLU:OE2	1.92	0.68
3:A:259:LEU:HD12	3:A:260:ILE:H	1.58	0.68
3:A:180:SER:CB	3:A:183:ARG:HH21	1.96	0.68
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.75	0.67
3:A:268:GLY:O	3:A:271:TYR:HB3	1.94	0.67
3:A:12:ASN:HA	6:A:553:HOH:O	1.93	0.67
3:A:323:ILE:C	3:A:324:GLN:HG2	2.18	0.67
3:A:59:ALA:O	3:A:65:VAL:HG21	1.95	0.67
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.76	0.67
3:A:182:ARG:HH11	3:A:273:THR:CG2	2.08	0.66
3:A:152:ARG:NE	3:A:184:GLY:O	2.29	0.66
3:A:286:ALA:O	3:A:291:PHE:N	2.28	0.66
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.25	0.66
3:A:182:ARG:HH11	3:A:182:ARG:HG2	1.61	0.65
3:A:254:ARG:NH2	3:A:256:ASP:OD1	2.29	0.65
2:P:5:DA:C2'	2:P:6:DT:H5''	2.24	0.65
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.11	0.65
3:A:330:PRO:CA	3:A:333:ARG:HG2	2.20	0.65
1:T:6:DG:N7	6:T:652:HOH:O	2.30	0.64
3:A:35:LYS:O	3:A:38:ALA:HB3	1.97	0.64
3:A:165:GLU:O	3:A:168:LYS:N	2.29	0.64
1:T:3:DT:OP2	6:T:659:HOH:O	2.15	0.64
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.64
3:A:302:GLY:HA3	3:A:307:ALA:HB2	1.79	0.64
3:A:207:GLN:O	3:A:210:LEU:HB2	1.98	0.64
3:A:321:ASP:O	3:A:324:GLN:N	2.28	0.64
3:A:317:LYS:O	3:A:320:PHE:N	2.32	0.63
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.34	0.63
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.81	0.63
3:A:262:LYS:O	3:A:262:LYS:HG3	1.95	0.63
3:A:93:THR:HG22	3:A:94:SER:N	2.14	0.63
3:A:181:PHE:HA	6:A:530:HOH:O	1.97	0.63
3:A:278:PHE:CD2	3:A:333:ARG:HB3	2.34	0.63
3:A:124:ASP:O	3:A:128:ASN:ND2	2.30	0.62
3:A:155:MET:CA	3:A:158:MET:HE3	2.23	0.62
3:A:277:ILE:HG13	3:A:335:GLU:HB2	1.80	0.62
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.47	0.62
6:T:617:HOH:O	3:A:234:LYS:HD3	1.99	0.62
3:A:182:ARG:HG2	3:A:273:THR:CG2	2.30	0.62
3:A:328:ARG:HB2	3:A:333:ARG:HD3	1.81	0.61
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.66	0.61
3:A:306:VAL:HG22	6:A:650:HOH:O	2.00	0.60
3:A:243:SER:OG	3:A:249:GLU:HG3	2.01	0.60
3:A:260:ILE:HG23	3:A:261:PRO:HD2	1.84	0.60
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.36	0.60
3:A:172:GLU:HB3	3:A:197:HIS:HE2	1.65	0.60
3:A:200:PHE:HB2	6:A:625:HOH:O	2.01	0.60
3:A:11:LEU:HD23	3:A:11:LEU:H	1.66	0.60
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.84	0.60
3:A:288:GLU:C	3:A:290:GLY:H	2.09	0.60
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.83	0.59
3:A:119:ILE:HG22	3:A:124:ASP:HB3	1.85	0.59
3:A:56:GLY:O	3:A:59:ALA:HB3	2.02	0.59
3:A:172:GLU:HG3	3:A:198:PRO:CG	2.33	0.58
3:A:279:ASN:O	3:A:283:ARG:N	2.29	0.58
3:A:103:VAL:HG22	3:A:143:PHE:CD2	2.37	0.58
2:P:5:DA:H2'	2:P:6:DT:H71	1.84	0.58
1:T:6:DG:N3	6:T:651:HOH:O	2.32	0.58
3:A:152:ARG:NH2	3:A:181:PHE:O	2.28	0.58
3:A:204:SER:O	3:A:206:LYS:N	2.36	0.58
3:A:279:ASN:O	3:A:283:ARG:HG3	2.03	0.58
1:T:6:DG:H2''	1:T:7:DA:C8	2.39	0.57
3:A:191:MET:CG	3:A:255:ILE:HG13	2.33	0.57
3:A:211:LEU:HD12	3:A:211:LEU:O	2.05	0.57
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.85	0.57
3:A:212:HIS:H	3:A:212:HIS:CD2	2.22	0.57
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.34	0.57
3:A:11:LEU:HD23	3:A:11:LEU:N	2.18	0.56
3:A:12:ASN:HD21	3:A:53:ILE:H	1.53	0.56
3:A:259:LEU:HD12	3:A:260:ILE:N	2.19	0.56
3:A:278:PHE:HB2	3:A:333:ARG:O	2.04	0.56
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.31	0.56
3:A:200:PHE:O	3:A:262:LYS:N	2.38	0.56
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.41	0.56
3:A:18:MET:HE2	3:A:82:LEU:CD1	2.30	0.56
3:A:255:ILE:HG12	3:A:256:ASP:N	2.21	0.55
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.87	0.55
3:A:155:MET:CE	3:A:188:SER:HB2	2.27	0.55
3:A:328:ARG:O	3:A:333:ARG:NE	2.29	0.55
3:A:11:LEU:H	3:A:11:LEU:CD2	2.19	0.55
3:A:15:ILE:HD13	3:A:73:ILE:CG2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.41	0.55
3:A:41:LYS:NZ	3:A:64:GLY:O	2.33	0.55
3:A:211:LEU:HD12	3:A:211:LEU:C	2.32	0.55
3:A:155:MET:HE2	3:A:188:SER:CB	2.29	0.54
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.90	0.54
3:A:56:GLY:N	3:A:74:ASP:OD1	2.35	0.54
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.40	0.54
3:A:218:LEU:N	3:A:218:LEU:HD13	2.23	0.54
3:A:273:THR:HG22	3:A:273:THR:O	2.08	0.54
3:A:18:MET:HE3	3:A:76:PHE:CB	2.37	0.53
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.43	0.53
3:A:114:PHE:HB3	3:A:119:ILE:HB	1.90	0.53
3:A:270:LEU:CD2	3:A:282:MET:HE1	2.36	0.53
3:A:196:THR:HB	3:A:265:TYR:CD1	2.43	0.53
3:A:243:SER:HB3	3:A:249:GLU:HA	1.89	0.53
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.39	0.52
3:A:114:PHE:O	3:A:119:ILE:HG12	2.09	0.52
3:A:182:ARG:HG2	3:A:273:THR:HG21	1.91	0.52
3:A:195:LEU:O	3:A:260:ILE:N	2.40	0.52
3:A:28:ASN:N	3:A:28:ASN:ND2	2.46	0.52
3:A:111:ALA:O	3:A:115:VAL:HG23	2.10	0.52
3:A:248:LYS:O	3:A:248:LYS:HG2	2.09	0.52
3:A:25:PHE:CG	3:A:88:ILE:HD13	2.45	0.52
3:A:41:LYS:O	3:A:45:VAL:HG13	2.10	0.52
3:A:189:GLY:N	4:A:338:SO4:O3	2.32	0.52
3:A:166:VAL:O	3:A:169:VAL:HG13	2.09	0.51
3:A:103:VAL:HG22	3:A:143:PHE:HD2	1.74	0.51
3:A:332:ASP:C	3:A:334:SER:H	2.16	0.51
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.91	0.51
3:A:277:ILE:CG1	3:A:335:GLU:HB2	2.41	0.51
3:A:170:ASP:OD1	3:A:171:SER:N	2.44	0.51
3:A:151:PRO:CG	3:A:154:GLU:HG3	2.32	0.51
3:A:182:ARG:HG2	3:A:273:THR:HG23	1.92	0.51
3:A:292:THR:HG22	3:A:299:ARG:O	2.10	0.51
3:A:286:ALA:CA	3:A:323:ILE:HG21	2.40	0.51
3:A:83:ARG:O	3:A:86:GLU:N	2.43	0.51
3:A:36:TYR:CD2	3:A:37:ASN:N	2.79	0.50
3:A:254:ARG:NH1	3:A:255:ILE:N	2.57	0.50
3:A:271:TYR:CD1	3:A:283:ARG:NH2	2.79	0.50
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.45	0.50
3:A:148:LYS:HB3	6:A:620:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.42	0.50
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.46	0.50
3:A:74:ASP:O	3:A:78:ALA:N	2.30	0.50
3:A:159:GLN:HG2	3:A:160:ASP:N	2.26	0.50
3:A:200:PHE:CE2	3:A:261:PRO:N	2.79	0.50
3:A:212:HIS:CD2	3:A:212:HIS:N	2.79	0.50
3:A:122:LEU:O	3:A:125:LEU:HB2	2.11	0.50
3:A:29:VAL:HG22	3:A:97:ILE:HD12	1.92	0.50
3:A:282:MET:HE3	6:A:555:HOH:O	2.13	0.49
3:A:38:ALA:O	3:A:41:LYS:HD3	2.12	0.49
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.26	0.49
3:A:302:GLY:HA3	3:A:307:ALA:CB	2.42	0.49
3:A:58:GLU:O	3:A:61:LYS:HG3	2.12	0.49
3:A:271:TYR:CE1	3:A:283:ARG:NH2	2.81	0.49
3:A:180:SER:O	3:A:185:ALA:HB3	2.12	0.49
2:P:5:DA:C2'	2:P:6:DT:H71	2.42	0.49
3:A:21:GLU:OE1	3:A:85:LEU:HD21	2.13	0.49
3:A:270:LEU:HD13	3:A:316:GLU:OE2	2.12	0.49
3:A:41:LYS:HD3	3:A:42:ALA:N	2.28	0.49
3:A:218:LEU:HB2	3:A:224:ILE:HD12	1.94	0.49
1:T:4:DT:H2''	1:T:5:DA:C8	2.48	0.49
3:A:226:ASP:OD1	3:A:238:VAL:HB	2.13	0.49
3:A:229:SER:O	3:A:236:MET:N	2.45	0.49
3:A:65:VAL:HG23	3:A:65:VAL:O	2.12	0.48
3:A:32:ALA:O	3:A:36:TYR:HB3	2.13	0.48
1:T:5:DA:H2	2:P:3:DT:O2	1.95	0.48
2:P:5:DA:H2'	2:P:6:DT:C7	2.44	0.48
3:A:306:VAL:HG23	3:A:307:ALA:N	2.29	0.47
2:P:5:DA:OP2	3:A:109:SER:N	2.41	0.47
3:A:194:LEU:O	3:A:265:TYR:OH	2.29	0.47
3:A:201:THR:HA	3:A:261:PRO:CB	2.43	0.47
3:A:303:VAL:C	3:A:305:GLY:H	2.21	0.47
3:A:285:HIS:CD2	3:A:323:ILE:HD12	2.38	0.47
3:A:62:LEU:O	3:A:65:VAL:HG22	2.14	0.47
3:A:326:LYS:HG3	3:A:326:LYS:O	2.15	0.47
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.96	0.47
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.44	0.47
3:A:188:SER:HB3	6:A:522:HOH:O	2.15	0.46
3:A:274:GLY:O	3:A:278:PHE:HD2	1.99	0.46
3:A:92:ASP:O	3:A:96:SER:N	2.46	0.46
3:A:62:LEU:CD1	3:A:62:LEU:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASN:ND2	3:A:245:ASN:N	2.43	0.46
1:T:6:DG:C2'	1:T:7:DA:C8	2.99	0.46
3:A:180:SER:HB2	3:A:185:ALA:CB	2.45	0.46
3:A:196:THR:CG2	3:A:265:TYR:CD1	2.99	0.46
3:A:251:PRO:O	3:A:253:ARG:HD2	2.16	0.46
3:A:59:ALA:C	3:A:65:VAL:HG21	2.39	0.46
3:A:260:ILE:CG2	3:A:261:PRO:HD2	2.46	0.46
3:A:16:THR:HG23	3:A:46:ILE:HG13	1.98	0.45
3:A:285:HIS:NE2	3:A:323:ILE:O	2.41	0.45
3:A:276:ASP:O	3:A:280:LYS:HG3	2.16	0.45
3:A:277:ILE:HD13	3:A:277:ILE:H	1.80	0.45
3:A:85:LEU:HD12	3:A:85:LEU:HA	1.57	0.45
3:A:149:ARG:HH21	3:A:187:SER:C	2.25	0.45
3:A:263:ASP:C	3:A:264:GLN:HG2	2.41	0.45
3:A:292:THR:O	3:A:298:ILE:HA	2.15	0.45
2:P:5:DA:H2''	2:P:6:DT:H5'	1.96	0.45
3:A:11:LEU:N	3:A:11:LEU:CD2	2.79	0.45
3:A:211:LEU:HB3	3:A:212:HIS:HD2	1.81	0.45
3:A:243:SER:O	3:A:244:LYS:O	2.34	0.45
3:A:303:VAL:O	3:A:305:GLY:N	2.50	0.45
3:A:54:LYS:HA	3:A:54:LYS:HD2	1.55	0.45
3:A:121:THR:O	3:A:124:ASP:HB2	2.17	0.45
3:A:75:GLU:O	3:A:75:GLU:HG2	2.16	0.45
3:A:165:GLU:HG3	3:A:217:GLN:HG3	1.98	0.45
3:A:196:THR:OG1	3:A:197:HIS:N	2.49	0.45
3:A:243:SER:CB	3:A:249:GLU:HA	2.47	0.44
3:A:158:MET:O	3:A:161:ILE:N	2.50	0.44
3:A:125:LEU:HD23	3:A:125:LEU:HA	1.57	0.44
1:T:6:DG:H1'	6:T:651:HOH:O	2.18	0.44
3:A:214:VAL:HG23	3:A:215:VAL:N	2.31	0.44
3:A:178:CYS:HA	3:A:182:ARG:HD3	1.99	0.44
3:A:200:PHE:C	3:A:201:THR:HG22	2.42	0.44
3:A:16:THR:CG2	3:A:46:ILE:HG13	2.48	0.44
3:A:122:LEU:HD22	3:A:126:ARG:CZ	2.48	0.44
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.29	0.44
3:A:214:VAL:CG2	3:A:215:VAL:N	2.80	0.43
3:A:152:ARG:HA	3:A:155:MET:HB2	2.00	0.43
3:A:253:ARG:NH2	6:A:620:HOH:O	2.28	0.43
3:A:172:GLU:HB3	3:A:197:HIS:CD2	2.53	0.43
3:A:207:GLN:HB3	3:A:210:LEU:HG	2.00	0.43
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:LEU:HB2	3:A:250:TYR:CD2	2.54	0.43
3:A:15:ILE:CD1	3:A:77:LEU:HD11	2.36	0.43
2:P:6:DT:H2"	2:P:7:DG:C8	2.53	0.43
3:A:230:LYS:HE2	3:A:230:LYS:HB3	1.71	0.43
3:A:315:SER:C	3:A:317:LYS:H	2.27	0.43
3:A:133:ASN:O	3:A:137:ARG:HG3	2.18	0.42
3:A:223:PHE:O	3:A:239:CYS:HA	2.19	0.42
3:A:228:LEU:O	3:A:229:SER:HB3	2.19	0.42
3:A:154:GLU:C	3:A:158:MET:HE2	2.45	0.42
3:A:122:LEU:HD22	3:A:126:ARG:NH1	2.34	0.42
3:A:254:ARG:HH11	3:A:255:ILE:H	1.62	0.42
2:P:5:DA:P	3:A:107:GLY:HA3	2.59	0.42
3:A:15:ILE:HG22	3:A:19:LEU:HD22	2.00	0.42
3:A:119:ILE:HG22	3:A:124:ASP:CB	2.49	0.42
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.77	0.42
3:A:194:LEU:HA	3:A:194:LEU:HD12	1.12	0.42
1:T:4:DT:H2"	1:T:5:DA:H8	1.83	0.42
3:A:25:PHE:CD2	3:A:88:ILE:HD13	2.55	0.42
3:A:45:VAL:CG2	3:A:46:ILE:N	2.83	0.42
3:A:195:LEU:O	3:A:259:LEU:HD12	2.20	0.42
3:A:250:TYR:HB3	6:A:577:HOH:O	2.19	0.42
3:A:260:ILE:HG23	3:A:260:ILE:HD12	1.75	0.42
3:A:302:GLY:N	3:A:307:ALA:CB	2.79	0.42
3:A:41:LYS:HD3	3:A:42:ALA:H	1.84	0.42
3:A:92:ASP:HA	3:A:95:SER:HB2	2.01	0.42
3:A:99:PHE:CD2	3:A:99:PHE:C	2.97	0.42
3:A:200:PHE:CD2	3:A:261:PRO:CA	3.01	0.42
3:A:121:THR:HG23	3:A:124:ASP:CG	2.45	0.42
3:A:44:SER:O	3:A:47:ALA:HB3	2.19	0.42
3:A:330:PRO:C	3:A:333:ARG:HG2	2.44	0.42
3:A:196:THR:HB	3:A:265:TYR:HD1	1.85	0.41
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.55	0.41
3:A:294:ASN:O	3:A:296:TYR:N	2.52	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.78	0.41
3:A:326:LYS:O	3:A:328:ARG:HG2	2.20	0.41
3:A:122:LEU:CD2	3:A:126:ARG:CZ	2.98	0.41
3:A:128:ASN:ND2	3:A:128:ASN:N	2.68	0.41
3:A:205:THR:O	3:A:206:LYS:HB2	2.19	0.41
3:A:327:TYR:C	3:A:327:TYR:CD1	2.98	0.41
3:A:183:ARG:HH11	3:A:275:SER:HB3	1.85	0.41
3:A:211:LEU:O	3:A:214:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:LYS:C	3:A:62:LEU:N	2.79	0.41
3:A:135:HIS:CD2	3:A:135:HIS:C	2.98	0.41
3:A:244:LYS:H	3:A:244:LYS:HG2	1.66	0.41
3:A:60:LYS:CA	3:A:65:VAL:CG2	2.97	0.41
3:A:197:HIS:CD2	3:A:198:PRO:HD2	2.55	0.41
3:A:92:ASP:HB3	6:A:647:HOH:O	2.20	0.41
3:A:209:LYS:HA	3:A:212:HIS:HB2	2.02	0.41
3:A:254:ARG:HD2	3:A:254:ARG:HA	1.95	0.41
3:A:11:LEU:O	3:A:12:ASN:ND2	2.54	0.41
3:A:26:GLU:O	3:A:30:SER:O	2.38	0.41
3:A:79:THR:C	3:A:81:LYS:H	2.26	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.40	0.41
3:A:127:LYS:N	3:A:127:LYS:HD2	2.36	0.41
3:A:286:ALA:O	3:A:291:PHE:HB2	2.21	0.41
3:A:288:GLU:O	3:A:290:GLY:N	2.53	0.41
3:A:31:GLN:HE21	3:A:112:ARG:NH1	2.09	0.40
3:A:210:LEU:HB3	3:A:259:LEU:HD21	2.02	0.40
3:A:263:ASP:O	3:A:264:GLN:HG2	2.21	0.40
3:A:149:ARG:NH2	3:A:188:SER:HA	2.36	0.40
3:A:291:PHE:CD1	3:A:300:PRO:HA	2.56	0.40
2:P:6:DT:H6	2:P:6:DT:H2'	1.44	0.40
3:A:52:LYS:HE3	6:A:642:HOH:O	2.21	0.40
3:A:150:ILE:O	3:A:187:SER:HA	2.22	0.40
3:A:255:ILE:HG12	3:A:256:ASP:H	1.87	0.40
3:A:288:GLU:C	3:A:290:GLY:N	2.79	0.40
3:A:15:ILE:HB	3:A:46:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	325/335 (97%)	268 (82%)	39 (12%)	18 (6%)	1 9

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	80	GLY
3	A	202	SER
3	A	205	THR
3	A	244	LYS
3	A	246	ASP
3	A	247	GLU
3	A	289	LYS
3	A	295	GLU
3	A	304	THR
3	A	13	GLY
3	A	185	ALA
3	A	204	SER
3	A	262	LYS
3	A	310	PRO
3	A	206	LYS
3	A	222	HIS
3	A	309	GLU
3	A	166	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	214 (74%)	74 (26%)	0 2

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	18	MET
3	A	19	LEU

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Mol	Chain	Res	Type
3	A	22	LEU
3	A	30	SER
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	52	LYS
3	A	61	LYS
3	A	65	VAL
3	A	67	THR
3	A	77	LEU
3	A	79	THR
3	A	81	LYS
3	A	83	ARG
3	A	89	ARG
3	A	92	ASP
3	A	94	SER
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	121	THR
3	A	128	ASN
3	A	138	ILE
3	A	153	GLU
3	A	161	ILE
3	A	165	GLU
3	A	169	VAL
3	A	174	ILE
3	A	182	ARG
3	A	191	MET
3	A	193	VAL
3	A	194	LEU
3	A	201	THR
3	A	202	SER
3	A	203	GLU
3	A	205	THR
3	A	209	LYS
3	A	211	LEU
3	A	213	GLN
3	A	217	GLN
3	A	218	LEU
3	A	219	GLN

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Mol	Chain	Res	Type
3	A	221	VAL
3	A	226	ASP
3	A	228	LEU
3	A	230	LYS
3	A	232	GLU
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	259	LEU
3	A	264	GLN
3	A	269	VAL
3	A	277	ILE
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	324	GLN
3	A	325	TRP
3	A	328	ARG
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	98	ASN
3	A	134	HIS
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN

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Mol	Chain	Res	Type
3	A	245	ASN
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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	338	-	4,4,4	0.81	0	6,6,6	0.89	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	338	SO4	1	0

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%)	-0.21	1 (12%) 8 5	20, 43, 69, 100	1 (12%)
2	P	7/7 (100%)	-0.82	0 100 100	19, 26, 38, 99	0
3	A	325/335 (97%)	-0.96	0 100 100	4, 33, 83, 100	0
All	All	340/350 (97%)	-0.94	1 (0%) 90 80	4, 33, 85, 100	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1	DC	2.9

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	SO4	A	338	5/5	0.79	0.17	68,68,69,69	5
5	NA	A	342	1/1	0.91	0.08	54,54,54,54	0
5	NA	A	341	1/1	0.97	0.05	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.