



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:16 PM UTC

PDB ID : 1RTD / pdb_00001rtd
Title : STRUCTURE OF A CATALYTIC COMPLEX OF HIV-1 REVERSE TRANSCRIPTASE: IMPLICATIONS FOR NUCLEOSIDE ANALOG DRUG RESISTANCE
Authors : Chopra, R.; Huang, H.; Verdine, G.L.; Harrison, S.C.
Deposited on : 1998-08-26
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

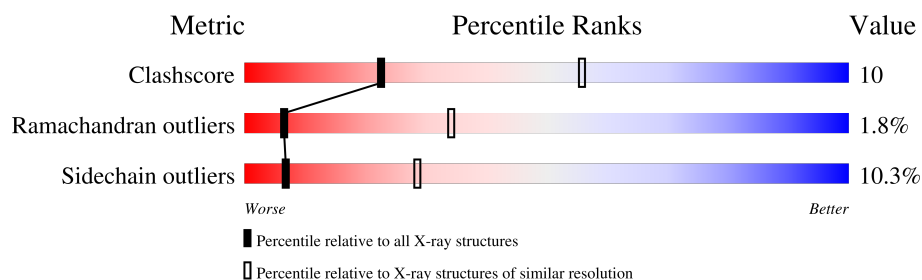
1 Overall quality at a glance

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	E	27	 7% 26% 59% 7%
1	G	27	 33% 56% 7%
2	F	21	 5% 43% 52%
2	H	21	 5% 43% 52%
3	A	554	 72% 23% . .
3	C	554	 72% 22% 6%
4	B	440	 71% 19% . 6%
4	D	440	 69% 21% . 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17784 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 TEMPLATE FOR REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	25	Total	C	N	O	P	0	0	0
			512	242	100	146	24			
1	G	25	Total	C	N	O	P	0	0	0
			512	242	100	146	24			

- Molecule 2 is a DNA chain called DNA PRIMER FOR REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			424	202	77	125	20			
2	H	21	Total	C	N	O	P	0	0	0
			424	202	77	125	20			

- Molecule 3 is a protein called PROTEIN (REVERSE TRANSCRIPTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	554	Total	C	N	O	S	0	0	0
			4510	2917	751	833	9			
3	C	554	Total	C	N	O	S	0	0	0
			4508	2915	751	833	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LYS	PRO	engineered mutation	UNP P03366
A	172	ARG	LYS	conflict	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	471	ASP	ASN	conflict	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366
A	512	GLU	LYS	conflict	UNP P03366
C	1	LYS	PRO	engineered mutation	UNP P03366
C	172	ARG	LYS	conflict	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
C	258	CYS	GLN	engineered mutation	UNP P03366
C	471	ASP	ASN	conflict	UNP P03366
C	478	GLN	GLU	engineered mutation	UNP P03366
C	512	GLU	LYS	conflict	UNP P03366

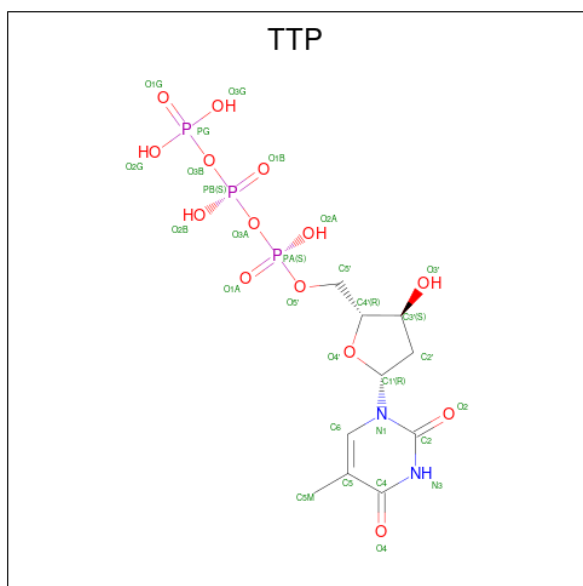
- Molecule 4 is a protein called PROTEIN (REVERSE TRANSCRIPTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	414	Total	C	N	O	S	0	0	0
			3415	2221	567	620	7			
4	D	414	Total	C	N	O	S	0	0	0
			3415	2221	567	620	7			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Mg	0	0
			4	4		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

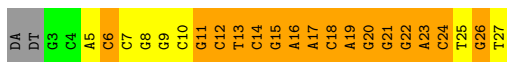
3 Residue-property plots

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.

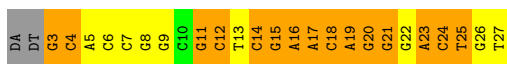
• Molecule 1: DNA TEMPLATE FOR REVERSE TRANSCRIPTASE

Chain E: 



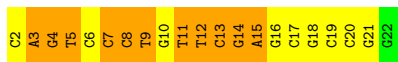
• Molecule 1: DNA TEMPLATE FOR REVERSE TRANSCRIPTASE

Chain G: 



• Molecule 2: DNA PRIMER FOR REVERSE TRANSCRIPTASE

Chain F: 



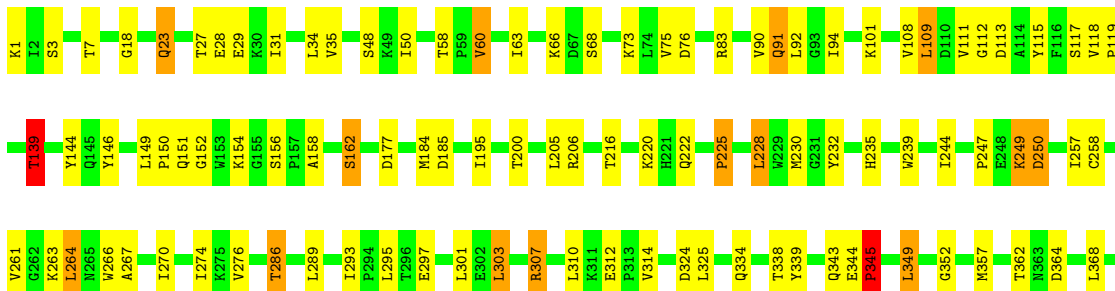
• Molecule 2: DNA PRIMER FOR REVERSE TRANSCRIPTASE

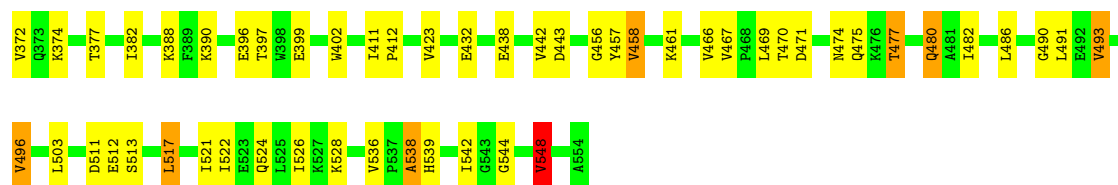
Chain H: 



• Molecule 3: PROTEIN (REVERSE TRANSCRIPTASE)

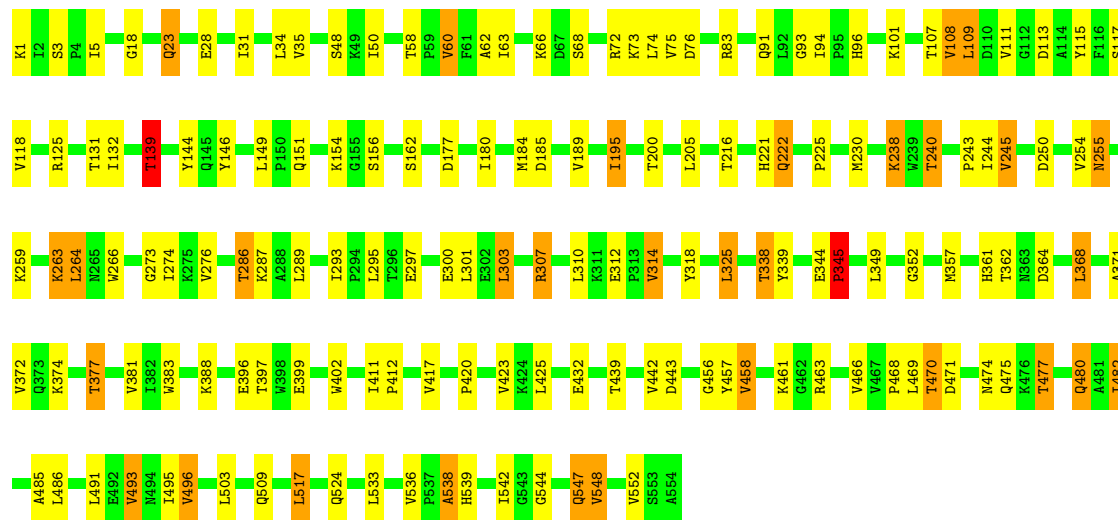
Chain A: 





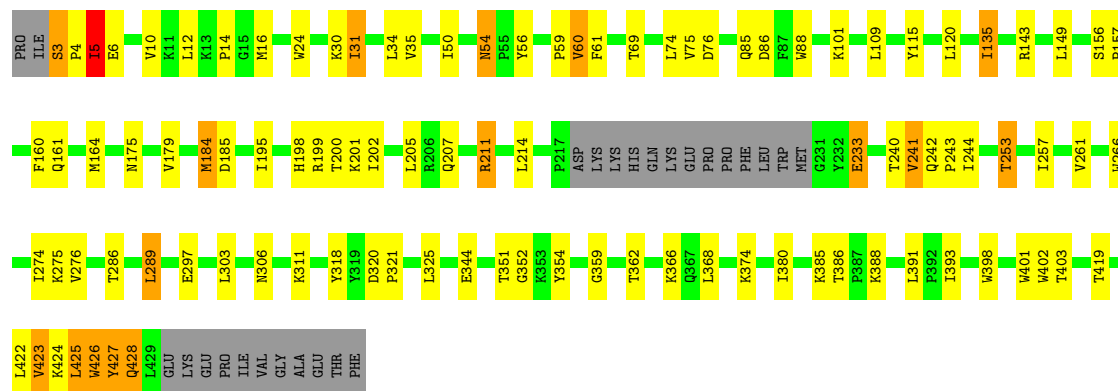
• Molecule 3: PROTEIN (REVERSE TRANSCRIPTASE)

Chain C: 72% 22% 6%



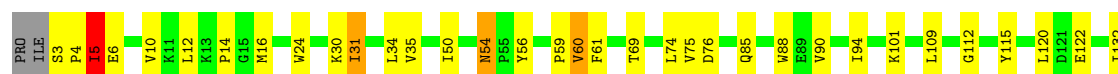
• Molecule 4: PROTEIN (REVERSE TRANSCRIPTASE)

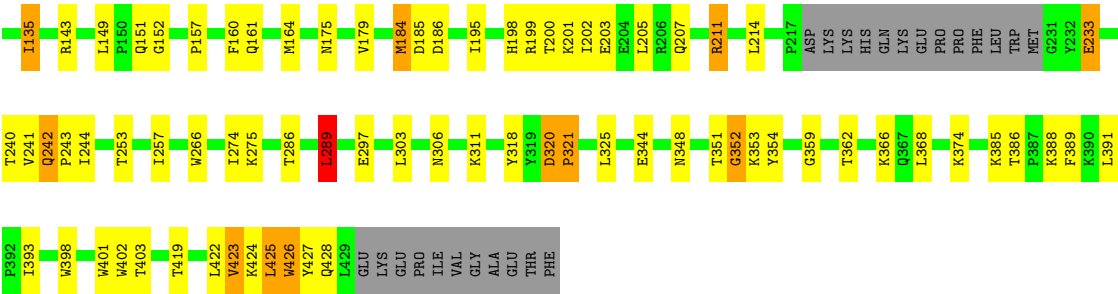
Chain B: 71% 19% 6%



• Molecule 4: PROTEIN (REVERSE TRANSCRIPTASE)

Chain D: 69% 21% 6%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.84Å 150.70Å 280.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.2 (12.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.224 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17784	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP

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	E	0.51	0/575	1.66	26/886 (2.9%)
1	G	0.41	0/575	1.47	18/886 (2.0%)
2	F	0.53	0/474	1.56	16/729 (2.2%)
2	H	0.40	0/474	1.39	13/729 (1.8%)
3	A	0.83	6/4627 (0.1%)	1.30	40/6286 (0.6%)
3	C	0.89	10/4624 (0.2%)	1.30	38/6281 (0.6%)
4	B	0.79	2/3512 (0.1%)	1.28	34/4774 (0.7%)
4	D	0.81	3/3512 (0.1%)	1.29	35/4774 (0.7%)
All	All	0.80	21/18373 (0.1%)	1.32	220/25345 (0.9%)

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	C	0	1
4	B	0	1
4	D	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	293	ILE	CA-CB	7.23	1.59	1.54
4	D	94	ILE	CA-CB	7.00	1.63	1.54
4	D	5	ILE	CA-CB	6.61	1.63	1.54
4	B	5	ILE	CA-CB	6.61	1.63	1.54
3	C	5	ILE	CA-CB	6.32	1.60	1.54
3	C	245	VAL	CA-CB	6.25	1.61	1.54
3	C	132	ILE	CA-CB	6.24	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	513	SER	N-CA	6.20	1.53	1.46
3	A	293	ILE	CA-CB	6.10	1.59	1.54
3	A	274	ILE	CA-CB	5.88	1.60	1.54
3	C	118	VAL	CA-CB	5.83	1.59	1.54
3	A	511	ASP	C-N	-5.54	1.26	1.33
3	A	118	VAL	CA-CB	5.45	1.59	1.54
4	B	241	VAL	CA-CB	5.38	1.61	1.53
3	C	496	VAL	CA-CB	5.23	1.60	1.53
3	A	496	VAL	CA-CB	5.18	1.60	1.53
3	C	461	LYS	CE-NZ	-5.17	1.33	1.49
3	C	274	ILE	CA-CB	5.14	1.60	1.54
4	D	132	ILE	CA-CB	5.11	1.60	1.54
3	C	420	PRO	CA-C	5.09	1.56	1.52
3	C	417	VAL	CA-CB	5.09	1.60	1.54

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	DG	N9-C1'-C2'	12.09	131.63	113.50
1	G	16	DA	N9-C1'-C2'	11.30	130.45	113.50
4	B	4	PRO	N-CA-C	10.80	128.87	111.26
1	G	18	DC	N1-C1'-C2'	10.33	129.00	113.50
2	F	8	DC	N1-C1'-C2'	9.63	127.94	113.50
2	H	15	DA	N9-C1'-C2'	9.59	127.88	113.50
3	C	310	LEU	N-CA-C	9.57	122.93	111.82
3	A	225	PRO	CA-C-N	-9.46	108.02	119.84
3	A	225	PRO	C-N-CA	-9.46	108.02	119.84
1	E	21	DG	N9-C1'-C2'	9.24	127.37	113.50
1	G	15	DG	N9-C1'-C2'	9.14	127.21	113.50
1	E	15	DG	C2'-C3'-O3'	-9.12	97.82	111.50
2	H	9	DT	N1-C1'-C2'	9.10	127.15	113.50
2	F	12	DT	N1-C1'-C2'	9.04	127.06	113.50
3	C	468	PRO	N-CA-CB	8.95	112.42	102.67
2	F	9	DT	N1-C1'-C2'	8.94	126.91	113.50
2	H	8	DC	N1-C1'-C2'	8.92	126.88	113.50
3	A	310	LEU	N-CA-C	8.76	123.22	112.54
2	F	14	DG	N9-C1'-C2'	8.67	126.50	113.50
1	G	4	DC	N1-C1'-C2'	8.66	126.49	113.50
2	H	5	DT	N1-C1'-C2'	8.63	126.45	113.50
1	G	21	DG	N9-C1'-C2'	8.62	126.44	113.50
3	A	139	THR	CA-C-N	-8.57	111.19	119.85
3	A	139	THR	C-N-CA	-8.57	111.19	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	DC	N1-C1'-C2'	8.55	126.33	113.50
2	F	13	DC	N1-C1'-C2'	8.53	126.30	113.50
1	E	15	DG	N9-C1'-C2'	8.46	126.20	113.50
1	G	17	DA	N9-C1'-C2'	8.46	126.18	113.50
3	C	225	PRO	N-CA-C	8.40	120.95	110.70
3	C	139	THR	CA-C-N	-8.39	111.38	119.85
3	C	139	THR	C-N-CA	-8.39	111.38	119.85
4	D	88	TRP	N-CA-C	8.37	123.15	113.19
1	E	11	DG	C2'-C3'-O3'	-8.36	98.96	111.50
2	F	11	DT	N1-C1'-C2'	8.11	125.67	113.50
3	C	230	MET	N-CA-C	8.10	122.59	111.90
4	D	391	LEU	N-CA-C	8.06	119.81	109.65
1	E	19	DA	N9-C1'-C2'	7.97	125.46	113.50
4	B	391	LEU	N-CA-C	7.92	119.63	109.65
2	F	4	DG	N9-C1'-C2'	7.83	125.24	113.50
1	G	14	DC	N1-C1'-C2'	7.82	125.23	113.50
4	D	4	PRO	N-CA-C	7.81	128.56	112.47
1	E	17	DA	N9-C1'-C2'	7.80	125.20	113.50
1	E	14	DC	C2'-C3'-O3'	-7.79	99.82	111.50
2	H	13	DC	N1-C1'-C2'	7.74	125.11	113.50
2	F	3	DA	N9-C1'-C2'	7.67	125.00	113.50
1	E	16	DA	N9-C1'-C2'	7.62	124.93	113.50
3	C	238	LYS	N-CA-C	7.52	118.19	108.34
4	D	386	THR	CA-C-N	-7.39	112.60	120.66
4	D	386	THR	C-N-CA	-7.39	112.60	120.66
1	E	18	DC	N1-C1'-C2'	7.37	124.56	113.50
3	A	493	VAL	CB-CA-C	-7.35	100.31	110.90
2	H	11	DT	N1-C1'-C2'	7.29	124.43	113.50
3	C	156	SER	N-CA-C	7.28	122.72	113.25
1	E	24	DC	N1-C1'-C2'	7.27	124.40	113.50
2	F	8	DC	C4'-C3'-O3'	-7.25	99.13	110.00
1	E	21	DG	C4'-C3'-O3'	-7.23	99.15	110.00
1	E	20	DG	N9-C1'-C2'	7.23	124.34	113.50
1	E	20	DG	C4'-C3'-O3'	-7.22	99.16	110.00
3	A	156	SER	N-CA-C	7.18	122.58	113.25
2	F	15	DA	N9-C1'-C2'	7.16	124.23	113.50
1	G	16	DA	C4'-C3'-O3'	-7.15	99.27	110.00
4	B	244	ILE	N-CA-C	-7.11	98.06	108.87
3	C	297	GLU	N-CA-C	7.08	119.61	111.11
3	C	493	VAL	CB-CA-C	-7.08	99.79	110.55
3	A	297	GLU	N-CA-C	7.03	119.54	111.11
4	D	427	TYR	N-CA-C	6.97	121.54	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	244	ILE	N-CA-C	-6.88	98.41	108.87
1	G	25	DT	N1-C1'-C2'	6.85	123.78	113.50
4	B	233	GLU	N-CA-C	6.80	119.83	110.24
2	H	14	DG	N9-C1'-C2'	6.75	123.63	113.50
2	F	9	DT	C4'-C3'-O3'	-6.75	99.87	110.00
4	B	366	LYS	N-CA-C	-6.73	103.95	111.28
4	B	243	PRO	N-CA-C	6.72	120.63	111.22
2	F	5	DT	N1-C1'-C2'	6.65	123.47	113.50
4	B	344	GLU	N-CA-C	-6.63	98.79	109.40
1	E	23	DA	N9-C1'-C2'	6.61	123.42	113.50
4	B	12	LEU	N-CA-C	-6.61	98.63	109.40
4	D	12	LEU	N-CA-C	-6.60	98.65	109.40
4	D	233	GLU	N-CA-C	6.60	119.54	110.24
1	G	11	DG	N9-C1'-C2'	6.59	123.39	113.50
3	A	456	GLY	N-CA-C	6.55	120.69	111.19
1	E	22	DG	N9-C1'-C2'	6.55	123.32	113.50
4	D	31	ILE	N-CA-C	-6.54	103.87	111.00
1	E	17	DA	C2'-C3'-O3'	-6.52	101.72	111.50
4	D	244	ILE	CB-CA-C	-6.52	102.27	111.21
4	B	88	TRP	N-CA-C	6.52	121.23	113.28
4	B	244	ILE	CB-CA-C	-6.52	102.28	111.21
2	H	3	DA	N9-C1'-C2'	6.51	123.26	113.50
4	D	366	LYS	N-CA-C	-6.51	104.19	111.28
1	G	3	DG	N9-C1'-C2'	6.47	123.21	113.50
4	D	85	GLN	N-CA-C	6.47	120.27	112.38
4	B	31	ILE	N-CA-C	-6.45	103.97	111.00
3	A	18	GLY	CA-C-N	6.41	126.17	119.76
3	A	18	GLY	C-N-CA	6.41	126.17	119.76
1	E	6	DC	C2'-C3'-O3'	-6.39	101.91	111.50
3	A	344	GLU	CA-C-N	6.38	127.81	119.84
3	A	344	GLU	C-N-CA	6.38	127.81	119.84
4	D	101	LYS	N-CA-C	-6.36	104.27	111.14
3	C	18	GLY	CA-C-N	6.36	126.12	119.76
3	C	18	GLY	C-N-CA	6.36	126.12	119.76
4	B	427	TYR	N-CA-C	6.36	120.24	112.23
4	D	198	HIS	N-CA-C	-6.32	104.08	110.97
2	H	16	DG	N9-C1'-C2'	6.31	122.97	113.50
3	C	344	GLU	CA-C-N	6.30	127.71	119.84
3	C	344	GLU	C-N-CA	6.30	127.71	119.84
3	A	512	GLU	CA-C-O	-6.28	114.55	121.33
1	G	23	DA	N9-C1'-C2'	6.26	122.89	113.50
3	A	345	PRO	N-CA-C	6.25	125.34	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	247	PRO	N-CA-C	6.21	120.18	110.80
3	A	513	SER	N-CA-CB	-6.21	101.90	111.46
3	C	456	GLY	N-CA-C	6.20	120.18	111.19
4	B	289	LEU	N-CA-C	6.15	119.63	111.75
3	A	235	HIS	N-CA-C	-6.15	101.61	110.40
4	D	243	PRO	N-CA-C	6.15	119.83	111.22
2	F	7	DC	N1-C1'-C2'	6.13	122.70	113.50
1	G	24	DC	N1-C1'-C2'	6.12	122.67	113.50
1	E	19	DA	C4'-C3'-O3'	-6.10	100.85	110.00
4	D	289	LEU	N-CA-C	6.09	119.54	111.75
3	C	345	PRO	N-CA-C	6.08	124.99	112.47
4	D	352	GLY	N-CA-C	6.07	119.44	110.63
1	E	26	DG	N9-C1'-C2'	6.07	122.60	113.50
3	C	402	TRP	N-CA-C	6.06	117.88	111.28
4	D	90	VAL	N-CA-C	6.03	121.88	109.34
4	B	85	GLN	N-CA-C	6.03	119.73	112.38
4	B	386	THR	CA-C-N	-6.02	114.10	120.66
4	B	386	THR	C-N-CA	-6.02	114.10	120.66
3	A	250	ASP	N-CA-C	6.01	117.84	111.28
4	D	402	TRP	N-CA-C	6.01	117.84	111.28
3	A	325	LEU	N-CA-C	5.97	118.46	108.73
3	A	249	LYS	CA-C-N	5.94	128.25	120.28
3	A	249	LYS	C-N-CA	5.94	128.25	120.28
3	A	482	ILE	N-CA-C	-5.94	104.52	111.00
4	B	198	HIS	N-CA-C	-5.94	104.44	111.03
3	A	402	TRP	N-CA-C	5.92	117.74	111.28
3	C	349	LEU	N-CA-C	-5.90	105.08	112.93
1	G	19	DA	N9-C1'-C2'	5.90	122.36	113.50
1	G	12	DC	N1-C1'-C2'	5.90	122.34	113.50
3	A	390	LYS	N-CA-C	-5.89	97.72	108.02
3	C	388	LYS	N-CA-C	-5.87	99.71	109.46
3	A	538	ALA	N-CA-C	5.84	123.25	110.80
3	A	349	LEU	N-CA-C	-5.84	105.16	112.93
1	E	12	DC	N1-C1'-C2'	5.83	122.24	113.50
3	C	482	ILE	N-CA-C	-5.79	104.68	111.00
1	E	21	DG	C2'-C3'-O3'	-5.79	102.82	111.50
1	G	3	DG	C2'-C3'-O3'	5.78	120.17	111.50
4	B	352	GLY	N-CA-C	5.78	119.20	110.18
1	E	23	DA	C2'-C3'-O3'	-5.75	102.87	111.50
3	A	225	PRO	N-CA-C	5.75	117.72	110.70
4	B	86	ASP	N-CA-C	-5.73	105.11	111.36
2	H	4	DG	N9-C1'-C2'	5.72	122.08	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	388	LYS	N-CA-C	-5.71	99.98	109.46
3	A	230	MET	N-CA-C	5.69	119.80	112.86
3	C	325	LEU	N-CA-C	5.67	117.97	108.73
1	E	13	DT	C2'-C3'-O3'	-5.66	103.01	111.50
4	B	101	LYS	N-CA-C	-5.62	105.24	111.36
3	C	146	TYR	N-CA-C	5.61	118.96	109.76
3	C	96	HIS	CA-C-N	5.58	125.25	119.56
3	C	96	HIS	C-N-CA	5.58	125.25	119.56
4	B	202	ILE	N-CA-C	-5.57	105.10	110.72
4	D	388	LYS	N-CA-C	-5.57	100.22	109.46
3	A	388	LYS	N-CA-C	-5.56	100.23	109.46
3	C	538	ALA	N-CA-C	5.55	122.63	110.80
3	C	255	ASN	N-CA-C	-5.55	105.31	111.36
4	D	320	ASP	CA-C-N	5.53	126.75	119.84
4	D	320	ASP	C-N-CA	5.53	126.75	119.84
2	F	13	DC	C4'-C3'-O3'	-5.50	101.75	110.00
4	D	202	ILE	N-CA-C	-5.48	105.19	110.72
4	B	54	ASN	N-CA-C	-5.46	98.87	108.69
1	E	16	DA	C4'-C3'-O3'	-5.43	101.85	110.00
4	D	186	ASP	N-CA-C	5.42	118.83	110.42
3	A	458	VAL	N-CA-C	-5.42	101.20	108.35
2	F	15	DA	C4'-C3'-O3'	-5.42	101.88	110.00
3	C	3	SER	N-CA-C	5.40	116.50	109.64
3	A	382	ILE	N-CA-C	5.39	116.05	110.82
3	C	539	HIS	N-CA-C	5.36	120.49	113.20
3	A	66	LYS	N-CA-C	5.36	117.81	111.33
2	F	7	DC	C4'-C3'-O3'	-5.33	102.00	110.00
4	D	69	THR	N-CA-C	-5.33	106.16	113.30
1	G	11	DG	C4'-C3'-O3'	-5.31	102.03	110.00
3	C	458	VAL	N-CA-C	-5.30	101.35	108.35
3	A	146	TYR	N-CA-C	5.29	118.44	109.76
3	A	397	THR	N-CA-C	-5.29	105.43	111.14
4	B	380	ILE	N-CA-C	-5.29	105.45	110.42
3	C	368	LEU	N-CA-C	-5.26	105.63	111.36
4	B	359	GLY	N-CA-C	5.24	120.93	114.69
1	E	13	DT	N1-C1'-C2'	5.24	121.35	113.50
3	C	263	LYS	N-CA-C	-5.24	105.49	111.14
3	A	3	SER	N-CA-C	5.20	116.25	109.64
2	H	9	DT	C4'-C3'-O3'	-5.19	102.21	110.00
2	H	7	DC	C4'-C3'-O3'	-5.19	102.22	110.00
4	B	56	TYR	N-CA-C	5.15	118.14	110.52
4	D	344	GLU	CA-C-N	5.15	126.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	344	GLU	C-N-CA	5.15	126.28	119.84
1	E	12	DC	C4'-C3'-O3'	-5.14	102.28	110.00
4	B	401	TRP	N-CA-C	5.13	121.31	113.61
4	B	3	SER	CA-C-N	5.12	125.41	119.93
4	B	3	SER	C-N-CA	5.12	125.41	119.93
3	A	548	VAL	CB-CA-C	-5.12	103.96	112.26
3	C	443	ASP	N-CA-C	-5.12	101.34	108.96
4	D	389	PHE	N-CA-C	5.09	117.54	109.24
4	D	401	TRP	N-CA-C	5.09	121.25	113.61
4	B	320	ASP	CA-C-N	5.09	126.20	119.84
4	B	320	ASP	C-N-CA	5.09	126.20	119.84
3	C	371	ALA	N-CA-C	-5.09	105.19	111.40
4	D	54	ASN	N-CA-C	-5.09	99.36	108.47
3	A	539	HIS	N-CA-C	5.09	120.12	113.20
3	A	443	ASP	N-CA-C	-5.08	101.72	108.74
3	C	397	THR	N-CA-C	-5.08	105.65	111.14
4	D	56	TYR	N-CA-C	5.08	118.04	110.52
3	A	150	PRO	N-CA-C	5.08	119.16	111.19
4	B	402	TRP	N-CA-C	5.07	117.54	111.71
3	C	93	GLY	N-CA-C	5.05	118.13	110.75
4	D	362	THR	N-CA-C	5.05	116.43	109.15
3	C	125	ARG	N-CA-C	5.04	118.53	112.38
3	C	240	THR	N-CA-C	-5.04	101.74	108.34
4	D	348	ASN	N-CA-C	5.03	117.76	109.76
4	D	359	GLY	N-CA-C	5.02	120.67	114.69
4	B	69	THR	N-CA-C	-5.02	106.57	113.30
4	B	362	THR	N-CA-C	5.01	116.36	109.15
3	C	66	LYS	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	354	TYR	Sidechain
3	C	318	TYR	Sidechain
4	D	354	TYR	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	E	512	0	280	61	0
1	G	512	0	280	58	0
2	F	424	0	235	50	0
2	H	424	0	235	48	0
3	A	4510	0	4566	53	0
3	C	4508	0	4560	58	0
4	B	3415	0	3448	34	0
4	D	3415	0	3448	37	0
5	A	4	0	0	0	0
5	C	2	0	0	0	0
6	A	29	0	13	1	0
6	C	29	0	13	2	0
All	All	17784	0	17078	366	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 10.

All (366) 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:F:3:DA:H2'	2:F:4:DG:C8	1.91	1.05
1:E:24:DC:H2''	1:E:25:DT:O5'	1.55	1.05
1:G:25:DT:H2''	1:G:26:DG:O5'	1.59	1.03
1:G:24:DC:H2''	1:G:25:DT:O5'	1.56	1.02
1:E:5:DA:H2''	1:E:6:DC:H5'	1.46	0.97
1:E:12:DC:H2'	1:E:13:DT:H71	1.46	0.96
2:H:2:DC:H2'	2:H:3:DA:C8	2.03	0.93
1:G:16:DA:H2'	1:G:17:DA:C8	2.04	0.93
2:H:3:DA:H2'	2:H:4:DG:C8	2.05	0.92
2:H:13:DC:H2'	2:H:14:DG:C8	2.05	0.92
2:H:3:DA:H2'	2:H:4:DG:H8	1.34	0.91
2:F:3:DA:H2'	2:F:4:DG:H8	1.29	0.91
1:G:23:DA:H2'	1:G:24:DC:C6	2.05	0.91
1:G:22:DG:H2'	1:G:23:DA:C8	2.10	0.86
3:A:544:GLY:HA2	4:B:286:THR:HG22	1.57	0.86
1:E:19:DA:H2''	1:E:20:DG:O5'	1.75	0.86
1:E:20:DG:H2''	1:E:21:DG:O5'	1.75	0.85
1:G:13:DT:H2'	1:G:14:DC:C6	2.12	0.84
2:F:14:DG:H2''	2:F:15:DA:O5'	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:DA:H2'	1:G:24:DC:H6	1.41	0.84
1:G:19:DA:H2''	1:G:20:DG:O5'	1.79	0.81
2:F:3:DA:C2'	2:F:4:DG:C8	2.64	0.80
1:G:26:DG:H2''	1:G:27:DT:O5'	1.80	0.80
3:C:486:LEU:HB3	3:C:524:GLN:HG2	1.62	0.79
2:F:13:DC:H2'	2:F:14:DG:C8	2.18	0.79
1:G:19:DA:H2'	1:G:20:DG:C8	2.18	0.78
2:H:5:DT:H2'	2:H:6:DC:C6	2.18	0.78
2:F:7:DC:H2''	2:F:8:DC:O5'	1.83	0.78
3:A:486:LEU:HB3	3:A:524:GLN:HG2	1.65	0.78
2:F:17:DC:H2'	2:F:18:DG:H8	1.49	0.78
3:C:544:GLY:HA2	4:D:286:THR:HG22	1.66	0.78
1:E:18:DC:H2''	1:E:19:DA:O5'	1.83	0.77
1:E:17:DA:H2''	1:E:18:DC:O5'	1.85	0.77
1:G:8:DG:H2'	1:G:9:DG:C8	2.19	0.77
2:F:10:DG:H2''	2:F:11:DT:O5'	1.84	0.76
1:G:16:DA:H2'	1:G:17:DA:H8	1.48	0.76
1:E:6:DC:H2'	1:E:7:DC:C6	2.21	0.76
2:H:16:DG:H2'	2:H:17:DC:C6	2.21	0.76
2:F:6:DC:H2''	2:F:7:DC:O5'	1.85	0.76
1:G:12:DC:H2'	1:G:13:DT:C6	2.20	0.76
1:E:13:DT:H2''	1:E:14:DC:O5'	1.85	0.75
1:E:5:DA:C2'	1:E:6:DC:H5'	2.16	0.75
1:G:8:DG:H2'	1:G:9:DG:H8	1.53	0.74
1:G:5:DA:H4'	3:C:76:ASP:OD1	1.88	0.73
1:G:22:DG:H2'	1:G:23:DA:H8	1.50	0.73
2:H:7:DC:H2''	2:H:8:DC:O5'	1.89	0.73
2:F:12:DT:H2''	2:F:13:DC:O5'	1.87	0.72
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.70	0.72
1:E:8:DG:H2'	1:E:9:DG:C8	2.24	0.72
1:G:14:DC:H2'	1:G:15:DG:C8	2.25	0.71
4:D:266:TRP:HB3	4:D:426:TRP:HE1	1.55	0.71
1:E:14:DC:H2'	1:E:15:DG:C8	2.25	0.71
2:F:5:DT:H2''	2:F:6:DC:O5'	1.89	0.71
1:E:26:DG:OP2	1:E:26:DG:H3'	1.90	0.71
1:G:6:DC:H2'	1:G:7:DC:C6	2.25	0.70
2:H:6:DC:H2'	2:H:7:DC:C6	2.26	0.70
1:G:18:DC:H2''	1:G:19:DA:O5'	1.92	0.70
1:G:13:DT:H2'	1:G:14:DC:H6	1.57	0.70
1:G:24:DC:C2'	1:G:25:DT:O5'	2.39	0.69
2:H:11:DT:H2'	2:H:12:DT:C6	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:DC:H2'	2:F:18:DG:C8	2.27	0.69
3:C:364:ASP:HB3	3:C:423:VAL:HG13	1.74	0.69
2:F:15:DA:H2''	2:F:16:DG:O5'	1.92	0.68
4:D:112:GLY:HA3	4:D:151:GLN:HE21	1.58	0.68
1:E:5:DA:H4'	3:A:76:ASP:OD1	1.94	0.68
2:H:6:DC:H2''	2:H:7:DC:O5'	1.93	0.68
2:H:2:DC:H2''	2:H:3:DA:O5'	1.93	0.68
1:E:16:DA:H2'	1:E:17:DA:C8	2.31	0.66
2:F:8:DC:H2''	2:F:9:DT:C5'	2.25	0.66
2:F:2:DC:H2''	2:F:3:DA:O5'	1.93	0.66
4:D:175:ASN:ND2	4:D:201:LYS:HE3	2.10	0.66
2:F:8:DC:H2''	2:F:9:DT:H5'	1.76	0.66
4:B:175:ASN:ND2	4:B:201:LYS:HE3	2.10	0.66
2:F:4:DG:C2'	2:F:5:DT:O5'	2.44	0.66
2:H:20:DC:H4'	3:C:266:TRP:CE2	2.31	0.66
1:E:14:DC:H4'	3:A:286:THR:HG22	1.77	0.65
3:C:469:LEU:HD12	3:C:477:THR:HG22	1.78	0.65
1:E:22:DG:H2'	1:E:23:DA:H8	1.62	0.65
2:F:15:DA:C2'	2:F:16:DG:O5'	2.44	0.65
2:H:20:DC:H4'	3:C:266:TRP:CD2	2.31	0.65
3:A:458:VAL:HG12	3:A:548:VAL:HG22	1.78	0.65
2:H:9:DT:H2'	2:H:10:DG:C8	2.31	0.65
1:G:15:DG:H2'	1:G:16:DA:C8	2.32	0.65
2:H:14:DG:H2'	2:H:15:DA:C8	2.32	0.65
2:H:16:DG:H2'	2:H:17:DC:H6	1.58	0.65
3:A:438:GLU:CD	3:A:461:LYS:HD2	2.21	0.64
1:E:16:DA:H2'	1:E:17:DA:H8	1.62	0.64
1:G:13:DT:H2''	1:G:14:DC:O5'	1.97	0.64
1:E:9:DG:H2'	1:E:10:DC:C6	2.33	0.64
3:A:31:ILE:O	3:A:35:VAL:HG23	1.98	0.64
4:B:175:ASN:HD21	4:B:201:LYS:HE3	1.62	0.64
3:C:31:ILE:O	3:C:35:VAL:HG23	1.98	0.63
1:E:16:DA:H2''	1:E:17:DA:O5'	1.96	0.63
2:F:6:DC:C2'	2:F:7:DC:O5'	2.46	0.63
3:A:469:LEU:HD12	3:A:477:THR:HG22	1.79	0.63
2:H:5:DT:C2'	2:H:6:DC:C6	2.81	0.63
4:D:24:TRP:CH2	4:D:403:THR:HG21	2.33	0.63
1:G:3:DG:H4'	1:G:4:DC:OP2	1.99	0.63
4:D:175:ASN:HD21	4:D:201:LYS:HE3	1.64	0.62
3:C:107:THR:HG22	3:C:222:GLN:O	2.00	0.62
1:E:8:DG:H2'	1:E:9:DG:H8	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:DG:H1'	3:C:94:ILE:HD11	1.82	0.61
1:G:15:DG:H2'	1:G:16:DA:H8	1.63	0.61
2:F:2:DC:H4'	2:F:3:DA:OP1	1.99	0.61
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.82	0.61
3:A:239:TRP:HZ2	3:A:349:LEU:O	1.83	0.61
1:E:9:DG:H2'	1:E:10:DC:H6	1.65	0.61
2:H:9:DT:H2''	2:H:10:DG:O4'	2.00	0.61
2:H:18:DG:H2'	2:H:19:DC:C6	2.36	0.61
1:E:6:DC:H2'	1:E:7:DC:H6	1.63	0.61
1:E:22:DG:H2'	1:E:23:DA:C8	2.36	0.61
1:G:21:DG:C2'	1:G:22:DG:O5'	2.48	0.61
3:C:111:VAL:HB	3:C:185:ASP:HB2	1.82	0.61
2:H:5:DT:H2''	2:H:6:DC:O5'	2.00	0.60
2:H:8:DC:H1'	3:C:475:GLN:HE22	1.66	0.60
4:D:59:PRO:HG2	4:D:76:ASP:HB3	1.83	0.60
2:F:15:DA:H2'	2:F:16:DG:C8	2.36	0.60
2:F:20:DC:H4'	3:A:266:TRP:CE2	2.37	0.60
1:G:23:DA:C4	1:G:24:DC:C5	2.90	0.60
2:H:5:DT:H2'	2:H:6:DC:H6	1.66	0.59
3:C:548:VAL:O	3:C:552:VAL:HG22	2.02	0.59
4:D:157:PRO:HG3	4:D:184:MET:HA	1.83	0.59
2:F:9:DT:H2''	2:F:10:DG:O5'	2.02	0.59
2:F:12:DT:C2'	2:F:13:DC:O5'	2.50	0.59
3:A:111:VAL:HB	3:A:185:ASP:HB2	1.83	0.59
2:H:14:DG:H2'	2:H:15:DA:H8	1.67	0.59
4:D:31:ILE:O	4:D:35:VAL:HG23	2.02	0.59
2:H:12:DT:H2''	2:H:13:DC:O5'	2.02	0.58
2:H:17:DC:H4'	3:C:289:LEU:HD21	1.84	0.58
4:D:115:TYR:HB3	4:D:149:LEU:HB2	1.84	0.58
1:G:13:DT:C2'	1:G:14:DC:O5'	2.52	0.58
2:H:12:DT:H2'	2:H:13:DC:C6	2.38	0.58
2:H:9:DT:H2'	2:H:10:DG:H8	1.68	0.58
1:E:12:DC:H2'	1:E:13:DT:C7	2.29	0.58
4:B:157:PRO:HG3	4:B:184:MET:HA	1.85	0.58
4:B:266:TRP:HB3	4:B:426:TRP:HE1	1.69	0.58
2:H:17:DC:H2'	2:H:18:DG:H8	1.69	0.58
2:F:7:DC:C2'	2:F:8:DC:O5'	2.51	0.57
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.86	0.57
2:H:3:DA:C2'	2:H:4:DG:C8	2.85	0.57
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.87	0.57
4:B:31:ILE:O	4:B:35:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:VAL:HG12	4:D:75:VAL:HG22	1.86	0.56
2:H:18:DG:H2'	2:H:19:DC:H6	1.70	0.56
1:E:12:DC:H2''	1:E:13:DT:O5'	2.04	0.56
1:G:21:DG:H2'	1:G:22:DG:C8	2.41	0.56
3:C:72:ARG:NH2	6:C:705:TTP:O2A	2.38	0.56
3:A:112:GLY:HA2	6:A:700:TTP:O1G	2.06	0.56
1:E:5:DA:C2'	1:E:6:DC:C5'	2.84	0.56
1:G:4:DC:H2'	1:G:4:DC:O2	2.05	0.56
1:G:26:DG:H2'	1:G:27:DT:H71	1.88	0.56
2:H:13:DC:H2'	2:H:14:DG:H8	1.65	0.56
2:F:12:DT:H2'	2:F:13:DC:C6	2.41	0.55
1:E:7:DC:H2'	1:E:8:DG:H8	1.71	0.55
2:F:14:DG:C2'	2:F:15:DA:O5'	2.52	0.55
1:E:25:DT:OP2	1:E:25:DT:H3'	2.07	0.55
2:F:3:DA:C2'	2:F:4:DG:H8	2.11	0.55
2:F:8:DC:H1'	3:A:475:GLN:HE22	1.71	0.55
3:C:273:GLY:HA2	3:C:338:THR:HG21	1.89	0.55
4:D:207:GLN:O	4:D:211:ARG:HB2	2.06	0.55
1:G:14:DC:H4'	3:C:286:THR:HG22	1.89	0.54
1:G:12:DC:H2'	1:G:13:DT:H6	1.68	0.54
2:H:17:DC:H2'	2:H:18:DG:C8	2.42	0.54
2:F:17:DC:H4'	3:A:289:LEU:HD21	1.89	0.54
1:G:23:DA:H2''	1:G:24:DC:O5'	2.07	0.54
2:F:3:DA:H2''	2:F:4:DG:O4'	2.08	0.54
1:G:21:DG:C6	1:G:22:DG:C6	2.96	0.54
3:C:442:VAL:HG12	3:C:457:TYR:HB3	1.89	0.54
1:E:17:DA:H2''	1:E:18:DC:C5'	2.37	0.54
3:A:109:LEU:HD23	3:A:216:THR:HG21	1.90	0.53
1:E:21:DG:H2'	1:E:22:DG:C8	2.43	0.53
2:F:11:DT:H2'	2:F:12:DT:C6	2.44	0.53
2:F:15:DA:H2'	2:F:16:DG:H8	1.73	0.53
3:A:34:LEU:HD11	3:A:73:LYS:HG3	1.90	0.53
2:F:4:DG:H2'	2:F:5:DT:O5'	2.08	0.53
3:C:115:TYR:OH	3:C:184:MET:HE1	2.08	0.53
1:G:19:DA:H2'	1:G:20:DG:H8	1.71	0.53
4:D:152:GLY:O	4:D:184:MET:HE3	2.09	0.53
1:G:22:DG:C2'	1:G:23:DA:C8	2.89	0.52
3:A:257:ILE:O	3:A:261:VAL:HG23	2.09	0.52
4:D:266:TRP:HB3	4:D:426:TRP:NE1	2.22	0.52
1:G:22:DG:H2''	1:G:23:DA:O5'	2.09	0.52
1:E:15:DG:H2''	1:E:16:DA:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:DA:H2''	1:E:17:DA:C5'	2.39	0.52
1:G:9:DG:H1'	3:C:94:ILE:CD1	2.40	0.52
3:C:34:LEU:HD11	3:C:73:LYS:HG3	1.90	0.52
2:F:8:DC:C2'	2:F:9:DT:O5'	2.57	0.52
2:F:20:DC:H4'	3:A:266:TRP:CD2	2.43	0.52
1:G:21:DG:H2'	1:G:22:DG:H8	1.74	0.52
3:A:503:LEU:HD23	4:B:422:LEU:HD22	1.91	0.52
3:C:240:THR:HG22	3:C:314:VAL:O	2.09	0.52
1:E:21:DG:H2'	1:E:22:DG:H8	1.75	0.52
3:A:23:GLN:HE21	3:A:60:VAL:H	1.57	0.52
4:B:34:LEU:HD21	4:B:61:PHE:O	2.11	0.51
2:H:4:DG:C2'	2:H:5:DT:O5'	2.59	0.51
1:G:24:DC:H2'	1:G:25:DT:C6	2.46	0.51
2:H:12:DT:C2'	2:H:13:DC:O5'	2.58	0.51
1:E:23:DA:H2'	1:E:24:DC:C6	2.46	0.51
2:H:10:DG:OP1	3:C:361:HIS:NE2	2.40	0.51
1:E:7:DC:H2''	1:E:8:DG:H5'	1.92	0.50
1:G:21:DG:H2''	1:G:22:DG:O5'	2.12	0.50
3:A:490:GLY:O	3:A:528:LYS:NZ	2.41	0.50
4:B:207:GLN:O	4:B:211:ARG:HB2	2.12	0.50
1:E:16:DA:C2'	1:E:17:DA:O5'	2.60	0.50
2:F:17:DC:C2'	2:F:18:DG:O5'	2.59	0.50
1:E:13:DT:H2''	1:E:14:DC:C5'	2.41	0.50
2:H:5:DT:H2'	2:H:6:DC:C5	2.46	0.50
4:B:115:TYR:HB3	4:B:149:LEU:HB2	1.94	0.50
3:C:503:LEU:HD23	4:D:422:LEU:HD22	1.94	0.49
2:H:6:DC:C2'	2:H:7:DC:O5'	2.58	0.49
1:G:20:DG:H2'	1:G:21:DG:C8	2.48	0.49
3:C:439:THR:HG21	4:D:289:LEU:HD13	1.92	0.49
1:G:11:DG:C2'	1:G:12:DC:O5'	2.60	0.49
3:C:255:ASN:HB2	3:C:289:LEU:O	2.13	0.49
3:C:372:VAL:HG11	3:C:411:ILE:HG23	1.94	0.49
1:E:26:DG:H2''	1:E:27:DT:O5'	2.11	0.49
2:H:18:DG:O3'	3:C:259:LYS:HG2	2.13	0.48
3:A:206:ARG:NH1	3:A:220:LYS:HE2	2.28	0.48
3:C:458:VAL:HG12	3:C:548:VAL:HG22	1.95	0.48
1:E:26:DG:C2'	1:E:27:DT:OP2	2.62	0.48
3:C:303:LEU:HD11	3:C:307:ARG:HH11	1.79	0.48
2:F:16:DG:H2''	2:F:17:DC:H5'	1.95	0.48
4:B:393:ILE:HD13	4:B:398:TRP:HB2	1.96	0.48
3:C:109:LEU:HD23	3:C:216:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:DT:H2'	2:F:10:DG:H8	1.79	0.47
1:G:18:DC:C2'	1:G:19:DA:O5'	2.62	0.47
3:A:442:VAL:HG12	3:A:457:TYR:HB3	1.96	0.47
2:F:14:DG:H2'	2:F:15:DA:C8	2.50	0.47
1:G:26:DG:H2'	1:G:27:DT:C7	2.43	0.47
3:A:372:VAL:HG11	3:A:411:ILE:HG23	1.97	0.47
4:B:24:TRP:CH2	4:B:403:THR:HG21	2.49	0.47
3:C:536:VAL:HB	3:C:542:ILE:HD13	1.95	0.47
1:E:7:DC:H2'	1:E:8:DG:C8	2.50	0.47
3:A:60:VAL:HG12	3:A:75:VAL:HG22	1.97	0.47
4:D:54:ASN:HB3	4:D:143:ARG:HH21	1.79	0.47
1:G:18:DC:H2'	1:G:19:DA:C8	2.49	0.47
2:H:10:DG:H2'	2:H:11:DT:OP2	2.15	0.47
4:D:34:LEU:HD21	4:D:61:PHE:O	2.15	0.47
2:F:9:DT:H2'	2:F:10:DG:C8	2.51	0.46
2:H:15:DA:H2'	2:H:16:DG:C8	2.50	0.46
3:C:439:THR:HG23	4:D:289:LEU:HD22	1.98	0.46
4:B:423:VAL:O	4:B:425:LEU:N	2.49	0.46
2:F:9:DT:C2'	2:F:10:DG:O5'	2.63	0.46
3:A:23:GLN:NE2	3:A:60:VAL:H	2.14	0.46
4:B:135:ILE:HD12	4:B:135:ILE:H	1.81	0.46
3:A:438:GLU:HG3	3:A:461:LYS:HE3	1.97	0.46
4:B:266:TRP:HB3	4:B:426:TRP:NE1	2.30	0.46
1:G:14:DC:H4'	3:C:286:THR:CG2	2.46	0.46
3:C:108:VAL:HG22	3:C:221:HIS:HB2	1.98	0.46
1:E:25:DT:H2''	1:E:26:DG:O5'	2.12	0.46
4:D:195:ILE:HG12	4:D:199:ARG:NH1	2.30	0.46
2:H:19:DC:H5'	3:C:259:LYS:HA	1.98	0.46
4:B:54:ASN:HB3	4:B:143:ARG:HH21	1.79	0.46
4:B:241:VAL:HG13	4:B:351:THR:OG1	2.16	0.45
3:C:442:VAL:HG11	3:C:485:ALA:HB2	1.98	0.45
1:E:5:DA:H2''	1:E:6:DC:C5'	2.31	0.45
1:E:8:DG:H4'	3:A:91:GLN:O	2.16	0.45
3:A:480:GLN:HG2	3:A:517:LEU:HD11	1.97	0.45
3:A:303:LEU:HD11	3:A:307:ARG:HH11	1.81	0.45
3:A:536:VAL:HB	3:A:542:ILE:HD13	1.97	0.45
3:C:180:ILE:HG12	3:C:189:VAL:HG13	1.98	0.45
1:E:13:DT:H2'	1:E:14:DC:C6	2.52	0.45
4:D:423:VAL:O	4:D:425:LEU:N	2.50	0.45
4:B:54:ASN:HB3	4:B:143:ARG:NH2	2.31	0.45
3:A:239:TRP:CH2	3:A:270:ILE:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:438:GLU:OE2	3:A:461:LYS:HD2	2.16	0.45
1:E:20:DG:C2'	1:E:21:DG:C8	3.00	0.45
3:C:23:GLN:HE21	3:C:60:VAL:H	1.63	0.45
3:C:115:TYR:CZ	6:C:705:TTP:H2'1	2.52	0.45
1:E:6:DC:H2''	1:E:7:DC:H5'	1.98	0.44
4:D:135:ILE:HD12	4:D:135:ILE:H	1.80	0.44
1:E:11:DG:H2'	1:E:12:DC:C6	2.52	0.44
1:G:6:DC:H2'	1:G:7:DC:H6	1.77	0.44
4:B:195:ILE:HG12	4:B:199:ARG:NH1	2.32	0.44
4:D:241:VAL:HG13	4:D:351:THR:OG1	2.17	0.44
4:D:253:THR:O	4:D:257:ILE:HG12	2.17	0.44
2:F:5:DT:C2'	2:F:6:DC:O5'	2.62	0.44
3:A:115:TYR:OH	3:A:184:MET:HE1	2.17	0.44
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.52	0.44
3:A:264:LEU:HD23	3:A:276:VAL:HG12	2.00	0.44
1:E:23:DA:H2''	1:E:24:DC:O5'	2.18	0.44
4:B:425:LEU:C	4:B:427:TYR:N	2.76	0.44
3:C:547:GLN:H	3:C:547:GLN:HG2	1.38	0.44
1:E:5:DA:C5'	3:A:76:ASP:OD1	2.66	0.44
4:D:233:GLU:CD	4:D:233:GLU:H	2.26	0.44
3:C:325:LEU:HD21	3:C:383:TRP:CE3	2.52	0.44
2:F:19:DC:H2''	2:F:20:DC:H5'	2.00	0.43
2:H:8:DC:C2'	2:H:9:DT:O5'	2.66	0.43
3:A:517:LEU:O	3:A:521:ILE:HG13	2.18	0.43
4:D:274:ILE:HG23	4:D:306:ASN:OD1	2.18	0.43
2:F:19:DC:C2'	2:F:20:DC:H5'	2.48	0.43
3:C:23:GLN:NE2	3:C:60:VAL:H	2.16	0.43
4:B:425:LEU:C	4:B:427:TYR:H	2.25	0.43
3:C:34:LEU:HD13	3:C:62:ALA:HB2	2.00	0.43
2:H:6:DC:H2'	2:H:7:DC:H6	1.80	0.43
1:E:17:DA:C2'	1:E:18:DC:O5'	2.62	0.43
1:E:19:DA:H2'	1:E:20:DG:C8	2.54	0.43
2:F:4:DG:H2''	2:F:5:DT:H5'	2.00	0.43
4:D:184:MET:HB3	4:D:185:ASP:H	1.69	0.43
2:F:16:DG:H2'	2:F:17:DC:C6	2.54	0.43
2:H:10:DG:C2'	2:H:11:DT:OP2	2.67	0.43
4:D:160:PHE:HE2	4:D:164:MET:HE2	1.83	0.42
4:D:242:GLN:HE21	4:D:353:LYS:HE3	1.84	0.42
1:E:14:DC:H4'	3:A:286:THR:CG2	2.45	0.42
1:G:5:DA:C5'	3:C:76:ASP:OD1	2.67	0.42
4:D:54:ASN:HB3	4:D:143:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:GLN:HG2	3:C:517:LEU:HD11	2.01	0.42
1:G:26:DG:H2'	1:G:27:DT:C5	2.55	0.42
4:B:274:ILE:HG23	4:B:306:ASN:OD1	2.20	0.42
4:D:242:GLN:HG3	4:D:352:GLY:HA2	2.01	0.42
3:A:228:LEU:HA	3:A:232:TYR:O	2.20	0.42
3:C:295:LEU:HD23	3:C:300:GLU:OE1	2.19	0.42
3:A:467:VAL:HG13	3:C:463:ARG:NH1	2.35	0.42
4:B:5:ILE:HG23	4:B:6:GLU:H	1.84	0.42
2:F:5:DT:H2'	2:F:6:DC:C6	2.55	0.42
2:H:5:DT:C2'	2:H:6:DC:H6	2.28	0.42
3:C:287:LYS:HA	3:C:287:LYS:HD3	1.93	0.42
4:D:320:ASP:HA	4:D:321:PRO:HD2	1.89	0.42
3:C:425:LEU:HD22	3:C:509:GLN:NE2	2.34	0.42
1:E:9:DG:H1'	3:A:94:ILE:CD1	2.50	0.42
1:G:11:DG:H2'	1:G:12:DC:C6	2.55	0.42
1:G:25:DT:C2'	1:G:26:DG:O5'	2.45	0.42
3:C:264:LEU:HD23	3:C:276:VAL:HG12	2.01	0.42
3:C:377:THR:O	3:C:381:VAL:HG23	2.20	0.42
1:E:7:DC:H2''	1:E:8:DG:C5'	2.49	0.41
1:E:25:DT:H2''	1:E:26:DG:OP2	2.15	0.41
2:H:18:DG:C4	2:H:19:DC:C5	3.07	0.41
3:A:206:ARG:HH12	3:A:220:LYS:HE2	1.83	0.41
1:E:6:DC:C2	1:E:7:DC:C5	3.08	0.41
1:E:20:DG:H2'	1:E:21:DG:C8	2.55	0.41
1:G:5:DA:C5	3:C:74:LEU:HD13	2.56	0.41
2:H:2:DC:H2'	2:H:3:DA:H8	1.75	0.41
4:B:261:VAL:HG13	4:B:276:VAL:HG21	2.01	0.41
3:C:339:TYR:CZ	3:C:352:GLY:HA3	2.55	0.41
4:D:5:ILE:HG23	4:D:6:GLU:H	1.85	0.41
1:G:23:DA:C2'	1:G:24:DC:O5'	2.68	0.41
1:E:5:DA:N3	3:A:152:GLY:HA2	2.34	0.41
3:A:158:ALA:O	3:A:162:SER:HB2	2.21	0.41
3:A:522:ILE:O	3:A:526:ILE:HG13	2.21	0.41
4:D:393:ILE:HD13	4:D:398:TRP:HB2	2.01	0.41
2:H:20:DC:H2''	2:H:21:DG:H5'	2.02	0.41
4:B:160:PHE:HE2	4:B:164:MET:HE2	1.86	0.41
4:B:184:MET:HB3	4:B:185:ASP:H	1.70	0.41
4:B:233:GLU:CD	4:B:233:GLU:H	2.29	0.41
3:C:442:VAL:HG21	3:C:482:ILE:HD13	2.02	0.41
3:A:249:LYS:HB3	3:A:249:LYS:HE2	1.88	0.41
4:D:203:GLU:O	4:D:207:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:156:SER:HB2	4:B:157:PRO:HD3	2.03	0.41
4:B:253:THR:O	4:B:257:ILE:HG12	2.20	0.41
4:B:425:LEU:O	4:B:427:TYR:N	2.54	0.41
3:C:60:VAL:HG12	3:C:75:VAL:HG22	2.03	0.41
3:C:195:ILE:H	3:C:195:ILE:HG13	1.55	0.41
4:D:74:LEU:HD12	4:D:74:LEU:HA	1.93	0.41
1:E:5:DA:C4'	3:A:76:ASP:OD1	2.66	0.41
3:C:495:ILE:O	3:C:533:LEU:HD12	2.21	0.41
4:B:74:LEU:HD12	4:B:74:LEU:HA	1.92	0.40
1:E:25:DT:C2'	1:E:26:DG:C8	3.05	0.40
1:G:4:DC:OP1	1:G:4:DC:O4'	2.38	0.40
3:A:7:THR:HG22	3:A:119:PRO:HB2	2.02	0.40
3:A:324:ASP:O	3:A:343:GLN:HG2	2.21	0.40
2:F:8:DC:H2''	2:F:9:DT:O5'	2.19	0.40
1:G:17:DA:H2''	1:G:18:DC:C5'	2.51	0.40
3:A:27:THR:HG22	3:A:29:GLU:H	1.86	0.40
2:F:20:DC:H2'	2:F:21:DG:O5'	2.22	0.40
4:B:423:VAL:HG23	4:B:426:TRP:CZ2	2.57	0.40
4:D:160:PHE:CE2	4:D:164:MET:HE2	2.56	0.40

There are no symmetry-related clashes.

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	552/554 (100%)	514 (93%)	30 (5%)	8 (1%)	9	39
3	C	552/554 (100%)	509 (92%)	33 (6%)	10 (2%)	6	34
4	B	410/440 (93%)	384 (94%)	18 (4%)	8 (2%)	6	31
4	D	410/440 (93%)	383 (93%)	19 (5%)	8 (2%)	6	31
All	All	1924/1988 (97%)	1790 (93%)	100 (5%)	34 (2%)	6	34

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	345	PRO
3	A	412	PRO
3	A	538	ALA
4	B	5	ILE
4	B	240	THR
4	B	424	LYS
4	B	425	LEU
4	B	426	TRP
4	B	428	GLN
3	C	222	GLN
3	C	345	PRO
3	C	412	PRO
3	C	538	ALA
4	D	5	ILE
4	D	240	THR
4	D	424	LYS
4	D	425	LEU
4	D	426	TRP
3	A	117	SER
3	A	286	THR
3	C	117	SER
3	C	243	PRO
3	C	286	THR
4	D	428	GLN
3	A	139	THR
3	C	139	THR
3	C	470	THR
3	A	144	TYR
3	C	144	TYR
3	A	222	GLN
4	D	321	PRO
4	B	321	PRO
4	B	14	PRO
4	D	14	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	495/495 (100%)	435 (88%)	60 (12%)	5	22
3	C	494/495 (100%)	435 (88%)	59 (12%)	5	23
4	B	376/400 (94%)	345 (92%)	31 (8%)	10	39
4	D	376/400 (94%)	346 (92%)	30 (8%)	11	40
All	All	1741/1790 (97%)	1561 (90%)	180 (10%)	7	28

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	LYS
3	A	23	GLN
3	A	28	GLU
3	A	48	SER
3	A	50	ILE
3	A	58	THR
3	A	60	VAL
3	A	63	ILE
3	A	68	SER
3	A	83	ARG
3	A	90	VAL
3	A	91	GLN
3	A	92	LEU
3	A	101	LYS
3	A	108	VAL
3	A	109	LEU
3	A	113	ASP
3	A	139	THR
3	A	149	LEU
3	A	151	GLN
3	A	154	LYS
3	A	162	SER
3	A	177	ASP
3	A	195	ILE
3	A	200	THR
3	A	205	LEU
3	A	225	PRO
3	A	228	LEU
3	A	250	ASP
3	A	258	CYS
3	A	263	LYS

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Mol	Chain	Res	Type
3	A	264	LEU
3	A	295	LEU
3	A	301	LEU
3	A	303	LEU
3	A	307	ARG
3	A	312	GLU
3	A	314	VAL
3	A	334	GLN
3	A	338	THR
3	A	345	PRO
3	A	357	MET
3	A	362	THR
3	A	368	LEU
3	A	374	LYS
3	A	377	THR
3	A	396	GLU
3	A	399	GLU
3	A	432	GLU
3	A	466	VAL
3	A	470	THR
3	A	471	ASP
3	A	474	ASN
3	A	477	THR
3	A	480	GLN
3	A	491	LEU
3	A	493	VAL
3	A	496	VAL
3	A	517	LEU
3	A	548	VAL
4	B	3	SER
4	B	10	VAL
4	B	16	MET
4	B	30	LYS
4	B	50	ILE
4	B	60	VAL
4	B	109	LEU
4	B	120	LEU
4	B	135	ILE
4	B	161	GLN
4	B	179	VAL
4	B	184	MET
4	B	200	THR

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Mol	Chain	Res	Type
4	B	205	LEU
4	B	211	ARG
4	B	214	LEU
4	B	242	GLN
4	B	253	THR
4	B	275	LYS
4	B	289	LEU
4	B	297	GLU
4	B	303	LEU
4	B	311	LYS
4	B	318	TYR
4	B	325	LEU
4	B	368	LEU
4	B	374	LYS
4	B	385	LYS
4	B	419	THR
4	B	423	VAL
4	B	428	GLN
3	C	1	LYS
3	C	23	GLN
3	C	28	GLU
3	C	48	SER
3	C	50	ILE
3	C	58	THR
3	C	60	VAL
3	C	63	ILE
3	C	68	SER
3	C	83	ARG
3	C	91	GLN
3	C	101	LYS
3	C	108	VAL
3	C	109	LEU
3	C	113	ASP
3	C	131	THR
3	C	139	THR
3	C	149	LEU
3	C	151	GLN
3	C	154	LYS
3	C	162	SER
3	C	177	ASP
3	C	195	ILE
3	C	200	THR

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Mol	Chain	Res	Type
3	C	205	LEU
3	C	238	LYS
3	C	244	ILE
3	C	245	VAL
3	C	250	ASP
3	C	254	VAL
3	C	263	LYS
3	C	264	LEU
3	C	301	LEU
3	C	303	LEU
3	C	307	ARG
3	C	312	GLU
3	C	314	VAL
3	C	338	THR
3	C	345	PRO
3	C	357	MET
3	C	362	THR
3	C	368	LEU
3	C	374	LYS
3	C	377	THR
3	C	396	GLU
3	C	399	GLU
3	C	432	GLU
3	C	466	VAL
3	C	470	THR
3	C	471	ASP
3	C	474	ASN
3	C	477	THR
3	C	480	GLN
3	C	491	LEU
3	C	493	VAL
3	C	496	VAL
3	C	517	LEU
3	C	547	GLN
3	C	548	VAL
4	D	3	SER
4	D	10	VAL
4	D	16	MET
4	D	30	LYS
4	D	50	ILE
4	D	60	VAL
4	D	109	LEU

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Mol	Chain	Res	Type
4	D	120	LEU
4	D	122	GLU
4	D	135	ILE
4	D	161	GLN
4	D	179	VAL
4	D	184	MET
4	D	200	THR
4	D	205	LEU
4	D	211	ARG
4	D	214	LEU
4	D	242	GLN
4	D	275	LYS
4	D	289	LEU
4	D	297	GLU
4	D	303	LEU
4	D	311	LYS
4	D	318	TYR
4	D	325	LEU
4	D	368	LEU
4	D	374	LYS
4	D	385	LYS
4	D	419	THR
4	D	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	54	ASN
3	A	182	GLN
3	A	221	HIS
3	A	255	ASN
3	A	315	HIS
3	A	336	GLN
3	A	373	GLN
3	A	480	GLN
4	B	137	ASN
4	B	145	GLN
4	B	147	ASN
4	B	175	ASN
4	B	242	GLN
4	B	255	ASN

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Mol	Chain	Res	Type
4	B	265	ASN
3	C	23	GLN
3	C	54	ASN
3	C	136	ASN
3	C	182	GLN
3	C	255	ASN
3	C	332	GLN
3	C	373	GLN
3	C	464	GLN
3	C	475	GLN
3	C	480	GLN
3	C	509	GLN
4	D	145	GLN
4	D	147	ASN
4	D	151	GLN
4	D	175	ASN
4	D	235	HIS
4	D	242	GLN
4	D	255	ASN
4	D	265	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	TTP	A	700	5	29,30,30	2.66	4 (13%)	43,47,47	1.36	7 (16%)
6	TTP	C	705	5	29,30,30	2.97	4 (13%)	43,47,47	1.05	4 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TTP	A	700	5	-	6/22/34/34	0/2/2/2
6	TTP	C	705	5	-	2/22/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	705	TTP	PA-O3A	9.28	1.69	1.59
6	C	705	TTP	PB-O3B	8.83	1.69	1.59
6	C	705	TTP	PB-O3A	8.74	1.68	1.59
6	A	700	TTP	PA-O3A	8.34	1.68	1.59
6	A	700	TTP	PB-O3B	-7.24	1.51	1.59
6	A	700	TTP	PG-O3G	6.92	1.80	1.54
6	A	700	TTP	PB-O3A	4.95	1.64	1.59
6	C	705	TTP	PG-O3G	2.10	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	700	TTP	O2A-PA-O3A	4.65	119.83	107.27
6	A	700	TTP	O3G-PG-O2G	3.52	121.02	107.80
6	C	705	TTP	O2A-PA-O3A	3.38	116.41	107.27
6	A	700	TTP	O2G-PG-O3B	-2.90	94.90	104.64
6	A	700	TTP	O3A-PB-O1B	2.73	118.91	110.70
6	A	700	TTP	O3B-PB-O1B	-2.60	102.89	110.70
6	A	700	TTP	O2B-PB-O3B	-2.50	100.52	107.27
6	A	700	TTP	O2G-PG-O1G	2.21	119.47	110.83
6	C	705	TTP	O2G-PG-O1G	2.18	119.34	110.83
6	C	705	TTP	O3G-PG-O1G	-2.18	102.35	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	TTP	O3A-PA-O1A	-2.02	104.63	110.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

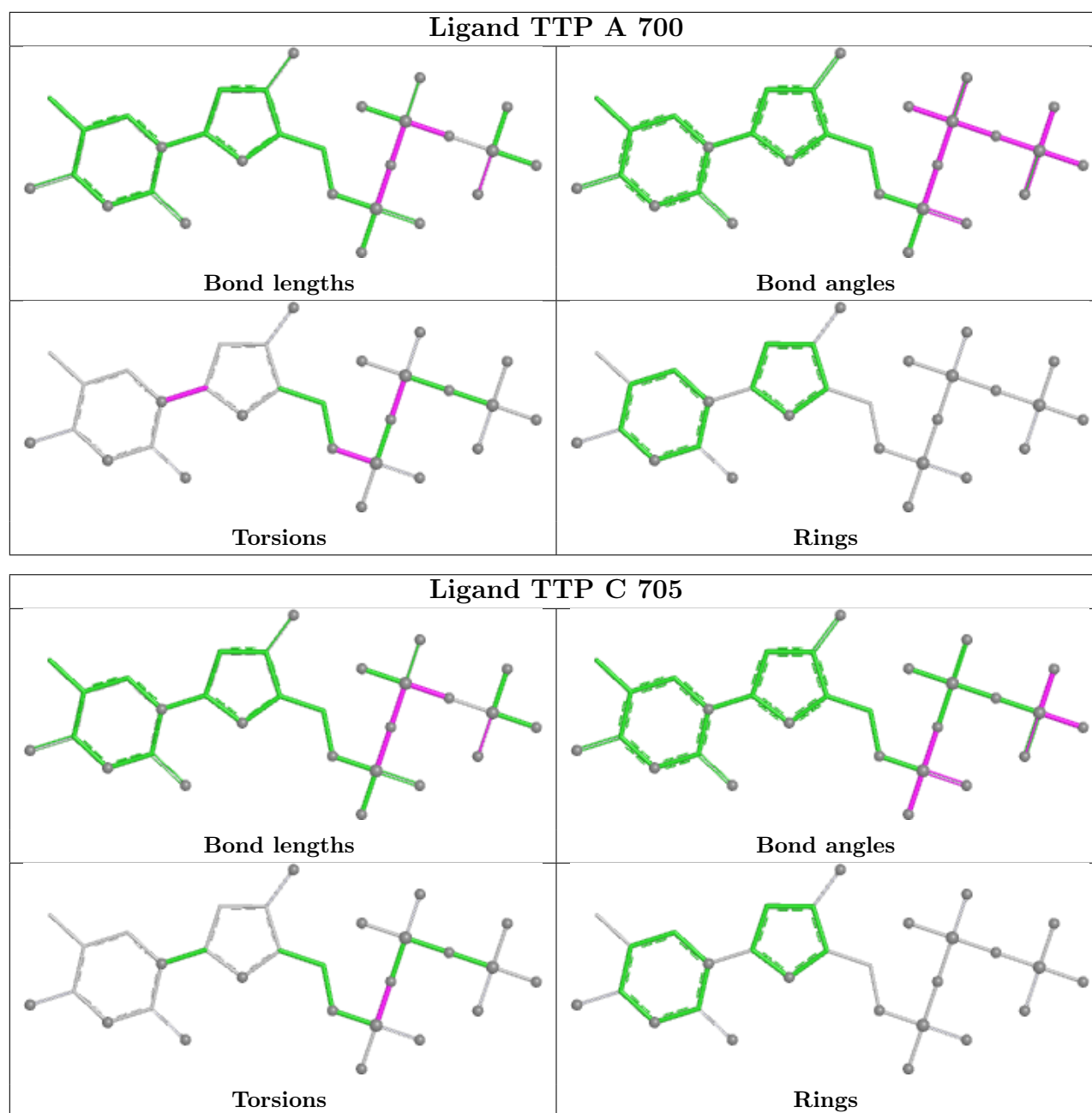
Mol	Chain	Res	Type	Atoms
6	A	700	TTP	C5'-O5'-PA-O1A
6	C	705	TTP	PB-O3A-PA-O1A
6	A	700	TTP	C5'-O5'-PA-O2A
6	A	700	TTP	C5'-O5'-PA-O3A
6	A	700	TTP	C2'-C1'-N1-C2
6	A	700	TTP	PA-O3A-PB-O2B
6	A	700	TTP	PA-O3A-PB-O1B
6	C	705	TTP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	700	TTP	1	0
6	C	705	TTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.