



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 1ZQQ / pdb_00001zqq
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SEVEN BASE PAIRS OF DNA; SOAKED IN THE PRESENCE OF MNCL2 (15 MILLIMOLAR) AND NACL (15 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-12
Resolution : 3.30 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
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

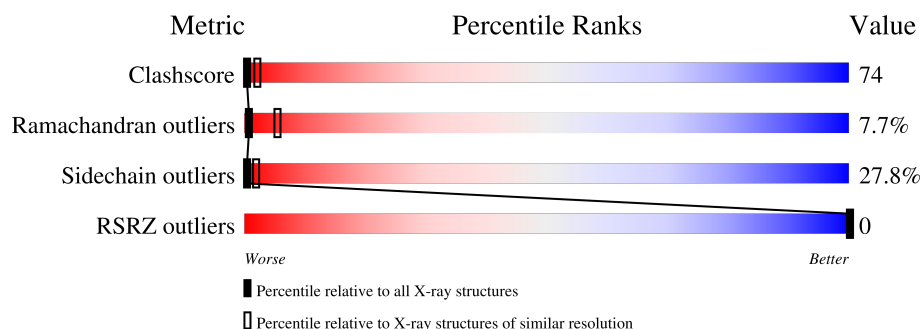
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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% 38% 50%
2	P	7	43% 57%
3	A	335	16% 41% 33% 7% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3057 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 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	22	Total 22	O 22	0	0
6	A	103	Total 103	O 103	0	0

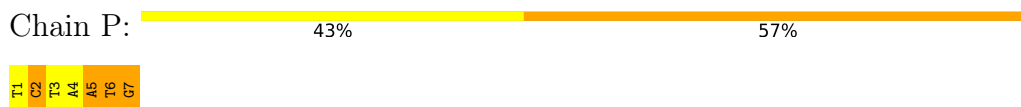
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

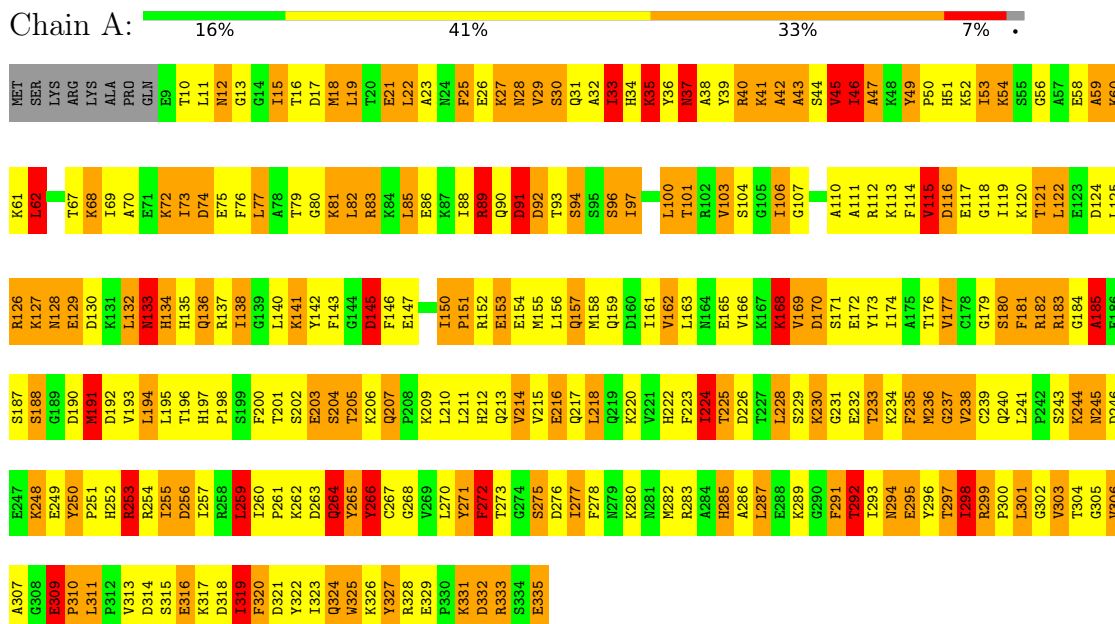
- Molecule 1: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*A)-3')



- 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	180.06Å 57.37Å 47.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	75.0 (20.00-3.30) 74.5 (20.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 2.68Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.163 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.86 , 505.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3057	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	1.06	0/162	4.25	18/249 (7.2%)
2	P	1.25	1/160 (0.6%)	2.49	11/243 (4.5%)
3	A	1.44	7/2672 (0.3%)	2.19	119/3590 (3.3%)
All	All	1.41	8/2994 (0.3%)	2.38	148/4082 (3.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	238	VAL	N-CA	-6.39	1.39	1.46
2	P	1	DT	OP3-P	6.35	1.61	1.48
3	A	150	ILE	C-N	6.01	1.40	1.33
3	A	216	GLU	N-CA	-5.73	1.39	1.46
3	A	157	GLN	CA-C	-5.72	1.45	1.52
3	A	17	ASP	N-CA	-5.42	1.40	1.46
3	A	90	GLN	CA-CB	5.10	1.61	1.53
3	A	53	ILE	N-CA	-5.06	1.40	1.46

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	7	DA	C4-N9-C1'	-26.92	86.68	127.05
1	T	7	DA	C8-N9-C1'	25.09	164.68	127.05
1	T	4	DT	C6-N1-C1'	-20.41	88.73	119.35
1	T	4	DT	C2-N1-C1'	19.23	148.20	119.35
1	T	3	DT	C6-N1-C1'	18.36	146.90	119.35
1	T	2	DA	C8-N9-C1'	18.26	154.44	127.05
1	T	2	DA	C4-N9-C1'	-17.87	100.24	127.05
1	T	3	DT	C2-N1-C1'	-17.43	93.20	119.35
2	P	7	DG	C4-N9-C1'	-14.44	105.34	127.00
2	P	7	DG	C8-N9-C1'	13.86	147.79	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	DC	C6-N1-C1'	-11.17	102.94	119.70
3	A	181	PHE	CA-CB-CG	-10.24	103.56	113.80
3	A	157	GLN	N-CA-CB	9.82	125.49	110.28
3	A	40	ARG	N-CA-C	9.55	122.68	111.02
2	P	2	DC	C2-N1-C1'	9.49	133.93	119.70
1	T	1	DC	C2-N1-C1'	-9.48	105.48	119.70
1	T	7	DA	O5'-C5'-C4'	-9.12	97.12	110.80
3	A	25	PHE	CA-CB-CG	-8.75	105.05	113.80
3	A	130	ASP	CA-CB-CG	8.72	121.32	112.60
3	A	46	ILE	N-CA-CB	8.71	122.38	110.54
2	P	7	DG	P-O5'-C5'	-8.69	106.97	120.00
3	A	21	GLU	N-CA-C	-8.65	101.81	111.07
3	A	236	MET	CA-C-N	-8.59	111.61	121.83
3	A	236	MET	C-N-CA	-8.59	111.61	121.83
1	T	1	DC	C6-N1-C1'	8.51	132.47	119.70
3	A	146	PHE	N-CA-CB	8.49	122.73	110.16
3	A	17	ASP	CB-CA-C	8.45	124.15	110.88
1	T	6	DG	C8-N9-C1'	-8.42	114.37	127.00
3	A	49	TYR	CB-CA-C	8.28	122.11	109.60
3	A	272	PHE	CA-CB-CG	-8.27	105.53	113.80
3	A	59	ALA	N-CA-C	-8.12	102.37	111.14
3	A	297	THR	CB-CA-C	-7.91	102.93	114.87
3	A	253	ARG	N-CA-C	7.88	121.76	109.07
3	A	129	GLU	CA-C-N	7.68	130.90	120.54
3	A	129	GLU	C-N-CA	7.68	130.90	120.54
3	A	53	ILE	N-CA-C	-7.57	98.85	108.84
3	A	49	TYR	CA-C-N	7.55	129.28	119.84
3	A	49	TYR	C-N-CA	7.55	129.28	119.84
3	A	168	LYS	N-CA-CB	7.51	121.33	110.06
1	T	6	DG	C4-N9-C1'	7.45	138.17	127.00
3	A	319	ILE	N-CA-C	-7.17	103.54	110.42
3	A	224	ILE	CB-CA-C	7.10	119.55	110.96
3	A	299	ARG	CA-C-N	6.99	128.58	119.84
3	A	299	ARG	C-N-CA	6.99	128.58	119.84
3	A	151	PRO	CB-CA-C	-6.99	102.63	111.71
3	A	33	ILE	CA-C-N	6.98	130.50	120.79
3	A	33	ILE	C-N-CA	6.98	130.50	120.79
3	A	69	ILE	N-CA-CB	6.93	122.13	110.56
1	T	5	DA	O5'-C5'-C4'	6.93	121.19	110.80
3	A	106	ILE	N-CA-C	6.82	117.69	107.80
3	A	299	ARG	O-C-N	6.82	127.34	121.20
3	A	59	ALA	CB-CA-C	-6.79	100.17	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	333	ARG	N-CA-C	-6.69	105.10	112.72
3	A	97	ILE	CB-CA-C	-6.68	103.46	111.81
3	A	134	HIS	CA-CB-CG	-6.64	107.16	113.80
3	A	332	ASP	N-CA-C	6.63	121.26	112.25
3	A	42	ALA	N-CA-C	-6.55	104.22	111.36
3	A	17	ASP	N-CA-C	6.54	118.07	111.07
3	A	250	TYR	N-CA-C	6.50	118.84	110.39
3	A	291	PHE	N-CA-C	6.47	117.67	108.74
3	A	193	VAL	CA-C-N	6.47	130.76	121.50
3	A	193	VAL	C-N-CA	6.47	130.76	121.50
1	T	4	DT	O4'-C1'-N1	6.43	118.04	108.40
3	A	59	ALA	O-C-N	6.42	129.02	122.09
3	A	297	THR	O-C-N	6.39	127.90	123.11
3	A	43	ALA	CB-CA-C	6.36	120.98	110.81
3	A	62	LEU	N-CA-C	6.35	118.84	110.08
3	A	91	ASP	CA-C-N	6.34	129.64	120.38
3	A	91	ASP	C-N-CA	6.34	129.64	120.38
3	A	103	VAL	N-CA-CB	6.31	119.98	110.13
3	A	266	TYR	CA-CB-CG	-6.29	102.58	113.90
3	A	35	LYS	N-CA-C	-6.21	104.51	111.28
3	A	37	ASN	N-CA-C	-6.21	103.65	111.11
3	A	83	ARG	N-CA-CB	6.15	119.29	110.06
3	A	285	HIS	CA-CB-CG	-6.12	107.67	113.80
3	A	103	VAL	CA-C-N	-6.08	114.09	122.30
3	A	103	VAL	C-N-CA	-6.08	114.09	122.30
3	A	185	ALA	N-CA-C	6.08	123.74	110.80
3	A	309	GLU	CA-C-N	6.05	127.41	119.84
3	A	309	GLU	C-N-CA	6.05	127.41	119.84
3	A	60	LYS	N-CA-CB	6.05	120.71	110.49
3	A	72	LYS	N-CA-CB	6.04	119.53	110.22
2	P	6	DT	C5'-C4'-O4'	-6.01	100.38	109.40
3	A	292	THR	CB-CA-C	6.00	120.15	109.65
3	A	145	ASP	CA-C-N	-5.98	111.79	120.29
3	A	145	ASP	C-N-CA	-5.98	111.79	120.29
3	A	101	THR	N-CA-CB	-5.91	100.51	110.49
2	P	7	DG	O5'-C5'-C4'	5.85	119.57	110.80
3	A	225	THR	N-CA-CB	-5.82	102.58	110.67
3	A	114	PHE	CA-C-N	5.79	128.36	120.77
3	A	114	PHE	C-N-CA	5.79	128.36	120.77
3	A	138	ILE	N-CA-C	-5.78	105.48	110.74
3	A	320	PHE	CA-CB-CG	-5.78	108.02	113.80
3	A	177	VAL	N-CA-C	-5.77	98.92	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	68	LYS	N-CA-C	5.74	117.53	111.28
3	A	237	GLY	CA-C-N	-5.65	114.67	122.69
3	A	237	GLY	C-N-CA	-5.65	114.67	122.69
2	P	3	DT	N1-C1'-C2'	5.64	121.97	113.50
3	A	62	LEU	CA-C-N	5.64	127.17	120.23
3	A	62	LEU	C-N-CA	5.64	127.17	120.23
3	A	259	LEU	N-CA-C	5.60	117.82	109.25
3	A	12	ASN	N-CA-C	5.59	120.25	113.38
1	T	7	DA	C5'-C4'-C3'	-5.58	106.53	114.90
3	A	275	SER	CB-CA-C	-5.56	99.53	110.10
3	A	45	VAL	O-C-N	5.56	127.36	121.91
3	A	228	LEU	N-CA-CB	5.55	118.28	110.12
3	A	235	PHE	CA-C-N	-5.55	114.95	122.77
3	A	235	PHE	C-N-CA	-5.55	114.95	122.77
3	A	49	TYR	CA-C-O	5.54	124.41	119.59
3	A	191	MET	N-CA-CB	5.50	119.40	110.17
3	A	73	ILE	CB-CA-C	5.49	119.22	112.02
3	A	90	GLN	CB-CG-CD	5.46	121.89	112.60
3	A	127	LYS	CA-C-N	-5.44	114.69	123.23
3	A	127	LYS	C-N-CA	-5.44	114.69	123.23
3	A	89	ARG	CA-C-N	5.42	129.66	120.88
3	A	89	ARG	C-N-CA	5.42	129.66	120.88
3	A	96	SER	N-CA-CB	5.41	118.00	109.94
3	A	28	ASN	CA-CB-CG	-5.40	107.20	112.60
3	A	47	ALA	N-CA-C	5.37	117.83	111.33
3	A	126	ARG	O-C-N	5.36	127.60	122.03
3	A	110	ALA	N-CA-CB	5.34	118.07	110.16
3	A	256	ASP	CA-CB-CG	5.33	117.93	112.60
3	A	116	ASP	CB-CA-C	5.32	120.78	110.46
2	P	5	DA	C4-N9-C1'	5.31	135.02	127.05
3	A	74	ASP	N-CA-C	5.31	117.76	111.33
2	P	6	DT	C6-N1-C1'	-5.30	111.39	119.35
3	A	170	ASP	CA-C-N	5.30	129.16	120.63
3	A	170	ASP	C-N-CA	5.30	129.16	120.63
3	A	52	LYS	N-CA-CB	5.26	118.45	109.87
3	A	162	VAL	N-CA-CB	5.26	116.70	110.55
1	T	7	DA	N9-C1'-C2'	-5.25	105.62	113.50
1	T	4	DT	N1-C1'-C2'	5.22	121.33	113.50
3	A	327	TYR	N-CA-CB	5.21	119.29	110.49
3	A	133	ASN	N-CA-CB	5.21	119.12	110.63
3	A	180	SER	N-CA-C	-5.20	105.69	111.36
3	A	190	ASP	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	DC	O3'-P-O5'	-5.17	96.24	104.00
3	A	28	ASN	N-CA-C	5.14	119.01	111.04
3	A	103	VAL	N-CA-C	-5.14	102.95	109.58
3	A	151	PRO	N-CA-CB	5.14	107.74	103.17
3	A	266	TYR	N-CA-C	5.10	121.67	110.80
3	A	168	LYS	N-CA-C	5.06	117.46	111.33
3	A	70	ALA	N-CA-C	-5.06	105.76	111.28
3	A	224	ILE	CA-CB-CG1	-5.06	101.80	110.40
3	A	17	ASP	CA-CB-CG	-5.05	107.55	112.60
3	A	264	GLN	CB-CA-C	5.03	117.90	109.80
3	A	115	VAL	CB-CA-C	-5.03	105.26	111.70
3	A	257	ILE	CA-CB-CG2	-5.02	101.96	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	145	0	80	7	0
2	P	144	0	81	16	0
3	A	2623	0	2641	401	1
4	A	2	0	0	0	0
5	A	2	0	0	0	0
6	A	103	0	0	24	0
6	P	22	0	0	1	0
6	T	16	0	0	0	0
All	All	3057	0	2802	419	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 74.

All (419) 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:316:GLU:HA	3:A:319:ILE:HD12	1.35	1.07
2:P:6:DT:H2''	2:P:7:DG:H5''	1.40	1.00
3:A:128:ASN:N	3:A:128:ASN:HD22	1.60	0.98
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.45	0.97
3:A:243:SER:HB3	3:A:249:GLU:HA	1.46	0.97
3:A:151:PRO:HG2	3:A:154:GLU:HG3	1.44	0.96
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.44	0.95
3:A:155:MET:HE2	3:A:188:SER:HB2	1.50	0.93
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.50	0.93
3:A:172:GLU:HB3	3:A:197:HIS:NE2	1.83	0.93
3:A:31:GLN:HE21	3:A:112:ARG:HH12	1.15	0.93
3:A:29:VAL:HA	3:A:97:ILE:HD12	1.55	0.89
3:A:259:LEU:HD12	3:A:260:ILE:H	1.35	0.88
3:A:245:ASN:N	3:A:245:ASN:HD22	1.69	0.88
1:T:6:DG:H2''	1:T:7:DA:C8	2.09	0.87
3:A:326:LYS:HE3	3:A:328:ARG:HE	1.40	0.85
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.41	0.85
3:A:245:ASN:HD22	3:A:245:ASN:H	1.22	0.85
3:A:299:ARG:CD	3:A:310:PRO:HD3	2.07	0.85
3:A:15:ILE:HG22	3:A:19:LEU:HD22	1.59	0.84
3:A:326:LYS:HE3	3:A:328:ARG:NE	1.92	0.84
3:A:49:TYR:CD2	3:A:50:PRO:HD2	2.13	0.84
3:A:299:ARG:HD2	3:A:310:PRO:HD3	1.62	0.82
3:A:313:VAL:HG13	3:A:318:ASP:HB2	1.61	0.81
2:P:6:DT:H2''	2:P:7:DG:C5'	2.09	0.81
3:A:286:ALA:CB	3:A:323:ILE:HG21	2.11	0.81
2:P:5:DA:H2''	2:P:6:DT:C5'	2.10	0.81
3:A:270:LEU:HD21	3:A:282:MET:HE1	1.61	0.81
3:A:180:SER:HA	3:A:183:ARG:HE	1.45	0.81
3:A:259:LEU:HD12	3:A:260:ILE:N	1.95	0.80
3:A:282:MET:HB2	3:A:325:TRP:CZ3	2.17	0.80
3:A:165:GLU:OE2	3:A:168:LYS:HD3	1.82	0.80
3:A:15:ILE:HB	3:A:46:ILE:CD1	2.13	0.79
3:A:151:PRO:HG2	3:A:154:GLU:CG	2.12	0.79
3:A:191:MET:HA	6:A:502:HOH:O	1.82	0.79
3:A:158:MET:HG3	3:A:241:LEU:HD21	1.64	0.79
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.14	0.78
3:A:151:PRO:HB2	3:A:153:GLU:HG2	1.66	0.77
3:A:129:GLU:O	3:A:132:LEU:HB2	1.84	0.77
3:A:91:ASP:HB3	3:A:94:SER:HB3	1.66	0.77
3:A:270:LEU:HD22	3:A:319:ILE:HD13	1.67	0.77
3:A:323:ILE:O	3:A:324:GLN:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:259:LEU:O	3:A:260:ILE:HD13	1.85	0.76
3:A:29:VAL:HA	3:A:97:ILE:CD1	2.14	0.76
3:A:37:ASN:HB3	6:A:551:HOH:O	1.84	0.76
3:A:25:PHE:CE1	3:A:29:VAL:HG11	2.20	0.76
3:A:138:ILE:HG21	3:A:228:LEU:HD11	1.68	0.76
3:A:277:ILE:HD11	3:A:335:GLU:HB3	1.66	0.76
3:A:286:ALA:HB2	3:A:323:ILE:HG21	1.66	0.76
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.68	0.75
3:A:133:ASN:ND2	3:A:135:HIS:H	1.83	0.75
3:A:15:ILE:HB	3:A:46:ILE:HD11	1.68	0.74
3:A:243:SER:CB	3:A:249:GLU:HA	2.15	0.74
3:A:331:LYS:HG2	3:A:332:ASP:N	2.00	0.74
3:A:245:ASN:H	3:A:245:ASN:ND2	1.85	0.74
3:A:128:ASN:N	3:A:128:ASN:ND2	2.29	0.74
3:A:299:ARG:HG2	3:A:310:PRO:N	2.02	0.74
3:A:306:VAL:HG22	6:A:632:HOH:O	1.87	0.74
2:P:5:DA:H2''	2:P:6:DT:H5'	1.70	0.73
2:P:5:DA:H2'	2:P:6:DT:H71	1.70	0.73
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.00	0.73
3:A:217:GLN:HE21	3:A:217:GLN:HA	1.53	0.73
3:A:76:PHE:HD1	3:A:77:LEU:HD12	1.53	0.72
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.71	0.72
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.25	0.71
3:A:155:MET:HA	3:A:158:MET:CE	2.20	0.70
3:A:194:LEU:HD21	3:A:272:PHE:HD2	1.56	0.70
3:A:103:VAL:HB	3:A:106:ILE:CD1	2.22	0.70
3:A:73:ILE:CG2	3:A:77:LEU:HD22	2.22	0.70
3:A:97:ILE:HG23	3:A:111:ALA:HB1	1.73	0.70
3:A:147:GLU:HG2	6:A:505:HOH:O	1.92	0.70
3:A:127:LYS:HE3	3:A:127:LYS:HA	1.73	0.70
3:A:18:MET:HE1	3:A:76:PHE:CB	2.23	0.69
3:A:76:PHE:HD1	3:A:77:LEU:CD1	2.05	0.69
3:A:289:LYS:HD3	3:A:289:LYS:N	2.06	0.69
1:T:4:DT:H5''	3:A:231:GLY:HA3	1.75	0.68
3:A:316:GLU:HA	3:A:319:ILE:CD1	2.19	0.68
3:A:152:ARG:NH2	3:A:184:GLY:HA2	2.08	0.68
3:A:191:MET:HG2	3:A:255:ILE:CG1	2.21	0.68
3:A:211:LEU:O	3:A:214:VAL:HG22	1.93	0.68
3:A:295:GLU:HG2	3:A:296:TYR:CE2	2.27	0.68
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.27	0.67
3:A:236:MET:HG2	3:A:254:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DT:C2'	2:P:7:DG:H5''	2.22	0.67
3:A:294:ASN:O	3:A:296:TYR:N	2.27	0.67
3:A:177:VAL:O	3:A:182:ARG:HD3	1.95	0.67
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.92	0.67
3:A:11:LEU:HD23	3:A:12:ASN:H	1.59	0.66
3:A:298:ILE:N	6:A:569:HOH:O	2.29	0.66
3:A:253:ARG:NH1	6:A:503:HOH:O	2.27	0.66
3:A:29:VAL:HG12	3:A:30:SER:N	2.10	0.66
3:A:264:GLN:HB3	3:A:296:TYR:O	1.96	0.66
3:A:300:PRO:HD3	3:A:311:LEU:HD22	1.75	0.66
3:A:128:ASN:HD22	3:A:128:ASN:H	1.39	0.66
3:A:163:LEU:HD23	3:A:163:LEU:N	2.11	0.66
3:A:240:GLN:NE2	3:A:250:TYR:O	2.29	0.66
3:A:173:TYR:OH	3:A:213:GLN:NE2	2.29	0.66
3:A:218:LEU:HB3	3:A:224:ILE:HG13	1.76	0.65
1:T:6:DG:N2	2:P:2:DC:O2	2.28	0.65
3:A:228:LEU:N	3:A:236:MET:O	2.30	0.65
3:A:18:MET:HG2	3:A:19:LEU:N	2.09	0.65
3:A:44:SER:OG	3:A:45:VAL:N	2.29	0.65
3:A:41:LYS:HD3	3:A:42:ALA:H	1.62	0.65
3:A:133:ASN:H	3:A:136:GLN:HE21	1.42	0.65
3:A:155:MET:HA	3:A:158:MET:HE3	1.78	0.64
3:A:285:HIS:NE2	6:A:574:HOH:O	2.29	0.64
3:A:103:VAL:CB	3:A:106:ILE:HD12	2.26	0.64
3:A:133:ASN:HD22	3:A:135:HIS:H	1.45	0.64
3:A:73:ILE:HG23	3:A:77:LEU:HD22	1.78	0.64
3:A:44:SER:O	3:A:47:ALA:HB3	1.98	0.64
3:A:298:ILE:HA	6:A:581:HOH:O	1.97	0.64
3:A:328:ARG:O	3:A:333:ARG:NE	2.27	0.64
3:A:275:SER:OG	3:A:278:PHE:N	2.27	0.64
3:A:11:LEU:HD23	3:A:11:LEU:H	1.63	0.64
3:A:27:LYS:CE	3:A:28:ASN:HD21	2.11	0.64
3:A:141:LYS:HE2	3:A:142:TYR:CZ	2.32	0.64
2:P:5:DA:H2''	2:P:6:DT:H5''	1.79	0.64
3:A:277:ILE:HD11	3:A:335:GLU:CB	2.27	0.63
3:A:115:VAL:HG12	3:A:116:ASP:N	2.12	0.63
3:A:38:ALA:O	3:A:41:LYS:NZ	2.29	0.63
3:A:282:MET:HB2	3:A:325:TRP:HZ3	1.60	0.63
2:P:4:DA:H5'	6:P:563:HOH:O	1.99	0.62
3:A:88:ILE:HG22	3:A:89:ARG:N	2.12	0.62
3:A:323:ILE:C	3:A:324:GLN:HG2	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:ARG:HG2	3:A:310:PRO:CA	2.30	0.62
3:A:165:GLU:HB3	3:A:217:GLN:HG2	1.80	0.62
3:A:250:TYR:HD1	3:A:251:PRO:HD2	1.64	0.62
3:A:26:GLU:HA	3:A:30:SER:OG	1.99	0.62
3:A:49:TYR:CE1	3:A:51:HIS:HB2	2.34	0.62
3:A:254:ARG:NH1	3:A:255:ILE:O	2.31	0.62
3:A:214:VAL:O	3:A:217:GLN:N	2.31	0.62
3:A:15:ILE:HG22	3:A:19:LEU:CD2	2.28	0.61
3:A:97:ILE:HG23	3:A:111:ALA:CB	2.29	0.61
3:A:180:SER:HB3	3:A:183:ARG:HH21	1.65	0.61
3:A:154:GLU:C	3:A:158:MET:HE2	2.26	0.61
3:A:292:THR:N	3:A:299:ARG:O	2.33	0.61
3:A:179:GLY:H	3:A:273:THR:HA	1.66	0.61
3:A:299:ARG:HG2	3:A:310:PRO:HA	1.83	0.61
3:A:326:LYS:HE3	3:A:328:ARG:CZ	2.29	0.61
3:A:217:GLN:HE21	3:A:217:GLN:CA	2.09	0.61
3:A:12:ASN:ND2	6:A:624:HOH:O	2.34	0.60
3:A:326:LYS:HE3	3:A:328:ARG:NH2	2.17	0.60
3:A:33:ILE:HG23	3:A:34:HIS:H	1.65	0.60
3:A:133:ASN:ND2	3:A:135:HIS:N	2.50	0.60
3:A:177:VAL:HG12	3:A:181:PHE:CD2	2.38	0.59
3:A:18:MET:CE	3:A:76:PHE:HB2	2.32	0.59
3:A:27:LYS:HE2	3:A:28:ASN:HD21	1.67	0.59
3:A:79:THR:C	3:A:81:LYS:H	2.10	0.59
3:A:39:TYR:OH	3:A:72:LYS:HE3	2.03	0.59
3:A:121:THR:HG23	3:A:124:ASP:OD2	2.02	0.59
3:A:212:HIS:O	3:A:216:GLU:HB2	2.03	0.59
3:A:291:PHE:CD2	3:A:323:ILE:HG22	2.38	0.59
3:A:196:THR:HB	3:A:265:TYR:CD1	2.37	0.59
3:A:278:PHE:HB2	3:A:333:ARG:O	2.03	0.59
3:A:121:THR:HG23	3:A:124:ASP:CG	2.28	0.58
1:T:6:DG:H2''	1:T:7:DA:H8	1.63	0.58
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.95	0.58
3:A:165:GLU:HA	3:A:168:LYS:HG2	1.84	0.58
3:A:292:THR:O	3:A:298:ILE:HA	2.03	0.58
3:A:19:LEU:HB3	3:A:43:ALA:HB2	1.85	0.58
3:A:79:THR:O	3:A:81:LYS:N	2.36	0.58
3:A:249:GLU:HG3	3:A:250:TYR:N	2.19	0.58
3:A:33:ILE:O	3:A:36:TYR:HB3	2.02	0.57
3:A:326:LYS:HG3	3:A:326:LYS:O	2.04	0.57
3:A:13:GLY:HA2	3:A:16:THR:OG1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HB	3:A:46:ILE:HD13	1.83	0.57
3:A:251:PRO:O	3:A:253:ARG:HD2	2.03	0.57
3:A:298:ILE:HG22	6:A:569:HOH:O	2.05	0.57
3:A:58:GLU:O	3:A:61:LYS:HG3	2.04	0.57
3:A:180:SER:CA	3:A:183:ARG:HH21	2.17	0.56
3:A:253:ARG:HH11	3:A:253:ARG:CG	2.19	0.56
3:A:217:GLN:HA	3:A:217:GLN:NE2	2.19	0.56
3:A:299:ARG:HG2	3:A:310:PRO:CD	2.35	0.56
3:A:317:LYS:O	3:A:321:ASP:N	2.32	0.56
3:A:210:LEU:HB3	3:A:259:LEU:HD21	1.88	0.56
3:A:124:ASP:O	3:A:128:ASN:ND2	2.39	0.56
3:A:173:TYR:C	3:A:174:ILE:HG13	2.31	0.56
3:A:278:PHE:CE2	3:A:333:ARG:HD2	2.40	0.56
3:A:317:LYS:O	3:A:320:PHE:N	2.38	0.55
3:A:36:TYR:CD2	3:A:37:ASN:N	2.74	0.55
3:A:177:VAL:HA	3:A:192:ASP:O	2.05	0.55
3:A:298:ILE:HG23	3:A:298:ILE:O	2.07	0.55
3:A:40:ARG:O	3:A:43:ALA:HB3	2.06	0.55
3:A:152:ARG:HA	3:A:155:MET:HB2	1.88	0.55
3:A:100:LEU:O	3:A:103:VAL:HG23	2.06	0.55
3:A:230:LYS:HB2	3:A:235:PHE:HD1	1.71	0.55
3:A:210:LEU:HB3	3:A:259:LEU:CD2	2.37	0.55
3:A:278:PHE:HZ	3:A:320:PHE:HZ	1.54	0.54
3:A:291:PHE:O	3:A:301:LEU:HD22	2.07	0.54
3:A:302:GLY:N	3:A:307:ALA:HB3	2.20	0.54
3:A:81:LYS:NZ	3:A:86:GLU:HB3	2.23	0.54
3:A:151:PRO:HG2	3:A:154:GLU:CD	2.32	0.54
3:A:156:LEU:N	3:A:156:LEU:HD23	2.22	0.54
3:A:91:ASP:CB	3:A:94:SER:HB3	2.34	0.54
3:A:150:ILE:HG12	3:A:253:ARG:HG2	1.90	0.54
3:A:248:LYS:O	3:A:248:LYS:HG2	2.07	0.54
3:A:282:MET:HG3	3:A:323:ILE:HD11	1.89	0.54
3:A:195:LEU:O	3:A:260:ILE:N	2.38	0.54
3:A:240:GLN:NE2	3:A:252:HIS:CE1	2.75	0.54
3:A:12:ASN:OD1	3:A:51:HIS:O	2.25	0.54
3:A:125:LEU:HD22	3:A:132:LEU:HD21	1.87	0.54
3:A:236:MET:HG2	3:A:254:ARG:HH22	1.73	0.54
3:A:180:SER:CB	3:A:183:ARG:HH21	2.21	0.54
3:A:302:GLY:H	3:A:307:ALA:HB3	1.71	0.54
3:A:44:SER:HB2	6:A:594:HOH:O	2.07	0.54
3:A:249:GLU:HG3	3:A:250:TYR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:295:GLU:N	3:A:295:GLU:OE1	2.40	0.54
3:A:326:LYS:HE3	3:A:328:ARG:HH21	1.72	0.54
3:A:311:LEU:HB3	3:A:322:TYR:CE2	2.44	0.53
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.91	0.53
3:A:180:SER:HA	3:A:183:ARG:HB2	1.89	0.53
3:A:204:SER:O	3:A:206:LYS:N	2.42	0.53
3:A:300:PRO:HD2	3:A:309:GLU:O	2.08	0.53
3:A:11:LEU:HD23	3:A:11:LEU:N	2.24	0.53
3:A:266:TYR:O	3:A:270:LEU:HB2	2.08	0.53
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.44	0.53
3:A:165:GLU:CD	3:A:168:LYS:HD3	2.34	0.53
3:A:180:SER:HA	3:A:183:ARG:NE	2.21	0.53
3:A:244:LYS:HB2	3:A:248:LYS:HD3	1.91	0.53
3:A:15:ILE:HG21	3:A:73:ILE:HD11	1.91	0.53
3:A:293:ILE:O	3:A:294:ASN:HB3	2.08	0.52
2:P:6:DT:H5'	2:P:6:DT:H6	1.75	0.52
2:P:6:DT:H2'	2:P:7:DG:C8	2.44	0.52
3:A:18:MET:O	3:A:22:LEU:HD22	2.09	0.52
3:A:278:PHE:CD2	3:A:333:ARG:HB3	2.45	0.52
3:A:103:VAL:CG2	3:A:106:ILE:HD12	2.39	0.52
3:A:238:VAL:HA	3:A:253:ARG:O	2.09	0.52
3:A:232:GLU:O	3:A:233:THR:HG23	2.09	0.52
3:A:266:TYR:CD1	3:A:315:SER:HA	2.45	0.52
3:A:49:TYR:CZ	3:A:51:HIS:HB2	2.45	0.52
3:A:207:GLN:HB3	3:A:210:LEU:CG	2.39	0.52
3:A:234:LYS:NZ	6:A:643:HOH:O	2.41	0.52
3:A:25:PHE:HE1	3:A:29:VAL:HG11	1.69	0.51
3:A:278:PHE:CZ	3:A:333:ARG:HD2	2.45	0.51
3:A:278:PHE:HE1	3:A:328:ARG:HD3	1.74	0.51
2:P:6:DT:C4	2:P:7:DG:C6	2.99	0.51
3:A:170:ASP:HB3	3:A:173:TYR:CE2	2.45	0.51
3:A:11:LEU:H	3:A:11:LEU:CD2	2.22	0.51
1:T:5:DA:H2'	1:T:6:DG:C8	2.45	0.51
3:A:182:ARG:HH11	3:A:182:ARG:CG	2.19	0.51
3:A:237:GLY:O	3:A:254:ARG:NH1	2.43	0.51
3:A:270:LEU:HD22	3:A:319:ILE:CD1	2.39	0.51
3:A:157:GLN:HG3	3:A:241:LEU:HD22	1.93	0.51
3:A:195:LEU:O	3:A:259:LEU:HD12	2.09	0.51
3:A:275:SER:H	3:A:278:PHE:HB3	1.76	0.51
3:A:152:ARG:HH22	3:A:184:GLY:HA2	1.76	0.50
3:A:103:VAL:HG12	3:A:104:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.40	0.50
3:A:19:LEU:O	3:A:23:ALA:N	2.40	0.50
3:A:26:GLU:HB3	3:A:32:ALA:HB3	1.93	0.50
3:A:315:SER:O	3:A:317:LYS:N	2.44	0.50
3:A:315:SER:C	3:A:317:LYS:H	2.20	0.50
3:A:299:ARG:CG	3:A:310:PRO:HD3	2.41	0.50
3:A:41:LYS:HD3	3:A:42:ALA:N	2.27	0.50
3:A:214:VAL:HG23	3:A:215:VAL:N	2.26	0.50
1:T:5:DA:C2	2:P:4:DA:C2	3.00	0.49
3:A:329:GLU:O	3:A:333:ARG:HG2	2.11	0.49
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.42	0.49
3:A:265:TYR:HB3	3:A:266:TYR:CD2	2.47	0.49
3:A:89:ARG:HD3	3:A:89:ARG:C	2.37	0.49
3:A:59:ALA:O	3:A:62:LEU:HB2	2.12	0.49
3:A:180:SER:HB2	3:A:185:ALA:HB3	1.94	0.49
3:A:36:TYR:OH	3:A:40:ARG:HD2	2.13	0.49
3:A:243:SER:O	3:A:244:LYS:O	2.31	0.49
3:A:91:ASP:CG	3:A:94:SER:H	2.20	0.49
3:A:196:THR:HB	3:A:265:TYR:CE1	2.48	0.49
3:A:267:CYS:HB3	6:A:580:HOH:O	2.11	0.49
3:A:212:HIS:N	3:A:212:HIS:CD2	2.79	0.49
3:A:217:GLN:O	3:A:220:LYS:HB3	2.12	0.49
3:A:217:GLN:O	3:A:220:LYS:N	2.46	0.48
3:A:12:ASN:HD21	3:A:53:ILE:H	1.61	0.48
3:A:133:ASN:HD22	3:A:134:HIS:N	2.12	0.48
3:A:141:LYS:HE2	3:A:142:TYR:OH	2.13	0.48
3:A:250:TYR:HD1	3:A:251:PRO:CD	2.25	0.48
3:A:214:VAL:CG2	3:A:215:VAL:N	2.77	0.48
3:A:122:LEU:O	3:A:126:ARG:HG3	2.14	0.48
3:A:282:MET:O	3:A:285:HIS:HB3	2.13	0.48
3:A:73:ILE:HG22	3:A:77:LEU:HD22	1.93	0.47
3:A:299:ARG:HG2	3:A:310:PRO:HD3	1.96	0.47
3:A:223:PHE:O	3:A:239:CYS:HB2	2.13	0.47
3:A:236:MET:HG3	3:A:256:ASP:OD1	2.15	0.47
3:A:276:ASP:O	3:A:280:LYS:HG3	2.14	0.47
3:A:286:ALA:O	3:A:291:PHE:N	2.47	0.47
3:A:23:ALA:HB2	3:A:39:TYR:HB3	1.95	0.47
3:A:31:GLN:O	3:A:31:GLN:HG2	2.13	0.47
3:A:112:ARG:O	3:A:115:VAL:HB	2.14	0.47
3:A:81:LYS:O	3:A:82:LEU:HB2	2.14	0.47
3:A:122:LEU:O	3:A:125:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:249:GLU:CG	3:A:250:TYR:N	2.77	0.47
3:A:278:PHE:CE1	3:A:328:ARG:HD3	2.50	0.47
3:A:56:GLY:O	3:A:59:ALA:HB3	2.14	0.47
3:A:165:GLU:HB3	3:A:217:GLN:CG	2.45	0.47
3:A:299:ARG:HG2	3:A:309:GLU:C	2.39	0.47
3:A:140:LEU:HB3	6:A:607:HOH:O	2.14	0.47
3:A:200:PHE:HB2	6:A:610:HOH:O	2.14	0.47
3:A:270:LEU:HA	3:A:316:GLU:OE2	2.14	0.47
3:A:283:ARG:HA	3:A:293:ILE:HG13	1.95	0.47
3:A:283:ARG:HG3	6:A:550:HOH:O	2.14	0.47
3:A:218:LEU:N	3:A:218:LEU:CD1	2.78	0.46
3:A:217:GLN:CA	3:A:217:GLN:NE2	2.77	0.46
3:A:154:GLU:O	3:A:158:MET:HE2	2.16	0.46
3:A:19:LEU:HD12	3:A:19:LEU:HA	1.71	0.46
3:A:38:ALA:O	3:A:41:LYS:HD3	2.16	0.46
3:A:145:ASP:OD1	3:A:145:ASP:N	2.48	0.46
3:A:275:SER:N	3:A:278:PHE:HB3	2.31	0.46
3:A:197:HIS:HA	3:A:198:PRO:HD3	1.83	0.46
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.98	0.46
3:A:301:LEU:HD12	3:A:301:LEU:HA	1.62	0.46
3:A:41:LYS:CG	3:A:42:ALA:N	2.79	0.46
3:A:143:PHE:CD1	3:A:143:PHE:C	2.94	0.45
3:A:198:PRO:C	3:A:200:PHE:H	2.23	0.45
3:A:203:GLU:CD	3:A:203:GLU:H	2.23	0.45
3:A:297:THR:HB	3:A:298:ILE:H	1.42	0.45
3:A:316:GLU:O	3:A:320:PHE:HD2	1.99	0.45
3:A:77:LEU:CD1	3:A:77:LEU:N	2.79	0.45
3:A:306:VAL:O	3:A:307:ALA:HB2	2.15	0.45
3:A:127:LYS:HB2	3:A:128:ASN:ND2	2.31	0.45
3:A:155:MET:CE	3:A:188:SER:HB2	2.33	0.45
3:A:56:GLY:N	3:A:74:ASP:OD1	2.49	0.45
3:A:196:THR:OG1	3:A:197:HIS:N	2.47	0.45
3:A:246:ASP:C	3:A:248:LYS:H	2.25	0.45
3:A:81:LYS:NZ	3:A:86:GLU:CB	2.79	0.45
3:A:158:MET:CG	3:A:241:LEU:HD21	2.43	0.45
3:A:180:SER:OG	3:A:181:PHE:N	2.49	0.45
3:A:207:GLN:HB3	3:A:210:LEU:CD1	2.47	0.45
3:A:223:PHE:O	3:A:239:CYS:HA	2.17	0.45
3:A:62:LEU:HD12	3:A:62:LEU:HA	1.74	0.45
3:A:286:ALA:HB1	3:A:291:PHE:HB2	1.99	0.45
2:P:5:DA:P	3:A:107:GLY:HA3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:LEU:HB3	6:A:577:HOH:O	2.16	0.44
3:A:75:GLU:OE2	3:A:82:LEU:HA	2.18	0.44
3:A:209:LYS:O	3:A:213:GLN:HG3	2.17	0.44
3:A:91:ASP:CG	3:A:94:SER:HB3	2.42	0.44
3:A:35:LYS:O	3:A:39:TYR:N	2.45	0.44
3:A:263:ASP:C	3:A:264:GLN:HG2	2.42	0.44
3:A:320:PHE:CE1	3:A:328:ARG:HG3	2.53	0.44
3:A:73:ILE:HG23	3:A:77:LEU:CD2	2.44	0.44
3:A:158:MET:O	3:A:162:VAL:HG23	2.17	0.44
3:A:282:MET:HG3	3:A:323:ILE:CD1	2.48	0.44
3:A:286:ALA:HB1	3:A:323:ILE:HG21	1.95	0.44
3:A:203:GLU:O	3:A:205:THR:N	2.51	0.44
3:A:268:GLY:O	3:A:271:TYR:HB3	2.17	0.44
3:A:291:PHE:HD2	3:A:323:ILE:HG22	1.79	0.44
3:A:327:TYR:HD1	3:A:328:ARG:N	2.16	0.44
3:A:15:ILE:O	3:A:19:LEU:HD22	2.18	0.43
3:A:171:SER:HB2	6:A:548:HOH:O	2.18	0.43
1:T:5:DA:C2'	1:T:6:DG:C8	3.02	0.43
3:A:27:LYS:CE	3:A:28:ASN:ND2	2.79	0.43
3:A:180:SER:HB3	6:A:638:HOH:O	2.17	0.43
3:A:253:ARG:HH11	3:A:253:ARG:HG3	1.82	0.43
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.53	0.43
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.55	0.43
3:A:141:LYS:O	3:A:141:LYS:HG3	2.17	0.43
3:A:150:ILE:O	3:A:188:SER:N	2.45	0.43
3:A:176:THR:O	3:A:194:LEU:N	2.36	0.43
3:A:182:ARG:NE	6:A:567:HOH:O	2.41	0.43
3:A:327:TYR:HD1	3:A:327:TYR:C	2.26	0.43
3:A:11:LEU:HD23	3:A:12:ASN:N	2.30	0.43
3:A:28:ASN:HD22	3:A:28:ASN:HA	1.49	0.43
3:A:183:ARG:HE	3:A:183:ARG:HB2	1.43	0.43
3:A:315:SER:C	3:A:317:LYS:N	2.75	0.43
3:A:92:ASP:HB3	6:A:629:HOH:O	2.19	0.43
3:A:133:ASN:HD21	3:A:135:HIS:CB	2.31	0.43
3:A:76:PHE:CD1	3:A:77:LEU:HD12	2.43	0.43
3:A:261:PRO:HB2	3:A:264:GLN:HG3	2.01	0.43
3:A:328:ARG:HB2	3:A:333:ARG:HD3	2.00	0.43
3:A:54:LYS:HA	3:A:54:LYS:HD2	1.59	0.42
3:A:326:LYS:CE	3:A:328:ARG:HH21	2.31	0.42
3:A:41:LYS:O	3:A:44:SER:OG	2.33	0.42
3:A:41:LYS:HG2	3:A:42:ALA:N	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:LEU:CB	3:A:259:LEU:CD2	2.97	0.42
3:A:229:SER:OG	3:A:236:MET:HE2	2.19	0.42
3:A:41:LYS:O	3:A:45:VAL:HG13	2.20	0.42
3:A:140:LEU:HD12	3:A:140:LEU:HA	1.77	0.42
3:A:174:ILE:HB	3:A:196:THR:HG22	2.01	0.42
3:A:321:ASP:O	3:A:324:GLN:N	2.50	0.42
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.60	0.42
3:A:327:TYR:C	3:A:327:TYR:CD1	2.98	0.42
3:A:316:GLU:CA	3:A:319:ILE:HD12	2.26	0.42
3:A:251:PRO:HG2	3:A:253:ARG:CZ	2.50	0.42
3:A:282:MET:CB	3:A:325:TRP:CZ3	2.98	0.42
3:A:303:VAL:C	3:A:305:GLY:N	2.76	0.42
3:A:133:ASN:HD22	3:A:135:HIS:N	2.13	0.42
3:A:135:HIS:C	3:A:135:HIS:CD2	2.97	0.42
2:P:6:DT:C2'	2:P:7:DG:C8	3.03	0.41
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.49	0.41
3:A:152:ARG:NH2	3:A:184:GLY:CA	2.81	0.41
3:A:283:ARG:HG2	3:A:293:ILE:HB	2.02	0.41
3:A:326:LYS:CE	3:A:328:ARG:HE	2.23	0.41
2:P:5:DA:O5'	3:A:107:GLY:HA3	2.20	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.64	0.41
3:A:293:ILE:HA	6:A:581:HOH:O	2.20	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.68	0.41
3:A:158:MET:HE3	3:A:158:MET:HB2	1.76	0.41
3:A:97:ILE:HD13	3:A:97:ILE:HG21	1.70	0.41
3:A:135:HIS:NE2	3:A:228:LEU:HD23	2.35	0.41
3:A:228:LEU:H	3:A:237:GLY:HA2	1.86	0.41
3:A:169:VAL:HG13	3:A:170:ASP:N	2.35	0.41
3:A:265:TYR:HB3	3:A:266:TYR:H	1.60	0.41
3:A:306:VAL:HG23	3:A:307:ALA:N	2.36	0.41
3:A:230:LYS:HB2	3:A:235:PHE:CD1	2.52	0.41
3:A:150:ILE:O	3:A:187:SER:HA	2.20	0.41
3:A:104:SER:HB2	6:A:640:HOH:O	2.21	0.41
3:A:237:GLY:O	3:A:254:ARG:HD2	2.21	0.41
3:A:27:LYS:CB	3:A:36:TYR:CD1	3.03	0.40
3:A:85:LEU:HA	3:A:85:LEU:HD12	1.55	0.40
3:A:194:LEU:HD12	3:A:194:LEU:HA	1.35	0.40
3:A:240:GLN:HA	6:A:568:HOH:O	2.21	0.40
3:A:295:GLU:HG2	3:A:296:TYR:CZ	2.56	0.40
3:A:25:PHE:CE1	3:A:29:VAL:CG1	2.98	0.40
3:A:133:ASN:ND2	3:A:133:ASN:C	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:GLY:O	3:A:183:ARG:HB2	2.22	0.40
3:A:125:LEU:HA	3:A:125:LEU:HD23	1.81	0.40
3:A:228:LEU:HD22	3:A:254:ARG:NE	2.35	0.40
3:A:133:ASN:O	3:A:137:ARG:N	2.47	0.40
3:A:243:SER:OG	3:A:249:GLU:HG3	2.22	0.40
3:A:270:LEU:HA	3:A:270:LEU:HD12	1.71	0.40
3:A:75:GLU:O	3:A:79:THR:O	2.39	0.40
3:A:115:VAL:O	3:A:118:GLY:N	2.43	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:CG[3_558]	2.10	0.10

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%)	257 (79%)	43 (13%)	25 (8%)	1 5

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	204	SER
3	A	205	THR
3	A	222	HIS
3	A	244	LYS
3	A	265	TYR
3	A	295	GLU
3	A	60	LYS
3	A	80	GLY

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Mol	Chain	Res	Type
3	A	91	ASP
3	A	141	LYS
3	A	185	ALA
3	A	202	SER
3	A	272	PHE
3	A	316	GLU
3	A	82	LEU
3	A	207	GLN
3	A	266	TYR
3	A	294	ASN
3	A	298	ILE
3	A	233	THR
3	A	271	TYR
3	A	304	THR
3	A	303	VAL
3	A	309	GLU
3	A	310	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	208 (72%)	80 (28%)	0 2

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	10	THR
3	A	15	ILE
3	A	18	MET
3	A	19	LEU
3	A	21	GLU
3	A	22	LEU
3	A	27	LYS
3	A	29	VAL
3	A	30	SER

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Mol	Chain	Res	Type
3	A	33	ILE
3	A	35	LYS
3	A	37	ASN
3	A	41	LYS
3	A	45	VAL
3	A	46	ILE
3	A	54	LYS
3	A	62	LEU
3	A	67	THR
3	A	68	LYS
3	A	77	LEU
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	96	SER
3	A	100	LEU
3	A	101	THR
3	A	113	LYS
3	A	115	VAL
3	A	119	ILE
3	A	120	LYS
3	A	121	THR
3	A	122	LEU
3	A	128	ASN
3	A	132	LEU
3	A	133	ASN
3	A	136	GLN
3	A	145	ASP
3	A	153	GLU
3	A	159	GLN
3	A	161	ILE
3	A	166	VAL
3	A	168	LYS
3	A	169	VAL
3	A	182	ARG
3	A	183	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU

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Mol	Chain	Res	Type
3	A	201	THR
3	A	203	GLU
3	A	214	VAL
3	A	218	LEU
3	A	224	ILE
3	A	225	THR
3	A	226	ASP
3	A	230	LYS
3	A	245	ASN
3	A	248	LYS
3	A	253	ARG
3	A	255	ILE
3	A	259	LEU
3	A	262	LYS
3	A	264	GLN
3	A	277	ILE
3	A	287	LEU
3	A	292	THR
3	A	298	ILE
3	A	301	LEU
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	319	ILE
3	A	324	GLN
3	A	325	TRP
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	128	ASN
3	A	133	ASN
3	A	134	HIS
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS

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Mol	Chain	Res	Type
3	A	213	GLN
3	A	217	GLN
3	A	240	GLN
3	A	245	ASN
3	A	279	ASN
3	A	281	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.22	0 100 100	19, 38, 97, 100	0
2	P	7/7 (100%)	-0.56	0 100 100	16, 28, 43, 64	0
3	A	325/335 (97%)	-0.68	0 100 100	4, 32, 83, 99	0
All	All	340/350 (97%)	-0.67	0 100 100	4, 33, 84, 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
4	MN	A	340	1/1	0.97	0.13	48,48,48,48	0
4	MN	A	343	1/1	0.98	0.10	82,82,82,82	0
5	NA	A	341	1/1	0.99	0.07	4,4,4,4	0
5	NA	A	342	1/1	0.99	0.06	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.