



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:15 AM UTC

PDB ID : 1KLN / pdb_00001klh
Title : DNA POLYMERASE I KLENOW FRAGMENT (E.C.2.7.7.7) MUTANT/DNA COMPLEX
Authors : Beese, L.S.; Derbyshire, V.; Steitz, T.A.
Deposited on : 1994-05-24
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

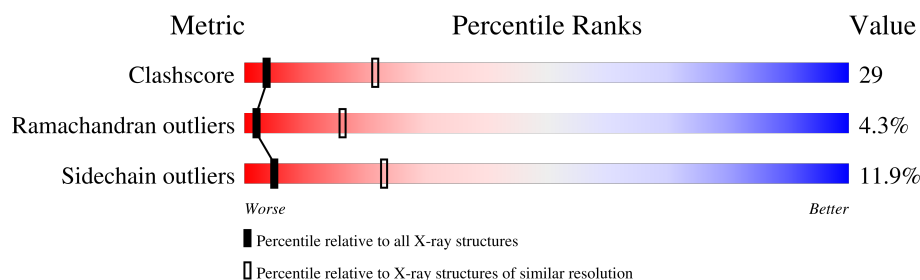
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	13	
2	C	10	
3	A	605	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5171 atoms, of which 31 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(*GP*CP*CP*TP*CP*GP*CP*GP*GP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	13	Total	C	N	O	P	0	0	0
			263	124	50	77	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			207	96	42	59	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	595	Total	C	H	N	O	S	0	0
			4700	2951	31	818	885	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	ALA	ASP	engineered mutation	UNP P00582

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

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

Chain B: 



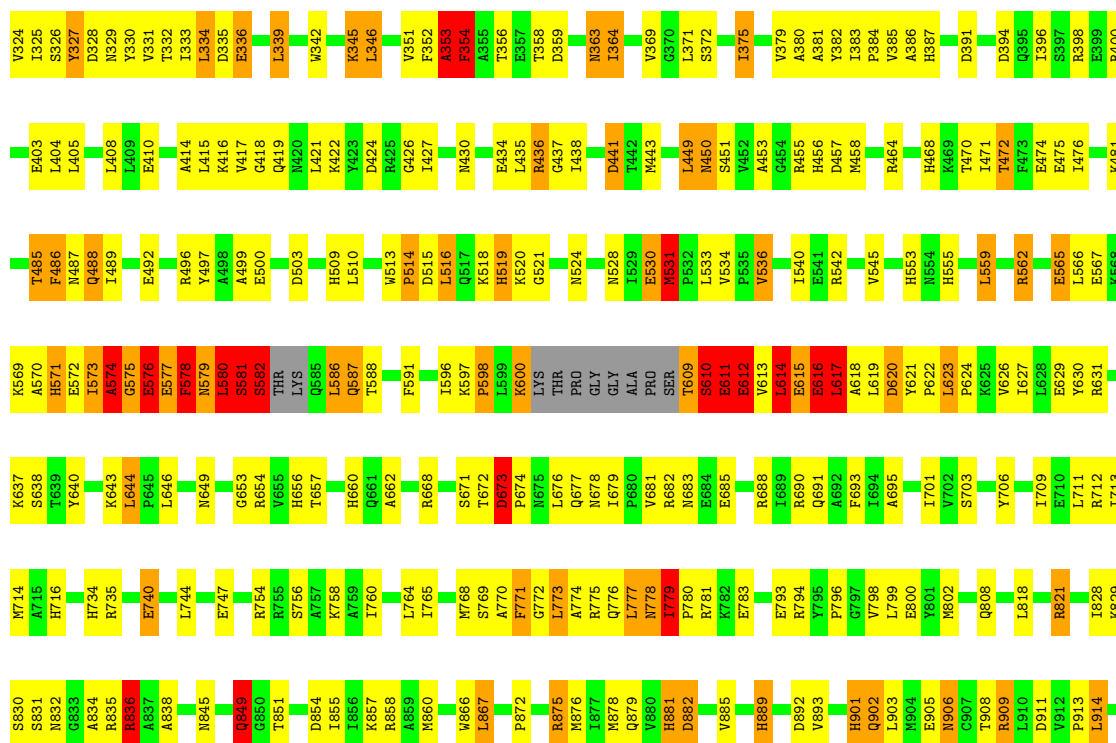
- Molecule 2: DNA (5'-D(*GP*CP*CP*GP*CP*GP*AP*GP*GP*C)-3')

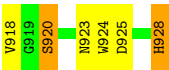
Chain C: 



- Molecule 3: PROTEIN (DNA POLYMERASE I KLENOW FRAGMENT (E.C.2.7.7.7))

Chain A: 





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	104.30 Å 104.30 Å 86.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5171	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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: ZN

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	B	0.95	0/294	3.77	38/452 (8.4%)
2	C	1.62	1/232 (0.4%)	2.49	21/356 (5.9%)
3	A	1.15	26/4751 (0.5%)	1.83	105/6431 (1.6%)
All	All	1.17	27/5277 (0.5%)	2.04	164/7239 (2.3%)

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
1	B	0	1
2	C	0	2
3	A	0	9
All	All	0	12

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	567	GLU	N-CA	-32.20	1.07	1.46
2	C	19	DG	O3'-P	21.26	1.93	1.61
3	A	600	LYS	CA-CB	12.07	1.77	1.53
3	A	581	SER	C-N	-11.66	1.17	1.33
3	A	582	SER	N-CA	-9.18	1.28	1.46
3	A	734	HIS	CD2-NE2	-6.90	1.30	1.37
3	A	387	HIS	CD2-NE2	-6.84	1.30	1.37
3	A	581	SER	N-CA	-6.81	1.37	1.46
3	A	353	ALA	C-N	6.77	1.43	1.33
3	A	456	HIS	CD2-NE2	-6.75	1.30	1.37
3	A	889	HIS	CD2-NE2	-6.70	1.30	1.37
3	A	656	HIS	CD2-NE2	-6.65	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	571	HIS	CD2-NE2	-6.58	1.30	1.37
3	A	716	HIS	CD2-NE2	-6.50	1.30	1.37
3	A	509	HIS	CD2-NE2	-6.45	1.30	1.37
3	A	881	HIS	CD2-NE2	-6.33	1.30	1.37
3	A	555	HIS	CD2-NE2	-6.19	1.31	1.37
3	A	660	HIS	CD2-NE2	-6.19	1.31	1.37
3	A	580	LEU	CA-C	-6.17	1.44	1.52
3	A	928	HIS	CD2-NE2	-6.06	1.31	1.37
3	A	468	HIS	CD2-NE2	-6.01	1.31	1.37
3	A	901	HIS	CD2-NE2	-5.78	1.31	1.37
3	A	534	VAL	CA-CB	5.68	1.56	1.54
3	A	779	ILE	CA-CB	5.47	1.61	1.54
3	A	553	HIS	CD2-NE2	-5.47	1.31	1.37
3	A	519	HIS	CD2-NE2	-5.45	1.31	1.37
3	A	536	VAL	CA-CB	5.02	1.61	1.54

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	DG	O3'-P-O5'	-33.88	53.18	104.00
3	A	581	SER	O-C-N	26.48	157.81	122.59
1	B	9	DG	O3'-P-O5'	23.29	138.94	104.00
1	B	2	DG	O3'-P-O5'	17.97	130.96	104.00
1	B	13	DG	OP1-P-O3'	-17.33	56.00	108.00
3	A	580	LEU	O-C-N	15.99	143.85	122.59
1	B	13	DG	OP2-P-O3'	15.49	154.48	108.00
1	B	4	DC	O3'-P-O5'	-14.96	81.56	104.00
2	C	23	DG	O3'-P-O5'	14.22	125.34	104.00
3	A	353	ALA	O-C-N	-14.12	103.28	121.78
1	B	7	DG	OP2-P-O3'	13.52	148.55	108.00
1	B	10	DG	OP1-P-O3'	13.19	147.56	108.00
1	B	5	DT	OP2-P-O3'	-12.32	71.03	108.00
3	A	881	HIS	CA-CB-CG	12.06	125.86	113.80
3	A	581	SER	CA-C-N	12.03	143.35	121.70
3	A	581	SER	C-N-CA	12.03	143.35	121.70
1	B	12	DG	OP1-P-O3'	-12.02	71.95	108.00
1	B	3	DC	O3'-P-O5'	11.86	121.79	104.00
1	B	3	DC	OP1-P-O3'	-11.82	72.53	108.00
1	B	5	DT	O3'-P-O5'	11.71	121.56	104.00
1	B	11	DC	O3'-P-O5'	-11.67	86.50	104.00
1	B	10	DG	OP2-P-O3'	-11.24	74.28	108.00
1	B	9	DG	OP1-P-O3'	-10.82	75.54	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	DC	OP2-P-O3'	10.62	139.86	108.00
1	B	7	DG	O3'-P-O5'	-10.52	88.22	104.00
2	C	20	DC	O3'-P-O5'	10.52	119.78	104.00
3	A	882	ASP	CA-CB-CG	10.40	123.00	112.60
2	C	26	DA	O3'-P-O5'	-10.24	88.64	104.00
3	A	567	GLU	N-CA-C	-10.15	100.17	111.14
2	C	21	DC	OP1-P-O3'	-10.00	77.99	108.00
3	A	610	SER	O-C-N	9.95	135.82	122.59
1	B	7	DG	OP1-P-O3'	-9.93	78.21	108.00
3	A	582	SER	N-CA-C	9.78	138.37	111.00
2	C	24	DC	O3'-P-O5'	9.77	118.66	104.00
2	C	19	DG	O3'-P-O5'	-9.75	89.37	104.00
3	A	328	ASP	CA-CB-CG	9.70	122.30	112.60
3	A	836	ARG	N-CA-C	-9.61	100.67	111.82
3	A	329	ASN	CA-CB-CG	9.02	121.62	112.60
2	C	29	DC	C4'-C3'-C2'	-8.94	88.98	102.40
2	C	28	DG	P-O3'-C3'	8.65	133.17	120.20
1	B	12	DG	OP2-P-O3'	8.58	133.75	108.00
1	B	13	DG	P-O3'-C3'	-8.38	107.63	120.20
3	A	359	ASP	CA-CB-CG	8.33	120.93	112.60
3	A	777	LEU	N-CA-C	-8.26	97.23	109.62
3	A	600	LYS	CB-CA-C	-8.17	94.58	110.10
1	B	8	DC	P-O3'-C3'	8.02	132.22	120.20
2	C	23	DG	P-O3'-C3'	8.01	132.22	120.20
2	C	21	DC	OP2-P-O3'	7.92	131.75	108.00
3	A	567	GLU	N-CA-CB	7.91	121.54	110.07
3	A	609	THR	O-C-N	7.91	135.65	123.00
3	A	911	ASP	CA-CB-CG	7.88	120.48	112.60
3	A	600	LYS	N-CA-CB	7.87	123.87	110.50
3	A	611	GLU	O-C-N	7.65	132.76	122.59
1	B	10	DG	O3'-P-O5'	-7.55	92.68	104.00
3	A	800	GLU	N-CA-C	-7.40	103.15	111.07
1	B	14	DC	O5'-C5'-C4'	7.27	121.71	110.80
1	B	6	DC	O3'-P-O5'	7.27	114.90	104.00
3	A	488	GLN	OE1-CD-NE2	-7.23	115.37	122.60
2	C	20	DC	P-O3'-C3'	7.20	130.99	120.20
3	A	582	SER	CB-CA-C	-7.18	96.45	110.10
3	A	578	PHE	CA-CB-CG	7.08	120.88	113.80
2	C	24	DC	OP1-P-O3'	-7.07	86.78	108.00
3	A	598	PRO	N-CA-CB	7.07	110.67	103.25
2	C	25	DG	P-O5'-C5'	6.98	130.47	120.00
2	C	29	DC	O4'-C1'-N1	6.98	118.87	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	19	DG	OP2-P-O3'	6.94	128.83	108.00
3	A	572	GLU	N-CA-C	-6.86	103.86	111.82
1	B	2	DG	P-O3'-C3'	6.72	130.27	120.20
3	A	531	MET	CG-SD-CE	-6.64	86.29	100.90
3	A	364	ILE	CB-CA-C	6.61	118.08	110.88
3	A	923	ASN	CA-CB-CG	6.53	119.12	112.60
3	A	364	ILE	N-CA-CB	-6.50	103.38	112.35
3	A	609	THR	CA-C-N	6.45	133.87	121.54
3	A	609	THR	C-N-CA	6.45	133.87	121.54
3	A	821	ARG	NE-CZ-NH2	6.44	124.99	119.20
3	A	345	LYS	CA-CB-CG	6.38	126.86	114.10
2	C	21	DC	P-O3'-C3'	6.37	129.75	120.20
3	A	458	MET	CA-CB-CG	-6.34	101.42	114.10
3	A	879	GLN	OE1-CD-NE2	-6.30	116.30	122.60
3	A	327	TYR	N-CA-C	6.27	120.03	112.38
1	B	8	DC	O5'-C5'-C4'	6.25	120.18	110.80
3	A	528	ASN	OD1-CG-ND2	-6.25	116.35	122.60
3	A	486	PHE	CA-CB-CG	-6.22	107.58	113.80
3	A	616	GLU	N-CA-C	-6.20	105.72	113.28
3	A	808	GLN	OE1-CD-NE2	-6.18	116.42	122.60
3	A	875	ARG	CA-CB-CG	6.17	126.44	114.10
3	A	486	PHE	N-CA-C	6.15	118.77	111.33
1	B	14	DC	O5'-P-OP1	-6.13	90.62	109.00
3	A	673	ASP	N-CA-C	-6.09	96.34	109.81
1	B	10	DG	N9-C1'-C2'	-6.09	104.37	113.50
3	A	771	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	7	DG	P-O5'-C5'	5.99	128.99	120.00
3	A	882	ASP	N-CA-CB	5.99	120.61	110.49
3	A	673	ASP	CA-C-O	-5.98	111.97	120.16
3	A	424	ASP	CA-CB-CG	5.97	118.57	112.60
2	C	29	DC	N1-C1'-C2'	-5.91	104.64	113.50
3	A	464	ARG	NE-CZ-NH2	5.90	124.51	119.20
3	A	893	VAL	N-CA-C	5.78	117.20	110.62
1	B	13	DG	P-O5'-C5'	5.77	128.66	120.00
3	A	612	GLU	O-C-N	5.75	130.23	122.59
3	A	881	HIS	O-C-N	-5.74	114.95	122.59
3	A	579	ASN	O-C-N	5.71	130.18	122.59
3	A	450	ASN	OD1-CG-ND2	-5.68	116.92	122.60
3	A	882	ASP	CB-CA-C	-5.68	99.12	110.42
3	A	906	ASN	CA-CB-CG	5.66	118.26	112.60
3	A	914	LEU	N-CA-C	5.66	119.04	109.76
3	A	385	VAL	CB-CA-C	-5.64	105.33	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	DC	P-O5'-C5'	5.63	128.44	120.00
3	A	677	GLN	OE1-CD-NE2	-5.61	116.99	122.60
3	A	902	GLN	CA-C-O	-5.61	112.49	120.51
3	A	821	ARG	NE-CZ-NH1	-5.60	115.90	121.50
3	A	542	ARG	NE-CZ-NH2	5.60	124.24	119.20
2	C	29	DC	O4'-C1'-C2'	-5.59	98.02	106.40
3	A	714	MET	CA-CB-CG	-5.55	102.99	114.10
2	C	25	DG	O5'-C5'-C4'	5.54	119.11	110.80
1	B	11	DC	OP2-P-O3'	5.54	124.62	108.00
3	A	653	GLY	N-CA-C	-5.53	106.38	114.90
3	A	906	ASN	OD1-CG-ND2	-5.53	117.07	122.60
3	A	881	HIS	N-CA-C	5.53	122.57	110.80
3	A	336	GLU	N-CA-C	5.51	117.72	111.11
3	A	828	ILE	N-CA-C	-5.50	105.17	110.72
3	A	668	ARG	NE-CZ-NH2	5.47	124.12	119.20
3	A	485	THR	CA-CB-OG1	-5.47	101.40	109.60
3	A	488	GLN	CG-CD-NE2	5.46	124.59	116.40
3	A	329	ASN	CB-CA-C	-5.46	101.61	110.79
3	A	571	HIS	CA-CB-CG	-5.45	108.35	113.80
3	A	464	ARG	NE-CZ-NH1	-5.44	116.06	121.50
3	A	542	ARG	NE-CZ-NH1	-5.43	116.06	121.50
3	A	673	ASP	CA-CB-CG	-5.40	107.20	112.60
3	A	472	THR	CA-CB-OG1	-5.39	101.52	109.60
3	A	617	LEU	O-C-N	5.36	129.72	122.59
3	A	441	ASP	CA-CB-CG	5.35	117.95	112.60
3	A	901	HIS	O-C-N	-5.34	116.46	122.12
3	A	649	ASN	CA-C-N	5.33	125.65	119.47
3	A	649	ASN	C-N-CA	5.33	125.65	119.47
1	B	2	DG	OP2-P-O3'	-5.29	92.14	108.00
3	A	866	TRP	CG-CD1-NE1	-5.27	103.35	110.20
3	A	849	GLN	CA-C-N	5.27	125.69	119.94
3	A	849	GLN	C-N-CA	5.27	125.69	119.94
3	A	534	VAL	O-C-N	-5.26	117.05	120.42
1	B	10	DG	O4'-C1'-N9	5.25	116.28	108.40
3	A	580	LEU	N-CA-C	5.25	121.97	110.80
2	C	23	DG	OP1-P-O3'	-5.25	92.27	108.00
2	C	23	DG	C5'-C4'-O4'	-5.24	101.54	109.40
3	A	683	ASN	OD1-CG-ND2	-5.22	117.38	122.60
3	A	596	ILE	O-C-N	5.21	129.09	122.57
3	A	419	GLN	OE1-CD-NE2	-5.21	117.39	122.60
3	A	379	VAL	N-CA-CB	-5.21	107.01	112.06
1	B	8	DC	O3'-P-O5'	-5.19	96.22	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	375	ILE	CA-C-O	5.18	123.46	118.90
3	A	866	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	B	6	DC	OP1-P-O3'	-5.12	92.63	108.00
3	A	778	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	B	4	DC	OP1-P-O3'	-5.09	92.73	108.00
3	A	679	ILE	CA-C-N	5.09	126.20	119.84
3	A	679	ILE	C-N-CA	5.09	126.20	119.84
3	A	430	ASN	CA-CB-CG	5.08	117.69	112.60
3	A	521	GLY	CA-C-N	5.07	124.24	118.97
3	A	521	GLY	C-N-CA	5.07	124.24	118.97
3	A	398	ARG	NE-CZ-NH2	5.06	123.75	119.20
3	A	436	ARG	N-CA-C	5.03	120.27	114.04
3	A	908	THR	N-CA-CB	-5.02	102.01	110.49
3	A	838	ALA	N-CA-C	-5.02	105.89	111.36
3	A	391	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	353	ALA	Mainchain
3	A	497	TYR	Sidechain
3	A	574	ALA	Peptide
3	A	575	GLY	Peptide
3	A	576	GLU	Peptide
3	A	577	GLU	Peptide
3	A	578	PHE	Peptide
3	A	580	LEU	Peptide
3	A	581	SER	Peptide
1	B	6	DC	Sidechain
2	C	19	DG	Sidechain
2	C	28	DG	Sidechain

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	B	263	0	146	21	0
2	C	207	0	111	6	0
3	A	4669	31	4628	285	0
4	B	1	0	0	0	0
All	All	5140	31	4885	292	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 29.

All (292) 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:600:LYS:CB	3:A:600:LYS:CA	1.77	1.60
3:A:612:GLU:CG	3:A:613:VAL:N	1.71	1.34
3:A:616:GLU:OE1	3:A:618:ALA:HB3	1.10	1.27
3:A:580:LEU:HD21	3:A:581:SER:O	1.42	1.16
3:A:619:LEU:HD21	3:A:620:ASP:OD1	1.48	1.13
3:A:573:ILE:CG1	3:A:622:PRO:HB2	1.64	1.12
3:A:616:GLU:OE1	3:A:618:ALA:CB	2.00	1.09
3:A:610:SER:HB2	3:A:631:ARG:NH2	1.68	1.09
3:A:326:SER:HA	3:A:496:ARG:HG2	1.38	1.06
3:A:580:LEU:HD11	3:A:581:SER:O	1.56	1.05
1:B:7:DG:OP2	3:A:609:THR:OG1	1.73	1.04
3:A:619:LEU:CD2	3:A:620:ASP:OD1	2.05	1.04
3:A:620:ASP:C	3:A:621:TYR:N	2.16	1.03
3:A:330:TYR:CD1	3:A:380:ALA:HB3	1.93	1.03
3:A:580:LEU:CD2	3:A:581:SER:O	2.05	1.03
3:A:612:GLU:HG3	3:A:613:VAL:CA	1.88	1.02
3:A:573:ILE:CD1	3:A:622:PRO:HB2	1.89	1.00
3:A:620:ASP:C	3:A:621:TYR:C	2.28	1.00
3:A:346:LEU:HD23	3:A:408:LEU:CD2	1.93	0.99
3:A:332:THR:HA	3:A:382:TYR:O	1.63	0.99
3:A:612:GLU:HG3	3:A:613:VAL:N	0.90	0.98
3:A:570:ALA:HA	3:A:626:VAL:HG21	1.46	0.97
3:A:610:SER:CB	3:A:631:ARG:NH2	2.28	0.97
3:A:620:ASP:C	3:A:621:TYR:CA	2.39	0.96
3:A:580:LEU:CG	3:A:581:SER:O	2.13	0.96
3:A:565:GLU:O	3:A:569:LYS:N	2.00	0.94
3:A:573:ILE:HG12	3:A:622:PRO:HB2	1.49	0.94
3:A:580:LEU:CD1	3:A:581:SER:O	2.16	0.93
3:A:333:ILE:HB	3:A:383:ILE:HG12	1.51	0.93
1:B:7:DG:P	3:A:609:THR:HA	2.11	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:600:LYS:CB	3:A:600:LYS:C	2.43	0.91
3:A:612:GLU:CD	3:A:613:VAL:HG23	1.96	0.91
3:A:573:ILE:CG1	3:A:622:PRO:CB	2.49	0.91
3:A:352:PHE:CE2	3:A:414:ALA:HB1	2.06	0.90
2:C:28:DG:H3'	2:C:29:DC:H5''	1.53	0.89
3:A:573:ILE:HD13	3:A:622:PRO:HB2	1.53	0.89
3:A:352:PHE:O	3:A:416:LYS:HA	1.72	0.89
3:A:573:ILE:HD11	3:A:626:VAL:HG11	1.56	0.88
3:A:331:VAL:CG1	3:A:381:ALA:HB2	2.04	0.87
3:A:573:ILE:HG12	3:A:622:PRO:CB	2.05	0.86
1:B:7:DG:OP1	3:A:609:THR:HA	1.76	0.85
3:A:331:VAL:HG13	3:A:381:ALA:CB	2.08	0.84
3:A:616:GLU:OE1	3:A:616:GLU:O	1.96	0.83
3:A:331:VAL:O	3:A:382:TYR:N	2.13	0.82
3:A:610:SER:HB2	3:A:631:ARG:CZ	2.10	0.82
3:A:610:SER:HB2	3:A:631:ARG:HH22	1.45	0.80
3:A:613:VAL:O	3:A:614:LEU:HB2	1.79	0.80
3:A:441:ASP:HB2	3:A:531:MET:HE1	1.64	0.79
3:A:578:PHE:HD1	3:A:580:LEU:HB3	1.46	0.79
1:B:7:DG:P	3:A:609:THR:HG1	2.06	0.79
3:A:331:VAL:HG13	3:A:381:ALA:HB1	1.65	0.79
3:A:351:VAL:HG12	3:A:415:LEU:HB2	1.65	0.78
3:A:620:ASP:O	3:A:621:TYR:C	2.27	0.78
3:A:566:LEU:O	3:A:570:ALA:CB	2.32	0.78
3:A:331:VAL:HG12	3:A:381:ALA:HB2	1.63	0.77
3:A:573:ILE:HD11	3:A:626:VAL:CG1	2.14	0.77
3:A:330:TYR:CE1	3:A:380:ALA:HB3	2.20	0.77
3:A:352:PHE:HE2	3:A:414:ALA:HB1	1.49	0.76
3:A:352:PHE:CZ	3:A:416:LYS:HE3	2.21	0.75
3:A:578:PHE:CD1	3:A:580:LEU:HB3	2.21	0.75
3:A:573:ILE:O	3:A:574:ALA:HB2	1.86	0.74
1:B:12:DG:H22	3:A:422:LYS:NZ	1.86	0.74
3:A:330:TYR:CG	3:A:499:ALA:HB1	2.22	0.74
3:A:331:VAL:CG1	3:A:381:ALA:CB	2.65	0.73
3:A:579:ASN:HD22	3:A:580:LEU:N	1.87	0.73
3:A:576:GLU:HB3	3:A:577:GLU:HA	1.70	0.73
3:A:616:GLU:O	3:A:618:ALA:O	2.08	0.72
3:A:832:ASN:HA	3:A:836:ARG:HD3	1.71	0.71
2:C:28:DG:H2'	2:C:29:DC:O4'	1.91	0.71
3:A:330:TYR:CD2	3:A:499:ALA:HB3	2.26	0.71
3:A:450:ASN:HB3	3:A:453:ALA:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325:ILE:HD13	3:A:500:GLU:HG3	1.73	0.70
1:B:7:DG:OP1	3:A:609:THR:CA	2.40	0.69
3:A:695:ALA:HB2	3:A:701:ILE:HG12	1.73	0.69
3:A:346:LEU:HD23	3:A:408:LEU:HD22	1.71	0.68
3:A:905:GLU:HA	3:A:914:LEU:HD23	1.75	0.68
3:A:333:ILE:N	3:A:382:TYR:O	2.26	0.68
3:A:336:GLU:CD	3:A:400:ARG:HE	2.01	0.68
3:A:332:THR:CA	3:A:382:TYR:O	2.40	0.68
3:A:760:ILE:HG12	3:A:773:LEU:HD11	1.75	0.68
3:A:325:ILE:HD11	3:A:330:TYR:HE2	1.58	0.68
3:A:325:ILE:CD1	3:A:500:GLU:HB2	2.25	0.67
3:A:573:ILE:CD1	3:A:626:VAL:HG21	2.24	0.67
3:A:325:ILE:HD13	3:A:500:GLU:CG	2.23	0.67
3:A:325:ILE:HG23	3:A:471:ILE:HD11	1.76	0.67
3:A:486:PHE:HA	3:A:489:ILE:HD12	1.77	0.67
3:A:334:LEU:HD13	3:A:384:PRO:HD2	1.77	0.67
3:A:573:ILE:HD13	3:A:622:PRO:C	2.19	0.67
3:A:610:SER:HB3	3:A:631:ARG:NH2	2.08	0.66
3:A:612:GLU:CG	3:A:613:VAL:HG23	2.25	0.66
3:A:325:ILE:HD13	3:A:500:GLU:HB2	1.77	0.66
3:A:330:TYR:HA	3:A:380:ALA:O	1.95	0.66
3:A:443:MET:HE2	3:A:662:ALA:HB3	1.78	0.66
3:A:566:LEU:O	3:A:570:ALA:HB2	1.95	0.65
3:A:616:GLU:OE2	3:A:620:ASP:C	2.39	0.65
3:A:711:LEU:HD13	3:A:765:ILE:HD11	1.78	0.65
3:A:575:GLY:O	3:A:576:GLU:O	2.14	0.65
3:A:623:LEU:HB3	3:A:624:PRO:HD3	1.79	0.65
3:A:354:PHE:HE1	3:A:371:LEU:HD23	1.62	0.65
3:A:485:THR:HG23	3:A:487:ASN:OD1	1.96	0.65
3:A:579:ASN:HD22	3:A:579:ASN:C	2.03	0.65
1:B:12:DG:H22	3:A:422:LYS:HZ1	1.44	0.64
3:A:346:LEU:HD23	3:A:408:LEU:HD21	1.79	0.64
3:A:325:ILE:CD1	3:A:500:GLU:HG3	2.27	0.64
3:A:331:VAL:O	3:A:381:ALA:HB1	1.98	0.64
3:A:620:ASP:O	3:A:621:TYR:O	2.16	0.64
3:A:573:ILE:O	3:A:574:ALA:CB	2.46	0.63
3:A:616:GLU:OE1	3:A:616:GLU:CA	2.46	0.63
3:A:619:LEU:N	3:A:619:LEU:HD23	2.14	0.63
3:A:616:GLU:CD	3:A:618:ALA:O	2.43	0.62
3:A:533:LEU:HD22	3:A:857:LYS:HD3	1.80	0.61
3:A:619:LEU:HG	3:A:620:ASP:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:DG:H5''	3:A:457:ASP:HB3	1.82	0.61
3:A:573:ILE:CD1	3:A:626:VAL:CG2	2.79	0.61
3:A:330:TYR:CG	3:A:499:ALA:CB	2.83	0.61
3:A:610:SER:CB	3:A:631:ARG:CZ	2.75	0.60
3:A:559:LEU:HD12	3:A:637:LYS:HB2	1.83	0.60
3:A:616:GLU:OE1	3:A:616:GLU:HA	2.00	0.60
3:A:774:ALA:O	3:A:778:ASN:HA	2.01	0.60
3:A:579:ASN:C	3:A:579:ASN:ND2	2.60	0.60
3:A:325:ILE:HD11	3:A:330:TYR:CE2	2.37	0.59
3:A:713:ILE:HD11	3:A:855:ILE:HD12	1.84	0.59
3:A:878:MET:HG2	3:A:885:VAL:HB	1.84	0.59
3:A:330:TYR:CD2	3:A:499:ALA:CB	2.86	0.59
3:A:580:LEU:CD2	3:A:581:SER:C	2.72	0.59
3:A:352:PHE:CE1	3:A:416:LYS:HG3	2.39	0.58
2:C:28:DG:C3'	2:C:29:DC:H5''	2.31	0.58
3:A:330:TYR:CE2	3:A:500:GLU:HA	2.39	0.58
3:A:616:GLU:OE2	3:A:618:ALA:O	2.22	0.58
3:A:616:GLU:OE1	3:A:616:GLU:C	2.46	0.58
3:A:619:LEU:HD23	3:A:620:ASP:H	1.69	0.58
3:A:772:GLY:HA2	3:A:775:ARG:NE	2.19	0.58
3:A:533:LEU:O	3:A:536:VAL:HG22	2.04	0.58
3:A:616:GLU:OE2	3:A:621:TYR:N	2.38	0.57
3:A:327:TYR:CD1	3:A:492:GLU:HB3	2.40	0.57
3:A:799:LEU:HA	3:A:802:MET:HB2	1.87	0.56
3:A:623:LEU:O	3:A:627:ILE:HG12	2.04	0.56
3:A:540:ILE:HD11	3:A:876:MET:HE3	1.87	0.56
3:A:777:LEU:O	3:A:780:PRO:HD2	2.05	0.56
3:A:421:LEU:HD23	3:A:438:ILE:HG23	1.87	0.56
3:A:520:LYS:HE3	3:A:524:ASN:HB2	1.87	0.56
3:A:326:SER:HA	3:A:496:ARG:CG	2.25	0.55
3:A:573:ILE:HG12	3:A:622:PRO:HB3	1.86	0.55
3:A:325:ILE:HD13	3:A:500:GLU:CB	2.35	0.55
3:A:616:GLU:CD	3:A:621:TYR:N	2.65	0.55
2:C:21:DC:H1'	2:C:23:DG:C5'	2.37	0.55
3:A:545:VAL:HG21	3:A:693:PHE:HD2	1.72	0.55
3:A:619:LEU:CG	3:A:620:ASP:OD1	2.54	0.55
3:A:485:THR:HG22	3:A:488:GLN:HE21	1.72	0.55
3:A:573:ILE:HD11	3:A:626:VAL:CG2	2.36	0.54
3:A:612:GLU:HG3	3:A:613:VAL:CB	2.37	0.54
3:A:855:ILE:HG12	3:A:909:ARG:HB2	1.88	0.54
3:A:369:VAL:HA	3:A:386:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:740:GLU:HG3	3:A:794:ARG:HG2	1.90	0.54
3:A:612:GLU:CG	3:A:613:VAL:CB	2.85	0.54
3:A:690:ARG:HB3	3:A:925:ASP:HB2	1.89	0.54
3:A:566:LEU:O	3:A:570:ALA:N	2.37	0.53
3:A:573:ILE:HD12	3:A:626:VAL:HG21	1.91	0.53
3:A:580:LEU:CD1	3:A:581:SER:C	2.76	0.53
3:A:363:ASN:HD21	3:A:426:GLY:HA3	1.73	0.53
3:A:573:ILE:HD11	3:A:626:VAL:HG21	1.90	0.53
3:A:334:LEU:CD1	3:A:384:PRO:HD2	2.39	0.52
3:A:712:ARG:HD3	3:A:913:PRO:O	2.09	0.52
3:A:619:LEU:CD2	3:A:619:LEU:N	2.72	0.52
1:B:2:DG:H1'	1:B:3:DC:O5'	2.09	0.52
3:A:566:LEU:HB2	3:A:630:TYR:HD1	1.74	0.52
3:A:764:LEU:HD13	3:A:798:VAL:HG11	1.92	0.52
3:A:845:ASN:HD21	3:A:849:GLN:NE2	2.07	0.52
3:A:573:ILE:HD13	3:A:622:PRO:CB	2.31	0.52
3:A:902:GLN:O	3:A:906:ASN:OD1	2.28	0.52
3:A:616:GLU:OE1	3:A:618:ALA:CA	2.58	0.51
3:A:769:SER:O	3:A:771:PHE:N	2.43	0.51
3:A:336:GLU:OE1	3:A:400:ARG:NE	2.39	0.51
3:A:619:LEU:HG	3:A:620:ASP:CG	2.35	0.51
1:B:8:DC:OP1	3:A:631:ARG:NH2	2.43	0.51
3:A:346:LEU:CG	3:A:408:LEU:HD21	2.41	0.51
3:A:414:ALA:O	3:A:437:GLY:HA3	2.10	0.51
3:A:619:LEU:CD2	3:A:619:LEU:H	2.24	0.51
3:A:640:TYR:O	3:A:644:LEU:HB2	2.10	0.51
3:A:332:THR:CG2	3:A:384:PRO:HD3	2.41	0.51
3:A:325:ILE:CG2	3:A:471:ILE:HD11	2.41	0.50
3:A:619:LEU:CG	3:A:620:ASP:N	2.75	0.50
3:A:352:PHE:CZ	3:A:414:ALA:HB1	2.46	0.50
3:A:706:TYR:HB3	3:A:709:ILE:HB	1.94	0.50
3:A:566:LEU:O	3:A:570:ALA:HB3	2.12	0.49
3:A:331:VAL:H	3:A:381:ALA:HA	1.77	0.49
3:A:418:GLY:HA3	3:A:421:LEU:HD13	1.94	0.49
3:A:325:ILE:CD1	3:A:500:GLU:CB	2.91	0.49
3:A:610:SER:C	3:A:612:GLU:H	2.15	0.49
3:A:330:TYR:CZ	3:A:500:GLU:HA	2.46	0.49
3:A:575:GLY:C	3:A:576:GLU:O	2.55	0.49
3:A:566:LEU:HD23	3:A:569:LYS:HD2	1.93	0.49
3:A:616:GLU:O	3:A:616:GLU:CD	2.56	0.49
3:A:346:LEU:CD2	3:A:408:LEU:HD21	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:DC:OP1	3:A:610:SER:O	2.30	0.48
1:B:7:DG:OP1	3:A:609:THR:CB	2.61	0.48
3:A:332:THR:HG23	3:A:384:PRO:HD3	1.94	0.48
3:A:530:GLU:CD	3:A:821:ARG:HH12	2.22	0.48
3:A:616:GLU:CB	3:A:624:PRO:O	2.62	0.48
1:B:7:DG:P	3:A:609:THR:CB	3.02	0.48
3:A:352:PHE:CE2	3:A:408:LEU:HD11	2.49	0.47
3:A:612:GLU:HG2	3:A:613:VAL:HB	1.95	0.47
1:B:8:DC:P	3:A:610:SER:O	2.72	0.47
3:A:400:ARG:HA	3:A:403:GLU:HG2	1.96	0.47
3:A:703:SER:O	3:A:918:VAL:HA	2.14	0.47
3:A:331:VAL:O	3:A:381:ALA:CA	2.63	0.47
3:A:346:LEU:CD2	3:A:408:LEU:CD2	2.79	0.46
3:A:570:ALA:HA	3:A:626:VAL:CG2	2.33	0.46
3:A:901:HIS:O	3:A:905:GLU:HG2	2.15	0.46
3:A:351:VAL:HG12	3:A:415:LEU:HD12	1.97	0.46
3:A:353:ALA:O	3:A:354:PHE:CB	2.57	0.46
3:A:449:LEU:HD13	3:A:516:LEU:HG	1.98	0.46
3:A:854:ASP:HB3	3:A:909:ARG:HH22	1.80	0.46
1:B:10:DG:H2'	1:B:11:DC:C6	2.51	0.46
3:A:905:GLU:HG3	3:A:906:ASN:OD1	2.16	0.46
3:A:709:ILE:HD11	3:A:855:ILE:HG21	1.99	0.45
3:A:330:TYR:OH	3:A:503:ASP:CB	2.64	0.45
3:A:690:ARG:HG2	3:A:924:TRP:CD2	2.52	0.45
3:A:330:TYR:CB	3:A:499:ALA:CB	2.95	0.45
3:A:638:SER:HB2	3:A:643:LYS:NZ	2.31	0.45
3:A:673:ASP:HB3	3:A:674:PRO:HD3	1.99	0.45
3:A:324:VAL:HG13	3:A:325:ILE:H	1.80	0.45
3:A:586:LEU:C	3:A:588:THR:N	2.75	0.45
3:A:830:SER:O	3:A:832:ASN:N	2.50	0.45
3:A:352:PHE:N	3:A:415:LEU:O	2.46	0.45
3:A:580:LEU:HD11	3:A:581:SER:C	2.36	0.45
3:A:612:GLU:CG	3:A:613:VAL:CG2	2.94	0.45
3:A:780:PRO:HB2	3:A:783:GLU:HB2	1.97	0.45
3:A:354:PHE:HA	3:A:372:SER:O	2.16	0.45
1:B:7:DG:OP2	3:A:609:THR:CB	2.64	0.45
3:A:613:VAL:CG1	3:A:614:LEU:N	2.80	0.45
3:A:330:TYR:OH	3:A:503:ASP:HB3	2.17	0.44
3:A:331:VAL:O	3:A:381:ALA:CB	2.64	0.44
3:A:335:ASP:C	3:A:396:ILE:HD11	2.42	0.44
1:B:12:DG:H5'	3:A:455:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:610:SER:O	3:A:611:GLU:HB2	2.16	0.44
3:A:614:LEU:HD22	3:A:614:LEU:HA	1.73	0.44
3:A:657:THR:HA	3:A:674:PRO:HD2	2.00	0.44
3:A:332:THR:CG2	3:A:384:PRO:CG	2.96	0.44
3:A:533:LEU:CD2	3:A:857:LYS:HD3	2.47	0.44
3:A:851:THR:O	3:A:855:ILE:HG13	2.17	0.44
3:A:867:LEU:HD12	3:A:872:PRO:HD2	1.99	0.43
3:A:681:VAL:HG13	3:A:682:ARG:H	1.82	0.43
3:A:779:ILE:H	3:A:780:PRO:HD2	1.83	0.43
3:A:610:SER:HB2	3:A:631:ARG:NH1	2.33	0.43
3:A:351:VAL:HG12	3:A:415:LEU:CB	2.43	0.43
1:B:12:DG:N2	3:A:422:LYS:NZ	2.61	0.43
3:A:619:LEU:CD2	3:A:620:ASP:H	2.30	0.43
3:A:325:ILE:HD11	3:A:500:GLU:HB2	1.99	0.43
3:A:775:ARG:O	3:A:778:ASN:HB2	2.19	0.43
3:A:339:LEU:HD12	3:A:404:LEU:HD12	2.00	0.43
3:A:781:ARG:HA	3:A:781:ARG:NE	2.34	0.42
1:B:7:DG:OP1	3:A:609:THR:HB	2.18	0.42
3:A:330:TYR:OH	3:A:500:GLU:HA	2.19	0.42
3:A:627:ILE:O	3:A:631:ARG:HG3	2.19	0.42
3:A:796:PRO:O	3:A:799:LEU:HD12	2.19	0.42
3:A:330:TYR:CE2	3:A:500:GLU:CA	3.02	0.42
3:A:515:ASP:O	3:A:518:LYS:HB2	2.19	0.42
3:A:562:ARG:O	3:A:566:LEU:HG	2.19	0.42
3:A:638:SER:O	3:A:643:LYS:HG2	2.20	0.42
3:A:513:TRP:HB3	3:A:514:PRO:HD3	2.02	0.42
2:C:27:DG:OP1	3:A:582:SER:OG	2.27	0.42
3:A:889:HIS:HB3	3:A:892:ASP:OD2	2.20	0.42
3:A:330:TYR:CB	3:A:499:ALA:HB1	2.49	0.42
3:A:901:HIS:O	3:A:902:GLN:O	2.37	0.42
3:A:580:LEU:HD22	3:A:588:THR:CB	2.49	0.42
3:A:586:LEU:C	3:A:588:THR:H	2.28	0.41
3:A:325:ILE:CD1	3:A:500:GLU:CG	2.94	0.41
3:A:352:PHE:CE1	3:A:416:LYS:CG	3.03	0.41
3:A:472:THR:HG22	3:A:475:GLU:OE2	2.21	0.41
3:A:701:ILE:O	3:A:920:SER:HA	2.20	0.41
3:A:830:SER:HB3	3:A:836:ARG:HB3	2.02	0.41
3:A:330:TYR:CE2	3:A:500:GLU:N	2.89	0.41
2:C:23:DG:H5'	2:C:23:DG:C8	2.56	0.41
3:A:857:LYS:HA	3:A:860:MET:HE3	2.02	0.41
3:A:330:TYR:OH	3:A:503:ASP:OD2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:735:ARG:HG3	3:A:754:ARG:HG3	2.03	0.41
3:A:587:GLN:O	3:A:591:PHE:N	2.54	0.41
3:A:756:SER:O	3:A:760:ILE:HG13	2.21	0.41
3:A:835:ARG:O	3:A:835:ARG:HG3	2.20	0.41
3:A:688:ARG:O	3:A:691:GLN:HB2	2.21	0.41
3:A:410:GLU:O	3:A:436:ARG:HD2	2.20	0.40
3:A:578:PHE:HE1	3:A:580:LEU:C	2.29	0.40
3:A:654:ARG:HH11	3:A:875:ARG:HH11	1.69	0.40
3:A:342:TRP:HA	3:A:345:LYS:HG2	2.04	0.40
3:A:682:ARG:HH22	3:A:758:LYS:NZ	2.19	0.40
3:A:358:THR:HG21	3:A:427:ILE:HD12	2.02	0.40
3:A:571:HIS:HA	3:A:574:ALA:O	2.21	0.40
1:B:7:DG:P	3:A:609:THR:CA	2.97	0.40
1:B:10:DG:O3'	3:A:672:THR:HG21	2.21	0.40
3:A:353:ALA:HA	3:A:417:VAL:O	2.21	0.40
3:A:586:LEU:O	3:A:588:THR:N	2.54	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	587/605 (97%)	512 (87%)	50 (8%)	25 (4%)	2 16

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	574	ALA
3	A	576	GLU
3	A	578	PHE
3	A	581	SER
3	A	610	SER

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Mol	Chain	Res	Type
3	A	614	LEU
3	A	617	LEU
3	A	673	ASP
3	A	770	ALA
3	A	779	ILE
3	A	831	SER
3	A	881	HIS
3	A	882	ASP
3	A	354	PHE
3	A	580	LEU
3	A	587	GLN
3	A	611	GLU
3	A	615	GLU
3	A	834	ALA
3	A	586	LEU
3	A	598	PRO
3	A	363	ASN
3	A	612	GLU
3	A	903	LEU
3	A	597	LYS

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	486/509 (96%)	428 (88%)	58 (12%)	5	23

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	334	LEU
3	A	339	LEU
3	A	346	LEU
3	A	354	PHE
3	A	356	THR
3	A	364	ILE

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Mol	Chain	Res	Type
3	A	375	ILE
3	A	394	ASP
3	A	405	LEU
3	A	434	GLU
3	A	435	LEU
3	A	449	LEU
3	A	451	SER
3	A	470	THR
3	A	474	GLU
3	A	476	ILE
3	A	481	LYS
3	A	510	LEU
3	A	514	PRO
3	A	516	LEU
3	A	519	HIS
3	A	530	GLU
3	A	531	MET
3	A	559	LEU
3	A	562	ARG
3	A	565	GLU
3	A	573	ILE
3	A	582	SER
3	A	612	GLU
3	A	614	LEU
3	A	615	GLU
3	A	616	GLU
3	A	617	LEU
3	A	620	ASP
3	A	623	LEU
3	A	629	GLU
3	A	644	LEU
3	A	646	LEU
3	A	671	SER
3	A	676	LEU
3	A	678	ASN
3	A	685	GLU
3	A	740	GLU
3	A	744	LEU
3	A	747	GLU
3	A	768	MET
3	A	773	LEU
3	A	776	GLN

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Mol	Chain	Res	Type
3	A	793	GLU
3	A	818	LEU
3	A	829	LYS
3	A	836	ARG
3	A	849	GLN
3	A	858	ARG
3	A	867	LEU
3	A	909	ARG
3	A	920	SER
3	A	928	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	420	ASN
3	A	456	HIS
3	A	488	GLN
3	A	524	ASN
3	A	543	ASN
3	A	677	GLN
3	A	691	GLN
3	A	808	GLN
3	A	812	GLN
3	A	845	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 [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	2
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	620:ASP	C	621:TYR	N	2.16
1	C	19:DG	O3'	20:DC	P	1.93
1	A	581:SER	C	582:SER	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.