



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:01 PM UTC

PDB ID : 1HAP / pdb_00001hap
Title : COMPLEX OF HUMAN ALPHA-THROMBIN WITH A 15MER OLIGONUCLEOTIDE GGTTGGTGTGGTTGG (BASED ON X-RAY MODEL OF DNA)
Authors : Padmanabhan, K.; Tulinsky, A.
Deposited on : 1995-10-03
Resolution : 2.80 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)
Xtrriage (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

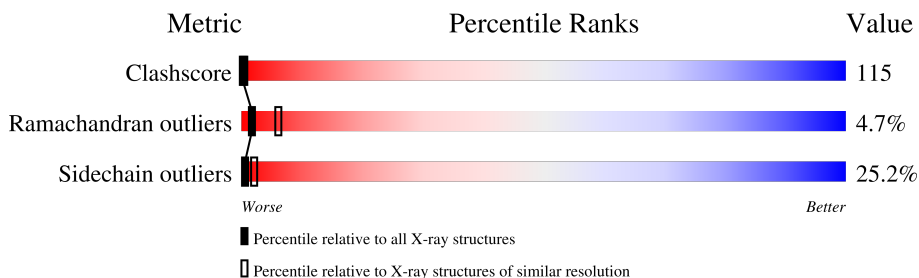
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	D	15	20% 73% 7%
2	L	36	28% 39% 6% 25%
3	H	259	6% 31% 50% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OG6	H	297	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2771 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(*GP*GP*TP*TP*GP*GP*TP*GP*TP*GP*GP*TP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	D	15	315	150	57	94	14	0	0	0

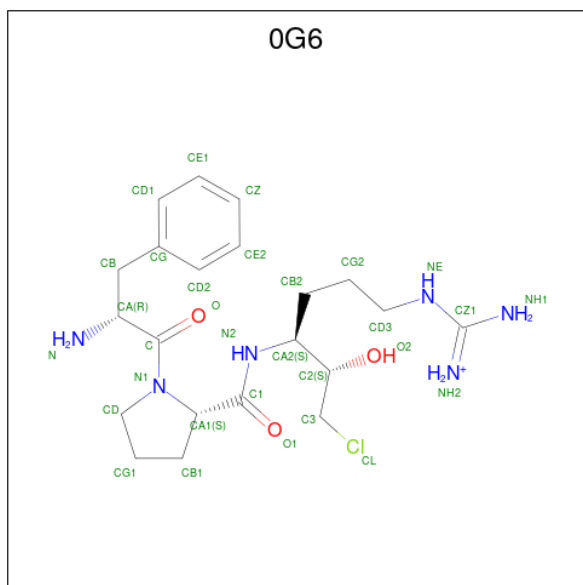
- Molecule 2 is a protein called Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	27	222	140	36	45	1	0	0	0

- Molecule 3 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	253	2053	1310	362	367	14	0	0	0

- Molecule 4 is D-phenylalanyl-N-[(2S,3S)-6-{{[amino(iminio)methyl]amino}}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	30	21	6	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	16	Total	O	0	0
			16	16		
5	L	10	Total	O	0	0
			10	10		
5	H	125	Total	O	0	0
			125	125		

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: 5'-D>(*GP*GP*TP*TP*GP*GP*TP*GP*TP*GP*GP*TP*TP*GP*G)-3'

Chain D: 



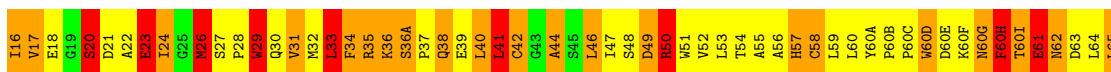
- Molecule 2: Thrombin light chain

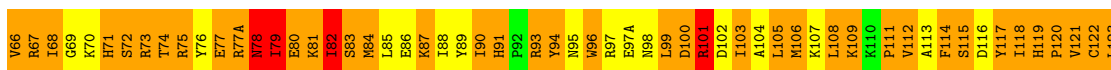
Chain L: 



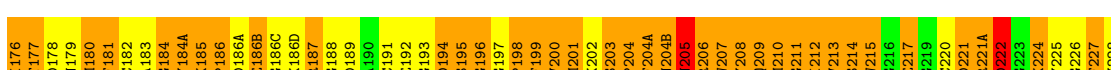
- Molecule 3: Thrombin heavy chain

Chain H: 











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	58.28Å 77.61Å 100.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	68.0 (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLIN, PROLSQ	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2771	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: 0G6

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	D	0.93	0/353	2.94	41/547 (7.5%)
2	L	1.21	2/224 (0.9%)	2.64	24/298 (8.1%)
3	H	1.28	7/2107 (0.3%)	2.88	255/2846 (9.0%)
All	All	1.23	9/2684 (0.3%)	2.87	320/3691 (8.7%)

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	D	0	1
2	L	0	1
3	H	0	2
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	220	CYS	CA-C	-5.81	1.46	1.52
3	H	141	TRP	NE1-CE2	-5.79	1.31	1.37
3	H	44	ALA	C-N	-5.65	1.25	1.33
3	H	50	ARG	C-N	-5.54	1.25	1.33
3	H	60(D)	TRP	C-N	-5.49	1.21	1.34
2	L	10	LYS	N-CA	5.23	1.52	1.46
2	L	7	PHE	C-N	-5.22	1.27	1.33
3	H	100	ASP	N-CA	5.22	1.52	1.46
3	H	96	TRP	C-N	-5.03	1.27	1.33

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	404	DT	P-O3'-C3'	21.05	151.78	120.20
1	D	405	DG	P-O3'-C3'	15.01	142.72	120.20
3	H	160	LEU	O-C-N	14.36	135.50	121.57
3	H	170	ASP	CA-CB-CG	-14.14	98.45	112.60
3	H	62	ASN	CA-CB-CG	13.87	126.47	112.60
1	D	414	DG	P-O5'-C5'	13.59	140.39	120.00
3	H	63	ASP	CA-CB-CG	12.01	124.61	112.60
3	H	237	TRP	N-CA-C	-11.89	98.30	111.14
1	D	401	DG	O5'-C5'-C4'	11.69	128.33	110.80
3	H	242	ILE	O-C-N	11.58	133.75	121.83
3	H	18	GLU	CA-C-O	-11.57	108.11	121.65
1	D	404	DT	C5'-C4'-O4'	-11.46	92.20	109.40
1	D	404	DT	C5'-C4'-C3'	11.36	131.94	114.90
3	H	194	ASP	N-CA-C	11.12	123.40	111.28
3	H	221(A)	ARG	O-C-N	10.88	135.78	123.16
3	H	17	VAL	CA-C-N	10.78	137.32	122.34
3	H	17	VAL	C-N-CA	10.78	137.32	122.34
1	D	403	DT	O3'-P-O5'	10.77	120.16	104.00
3	H	35	ARG	CD-NE-CZ	10.75	139.45	124.40
1	D	415	DG	P-O5'-C5'	10.63	135.94	120.00
1	D	403	DT	C4'-C3'-O3'	10.54	125.82	110.00
3	H	31	VAL	O-C-N	10.34	134.16	123.10
1	D	404	DT	C4'-C3'-O3'	10.34	125.50	110.00
3	H	83	SER	CA-C-N	10.30	137.55	122.41
3	H	83	SER	C-N-CA	10.30	137.55	122.41
1	D	413	DT	P-O5'-C5'	10.16	135.25	120.00
3	H	193	GLY	CA-C-N	10.08	133.78	120.28
3	H	193	GLY	C-N-CA	10.08	133.78	120.28
3	H	153	SER	N-CA-C	-9.82	101.30	113.28
3	H	207	TRP	CA-C-O	-9.62	109.93	121.28
3	H	65	LEU	CA-C-O	-9.45	109.26	120.60
3	H	184	GLY	N-CA-C	9.42	124.88	110.18
2	L	14(G)	LEU	CB-CA-C	9.41	126.96	110.01
2	L	14(B)	THR	N-CA-CB	-9.37	98.53	111.00
3	H	221(A)	ARG	CA-C-O	-9.37	110.15	120.92
3	H	106	MET	CA-C-O	-9.27	109.49	120.43
3	H	242	ILE	N-CA-C	-9.15	101.48	110.72
3	H	135	LYS	CA-C-N	9.11	130.74	121.35
3	H	135	LYS	C-N-CA	9.11	130.74	121.35
3	H	173	ARG	CA-C-N	-9.06	107.76	120.35
3	H	173	ARG	C-N-CA	-9.06	107.76	120.35
3	H	230	HIS	CA-CB-CG	9.06	122.86	113.80
3	H	210	MET	CA-C-O	8.98	130.31	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	91	HIS	O-C-N	8.97	130.93	121.42
3	H	33	LEU	CB-CA-C	8.78	124.23	109.75
3	H	194	ASP	CA-CB-CG	-8.75	103.85	112.60
3	H	207	TRP	O-C-N	8.72	133.13	123.10
2	L	14(I)	SER	N-CA-CB	-8.67	97.33	110.07
3	H	156	GLN	O-C-N	8.65	133.05	123.10
3	H	41	LEU	CB-CA-C	8.63	124.16	109.65
3	H	196	GLY	CA-C-O	8.62	128.50	119.10
3	H	212	ILE	CA-C-O	-8.62	112.32	121.19
3	H	105	LEU	N-CA-C	-8.59	97.75	110.46
3	H	184(A)	TYR	CA-C-O	-8.58	111.05	120.92
3	H	160	LEU	CA-C-O	-8.33	110.50	120.41
3	H	157	VAL	CA-C-O	-8.27	111.41	120.67
3	H	18	GLU	O-C-N	8.24	132.47	122.58
3	H	133	GLY	N-CA-C	-8.24	103.98	114.37
1	D	414	DG	O3'-P-O5'	8.19	116.28	104.00
3	H	101	ARG	O-C-N	8.17	132.66	122.86
3	H	40	LEU	CA-C-O	-8.16	111.54	120.92
3	H	151	GLN	N-CA-CB	8.16	122.11	110.77
1	D	412	DT	P-O3'-C3'	8.12	132.37	120.20
3	H	122	CYS	O-C-N	8.11	132.58	123.01
3	H	247	GLU	CB-CG-CD	8.01	126.22	112.60
3	H	198	PRO	CB-CA-C	-8.00	99.57	110.85
3	H	67	ARG	CA-C-O	7.98	130.30	120.25
3	H	18	GLU	CB-CA-C	-7.93	101.24	111.86
3	H	156	GLN	CA-C-O	-7.91	111.94	121.28
3	H	68	ILE	O-C-N	7.90	131.31	122.93
3	H	206	ARG	N-CA-C	-7.87	98.87	110.52
3	H	30	GLN	CB-CG-CD	7.82	125.89	112.60
3	H	61	GLU	CB-CG-CD	7.78	125.83	112.60
3	H	184	GLY	CA-C-O	7.77	129.24	121.62
1	D	406	DG	O4'-C1'-N9	7.75	120.02	108.40
3	H	204(A)	PHE	CA-CB-CG	-7.73	106.07	113.80
2	L	14(I)	SER	CA-C-O	7.72	128.90	120.80
3	H	117	TYR	N-CA-C	7.69	122.97	112.90
2	L	14(B)	THR	CB-CA-C	7.64	121.05	109.13
3	H	137	ARG	CD-NE-CZ	7.64	135.09	124.40
3	H	181	PHE	CA-CB-CG	7.62	121.42	113.80
3	H	185	LYS	CB-CA-C	7.59	121.44	109.37
3	H	74	THR	CB-CA-C	-7.55	95.39	110.42
3	H	140	GLY	N-CA-C	7.53	119.92	110.96
3	H	137	ARG	NE-CZ-NH1	7.50	129.00	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	44	ALA	CA-C-N	-7.49	112.43	122.99
3	H	44	ALA	C-N-CA	-7.49	112.43	122.99
1	D	402	DG	O5'-C5'-C4'	-7.48	99.58	110.80
3	H	102	ASP	CA-C-N	-7.47	110.88	122.68
3	H	102	ASP	C-N-CA	-7.47	110.88	122.68
3	H	106	MET	O-C-N	7.45	131.98	123.48
3	H	18	GLU	N-CA-CB	7.45	123.24	111.91
3	H	112	VAL	N-CA-CB	7.44	118.64	110.53
3	H	95	ASN	CA-CB-CG	7.43	120.03	112.60
3	H	22	ALA	N-CA-C	-7.41	99.51	110.48
3	H	206	ARG	O-C-N	7.34	131.16	122.94
3	H	209	GLN	CA-C-O	-7.31	112.35	120.69
3	H	97(A)	GLU	N-CA-C	7.31	122.75	111.56
3	H	73	ARG	O-C-N	7.27	129.59	122.03
3	H	215	TRP	CA-C-N	7.22	135.57	121.41
3	H	215	TRP	C-N-CA	7.22	135.57	121.41
1	D	410	DG	O5'-C5'-C4'	-7.19	100.02	110.80
3	H	105	LEU	O-C-N	7.18	131.17	122.84
3	H	79	ILE	O-C-N	7.16	127.50	121.98
1	D	407	DT	C4'-C3'-O3'	7.14	120.70	110.00
3	H	115	SER	CA-C-O	7.12	128.90	121.28
3	H	124	PRO	N-CA-CB	7.10	109.66	103.27
3	H	221	ASP	CA-C-O	-7.09	112.96	121.40
3	H	42	CYS	N-CA-C	7.03	117.87	108.38
3	H	181	PHE	CA-C-O	-7.03	112.58	120.66
3	H	154	VAL	N-CA-C	7.02	120.56	108.90
1	D	403	DT	P-O5'-C5'	7.02	130.53	120.00
3	H	60(D)	TRP	CB-CA-C	-7.01	99.57	110.37
3	H	206	ARG	CD-NE-CZ	7.00	134.20	124.40
3	H	135	LYS	CB-CA-C	6.99	122.06	109.83
3	H	154	VAL	CA-C-O	6.94	128.50	121.63
3	H	238	ILE	N-CA-CB	6.93	118.21	110.51
3	H	182	CYS	CA-CB-SG	6.87	130.19	114.40
1	D	402	DG	P-O5'-C5'	-6.86	109.71	120.00
2	L	14(K)	ILE	CA-C-O	-6.83	109.18	120.80
3	H	211	GLY	CA-C-N	6.81	132.04	122.23
3	H	211	GLY	C-N-CA	6.81	132.04	122.23
3	H	158	VAL	CA-C-O	-6.80	114.07	121.28
3	H	236	LYS	CB-CA-C	6.80	122.08	110.79
3	H	83	SER	CA-C-O	6.77	128.76	121.11
3	H	131	GLN	CA-C-N	6.74	134.42	121.54
3	H	131	GLN	C-N-CA	6.74	134.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	117	TYR	CA-C-N	6.71	131.85	123.12
3	H	117	TYR	C-N-CA	6.71	131.85	123.12
3	H	151	GLN	O-C-N	6.68	127.04	121.83
3	H	23	GLU	CA-CB-CG	6.68	127.45	114.10
2	L	14(E)	GLU	CB-CG-CD	6.66	123.91	112.60
3	H	200	VAL	CA-C-N	6.63	133.24	122.29
3	H	200	VAL	C-N-CA	6.63	133.24	122.29
3	H	215	TRP	N-CA-C	-6.63	99.08	108.23
3	H	23	GLU	N-CA-C	-6.63	100.71	110.52
3	H	246	GLY	CA-C-O	-6.63	115.65	122.28
1	D	415	DG	N9-C1'-C2'	-6.61	103.59	113.50
3	H	144	LEU	CB-CA-C	6.56	122.87	109.55
3	H	115	SER	N-CA-C	6.55	118.10	108.14
1	D	413	DT	N1-C1'-C2'	-6.53	103.71	113.50
1	D	407	DT	N1-C1'-C2'	-6.52	103.72	113.50
3	H	55	ALA	CB-CA-C	6.50	120.52	109.53
3	H	222	ASP	N-CA-C	-6.48	100.25	109.96
3	H	209	GLN	OE1-CD-NE2	6.45	129.04	122.60
1	D	408	DG	P-O3'-C3'	6.41	129.82	120.20
3	H	137	ARG	CA-CB-CG	6.38	126.86	114.10
3	H	159	ASN	CA-CB-CG	-6.37	106.23	112.60
3	H	196	GLY	N-CA-C	-6.30	107.02	115.21
3	H	226	GLY	O-C-N	6.30	128.31	122.77
3	H	29	TRP	O-C-N	6.29	129.78	122.17
1	D	406	DG	C4'-C3'-O3'	6.28	119.42	110.00
3	H	156	GLN	CA-C-N	6.26	131.65	122.94
3	H	156	GLN	C-N-CA	6.26	131.65	122.94
3	H	152	PRO	O-C-N	6.25	131.00	123.13
3	H	186	PRO	C-N-CA	6.24	137.29	121.70
3	H	26	MET	CA-C-O	6.22	127.02	119.31
3	H	245	PHE	CA-CB-CG	6.22	120.02	113.80
3	H	232	PHE	CA-CB-CG	-6.21	107.59	113.80
3	H	81	LYS	CA-C-N	6.21	130.85	122.90
3	H	81	LYS	C-N-CA	6.21	130.85	122.90
3	H	94	TYR	CB-CA-C	6.21	119.58	109.90
3	H	172	THR	CB-CA-C	-6.17	98.54	109.70
3	H	203	SER	O-C-N	6.16	126.78	121.30
3	H	20	SER	N-CA-C	6.15	117.54	108.86
3	H	151	GLN	CB-CG-CD	-6.13	102.17	112.60
3	H	201	MET	CA-C-O	6.12	128.16	121.06
3	H	26	MET	O-C-N	-6.11	114.03	122.46
2	L	14(B)	THR	CA-CB-OG1	-6.09	100.46	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	172	THR	CA-CB-OG1	-6.09	100.46	109.60
3	H	200	VAL	N-CA-C	6.09	117.92	109.45
3	H	55	ALA	N-CA-CB	-6.09	100.87	110.06
3	H	55	ALA	N-CA-C	-6.08	100.59	110.20
3	H	245	PHE	O-C-N	6.08	130.67	122.59
3	H	21	ASP	N-CA-CB	6.07	118.91	110.17
3	H	111	PRO	N-CA-C	6.06	121.13	111.26
3	H	208	TYR	N-CA-C	6.05	119.34	109.24
3	H	232	PHE	CB-CA-C	-6.04	98.40	110.42
3	H	212	ILE	N-CA-CB	6.04	123.09	111.62
3	H	93	ARG	NE-CZ-NH2	6.02	124.62	119.20
3	H	170	ASP	O-C-N	6.02	130.12	122.06
3	H	204	PRO	N-CA-C	-5.99	100.14	112.47
3	H	54	THR	CA-C-N	5.98	129.98	121.42
3	H	54	THR	C-N-CA	5.98	129.98	121.42
2	L	1	CYS	CA-C-N	5.97	133.12	121.41
2	L	1	CYS	C-N-CA	5.97	133.12	121.41
3	H	33	LEU	N-CA-CB	-5.96	100.72	110.43
3	H	148	TRP	CA-CB-CG	5.96	124.92	113.60
3	H	127	GLU	CB-CG-CD	5.96	122.72	112.60
3	H	122	CYS	CA-C-O	-5.95	114.26	121.05
1	D	411	DG	O4'-C1'-N9	5.93	117.30	108.40
1	D	402	DG	C2'-C3'-O3'	5.92	120.39	111.50
3	H	230	HIS	CA-C-O	-5.90	115.22	122.36
3	H	222	ASP	N-CA-CB	5.89	118.63	109.85
3	H	129(B)	SER	CA-CB-OG	-5.88	99.34	111.10
3	H	221(A)	ARG	N-CA-CB	5.87	119.75	110.23
3	H	181	PHE	CB-CA-C	5.86	120.94	109.35
3	H	78	ASN	CA-CB-CG	-5.85	106.75	112.60
3	H	214	SER	N-CA-C	5.81	119.90	112.12
3	H	141	TRP	O-C-N	-5.75	114.94	122.59
2	L	14(C)	GLU	CB-CG-CD	-5.74	102.84	112.60
2	L	14(F)	LEU	N-CA-C	5.74	117.53	111.28
3	H	204(B)	ASN	CA-CB-CG	-5.74	106.86	112.60
3	H	97(A)	GLU	CB-CA-C	-5.71	100.36	111.03
3	H	35	ARG	N-CA-C	5.70	117.65	110.24
3	H	38	GLN	CG-CD-NE2	-5.70	107.85	116.40
3	H	237	TRP	CB-CA-C	5.70	119.90	110.90
3	H	247	GLU	N-CA-CB	5.69	120.18	110.50
3	H	94	TYR	N-CA-C	-5.69	101.63	110.10
3	H	217	GLU	CA-C-O	5.67	126.81	120.92
3	H	90	ILE	N-CA-C	-5.66	103.88	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	232	PHE	CA-C-O	5.66	128.60	120.51
3	H	231	VAL	CA-C-O	-5.65	113.72	120.78
2	L	14(C)	GLU	OE1-CD-OE2	5.63	136.41	122.90
2	L	7	PHE	CA-CB-CG	-5.63	108.17	113.80
3	H	227	PHE	CB-CA-C	5.62	119.29	110.19
3	H	118	ILE	CA-C-O	5.60	126.52	120.53
1	D	406	DG	N9-C1'-C2'	-5.59	105.11	113.50
2	L	14(G)	LEU	O-C-N	-5.59	113.76	122.70
3	H	62	ASN	CA-C-N	5.59	132.48	121.58
3	H	62	ASN	C-N-CA	5.59	132.48	121.58
3	H	27	SER	O-C-N	5.56	127.72	121.32
3	H	61	GLU	CG-CD-OE1	5.55	131.18	118.40
1	D	415	DG	C4'-C3'-O3'	5.55	118.33	110.00
3	H	93	ARG	N-CA-C	5.54	119.59	113.21
1	D	409	DT	P-O3'-C3'	5.53	128.50	120.20
2	L	1(A)	ASP	CB-CA-C	5.52	119.30	111.74
3	H	212	ILE	O-C-N	5.52	129.07	123.00
3	H	206	ARG	NH1-CZ-NH2	-5.50	112.15	119.30
3	H	221	ASP	CA-CB-CG	5.50	118.10	112.60
3	H	114	PHE	CA-C-O	-5.49	115.25	121.72
3	H	243	ASP	CA-CB-CG	5.49	118.09	112.60
3	H	29	TRP	CA-CB-CG	5.48	124.02	113.60
1	D	401	DG	C4'-C3'-O3'	5.47	118.21	110.00
3	H	240	LYS	CB-CG-CD	5.47	123.89	111.30
2	L	14	ASP	CA-CB-CG	5.47	118.07	112.60
3	H	74	THR	N-CA-C	5.47	122.45	110.80
1	D	411	DG	C3'-C2'-C1'	-5.46	93.41	101.60
3	H	205	ASN	N-CA-CB	-5.46	103.55	113.10
3	H	58	CYS	N-CA-C	-5.45	105.76	112.90
1	D	409	DT	C4'-C3'-O3'	5.44	118.17	110.00
3	H	204(B)	ASN	CA-C-N	-5.44	115.56	123.93
3	H	204(B)	ASN	C-N-CA	-5.44	115.56	123.93
3	H	60(I)	THR	O-C-N	5.43	129.57	123.27
3	H	35	ARG	O-C-N	5.42	129.76	122.82
3	H	161	PRO	CA-C-O	-5.41	110.75	120.60
3	H	71	HIS	CA-C-O	-5.40	112.79	120.51
1	D	402	DG	O3'-P-O5'	5.39	112.08	104.00
3	H	106	MET	CA-C-N	-5.37	115.59	123.00
3	H	106	MET	C-N-CA	-5.37	115.59	123.00
3	H	161	PRO	CB-CA-C	-5.36	102.72	111.56
3	H	130	LEU	CB-CA-C	5.33	121.03	110.42
3	H	140	GLY	O-C-N	5.33	129.09	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	30	GLN	OE1-CD-NE2	-5.33	117.27	122.60
3	H	129(B)	SER	N-CA-CB	-5.33	102.26	110.20
1	D	406	DG	C3'-C2'-C1'	-5.33	93.61	101.60
3	H	129(C)	LEU	N-CA-CB	-5.32	101.94	110.19
1	D	403	DT	P-O3'-C3'	5.31	128.17	120.20
3	H	124	PRO	CA-C-N	-5.29	113.65	122.64
3	H	124	PRO	C-N-CA	-5.29	113.65	122.64
3	H	214	SER	CA-CB-OG	-5.26	100.58	111.10
2	L	1(B)	ALA	CA-C-N	-5.25	105.65	117.20
3	H	82	ILE	N-CA-C	5.25	115.65	107.99
3	H	238	ILE	CB-CA-C	-5.25	105.16	111.88
3	H	106	MET	N-CA-C	-5.25	100.05	108.55
2	L	14(E)	GLU	N-CA-C	-5.24	105.46	111.07
3	H	213	VAL	CB-CA-C	5.24	117.97	111.15
3	H	125	ASP	N-CA-C	-5.24	101.74	110.17
3	H	60(G)	ASN	N-CA-CB	5.24	119.34	110.49
3	H	101	ARG	NE-CZ-NH2	5.24	123.91	119.20
3	H	221(A)	ARG	CA-C-N	-5.23	113.63	120.95
3	H	221(A)	ARG	C-N-CA	-5.23	113.63	120.95
3	H	65	LEU	O-C-N	5.22	129.65	123.33
3	H	204(B)	ASN	OD1-CG-ND2	5.22	127.82	122.60
1	D	413	DT	C4'-C3'-O3'	5.22	117.83	110.00
3	H	125	ASP	CB-CA-C	5.22	118.31	109.50
3	H	154	VAL	N-CA-CB	-5.22	102.71	112.36
3	H	135	LYS	CA-C-O	-5.21	115.57	121.72
3	H	60(D)	TRP	CA-CB-CG	5.21	123.50	113.60
3	H	165	ARG	CA-C-N	5.21	126.35	119.84
3	H	165	ARG	C-N-CA	5.21	126.35	119.84
3	H	123	LEU	CB-CA-C	5.20	115.71	109.31
2	L	9	LYS	O-C-N	-5.19	115.69	122.59
3	H	194	ASP	CB-CG-OD1	-5.18	106.49	118.40
3	H	124	PRO	O-C-N	5.17	128.95	123.01
3	H	33	LEU	N-CA-C	-5.16	100.83	109.24
3	H	79	ILE	N-CA-C	-5.16	107.55	111.62
3	H	129(B)	SER	N-CA-C	5.14	118.02	111.69
3	H	119	HIS	O-C-N	5.14	125.85	121.84
3	H	23	GLU	N-CA-CB	5.14	118.68	110.46
3	H	55	ALA	CA-C-O	-5.14	115.19	121.05
1	D	405	DG	P-O5'-C5'	-5.13	112.30	120.00
3	H	18	GLU	CB-CG-CD	5.13	121.31	112.60
3	H	156	GLN	CA-CB-CG	-5.13	103.85	114.10
3	H	73	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	121	VAL	CA-C-O	5.12	128.10	121.80
3	H	187	ARG	N-CA-C	5.12	116.08	108.86
3	H	108	LEU	N-CA-CB	-5.12	102.94	110.26
1	D	411	DG	C4'-C3'-O3'	5.11	117.66	110.00
2	L	1(B)	ALA	CA-C-O	5.10	129.47	120.80
3	H	134	TYR	N-CA-CB	5.09	117.46	109.97
2	L	3	LEU	O-C-N	5.09	129.75	123.14
1	D	413	DT	O3'-P-O5'	5.08	111.62	104.00
3	H	21	ASP	O-C-N	5.08	128.85	122.86
3	H	224	LYS	CB-CA-C	5.07	119.32	109.33
3	H	225	TYR	CA-C-N	5.07	125.80	120.43
3	H	225	TYR	C-N-CA	5.07	125.80	120.43
3	H	235	LYS	O-C-N	5.07	129.55	122.36
2	L	1	CYS	N-CA-CB	5.06	117.36	110.38
1	D	411	DG	O5'-C5'-C4'	-5.05	103.22	110.80
3	H	120	PRO	CB-CA-C	5.05	117.50	110.17
3	H	40	LEU	O-C-N	5.05	129.02	123.16
3	H	91	HIS	CA-CB-CG	5.05	118.85	113.80
2	L	13	GLU	OE1-CD-OE2	5.04	135.01	122.90
1	D	403	DT	C5'-C4'-C3'	5.04	122.45	114.90
3	H	137	ARG	N-CA-C	5.03	116.61	108.41
3	H	114	PHE	O-C-N	5.03	128.57	122.94
3	H	173	ARG	NE-CZ-NH1	-5.02	116.48	121.50
3	H	60(H)	PHE	CA-C-N	-5.02	106.17	117.20
3	H	246	GLY	O-C-N	5.01	127.64	122.88

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	401	DG	Sidechain
3	H	60(H)	PHE	Mainchain
3	H	78	ASN	Mainchain
2	L	14(D)	ARG	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	D	315	0	173	33	8
2	L	222	0	225	51	0
3	H	2053	0	2018	508	8
4	H	30	0	30	16	0
5	D	16	0	0	1	0
5	H	125	0	0	11	0
5	L	10	0	0	1	0
All	All	2771	0	2446	568	8

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 115.

All (568) 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:H:162:ILE:HD11	3:H:199:PHE:CZ	1.66	1.30
3:H:51:TRP:NE1	3:H:247:GLU:H	1.30	1.28
3:H:172:THR:CG2	3:H:176:ILE:HD11	1.69	1.22
3:H:51:TRP:HE1	3:H:247:GLU:N	1.38	1.21
3:H:51:TRP:CZ2	3:H:246:GLY:HA2	1.78	1.19
3:H:50:ARG:HB2	3:H:247:GLU:HG2	1.21	1.16
3:H:91:HIS:CE1	3:H:101:ARG:HD3	1.80	1.15
3:H:60(B):PRO:HG2	3:H:96:TRP:CE2	1.83	1.14
1:D:402:DG:N2	1:D:405:DG:N7	1.96	1.13
3:H:84:MET:HB2	3:H:109:LYS:HB2	1.22	1.13
1:D:407:DT:H1'	3:H:79:ILE:HG21	1.26	1.12
1:D:409:DT:H5'	3:H:77(A):ARG:HD3	1.27	1.12
3:H:34:PHE:HB2	3:H:40:LEU:HA	1.22	1.12
3:H:240:LYS:HE2	3:H:244:GLN:HG3	1.12	1.11
2:L:14:ASP:CG	3:H:137:ARG:HH22	1.57	1.10
1:D:413:DT:C2'	1:D:414:DG:OP2	1.96	1.10
3:H:24:ILE:HD13	3:H:24:ILE:N	1.64	1.09
3:H:17:VAL:O	3:H:188:GLY:HA2	1.52	1.08
3:H:144:LEU:HD21	3:H:152:PRO:HD3	1.26	1.08
3:H:124:PRO:HB3	3:H:210:MET:HE1	1.16	1.07
3:H:51:TRP:HZ2	3:H:246:GLY:HA2	1.14	1.06
3:H:124:PRO:HB3	3:H:210:MET:CE	1.86	1.05
3:H:124:PRO:HG3	3:H:210:MET:HE2	1.37	1.05
3:H:195:SER:CB	4:H:297:OG6:O2	2.04	1.05
3:H:60(B):PRO:HG2	3:H:96:TRP:CD2	1.90	1.05
3:H:144:LEU:HD21	3:H:152:PRO:CD	1.86	1.05
3:H:50:ARG:HB2	3:H:247:GLU:CG	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:85:LEU:HD21	3:H:106:MET:CE	1.88	1.04
3:H:85:LEU:CD2	3:H:106:MET:CE	2.36	1.04
3:H:33:LEU:HD12	3:H:42:CYS:HB2	1.38	1.04
2:L:8:GLU:OE2	3:H:202:LYS:NZ	1.90	1.03
3:H:85:LEU:HD23	3:H:106:MET:HE2	1.41	1.02
3:H:162:ILE:CD1	3:H:199:PHE:HZ	1.74	1.01
3:H:204(B):ASN:HD22	3:H:205:ASN:N	1.58	1.01
3:H:101:ARG:HB3	3:H:234:LEU:CD1	1.91	1.00
3:H:101:ARG:HB3	3:H:234:LEU:HD11	1.05	1.00
3:H:234:LEU:O	3:H:238:ILE:HG13	1.60	1.00
3:H:73:ARG:HD3	3:H:152:PRO:O	1.61	1.00
3:H:84:MET:HB2	3:H:109:LYS:CB	1.91	0.99
3:H:143:ASN:CG	3:H:148:TRP:HH2	1.68	0.99
3:H:143:ASN:CG	3:H:148:TRP:CH2	2.41	0.99
1:D:409:DT:H2'	1:D:409:DT:O2	1.59	0.99
3:H:204(B):ASN:HD22	3:H:204(B):ASN:C	1.66	0.99
1:D:409:DT:H3'	3:H:78:ASN:HB2	1.43	0.99
1:D:413:DT:H2''	1:D:414:DG:OP2	1.19	0.98
3:H:162:ILE:HD11	3:H:199:PHE:HZ	0.82	0.97
3:H:210:MET:O	3:H:231:VAL:HG23	1.61	0.97
3:H:60(F):LYS:HG3	3:H:60(H):PHE:HE2	1.26	0.97
3:H:178:ASP:HB3	3:H:233:ARG:NH1	1.80	0.97
3:H:180:MET:HE2	3:H:215:TRP:HE1	1.28	0.96
3:H:35:ARG:HD3	3:H:36(A):SER:C	1.90	0.96
3:H:165:ARG:HB3	3:H:166:PRO:HD3	1.47	0.96
3:H:58:CYS:C	3:H:60(F):LYS:HD3	1.91	0.95
3:H:140:GLY:CA	5:H:579:HOH:O	2.11	0.95
3:H:195:SER:CB	4:H:297:OG6:C2	2.44	0.95
3:H:60(F):LYS:HG3	3:H:60(H):PHE:CE2	2.01	0.95
3:H:240:LYS:HE2	3:H:244:GLN:CG	1.96	0.95
3:H:240:LYS:CE	3:H:244:GLN:HG3	1.95	0.94
3:H:195:SER:HB2	4:H:297:OG6:O2	1.65	0.94
3:H:140:GLY:HA2	5:H:579:HOH:O	1.67	0.94
3:H:85:LEU:CD2	3:H:106:MET:HE2	1.98	0.93
3:H:89:TYR:CE2	3:H:245:PHE:CZ	2.56	0.93
3:H:51:TRP:CD1	3:H:247:GLU:H	1.89	0.90
3:H:91:HIS:CE1	3:H:101:ARG:CD	2.55	0.90
3:H:195:SER:OG	4:H:297:OG6:O2	1.89	0.90
1:D:402:DG:O6	1:D:414:DG:N1	2.04	0.90
3:H:51:TRP:NE1	3:H:247:GLU:N	2.05	0.89
3:H:89:TYR:CE2	3:H:245:PHE:CE1	2.61	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:122:CYS:HB3	3:H:208:TYR:CE1	2.08	0.88
3:H:60(A):TYR:CZ	3:H:60(C):PRO:HG2	2.07	0.88
3:H:84:MET:O	3:H:109:LYS:HB2	1.74	0.88
1:D:414:DG:H5''	1:D:414:DG:N3	1.89	0.87
3:H:101:ARG:CB	3:H:234:LEU:HD11	2.00	0.87
3:H:84:MET:O	3:H:109:LYS:N	2.07	0.87
3:H:50:ARG:HB2	3:H:247:GLU:CB	2.05	0.87
3:H:144:LEU:CD2	3:H:152:PRO:HD3	2.04	0.87
3:H:103:ILE:HG13	3:H:104:ALA:H	1.40	0.86
3:H:172:THR:HG23	3:H:176:ILE:HD11	1.56	0.86
3:H:114:PHE:CZ	3:H:120:PRO:HG3	2.11	0.86
1:D:407:DT:O4'	1:D:409:DT:N3	2.09	0.86
3:H:41:LEU:HD21	3:H:64:LEU:CD2	2.06	0.85
1:D:405:DG:H2''	1:D:405:DG:N3	1.88	0.85
1:D:407:DT:C1'	3:H:79:ILE:HG21	2.04	0.85
3:H:204(B):ASN:ND2	3:H:206:ARG:H	1.75	0.85
3:H:203:SER:OG	3:H:204(A):PHE:HB2	1.77	0.84
3:H:103:ILE:HG13	3:H:104:ALA:N	1.92	0.84
3:H:51:TRP:HE1	3:H:246:GLY:C	1.85	0.84
1:D:407:DT:H1'	3:H:79:ILE:CG2	2.05	0.84
3:H:162:ILE:CD1	3:H:199:PHE:CZ	2.56	0.84
3:H:24:ILE:N	3:H:24:ILE:CD1	2.40	0.84
3:H:50:ARG:CB	3:H:247:GLU:HB2	2.07	0.84
3:H:50:ARG:CB	3:H:247:GLU:CB	2.56	0.83
2:L:6:LEU:HD11	3:H:116:ASP:CG	2.04	0.83
3:H:97:ARG:NH2	5:H:550:HOH:O	2.04	0.83
3:H:143:ASN:OD1	3:H:148:TRP:HH2	1.61	0.83
3:H:210:MET:C	3:H:231:VAL:HG23	2.04	0.82
3:H:51:TRP:HE1	3:H:246:GLY:CA	1.92	0.82
3:H:58:CYS:O	3:H:60(F):LYS:HD3	1.79	0.82
3:H:51:TRP:HE1	3:H:247:GLU:H	0.87	0.82
3:H:60(A):TYR:C	3:H:60(C):PRO:HD2	2.05	0.81
3:H:50:ARG:HB3	3:H:247:GLU:HB2	1.63	0.81
3:H:34:PHE:HE1	3:H:65:LEU:HD23	1.45	0.81
3:H:98:ASN:O	3:H:180:MET:HE1	1.81	0.81
3:H:172:THR:HG21	3:H:176:ILE:HD11	1.62	0.81
3:H:24:ILE:HD13	3:H:24:ILE:H	1.44	0.80
3:H:33:LEU:CD1	3:H:42:CYS:HB2	2.11	0.80
3:H:26:MET:HE2	3:H:137:ARG:CZ	2.12	0.80
3:H:85:LEU:HD23	3:H:106:MET:CE	2.09	0.80
3:H:60(B):PRO:CG	3:H:96:TRP:CE2	2.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:DT:H3'	3:H:78:ASN:CB	2.12	0.79
3:H:60:LEU:HD23	3:H:94:TYR:HE2	1.47	0.79
3:H:172:THR:OG1	3:H:174:ILE:N	2.15	0.79
3:H:115:SER:O	3:H:116:ASP:C	2.25	0.78
3:H:138:VAL:HG22	3:H:199:PHE:HB2	1.63	0.78
1:D:409:DT:C5'	3:H:77(A):ARG:HD3	2.09	0.78
3:H:103:ILE:CG1	3:H:104:ALA:N	2.46	0.78
3:H:148:TRP:HZ2	3:H:151:GLN:HE21	1.32	0.78
3:H:144:LEU:HD21	3:H:152:PRO:CG	2.14	0.77
1:D:409:DT:H1'	1:D:410:DG:OP2	1.84	0.77
3:H:81:LYS:NZ	3:H:113:ALA:HB3	1.99	0.77
3:H:153:SER:HB3	5:H:640:HOH:O	1.84	0.77
3:H:172:THR:HG23	3:H:172:THR:O	1.84	0.77
3:H:191:CYS:N	3:H:194:ASP:OD2	2.18	0.77
3:H:199:PHE:HD1	3:H:199:PHE:O	1.68	0.77
3:H:212:ILE:O	3:H:228:TYR:HB3	1.85	0.76
3:H:230:HIS:HB3	3:H:233:ARG:HB2	1.68	0.76
3:H:183:ALA:HB3	3:H:228:TYR:HE2	1.49	0.76
3:H:185:LYS:H	3:H:186(B):GLU:HG3	1.48	0.76
3:H:71:HIS:N	3:H:77:GLU:OE2	2.18	0.76
3:H:195:SER:OG	4:H:297:OG6:CA2	2.34	0.76
3:H:26:MET:HE2	3:H:137:ARG:NH2	2.01	0.76
3:H:241:VAL:HA	3:H:244:GLN:HB2	1.68	0.76
2:L:14(I):SER:O	2:L:14(K):ILE:HG13	1.86	0.75
3:H:204(B):ASN:C	3:H:204(B):ASN:ND2	2.45	0.75
3:H:178:ASP:HB3	3:H:233:ARG:CZ	2.16	0.75
3:H:51:TRP:CD1	3:H:242:ILE:CG2	2.69	0.75
3:H:85:LEU:CD2	3:H:106:MET:HE3	2.14	0.75
3:H:150:GLY:O	3:H:151:GLN:HG3	1.87	0.75
3:H:51:TRP:CD1	3:H:242:ILE:HG23	2.22	0.75
3:H:51:TRP:CE2	3:H:246:GLY:HA2	2.20	0.75
3:H:49:ASP:OD2	3:H:247:GLU:OE2	2.05	0.75
3:H:124:PRO:CG	3:H:210:MET:HE2	2.14	0.75
3:H:157:VAL:CG2	3:H:157:VAL:O	2.35	0.75
3:H:70:LYS:HE3	3:H:80:GLU:OE1	1.87	0.74
1:D:409:DT:O2	1:D:409:DT:C2'	2.34	0.74
2:L:7:PHE:CE2	2:L:14:ASP:HB3	2.22	0.74
3:H:34:PHE:CE1	3:H:65:LEU:HD23	2.21	0.74
3:H:46:LEU:HD11	3:H:112:VAL:HG21	1.68	0.74
3:H:180:MET:HE2	3:H:215:TRP:NE1	2.03	0.74
1:D:407:DT:O5'	1:D:409:DT:O4	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:ARG:HA	3:H:232:PHE:CZ	2.22	0.73
1:D:407:DT:C5'	1:D:409:DT:O4	2.36	0.73
3:H:60(A):TYR:CE2	3:H:60(C):PRO:HG2	2.23	0.73
3:H:29:TRP:O	3:H:31:VAL:HG23	1.88	0.73
3:H:187:ARG:NH1	3:H:221:ASP:CG	2.46	0.73
3:H:195:SER:CB	4:H:297:OG6:C3	2.66	0.73
2:L:14:ASP:CG	3:H:137:ARG:NH2	2.40	0.73
3:H:124:PRO:CB	3:H:210:MET:CE	2.64	0.73
3:H:235:LYS:O	3:H:239:GLN:N	2.21	0.73
3:H:89:TYR:CZ	3:H:245:PHE:CE1	2.77	0.72
3:H:195:SER:HB2	4:H:297:OG6:C3	2.20	0.72
1:D:405:DG:N3	1:D:405:DG:C2'	2.52	0.72
3:H:235:LYS:O	3:H:238:ILE:HB	1.90	0.72
3:H:60:LEU:HD23	3:H:94:TYR:CE2	2.25	0.72
3:H:195:SER:HB2	4:H:297:OG6:C2	2.16	0.71
3:H:57:HIS:O	3:H:60(F):LYS:HD2	1.90	0.71
3:H:199:PHE:O	3:H:199:PHE:CD1	2.44	0.71
2:L:7:PHE:HE2	2:L:14:ASP:N	1.88	0.71
3:H:52:VAL:CG2	3:H:108:LEU:HD11	2.20	0.71
3:H:51:TRP:CZ2	3:H:246:GLY:CA	2.67	0.71
3:H:187:ARG:NH1	3:H:221:ASP:OD2	2.24	0.71
2:L:7:PHE:HE2	2:L:14:ASP:CA	2.04	0.71
3:H:68:ILE:CG2	3:H:118:ILE:HD13	2.20	0.71
3:H:51:TRP:NE1	3:H:246:GLY:CA	2.54	0.70
3:H:181:PHE:CE2	3:H:211:GLY:HA2	2.26	0.70
3:H:187:ARG:HH11	3:H:221:ASP:CG	1.98	0.70
3:H:212:ILE:O	3:H:228:TYR:HA	1.90	0.70
3:H:172:THR:CG2	3:H:176:ILE:CD1	2.62	0.70
2:L:5:PRO:HA	2:L:9:LYS:HB2	1.74	0.70
3:H:122:CYS:HB3	3:H:208:TYR:CD1	2.26	0.69
3:H:201:MET:O	3:H:207:TRP:HA	1.92	0.69
1:D:402:DG:O6	1:D:414:DG:C6	2.46	0.69
3:H:60(B):PRO:N	3:H:60(C):PRO:CD	2.55	0.69
3:H:181:PHE:CZ	3:H:211:GLY:HA3	2.27	0.69
3:H:60(I):THR:O	3:H:62:ASN:N	2.26	0.68
3:H:60(I):THR:C	3:H:62:ASN:N	2.51	0.68
3:H:125:ASP:OD1	3:H:127:GLU:HB3	1.94	0.68
3:H:44:ALA:HB1	3:H:52:VAL:HG12	1.75	0.68
3:H:47:ILE:HD12	3:H:123:LEU:HD11	1.73	0.68
3:H:35:ARG:HD3	3:H:37:PRO:N	2.07	0.68
3:H:41:LEU:HD21	3:H:64:LEU:HD23	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:20:SER:O	3:H:156:GLN:HA	1.93	0.68
3:H:68:ILE:HG22	3:H:118:ILE:HD13	1.76	0.68
3:H:201:MET:O	3:H:208:TYR:N	2.25	0.68
3:H:69:GLY:O	3:H:79:ILE:HD11	1.94	0.68
3:H:178:ASP:CB	3:H:233:ARG:NH1	2.55	0.68
3:H:177:THR:OG1	3:H:178:ASP:N	2.19	0.68
3:H:84:MET:CB	3:H:109:LYS:HB2	2.15	0.67
3:H:181:PHE:HE2	3:H:211:GLY:HA2	1.59	0.67
3:H:230:HIS:CG	3:H:233:ARG:HB2	2.29	0.67
3:H:157:VAL:O	3:H:157:VAL:HG22	1.94	0.67
3:H:203:SER:OG	3:H:204(A):PHE:CB	2.42	0.67
3:H:144:LEU:HD21	3:H:152:PRO:HG3	1.74	0.67
3:H:35:ARG:HG2	3:H:36:LYS:N	2.09	0.66
3:H:44:ALA:HB1	3:H:52:VAL:CG1	2.26	0.66
3:H:172:THR:HG22	3:H:176:ILE:HD11	1.76	0.66
3:H:163:VAL:CG1	3:H:167:VAL:CG1	2.74	0.66
2:L:7:PHE:CE2	2:L:14:ASP:N	2.64	0.66
3:H:165:ARG:HB3	3:H:166:PRO:CD	2.25	0.66
3:H:230:HIS:HB3	3:H:233:ARG:CB	2.26	0.65
3:H:67:ARG:NE	3:H:80:GLU:OE2	2.28	0.65
3:H:181:PHE:CE2	3:H:211:GLY:CA	2.79	0.65
2:L:14(J):TYR:CD2	3:H:204:PRO:HG3	2.32	0.65
3:H:49:ASP:O	3:H:112:VAL:N	2.25	0.65
3:H:212:ILE:O	3:H:228:TYR:CB	2.44	0.65
3:H:221(A):ARG:HH11	3:H:221(A):ARG:CG	2.08	0.65
2:L:14:ASP:OD2	3:H:137:ARG:NH2	2.28	0.65
3:H:28:PRO:HB2	3:H:119:HIS:CB	2.27	0.65
3:H:52:VAL:HG21	3:H:108:LEU:HD11	1.77	0.64
3:H:204(B):ASN:O	3:H:205:ASN:CB	2.45	0.64
2:L:1(A):ASP:OD1	2:L:1(A):ASP:O	2.16	0.64
3:H:53:LEU:HD11	3:H:103:ILE:HD11	1.78	0.64
3:H:60(B):PRO:CG	3:H:96:TRP:CD2	2.77	0.64
3:H:140:GLY:HA2	3:H:155:LEU:CD1	2.28	0.64
3:H:67:ARG:HB3	3:H:82:ILE:HG13	1.79	0.64
3:H:212:ILE:O	3:H:228:TYR:CA	2.46	0.64
1:D:403:DT:H2"	1:D:404:DT:OP2	1.98	0.64
2:L:14:ASP:OD1	3:H:137:ARG:NH2	2.29	0.64
3:H:59:LEU:CD2	3:H:88:ILE:HG21	2.28	0.64
3:H:204(B):ASN:ND2	3:H:205:ASN:N	2.40	0.63
3:H:148:TRP:CZ2	3:H:151:GLN:NE2	2.66	0.63
3:H:143:ASN:OD1	3:H:148:TRP:CH2	2.48	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:72:SER:H	3:H:77:GLU:CD	2.07	0.63
3:H:85:LEU:HD21	3:H:106:MET:HE3	1.72	0.63
3:H:73:ARG:HG3	3:H:141:TRP:HB3	1.80	0.62
3:H:81:LYS:HD3	3:H:118:ILE:CD1	2.29	0.62
3:H:186(A):ASP:C	3:H:186(C):GLY:H	2.07	0.62
3:H:105:LEU:C	3:H:106:MET:HG3	2.24	0.62
3:H:237:TRP:CE3	3:H:238:ILE:N	2.67	0.62
3:H:163:VAL:CG1	3:H:167:VAL:HG11	2.28	0.62
3:H:181:PHE:HZ	3:H:211:GLY:HA3	1.63	0.62
2:L:3:LEU:HD13	5:H:531:HOH:O	1.97	0.62
3:H:67:ARG:CB	3:H:82:ILE:HG13	2.30	0.62
2:L:14:ASP:H	2:L:14(C):GLU:HG3	1.64	0.61
3:H:181:PHE:CZ	3:H:211:GLY:CA	2.83	0.61
3:H:33:LEU:HD22	3:H:64:LEU:HD22	1.81	0.61
3:H:49:ASP:HA	3:H:112:VAL:HG22	1.82	0.61
3:H:50:ARG:CB	3:H:247:GLU:CG	2.72	0.61
3:H:152:PRO:HB2	3:H:154:VAL:O	2.01	0.61
3:H:240:LYS:O	3:H:244:GLN:CG	2.48	0.61
3:H:185:LYS:HB3	3:H:186:PRO:HD2	1.82	0.61
3:H:34:PHE:CD1	3:H:34:PHE:C	2.78	0.61
3:H:60(A):TYR:H	3:H:60(F):LYS:HB3	1.64	0.61
3:H:91:HIS:NE2	3:H:101:ARG:HD3	2.15	0.61
2:L:14:ASP:N	2:L:14(C):GLU:HG3	2.16	0.61
3:H:122:CYS:HB2	3:H:207:TRP:O	1.99	0.61
3:H:163:VAL:HG13	3:H:167:VAL:HG11	1.82	0.61
3:H:79:ILE:HD12	3:H:117:TYR:CD1	2.35	0.60
3:H:33:LEU:CD2	3:H:64:LEU:HD22	2.31	0.60
3:H:168:CYS:O	3:H:171:SER:HB3	2.01	0.60
3:H:56:ALA:C	3:H:58:CYS:H	2.09	0.60
3:H:60(A):TYR:CE1	3:H:60(C):PRO:HG2	2.36	0.60
3:H:195:SER:OG	4:H:297:OG6:CB2	2.50	0.60
2:L:14:ASP:OD1	2:L:14(C):GLU:N	2.33	0.60
3:H:77(A):ARG:O	3:H:78:ASN:ND2	2.34	0.60
3:H:203:SER:OG	3:H:204(A):PHE:CD2	2.52	0.60
2:L:6:LEU:CD1	3:H:116:ASP:CG	2.75	0.60
2:L:14(J):TYR:HD2	3:H:204:PRO:HG3	1.65	0.60
3:H:81:LYS:HZ3	3:H:113:ALA:HB3	1.63	0.60
3:H:81:LYS:HZ1	3:H:113:ALA:HB3	1.67	0.60
3:H:160:LEU:HD23	3:H:184(A):TYR:CE2	2.36	0.59
3:H:66:VAL:CG1	3:H:68:ILE:HD11	2.32	0.59
3:H:209:GLN:HG2	3:H:231:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60(I):THR:O	3:H:61:GLU:C	2.46	0.59
2:L:7:PHE:CE2	2:L:14:ASP:CA	2.85	0.59
3:H:60(B):PRO:N	3:H:60(C):PRO:HD2	2.16	0.59
3:H:143:ASN:CG	3:H:148:TRP:CZ3	2.80	0.59
3:H:201:MET:SD	3:H:210:MET:HG3	2.42	0.59
3:H:16:ILE:HG21	3:H:158:VAL:HG12	1.83	0.59
3:H:203:SER:OG	3:H:204(A):PHE:CG	2.55	0.59
3:H:243:ASP:OD1	3:H:243:ASP:O	2.20	0.59
3:H:158:VAL:HG22	3:H:160:LEU:HG	1.84	0.59
3:H:161:PRO:HG2	3:H:184:GLY:O	2.03	0.59
3:H:236:LYS:HA	3:H:239:GLN:OE1	2.02	0.59
2:L:1(A):ASP:O	2:L:1(A):ASP:CG	2.45	0.59
3:H:28:PRO:HB2	3:H:119:HIS:HB3	1.85	0.59
3:H:76:TYR:O	3:H:77(A):ARG:N	2.36	0.59
2:L:14(A):LYS:C	2:L:14(B):THR:HG23	2.28	0.58
2:L:14(C):GLU:N	3:H:137:ARG:HH12	2.00	0.58
1:D:402:DG:O6	1:D:414:DG:O6	2.21	0.58
2:L:4:ARG:NH2	2:L:8:GLU:OE1	2.35	0.58
2:L:4:ARG:O	2:L:9:LYS:HB2	2.04	0.58
2:L:7:PHE:O	2:L:12:LEU:O	2.21	0.58
3:H:41:LEU:HD21	3:H:64:LEU:HD21	1.85	0.58
3:H:51:TRP:NE1	3:H:242:ILE:HG23	2.18	0.58
3:H:57:HIS:O	3:H:60(F):LYS:CD	2.52	0.58
3:H:172:THR:HG21	3:H:215:TRP:HH2	1.68	0.58
3:H:164:GLU:C	3:H:166:PRO:HD2	2.28	0.57
3:H:17:VAL:O	3:H:188:GLY:CA	2.39	0.57
3:H:230:HIS:CB	3:H:233:ARG:HB2	2.34	0.57
3:H:46:LEU:CD2	3:H:48:SER:O	2.53	0.57
3:H:51:TRP:CE2	3:H:246:GLY:CA	2.86	0.57
3:H:214:SER:HB3	3:H:227:PHE:O	2.03	0.57
3:H:214:SER:CB	3:H:227:PHE:O	2.53	0.57
3:H:89:TYR:CD2	3:H:245:PHE:CZ	2.92	0.57
3:H:162:ILE:HD13	3:H:162:ILE:N	2.20	0.57
3:H:212:ILE:H	3:H:228:TYR:HB3	1.69	0.56
3:H:28:PRO:HD2	3:H:29:TRP:CZ3	2.40	0.56
3:H:50:ARG:HB3	3:H:247:GLU:CB	2.27	0.56
2:L:14:ASP:OD1	3:H:137:ARG:NH1	2.36	0.56
2:L:14(I):SER:C	2:L:14(K):ILE:H	2.12	0.56
2:L:14(B):THR:O	2:L:14(C):GLU:C	2.48	0.56
3:H:56:ALA:HA	3:H:59:LEU:HD13	1.87	0.56
3:H:131:GLN:O	3:H:134:TYR:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:204(B):ASN:O	3:H:205:ASN:HB2	2.06	0.56
3:H:70:LYS:HD2	3:H:80:GLU:OE2	2.06	0.56
3:H:212:ILE:HG22	3:H:213:VAL:N	2.21	0.56
1:D:401:DG:H2'	1:D:401:DG:N3	2.20	0.56
1:D:409:DT:H5'	3:H:77(A):ARG:CD	2.17	0.56
1:D:410:DG:H5''	1:D:410:DG:N3	2.21	0.55
2:L:7:PHE:HE2	2:L:14:ASP:HA	1.72	0.55
3:H:17:VAL:HG22	3:H:144:LEU:O	2.05	0.55
3:H:59:LEU:CD2	3:H:88:ILE:CG2	2.84	0.55
3:H:67:ARG:HB3	3:H:82:ILE:CG1	2.36	0.55
3:H:142:GLY:O	3:H:144:LEU:HD23	2.05	0.55
3:H:172:THR:CG2	3:H:172:THR:O	2.55	0.55
3:H:203:SER:C	3:H:204(A):PHE:H	2.14	0.55
3:H:81:LYS:HD3	3:H:118:ILE:HD12	1.88	0.55
3:H:183:ALA:HB3	3:H:228:TYR:CE2	2.36	0.55
3:H:199:PHE:CD1	3:H:199:PHE:C	2.85	0.55
3:H:130:LEU:O	3:H:131:GLN:HG3	2.07	0.55
3:H:186(A):ASP:O	3:H:186(C):GLY:N	2.39	0.55
3:H:85:LEU:HD21	3:H:106:MET:HE1	1.84	0.55
2:L:6:LEU:HD11	3:H:116:ASP:OD2	2.07	0.55
3:H:165:ARG:HD3	3:H:165:ARG:C	2.32	0.55
3:H:242:ILE:HA	3:H:246:GLY:HA3	1.88	0.54
1:D:401:DG:H2''	1:D:402:DG:O5'	2.06	0.54
3:H:60(I):THR:C	3:H:62:ASN:H	2.15	0.54
2:L:14:ASP:CG	2:L:14(C):GLU:HG2	2.33	0.54
3:H:35:ARG:N	3:H:39:GLU:O	2.41	0.54
3:H:60(B):PRO:HG2	3:H:96:TRP:CZ2	2.38	0.54
3:H:84:MET:O	3:H:109:LYS:CB	2.52	0.54
3:H:140:GLY:CA	3:H:155:LEU:CD1	2.85	0.54
3:H:242:ILE:O	3:H:246:GLY:HA3	2.08	0.54
3:H:50:ARG:CB	3:H:247:GLU:HG2	2.14	0.54
3:H:60:LEU:HA	3:H:60(F):LYS:O	2.08	0.54
3:H:16:ILE:HG21	3:H:158:VAL:CG1	2.37	0.54
3:H:162:ILE:HD11	3:H:199:PHE:CE2	2.38	0.54
3:H:143:ASN:ND2	3:H:192:GLU:OE1	2.37	0.54
3:H:163:VAL:CG1	3:H:167:VAL:HG12	2.38	0.54
3:H:35:ARG:CD	3:H:37:PRO:HD2	2.38	0.53
3:H:58:CYS:O	3:H:60(F):LYS:CD	2.54	0.53
3:H:68:ILE:HG21	3:H:118:ILE:HG23	1.90	0.53
3:H:221(A):ARG:CG	3:H:221(A):ARG:NH1	2.65	0.53
3:H:215:TRP:HB2	4:H:297:OG6:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:143:ASN:HB3	3:H:148:TRP:CZ3	2.44	0.53
3:H:172:THR:OG1	3:H:174:ILE:HB	2.08	0.53
3:H:185:LYS:N	3:H:186(B):GLU:HG3	2.22	0.53
1:D:413:DT:H1'	1:D:414:DG:C2	2.44	0.53
3:H:77(A):ARG:O	3:H:77(A):ARG:HG2	2.08	0.53
3:H:96:TRP:CE3	3:H:96:TRP:C	2.87	0.53
3:H:221(A):ARG:HH11	3:H:221(A):ARG:HG2	1.73	0.53
3:H:161:PRO:HD3	3:H:184(A):TYR:CZ	2.44	0.53
3:H:186(A):ASP:C	3:H:186(C):GLY:N	2.66	0.53
3:H:68:ILE:CG2	3:H:118:ILE:HG23	2.38	0.53
3:H:115:SER:C	3:H:117:TYR:N	2.67	0.53
2:L:5:PRO:HA	2:L:9:LYS:CB	2.39	0.53
3:H:99:LEU:HD22	4:H:297:OG6:CE2	2.39	0.53
3:H:237:TRP:HZ3	3:H:238:ILE:HG12	1.72	0.53
3:H:66:VAL:HG11	3:H:68:ILE:HD11	1.91	0.52
3:H:137:ARG:O	3:H:200:VAL:HG22	2.08	0.52
3:H:237:TRP:CZ3	3:H:238:ILE:HG12	2.44	0.52
3:H:59:LEU:HD23	3:H:88:ILE:HG21	1.91	0.52
3:H:68:ILE:HG22	3:H:118:ILE:CD1	2.38	0.52
1:D:407:DT:O4'	1:D:409:DT:C4	2.62	0.52
3:H:32:MET:HB2	3:H:141:TRP:CZ3	2.45	0.52
3:H:51:TRP:CH2	3:H:107:LYS:HB3	2.45	0.52
3:H:172:THR:HG21	3:H:176:ILE:CD1	2.33	0.52
1:D:405:DG:H1'	1:D:406:DG:H5'	1.92	0.52
3:H:90:ILE:HG21	3:H:94:TYR:CD2	2.45	0.52
3:H:229:THR:O	3:H:231:VAL:N	2.42	0.52
3:H:35:ARG:HD3	3:H:36(A):SER:O	2.10	0.51
3:H:185:LYS:HB3	3:H:186:PRO:CD	2.40	0.51
1:D:402:DG:H2''	1:D:403:DT:H5'	1.92	0.51
3:H:128:THR:O	3:H:129(B):SER:OG	2.29	0.51
2:L:7:PHE:CE2	2:L:14:ASP:CB	2.93	0.51
3:H:51:TRP:CG	3:H:242:ILE:HG23	2.46	0.51
3:H:51:TRP:NE1	3:H:242:ILE:CG2	2.73	0.51
1:D:410:DG:H2''	1:D:411:DG:O5'	2.11	0.51
3:H:195:SER:HA	3:H:213:VAL:HB	1.92	0.51
3:H:98:ASN:O	3:H:180:MET:CE	2.56	0.50
3:H:99:LEU:HD22	4:H:297:OG6:HE2	1.93	0.50
2:L:3:LEU:CD1	5:H:531:HOH:O	2.55	0.50
3:H:67:ARG:NE	3:H:82:ILE:HD11	2.27	0.50
3:H:67:ARG:HE	3:H:82:ILE:HD11	1.76	0.50
2:L:14(I):SER:HB3	3:H:135:LYS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:204(B):ASN:HD21	3:H:206:ARG:H	1.57	0.50
3:H:172:THR:C	3:H:174:ILE:N	2.68	0.50
3:H:119:HIS:CD2	3:H:120:PRO:HD2	2.47	0.50
3:H:79:ILE:HD12	3:H:117:TYR:CG	2.46	0.50
3:H:168:CYS:O	3:H:171:SER:CB	2.59	0.50
3:H:232:PHE:O	3:H:235:LYS:N	2.44	0.50
2:L:14:ASP:CG	2:L:14(C):GLU:CG	2.85	0.49
3:H:153:SER:HB2	5:H:659:HOH:O	2.11	0.49
3:H:171:SER:OG	3:H:172:THR:N	2.42	0.49
3:H:165:ARG:CB	3:H:166:PRO:HD3	2.28	0.49
3:H:224:LYS:HE3	5:H:512:HOH:O	2.12	0.49
3:H:81:LYS:HD3	3:H:118:ILE:HD11	1.93	0.49
2:L:4:ARG:NE	2:L:8:GLU:OE1	2.44	0.49
2:L:14(I):SER:C	2:L:14(K):ILE:N	2.71	0.49
3:H:143:ASN:ND2	3:H:148:TRP:CH2	2.79	0.49
3:H:51:TRP:CE2	3:H:242:ILE:HG23	2.48	0.49
3:H:53:LEU:CD1	3:H:103:ILE:HD11	2.42	0.49
3:H:57:HIS:CE1	4:H:297:OG6:C3	2.87	0.48
3:H:144:LEU:HG	3:H:151:GLN:HA	1.95	0.48
2:L:4:ARG:HH21	2:L:8:GLU:CD	2.20	0.48
3:H:16:ILE:CG1	3:H:156:GLN:HB2	2.43	0.48
3:H:66:VAL:CG1	3:H:68:ILE:CD1	2.92	0.48
3:H:185:LYS:CB	3:H:186:PRO:HD2	2.44	0.48
3:H:204(B):ASN:HD22	3:H:206:ARG:H	1.60	0.48
3:H:235:LYS:O	3:H:235:LYS:HG3	2.13	0.48
3:H:98:ASN:O	3:H:99:LEU:HB2	2.13	0.48
3:H:107:LYS:O	3:H:107:LYS:CG	2.60	0.48
3:H:59:LEU:O	3:H:60(G):ASN:HA	2.13	0.48
3:H:72:SER:N	3:H:77:GLU:OE2	2.47	0.48
2:L:4:ARG:HG2	3:H:28:PRO:CD	2.44	0.48
3:H:73:ARG:N	3:H:153:SER:O	2.38	0.48
3:H:130:LEU:O	3:H:131:GLN:CG	2.62	0.48
5:D:656:HOH:O	3:H:75:ARG:NH1	2.47	0.48
3:H:215:TRP:HA	4:H:297:OG6:O	2.13	0.48
3:H:59:LEU:HD22	3:H:88:ILE:CG2	2.44	0.47
3:H:159:ASN:O	3:H:184(A):TYR:CE2	2.67	0.47
3:H:204(A):PHE:HD1	3:H:204(A):PHE:HA	1.53	0.47
3:H:31:VAL:CG2	3:H:46:LEU:HB2	2.44	0.47
3:H:31:VAL:HB	3:H:44:ALA:HB3	1.97	0.47
3:H:31:VAL:N	3:H:44:ALA:O	2.42	0.47
3:H:78:ASN:HD22	3:H:78:ASN:HA	1.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:240:LYS:O	3:H:244:GLN:HG2	2.13	0.47
3:H:165:ARG:N	3:H:166:PRO:HD2	2.29	0.47
3:H:232:PHE:C	3:H:234:LEU:N	2.72	0.47
3:H:98:ASN:OD1	3:H:98:ASN:N	2.47	0.47
3:H:23:GLU:O	3:H:26:MET:HB2	2.14	0.47
3:H:130:LEU:HD21	3:H:210:MET:HB3	1.96	0.47
2:L:13:GLU:HB3	2:L:14(C):GLU:OE2	2.15	0.47
3:H:140:GLY:N	3:H:155:LEU:HD11	2.30	0.47
3:H:151:GLN:HB3	3:H:152:PRO:HD2	1.95	0.47
3:H:185:LYS:H	3:H:186(B):GLU:CG	2.24	0.47
3:H:215:TRP:CB	4:H:297:OG6:O	2.63	0.47
1:D:407:DT:H5''	1:D:409:DT:O4	2.15	0.47
3:H:61:GLU:H	3:H:61:GLU:HG2	1.35	0.47
3:H:115:SER:O	3:H:117:TYR:N	2.48	0.47
3:H:186:PRO:HA	3:H:222:ASP:OD1	2.15	0.47
3:H:35:ARG:CG	3:H:36:LYS:N	2.77	0.47
3:H:52:VAL:CG2	3:H:108:LEU:CD1	2.91	0.47
3:H:124:PRO:CG	3:H:210:MET:CE	2.86	0.47
3:H:52:VAL:HG23	3:H:108:LEU:HG	1.97	0.46
3:H:93:ARG:HB2	3:H:101:ARG:HD2	1.97	0.46
3:H:130:LEU:HD21	3:H:210:MET:SD	2.54	0.46
3:H:41:LEU:O	3:H:42:CYS:SG	2.73	0.46
3:H:31:VAL:HG13	3:H:68:ILE:HG13	1.98	0.46
3:H:167:VAL:O	3:H:168:CYS:C	2.59	0.46
3:H:67:ARG:HH21	3:H:80:GLU:CD	2.23	0.46
3:H:56:ALA:C	3:H:58:CYS:N	2.68	0.46
3:H:79:ILE:CG1	3:H:80:GLU:N	2.77	0.46
3:H:165:ARG:N	3:H:166:PRO:CD	2.79	0.46
3:H:169:LYS:C	3:H:171:SER:H	2.22	0.46
3:H:57:HIS:CE1	3:H:195:SER:OG	2.70	0.45
3:H:130:LEU:C	3:H:131:GLN:HG3	2.42	0.45
3:H:213:VAL:HA	3:H:228:TYR:HD1	1.82	0.45
3:H:145:LYS:O	3:H:146:GLU:C	2.59	0.45
3:H:208:TYR:HB3	3:H:210:MET:HE3	1.99	0.45
3:H:77:GLU:HB2	3:H:80:GLU:HB3	1.99	0.45
3:H:58:CYS:CA	3:H:60(F):LYS:HD3	2.46	0.45
3:H:70:LYS:CE	3:H:80:GLU:OE1	2.63	0.45
3:H:148:TRP:HZ2	3:H:151:GLN:NE2	2.06	0.45
3:H:242:ILE:O	3:H:246:GLY:CA	2.65	0.45
3:H:34:PHE:CD1	3:H:34:PHE:O	2.70	0.45
3:H:127:GLU:O	3:H:129(A):ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:96:TRP:C	3:H:96:TRP:HE3	2.25	0.45
3:H:144:LEU:CD2	3:H:152:PRO:HG3	2.45	0.45
2:L:14:ASP:OD2	2:L:14(C):GLU:HG2	2.17	0.45
3:H:51:TRP:HZ2	3:H:246:GLY:CA	2.04	0.45
3:H:56:ALA:HB1	3:H:90:ILE:HD12	1.99	0.45
3:H:164:GLU:H	3:H:164:GLU:HG3	1.49	0.45
3:H:143:ASN:ND2	3:H:192:GLU:HB3	2.32	0.44
3:H:60(A):TYR:C	3:H:60(C):PRO:CD	2.80	0.44
3:H:60(D):TRP:O	3:H:60(E):ASP:HB2	2.17	0.44
2:L:14(C):GLU:O	2:L:14(F):LEU:HB2	2.18	0.44
3:H:28:PRO:CB	3:H:119:HIS:CB	2.95	0.44
3:H:35:ARG:CZ	3:H:60(H):PHE:HE1	2.30	0.44
3:H:129(C):LEU:HD23	3:H:129(C):LEU:HA	1.63	0.44
3:H:243:ASP:OD1	3:H:243:ASP:C	2.61	0.44
3:H:35:ARG:HD3	3:H:37:PRO:CD	2.47	0.44
3:H:76:TYR:O	3:H:76:TYR:CD2	2.70	0.44
3:H:200:VAL:CG2	5:H:503:HOH:O	2.64	0.44
3:H:31:VAL:HG21	3:H:46:LEU:HB2	2.00	0.44
3:H:196:GLY:O	3:H:197:GLY:C	2.61	0.44
3:H:97:ARG:HG2	5:H:544:HOH:O	2.18	0.44
3:H:121:VAL:HG22	3:H:122:CYS:N	2.33	0.44
3:H:210:MET:C	3:H:231:VAL:CG2	2.83	0.44
3:H:68:ILE:HG21	3:H:118:ILE:CG2	2.47	0.44
3:H:70:LYS:HD2	3:H:80:GLU:CD	2.42	0.44
3:H:189:ASP:OD2	4:H:297:OG6:NH2	2.50	0.44
3:H:160:LEU:HA	3:H:161:PRO:HD3	1.84	0.44
3:H:35:ARG:NE	3:H:37:PRO:HD2	2.33	0.43
3:H:60(B):PRO:HG2	3:H:96:TRP:CE3	2.48	0.43
3:H:191:CYS:O	3:H:194:ASP:HB2	2.18	0.43
3:H:41:LEU:C	3:H:42:CYS:SG	3.01	0.43
3:H:184(A):TYR:HB3	3:H:186(D):LYS:O	2.17	0.43
2:L:14:ASP:C	2:L:14(B):THR:H	2.25	0.43
3:H:142:GLY:O	3:H:143:ASN:C	2.62	0.43
3:H:67:ARG:CZ	3:H:80:GLU:OE2	2.67	0.43
2:L:14:ASP:C	2:L:14(B):THR:N	2.77	0.43
3:H:100:ASP:OD1	3:H:179:ASN:HB2	2.18	0.43
3:H:151:GLN:HB3	3:H:152:PRO:CD	2.48	0.43
3:H:230:HIS:ND1	3:H:233:ARG:HB2	2.33	0.43
3:H:178:ASP:O	3:H:233:ARG:HD2	2.19	0.43
3:H:48:SER:O	3:H:50:ARG:N	2.51	0.43
3:H:143:ASN:ND2	3:H:148:TRP:CZ3	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:128:THR:O	3:H:129(C):LEU:HB2	2.19	0.42
3:H:16:ILE:CG2	3:H:158:VAL:CG1	2.97	0.42
3:H:200:VAL:HA	3:H:208:TYR:O	2.19	0.42
3:H:28:PRO:CB	3:H:119:HIS:HB3	2.50	0.42
3:H:49:ASP:O	3:H:111:PRO:HA	2.18	0.42
3:H:138:VAL:CG2	3:H:199:PHE:HB2	2.42	0.42
3:H:163:VAL:HG11	3:H:167:VAL:HG12	2.00	0.42
3:H:212:ILE:CG2	3:H:213:VAL:N	2.82	0.42
3:H:53:LEU:HD12	3:H:53:LEU:HA	1.78	0.42
3:H:235:LYS:C	3:H:238:ILE:HB	2.44	0.42
3:H:141:TRP:N	5:H:579:HOH:O	1.90	0.42
3:H:236:LYS:HD2	3:H:239:GLN:OE1	2.19	0.42
3:H:34:PHE:CD2	3:H:39:GLU:C	2.97	0.42
3:H:107:LYS:O	3:H:107:LYS:HG3	2.14	0.42
3:H:217:GLU:OE1	3:H:224:LYS:NZ	2.40	0.42
3:H:121:VAL:HG22	3:H:122:CYS:H	1.85	0.42
3:H:163:VAL:HG11	3:H:167:VAL:CG1	2.49	0.42
3:H:201:MET:O	3:H:207:TRP:CA	2.63	0.42
3:H:185:LYS:CB	3:H:186:PRO:CD	2.95	0.41
3:H:88:ILE:HA	3:H:106:MET:HA	2.01	0.41
3:H:130:LEU:HD21	3:H:210:MET:CG	2.50	0.41
3:H:242:ILE:H	3:H:242:ILE:HG12	1.68	0.41
2:L:1(B):ALA:HB2	5:L:528:HOH:O	2.21	0.41
3:H:84:MET:O	3:H:109:LYS:CA	2.69	0.41
2:L:4:ARG:HB2	2:L:7:PHE:HB2	2.01	0.41
3:H:103:ILE:HG12	3:H:104:ALA:N	2.32	0.41
3:H:126:ARG:CD	3:H:126:ARG:C	2.93	0.41
3:H:28:PRO:HD2	3:H:29:TRP:CE3	2.55	0.41
3:H:51:TRP:HE1	3:H:246:GLY:HA3	1.80	0.41
3:H:57:HIS:HE1	3:H:195:SER:OG	2.04	0.41
3:H:47:ILE:O	3:H:48:SER:HB3	2.19	0.41
3:H:57:HIS:CE1	3:H:195:SER:HB3	2.55	0.41
3:H:67:ARG:HH21	3:H:76:TYR:HD1	1.69	0.41
3:H:87:LYS:O	3:H:107:LYS:N	2.51	0.41
2:L:14(J):TYR:CE2	3:H:204:PRO:HG3	2.56	0.41
3:H:160:LEU:HD23	3:H:184(A):TYR:HE2	1.84	0.40
3:H:176:ILE:HD12	3:H:227:PHE:CE2	2.56	0.40
3:H:16:ILE:HG13	3:H:156:GLN:HB2	2.02	0.40
3:H:143:ASN:CB	3:H:148:TRP:CZ3	3.04	0.40
3:H:143:ASN:HB2	3:H:191:CYS:SG	2.61	0.40
2:L:4:ARG:HG2	3:H:28:PRO:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:24:ILE:CD1	3:H:24:ILE:H	2.16	0.40
3:H:198:PRO:HB2	3:H:200:VAL:HG13	2.03	0.40
3:H:46:LEU:HD23	3:H:48:SER:O	2.21	0.40
3:H:90:ILE:HG22	3:H:91:HIS:N	2.36	0.40
3:H:202:LYS:HD2	3:H:205:ASN:C	2.46	0.40
3:H:67:ARG:NH2	3:H:80:GLU:CD	2.79	0.40
3:H:140:GLY:N	3:H:155:LEU:CD1	2.85	0.40
3:H:167:VAL:HG12	3:H:168:CYS:N	2.37	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:DT:OP2	3:H:101:ARG:NH1[2_564]	1.15	1.05
1:D:413:DT:P	3:H:101:ARG:NH1[2_564]	1.50	0.70
1:D:413:DT:C5'	3:H:101:ARG:NE[2_564]	1.58	0.62
1:D:413:DT:O5'	3:H:101:ARG:NH1[2_564]	1.72	0.48
1:D:413:DT:C5'	3:H:101:ARG:CZ[2_564]	1.80	0.40
1:D:413:DT:C5'	3:H:101:ARG:CD[2_564]	1.84	0.36
1:D:413:DT:O5'	3:H:101:ARG:CZ[2_564]	2.08	0.12
1:D:413:DT:C5'	3:H:101:ARG:NH1[2_564]	2.15	0.05

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	
2	L	25/36 (69%)	17 (68%)	6 (24%)	2 (8%)	1	1
3	H	249/259 (96%)	197 (79%)	41 (16%)	11 (4%)	2	7
All	All	274/295 (93%)	214 (78%)	47 (17%)	13 (5%)	2	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	233	ARG
2	L	2	GLY
3	H	49	ASP
3	H	61	GLU
3	H	77	GLU
3	H	186(B)	GLU
3	H	232	PHE
3	H	245	PHE
2	L	14(J)	TYR
3	H	38	GLN
3	H	77(A)	ARG
3	H	195	SER
3	H	57	HIS

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	
2	L	25/31 (81%)	19 (76%)	6 (24%)	1	2
3	H	221/225 (98%)	165 (75%)	56 (25%)	0	2
All	All	246/256 (96%)	184 (75%)	62 (25%)	0	2

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	1(A)	ASP
2	L	1	CYS
2	L	10	LYS
2	L	11	SER
2	L	12	LEU
2	L	13	GLU
3	H	16	ILE
3	H	20	SER
3	H	23	GLU
3	H	24	ILE
3	H	26	MET

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Mol	Chain	Res	Type
3	H	29	TRP
3	H	33	LEU
3	H	34	PHE
3	H	36	LYS
3	H	36(A)	SER
3	H	41	LEU
3	H	46	LEU
3	H	50	ARG
3	H	61	GLU
3	H	66	VAL
3	H	72	SER
3	H	74	THR
3	H	75	ARG
3	H	78	ASN
3	H	79	ILE
3	H	80	GLU
3	H	82	ILE
3	H	83	SER
3	H	84	MET
3	H	86	GLU
3	H	87	LYS
3	H	99	LEU
3	H	101	ARG
3	H	103	ILE
3	H	109	LYS
3	H	126	ARG
3	H	137	ARG
3	H	154	VAL
3	H	157	VAL
3	H	158	VAL
3	H	162	ILE
3	H	165	ARG
3	H	167	VAL
3	H	173	ARG
3	H	174	ILE
3	H	175	ARG
3	H	176	ILE
3	H	177	THR
3	H	180	MET
3	H	199	PHE
3	H	205	ASN
3	H	222	ASP

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Mol	Chain	Res	Type
3	H	233	ARG
3	H	234	LEU
3	H	235	LYS
3	H	236	LYS
3	H	237	TRP
3	H	239	GLN
3	H	241	VAL
3	H	242	ILE
3	H	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	38	GLN
3	H	57	HIS
3	H	71	HIS
3	H	95	ASN
3	H	156	GLN
3	H	204(B)	ASN
3	H	244	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	0G6	H	297	3	30,31,32	2.26	2 (6%)	37,41,42	1.45	5 (13%)

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
4	0G6	H	297	3	1/1/8/10	8/31/41/43	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	297	0G6	C3-C2	-9.14	1.25	1.51
4	H	297	0G6	O2-C2	-6.91	1.24	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	297	0G6	CA2-N2-C1	-3.18	117.72	123.25
4	H	297	0G6	CB2-CG2-CD3	2.95	120.58	112.07
4	H	297	0G6	O-C-N1	2.64	126.12	121.38
4	H	297	0G6	O2-C2-C3	2.44	116.99	109.68
4	H	297	0G6	C1-CA1-N1	-2.41	105.91	112.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	297	0G6	C2

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	297	0G6	O2-C2-CA2-CB2
4	H	297	0G6	C2-CA2-CB2-CG2

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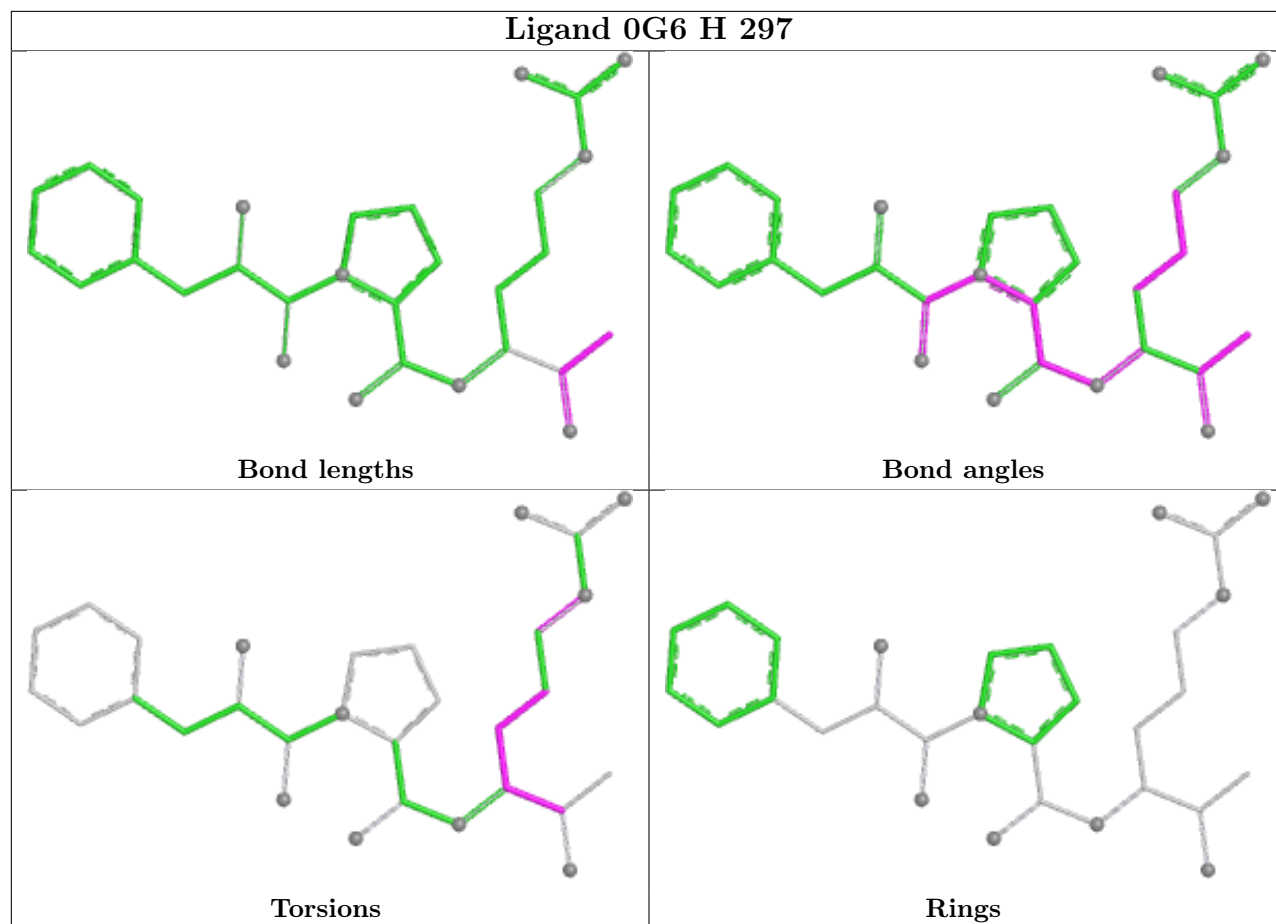
Mol	Chain	Res	Type	Atoms
4	H	297	0G6	C3-C2-CA2-N2
4	H	297	0G6	CA2-CB2-CG2-CD3
4	H	297	0G6	O2-C2-CA2-N2
4	H	297	0G6	N2-CA2-CB2-CG2
4	H	297	0G6	C3-C2-CA2-CB2
4	H	297	0G6	CG2-CD3-NE-CZ1

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	297	0G6	16	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.