



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:26 PM EDT

PDB ID : 1RTD
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

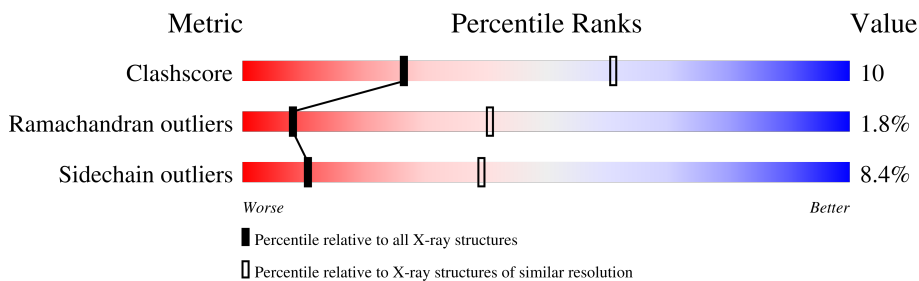
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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	
1	G	27	
2	F	21	
2	H	21	
3	A	554	
3	C	554	
4	B	440	
4	D	440	

2 Entry composition [i](#)

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
			Total	C	N	O	P			
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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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

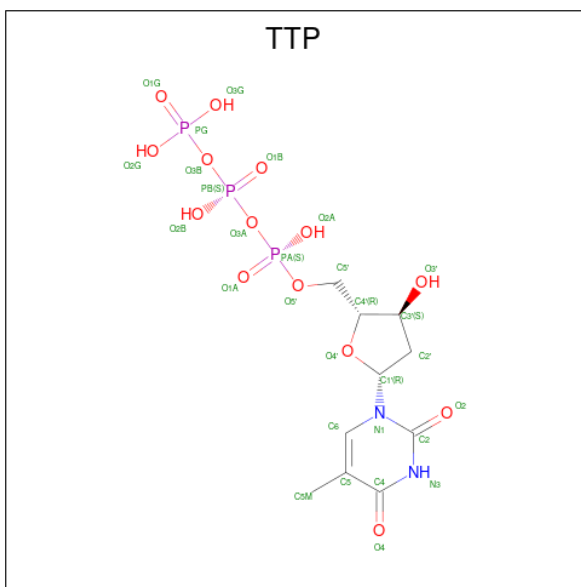
- Molecule 4 is a protein called PROTEIN (REVERSE TRANSCRIPTASE).

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 (three-letter code: 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 (three-letter code: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



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

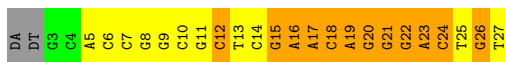
3 Residue-property plots

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: 



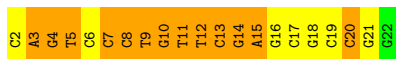
- Molecule 1: DNA TEMPLATE FOR REVERSE TRANSCRIPTASE

Chain G: 



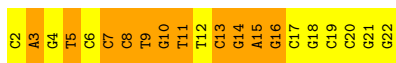
- Molecule 2: DNA PRIMER FOR REVERSE TRANSCRIPTASE

Chain F: 




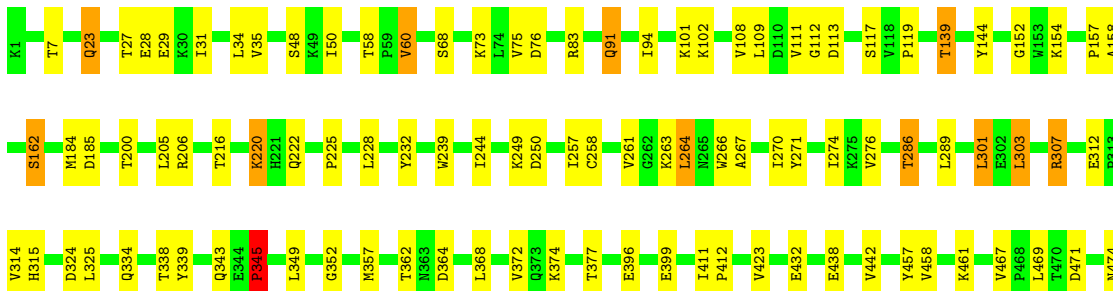
- Molecule 2: DNA PRIMER FOR REVERSE TRANSCRIPTASE

Chain H: 



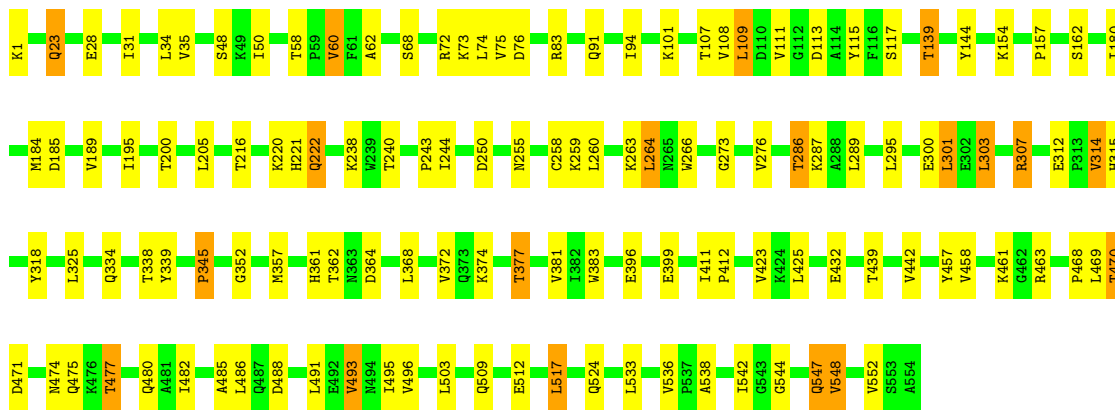
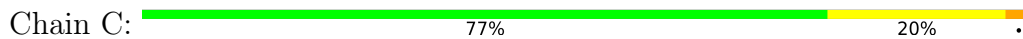
- Molecule 3: PROTEIN (REVERSE TRANSCRIPTASE)

Chain A: 

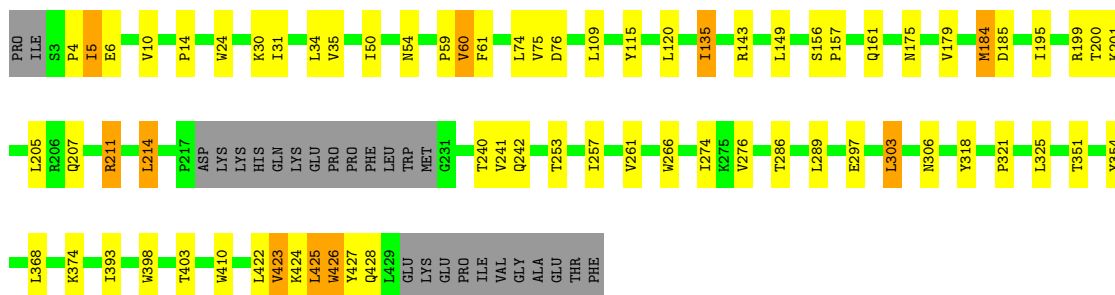
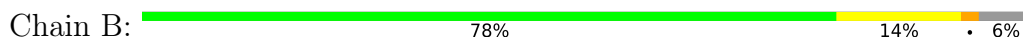




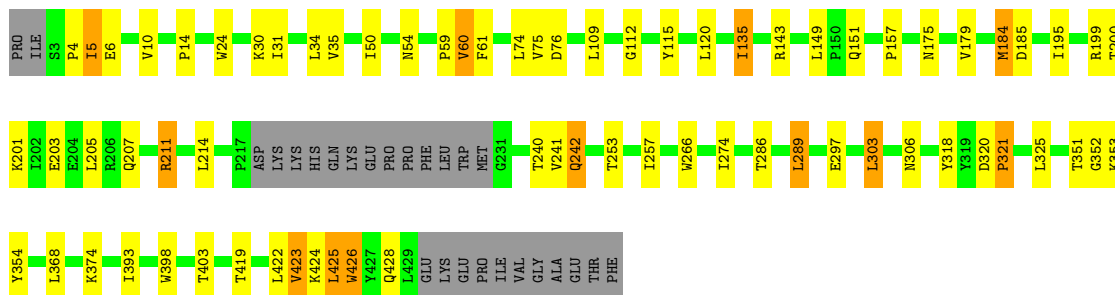
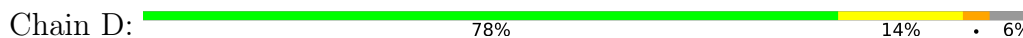
• Molecule 3: PROTEIN (REVERSE TRANSCRIPTASE)



• Molecule 4: PROTEIN (REVERSE TRANSCRIPTASE)



• Molecule 4: PROTEIN (REVERSE TRANSCRIPTASE)



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	17784	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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: 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	0.87	0/575	1.40	12/886 (1.4%)
1	G	0.76	0/575	1.53	20/886 (2.3%)
2	F	0.94	0/474	1.59	17/729 (2.3%)
2	H	0.69	0/474	1.48	13/729 (1.8%)
3	A	0.73	1/4627 (0.0%)	0.92	8/6286 (0.1%)
3	C	0.75	2/4624 (0.0%)	0.91	6/6281 (0.1%)
4	B	0.72	0/3512	0.89	3/4774 (0.1%)
4	D	0.72	0/3512	0.90	2/4774 (0.0%)
All	All	0.74	3/18373 (0.0%)	1.00	81/25345 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	512	GLU	CD-OE2	6.29	1.32	1.25
3	C	461	LYS	CE-NZ	-6.09	1.33	1.49
3	A	271	TYR	CD1-CE1	5.09	1.47	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	DG	N9-C1'-C2'	10.02	131.63	112.60
1	G	16	DA	N9-C1'-C2'	9.39	130.45	112.60
1	G	18	DC	N1-C1'-C2'	8.63	129.00	112.60
2	F	8	DC	N1-C1'-C2'	8.07	127.94	112.60
2	H	15	DA	N9-C1'-C2'	8.04	127.88	112.60
1	E	21	DG	N9-C1'-C2'	7.77	127.37	112.60
2	H	10	DG	O4'-C1'-N9	7.70	113.39	108.00
1	G	15	DG	N9-C1'-C2'	7.69	127.21	112.60
2	H	9	DT	N1-C1'-C2'	7.66	127.15	112.60
2	F	12	DT	N1-C1'-C2'	7.61	127.06	112.60
3	C	468	PRO	N-CA-CB	7.60	112.42	103.30
2	F	9	DT	N1-C1'-C2'	7.53	126.91	112.60
2	H	8	DC	N1-C1'-C2'	7.51	126.88	112.60
3	A	301	LEU	CA-CB-CG	7.47	132.49	115.30
2	F	14	DG	N9-C1'-C2'	7.32	126.50	112.60
1	G	4	DC	N1-C1'-C2'	7.31	126.49	112.60
2	H	5	DT	N1-C1'-C2'	7.29	126.45	112.60
1	G	21	DG	N9-C1'-C2'	7.28	126.44	112.60
3	C	301	LEU	CA-CB-CG	7.27	132.03	115.30
2	H	7	DC	N1-C1'-C2'	7.23	126.33	112.60
2	F	13	DC	N1-C1'-C2'	7.21	126.30	112.60
1	E	15	DG	N9-C1'-C2'	7.16	126.20	112.60
1	G	17	DA	N9-C1'-C2'	7.15	126.18	112.60
2	F	11	DT	N1-C1'-C2'	6.88	125.67	112.60
2	H	10	DG	O4'-C4'-C3'	-6.85	101.76	104.50
1	E	19	DA	N9-C1'-C2'	6.77	125.46	112.60
2	F	4	DG	N9-C1'-C2'	6.65	125.24	112.60
1	G	14	DC	N1-C1'-C2'	6.65	125.23	112.60
1	E	17	DA	N9-C1'-C2'	6.63	125.20	112.60
2	H	13	DC	N1-C1'-C2'	6.59	125.11	112.60
2	F	3	DA	N9-C1'-C2'	6.53	125.00	112.60
1	E	16	DA	N9-C1'-C2'	6.49	124.93	112.60
4	B	4	PRO	N-CA-C	6.45	128.87	112.10
1	G	18	DC	O4'-C1'-N1	6.45	112.52	108.00
4	D	4	PRO	N-CA-C	6.33	128.56	112.10
1	E	18	DC	N1-C1'-C2'	6.29	124.56	112.60
2	H	11	DT	N1-C1'-C2'	6.23	124.43	112.60
1	E	24	DC	N1-C1'-C2'	6.21	124.40	112.60
1	E	20	DG	N9-C1'-C2'	6.18	124.34	112.60
2	F	15	DA	N9-C1'-C2'	6.12	124.23	112.60
3	C	493	VAL	CB-CA-C	-6.11	99.79	111.40
1	G	7	DC	O4'-C1'-N1	6.08	112.26	108.00
2	F	14	DG	O4'-C1'-C2'	5.97	110.68	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	DT	N1-C1'-C2'	5.88	123.78	112.60
3	A	493	VAL	CB-CA-C	-5.84	100.31	111.40
2	H	14	DG	N9-C1'-C2'	5.80	123.63	112.60
1	G	20	DG	O4'-C1'-C2'	5.80	110.54	105.90
3	A	274	ILE	CG1-CB-CG2	-5.76	98.72	111.40
2	F	11	DT	O4'-C1'-C2'	5.76	110.51	105.90
3	A	513	SER	N-CA-CB	-5.73	101.90	110.50
2	F	5	DT	N1-C1'-C2'	5.72	123.47	112.60
3	C	303	LEU	CA-CB-CG	5.72	128.45	115.30
1	E	23	DA	N9-C1'-C2'	5.69	123.42	112.60
1	G	11	DG	N9-C1'-C2'	5.68	123.39	112.60
3	A	303	LEU	CA-CB-CG	5.68	128.36	115.30
3	C	260	LEU	CA-CB-CG	5.65	128.30	115.30
1	E	22	DG	N9-C1'-C2'	5.64	123.32	112.60
2	H	3	DA	N9-C1'-C2'	5.61	123.26	112.60
1	G	7	DC	O4'-C4'-C3'	-5.60	102.26	104.50
1	G	18	DC	O4'-C1'-C2'	5.58	110.37	105.90
1	G	3	DG	N9-C1'-C2'	5.58	123.21	112.60
3	A	491	LEU	CA-CB-CG	5.56	128.08	115.30
2	H	22	DG	O4'-C1'-N9	5.54	111.88	108.00
2	F	20	DC	O4'-C4'-C3'	-5.53	102.29	104.50
3	C	461	LYS	CD-CE-NZ	5.50	124.35	111.70
2	F	13	DC	O4'-C1'-C2'	5.49	110.29	105.90
2	H	16	DG	N9-C1'-C2'	5.46	122.97	112.60
1	G	23	DA	N9-C1'-C2'	5.41	122.89	112.60
2	F	7	DC	N1-C1'-C2'	5.32	122.70	112.60
1	G	24	DC	N1-C1'-C2'	5.30	122.67	112.60
1	E	26	DG	N9-C1'-C2'	5.26	122.60	112.60
3	A	325	LEU	CB-CG-CD2	-5.21	102.15	111.00
4	B	303	LEU	CA-CB-CG	5.14	127.12	115.30
1	G	19	DA	N9-C1'-C2'	5.13	122.36	112.60
1	G	12	DC	N1-C1'-C2'	5.13	122.34	112.60
3	A	345	PRO	N-CA-C	5.09	125.34	112.10
1	E	12	DC	N1-C1'-C2'	5.07	122.24	112.60
2	F	4	DG	O4'-C1'-C2'	5.05	109.94	105.90
2	F	10	DG	O4'-C1'-N9	5.03	111.52	108.00
4	D	303	LEU	CA-CB-CG	5.02	126.85	115.30
4	B	214	LEU	CA-CB-CG	5.01	126.83	115.30

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 [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	E	512	0	280	62	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	30	0
4	D	3415	0	3448	33	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	359	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 (359) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:12:DC:H2'	1:E:13:DT:C7	2.29	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
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:A:438:GLU:CD	3:A:461:LYS:HD2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:DT:H2'	2:H:10:DG:H8	1.68	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
1:E:12:DC:H2'	1:E:13:DT:H72	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:19:DA:H2'	1:G:20:DG:H8	1.71	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
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
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
1:E:12:DC:C6	1:E:13:DT:H72	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:157:PRO:HB3	3:A:184:MET:HE1	1.99	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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:490:GLY:O	3:A:528:LYS:NZ	2.41	0.42
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:184:MET:HB3	4:B:185:ASP:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:157:PRO:HB3	3:C:184:MET:HE1	2.02	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

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	552/554 (100%)	514 (93%)	30 (5%)	8 (1%)	11	46
3	C	552/554 (100%)	509 (92%)	33 (6%)	10 (2%)	8	41
4	B	410/440 (93%)	384 (94%)	18 (4%)	8 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	410/440 (93%)	383 (93%)	19 (5%)	8 (2%)	7	38
All	All	1924/1988 (97%)	1790 (93%)	100 (5%)	34 (2%)	8	41

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 [i](#)

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%)	446 (90%)	49 (10%)	8	30
3	C	494/495 (100%)	443 (90%)	51 (10%)	7	29
4	B	376/400 (94%)	352 (94%)	24 (6%)	17	52
4	D	376/400 (94%)	353 (94%)	23 (6%)	18	54
All	All	1741/1790 (97%)	1594 (92%)	147 (8%)	11	39

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	68	SER
3	A	83	ARG
3	A	91	GLN
3	A	101	LYS
3	A	102	LYS
3	A	108	VAL
3	A	113	ASP
3	A	139	THR
3	A	154	LYS
3	A	162	SER
3	A	200	THR
3	A	205	LEU
3	A	220	LYS
3	A	225	PRO
3	A	250	ASP
3	A	258	CYS
3	A	263	LYS
3	A	264	LEU

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Mol	Chain	Res	Type
3	A	301	LEU
3	A	307	ARG
3	A	312	GLU
3	A	314	VAL
3	A	315	HIS
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	471	ASP
3	A	474	ASN
3	A	477	THR
3	A	488	ASP
3	A	491	LEU
3	A	493	VAL
3	A	496	VAL
3	A	517	LEU
3	A	548	VAL
4	B	10	VAL
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
4	B	205	LEU
4	B	211	ARG
4	B	214	LEU
4	B	242	GLN
4	B	289	LEU
4	B	297	GLU

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Mol	Chain	Res	Type
4	B	303	LEU
4	B	318	TYR
4	B	325	LEU
4	B	368	LEU
4	B	374	LYS
4	B	410	TRP
4	B	423	VAL
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	68	SER
3	C	83	ARG
3	C	91	GLN
3	C	101	LYS
3	C	109	LEU
3	C	113	ASP
3	C	139	THR
3	C	154	LYS
3	C	162	SER
3	C	200	THR
3	C	205	LEU
3	C	220	LYS
3	C	238	LYS
3	C	244	ILE
3	C	250	ASP
3	C	258	CYS
3	C	263	LYS
3	C	264	LEU
3	C	301	LEU
3	C	307	ARG
3	C	312	GLU
3	C	314	VAL
3	C	315	HIS
3	C	334	GLN
3	C	345	PRO
3	C	357	MET
3	C	362	THR
3	C	368	LEU

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Mol	Chain	Res	Type
3	C	374	LYS
3	C	377	THR
3	C	396	GLU
3	C	399	GLU
3	C	432	GLU
3	C	470	THR
3	C	471	ASP
3	C	474	ASN
3	C	477	THR
3	C	488	ASP
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	10	VAL
4	D	30	LYS
4	D	50	ILE
4	D	60	VAL
4	D	109	LEU
4	D	120	LEU
4	D	135	ILE
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	289	LEU
4	D	297	GLU
4	D	303	LEU
4	D	318	TYR
4	D	325	LEU
4	D	368	LEU
4	D	374	LYS
4	D	419	THR
4	D	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	GLN
3	A	182	GLN
3	A	221	HIS
3	A	255	ASN
3	A	332	GLN
3	A	447	ASN
3	A	464	GLN
3	A	509	GLN
4	B	85	GLN
4	B	175	ASN
4	B	242	GLN
3	C	23	GLN
3	C	54	ASN
3	C	182	GLN
3	C	255	ASN
3	C	332	GLN
3	C	447	ASN
3	C	464	GLN
3	C	509	GLN
4	D	151	GLN
4	D	175	ASN
4	D	242	GLN

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 monosaccharides 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	23,30,30	1.78	3 (13%)	29,47,47	2.93	5 (17%)
6	TTP	C	705	5	23,30,30	1.23	4 (17%)	29,47,47	2.85	5 (17%)

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	-	5/19/34/34	0/2/2/2
6	TTP	C	705	5	-	1/19/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	700	TTP	PG-O3G	6.66	1.80	1.54
6	C	705	TTP	C4-N3	3.37	1.38	1.33
6	A	700	TTP	C4-N3	3.27	1.38	1.33
6	A	700	TTP	C6-C5	-2.37	1.33	1.40
6	C	705	TTP	C4-C5	2.32	1.46	1.41
6	C	705	TTP	C6-C5	-2.03	1.34	1.40
6	C	705	TTP	PG-O3G	2.02	1.62	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	700	TTP	C4-N3-C2	14.20	127.13	115.14
6	C	705	TTP	C4-N3-C2	13.86	126.84	115.14
6	A	700	TTP	O3G-PG-O2G	3.50	121.02	107.64
6	A	700	TTP	O2G-PG-O3B	-2.90	94.90	104.64
6	C	705	TTP	PB-O3B-PG	2.86	142.63	132.83
6	C	705	TTP	PB-O3A-PA	-2.50	124.26	132.83
6	A	700	TTP	PB-O3A-PA	-2.33	124.83	132.83
6	A	700	TTP	O2G-PG-O1G	2.24	119.47	110.68
6	C	705	TTP	O2G-PG-O1G	2.21	119.34	110.68
6	C	705	TTP	O3G-PG-O1G	-2.13	102.35	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

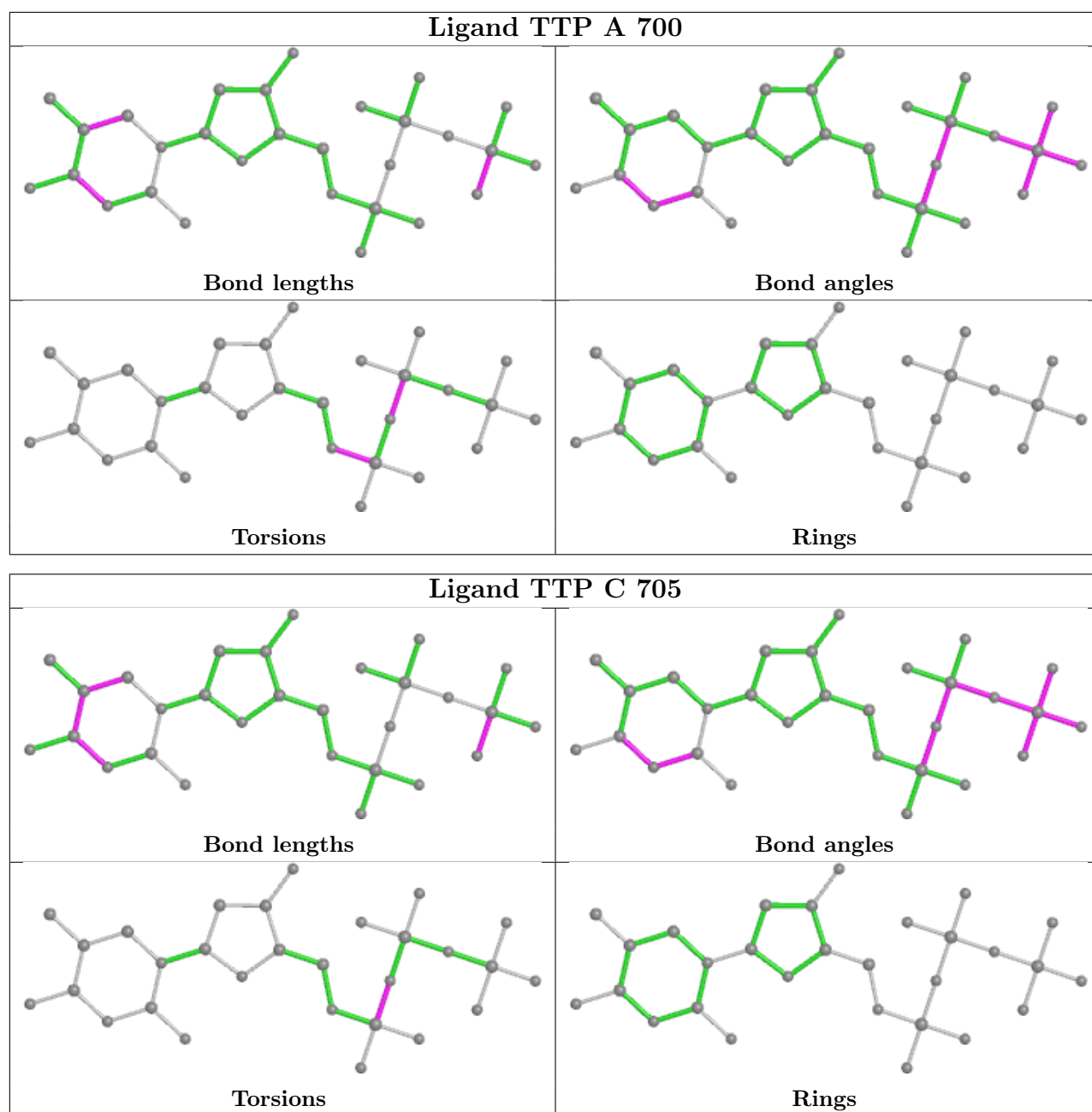
Mol	Chain	Res	Type	Atoms
6	A	700	TTP	C5'-O5'-PA-O1A
6	A	700	TTP	C5'-O5'-PA-O3A
6	C	705	TTP	PB-O3A-PA-O1A
6	A	700	TTP	C5'-O5'-PA-O2A
6	A	700	TTP	PA-O3A-PB-O2B
6	A	700	TTP	PA-O3A-PB-O1B

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.