



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:05 am BST

PDB ID : 1Z1C
Title : Structural Determinants of Tissue Tropism and In Vivo Pathogenicity for the Parvovirus Minute virus of Mice
Authors : Kontou, M.; Govindasamy, L.; Nam, H.J.; Bryant, N.; Llamas-Saiz, A.L.; Foces-Foces, C.; Hernando, E.; Rubio, M.P.; McKenna, R.; Almendral, J.M.; Agbandje-McKenna, M.
Deposited on : 2005-03-03
Resolution : 3.50 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)
Xtriage (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) : 2.11

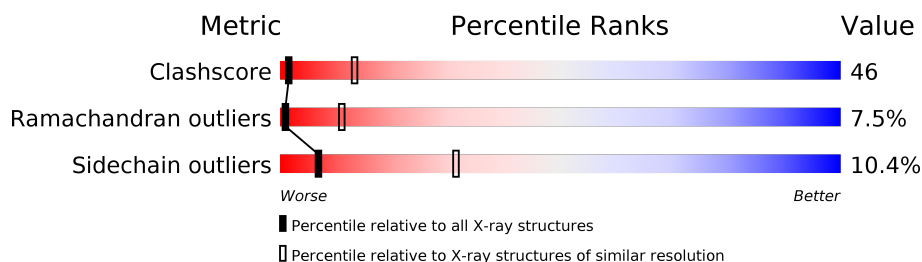
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 on 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	12	
2	C	9	
3	A	587	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4864 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 5'-D(*AP*TP*CP*CP*TP*CP*TP*AP*TP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			235	115	38	71	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			180	87	39	46	8			

- Molecule 3 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	549	Total	C	N	O	S	0	0	0
			4328	2727	751	830	20			

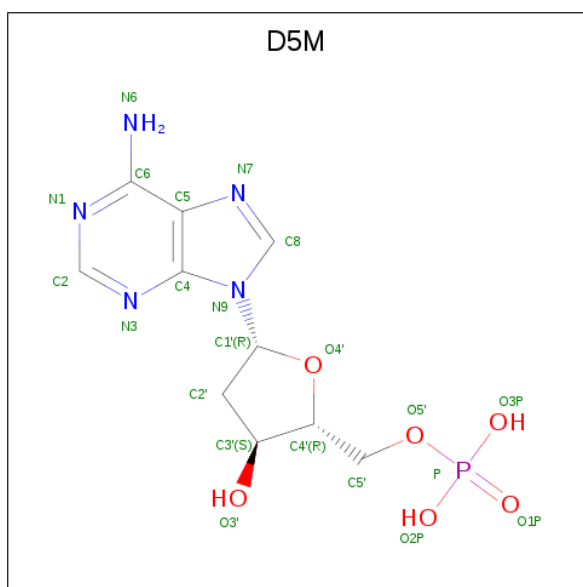
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	MET	VAL	SEE REMARK 999	UNP P07302
A	455	THR	ALA	SEE REMARK 999	UNP P07302

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C₁₀H₁₄N₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total	O	0	0
			5	5		
6	C	11	Total	O	0	0
			11	11		
6	A	85	Total	O	0	0
			85	85		


3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

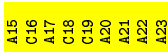
- Molecule 1: 5'-D(*AP*TP*CP*CP*TP*CP*TP*AP*TP*CP*AP*C)-3'

Chain B: 



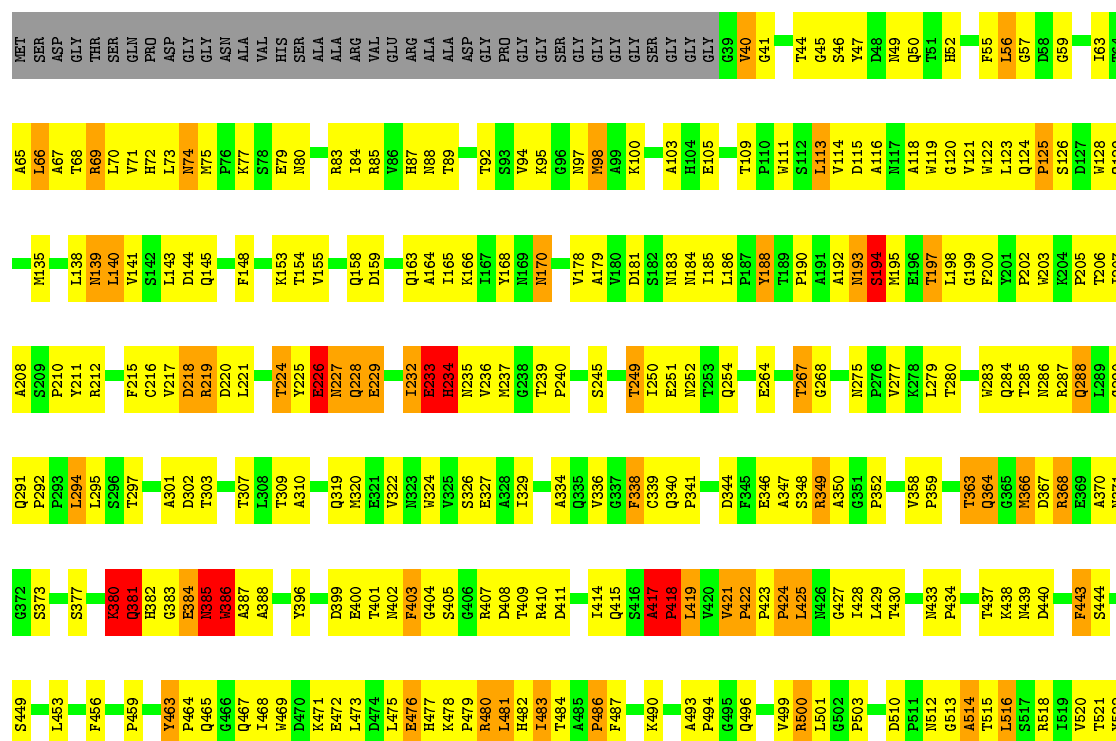
- Molecule 2: 5'-D(*AP*CP*AP*CP*CP*AP*AP*AP*A)-3'

Chain C: 



- Molecule 3: Coat protein VP2

Chain A: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	448.70 Å 416.70 Å 305.30 Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.325 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: CA, D5M

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	0.74	0/261	0.84	0/399
2	C	0.74	0/203	0.90	0/310
3	A	1.14	8/4452 (0.2%)	1.08	31/6088 (0.5%)
All	All	1.11	8/4916 (0.2%)	1.06	31/6797 (0.5%)

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
3	A	0	3
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	586	THR	N-CA	41.38	2.29	1.46
3	A	418	PRO	N-CD	37.60	2.00	1.47
3	A	234	HIS	N-CA	26.69	1.99	1.46
3	A	227	ASN	N-CA	13.98	1.74	1.46
3	A	581	PRO	N-CD	11.41	1.63	1.47
3	A	585	ASN	C-N	6.99	1.50	1.34
3	A	385	ASN	C-N	-5.29	1.21	1.34
3	A	385	ASN	N-CA	5.19	1.56	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	585	ASN	C-N-CA	-21.02	69.14	121.70
3	A	418	PRO	N-CA-CB	18.13	125.05	103.30
3	A	418	PRO	CA-N-CD	-17.05	87.63	111.50
3	A	233	GLU	C-N-CA	-14.67	85.02	121.70
3	A	586	THR	N-CA-CB	-14.06	83.58	110.30
3	A	380	LYS	O-C-N	-13.92	100.42	122.70
3	A	385	ASN	C-N-CA	-12.38	90.74	121.70
3	A	226	GLU	C-N-CA	-10.68	94.99	121.70
3	A	380	LYS	CA-C-N	9.79	138.74	117.20
3	A	585	ASN	O-C-N	9.76	138.32	122.70
3	A	364	GLN	N-CA-C	-8.64	87.67	111.00
3	A	229	GLU	N-CA-CB	-7.50	97.11	110.60
3	A	386	TRP	CE2-CD2-CG	6.95	112.86	107.30
3	A	385	ASN	CA-C-N	6.61	131.74	117.20
3	A	386	TRP	CB-CG-CD1	6.50	135.45	127.00
3	A	233	GLU	CB-CG-CD	-6.32	97.14	114.20
3	A	515	THR	N-CA-CB	6.18	122.04	110.30
3	A	229	GLU	N-CA-C	6.05	127.33	111.00
3	A	385	ASN	O-C-N	-6.02	113.07	122.70
3	A	380	LYS	C-N-CA	-5.99	106.72	121.70
3	A	227	ASN	N-CA-CB	-5.88	100.01	110.60
3	A	544	ASN	N-CA-C	-5.73	95.52	111.00
3	A	585	ASN	CA-C-N	-5.70	104.67	117.20
3	A	194	SER	O-C-N	-5.68	113.62	122.70
3	A	386	TRP	CG-CD2-CE3	-5.52	128.93	133.90
3	A	381	GLN	N-CA-C	5.51	125.89	111.00
3	A	419	LEU	CA-CB-CG	-5.42	102.82	115.30
3	A	66	LEU	CA-CB-CG	-5.24	103.26	115.30
3	A	197	THR	C-N-CA	-5.16	108.81	121.70
3	A	439	ASN	N-CA-C	5.12	124.84	111.00
3	A	515	THR	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	194	SER	Mainchain
3	A	363	THR	Peptide
3	A	417	ALA	Peptide
1	B	7	DT	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	235	0	138	30	0
2	C	180	0	101	19	0
3	A	4328	0	4124	384	0
4	B	2	0	0	0	0
5	B	18	0	12	3	0
6	A	85	0	0	0	0
6	B	5	0	0	0	0
6	C	11	0	0	0	0
All	All	4864	0	4375	421	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 46.

All (421) 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:227:ASN:CA	3:A:227:ASN:N	1.74	1.51
3:A:380:LYS:NZ	3:A:386:TRP:O	1.56	1.34
3:A:385:ASN:OD1	3:A:386:TRP:N	1.67	1.25
3:A:234:HIS:CA	3:A:234:HIS:N	1.99	1.25
3:A:418:PRO:CD	3:A:418:PRO:N	2.00	1.23
3:A:417:ALA:HB1	3:A:418:PRO:CD	1.71	1.19
3:A:421:VAL:HB	3:A:422:PRO:HD3	1.14	1.11
3:A:225:TYR:CE1	3:A:228:GLN:OE1	2.06	1.09
3:A:483:ILE:HD13	3:A:483:ILE:H	1.15	1.08
3:A:233:GLU:O	3:A:234:HIS:CA	2.04	1.06
3:A:380:LYS:HE2	3:A:384:GLU:HG2	1.36	1.05
3:A:585:ASN:C	3:A:586:THR:CA	2.24	1.05
3:A:578:ILE:HD12	3:A:578:ILE:H	1.18	1.03
3:A:226:GLU:C	3:A:227:ASN:CA	2.28	1.03
3:A:585:ASN:O	3:A:586:THR:CA	2.07	1.02
3:A:233:GLU:C	3:A:234:HIS:CA	2.29	1.00
3:A:339:CYS:H	3:A:449:SER:HB3	1.25	0.98
3:A:380:LYS:HZ3	3:A:388:ALA:H	1.07	0.98
3:A:158:GLN:HG2	3:A:159:ASP:H	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:363:THR:HG22	3:A:364:GLN:H	1.27	0.97
3:A:380:LYS:NZ	3:A:386:TRP:C	2.17	0.96
3:A:430:THR:H	3:A:433:ASN:ND2	1.64	0.95
3:A:586:THR:N	3:A:586:THR:CA	2.29	0.94
3:A:380:LYS:CE	3:A:384:GLU:HG2	1.99	0.91
3:A:421:VAL:CB	3:A:422:PRO:HD3	1.99	0.91
3:A:118:ALA:O	3:A:121:VAL:HG12	1.69	0.90
3:A:217:VAL:O	3:A:218:ASP:HB2	1.71	0.90
3:A:233:GLU:O	3:A:234:HIS:HA	1.70	0.90
3:A:417:ALA:CB	3:A:418:PRO:CD	2.50	0.89
3:A:561:VAL:HG23	3:A:562:THR:H	1.38	0.88
3:A:483:ILE:CD1	3:A:483:ILE:H	1.87	0.88
3:A:421:VAL:HB	3:A:422:PRO:CD	2.03	0.87
3:A:417:ALA:HB1	3:A:418:PRO:HD2	1.57	0.87
3:A:380:LYS:HE2	3:A:384:GLU:CG	2.04	0.87
3:A:585:ASN:O	3:A:586:THR:HA	1.72	0.86
3:A:49:ASN:HD22	3:A:68:THR:H	1.24	0.86
3:A:417:ALA:HB1	3:A:418:PRO:HD3	1.58	0.86
3:A:380:LYS:H	3:A:384:GLU:HB2	1.37	0.86
3:A:186:LEU:N	3:A:186:LEU:HD12	1.91	0.85
3:A:380:LYS:NZ	3:A:388:ALA:H	1.73	0.85
3:A:181:ASP:HA	3:A:254:GLN:NE2	1.92	0.84
3:A:69:ARG:NH2	3:A:202:PRO:HG3	1.93	0.83
3:A:225:TYR:CD1	3:A:228:GLN:OE1	2.32	0.83
3:A:115:ASP:O	3:A:198:LEU:HD13	1.79	0.83
3:A:226:GLU:O	3:A:227:ASN:CA	2.27	0.82
3:A:483:ILE:HD13	3:A:483:ILE:N	1.94	0.82
3:A:92:THR:HB	3:A:235:ASN:HD21	1.43	0.82
3:A:159:ASP:HB2	3:A:165:ILE:HG22	1.61	0.82
3:A:322:VAL:HB	3:A:324:TRP:NE1	1.93	0.82
3:A:367:ASP:HB3	3:A:370:ALA:HB3	1.61	0.82
3:A:56:LEU:HD12	3:A:56:LEU:N	1.95	0.81
3:A:380:LYS:CD	3:A:384:GLU:HG2	2.10	0.80
3:A:186:LEU:H	3:A:186:LEU:HD12	1.47	0.80
3:A:363:THR:CG2	3:A:364:GLN:H	1.94	0.79
3:A:226:GLU:O	3:A:227:ASN:HA	1.83	0.79
3:A:286:ASN:HD21	3:A:336:VAL:H	1.30	0.79
3:A:202:PRO:HD2	3:A:203:TRP:CZ3	2.17	0.78
3:A:285:THR:HG22	3:A:286:ASN:H	1.48	0.78
3:A:339:CYS:H	3:A:449:SER:CB	1.97	0.78
3:A:358:VAL:O	3:A:358:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:185:ILE:H	3:A:185:ILE:HD12	1.47	0.78
3:A:126:SER:O	3:A:129:GLN:HB3	1.84	0.77
3:A:385:ASN:CG	3:A:386:TRP:N	2.34	0.77
3:A:363:THR:HG22	3:A:364:GLN:N	1.94	0.77
3:A:145:GLN:H	3:A:267:THR:HG21	1.50	0.77
2:C:15:DA:H2''	2:C:16:DC:OP2	1.85	0.77
3:A:139:ASN:HD22	3:A:140:LEU:H	1.32	0.76
3:A:478:LYS:HB3	3:A:479:PRO:HD2	1.67	0.76
3:A:165:ILE:HG13	3:A:166:LYS:H	1.52	0.75
3:A:562:THR:HA	3:A:565:LEU:HD12	1.69	0.74
3:A:85:ARG:HD2	3:A:237:MET:HG2	1.69	0.74
3:A:141:VAL:HG23	3:A:533:MET:HA	1.70	0.74
3:A:227:ASN:N	3:A:227:ASN:CB	2.50	0.73
3:A:493:ALA:HB1	3:A:494:PRO:HD2	1.70	0.73
3:A:286:ASN:ND2	3:A:336:VAL:H	1.88	0.72
3:A:45:GLY:HA3	3:A:148:PHE:CD2	2.25	0.72
3:A:480:ARG:O	3:A:481:LEU:HB3	1.88	0.72
3:A:219:ARG:HG3	3:A:219:ARG:HH11	1.55	0.71
3:A:158:GLN:HG2	3:A:159:ASP:N	2.03	0.71
3:A:185:ILE:HD12	3:A:185:ILE:N	2.07	0.70
3:A:380:LYS:HZ3	3:A:388:ALA:N	1.86	0.70
3:A:358:VAL:O	3:A:358:VAL:CG2	2.40	0.70
3:A:586:THR:OG1	3:A:586:THR:N	2.24	0.69
3:A:385:ASN:OD1	3:A:387:ALA:N	2.25	0.69
3:A:228:GLN:HG3	3:A:229:GLU:H	1.58	0.69
3:A:567:THR:HG23	3:A:571:ASN:O	1.91	0.69
3:A:464:PRO:HD2	3:A:576:PRO:HA	1.75	0.69
3:A:181:ASP:OD2	3:A:184:ASN:HA	1.93	0.69
3:A:121:VAL:HG13	3:A:122:TRP:CD1	2.28	0.68
3:A:153:LYS:HG2	3:A:170:ASN:HB3	1.75	0.68
3:A:290:GLY:O	3:A:292:PRO:HD3	1.94	0.68
3:A:561:VAL:HG23	3:A:562:THR:N	2.08	0.68
1:B:6:DC:H2'	2:C:19:DC:C5	2.29	0.68
2:C:16:DC:H5'	2:C:17:DA:N3	2.09	0.68
3:A:380:LYS:O	3:A:381:GLN:C	2.26	0.68
3:A:139:ASN:HD22	3:A:140:LEU:N	1.91	0.68
1:B:11:DT:N3	2:C:17:DA:H2''	2.10	0.67
3:A:69:ARG:HH22	3:A:202:PRO:HG3	1.59	0.67
3:A:578:ILE:HD12	3:A:578:ILE:N	2.02	0.67
3:A:103:ALA:HB3	3:A:219:ARG:HD2	1.77	0.67
3:A:417:ALA:CB	3:A:418:PRO:HD2	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:285:THR:HG22	3:A:286:ASN:N	2.08	0.67
3:A:468:ILE:O	3:A:486:PRO:HD2	1.95	0.66
3:A:65:ALA:HB3	3:A:531:LEU:HB3	1.77	0.66
1:B:3:DA:H2''	1:B:4:DT:OP2	1.94	0.66
3:A:385:ASN:HA	3:A:573:GLN:HB3	1.78	0.65
3:A:579:THR:O	3:A:580:ARG:HB2	1.95	0.65
3:A:584:ARG:CG	3:A:585:ASN:H	2.10	0.65
3:A:236:VAL:HG12	3:A:237:MET:N	2.12	0.65
1:B:12:DC:O3'	1:B:13:DA:H4'	1.96	0.65
1:B:13:DA:H1'	5:B:231:D5M:N6	2.12	0.65
3:A:228:GLN:CG	3:A:229:GLU:N	2.60	0.64
3:A:234:HIS:ND1	3:A:234:HIS:N	2.46	0.64
3:A:44:THR:OG1	3:A:148:PHE:HB2	1.97	0.64
3:A:380:LYS:O	3:A:382:HIS:N	2.29	0.64
3:A:463:TYR:CD2	3:A:464:PRO:HD3	2.33	0.64
3:A:586:THR:CB	3:A:586:THR:N	2.60	0.64
3:A:185:ILE:HD13	3:A:254:GLN:HE22	1.63	0.64
3:A:380:LYS:H	3:A:384:GLU:CB	2.08	0.64
3:A:279:LEU:C	3:A:580:ARG:HG2	2.18	0.64
3:A:551:VAL:HG12	3:A:552:GLU:H	1.61	0.63
3:A:339:CYS:N	3:A:449:SER:HB3	2.07	0.63
3:A:186:LEU:H	3:A:186:LEU:CD1	2.11	0.63
3:A:200:PHE:HE2	3:A:465:GLN:H	1.47	0.63
3:A:159:ASP:HB2	3:A:165:ILE:CG2	2.27	0.63
3:A:217:VAL:HG23	3:A:218:ASP:H	1.63	0.63
3:A:219:ARG:HG2	3:A:220:ASP:N	2.14	0.62
3:A:183:ASN:HB2	3:A:185:ILE:HD11	1.81	0.62
3:A:194:SER:O	3:A:195:MET:C	2.38	0.62
3:A:465:GLN:OE1	3:A:576:PRO:HG3	2.00	0.62
3:A:92:THR:HB	3:A:235:ASN:ND2	2.15	0.62
1:B:10:DA:H1'	1:B:12:DC:H2'	1.82	0.62
3:A:186:LEU:N	3:A:186:LEU:CD1	2.63	0.62
3:A:143:LEU:HD12	3:A:144:ASP:H	1.65	0.61
3:A:190:PRO:HB3	3:A:467:GLN:NE2	2.15	0.61
3:A:239:THR:HB	3:A:240:PRO:HD2	1.80	0.61
3:A:280:THR:N	3:A:580:ARG:HG2	2.15	0.61
3:A:493:ALA:HB1	3:A:494:PRO:CD	2.30	0.61
3:A:89:THR:HA	3:A:92:THR:OG1	2.01	0.61
1:B:7:DT:O2	1:B:7:DT:H2'	2.00	0.61
3:A:434:PRO:HB3	3:A:438:LYS:O	2.00	0.60
3:A:49:ASN:ND2	3:A:69:ARG:HH21	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:210:PRO:O	3:A:212:ARG:NH1	2.35	0.60
3:A:50:GLN:O	3:A:66:LEU:HB2	2.01	0.60
3:A:584:ARG:O	3:A:585:ASN:HB2	2.02	0.60
3:A:380:LYS:HG2	3:A:384:GLU:HG2	1.83	0.60
3:A:566:PRO:HG3	3:A:572:MET:CE	2.30	0.60
3:A:464:PRO:CD	3:A:576:PRO:HA	2.32	0.60
3:A:143:LEU:HD12	3:A:144:ASP:N	2.17	0.59
3:A:138:LEU:HD11	3:A:533:MET:HB3	1.84	0.59
3:A:551:VAL:HG12	3:A:552:GLU:N	2.17	0.58
3:A:578:ILE:CD1	3:A:578:ILE:H	1.95	0.58
3:A:94:VAL:HB	3:A:97:ASN:HB2	1.85	0.58
3:A:111:TRP:CE3	3:A:500:ARG:HB3	2.39	0.58
3:A:70:LEU:HD12	3:A:71:VAL:N	2.19	0.58
3:A:380:LYS:CG	3:A:384:GLU:HG2	2.33	0.58
3:A:139:ASN:ND2	3:A:140:LEU:N	2.52	0.58
3:A:153:LYS:HB2	3:A:522:TYR:CE2	2.39	0.58
3:A:386:TRP:HB2	3:A:571:ASN:HB3	1.86	0.57
3:A:158:GLN:CG	3:A:159:ASP:H	2.01	0.57
3:A:170:ASN:ND2	3:A:170:ASN:H	2.02	0.57
3:A:363:THR:CG2	3:A:364:GLN:N	2.58	0.57
1:B:8:DC:H42	3:A:55:PHE:HE2	1.51	0.57
3:A:228:GLN:CG	3:A:229:GLU:H	2.18	0.57
3:A:124:GLN:HG2	3:A:125:PRO:HD2	1.86	0.57
3:A:383:GLY:O	3:A:384:GLU:O	2.23	0.57
3:A:165:ILE:HG13	3:A:166:LYS:N	2.18	0.57
3:A:218:ASP:OD2	3:A:349:ARG:HB3	2.04	0.57
3:A:49:ASN:HA	3:A:66:LEU:O	2.04	0.57
3:A:72:HIS:O	3:A:207:ILE:HG22	2.05	0.57
3:A:73:LEU:HD12	3:A:74:ASN:N	2.20	0.57
3:A:430:THR:H	3:A:433:ASN:HD22	1.49	0.57
3:A:155:VAL:HG22	3:A:520:VAL:HG11	1.86	0.57
1:B:11:DT:H4'	1:B:12:DC:H5'	1.87	0.57
3:A:153:LYS:HA	3:A:170:ASN:HA	1.87	0.57
3:A:339:CYS:HB2	3:A:449:SER:HB2	1.87	0.57
3:A:215:PHE:HE1	3:A:245:SER:HA	1.69	0.56
3:A:139:ASN:ND2	3:A:140:LEU:H	2.02	0.56
3:A:562:THR:CA	3:A:565:LEU:HD12	2.35	0.56
3:A:190:PRO:O	3:A:193:ASN:HB2	2.06	0.56
3:A:414:ILE:HG13	3:A:443:PHE:HE2	1.69	0.56
3:A:141:VAL:HB	3:A:532:THR:OG1	2.05	0.56
3:A:584:ARG:CG	3:A:585:ASN:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:63:ILE:N	3:A:63:ILE:HD12	2.20	0.56
3:A:546:VAL:HG22	3:A:547:TYR:N	2.21	0.56
3:A:46:SER:O	3:A:528:LYS:HE2	2.06	0.56
1:B:8:DC:H2''	1:B:9:DT:O5'	2.06	0.56
3:A:140:LEU:HD13	3:A:487:PHE:CE2	2.40	0.55
1:B:12:DC:H1'	1:B:13:DA:H4'	1.89	0.55
3:A:464:PRO:HG2	3:A:465:GLN:NE2	2.21	0.55
3:A:500:ARG:HG3	3:A:501:LEU:O	2.06	0.55
3:A:75:MET:HG3	3:A:521:THR:O	2.06	0.55
3:A:560:SER:O	3:A:561:VAL:C	2.44	0.55
3:A:49:ASN:ND2	3:A:68:THR:H	1.99	0.55
3:A:380:LYS:HD3	3:A:384:GLU:HB3	1.89	0.55
3:A:467:GLN:OE1	3:A:484:THR:HG22	2.07	0.55
3:A:560:SER:O	3:A:563:LYS:HG3	2.06	0.55
3:A:581:PRO:HG2	3:A:582:VAL:HG23	1.88	0.55
3:A:49:ASN:ND2	3:A:67:ALA:HA	2.22	0.55
3:A:584:ARG:HG2	3:A:585:ASN:H	1.71	0.55
3:A:138:LEU:HD12	3:A:139:ASN:H	1.72	0.55
3:A:383:GLY:C	3:A:384:GLU:O	2.42	0.55
1:B:8:DC:OP1	1:B:8:DC:H3'	2.06	0.55
3:A:144:ASP:HB2	3:A:530:LYS:HZ2	1.72	0.54
3:A:67:ALA:O	3:A:528:LYS:HA	2.07	0.54
1:B:12:DC:O5'	5:B:231:D5M:H5'2	2.06	0.54
3:A:285:THR:OG1	3:A:404:GLY:HA2	2.07	0.54
3:A:363:THR:HG21	3:A:408:ASP:HB2	1.88	0.54
3:A:69:ARG:NH1	3:A:199:GLY:O	2.40	0.54
3:A:49:ASN:HD21	3:A:69:ARG:HH21	1.55	0.54
3:A:144:ASP:OD1	3:A:267:THR:HG22	2.07	0.54
3:A:232:ILE:O	3:A:234:HIS:N	2.41	0.54
3:A:145:GLN:H	3:A:267:THR:CG2	2.20	0.54
3:A:219:ARG:HH21	3:A:221:LEU:HB2	1.73	0.54
3:A:192:ALA:C	3:A:194:SER:H	2.11	0.53
3:A:546:VAL:HG21	3:A:582:VAL:HG13	1.89	0.53
3:A:185:ILE:H	3:A:185:ILE:CD1	2.19	0.53
3:A:72:HIS:HE1	3:A:74:ASN:ND2	2.07	0.53
3:A:119:TRP:O	3:A:121:VAL:N	2.41	0.53
3:A:297:THR:HB	3:A:307:THR:H	1.73	0.53
3:A:280:THR:HB	3:A:584:ARG:HB2	1.90	0.53
1:B:6:DC:N4	2:C:18:DC:H4'	2.23	0.53
3:A:251:GLU:OE1	3:A:251:GLU:N	2.41	0.53
3:A:347:ALA:HB2	3:A:352:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:155:VAL:HG12	3:A:168:TYR:CD1	2.43	0.52
3:A:463:TYR:CG	3:A:464:PRO:N	2.76	0.52
1:B:9:DT:H2''	1:B:10:DA:C8	2.44	0.52
3:A:294:LEU:HD13	3:A:295:LEU:N	2.25	0.52
3:A:443:PHE:CD1	3:A:444:SER:N	2.78	0.52
3:A:475:LEU:O	3:A:477:HIS:N	2.43	0.52
3:A:530:LYS:HE2	3:A:532:THR:HG23	1.92	0.52
3:A:98:MET:C	3:A:100:LYS:H	2.13	0.51
3:A:384:GLU:O	3:A:573:GLN:HB3	2.10	0.51
3:A:178:VAL:HG12	3:A:179:ALA:N	2.25	0.51
3:A:472:GLU:OE1	3:A:473:LEU:N	2.41	0.51
1:B:14:DC:H2'	1:B:14:DC:O2	2.09	0.51
3:A:249:THR:HG23	3:A:252:ASN:HB2	1.93	0.51
1:B:13:DA:H2'	2:C:23:DA:H4'	1.93	0.51
3:A:400:GLU:HG3	3:A:402:ASN:OD1	2.11	0.51
3:A:84:ILE:O	3:A:105:GLU:HG3	2.10	0.51
3:A:118:ALA:O	3:A:119:TRP:C	2.48	0.51
3:A:510:ASP:H	3:A:516:LEU:HD11	1.75	0.51
2:C:19:DC:OP2	2:C:19:DC:H3'	2.11	0.51
3:A:367:ASP:HB3	3:A:370:ALA:CB	2.39	0.50
3:A:301:ALA:C	3:A:303:THR:H	2.14	0.50
3:A:277:VAL:HG23	3:A:487:PHE:CE1	2.47	0.50
3:A:326:SER:OG	3:A:329:ILE:HG12	2.11	0.50
3:A:206:THR:CB	3:A:381:GLN:HE22	2.24	0.50
1:B:13:DA:N6	2:C:22:DA:H2	2.09	0.50
3:A:98:MET:HE1	3:A:224:THR:H	1.76	0.50
3:A:542:THR:OG1	3:A:543:TRP:N	2.45	0.50
3:A:218:ASP:HA	3:A:349:ARG:O	2.12	0.50
3:A:186:LEU:HB3	3:A:211:TYR:OH	2.12	0.49
3:A:380:LYS:NZ	3:A:388:ALA:N	2.51	0.49
3:A:425:LEU:C	3:A:427:GLY:H	2.15	0.49
3:A:396:TYR:CD2	3:A:576:PRO:HG2	2.47	0.49
3:A:155:VAL:HG22	3:A:520:VAL:CG1	2.42	0.49
3:A:190:PRO:HB3	3:A:467:GLN:HE22	1.77	0.49
3:A:348:SER:O	3:A:350:ALA:N	2.45	0.49
3:A:287:ARG:HE	3:A:327:GLU:HB3	1.78	0.49
3:A:500:ARG:HH21	3:A:503:PRO:HD3	1.78	0.48
3:A:56:LEU:CD1	3:A:56:LEU:N	2.67	0.48
1:B:13:DA:H62	2:C:22:DA:H2	1.61	0.48
2:C:19:DC:H4'	2:C:20:DA:OP1	2.13	0.48
3:A:421:VAL:CB	3:A:422:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:DT:C2	2:C:17:DA:H2''	2.47	0.48
3:A:232:ILE:O	3:A:233:GLU:C	2.52	0.48
2:C:21:DA:H2''	2:C:22:DA:O5'	2.13	0.48
3:A:92:THR:CB	3:A:235:ASN:HD21	2.20	0.48
3:A:275:ASN:ND2	3:A:490:LYS:HE2	2.29	0.48
3:A:469:TRP:HA	3:A:487:PHE:O	2.13	0.48
3:A:475:LEU:O	3:A:478:LYS:HD3	2.13	0.48
3:A:135:MET:SD	3:A:537:LEU:HD23	2.54	0.48
3:A:236:VAL:CG1	3:A:237:MET:N	2.77	0.48
3:A:579:THR:O	3:A:580:ARG:CB	2.59	0.48
2:C:22:DA:H4'	2:C:23:DA:H5'	1.95	0.48
3:A:158:GLN:CG	3:A:159:ASP:N	2.71	0.48
3:A:414:ILE:HG13	3:A:443:PHE:CE2	2.48	0.47
3:A:562:THR:HA	3:A:565:LEU:CD1	2.43	0.47
3:A:429:LEU:C	3:A:429:LEU:HD23	2.34	0.47
3:A:543:TRP:CD1	3:A:543:TRP:C	2.86	0.47
3:A:45:GLY:HA3	3:A:148:PHE:CE2	2.49	0.47
3:A:73:LEU:HD12	3:A:74:ASN:H	1.78	0.47
3:A:481:LEU:HD12	3:A:482:HIS:N	2.29	0.47
1:B:12:DC:H1'	1:B:13:DA:C4'	2.44	0.47
2:C:22:DA:H4'	2:C:23:DA:C5'	2.44	0.47
3:A:215:PHE:CE1	3:A:245:SER:HA	2.49	0.47
3:A:586:THR:O	3:A:587:TYR:HB2	2.15	0.47
3:A:227:ASN:N	3:A:227:ASN:C	2.58	0.47
3:A:425:LEU:HD13	3:A:425:LEU:C	2.34	0.47
3:A:47:TYR:HA	3:A:68:THR:HG21	1.95	0.47
1:B:12:DC:H4'	1:B:14:DC:OP1	2.14	0.47
3:A:113:LEU:HD23	3:A:114:VAL:H	1.80	0.47
3:A:267:THR:HG23	3:A:268:GLY:N	2.30	0.47
3:A:371:ASN:HD21	3:A:407:ARG:H	1.62	0.47
3:A:322:VAL:HB	3:A:324:TRP:HE1	1.76	0.46
3:A:71:VAL:O	3:A:524:THR:HA	2.15	0.46
3:A:219:ARG:HG3	3:A:219:ARG:NH1	2.29	0.46
3:A:408:ASP:OD2	3:A:410:ARG:HD3	2.15	0.46
3:A:111:TRP:CD1	3:A:250:ILE:HG13	2.51	0.46
3:A:124:GLN:O	3:A:125:PRO:C	2.54	0.46
3:A:219:ARG:HG2	3:A:220:ASP:H	1.78	0.46
3:A:301:ALA:O	3:A:303:THR:N	2.49	0.46
3:A:373:SER:OG	3:A:399:ASP:HA	2.15	0.46
3:A:562:THR:N	3:A:565:LEU:HD12	2.31	0.46
3:A:75:MET:HB3	3:A:518:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:530:LYS:HZ2	3:A:530:LYS:HB3	1.80	0.46
3:A:98:MET:HE2	3:A:98:MET:HB3	1.93	0.46
3:A:135:MET:HB2	3:A:279:LEU:HD12	1.96	0.46
3:A:215:PHE:CD1	3:A:216:CYS:N	2.83	0.46
3:A:121:VAL:CG1	3:A:122:TRP:CD1	2.98	0.45
3:A:178:VAL:CG1	3:A:179:ALA:N	2.79	0.45
3:A:192:ALA:C	3:A:194:SER:N	2.69	0.45
3:A:206:THR:OG1	3:A:207:ILE:N	2.49	0.45
3:A:280:THR:OG1	3:A:584:ARG:HD3	2.16	0.45
3:A:430:THR:H	3:A:433:ASN:HD21	1.54	0.45
3:A:464:PRO:HG2	3:A:465:GLN:CD	2.36	0.45
3:A:334:ALA:HB1	3:A:453:LEU:O	2.15	0.45
3:A:66:LEU:HA	3:A:66:LEU:HD23	1.48	0.45
3:A:234:HIS:C	3:A:234:HIS:N	2.68	0.45
3:A:340:GLN:HA	3:A:341:PRO:HD3	1.83	0.45
3:A:284:GLN:HE22	3:A:587:TYR:HB3	1.81	0.45
3:A:40:VAL:HG22	3:A:41:GLY:H	1.82	0.45
3:A:480:ARG:O	3:A:481:LEU:CB	2.62	0.45
3:A:75:MET:HB3	3:A:518:ARG:NH1	2.31	0.45
3:A:363:THR:O	3:A:366:MET:N	2.43	0.45
3:A:386:TRP:HE3	3:A:571:ASN:HA	1.80	0.45
3:A:109:THR:OG1	3:A:211:TYR:HB3	2.17	0.45
3:A:540:ASN:HD22	3:A:541:THR:N	2.15	0.45
3:A:181:ASP:CG	3:A:186:LEU:HD13	2.38	0.45
3:A:188:TYR:HA	3:A:496:GLN:NE2	2.32	0.45
3:A:87:HIS:CE1	3:A:219:ARG:HH12	2.35	0.44
1:B:13:DA:N6	2:C:22:DA:C2	2.81	0.44
3:A:217:VAL:HG23	3:A:218:ASP:N	2.31	0.44
3:A:326:SER:O	3:A:327:GLU:C	2.56	0.44
3:A:433:ASN:HA	3:A:434:PRO:HD3	1.66	0.44
3:A:499:VAL:HG12	3:A:500:ARG:N	2.33	0.44
2:C:16:DC:H5'	2:C:17:DA:C2	2.52	0.44
3:A:45:GLY:CA	3:A:148:PHE:CD2	3.00	0.44
3:A:368:ARG:HH11	3:A:368:ARG:HG2	1.81	0.44
1:B:5:DC:C4	1:B:11:DT:H73	2.53	0.44
3:A:113:LEU:O	3:A:208:ALA:HB1	2.18	0.44
3:A:423:PRO:HA	3:A:424:PRO:HD3	1.87	0.44
3:A:513:GLY:O	3:A:514:ALA:C	2.55	0.44
1:B:12:DC:O4'	1:B:12:DC:O2	2.35	0.44
3:A:185:ILE:HB	3:A:186:LEU:HD12	1.99	0.44
3:A:438:LYS:HA	3:A:438:LYS:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:159:ASP:CB	3:A:165:ILE:HG22	2.39	0.43
3:A:368:ARG:C	3:A:370:ALA:N	2.71	0.43
3:A:98:MET:C	3:A:100:LYS:N	2.72	0.43
3:A:83:ARG:HD2	3:A:105:GLU:OE2	2.18	0.43
1:B:13:DA:H1'	5:B:231:D5M:HN61	1.82	0.43
3:A:138:LEU:HD12	3:A:139:ASN:N	2.32	0.43
3:A:170:ASN:ND2	3:A:170:ASN:N	2.63	0.43
3:A:410:ARG:HD2	3:A:410:ARG:H	1.83	0.43
3:A:456:PHE:N	3:A:456:PHE:CD1	2.85	0.43
1:B:11:DT:C4	2:C:17:DA:H2''	2.54	0.43
3:A:419:LEU:HD12	3:A:419:LEU:HA	1.61	0.43
3:A:98:MET:HE1	3:A:224:THR:N	2.34	0.43
3:A:288:GLN:N	3:A:288:GLN:OE1	2.52	0.43
3:A:322:VAL:HB	3:A:324:TRP:CD1	2.54	0.43
3:A:285:THR:HG23	3:A:404:GLY:O	2.19	0.43
3:A:546:VAL:CG2	3:A:547:TYR:N	2.82	0.43
1:B:10:DA:N3	1:B:12:DC:H2'	2.34	0.43
1:B:9:DT:O2	3:A:52:HIS:HB3	2.19	0.43
3:A:561:VAL:CG2	3:A:562:THR:H	2.19	0.43
3:A:285:THR:CG2	3:A:286:ASN:N	2.77	0.42
3:A:463:TYR:CD2	3:A:464:PRO:CD	3.02	0.42
3:A:123:LEU:HD12	3:A:128:TRP:HE3	1.84	0.42
3:A:219:ARG:CG	3:A:219:ARG:NH1	2.81	0.42
3:A:206:THR:HB	3:A:381:GLN:NE2	2.33	0.42
3:A:510:ASP:H	3:A:516:LEU:CD1	2.32	0.42
3:A:551:VAL:HG12	3:A:561:VAL:H	1.84	0.42
3:A:55:PHE:C	3:A:56:LEU:HD12	2.39	0.42
3:A:74:ASN:N	3:A:74:ASN:OD1	2.53	0.42
3:A:202:PRO:HD2	3:A:203:TRP:CE3	2.54	0.42
3:A:309:THR:HG22	3:A:310:ALA:N	2.35	0.42
3:A:154:THR:HG22	3:A:520:VAL:O	2.18	0.42
3:A:285:THR:O	3:A:288:GLN:OE1	2.38	0.42
3:A:338:PHE:CD1	3:A:338:PHE:N	2.86	0.42
3:A:368:ARG:O	3:A:370:ALA:N	2.53	0.42
3:A:70:LEU:HD11	3:A:524:THR:HB	2.01	0.42
3:A:348:SER:OG	3:A:349:ARG:N	2.52	0.42
3:A:430:THR:N	3:A:433:ASN:ND2	2.48	0.42
3:A:109:THR:C	3:A:111:TRP:H	2.24	0.42
3:A:348:SER:C	3:A:350:ALA:H	2.23	0.42
3:A:380:LYS:NZ	3:A:386:TRP:CA	2.82	0.42
3:A:553:ASP:O	3:A:555:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:VAL:HG12	3:A:95:LYS:N	2.35	0.42
3:A:138:LEU:CD1	3:A:533:MET:HB3	2.50	0.41
3:A:327:GLU:OE1	3:A:327:GLU:HA	2.20	0.41
3:A:364:GLN:O	3:A:366:MET:N	2.53	0.41
3:A:190:PRO:O	3:A:193:ASN:CB	2.68	0.41
3:A:463:TYR:HD2	3:A:464:PRO:HD3	1.83	0.41
3:A:88:ASN:OD1	3:A:88:ASN:N	2.52	0.41
2:C:15:DA:H1'	2:C:16:DC:H5''	2.01	0.41
3:A:577:LEU:HD23	3:A:577:LEU:HA	1.77	0.41
3:A:116:ALA:O	3:A:121:VAL:HG11	2.21	0.41
3:A:111:TRP:CG	3:A:250:ILE:HG13	2.55	0.41
3:A:57:GLY:C	3:A:59:GLY:N	2.72	0.41
3:A:250:ILE:HB	3:A:251:GLU:OE1	2.20	0.41
3:A:297:THR:HB	3:A:307:THR:HG23	2.03	0.41
1:B:6:DC:OP2	2:C:19:DC:N4	2.54	0.41
3:A:410:ARG:CD	3:A:410:ARG:H	2.33	0.41
3:A:155:VAL:HG12	3:A:168:TYR:HD1	1.83	0.41
3:A:234:HIS:CG	3:A:234:HIS:N	2.88	0.41
3:A:279:LEU:CA	3:A:580:ARG:HG2	2.50	0.41
3:A:279:LEU:HA	3:A:580:ARG:HG2	2.02	0.41
3:A:284:GLN:OE1	3:A:586:THR:N	2.54	0.41
3:A:348:SER:C	3:A:350:ALA:N	2.74	0.41
3:A:403:PHE:C	3:A:405:SER:H	2.23	0.41
3:A:386:TRP:CE3	3:A:571:ASN:HA	2.54	0.41
3:A:471:LYS:HG2	3:A:472:GLU:N	2.35	0.41
3:A:344:ASP:O	3:A:346:GLU:HG3	2.20	0.41
3:A:140:LEU:HD22	3:A:487:PHE:CG	2.56	0.41
3:A:516:LEU:N	3:A:516:LEU:HD23	2.36	0.41
3:A:493:ALA:CB	3:A:494:PRO:CD	2.97	0.40
3:A:197:THR:OG1	3:A:198:LEU:N	2.55	0.40
3:A:478:LYS:HB3	3:A:479:PRO:CD	2.43	0.40
3:A:481:LEU:HD12	3:A:482:HIS:C	2.42	0.40
3:A:283:TRP:O	3:A:404:GLY:HA3	2.22	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	547/587 (93%)	432 (79%)	74 (14%)	41 (8%)	1	11

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	218	ASP
3	A	226	GLU
3	A	233	GLU
3	A	380	LYS
3	A	381	GLN
3	A	417	ALA
3	A	418	PRO
3	A	424	PRO
3	A	463	TYR
3	A	542	THR
3	A	561	VAL
3	A	120	GLY
3	A	164	ALA
3	A	232	ILE
3	A	302	ASP
3	A	349	ARG
3	A	384	GLU
3	A	428	ILE
3	A	476	GLU
3	A	481	LEU
3	A	514	ALA
3	A	553	ASP
3	A	554	ASN
3	A	585	ASN
3	A	98	MET
3	A	163	GLN
3	A	480	ARG
3	A	543	TRP

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Mol	Chain	Res	Type
3	A	562	THR
3	A	403	PHE
3	A	422	PRO
3	A	425	LEU
3	A	459	PRO
3	A	545	PRO
3	A	228	GLN
3	A	421	VAL
3	A	580	ARG
3	A	205	PRO
3	A	125	PRO
3	A	291	GLN
3	A	486	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	472/492 (96%)	423 (90%)	49 (10%)	7 31

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	40	VAL
3	A	56	LEU
3	A	69	ARG
3	A	74	ASN
3	A	77	LYS
3	A	79	GLU
3	A	80	ASN
3	A	113	LEU
3	A	139	ASN
3	A	140	LEU
3	A	170	ASN
3	A	188	TYR
3	A	193	ASN

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Mol	Chain	Res	Type
3	A	219	ARG
3	A	224	THR
3	A	234	HIS
3	A	249	THR
3	A	264	GLU
3	A	267	THR
3	A	288	GLN
3	A	294	LEU
3	A	319	GLN
3	A	320	MET
3	A	338	PHE
3	A	359	PRO
3	A	366	MET
3	A	368	ARG
3	A	377	SER
3	A	385	ASN
3	A	386	TRP
3	A	401	THR
3	A	409	THR
3	A	411	ASP
3	A	415	GLN
3	A	437	THR
3	A	440	ASP
3	A	443	PHE
3	A	476	GLU
3	A	483	ILE
3	A	500	ARG
3	A	512	ASN
3	A	516	LEU
3	A	530	LYS
3	A	540	ASN
3	A	541	THR
3	A	562	THR
3	A	572	MET
3	A	578	ILE
3	A	584	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	49	ASN
3	A	50	GLN

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Mol	Chain	Res	Type
3	A	72	HIS
3	A	87	HIS
3	A	139	ASN
3	A	149	ASN
3	A	170	ASN
3	A	193	ASN
3	A	235	ASN
3	A	246	GLN
3	A	275	ASN
3	A	286	ASN
3	A	335	GLN
3	A	371	ASN
3	A	381	GLN
3	A	431	ASN
3	A	433	ASN
3	A	448	ASN
3	A	458	HIS
3	A	492	ASN
3	A	496	GLN
3	A	540	ASN
3	A	544	ASN
3	A	571	ASN
3	A	573	GLN
3	A	585	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	D5M	B	231	-	18,20,24	0.59	0	17,29,36	0.74	1 (5%)

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
5	D5M	B	231	-	-	0/2/18/22	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	231	D5M	C5-C6-N6	2.13	123.59	120.35

There are no chirality outliers.

There are no torsion outliers.

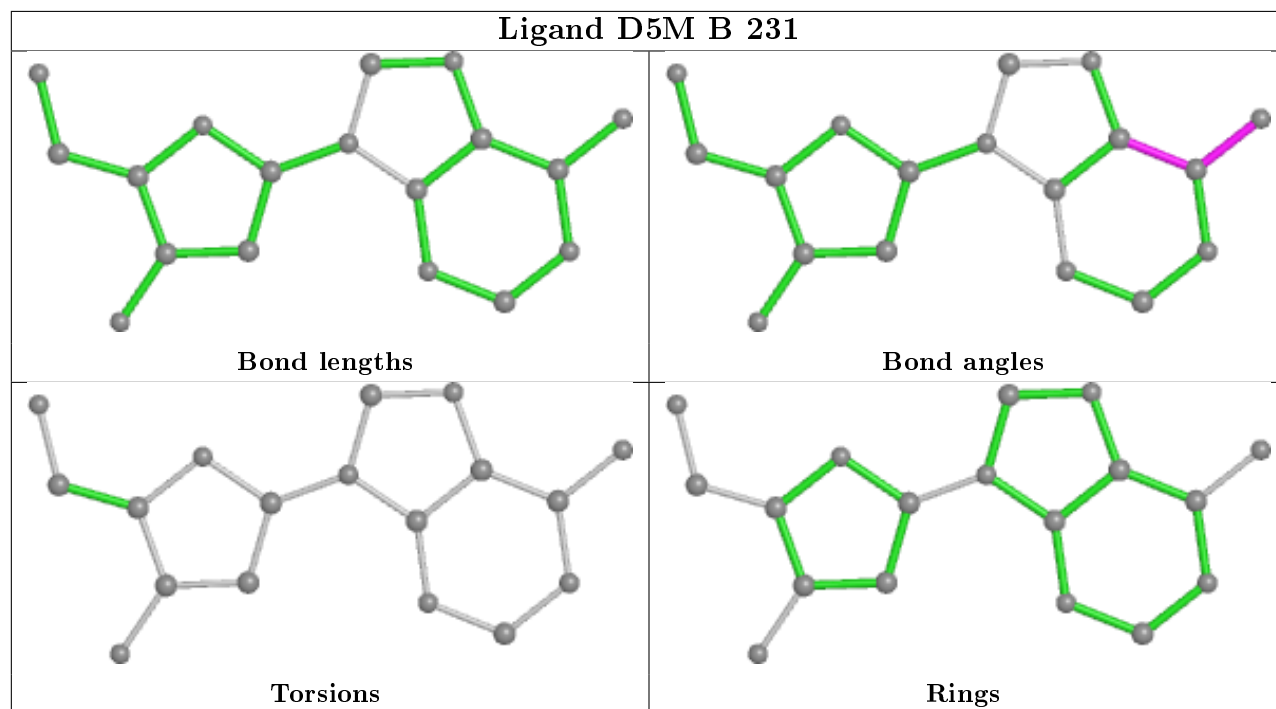
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	231	D5M	3	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.