



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 9ICW / pdb_00009icw
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7) COMPLEXED WITH SIX BASE PAIRS OF DNA; NATIVE STRUCTURE
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1995-12-16
Resolution : 2.60 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

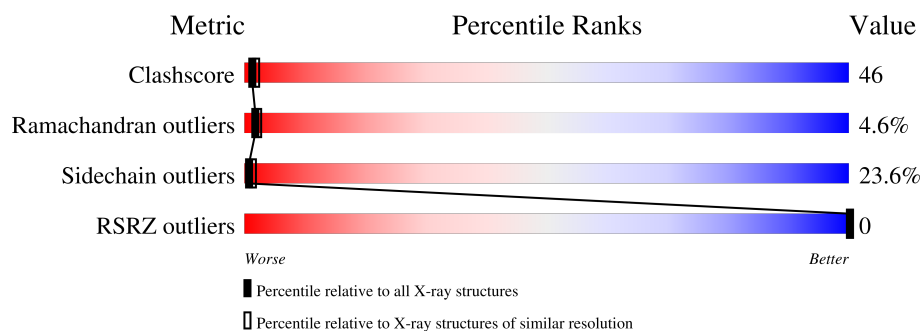
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	14% 57% 29%
2	P	6	17% 33% 50%
3	A	335	28% 39% 24% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3035 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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

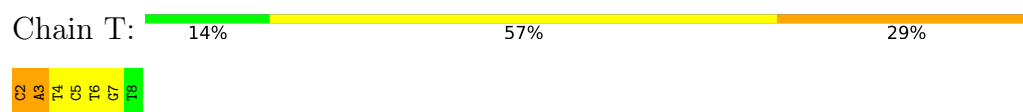
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	T	12	Total O 12 12	0	0
6	P	23	Total O 23 23	0	0
6	A	122	Total O 122 122	0	0

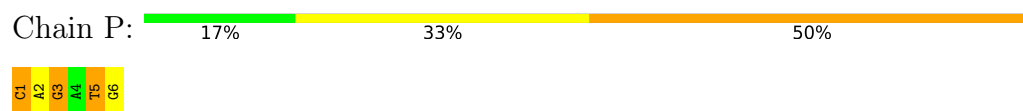
3 Residue-property plots [i](#)

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.

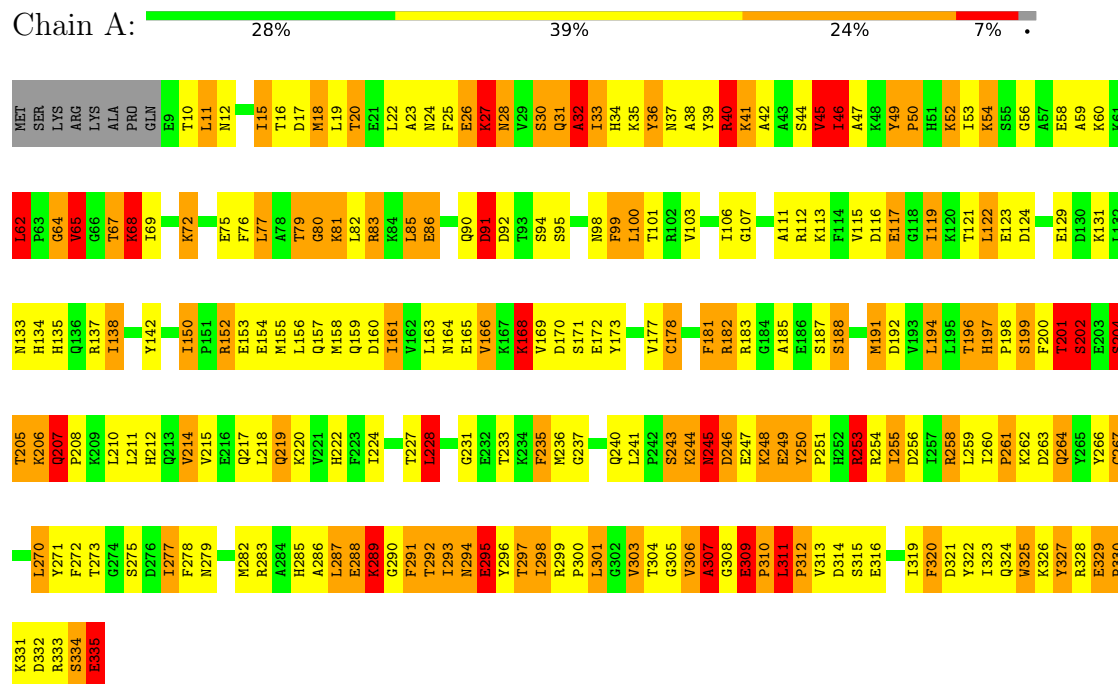
- Molecule 1: DNA (5'-D(*CP*AP*TP*CP*TP*GP*T)-3')



- 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	178.64Å 57.85Å 48.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.60) 94.2 (20.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.43Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	0.175 , (Not available) 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 237.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3035	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 5.65% 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, SO4

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	0.93	0/135	2.56	11/207 (5.3%)
2	P	1.23	2/141 (1.4%)	2.40	8/214 (3.7%)
3	A	1.74	31/2672 (1.2%)	2.15	105/3590 (2.9%)
All	All	1.69	33/2948 (1.1%)	2.19	124/4011 (3.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	1	0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	25	PHE	N-CA	-7.28	1.37	1.46
3	A	116	ASP	CA-C	-7.26	1.42	1.52
3	A	30	SER	C-N	-6.75	1.25	1.33
3	A	152	ARG	CA-C	-6.57	1.43	1.52
3	A	15	ILE	CA-CB	-6.48	1.47	1.54
3	A	24	ASN	C-N	-6.27	1.25	1.33
3	A	69	ILE	N-CA	-6.26	1.38	1.46
3	A	26	GLU	C-N	-6.24	1.25	1.33
2	P	5	DT	C1'-N1	6.19	1.68	1.49
3	A	58	GLU	CA-C	-6.10	1.45	1.52
2	P	1	DC	OP3-P	6.08	1.60	1.48
3	A	138	ILE	CA-CB	-5.99	1.47	1.54
3	A	330	PRO	N-CA	-5.99	1.39	1.47
3	A	178	CYS	CA-C	-5.96	1.46	1.53
3	A	31	GLN	N-CA	-5.95	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	122	LEU	CA-C	-5.94	1.45	1.52
3	A	116	ASP	C-N	-5.80	1.25	1.33
3	A	36	TYR	N-CA	-5.77	1.39	1.46
3	A	233	THR	CA-C	-5.64	1.46	1.52
3	A	15	ILE	CA-C	-5.58	1.46	1.52
3	A	222	HIS	CA-C	-5.48	1.45	1.52
3	A	160	ASP	C-O	-5.47	1.17	1.24
3	A	160	ASP	C-N	-5.44	1.26	1.33
3	A	27	LYS	N-CA	-5.41	1.40	1.46
3	A	91	ASP	CA-C	-5.36	1.45	1.52
3	A	129	GLU	CD-OE1	5.29	1.35	1.25
3	A	83	ARG	NE-CZ	5.29	1.38	1.33
3	A	249	GLU	CD-OE2	5.19	1.35	1.25
3	A	90	GLN	CA-C	-5.17	1.46	1.53
3	A	116	ASP	C-O	-5.09	1.17	1.24
3	A	160	ASP	CG-OD2	5.07	1.34	1.25
3	A	58	GLU	N-CA	-5.03	1.40	1.46
3	A	77	LEU	C-O	-5.00	1.18	1.24

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	C2-N1-C1'	16.52	144.13	119.35
1	T	4	DT	C6-N1-C1'	-16.28	94.93	119.35
2	P	5	DT	C6-N1-C1'	-16.06	95.26	119.35
1	T	4	DT	C2-N1-C1'	15.38	142.43	119.35
3	A	49	TYR	CA-C-N	12.71	132.27	119.82
3	A	49	TYR	C-N-CA	12.71	132.27	119.82
3	A	34	HIS	CA-CB-CG	-12.01	101.79	113.80
3	A	272	PHE	CA-CB-CG	-11.39	102.41	113.80
3	A	24	ASN	CA-CB-CG	-11.25	101.35	112.60
3	A	116	ASP	CA-CB-CG	-10.63	101.97	112.60
3	A	152	ARG	N-CA-CB	10.55	126.80	110.14
1	T	3	DA	C8-N9-C1'	10.02	142.08	127.05
1	T	3	DA	C4-N9-C1'	-9.11	113.39	127.05
3	A	64	GLY	N-CA-C	-8.75	104.28	114.69
3	A	291	PHE	N-CA-C	8.74	121.19	108.86
3	A	30	SER	CA-C-N	-8.37	109.37	122.67
3	A	30	SER	C-N-CA	-8.37	109.37	122.67
1	T	2	DC	C2-N1-C1'	8.28	132.12	119.70
3	A	65	VAL	N-CA-CB	8.26	121.73	111.41
1	T	5	DC	C6-N1-C1'	-8.18	107.42	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	40	ARG	N-CA-C	7.71	119.77	111.36
3	A	181	PHE	CB-CA-C	-7.70	97.59	110.68
3	A	204	SER	CA-C-N	-7.69	110.53	121.99
3	A	204	SER	C-N-CA	-7.69	110.53	121.99
3	A	312	PRO	CA-C-N	7.68	132.72	123.19
3	A	312	PRO	C-N-CA	7.68	132.72	123.19
3	A	49	TYR	O-C-N	7.41	127.25	121.47
3	A	65	VAL	N-CA-C	7.40	118.54	107.51
3	A	117	GLU	N-CA-C	-7.32	103.92	112.92
3	A	98	ASN	CA-CB-CG	-7.31	105.29	112.60
3	A	261	PRO	CB-CA-C	-7.26	101.55	111.21
3	A	27	LYS	N-CA-CB	-7.23	99.52	110.01
1	T	5	DC	C2-N1-C1'	7.20	130.50	119.70
3	A	32	ALA	N-CA-C	7.08	125.87	110.80
3	A	86	GLU	N-CA-CB	7.06	120.49	110.12
3	A	83	ARG	N-CA-CB	7.05	120.54	109.82
1	T	2	DC	C6-N1-C1'	-7.04	109.14	119.70
3	A	233	THR	O-C-N	7.03	129.09	121.85
3	A	214	VAL	N-CA-CB	6.94	118.67	110.55
3	A	335	GLU	N-CA-CB	6.86	122.16	110.50
3	A	220	LYS	N-CA-C	-6.83	102.68	111.02
3	A	20	THR	CB-CA-C	6.78	122.38	110.85
3	A	49	TYR	CA-C-O	6.73	125.45	119.59
3	A	197	HIS	CA-C-N	6.73	126.52	119.05
3	A	197	HIS	C-N-CA	6.73	126.52	119.05
3	A	138	ILE	CB-CA-C	-6.68	103.42	111.97
3	A	92	ASP	N-CA-CB	6.67	120.62	110.28
3	A	304	THR	N-CA-CB	-6.66	99.24	110.49
3	A	77	LEU	N-CA-C	-6.57	104.04	111.07
3	A	90	GLN	O-C-N	6.51	129.80	122.32
2	P	3	DG	P-O3'-C3'	6.50	129.94	120.20
3	A	291	PHE	CA-CB-CG	-6.48	107.32	113.80
3	A	31	GLN	N-CA-C	-6.47	104.70	112.59
3	A	99	PHE	CA-CB-CG	-6.35	107.45	113.80
3	A	297	THR	CB-CA-C	-6.34	99.54	110.95
3	A	168	LYS	N-CA-CB	6.33	119.37	109.94
3	A	28	ASN	N-CA-C	6.29	118.22	111.36
3	A	199	SER	N-CA-CB	-6.26	101.49	110.57
3	A	86	GLU	CB-CA-C	6.26	121.18	110.79
3	A	50	PRO	CB-CA-C	-6.24	102.51	111.62
1	T	6	DT	C6-N1-C1'	-6.23	110.01	119.35
3	A	30	SER	N-CA-C	-6.22	101.76	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	DT	O4'-C1'-C2'	-6.13	97.21	106.40
2	P	1	DC	O3'-P-O5'	-6.07	94.89	104.00
3	A	228	LEU	N-CA-C	-6.05	103.32	112.04
3	A	156	LEU	N-CA-CB	6.04	118.99	110.12
3	A	329	GLU	N-CA-C	-6.01	101.48	109.84
3	A	50	PRO	CA-C-N	-5.98	112.37	123.01
3	A	50	PRO	C-N-CA	-5.98	112.37	123.01
3	A	181	PHE	CA-C-N	5.95	130.79	120.68
3	A	181	PHE	C-N-CA	5.95	130.79	120.68
3	A	142	TYR	CB-CA-C	-5.82	101.77	111.13
3	A	327	TYR	N-CA-CB	5.78	118.64	109.51
3	A	36	TYR	CA-CB-CG	-5.73	103.59	113.90
1	T	4	DT	N1-C1'-C2'	5.71	122.07	113.50
3	A	310	PRO	N-CA-CB	5.69	109.23	103.25
3	A	166	VAL	CB-CA-C	-5.67	104.48	112.14
3	A	17	ASP	N-CA-CB	5.65	118.49	110.13
3	A	241	LEU	O-C-N	5.63	126.27	121.20
3	A	245	ASN	CA-CB-CG	5.61	118.21	112.60
3	A	313	VAL	N-CA-C	5.61	116.02	108.17
3	A	320	PHE	O-C-N	5.58	127.90	122.09
3	A	307	ALA	CB-CA-C	5.57	121.50	110.42
3	A	68	LYS	CA-CB-CG	-5.56	102.98	114.10
3	A	205	THR	N-CA-CB	5.48	118.70	109.94
2	P	6	DG	C4-N9-C1'	-5.45	118.83	127.00
3	A	295	GLU	CB-CG-CD	5.42	121.81	112.60
3	A	62	LEU	CA-C-N	5.42	125.18	119.76
3	A	62	LEU	C-N-CA	5.42	125.18	119.76
2	P	6	DG	C8-N9-C1'	5.40	135.09	127.00
3	A	45	VAL	N-CA-C	5.39	116.16	110.72
3	A	123	GLU	CB-CA-C	5.34	119.65	110.79
3	A	240	GLN	N-CA-C	5.31	117.03	108.32
3	A	250	TYR	CA-C-O	5.31	126.75	120.96
3	A	253	ARG	CD-NE-CZ	5.29	131.81	124.40
3	A	107	GLY	CA-C-N	5.28	124.91	119.05
3	A	107	GLY	C-N-CA	5.28	124.91	119.05
3	A	241	LEU	CB-CA-C	-5.26	101.38	109.85
1	T	7	DG	P-O5'-C5'	5.26	127.89	120.00
3	A	292	THR	N-CA-CB	5.24	120.61	111.13
3	A	243	SER	CB-CA-C	5.23	118.86	110.29
2	P	3	DG	P-O5'-C5'	5.21	127.82	120.00
3	A	266	TYR	N-CA-C	5.21	118.42	111.75
3	A	196	THR	N-CA-CB	5.21	120.00	111.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	LEU	CA-C-N	5.18	127.22	120.28
3	A	211	LEU	C-N-CA	5.18	127.22	120.28
3	A	152	ARG	N-CA-C	5.18	118.38	111.75
3	A	301	LEU	N-CA-C	5.18	117.05	108.20
3	A	20	THR	N-CA-CB	5.17	117.82	110.16
3	A	334	SER	CB-CA-C	5.17	120.72	110.42
3	A	270	LEU	CA-C-N	5.16	127.97	120.79
3	A	270	LEU	C-N-CA	5.16	127.97	120.79
3	A	307	ALA	N-CA-CB	5.16	119.20	110.49
3	A	231	GLY	CA-C-N	-5.15	114.41	122.65
3	A	231	GLY	C-N-CA	-5.15	114.41	122.65
3	A	192	ASP	CB-CA-C	-5.13	102.39	111.22
3	A	235	PHE	CA-C-O	-5.12	115.17	120.70
3	A	267	CYS	N-CA-C	-5.12	105.78	112.23
3	A	311	LEU	N-CA-C	-5.08	103.07	110.08
3	A	65	VAL	CB-CA-C	5.05	118.39	111.31
3	A	161	ILE	N-CA-C	5.02	115.25	110.53
3	A	201	THR	CA-C-N	5.01	131.11	121.54
3	A	201	THR	C-N-CA	5.01	131.11	121.54
3	A	46	ILE	N-CA-CB	5.00	119.21	110.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	65	VAL	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	3	0
2	P	126	0	68	15	0
3	A	2623	0	2641	238	1
4	A	5	0	0	0	0
5	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	122	0	0	11	0
6	P	23	0	0	3	0
6	T	12	0	0	2	0
All	All	3035	0	2778	256	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 46.

All (256) 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)
2:P:5:DT:N1	2:P:5:DT:C1'	1.68	1.54
2:P:5:DT:C1'	2:P:5:DT:C6	2.28	1.15
3:A:31:GLN:NE2	3:A:112:ARG:HH12	1.52	1.08
2:P:1:DC:H2''	2:P:2:DA:H5''	1.36	1.06
3:A:41:LYS:HE2	3:A:64:GLY:HA2	1.42	1.01
3:A:277:ILE:HG13	3:A:335:GLU:HB3	1.43	1.00
3:A:31:GLN:HE21	3:A:112:ARG:NH1	1.59	0.99
3:A:191:MET:HG2	3:A:255:ILE:HG13	1.49	0.91
3:A:293:ILE:CD1	3:A:298:ILE:HG13	2.01	0.90
3:A:31:GLN:HE21	3:A:112:ARG:HH12	0.91	0.88
3:A:245:ASN:H	3:A:245:ASN:HD22	1.20	0.87
3:A:150:ILE:HG21	3:A:158:MET:HE1	1.56	0.85
3:A:286:ALA:HA	3:A:323:ILE:HG21	1.57	0.85
3:A:60:LYS:HA	3:A:65:VAL:HG22	1.59	0.85
3:A:12:ASN:HB3	3:A:46:ILE:HD12	1.60	0.82
3:A:18:MET:HE1	3:A:76:PHE:HB2	1.61	0.81
3:A:49:TYR:CD1	3:A:50:PRO:HD2	2.14	0.81
3:A:294:ASN:HB2	3:A:295:GLU:OE2	1.82	0.80
3:A:12:ASN:HD21	3:A:53:ILE:H	1.27	0.79
3:A:11:LEU:HD23	3:A:11:LEU:H	1.48	0.79
3:A:300:PRO:HD3	3:A:311:LEU:HD13	1.65	0.79
3:A:27:LYS:HG3	3:A:28:ASN:N	1.98	0.79
3:A:23:ALA:HB2	3:A:39:TYR:HB2	1.63	0.78
3:A:286:ALA:HB1	3:A:293:ILE:HD11	1.64	0.77
3:A:60:LYS:HA	3:A:65:VAL:CG2	2.15	0.77
3:A:245:ASN:HD22	3:A:245:ASN:N	1.82	0.77
3:A:289:LYS:HD2	3:A:324:GLN:OE1	1.86	0.75
3:A:293:ILE:HD13	3:A:298:ILE:HG13	1.69	0.75
3:A:182:ARG:HG2	3:A:182:ARG:HH11	1.50	0.75
3:A:212:HIS:HB3	6:A:541:HOH:O	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:1:DC:C2'	2:P:2:DA:H5''	2.16	0.74
3:A:18:MET:HE1	3:A:76:PHE:CB	2.17	0.74
3:A:278:PHE:HB2	3:A:333:ARG:O	1.89	0.73
3:A:279:ASN:O	3:A:283:ARG:HG3	1.88	0.73
3:A:59:ALA:O	3:A:62:LEU:HB2	1.89	0.73
3:A:15:ILE:HG21	3:A:46:ILE:HD13	1.70	0.72
3:A:150:ILE:HG21	3:A:158:MET:CE	2.18	0.72
2:P:2:DA:C8	2:P:2:DA:H5'	2.23	0.72
3:A:172:GLU:HG2	3:A:198:PRO:HG2	1.70	0.72
3:A:292:THR:O	3:A:298:ILE:HA	1.90	0.72
3:A:197:HIS:ND1	3:A:198:PRO:HD2	2.05	0.72
3:A:41:LYS:HE2	3:A:64:GLY:CA	2.18	0.71
3:A:16:THR:O	3:A:20:THR:HG23	1.89	0.71
3:A:31:GLN:NE2	3:A:112:ARG:NH1	2.29	0.71
2:P:5:DT:C6	2:P:5:DT:C2'	2.73	0.71
3:A:119:ILE:HG23	3:A:124:ASP:HB3	1.73	0.71
3:A:68:LYS:O	3:A:72:LYS:HE3	1.91	0.70
3:A:293:ILE:HD12	3:A:298:ILE:HG13	1.72	0.70
3:A:237:GLY:O	3:A:254:ARG:NH1	2.25	0.69
3:A:277:ILE:HD13	3:A:277:ILE:H	1.56	0.69
3:A:286:ALA:HA	3:A:323:ILE:CG2	2.22	0.69
3:A:80:GLY:O	3:A:81:LYS:HG2	1.92	0.69
3:A:194:LEU:CD1	3:A:258:ARG:HD3	2.22	0.69
3:A:119:ILE:CG2	3:A:124:ASP:HB3	2.23	0.69
3:A:113:LYS:O	3:A:117:GLU:HG3	1.93	0.69
3:A:41:LYS:O	3:A:45:VAL:HG13	1.93	0.68
3:A:194:LEU:HD11	3:A:258:ARG:HD3	1.76	0.67
3:A:244:LYS:CB	3:A:245:ASN:HD22	2.08	0.67
3:A:15:ILE:CG2	3:A:46:ILE:HD13	2.25	0.67
3:A:201:THR:HA	3:A:261:PRO:HB3	1.77	0.67
3:A:292:THR:C	3:A:293:ILE:HD13	2.21	0.67
3:A:31:GLN:N	6:A:641:HOH:O	2.27	0.66
3:A:154:GLU:O	3:A:158:MET:HG3	1.94	0.66
3:A:155:MET:HE3	3:A:188:SER:OG	1.96	0.66
3:A:278:PHE:CE2	3:A:333:ARG:HD3	2.31	0.65
3:A:18:MET:HG2	3:A:19:LEU:N	2.11	0.65
3:A:12:ASN:HB3	3:A:46:ILE:CD1	2.26	0.65
3:A:201:THR:HA	3:A:261:PRO:CB	2.26	0.65
3:A:330:PRO:HA	3:A:333:ARG:HG3	1.78	0.65
3:A:326:LYS:HE2	3:A:328:ARG:HE	1.61	0.64
2:P:3:DG:N3	6:P:511:HOH:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:207:GLN:HB2	6:A:625:HOH:O	1.96	0.64
3:A:79:THR:O	3:A:81:LYS:N	2.30	0.63
3:A:172:GLU:CG	3:A:198:PRO:HG2	2.28	0.63
3:A:286:ALA:O	3:A:291:PHE:HB2	1.98	0.63
3:A:23:ALA:HB2	3:A:39:TYR:CB	2.28	0.63
3:A:255:ILE:HG12	3:A:256:ASP:N	2.14	0.63
3:A:306:VAL:HG23	3:A:307:ALA:N	2.14	0.63
3:A:178:CYS:SG	3:A:194:LEU:HD23	2.39	0.62
3:A:150:ILE:CD1	3:A:253:ARG:HG2	2.29	0.62
3:A:152:ARG:NH2	3:A:181:PHE:O	2.32	0.62
3:A:41:LYS:HD3	3:A:42:ALA:N	2.15	0.62
3:A:244:LYS:HB3	3:A:245:ASN:HD22	1.64	0.61
3:A:15:ILE:HD11	3:A:77:LEU:HD11	1.83	0.61
3:A:261:PRO:HG2	3:A:264:GLN:HG3	1.82	0.61
3:A:327:TYR:HD1	3:A:328:ARG:N	1.98	0.61
3:A:11:LEU:H	3:A:11:LEU:CD2	2.12	0.61
3:A:250:TYR:HB3	3:A:251:PRO:HD2	1.81	0.61
3:A:182:ARG:NH1	3:A:273:THR:OG1	2.34	0.60
3:A:155:MET:SD	3:A:158:MET:HE3	2.42	0.60
3:A:286:ALA:CB	3:A:293:ILE:HD11	2.31	0.59
3:A:200:PHE:HB2	6:A:625:HOH:O	2.02	0.59
3:A:197:HIS:CG	3:A:198:PRO:HD2	2.38	0.59
2:P:5:DT:H6	2:P:5:DT:H2'	1.68	0.59
3:A:202:SER:HB2	3:A:263:ASP:CG	2.28	0.59
3:A:182:ARG:NH1	3:A:273:THR:HG21	2.18	0.59
3:A:121:THR:O	3:A:124:ASP:HB2	2.03	0.58
3:A:157:GLN:O	3:A:161:ILE:HG13	2.02	0.58
3:A:243:SER:HB3	3:A:249:GLU:HA	1.84	0.58
2:P:5:DT:N1	2:P:5:DT:H1'	2.03	0.58
3:A:12:ASN:ND2	3:A:53:ILE:H	1.99	0.58
3:A:27:LYS:HG3	3:A:28:ASN:HD22	1.68	0.58
3:A:182:ARG:HG2	3:A:182:ARG:NH1	2.14	0.58
3:A:259:LEU:O	3:A:260:ILE:HD13	2.04	0.58
3:A:277:ILE:HG13	3:A:335:GLU:CB	2.28	0.57
3:A:16:THR:HG23	3:A:46:ILE:CG1	2.34	0.57
3:A:166:VAL:O	3:A:169:VAL:HG12	2.05	0.57
3:A:244:LYS:HB3	3:A:245:ASN:ND2	2.19	0.57
1:T:3:DA:H2''	6:T:573:HOH:O	2.05	0.57
3:A:245:ASN:H	3:A:245:ASN:ND2	1.98	0.57
3:A:177:VAL:HG11	3:A:191:MET:HE2	1.86	0.57
3:A:217:GLN:NE2	3:A:217:GLN:HA	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:HB	3:A:106:ILE:HD12	1.87	0.56
3:A:330:PRO:O	3:A:333:ARG:HG3	2.05	0.56
3:A:49:TYR:CG	3:A:50:PRO:HD2	2.41	0.55
3:A:248:LYS:O	3:A:248:LYS:HG2	2.06	0.55
3:A:183:ARG:NH1	3:A:275:SER:HA	2.21	0.55
3:A:196:THR:OG1	3:A:197:HIS:N	2.39	0.55
3:A:270:LEU:HD21	3:A:282:MET:HE2	1.88	0.55
3:A:23:ALA:O	3:A:36:TYR:HD1	1.89	0.54
3:A:277:ILE:CG1	3:A:335:GLU:HB3	2.29	0.54
3:A:68:LYS:HB2	3:A:68:LYS:NZ	2.21	0.54
3:A:197:HIS:ND1	3:A:199:SER:HB3	2.22	0.54
3:A:111:ALA:O	3:A:115:VAL:HG23	2.08	0.54
3:A:202:SER:HB2	3:A:263:ASP:OD2	2.07	0.54
3:A:207:GLN:HB3	3:A:210:LEU:HG	1.89	0.54
3:A:152:ARG:HB3	6:A:530:HOH:O	2.09	0.53
3:A:327:TYR:CD1	3:A:328:ARG:N	2.76	0.53
3:A:18:MET:CE	3:A:76:PHE:HB2	2.34	0.53
3:A:12:ASN:HA	6:A:642:HOH:O	2.08	0.53
3:A:321:ASP:O	3:A:324:GLN:N	2.39	0.53
3:A:308:GLY:O	3:A:309:GLU:HB2	2.09	0.53
3:A:79:THR:C	3:A:81:LYS:H	2.16	0.53
3:A:289:LYS:HG3	3:A:323:ILE:O	2.09	0.53
3:A:18:MET:HE2	3:A:82:LEU:HD13	1.92	0.52
3:A:319:ILE:O	3:A:322:TYR:HB2	2.10	0.52
3:A:261:PRO:HG2	3:A:264:GLN:CG	2.39	0.52
2:P:3:DG:H4'	6:P:569:HOH:O	2.08	0.52
3:A:325:TRP:HD1	6:A:583:HOH:O	1.90	0.52
3:A:81:LYS:NZ	3:A:86:GLU:OE1	2.33	0.52
2:P:5:DT:C6	2:P:5:DT:H2'	2.43	0.51
3:A:35:LYS:O	3:A:38:ALA:HB3	2.10	0.51
3:A:227:THR:HG23	3:A:235:PHE:CE2	2.46	0.51
3:A:262:LYS:O	3:A:262:LYS:HG3	2.11	0.51
3:A:210:LEU:CB	3:A:259:LEU:HD21	2.40	0.51
3:A:303:VAL:C	3:A:305:GLY:H	2.17	0.51
3:A:27:LYS:HB3	3:A:36:TYR:CD1	2.46	0.51
3:A:163:LEU:HD23	3:A:163:LEU:N	2.26	0.51
3:A:26:GLU:HG3	3:A:35:LYS:HB3	1.93	0.50
3:A:150:ILE:O	3:A:187:SER:HA	2.12	0.50
3:A:292:THR:O	3:A:293:ILE:HD13	2.10	0.50
3:A:60:LYS:CA	3:A:65:VAL:HG22	2.35	0.50
3:A:210:LEU:HB2	3:A:259:LEU:HD21	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:TYR:HB2	6:A:592:HOH:O	2.11	0.50
3:A:327:TYR:HE1	3:A:333:ARG:HH21	1.59	0.50
3:A:26:GLU:OE1	3:A:26:GLU:HA	2.12	0.49
3:A:267:CYS:SG	3:A:297:THR:HA	2.52	0.49
3:A:18:MET:HE2	3:A:82:LEU:HD22	1.94	0.49
3:A:309:GLU:OE1	3:A:309:GLU:HA	2.10	0.49
3:A:208:PRO:O	3:A:212:HIS:HD2	1.96	0.49
3:A:285:HIS:NE2	3:A:289:LYS:HG2	2.28	0.48
3:A:312:PRO:O	3:A:322:TYR:OH	2.29	0.48
3:A:194:LEU:HD12	3:A:258:ARG:CG	2.43	0.48
1:T:3:DA:H1'	6:T:617:HOH:O	2.13	0.48
3:A:75:GLU:O	3:A:79:THR:HG23	2.13	0.48
3:A:202:SER:HB2	3:A:263:ASP:OD1	2.14	0.47
3:A:68:LYS:NZ	3:A:68:LYS:CB	2.76	0.47
3:A:165:GLU:HB3	3:A:217:GLN:HG3	1.97	0.47
3:A:215:VAL:O	3:A:219:GLN:HG3	2.14	0.47
3:A:243:SER:CB	3:A:249:GLU:HA	2.45	0.47
3:A:164:ASN:O	3:A:168:LYS:HG2	2.14	0.47
3:A:295:GLU:CD	3:A:295:GLU:H	2.22	0.47
3:A:32:ALA:HB1	3:A:35:LYS:HB2	1.97	0.47
3:A:200:PHE:CD2	3:A:261:PRO:HA	2.50	0.47
3:A:82:LEU:HB3	3:A:85:LEU:HB2	1.97	0.47
3:A:244:LYS:HB2	3:A:245:ASN:HD22	1.79	0.47
1:T:2:DC:H2''	1:T:3:DA:C8	2.51	0.46
3:A:23:ALA:CB	3:A:39:TYR:HB2	2.38	0.46
3:A:155:MET:HA	3:A:158:MET:HE3	1.97	0.46
3:A:228:LEU:HA	3:A:228:LEU:HD12	1.54	0.46
3:A:228:LEU:HB2	3:A:236:MET:O	2.15	0.46
3:A:287:LEU:HD13	3:A:287:LEU:HA	1.54	0.46
2:P:1:DC:H2''	2:P:2:DA:C5'	2.27	0.46
3:A:178:CYS:SG	3:A:194:LEU:CD2	3.04	0.45
3:A:60:LYS:HE2	3:A:67:THR:CA	2.46	0.45
3:A:250:TYR:CB	3:A:251:PRO:HD2	2.47	0.45
3:A:264:GLN:HB3	3:A:296:TYR:O	2.16	0.45
3:A:159:GLN:O	3:A:163:LEU:HG	2.16	0.45
3:A:294:ASN:N	3:A:294:ASN:HD22	2.13	0.45
3:A:91:ASP:HB3	3:A:94:SER:HB3	1.99	0.45
3:A:182:ARG:NH1	3:A:273:THR:CG2	2.80	0.45
3:A:166:VAL:HG12	3:A:173:TYR:HB2	1.99	0.45
3:A:285:HIS:NE2	3:A:289:LYS:CG	2.80	0.45
3:A:11:LEU:CD2	3:A:11:LEU:N	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:316:GLU:CD	3:A:333:ARG:HH22	2.24	0.45
3:A:40:ARG:HE	3:A:40:ARG:HB2	1.57	0.44
3:A:150:ILE:HD11	3:A:253:ARG:HG2	2.00	0.44
3:A:315:SER:OG	3:A:316:GLU:N	2.50	0.44
3:A:16:THR:HG23	3:A:46:ILE:HG12	1.99	0.44
3:A:264:GLN:HA	6:A:536:HOH:O	2.17	0.44
3:A:295:GLU:HG2	3:A:296:TYR:CE1	2.53	0.44
2:P:5:DT:C2'	2:P:5:DT:H6	2.21	0.43
3:A:255:ILE:HG12	3:A:256:ASP:H	1.83	0.43
3:A:200:PHE:HB2	3:A:210:LEU:HD11	2.00	0.43
3:A:259:LEU:C	3:A:260:ILE:HD13	2.44	0.43
3:A:299:ARG:HB3	3:A:300:PRO:HD2	2.00	0.43
3:A:322:TYR:C	3:A:324:GLN:H	2.24	0.43
3:A:316:GLU:O	3:A:320:PHE:HD1	2.01	0.43
3:A:27:LYS:CB	3:A:36:TYR:CD1	3.02	0.43
3:A:197:HIS:CE1	3:A:198:PRO:HD2	2.52	0.43
3:A:299:ARG:HA	3:A:300:PRO:HD3	1.91	0.43
2:P:2:DA:N6	6:P:598:HOH:O	2.28	0.43
3:A:243:SER:OG	3:A:249:GLU:HG3	2.19	0.43
3:A:169:VAL:HG13	3:A:170:ASP:N	2.34	0.42
3:A:204:SER:O	3:A:204:SER:OG	2.30	0.42
3:A:288:GLU:C	3:A:290:GLY:H	2.27	0.42
3:A:16:THR:CG2	3:A:46:ILE:HG12	2.49	0.42
3:A:79:THR:C	3:A:81:LYS:N	2.77	0.42
3:A:99:PHE:CD2	3:A:99:PHE:C	2.98	0.42
3:A:135:HIS:C	3:A:135:HIS:CD2	2.97	0.42
3:A:264:GLN:HB3	3:A:264:GLN:HE21	1.58	0.42
3:A:194:LEU:HD12	3:A:258:ARG:HG2	2.01	0.42
3:A:150:ILE:HD13	3:A:253:ARG:HG2	2.02	0.42
3:A:273:THR:O	3:A:273:THR:HG22	2.20	0.42
3:A:301:LEU:HA	3:A:301:LEU:HD12	1.73	0.41
3:A:100:LEU:HD12	3:A:100:LEU:HA	1.76	0.41
3:A:52:LYS:HG2	6:A:554:HOH:O	2.21	0.41
3:A:227:THR:HG23	3:A:235:PHE:HE2	1.83	0.41
3:A:27:LYS:HB2	3:A:36:TYR:CG	2.55	0.41
3:A:133:ASN:O	3:A:137:ARG:HG3	2.20	0.41
3:A:270:LEU:HD21	3:A:282:MET:CE	2.50	0.41
3:A:294:ASN:HD22	3:A:294:ASN:H	1.68	0.41
3:A:54:LYS:HD2	3:A:54:LYS:HA	1.95	0.41
3:A:170:ASP:HB3	3:A:173:TYR:CD2	2.56	0.41
3:A:294:ASN:HD22	3:A:294:ASN:C	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:DA:H5'	2:P:2:DA:H2'	1.84	0.41
3:A:133:ASN:HD21	3:A:135:HIS:HB3	1.86	0.41
3:A:303:VAL:C	3:A:305:GLY:N	2.78	0.41
3:A:205:THR:HG23	3:A:205:THR:O	2.20	0.41
3:A:309:GLU:HA	3:A:310:PRO:HD2	1.97	0.41
3:A:32:ALA:O	3:A:36:TYR:HB3	2.20	0.41
3:A:44:SER:O	3:A:47:ALA:HB3	2.21	0.41
3:A:205:THR:O	3:A:206:LYS:O	2.38	0.41
3:A:150:ILE:N	3:A:188:SER:O	2.42	0.40
3:A:11:LEU:HD23	3:A:11:LEU:N	2.20	0.40
3:A:33:ILE:HG22	6:A:616:HOH:O	2.21	0.40
3:A:289:LYS:HA	3:A:289:LYS:HD3	1.76	0.40
3:A:166:VAL:CG1	3:A:173:TYR:CB	2.99	0.40
3:A:285:HIS:CE1	3:A:289:LYS:HE3	2.57	0.40
3:A:235:PHE:CD1	3:A:235:PHE:C	2.96	0.40
3:A:288:GLU:OE1	3:A:288:GLU:HA	2.08	0.40
3:A:332:ASP:C	3:A:334:SER:H	2.29	0.40
3:A:41:LYS:CE	3:A:64:GLY:HA2	2.31	0.40
3:A:56:GLY:O	3:A:59:ALA:N	2.55	0.40
3:A:134:HIS:O	3:A:138:ILE:HG12	2.22	0.40
3:A:330:PRO:C	3:A:333:ARG:HG3	2.47	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]	2.16	0.04

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%)	286 (88%)	24 (7%)	15 (5%)	2 2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	32	ALA
3	A	185	ALA
3	A	202	SER
3	A	206	LYS
3	A	244	LYS
3	A	309	GLU
3	A	80	GLY
3	A	247	GLU
3	A	289	LYS
3	A	307	ALA
3	A	10	THR
3	A	246	ASP
3	A	91	ASP
3	A	204	SER
3	A	207	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	288/295 (98%)	220 (76%)	68 (24%)	1 1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	18	MET
3	A	22	LEU
3	A	27	LYS
3	A	30	SER
3	A	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	85	LEU
3	A	95	SER
3	A	100	LEU
3	A	101	THR
3	A	119	ILE
3	A	122	LEU
3	A	131	LYS
3	A	150	ILE
3	A	153	GLU
3	A	168	LYS
3	A	171	SER
3	A	182	ARG
3	A	188	SER
3	A	191	MET
3	A	194	LEU
3	A	201	THR
3	A	202	SER
3	A	204	SER
3	A	207	GLN
3	A	214	VAL
3	A	218	LEU
3	A	219	GLN
3	A	224	ILE
3	A	228	LEU
3	A	245	ASN
3	A	246	ASP
3	A	248	LYS
3	A	253	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	255	ILE
3	A	258	ARG
3	A	264	GLN
3	A	277	ILE
3	A	287	LEU
3	A	288	GLU
3	A	289	LYS
3	A	293	ILE
3	A	294	ASN
3	A	295	GLU
3	A	298	ILE
3	A	303	VAL
3	A	306	VAL
3	A	309	GLU
3	A	311	LEU
3	A	314	ASP
3	A	325	TRP
3	A	329	GLU
3	A	331	LYS
3	A	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	28	ASN
3	A	31	GLN
3	A	90	GLN
3	A	98	ASN
3	A	136	GLN
3	A	157	GLN
3	A	212	HIS
3	A	213	GLN
3	A	217	GLN
3	A	245	ASN
3	A	264	GLN
3	A	279	ASN
3	A	281	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	0.99	0	6,6,6	0.87	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	7/7 (100%)	-1.19	0 100 100	25, 32, 65, 100	0
2	P	6/6 (100%)	-1.41	0 100 100	24, 30, 35, 42	0
3	A	324/335 (96%)	-0.81	0 100 100	10, 37, 83, 100	0
All	All	337/348 (96%)	-0.83	0 100 100	10, 36, 83, 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	SO4	A	338	5/5	0.91	0.12	10,29,66,74	5
5	NA	A	342	1/1	0.95	0.04	44,44,44,44	0
5	NA	A	341	1/1	0.98	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.