



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 PM UTC

PDB ID : 1HUT / pdb_00001hut
Title : THE STRUCTURE OF ALPHA-THROMBIN INHIBITED BY A 15-MER SINGLE-STRANDED DNA APTAMER
Authors : Padmanabhan, K.; Padmanabhan, K.P.; Ferrara, J.D.; Sadler, J.E.; Tulinsky, A.
Deposited on : 1993-05-27
Resolution : 2.90 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

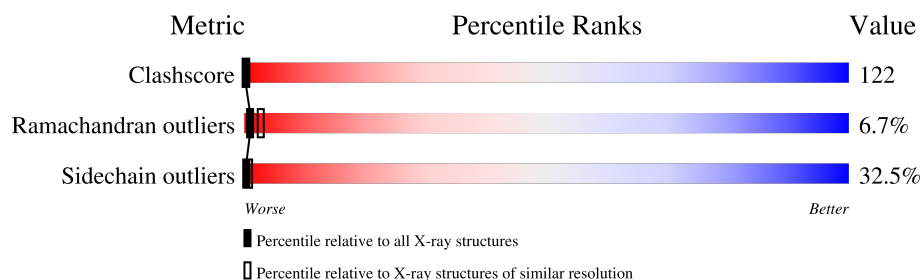
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	13% 87%
2	L	36	11% 36% 44% 8%
3	H	259	6% 35% 38% 18% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2815 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 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
1	D	15	Total	C	N	O	P	0	0	0
			315	150	57	94	14			

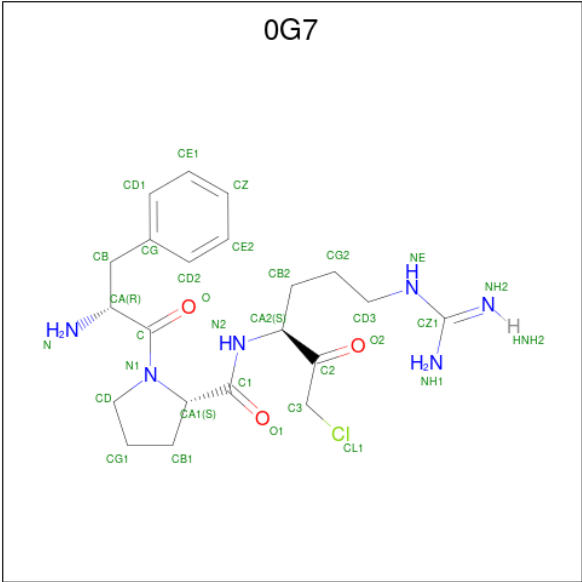
- Molecule 2 is a protein called ALPHA-Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 3 is a protein called ALPHA-Thrombin heavy chain.

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

- Molecule 4 is D-phenylalanyl-N-[(3S)-6-carbamimidamido-1-chloro-2-oxohexan-3-yl]-L-prolinamide (CCD ID: 0G7) (formula: C₂₁H₃₁ClN₆O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	25	Total	O	0	0
			25	25		
5	L	15	Total	O	0	0
			15	15		
5	H	90	Total	O	0	0
			90	90		

3 Residue-property plots

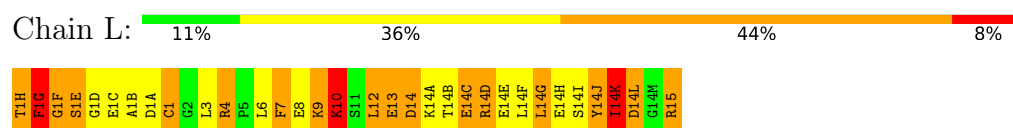
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

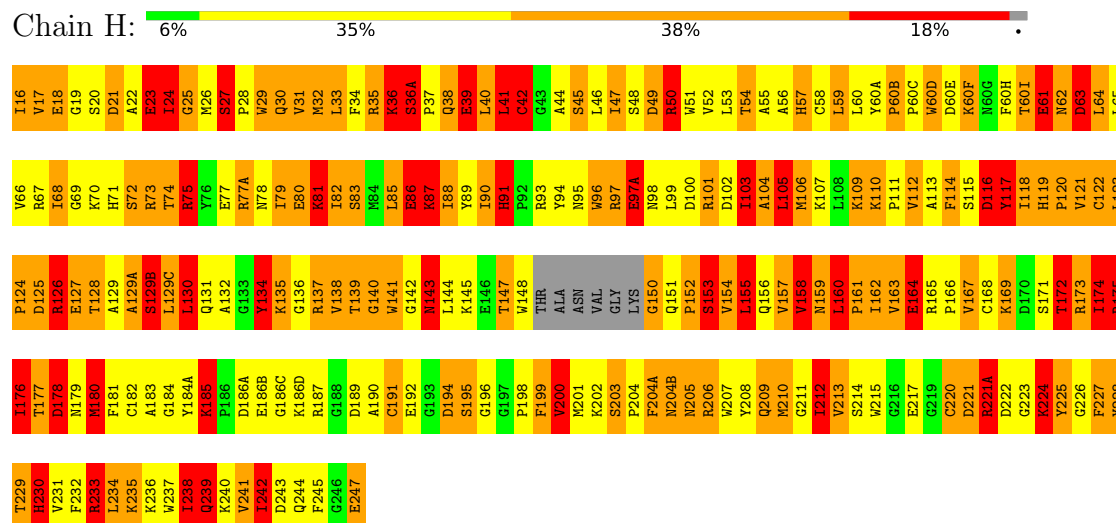
- Molecule 1: DNA 5'-D(*GP*GP*TP*TP*GP*GP*TP*GP*TP*GP*GP*TP*TP*GP*G)-3',



- Molecule 2: ALPHA-Thrombin light chain



- Molecule 3: ALPHA-Thrombin heavy chain



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.52Å 77.44Å 99.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2815	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: 0G7

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	1.33	1/353 (0.3%)	3.72	63/547 (11.5%)
2	L	1.47	3/290 (1.0%)	2.75	27/384 (7.0%)
3	H	1.45	17/2107 (0.8%)	2.76	223/2846 (7.8%)
All	All	1.43	21/2750 (0.8%)	2.91	313/3777 (8.3%)

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
2	L	0	1
3	H	0	6
All	All	0	7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	150	GLY	C-N	8.68	1.41	1.33
2	L	1(F)	GLY	C-N	7.53	1.51	1.34
3	H	180	MET	C-N	-7.43	1.24	1.33
3	H	135	LYS	C-N	-6.51	1.25	1.34
3	H	116	ASP	C-N	-6.48	1.24	1.33
3	H	200	VAL	C-N	6.13	1.42	1.33
3	H	68	ILE	CA-CB	5.99	1.61	1.54
3	H	117	TYR	C-N	-5.62	1.25	1.33
3	H	104	ALA	C-N	-5.52	1.25	1.33
3	H	247	GLU	C-OXT	5.37	1.34	1.23
3	H	140	GLY	C-N	-5.36	1.26	1.33
3	H	41	LEU	N-CA	5.28	1.52	1.46
2	L	14(B)	THR	CA-CB	5.27	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	109	LYS	C-O	5.24	1.30	1.24
2	L	13	GLU	C-N	5.23	1.40	1.33
3	H	210	MET	N-CA	5.19	1.53	1.46
3	H	60(F)	LYS	CA-C	5.18	1.59	1.52
1	D	407	DT	C3'-C2'	5.16	1.63	1.52
3	H	225	TYR	N-CA	5.13	1.52	1.45
3	H	224	LYS	N-CA	5.11	1.51	1.45
3	H	81	LYS	C-N	-5.11	1.28	1.33

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	135	LYS	CA-C-N	21.77	140.11	121.82
3	H	135	LYS	C-N-CA	21.77	140.11	121.82
1	D	412	DT	P-O3'-C3'	19.28	149.12	120.20
1	D	402	DG	P-O3'-C3'	15.56	143.54	120.20
1	D	406	DG	O4'-C1'-N9	15.44	131.56	108.40
1	D	405	DG	P-O3'-C3'	15.01	142.71	120.20
1	D	404	DT	P-O5'-C5'	14.65	141.97	120.00
1	D	404	DT	P-O3'-C3'	14.45	141.87	120.20
3	H	101	ARG	NE-CZ-NH1	13.49	134.99	121.50
1	D	412	DT	P-O5'-C5'	13.24	139.87	120.00
1	D	404	DT	C4'-C3'-O3'	13.04	129.56	110.00
1	D	403	DT	C4'-C3'-O3'	13.00	129.50	110.00
2	L	10	LYS	CA-C-N	12.73	145.85	121.54
2	L	10	LYS	C-N-CA	12.73	145.85	121.54
1	D	403	DT	O3'-P-O5'	12.67	123.01	104.00
1	D	406	DG	P-O5'-C5'	12.21	138.32	120.00
1	D	413	DT	P-O5'-C5'	12.03	138.04	120.00
1	D	412	DT	O4'-C1'-N1	11.94	126.31	108.40
3	H	157	VAL	CA-C-O	-11.90	109.78	120.96
3	H	196	GLY	CA-C-N	11.80	140.39	121.87
3	H	196	GLY	C-N-CA	11.80	140.39	121.87
3	H	40	LEU	CA-C-O	-11.79	108.28	120.54
1	D	404	DT	C5'-C4'-C3'	11.62	132.34	114.90
2	L	1(G)	PHE	CA-CB-CG	11.36	125.16	113.80
2	L	4	ARG	N-CA-C	11.24	126.06	109.42
1	D	407	DT	C4'-C3'-O3'	11.23	126.85	110.00
1	D	407	DT	N1-C1'-C2'	-10.71	97.44	113.50
1	D	404	DT	O4'-C1'-N1	10.43	124.05	108.40
3	H	226	GLY	CA-C-O	-10.31	110.53	120.64
3	H	159	ASN	CA-CB-CG	10.19	122.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	DG	P-O3'-C3'	10.09	135.33	120.20
3	H	30	GLN	O-C-N	9.99	134.56	123.27
3	H	105	LEU	O-C-N	-9.94	112.04	123.27
1	D	403	DT	O5'-C5'-C4'	9.85	125.58	110.80
1	D	410	DG	C1'-O4'-C4'	-9.80	95.00	109.70
2	L	14(J)	TYR	CA-C-O	-9.75	106.56	120.51
1	D	401	DG	O5'-C5'-C4'	9.71	125.36	110.80
3	H	131	GLN	CA-C-O	-9.65	109.86	120.38
3	H	36(A)	SER	CB-CA-C	-9.57	97.90	110.34
1	D	411	DG	O4'-C1'-N9	9.49	122.64	108.40
3	H	227	PHE	CA-C-O	-9.47	109.90	120.32
1	D	404	DT	C1'-O4'-C4'	-9.45	95.53	109.70
1	D	407	DT	C3'-C2'-C1'	-9.39	87.52	101.60
3	H	86	GLU	CA-CB-CG	9.38	132.85	114.10
3	H	123	LEU	CB-CA-C	9.35	122.84	109.38
1	D	410	DG	O4'-C1'-N9	9.14	122.11	108.40
3	H	129(B)	SER	N-CA-CB	-9.06	97.02	110.53
1	D	407	DT	O4'-C1'-N1	-8.87	95.10	108.40
3	H	229	THR	CA-C-O	8.79	130.47	120.54
3	H	116	ASP	O-C-N	-8.78	110.92	122.59
1	D	406	DG	N9-C1'-C2'	-8.65	100.52	113.50
1	D	403	DT	OP1-P-OP2	-8.64	94.07	120.00
3	H	96	TRP	CA-CB-CG	8.59	129.92	113.60
3	H	109	LYS	CA-C-O	-8.55	110.43	120.10
3	H	104	ALA	CA-C-N	8.54	134.50	122.72
3	H	104	ALA	C-N-CA	8.54	134.50	122.72
1	D	401	DG	C5'-C4'-O4'	8.44	122.06	109.40
1	D	412	DT	C4'-C3'-O3'	8.42	122.64	110.00
3	H	157	VAL	O-C-N	8.38	131.23	123.19
2	L	4	ARG	CD-NE-CZ	-8.36	112.69	124.40
1	D	402	DG	O5'-C5'-C4'	-8.33	98.31	110.80
3	H	164	GLU	CA-C-N	8.28	130.44	120.09
3	H	164	GLU	C-N-CA	8.28	130.44	120.09
3	H	68	ILE	N-CA-C	8.23	120.43	108.58
3	H	123	LEU	O-C-N	8.07	128.78	121.35
1	D	411	DG	C4'-C3'-O3'	8.05	122.07	110.00
3	H	102	ASP	CA-CB-CG	8.04	120.64	112.60
3	H	119	HIS	O-C-N	8.01	128.08	121.83
1	D	409	DT	P-O3'-C3'	7.98	132.17	120.20
3	H	160	LEU	N-CA-C	7.96	122.27	108.82
3	H	60(E)	ASP	CA-CB-CG	7.95	120.55	112.60
3	H	212	ILE	O-C-N	7.90	131.69	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	91	HIS	CB-CA-C	7.71	118.79	109.31
1	D	408	DG	P-O3'-C3'	7.66	131.69	120.20
3	H	192	GLU	CA-C-N	7.65	133.41	123.08
3	H	192	GLU	C-N-CA	7.65	133.41	123.08
3	H	60(F)	LYS	N-CA-CB	7.63	122.53	110.55
3	H	50	ARG	CD-NE-CZ	-7.63	113.72	124.40
3	H	129(B)	SER	N-CA-C	7.61	122.74	113.38
3	H	131	GLN	OE1-CD-NE2	7.56	130.16	122.60
3	H	101	ARG	NH1-CZ-NH2	-7.50	109.55	119.30
3	H	87	LYS	CA-C-O	7.49	129.75	120.54
1	D	402	DG	C1'-O4'-C4'	-7.49	98.46	109.70
3	H	178	ASP	CA-CB-CG	7.47	120.07	112.60
1	D	406	DG	O5'-C5'-C4'	7.44	121.96	110.80
3	H	60(B)	PRO	N-CA-C	7.43	119.77	110.70
3	H	49	ASP	CA-CB-CG	7.42	120.02	112.60
3	H	140	GLY	CA-C-N	7.41	134.64	123.23
3	H	140	GLY	C-N-CA	7.41	134.64	123.23
2	L	14(L)	ASP	CA-CB-CG	-7.41	105.19	112.60
3	H	131	GLN	O-C-N	7.38	132.00	123.29
3	H	101	ARG	CD-NE-CZ	7.37	134.72	124.40
3	H	192	GLU	CB-CG-CD	7.32	125.04	112.60
3	H	155	LEU	CA-C-O	7.30	128.92	120.96
3	H	209	GLN	CA-C-O	7.29	130.19	121.66
3	H	86	GLU	CA-C-O	-7.29	112.75	120.55
3	H	180	MET	CA-C-N	7.28	134.33	122.39
3	H	180	MET	C-N-CA	7.28	134.33	122.39
3	H	62	ASN	O-C-N	7.25	130.46	122.20
3	H	41	LEU	CA-C-O	-7.23	113.30	120.89
3	H	177	THR	CA-C-O	-7.23	112.69	121.36
3	H	27	SER	CA-C-O	-7.21	113.93	121.29
3	H	185	LYS	CB-CA-C	7.20	122.83	109.51
1	D	411	DG	N9-C1'-C2'	-7.17	102.74	113.50
3	H	152	PRO	O-C-N	7.16	131.31	122.71
3	H	159	ASN	CA-C-O	7.14	127.81	120.24
3	H	209	GLN	OE1-CD-NE2	7.13	129.73	122.60
3	H	224	LYS	CA-C-O	-7.12	112.95	121.56
1	D	411	DG	O3'-P-O5'	7.11	114.67	104.00
3	H	24	ILE	CB-CG1-CD1	7.11	128.73	113.80
1	D	403	DT	O4'-C1'-N1	7.08	119.02	108.40
3	H	162	ILE	CA-C-O	-7.07	113.58	121.36
3	H	224	LYS	N-CA-C	-7.06	99.19	110.14
3	H	36(A)	SER	CA-CB-OG	7.06	125.22	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	4	ARG	NE-CZ-NH2	7.02	125.52	119.20
3	H	62	ASN	CA-C-N	7.00	129.89	120.65
3	H	62	ASN	C-N-CA	7.00	129.89	120.65
3	H	121	VAL	O-C-N	-7.00	114.71	122.69
3	H	97(A)	GLU	CB-CG-CD	6.98	124.47	112.60
3	H	47	ILE	CA-C-O	-6.98	111.68	119.35
1	D	402	DG	P-O5'-C5'	-6.97	109.54	120.00
2	L	1(H)	THR	CA-CB-OG1	-6.97	99.14	109.60
3	H	27	SER	CB-CA-C	-6.93	101.85	111.41
1	D	407	DT	C4'-C3'-C2'	-6.92	92.02	102.40
1	D	410	DG	O4'-C4'-C3'	-6.89	95.07	105.40
2	L	14	ASP	CA-C-O	6.88	129.93	121.81
3	H	185	LYS	N-CA-C	-6.88	100.29	110.20
1	D	404	DT	O4'-C4'-C3'	-6.85	95.13	105.40
3	H	17	VAL	CB-CA-C	6.81	120.54	111.21
2	L	4	ARG	NE-CZ-NH1	-6.79	114.71	121.50
3	H	26	MET	CA-C-N	6.77	130.11	122.59
3	H	26	MET	C-N-CA	6.77	130.11	122.59
3	H	150	GLY	CA-C-N	-6.76	114.19	122.64
3	H	150	GLY	C-N-CA	-6.76	114.19	122.64
3	H	73	ARG	O-C-N	6.73	130.55	122.27
3	H	194	ASP	CA-CB-CG	-6.72	105.88	112.60
3	H	203	SER	O-C-N	6.71	126.66	121.23
3	H	103	ILE	CA-C-O	-6.66	115.11	121.64
3	H	225	TYR	CB-CA-C	6.65	122.75	110.24
3	H	45	SER	N-CA-C	6.65	119.36	108.52
1	D	412	DT	N1-C1'-C2'	-6.64	103.53	113.50
2	L	1	CYS	N-CA-C	-6.58	101.85	110.53
2	L	14(C)	GLU	O-C-N	6.56	133.19	122.70
3	H	38	GLN	CB-CG-CD	6.55	123.74	112.60
1	D	403	DT	C2'-C3'-O3'	-6.49	101.76	111.50
3	H	60(F)	LYS	O-C-N	6.47	133.04	122.70
3	H	129(B)	SER	CA-CB-OG	-6.47	98.17	111.10
3	H	126	ARG	NE-CZ-NH2	-6.46	113.39	119.20
3	H	194	ASP	N-CA-C	6.46	118.11	111.14
1	D	407	DT	C5'-C4'-C3'	6.42	124.53	114.90
3	H	138	VAL	CB-CA-C	-6.40	104.28	111.45
3	H	185	LYS	CB-CG-CD	6.40	126.02	111.30
3	H	83	SER	N-CA-C	6.38	119.12	109.23
1	D	407	DT	C1'-O4'-C4'	-6.38	100.14	109.70
3	H	225	TYR	CA-C-O	-6.37	114.17	121.68
3	H	68	ILE	CB-CA-C	-6.36	103.03	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	24	ILE	CB-CA-C	-6.35	101.78	111.69
2	L	14(B)	THR	CA-CB-OG1	-6.34	100.08	109.60
3	H	89	TYR	CA-CB-CG	6.34	125.32	113.90
3	H	30	GLN	N-CA-CB	6.33	120.74	110.43
3	H	42	CYS	N-CA-C	6.33	116.42	108.45
1	D	413	DT	N3-C4-O4	-6.31	113.14	122.60
3	H	97	ARG	CD-NE-CZ	6.30	133.22	124.40
3	H	36	LYS	O-C-N	-6.28	112.65	122.70
3	H	60(D)	TRP	CA-CB-CG	6.26	125.49	113.60
3	H	24	ILE	CA-C-O	-6.25	113.29	120.98
2	L	14(D)	ARG	NH1-CZ-NH2	-6.25	111.17	119.30
3	H	227	PHE	O-C-N	6.22	130.61	123.27
3	H	102	ASP	O-C-N	6.21	130.21	122.63
2	L	14	ASP	CA-C-N	-6.19	103.59	117.20
3	H	134	TYR	N-CA-C	-6.18	102.37	110.53
2	L	1	CYS	O-C-N	6.13	129.78	122.79
3	H	49	ASP	N-CA-C	-6.13	105.55	113.16
3	H	129(A)	ALA	C-N-CA	6.10	136.95	121.70
3	H	27	SER	O-C-N	6.09	126.32	121.20
3	H	223	GLY	O-C-N	6.08	128.84	122.51
1	D	407	DT	O5'-C5'-C4'	-6.07	101.70	110.80
3	H	54	THR	CA-CB-OG1	-6.06	100.51	109.60
1	D	405	DG	C5'-C4'-C3'	6.05	123.97	114.90
1	D	408	DG	N9-C1'-C2'	6.01	122.51	113.50
3	H	158	VAL	CA-C-O	-5.99	114.69	121.75
2	L	14(D)	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	H	224	LYS	N-CA-CB	5.96	120.03	110.85
2	L	14(K)	ILE	N-CA-CB	5.96	121.06	111.23
3	H	204(B)	ASN	CA-CB-CG	5.96	118.56	112.60
2	L	14(B)	THR	N-CA-C	5.93	119.78	111.30
2	L	14(B)	THR	N-CA-CB	-5.93	102.66	111.43
3	H	140	GLY	CA-C-O	5.93	127.83	121.61
1	D	410	DG	C4'-C3'-O3'	5.92	118.88	110.00
3	H	163	VAL	CA-C-O	5.91	126.60	120.39
3	H	120	PRO	CA-C-N	5.90	132.14	122.64
3	H	120	PRO	C-N-CA	5.90	132.14	122.64
1	D	401	DG	N9-C1'-C2'	5.88	122.32	113.50
3	H	30	GLN	CA-C-O	-5.87	114.03	120.43
3	H	185	LYS	CG-CD-CE	5.86	124.79	111.30
3	H	75	ARG	CD-NE-CZ	5.86	132.60	124.40
3	H	72	SER	N-CA-C	-5.85	100.46	109.76
3	H	160	LEU	O-C-N	5.84	126.03	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	176	ILE	CA-C-N	5.83	132.04	122.07
3	H	176	ILE	C-N-CA	5.83	132.04	122.07
1	D	411	DG	O4'-C1'-C2'	-5.83	97.66	106.40
3	H	80	GLU	N-CA-C	5.79	118.75	110.24
3	H	175	ARG	O-C-N	5.77	129.94	123.19
3	H	72	SER	CB-CA-C	5.75	119.22	109.84
3	H	243	ASP	O-C-N	5.74	128.20	122.12
3	H	239	GLN	N-CA-CB	5.74	120.18	110.49
3	H	87	LYS	N-CA-C	5.72	118.54	108.75
3	H	173	ARG	CA-C-O	-5.72	114.45	120.63
3	H	209	GLN	CA-CB-CG	-5.70	102.69	114.10
3	H	167	VAL	N-CA-CB	-5.69	106.97	111.64
3	H	45	SER	CB-CA-C	-5.68	100.88	110.19
3	H	47	ILE	CB-CA-C	5.68	115.97	110.63
3	H	29	TRP	CA-C-O	-5.67	112.56	119.43
3	H	176	ILE	N-CA-CB	-5.67	104.57	111.21
1	D	413	DT	O4'-C1'-N1	5.67	116.90	108.40
3	H	153	SER	CA-C-N	5.67	130.74	123.03
3	H	153	SER	C-N-CA	5.67	130.74	123.03
3	H	73	ARG	CB-CA-C	-5.67	99.79	110.67
3	H	36	LYS	C-N-CA	5.66	135.84	121.70
3	H	128	THR	CA-C-N	5.65	128.11	120.65
3	H	128	THR	C-N-CA	5.65	128.11	120.65
3	H	31	VAL	N-CA-C	5.64	117.25	109.46
3	H	172	THR	CA-C-N	5.63	128.09	120.38
3	H	172	THR	C-N-CA	5.63	128.09	120.38
3	H	23	GLU	CB-CG-CD	5.62	122.15	112.60
3	H	77(A)	ARG	NE-CZ-NH2	5.60	124.24	119.20
3	H	172	THR	O-C-N	5.60	130.10	123.33
2	L	7	PHE	CA-CB-CG	-5.58	108.22	113.80
3	H	137	ARG	CD-NE-CZ	5.57	132.20	124.40
3	H	17	VAL	CA-CB-CG1	5.54	119.82	110.40
2	L	14(J)	TYR	N-CA-C	-5.54	99.00	110.80
3	H	132	ALA	O-C-N	5.54	129.73	122.97
3	H	140	GLY	O-C-N	-5.54	117.01	123.44
3	H	224	LYS	O-C-N	5.53	130.24	123.10
3	H	173	ARG	O-C-N	5.53	127.98	122.12
3	H	161	PRO	O-C-N	5.50	130.07	122.64
3	H	126	ARG	CA-CB-CG	5.50	125.09	114.10
3	H	210	MET	CB-CA-C	5.50	121.79	110.31
3	H	161	PRO	CB-CA-C	-5.49	102.50	111.56
3	H	233	ARG	CA-C-N	5.49	130.17	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	233	ARG	C-N-CA	5.49	130.17	121.44
1	D	405	DG	P-O5'-C5'	-5.47	111.79	120.00
3	H	132	ALA	CA-C-O	-5.46	115.14	121.15
3	H	131	GLN	CB-CG-CD	-5.46	103.31	112.60
3	H	207	TRP	CA-C-O	-5.46	114.81	120.70
1	D	403	DT	P-O3'-C3'	-5.45	112.02	120.20
3	H	155	LEU	CA-C-N	5.45	132.65	122.74
3	H	155	LEU	C-N-CA	5.45	132.65	122.74
3	H	124	PRO	O-C-N	5.44	129.99	122.64
3	H	223	GLY	CA-C-N	-5.42	113.38	122.92
3	H	223	GLY	C-N-CA	-5.42	113.38	122.92
3	H	223	GLY	N-CA-C	-5.41	107.14	116.01
3	H	39	GLU	O-C-N	5.38	129.29	123.10
3	H	152	PRO	N-CA-C	5.38	119.03	111.33
3	H	242	ILE	CB-CA-C	5.36	119.62	112.22
3	H	241	VAL	O-C-N	5.35	127.14	121.89
3	H	187	ARG	NE-CZ-NH2	5.35	124.01	119.20
3	H	204(A)	PHE	N-CA-C	5.35	119.74	111.56
3	H	143	ASN	CA-CB-CG	-5.34	107.26	112.60
3	H	25	GLY	N-CA-C	5.34	122.57	114.61
3	H	226	GLY	O-C-N	5.33	129.35	123.49
3	H	238	ILE	CA-C-O	-5.32	114.13	120.78
3	H	97	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
3	H	23	GLU	CA-CB-CG	5.30	124.71	114.10
3	H	31	VAL	CA-C-N	-5.29	114.76	122.44
3	H	31	VAL	C-N-CA	-5.29	114.76	122.44
3	H	81	LYS	CA-C-N	5.29	129.52	122.01
3	H	81	LYS	C-N-CA	5.29	129.52	122.01
3	H	125	ASP	N-CA-C	-5.28	101.26	109.24
3	H	91	HIS	CA-C-O	5.26	125.50	119.61
2	L	14(L)	ASP	CA-C-N	-5.25	105.71	116.20
3	H	60(I)	THR	N-CA-C	5.25	118.36	109.76
3	H	123	LEU	N-CA-C	-5.24	101.95	109.24
3	H	50	ARG	NE-CZ-NH1	-5.24	116.26	121.50
3	H	141	TRP	CB-CA-C	-5.21	103.85	111.77
3	H	122	CYS	O-C-N	5.20	129.13	123.04
3	H	105	LEU	CA-C-N	-5.20	115.44	122.77
3	H	105	LEU	C-N-CA	-5.20	115.44	122.77
3	H	225	TYR	O-C-N	5.18	130.35	122.94
3	H	209	GLN	N-CA-C	5.18	117.75	108.17
1	D	410	DG	C5'-C4'-C3'	5.15	122.62	114.90
2	L	14	ASP	N-CA-C	5.14	117.49	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	212	ILE	CA-C-N	-5.13	114.61	121.80
3	H	212	ILE	C-N-CA	-5.13	114.61	121.80
1	D	402	DG	C2'-C3'-O3'	5.13	119.19	111.50
3	H	65	LEU	CA-C-N	-5.13	114.30	122.50
3	H	65	LEU	C-N-CA	-5.13	114.30	122.50
3	H	186(A)	ASP	N-CA-C	-5.13	104.43	111.81
3	H	114	PHE	CA-CB-CG	-5.12	108.68	113.80
3	H	127	GLU	CG-CD-OE2	-5.12	106.61	118.40
3	H	162	ILE	CA-CB-CG2	5.12	119.20	110.50
3	H	229	THR	O-C-N	-5.11	117.39	123.22
3	H	224	LYS	CA-C-N	-5.11	113.89	123.03
3	H	224	LYS	C-N-CA	-5.11	113.89	123.03
3	H	41	LEU	O-C-N	5.10	128.13	122.11
2	L	14(C)	GLU	CA-C-N	-5.10	105.98	117.20
3	H	60(D)	TRP	N-CA-CB	5.09	119.06	110.92
3	H	221(A)	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	411	DG	P-O5'-C5'	5.09	127.63	120.00
3	H	127	GLU	CA-CB-CG	-5.09	103.93	114.10
3	H	191	CYS	O-C-N	5.09	128.38	123.29
3	H	60(D)	TRP	N-CA-C	-5.08	106.39	112.59
3	H	60(I)	THR	CA-C-N	5.07	131.23	121.54
3	H	60(I)	THR	C-N-CA	5.07	131.23	121.54
3	H	35	ARG	CB-CA-C	5.07	118.09	109.53
2	L	14(D)	ARG	CA-C-O	-5.06	113.27	120.51
3	H	154	VAL	O-C-N	5.04	128.55	122.95
1	D	413	DT	OP1-P-OP2	-5.02	104.93	120.00
1	D	405	DG	O5'-C5'-C4'	5.02	118.33	110.80
3	H	226	GLY	N-CA-C	-5.01	101.78	110.71
3	H	80	GLU	CB-CA-C	-5.01	102.33	109.84
3	H	42	CYS	CA-C-O	5.00	126.30	121.14
1	D	413	DT	O4'-C1'-C2'	-5.00	98.90	106.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	153	SER	Mainchain
3	H	200	VAL	Mainchain
3	H	36	LYS	Mainchain
3	H	63	ASP	Mainchain
3	H	64	LEU	Mainchain
3	H	81	LYS	Mainchain

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Mol	Chain	Res	Type	Group
2	L	14(K)	ILE	Mainchain

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	107	0
2	L	287	0	278	78	0
3	H	2053	0	2020	525	0
4	H	30	0	27	20	0
5	D	25	0	0	2	0
5	H	90	0	0	6	0
5	L	15	0	0	2	0
All	All	2815	0	2498	630	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 122.

All (630) 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)
1:D:408:DG:C8	3:H:75:ARG:HD2	1.43	1.53
1:D:407:DT:H3'	1:D:407:DT:C6	1.41	1.44
1:D:408:DG:H8	3:H:75:ARG:CD	1.34	1.41
1:D:407:DT:C6	1:D:407:DT:C3'	2.09	1.34
3:H:60(I):THR:O	3:H:63:ASP:HB2	1.22	1.28
2:L:1(E):SER:HA	2:L:1:CYS:SG	1.78	1.21
3:H:25:GLY:O	3:H:28:PRO:HD3	1.36	1.19
1:D:404:DT:O4	1:D:412:DT:H5'	1.46	1.16
2:L:7:PHE:CE1	2:L:12:LEU:HD22	1.80	1.16
3:H:68:ILE:CG2	3:H:118:ILE:HG23	1.76	1.15
3:H:47:ILE:HG12	3:H:51:TRP:O	1.49	1.12
3:H:61:GLU:O	3:H:85:LEU:HD21	1.50	1.12
3:H:21:ASP:OD1	3:H:154:VAL:HG23	1.50	1.11
3:H:60:LEU:HD23	3:H:60(B):PRO:HD3	1.28	1.11
3:H:42:CYS:HB2	3:H:195:SER:O	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60:LEU:CD2	3:H:60(B):PRO:HD3	1.81	1.09
3:H:95:ASN:HB2	5:H:505:HOH:O	1.53	1.05
1:D:408:DG:H5''	3:H:75:ARG:NH2	1.70	1.04
3:H:169:LYS:HA	3:H:176:ILE:HD13	1.37	1.04
3:H:129:ALA:HA	3:H:210:MET:HE1	1.35	1.04
1:D:408:DG:C8	3:H:75:ARG:HB2	1.92	1.04
2:L:1(E):SER:HB3	5:L:501:HOH:O	1.57	1.03
3:H:234:LEU:HD23	3:H:237:TRP:HB3	1.40	1.03
3:H:103:ILE:HG12	3:H:237:TRP:HZ3	1.23	1.02
3:H:36:LYS:NZ	3:H:62:ASN:O	1.93	1.02
1:D:407:DT:C6	1:D:407:DT:C4'	2.40	1.01
2:L:7:PHE:HE1	2:L:12:LEU:HD22	1.17	1.01
3:H:103:ILE:HG12	3:H:237:TRP:CZ3	1.95	1.01
2:L:14(J):TYR:O	2:L:14(L):ASP:N	1.92	1.01
1:D:408:DG:C5'	3:H:75:ARG:NH2	2.24	1.01
3:H:60(A):TYR:H	3:H:60(F):LYS:HB2	1.25	1.00
3:H:60(A):TYR:HB3	3:H:60(F):LYS:HG3	1.41	1.00
1:D:408:DG:C8	3:H:75:ARG:CD	2.20	1.00
2:L:1(H):THR:HG22	2:L:1(G):PHE:H	1.22	1.00
1:D:410:DG:H1'	3:H:77(A):ARG:NH1	1.77	0.99
3:H:100:ASP:HB3	3:H:101:ARG:HH21	1.28	0.98
3:H:181:PHE:HE1	3:H:230:HIS:HA	1.22	0.98
3:H:160:LEU:HD23	3:H:184(A):TYR:CE1	1.99	0.98
1:D:405:DG:H2'	1:D:405:DG:N3	1.75	0.98
3:H:41:LEU:N	3:H:41:LEU:HD12	1.76	0.98
3:H:48:SER:HB3	3:H:51:TRP:H	1.29	0.98
2:L:14(J):TYR:CD1	3:H:134:TYR:CD2	2.52	0.97
3:H:128:THR:O	3:H:129(C):LEU:HB2	1.64	0.97
1:D:408:DG:H5''	3:H:75:ARG:CZ	1.94	0.96
3:H:110:LYS:HB3	3:H:111:PRO:HD2	1.48	0.96
2:L:15:ARG:HH11	2:L:15:ARG:HA	1.24	0.95
3:H:68:ILE:HG22	3:H:118:ILE:HG23	1.47	0.95
1:D:401:DG:H2''	1:D:402:DG:O5'	1.68	0.94
2:L:15:ARG:HA	2:L:15:ARG:NH1	1.82	0.94
3:H:42:CYS:CB	3:H:195:SER:O	2.16	0.92
3:H:71:HIS:CE1	3:H:154:VAL:HG11	2.03	0.92
3:H:211:GLY:HA2	3:H:231:VAL:HG23	1.51	0.92
1:D:406:DG:N7	1:D:410:DG:N2	2.17	0.92
2:L:14(F):LEU:HD11	3:H:159:ASN:ND2	1.83	0.92
1:D:408:DG:C8	3:H:75:ARG:CB	2.53	0.91
3:H:48:SER:HB2	3:H:51:TRP:HB2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:99:LEU:CD1	3:H:215:TRP:HB3	2.00	0.90
1:D:407:DT:H3	3:H:77:GLU:HG2	1.33	0.90
3:H:50:ARG:HD3	3:H:247:GLU:HB3	1.52	0.90
1:D:402:DG:N2	1:D:405:DG:N7	2.19	0.90
2:L:1(A):ASP:OD1	2:L:1(A):ASP:O	1.88	0.89
3:H:60(I):THR:O	3:H:63:ASP:CB	2.16	0.89
3:H:221(A):ARG:HB3	3:H:224:LYS:HB2	1.55	0.89
3:H:60(A):TYR:CZ	4:H:1:OG7:HG1	2.08	0.89
3:H:172:THR:CG2	3:H:174:ILE:HG13	2.04	0.88
3:H:147:THR:HG22	5:H:589:HOH:O	1.74	0.88
3:H:30:GLN:NE2	3:H:139:THR:O	2.07	0.88
3:H:48:SER:HB3	3:H:51:TRP:N	1.89	0.88
3:H:31:VAL:HG13	3:H:66:VAL:CG2	2.03	0.87
1:D:407:DT:O4'	1:D:409:DT:N3	2.07	0.87
3:H:213:VAL:HG13	3:H:228:TYR:CE2	2.09	0.87
1:D:407:DT:C4'	1:D:407:DT:H6	1.82	0.87
1:D:403:DT:C2'	1:D:404:DT:OP2	2.23	0.87
3:H:115:SER:O	3:H:118:ILE:CD1	2.22	0.86
2:L:14(G):LEU:HD11	3:H:202:LYS:HG2	1.56	0.86
3:H:103:ILE:HG13	3:H:104:ALA:N	1.91	0.85
3:H:32:MET:HB3	3:H:67:ARG:HB2	1.58	0.85
1:D:407:DT:C2	3:H:79:ILE:HG12	2.12	0.85
3:H:54:THR:HG22	3:H:55:ALA:H	1.41	0.85
3:H:162:ILE:HD11	3:H:201:MET:CE	2.06	0.85
1:D:403:DT:H2''	1:D:404:DT:OP2	1.77	0.85
3:H:58:CYS:C	3:H:59:LEU:HD12	2.02	0.84
3:H:212:ILE:O	3:H:228:TYR:HB3	1.76	0.84
3:H:157:VAL:HG23	3:H:157:VAL:O	1.78	0.84
3:H:77:GLU:CB	3:H:79:ILE:HB	2.06	0.83
3:H:41:LEU:N	3:H:41:LEU:CD1	2.40	0.83
1:D:410:DG:H4'	3:H:77(A):ARG:HH12	1.43	0.83
3:H:77:GLU:HB3	3:H:79:ILE:HB	1.61	0.83
3:H:103:ILE:HG13	3:H:104:ALA:H	1.44	0.83
3:H:144:LEU:HD21	3:H:152:PRO:HG3	1.61	0.83
1:D:402:DG:O6	1:D:414:DG:N1	2.12	0.83
3:H:57:HIS:CE1	4:H:1:OG7:O1	2.32	0.83
1:D:414:DG:H2'	1:D:415:DG:C8	2.14	0.82
3:H:61:GLU:OE2	3:H:87:LYS:HD3	1.79	0.82
1:D:403:DT:C2'	1:D:403:DT:O2	2.26	0.82
3:H:51:TRP:CE2	3:H:242:ILE:HG23	2.15	0.82
1:D:407:DT:H1'	1:D:409:DT:C2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60(A):TYR:C	3:H:60(C):PRO:HD2	2.05	0.82
3:H:185:LYS:O	3:H:186(B):GLU:HB3	1.79	0.82
1:D:404:DT:O4	1:D:412:DT:C5'	2.27	0.81
3:H:86:GLU:CB	3:H:109:LYS:HD3	2.10	0.81
3:H:35:ARG:NH2	3:H:36:LYS:HG2	1.95	0.81
3:H:169:LYS:HA	3:H:176:ILE:CD1	2.11	0.81
3:H:177:THR:HG22	3:H:179:ASN:H	1.45	0.81
2:L:1(F):GLY:HA2	3:H:123:LEU:O	1.80	0.81
1:D:407:DT:H3'	1:D:407:DT:C5	2.13	0.81
2:L:14(G):LEU:CD1	3:H:202:LYS:HG2	2.11	0.81
3:H:73:ARG:NH1	3:H:74:THR:HG23	1.95	0.81
1:D:411:DG:H1'	1:D:412:DT:H5''	1.63	0.81
3:H:91:HIS:HB3	3:H:103:ILE:HG23	1.62	0.80
3:H:94:TYR:HB2	3:H:101:ARG:O	1.80	0.80
2:L:1(H):THR:CG2	2:L:1(G):PHE:H	1.95	0.80
3:H:60(A):TYR:N	3:H:60(F):LYS:HB2	1.97	0.79
2:L:1(E):SER:CA	2:L:1:CYS:SG	2.68	0.79
3:H:157:VAL:O	3:H:157:VAL:CG2	2.30	0.79
3:H:46:LEU:O	3:H:121:VAL:HG12	1.83	0.79
3:H:190:ALA:CB	3:H:213:VAL:HG11	2.12	0.79
3:H:211:GLY:CA	3:H:231:VAL:HG23	2.12	0.79
3:H:164:GLU:HB2	3:H:166:PRO:HD2	1.65	0.79
1:D:405:DG:N3	1:D:405:DG:C2'	2.45	0.78
3:H:115:SER:O	3:H:118:ILE:HD12	1.83	0.78
3:H:86:GLU:HB2	3:H:109:LYS:HD3	1.63	0.78
3:H:127:GLU:O	3:H:129(B):SER:OG	2.02	0.77
1:D:407:DT:N3	3:H:77:GLU:HG2	1.99	0.77
3:H:60(B):PRO:HG2	3:H:96:TRP:CE2	2.19	0.77
1:D:405:DG:H1'	1:D:406:DG:H5'	1.67	0.77
3:H:32:MET:HE2	3:H:40:LEU:HD13	1.64	0.77
3:H:68:ILE:CG2	3:H:118:ILE:CG2	2.60	0.77
3:H:110:LYS:HB3	3:H:111:PRO:CD	2.15	0.77
3:H:46:LEU:HD21	3:H:114:PHE:CE1	2.20	0.77
3:H:85:LEU:O	3:H:85:LEU:HD23	1.83	0.77
1:D:408:DG:N7	3:H:75:ARG:HD2	1.96	0.77
2:L:14(J):TYR:HD1	3:H:134:TYR:CD2	2.03	0.76
3:H:21:ASP:OD1	3:H:154:VAL:CG2	2.31	0.76
3:H:183:ALA:HB3	3:H:228:TYR:CE1	2.19	0.76
3:H:25:GLY:HA2	5:H:506:HOH:O	1.86	0.76
3:H:136:GLY:HA3	3:H:199:PHE:CE1	2.20	0.76
3:H:244:GLN:OE1	3:H:244:GLN:HA	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:DT:H6	1:D:407:DT:C5'	1.99	0.75
3:H:77:GLU:O	3:H:77(A):ARG:C	2.29	0.75
2:L:14(J):TYR:O	2:L:14(K):ILE:C	2.29	0.75
3:H:99:LEU:HG	4:H:1:0G7:CZ	2.17	0.75
1:D:408:DG:N7	3:H:75:ARG:HB2	2.02	0.75
2:L:1(A):ASP:O	2:L:1(A):ASP:CG	2.29	0.75
3:H:177:THR:HG22	3:H:179:ASN:N	2.02	0.75
3:H:88:ILE:HG12	3:H:88:ILE:O	1.87	0.74
3:H:98:ASN:HA	4:H:1:0G7:HZ	1.69	0.74
3:H:98:ASN:ND2	3:H:175:ARG:O	2.20	0.74
3:H:41:LEU:CD1	3:H:41:LEU:H	2.01	0.74
3:H:162:ILE:HD11	3:H:201:MET:HE1	1.69	0.74
3:H:68:ILE:HG21	3:H:118:ILE:HG23	1.67	0.73
3:H:160:LEU:HD23	3:H:184(A):TYR:HE1	1.53	0.73
2:L:14(D):ARG:O	2:L:14(H):GLU:HG3	1.88	0.73
1:D:408:DG:H5'	3:H:75:ARG:NH2	2.04	0.73
3:H:181:PHE:CE1	3:H:230:HIS:HA	2.15	0.73
3:H:35:ARG:HE	3:H:36:LYS:N	1.86	0.73
3:H:204(B):ASN:ND2	3:H:206:ARG:HG3	2.03	0.73
3:H:48:SER:CB	3:H:51:TRP:HB2	2.18	0.73
3:H:73:ARG:HB2	3:H:141:TRP:CD1	2.24	0.73
3:H:164:GLU:OE1	3:H:167:VAL:HG23	1.89	0.73
3:H:172:THR:HG21	3:H:174:ILE:HG13	1.68	0.73
3:H:60(I):THR:O	3:H:64:LEU:HD12	1.89	0.72
3:H:189:ASP:CG	4:H:1:0G7:NH2	2.47	0.72
3:H:195:SER:OG	4:H:1:0G7:C3	2.37	0.72
1:D:408:DG:O4'	3:H:75:ARG:NE	2.23	0.72
1:D:409:DT:C5'	3:H:77(A):ARG:HB3	2.20	0.72
3:H:213:VAL:HG13	3:H:228:TYR:CD2	2.24	0.72
3:H:99:LEU:HD12	3:H:215:TRP:CG	2.24	0.72
1:D:408:DG:N7	3:H:75:ARG:CB	2.52	0.72
3:H:35:ARG:HE	3:H:36:LYS:H	1.38	0.72
3:H:165:ARG:HH12	3:H:178:ASP:HA	1.54	0.72
1:D:404:DT:H71	1:D:411:DG:H2''	1.71	0.71
3:H:55:ALA:O	3:H:58:CYS:HB2	1.88	0.71
3:H:165:ARG:NH1	3:H:178:ASP:HA	2.06	0.71
3:H:100:ASP:OD1	3:H:177:THR:HG21	1.89	0.71
3:H:87:LYS:O	3:H:107:LYS:N	2.23	0.71
3:H:144:LEU:C	3:H:145:LYS:HG2	2.12	0.71
1:D:404:DT:O4	1:D:412:DT:H3'	1.91	0.71
1:D:407:DT:C1'	1:D:409:DT:N3	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:54:THR:HG22	3:H:55:ALA:N	2.06	0.71
3:H:122:CYS:O	3:H:208:TYR:HA	1.91	0.71
3:H:66:VAL:CG1	3:H:83:SER:HB2	2.21	0.71
1:D:408:DG:H8	3:H:75:ARG:CG	2.03	0.71
2:L:3:LEU:HD22	3:H:206:ARG:HH11	1.55	0.71
3:H:67:ARG:NH2	3:H:80:GLU:OE2	2.24	0.70
3:H:211:GLY:HA2	3:H:231:VAL:CG2	2.20	0.70
2:L:1(G):PHE:CD1	3:H:239:GLN:HB2	2.27	0.70
3:H:128:THR:O	3:H:129(C):LEU:CB	2.40	0.70
3:H:61:GLU:C	3:H:85:LEU:HD21	2.16	0.70
3:H:95:ASN:HD21	3:H:97(A):GLU:CB	2.04	0.70
3:H:144:LEU:HD11	3:H:152:PRO:HD3	1.73	0.70
3:H:161:PRO:HD2	3:H:184:GLY:O	1.91	0.70
3:H:162:ILE:CD1	3:H:201:MET:HE1	2.22	0.69
3:H:17:VAL:HG22	3:H:144:LEU:C	2.17	0.69
3:H:87:LYS:O	3:H:106:MET:HA	1.91	0.69
3:H:95:ASN:HD21	3:H:97(A):GLU:HB2	1.57	0.69
3:H:68:ILE:HG21	3:H:118:ILE:CG2	2.22	0.69
1:D:407:DT:O4	3:H:71:HIS:HB2	1.93	0.69
3:H:47:ILE:HD13	3:H:53:LEU:HD23	1.74	0.69
3:H:211:GLY:CA	3:H:231:VAL:CG2	2.71	0.69
1:D:406:DG:C8	1:D:409:DT:OP2	2.47	0.68
2:L:14(F):LEU:C	2:L:14(H):GLU:H	1.98	0.68
1:D:401:DG:O5'	5:D:526:HOH:O	2.01	0.68
3:H:91:HIS:HB2	3:H:237:TRP:CE2	2.29	0.68
3:H:17:VAL:O	3:H:18:GLU:C	2.34	0.68
1:D:407:DT:H73	3:H:24:ILE:HG22	1.75	0.68
3:H:232:PHE:C	3:H:234:LEU:H	2.00	0.68
3:H:31:VAL:HG13	3:H:66:VAL:HG23	1.75	0.67
3:H:60(A):TYR:CE2	4:H:1:OG7:HG1	2.30	0.67
3:H:118:ILE:HD12	3:H:118:ILE:N	2.10	0.67
1:D:407:DT:H2'	1:D:408:DG:O5'	1.95	0.67
1:D:408:DG:C8	3:H:75:ARG:CG	2.76	0.67
3:H:21:ASP:CG	3:H:154:VAL:HG23	2.19	0.67
3:H:181:PHE:HE1	3:H:230:HIS:CA	2.02	0.67
1:D:408:DG:H8	3:H:75:ARG:NE	1.91	0.67
3:H:67:ARG:HG2	3:H:82:ILE:HG12	1.77	0.67
3:H:172:THR:HG23	3:H:174:ILE:HG13	1.76	0.67
3:H:189:ASP:OD2	4:H:1:OG7:NH2	2.27	0.67
2:L:1(H):THR:O	2:L:1(G):PHE:O	2.13	0.67
3:H:46:LEU:HD21	3:H:114:PHE:HE1	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:15:ARG:NH1	3:H:204:PRO:O	2.28	0.66
3:H:31:VAL:HB	3:H:44:ALA:O	1.94	0.66
3:H:60:LEU:HD23	3:H:60:LEU:C	2.20	0.66
3:H:66:VAL:HG12	3:H:83:SER:HB2	1.76	0.66
3:H:87:LYS:HD3	3:H:88:ILE:H	1.60	0.66
3:H:60(B):PRO:HG2	3:H:96:TRP:CD2	2.30	0.66
1:D:401:DG:H2''	1:D:402:DG:O4'	1.95	0.66
3:H:31:VAL:CG1	3:H:66:VAL:HG23	2.26	0.66
1:D:408:DG:H1'	3:H:77:GLU:HA	1.78	0.66
3:H:99:LEU:HD12	3:H:215:TRP:CB	2.26	0.66
3:H:17:VAL:HG22	3:H:144:LEU:O	1.96	0.65
3:H:35:ARG:N	3:H:41:LEU:HD11	2.12	0.65
3:H:144:LEU:HD12	3:H:150:GLY:C	2.21	0.65
2:L:8:GLU:C	2:L:10:LYS:H	2.04	0.65
3:H:177:THR:CG2	3:H:179:ASN:HB2	2.27	0.65
3:H:45:SER:O	3:H:47:ILE:HG23	1.95	0.65
1:D:402:DG:C2'	1:D:403:DT:H5''	2.27	0.65
2:L:14(F):LEU:C	2:L:14(H):GLU:N	2.54	0.65
2:L:14(F):LEU:CD1	3:H:159:ASN:ND2	2.58	0.65
3:H:100:ASP:CB	3:H:101:ARG:HH21	2.08	0.65
2:L:14(I):SER:O	5:L:521:HOH:O	2.13	0.64
1:D:406:DG:N2	3:H:75:ARG:NH2	2.45	0.64
3:H:22:ALA:HB2	3:H:157:VAL:CG1	2.28	0.64
1:D:407:DT:H1'	1:D:409:DT:O2	1.96	0.64
3:H:99:LEU:CD1	3:H:215:TRP:CB	2.75	0.64
1:D:402:DG:H2'	1:D:403:DT:H5''	1.78	0.64
3:H:41:LEU:HD12	3:H:41:LEU:H	1.58	0.64
3:H:99:LEU:HD13	3:H:215:TRP:HB3	1.79	0.64
3:H:234:LEU:CD2	3:H:237:TRP:HB3	2.21	0.64
3:H:103:ILE:CG1	3:H:104:ALA:N	2.61	0.64
3:H:31:VAL:CG1	3:H:66:VAL:CG2	2.76	0.64
1:D:411:DG:N2	1:D:412:DT:H2'	2.12	0.63
1:D:406:DG:C2	3:H:75:ARG:NH2	2.66	0.63
2:L:14(F):LEU:O	2:L:14(H):GLU:N	2.32	0.63
3:H:35:ARG:HH21	3:H:36:LYS:H	1.44	0.63
3:H:56:ALA:O	3:H:59:LEU:N	2.31	0.63
3:H:99:LEU:HD12	3:H:215:TRP:HB3	1.80	0.63
3:H:142:GLY:O	3:H:143:ASN:C	2.42	0.63
3:H:177:THR:HG22	3:H:179:ASN:HB2	1.81	0.63
3:H:56:ALA:HB2	3:H:90:ILE:HG22	1.81	0.63
1:D:403:DT:O2	1:D:403:DT:H2'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:PHE:CD1	2:L:12:LEU:HB3	2.34	0.63
1:D:407:DT:O2	3:H:77:GLU:HG3	1.98	0.63
3:H:91:HIS:C	3:H:91:HIS:CD2	2.77	0.63
3:H:214:SER:OG	3:H:229:THR:HG23	1.99	0.63
2:L:8:GLU:O	2:L:10:LYS:N	2.32	0.62
3:H:162:ILE:HD11	3:H:201:MET:HE3	1.80	0.62
3:H:30:GLN:HE22	3:H:139:THR:C	2.04	0.62
3:H:115:SER:O	3:H:118:ILE:HD13	1.96	0.62
3:H:130:LEU:HD12	3:H:130:LEU:O	1.99	0.62
3:H:115:SER:O	3:H:117:TYR:N	2.32	0.62
3:H:21:ASP:CG	3:H:154:VAL:CG2	2.73	0.62
3:H:190:ALA:H	4:H:1:OG7:HNHA	1.45	0.62
3:H:60(B):PRO:N	3:H:60(C):PRO:CD	2.62	0.62
3:H:86:GLU:HB3	3:H:109:LYS:HD3	1.80	0.62
2:L:14(F):LEU:HD11	3:H:159:ASN:HD22	1.63	0.62
3:H:33:LEU:HD12	3:H:42:CYS:SG	2.40	0.62
3:H:150:GLY:N	3:H:151:GLN:NE2	2.47	0.62
3:H:16:ILE:HG12	3:H:158:VAL:HG12	1.82	0.61
3:H:123:LEU:HG	3:H:235:LYS:HD3	1.82	0.61
3:H:73:ARG:HH12	3:H:74:THR:HG23	1.61	0.61
1:D:409:DT:H5'	3:H:77(A):ARG:HB3	1.81	0.61
3:H:91:HIS:HB3	3:H:103:ILE:CG2	2.30	0.61
1:D:407:DT:O4'	1:D:409:DT:C4	2.54	0.61
3:H:60(B):PRO:N	3:H:60(C):PRO:HD2	2.15	0.61
2:L:1(H):THR:HG22	2:L:1(G):PHE:CD1	2.36	0.61
3:H:47:ILE:CD1	3:H:53:LEU:HD23	2.30	0.61
3:H:31:VAL:CG1	3:H:44:ALA:HB3	2.31	0.61
3:H:54:THR:CG2	3:H:55:ALA:H	2.09	0.61
3:H:61:GLU:O	3:H:85:LEU:CD2	2.39	0.61
3:H:22:ALA:HB2	3:H:157:VAL:HG13	1.82	0.60
2:L:1(F):GLY:O	2:L:1(D):GLY:N	2.34	0.60
3:H:51:TRP:HZ2	3:H:245:PHE:O	1.84	0.60
1:D:403:DT:H2''	1:D:403:DT:O2	2.00	0.60
2:L:6:LEU:HD12	3:H:24:ILE:HB	1.82	0.60
3:H:211:GLY:HA2	3:H:229:THR:O	2.00	0.60
3:H:110:LYS:NZ	5:H:518:HOH:O	2.34	0.60
1:D:413:DT:H1'	1:D:414:DG:N2	2.16	0.60
3:H:35:ARG:N	3:H:39:GLU:O	2.34	0.60
3:H:73:ARG:HB2	3:H:141:TRP:HD1	1.64	0.60
2:L:1:CYS:C	3:H:122:CYS:SG	2.84	0.60
3:H:186(B):GLU:O	3:H:186(D):LYS:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:PRO:HB2	3:H:119:HIS:HB3	1.84	0.60
3:H:221:ASP:O	3:H:221(A):ARG:C	2.44	0.59
3:H:129:ALA:HA	3:H:210:MET:CE	2.21	0.59
3:H:190:ALA:HB3	3:H:213:VAL:HG11	1.84	0.59
3:H:137:ARG:HG3	3:H:137:ARG:O	2.01	0.59
3:H:86:GLU:HB2	3:H:109:LYS:CD	2.33	0.59
1:D:407:DT:O2	3:H:77:GLU:CG	2.50	0.59
3:H:164:GLU:OE1	3:H:167:VAL:CG2	2.51	0.59
3:H:60(A):TYR:CB	3:H:60(F):LYS:HG3	2.26	0.59
2:L:13:GLU:OE2	2:L:14(D):ARG:HG3	2.03	0.59
3:H:31:VAL:HB	3:H:44:ALA:HB3	1.83	0.59
3:H:56:ALA:HB1	3:H:90:ILE:HG21	1.85	0.59
1:D:407:DT:C2	3:H:77:GLU:HG2	2.38	0.59
3:H:234:LEU:O	3:H:238:ILE:HD12	2.03	0.58
3:H:24:ILE:HG12	3:H:24:ILE:O	2.03	0.58
3:H:211:GLY:N	3:H:231:VAL:HG23	2.19	0.58
1:D:411:DG:N2	1:D:412:DT:C2'	2.67	0.58
3:H:147:THR:HG23	3:H:148:TRP:H	1.69	0.58
3:H:232:PHE:O	3:H:235:LYS:N	2.20	0.58
1:D:411:DG:H21	1:D:412:DT:H2'	1.69	0.58
3:H:49:ASP:O	3:H:111:PRO:HA	2.04	0.57
3:H:56:ALA:HB1	3:H:90:ILE:CG2	2.34	0.57
3:H:56:ALA:CB	3:H:90:ILE:CG2	2.82	0.57
2:L:1(F):GLY:C	2:L:1(D):GLY:N	2.60	0.57
3:H:35:ARG:HH22	3:H:36:LYS:HG2	1.69	0.57
3:H:234:LEU:O	3:H:238:ILE:CD1	2.52	0.57
3:H:86:GLU:HG2	3:H:107:LYS:HG2	1.87	0.57
1:D:406:DG:N7	1:D:409:DT:OP2	2.37	0.57
1:D:411:DG:C2	1:D:412:DT:H2'	2.39	0.57
3:H:57:HIS:NE2	4:H:1:OG7:C3	2.68	0.57
3:H:88:ILE:HG22	3:H:106:MET:HG2	1.86	0.57
3:H:183:ALA:HB2	3:H:199:PHE:HE2	1.70	0.57
3:H:36:LYS:CE	3:H:62:ASN:O	2.51	0.57
2:L:14(G):LEU:HD11	3:H:202:LYS:CG	2.31	0.57
3:H:147:THR:CG2	3:H:148:TRP:N	2.68	0.56
2:L:8:GLU:C	2:L:10:LYS:N	2.61	0.56
3:H:91:HIS:HB2	3:H:237:TRP:CD2	2.39	0.56
1:D:409:DT:O4'	1:D:409:DT:P	2.64	0.56
2:L:14:ASP:O	2:L:14(A):LYS:C	2.47	0.56
2:L:14(J):TYR:CD1	3:H:134:TYR:HD2	2.21	0.56
3:H:159:ASN:C	3:H:160:LEU:HG	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:177:THR:C	3:H:179:ASN:H	2.13	0.56
3:H:209:GLN:O	3:H:231:VAL:HB	2.06	0.56
3:H:61:GLU:OE2	3:H:88:ILE:HD13	2.05	0.55
3:H:160:LEU:CD2	3:H:184(A):TYR:CE1	2.83	0.55
3:H:162:ILE:CD1	3:H:201:MET:CE	2.80	0.55
3:H:163:VAL:HB	3:H:182:CYS:SG	2.46	0.55
3:H:172:THR:CG2	3:H:174:ILE:CG1	2.82	0.55
1:D:404:DT:C7	1:D:411:DG:H2''	2.34	0.55
3:H:95:ASN:OD1	3:H:97(A):GLU:N	2.37	0.55
3:H:150:GLY:C	3:H:151:GLN:NE2	2.64	0.55
1:D:407:DT:C7	3:H:24:ILE:HG22	2.37	0.55
3:H:24:ILE:HD13	3:H:24:ILE:H	1.71	0.55
3:H:123:LEU:CD2	3:H:235:LYS:HD3	2.36	0.55
3:H:144:LEU:HD21	3:H:152:PRO:CG	2.35	0.55
3:H:60(D):TRP:HE3	3:H:60(F):LYS:HE3	1.72	0.55
3:H:180:MET:CE	3:H:215:TRP:HE1	2.20	0.55
3:H:56:ALA:CB	3:H:90:ILE:HG22	2.36	0.55
3:H:234:LEU:HD23	3:H:237:TRP:CB	2.26	0.55
3:H:126:ARG:O	3:H:129(A):ALA:HB2	2.06	0.55
3:H:234:LEU:C	3:H:236:LYS:N	2.64	0.55
2:L:4:ARG:HG2	3:H:28:PRO:CG	2.37	0.55
3:H:31:VAL:HG13	3:H:66:VAL:HG22	1.87	0.55
3:H:212:ILE:C	3:H:228:TYR:HB3	2.31	0.55
3:H:42:CYS:HB3	3:H:195:SER:O	2.02	0.55
3:H:91:HIS:CD2	3:H:93:ARG:H	2.25	0.55
3:H:169:LYS:C	3:H:171:SER:H	2.15	0.55
3:H:61:GLU:OE2	3:H:87:LYS:CD	2.54	0.54
3:H:60(D):TRP:CE3	3:H:60(F):LYS:HE3	2.43	0.54
3:H:31:VAL:CG1	3:H:32:MET:N	2.70	0.54
3:H:60(H):PHE:HB3	3:H:64:LEU:HD21	1.88	0.54
3:H:35:ARG:HG2	3:H:39:GLU:OE2	2.08	0.54
3:H:60(A):TYR:N	3:H:60(F):LYS:O	2.40	0.54
1:D:408:DG:N7	3:H:75:ARG:HB3	2.23	0.54
1:D:413:DT:H1'	1:D:414:DG:H21	1.73	0.54
2:L:4:ARG:HG2	3:H:28:PRO:HG2	1.90	0.54
3:H:206:ARG:HB2	3:H:208:TYR:HE1	1.72	0.54
1:D:407:DT:O2	3:H:79:ILE:HG12	2.08	0.53
3:H:123:LEU:HD21	3:H:238:ILE:HG21	1.90	0.53
1:D:408:DG:C8	3:H:75:ARG:NE	2.71	0.53
3:H:98:ASN:O	3:H:99:LEU:C	2.52	0.53
1:D:411:DG:N3	1:D:412:DT:H2'	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:TRP:NE1	3:H:242:ILE:HG23	2.22	0.53
3:H:177:THR:HG22	3:H:179:ASN:CB	2.38	0.53
3:H:31:VAL:CB	3:H:44:ALA:O	2.57	0.53
3:H:57:HIS:C	3:H:57:HIS:CD2	2.86	0.53
2:L:1(G):PHE:HA	3:H:235:LYS:NZ	2.24	0.53
2:L:14:ASP:N	2:L:14(C):GLU:OE1	2.36	0.53
3:H:144:LEU:CD2	3:H:152:PRO:HG3	2.36	0.53
3:H:144:LEU:HD11	3:H:152:PRO:CD	2.39	0.53
1:D:407:DT:H3	3:H:77:GLU:CG	2.12	0.53
1:D:408:DG:H2"	3:H:77(A):ARG:H	1.74	0.52
2:L:1(H):THR:HG22	2:L:1(G):PHE:N	2.06	0.52
3:H:22:ALA:HB3	3:H:155:LEU:HG	1.91	0.52
2:L:1(F):GLY:CA	3:H:123:LEU:O	2.56	0.52
2:L:14(A):LYS:HG3	3:H:23:GLU:OE1	2.09	0.52
3:H:18:GLU:HA	3:H:18:GLU:OE1	2.09	0.52
3:H:33:LEU:HB2	3:H:42:CYS:O	2.09	0.52
3:H:35:ARG:NH2	3:H:36:LYS:H	2.06	0.52
3:H:206:ARG:HB2	3:H:208:TYR:CE1	2.44	0.52
3:H:144:LEU:CD1	3:H:152:PRO:HD3	2.37	0.52
3:H:20:SER:O	3:H:157:VAL:HG22	2.08	0.52
1:D:407:DT:H6	1:D:407:DT:H5"	1.74	0.52
3:H:34:PHE:HA	3:H:39:GLU:O	2.10	0.52
3:H:129:ALA:CA	3:H:210:MET:HE1	2.25	0.52
3:H:165:ARG:N	3:H:166:PRO:HD2	2.25	0.52
3:H:232:PHE:O	3:H:234:LEU:N	2.42	0.52
3:H:183:ALA:HB3	3:H:228:TYR:HE1	1.73	0.51
3:H:60(I):THR:HG22	3:H:63:ASP:OD1	2.10	0.51
2:L:14(I):SER:HB3	3:H:135:LYS:HG3	1.91	0.51
3:H:31:VAL:HG12	3:H:32:MET:N	2.25	0.51
3:H:58:CYS:O	3:H:59:LEU:HD12	2.10	0.51
3:H:35:ARG:NE	3:H:36:LYS:H	2.06	0.51
3:H:235:LYS:HA	3:H:238:ILE:HD13	1.92	0.51
3:H:212:ILE:O	3:H:228:TYR:CB	2.52	0.51
3:H:35:ARG:HD2	3:H:60(H):PHE:CZ	2.46	0.51
2:L:8:GLU:OE1	2:L:14(C):GLU:OE2	2.29	0.51
3:H:60:LEU:CD2	3:H:60(B):PRO:CD	2.74	0.51
3:H:61:GLU:OE2	3:H:88:ILE:CD1	2.59	0.51
1:D:404:DT:C4	1:D:411:DG:C5	2.99	0.50
2:L:14:ASP:OD1	2:L:14(C):GLU:OE1	2.29	0.50
2:L:14(G):LEU:HD12	3:H:202:LYS:HG2	1.93	0.50
3:H:95:ASN:ND2	3:H:97(A):GLU:HB2	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:195:SER:HG	4:H:1:0G7:C3	2.24	0.50
3:H:210:MET:C	3:H:231:VAL:HG23	2.36	0.50
2:L:6:LEU:HD21	3:H:116:ASP:HB3	1.93	0.50
3:H:22:ALA:CB	3:H:155:LEU:HG	2.41	0.50
3:H:189:ASP:OD1	4:H:1:0G7:NH2	2.45	0.50
3:H:198:PRO:HB2	3:H:200:VAL:HG13	1.93	0.50
3:H:199:PHE:CD1	3:H:199:PHE:C	2.89	0.50
1:D:410:DG:C4'	3:H:77(A):ARG:HH12	2.19	0.50
3:H:31:VAL:HB	3:H:44:ALA:C	2.37	0.50
3:H:60:LEU:CD2	3:H:60:LEU:C	2.84	0.50
2:L:14(F):LEU:CD1	3:H:159:ASN:HD22	2.21	0.50
3:H:204(B):ASN:ND2	3:H:208:TYR:OH	2.40	0.50
3:H:221(A):ARG:O	3:H:224:LYS:N	2.40	0.50
2:L:14(F):LEU:N	2:L:14(F):LEU:HD12	2.26	0.50
3:H:49:ASP:HA	3:H:114:PHE:HZ	1.76	0.50
3:H:85:LEU:HD23	3:H:85:LEU:C	2.37	0.49
3:H:238:ILE:HD12	3:H:238:ILE:H	1.77	0.49
3:H:60(H):PHE:HB3	3:H:64:LEU:HD11	1.94	0.49
3:H:203:SER:C	3:H:204(A):PHE:H	2.19	0.49
3:H:51:TRP:CZ2	3:H:245:PHE:O	2.65	0.49
3:H:160:LEU:CD2	3:H:184(A):TYR:HE1	2.20	0.49
3:H:191:CYS:N	3:H:194:ASP:OD2	2.45	0.49
3:H:60(A):TYR:CE2	4:H:1:0G7:CG1	2.95	0.49
3:H:165:ARG:N	3:H:166:PRO:CD	2.75	0.49
3:H:186(B):GLU:C	3:H:186(D):LYS:H	2.20	0.49
1:D:407:DT:H1'	1:D:409:DT:N3	2.23	0.49
1:D:411:DG:H21	1:D:412:DT:C2'	2.23	0.49
3:H:103:ILE:O	3:H:104:ALA:HB2	2.12	0.49
3:H:199:PHE:C	3:H:199:PHE:HD1	2.20	0.49
3:H:136:GLY:HA3	3:H:199:PHE:HE1	1.76	0.49
3:H:100:ASP:HB3	3:H:101:ARG:NH2	2.12	0.49
3:H:211:GLY:N	3:H:231:VAL:CG2	2.76	0.49
3:H:81:LYS:NZ	3:H:115:SER:HB3	2.28	0.48
1:D:407:DT:C2	3:H:77:GLU:CG	2.96	0.48
3:H:45:SER:O	3:H:47:ILE:CG2	2.62	0.48
3:H:28:PRO:HB2	3:H:119:HIS:CB	2.43	0.48
3:H:214:SER:HB2	3:H:227:PHE:O	2.14	0.48
3:H:34:PHE:CD1	3:H:39:GLU:O	2.67	0.48
3:H:70:LYS:NZ	3:H:75:ARG:O	2.47	0.48
3:H:172:THR:HG22	3:H:174:ILE:HB	1.94	0.48
3:H:35:ARG:HE	3:H:35:ARG:CA	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:228:TYR:CD1	3:H:228:TYR:N	2.82	0.47
2:L:1:CYS:O	3:H:206:ARG:HD2	2.14	0.47
3:H:29:TRP:O	3:H:45:SER:HA	2.14	0.47
1:D:414:DG:N3	1:D:414:DG:O4'	2.46	0.47
3:H:33:LEU:HD22	3:H:41:LEU:HD22	1.96	0.47
3:H:77:GLU:CG	3:H:79:ILE:HB	2.44	0.47
3:H:212:ILE:O	3:H:228:TYR:HA	2.15	0.47
3:H:69:GLY:O	3:H:79:ILE:HG22	2.13	0.47
3:H:167:VAL:HG12	3:H:225:TYR:CE2	2.49	0.47
1:D:407:DT:C1'	1:D:409:DT:H3	2.22	0.47
3:H:46:LEU:C	3:H:47:ILE:CG2	2.86	0.47
3:H:172:THR:HG23	3:H:174:ILE:H	1.79	0.47
1:D:404:DT:H71	1:D:412:DT:H5'	1.97	0.47
1:D:409:DT:H5'	3:H:77(A):ARG:HD3	1.97	0.47
2:L:1(G):PHE:O	3:H:123:LEU:HB3	2.15	0.47
3:H:25:GLY:C	3:H:27:SER:N	2.72	0.47
3:H:114:PHE:CZ	3:H:120:PRO:HG3	2.50	0.47
3:H:147:THR:HG23	3:H:148:TRP:N	2.28	0.47
3:H:177:THR:HG21	3:H:179:ASN:HB2	1.97	0.47
2:L:14(A):LYS:HB2	3:H:23:GLU:OE1	2.14	0.47
3:H:71:HIS:CE1	3:H:154:VAL:CG1	2.89	0.47
3:H:160:LEU:HA	3:H:161:PRO:HD3	1.65	0.47
3:H:217:GLU:HB2	3:H:224:LYS:HD3	1.96	0.47
3:H:95:ASN:ND2	3:H:97(A):GLU:CB	2.74	0.47
1:D:406:DG:C6	1:D:408:DG:H3'	2.49	0.46
1:D:413:DT:O4'	1:D:413:DT:O2	2.30	0.46
3:H:60(I):THR:C	3:H:64:LEU:HD12	2.39	0.46
3:H:99:LEU:HD12	3:H:215:TRP:CD1	2.48	0.46
1:D:406:DG:O3'	1:D:407:DT:H4'	2.15	0.46
2:L:7:PHE:HB3	2:L:8:GLU:OE2	2.15	0.46
3:H:191:CYS:CA	4:H:1:OG7:HD3	2.45	0.46
3:H:33:LEU:HB3	3:H:42:CYS:H	1.79	0.46
3:H:163:VAL:N	3:H:182:CYS:O	2.41	0.46
3:H:177:THR:C	3:H:179:ASN:N	2.74	0.46
3:H:184:GLY:CA	5:H:562:HOH:O	2.63	0.46
2:L:14:ASP:OD2	3:H:137:ARG:NH2	2.43	0.46
3:H:135:LYS:HA	3:H:161:PRO:HA	1.97	0.46
3:H:190:ALA:C	4:H:1:OG7:NH1	2.74	0.46
3:H:191:CYS:HA	4:H:1:OG7:HD3	1.96	0.46
2:L:14(J):TYR:CE1	3:H:134:TYR:HD2	2.34	0.46
3:H:30:GLN:NE2	3:H:140:GLY:HA2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:85:LEU:HD23	3:H:85:LEU:H	1.81	0.46
1:D:410:DG:H1'	3:H:77(A):ARG:HH12	1.76	0.46
3:H:16:ILE:HG22	3:H:19:GLY:HA3	1.97	0.46
3:H:87:LYS:O	3:H:106:MET:CA	2.63	0.46
3:H:118:ILE:HD12	3:H:118:ILE:H	1.78	0.46
3:H:176:ILE:HG23	3:H:227:PHE:CE2	2.51	0.46
3:H:212:ILE:O	3:H:228:TYR:CA	2.64	0.46
1:D:409:DT:O4'	1:D:409:DT:OP1	2.34	0.45
3:H:159:ASN:O	3:H:184(A):TYR:OH	2.24	0.45
3:H:203:SER:C	3:H:204(A):PHE:N	2.72	0.45
2:L:14(J):TYR:CE1	3:H:134:TYR:CD2	3.04	0.45
3:H:172:THR:CG2	3:H:174:ILE:HB	2.46	0.45
3:H:238:ILE:HD12	3:H:238:ILE:N	2.32	0.45
3:H:105:LEU:HD12	3:H:241:VAL:HB	1.97	0.45
2:L:14(E):GLU:HG3	2:L:14(F):LEU:HD12	1.97	0.45
3:H:215:TRP:HA	4:H:1:0G7:HB2A	1.99	0.45
3:H:31:VAL:CB	3:H:44:ALA:HB3	2.47	0.45
3:H:85:LEU:CD2	3:H:85:LEU:H	2.30	0.45
3:H:105:LEU:C	3:H:106:MET:HG3	2.42	0.45
3:H:33:LEU:CB	3:H:42:CYS:H	2.30	0.45
3:H:41:LEU:H	3:H:41:LEU:HD13	1.81	0.45
3:H:61:GLU:CD	3:H:87:LYS:HD3	2.41	0.45
1:D:401:DG:O6	1:D:406:DG:O6	2.35	0.45
3:H:181:PHE:CZ	3:H:210:MET:O	2.70	0.45
3:H:31:VAL:N	3:H:44:ALA:O	2.47	0.45
3:H:73:ARG:HD3	3:H:152:PRO:O	2.17	0.45
3:H:128:THR:O	3:H:129(C):LEU:CG	2.65	0.45
3:H:60(B):PRO:CG	3:H:96:TRP:CE2	2.97	0.44
3:H:46:LEU:CD2	3:H:114:PHE:CE1	2.97	0.44
3:H:51:TRP:CD2	3:H:242:ILE:HG23	2.52	0.44
3:H:181:PHE:HZ	3:H:210:MET:O	2.00	0.44
3:H:31:VAL:CG1	3:H:32:MET:H	2.30	0.44
1:D:408:DG:OP2	3:H:71:HIS:HB3	2.17	0.44
2:L:6:LEU:CD2	3:H:116:ASP:OD2	2.66	0.44
3:H:123:LEU:HD12	3:H:124:PRO:HD2	2.00	0.44
3:H:129(C):LEU:HD23	3:H:129(C):LEU:HA	1.72	0.44
3:H:233:ARG:HG3	3:H:233:ARG:O	2.16	0.44
3:H:116:ASP:O	3:H:117:TYR:CG	2.71	0.44
3:H:180:MET:HE1	3:H:215:TRP:HE1	1.83	0.44
3:H:61:GLU:OE2	3:H:87:LYS:HE3	2.17	0.44
3:H:68:ILE:HG22	3:H:118:ILE:CG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:77:GLU:HG2	3:H:79:ILE:HB	1.99	0.44
3:H:230:HIS:C	3:H:232:PHE:H	2.25	0.44
2:L:1(G):PHE:HA	3:H:235:LYS:HZ3	1.81	0.44
2:L:14(C):GLU:C	2:L:14(E):GLU:N	2.76	0.44
3:H:69:GLY:HA3	3:H:118:ILE:HG13	2.00	0.44
3:H:234:LEU:C	3:H:236:LYS:H	2.25	0.44
1:D:404:DT:C4	1:D:412:DT:H5'	2.43	0.44
3:H:29:TRP:HB3	3:H:119:HIS:O	2.17	0.44
3:H:129:ALA:O	3:H:130:LEU:HB2	2.18	0.44
3:H:184:GLY:HA3	5:H:562:HOH:O	2.17	0.44
3:H:190:ALA:N	4:H:1:OG7:NH1	2.65	0.44
3:H:22:ALA:N	3:H:155:LEU:O	2.48	0.43
3:H:73:ARG:O	3:H:73:ARG:CG	2.59	0.43
3:H:144:LEU:O	3:H:145:LYS:HG2	2.16	0.43
3:H:158:VAL:CG2	3:H:160:LEU:HD11	2.47	0.43
1:D:404:DT:O4	1:D:412:DT:C3'	2.63	0.43
2:L:1(F):GLY:O	2:L:1(E):SER:C	2.61	0.43
3:H:112:VAL:HG23	3:H:113:ALA:O	2.18	0.43
3:H:123:LEU:CG	3:H:235:LYS:HD3	2.49	0.43
3:H:27:SER:OG	3:H:139:THR:HG21	2.19	0.43
3:H:158:VAL:HG22	3:H:159:ASN:N	2.33	0.43
3:H:56:ALA:HB2	3:H:103:ILE:O	2.19	0.43
3:H:86:GLU:HB3	3:H:109:LYS:HA	2.01	0.43
3:H:94:TYR:CD1	3:H:94:TYR:C	2.96	0.43
3:H:49:ASP:HA	3:H:114:PHE:CZ	2.53	0.43
3:H:77:GLU:O	3:H:78:ASN:N	2.52	0.43
3:H:215:TRP:CE3	4:H:1:OG7:HD2	2.54	0.43
2:L:15:ARG:HH11	2:L:15:ARG:CA	2.12	0.43
3:H:91:HIS:O	3:H:94:TYR:HB3	2.19	0.43
1:D:413:DT:H2''	1:D:414:DG:OP2	2.11	0.43
3:H:35:ARG:CZ	3:H:36(A):SER:H	2.32	0.43
3:H:40:LEU:C	3:H:41:LEU:HD12	2.42	0.43
3:H:61:GLU:OE2	3:H:87:LYS:CE	2.67	0.43
3:H:67:ARG:NE	3:H:80:GLU:OE2	2.51	0.42
3:H:70:LYS:HD2	3:H:80:GLU:CD	2.44	0.42
3:H:230:HIS:C	3:H:232:PHE:N	2.77	0.42
3:H:45:SER:OG	3:H:53:LEU:HG	2.19	0.42
3:H:118:ILE:CD1	3:H:118:ILE:N	2.77	0.42
3:H:190:ALA:O	4:H:1:OG7:NH1	2.52	0.42
3:H:209:GLN:NE2	3:H:212:ILE:HG12	2.34	0.42
1:D:409:DT:O2	1:D:409:DT:OP1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1(C):GLU:HG3	3:H:120:PRO:HG2	2.00	0.42
1:D:402:DG:H4'	5:D:544:HOH:O	2.19	0.42
1:D:406:DG:H2''	1:D:407:DT:H2''	2.01	0.42
3:H:25:GLY:C	3:H:27:SER:H	2.27	0.42
2:L:1(H):THR:CG2	2:L:1(G):PHE:CD1	3.02	0.42
2:L:14(F):LEU:O	2:L:14(I):SER:N	2.33	0.42
3:H:41:LEU:CD2	3:H:64:LEU:HD23	2.49	0.42
1:D:407:DT:C1'	1:D:409:DT:C2	2.90	0.42
3:H:98:ASN:HD21	3:H:175:ARG:HH11	1.68	0.42
3:H:106:MET:HE2	3:H:106:MET:HB2	1.70	0.42
3:H:119:HIS:HA	3:H:120:PRO:HD3	1.63	0.42
3:H:35:ARG:HH21	3:H:36:LYS:HG2	1.80	0.41
3:H:35:ARG:HG3	3:H:37:PRO:O	2.19	0.41
3:H:35:ARG:HE	3:H:35:ARG:C	2.28	0.41
3:H:55:ALA:O	3:H:59:LEU:HD13	2.20	0.41
3:H:144:LEU:HD12	3:H:150:GLY:O	2.19	0.41
1:D:408:DG:H4'	3:H:77:GLU:HG3	2.00	0.41
3:H:209:GLN:HE22	3:H:212:ILE:HG12	1.86	0.41
3:H:16:ILE:CG2	3:H:158:VAL:HB	2.50	0.41
3:H:156:GLN:C	3:H:157:VAL:HG13	2.45	0.41
3:H:124:PRO:HA	3:H:208:TYR:HD2	1.85	0.41
3:H:163:VAL:HG12	3:H:168:CYS:SG	2.61	0.41
3:H:189:ASP:OD2	3:H:220:CYS:HA	2.21	0.41
3:H:51:TRP:NE1	3:H:242:ILE:CG2	2.83	0.41
3:H:233:ARG:HA	3:H:233:ARG:HD3	1.98	0.41
3:H:24:ILE:H	3:H:24:ILE:CD1	2.32	0.41
2:L:3:LEU:HD22	3:H:206:ARG:NH1	2.30	0.41
3:H:128:THR:O	3:H:129(C):LEU:HG	2.21	0.41
3:H:203:SER:O	3:H:205:ASN:HA	2.21	0.41
3:H:94:TYR:HA	3:H:100:ASP:O	2.21	0.40
3:H:41:LEU:HD21	3:H:64:LEU:HD23	2.03	0.40
3:H:139:THR:HG22	3:H:157:VAL:HG12	2.02	0.40
3:H:163:VAL:O	3:H:182:CYS:SG	2.79	0.40
3:H:164:GLU:C	3:H:166:PRO:HD2	2.46	0.40
3:H:172:THR:CG2	3:H:174:ILE:CB	3.00	0.40
3:H:130:LEU:C	3:H:130:LEU:CD1	2.95	0.40
3:H:221:ASP:O	3:H:222:ASP:N	2.55	0.40
2:L:3:LEU:HD12	2:L:3:LEU:HA	1.84	0.40
2:L:8:GLU:HG3	3:H:202:LYS:NZ	2.37	0.40
2:L:14(E):GLU:HG2	3:H:159:ASN:HD22	1.86	0.40
2:L:14(J):TYR:HD1	3:H:134:TYR:CG	2.39	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	
2	L	34/36 (94%)	16 (47%)	12 (35%)	6 (18%)	0	0
3	H	249/259 (96%)	182 (73%)	54 (22%)	13 (5%)	1	5
All	All	283/295 (96%)	198 (70%)	66 (23%)	19 (7%)	1	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	1(G)	PHE
2	L	14(K)	ILE
3	H	116	ASP
3	H	186(C)	GLY
3	H	233	ARG
2	L	1(B)	ALA
2	L	14(G)	LEU
3	H	230	HIS
2	L	9	LYS
3	H	50	ARG
3	H	195	SER
3	H	117	TYR
3	H	238	ILE
3	H	21	ASP
3	H	61	GLU
3	H	130	LEU
3	H	143	ASN
2	L	1(E)	SER
3	H	174	ILE

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	
2	L	31/31 (100%)	27 (87%)	4 (13%)	4	13
3	H	221/225 (98%)	143 (65%)	78 (35%)	0	0
All	All	252/256 (98%)	170 (68%)	82 (32%)	0	1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	9	LYS
2	L	10	LYS
2	L	12	LEU
2	L	15	ARG
3	H	16	ILE
3	H	18	GLU
3	H	23	GLU
3	H	24	ILE
3	H	27	SER
3	H	32	MET
3	H	33	LEU
3	H	36	LYS
3	H	36(A)	SER
3	H	38	GLN
3	H	39	GLU
3	H	41	LEU
3	H	42	CYS
3	H	52	VAL
3	H	57	HIS
3	H	59	LEU
3	H	61	GLU
3	H	63	ASP
3	H	72	SER
3	H	74	THR
3	H	75	ARG
3	H	79	ILE
3	H	82	ILE

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Mol	Chain	Res	Type
3	H	85	LEU
3	H	86	GLU
3	H	87	LYS
3	H	88	ILE
3	H	90	ILE
3	H	91	HIS
3	H	97	ARG
3	H	97(A)	GLU
3	H	103	ILE
3	H	105	LEU
3	H	106	MET
3	H	110	LYS
3	H	112	VAL
3	H	117	TYR
3	H	118	ILE
3	H	125	ASP
3	H	126	ARG
3	H	129(B)	SER
3	H	129(C)	LEU
3	H	130	LEU
3	H	134	TYR
3	H	138	VAL
3	H	139	THR
3	H	143	ASN
3	H	147	THR
3	H	153	SER
3	H	155	LEU
3	H	158	VAL
3	H	160	LEU
3	H	164	GLU
3	H	169	LYS
3	H	172	THR
3	H	173	ARG
3	H	174	ILE
3	H	175	ARG
3	H	176	ILE
3	H	178	ASP
3	H	180	MET
3	H	185	LYS
3	H	199	PHE
3	H	205	ASN
3	H	206	ARG

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Mol	Chain	Res	Type
3	H	212	ILE
3	H	213	VAL
3	H	220	CYS
3	H	221	ASP
3	H	221(A)	ARG
3	H	224	LYS
3	H	228	TYR
3	H	230	HIS
3	H	234	LEU
3	H	235	LYS
3	H	239	GLN
3	H	240	LYS
3	H	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	38	GLN
3	H	62	ASN
3	H	71	HIS
3	H	143	ASN
3	H	151	GLN
3	H	159	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0G7	H	1	-	30,31,32	2.38	3 (10%)	36,41,42	2.16	11 (30%)

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	0G7	H	1	-	-	5/31/41/43	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	0G7	C3-C2	-11.28	1.22	1.49
4	H	1	0G7	O1-C1	4.34	1.31	1.23
4	H	1	0G7	C1-N2	-2.92	1.27	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G7	CA1-C1-N2	7.46	132.90	116.52
4	H	1	0G7	O1-C1-N2	-4.53	114.84	122.96
4	H	1	0G7	CG-CB-CA	4.31	122.94	114.13
4	H	1	0G7	O1-C1-CA1	-3.51	112.23	120.69
4	H	1	0G7	C1-CA1-N1	3.46	121.94	112.50
4	H	1	0G7	CB2-CA2-N2	2.69	116.24	110.91
4	H	1	0G7	CB-CA-C	2.42	115.90	109.43
4	H	1	0G7	CG2-CB2-CA2	2.28	120.82	113.80
4	H	1	0G7	CB2-CG2-CD3	2.23	118.52	112.07
4	H	1	0G7	CB1-CA1-C1	2.23	115.95	111.21
4	H	1	0G7	CA2-N2-C1	2.00	125.95	121.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

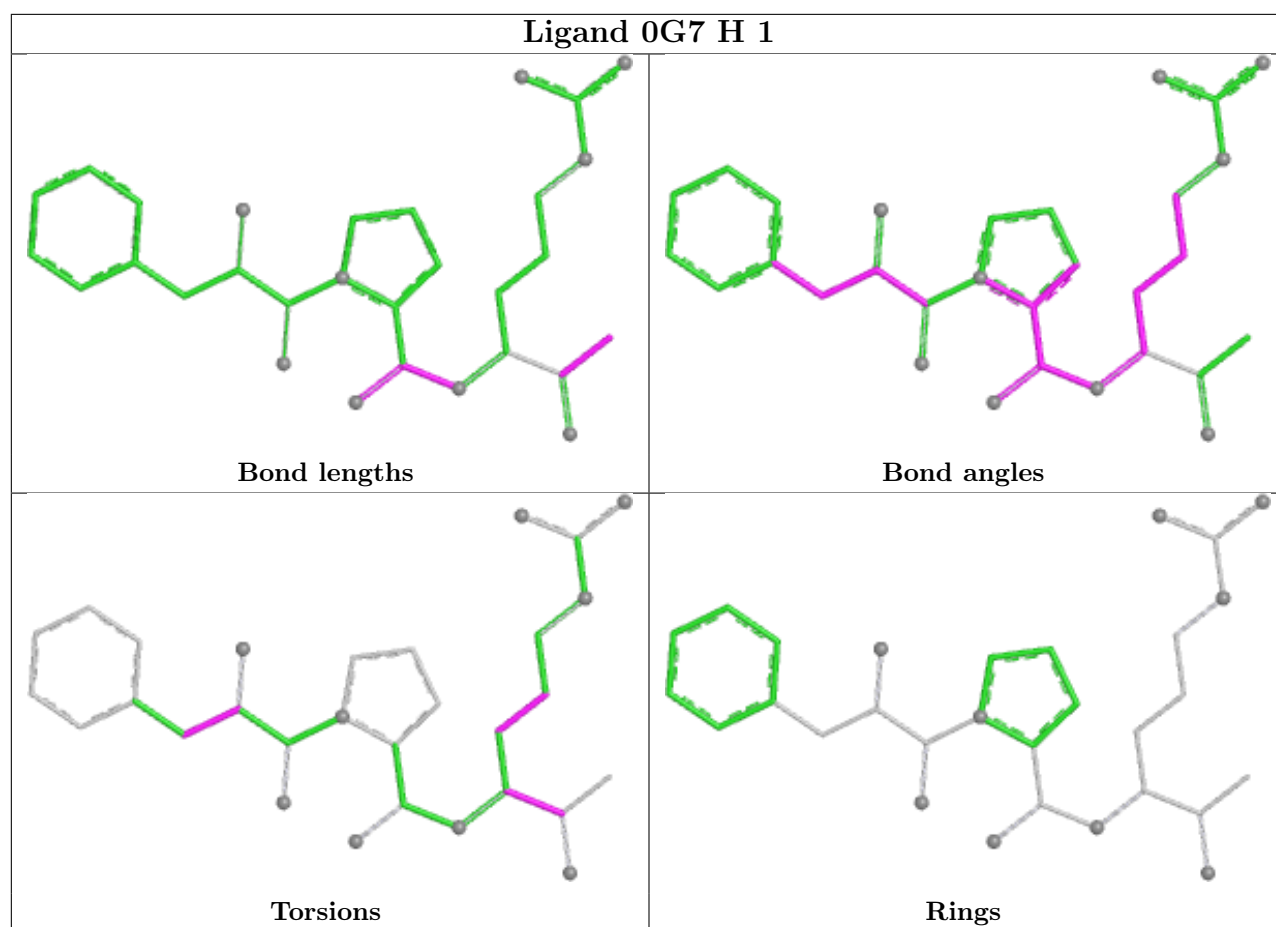
Mol	Chain	Res	Type	Atoms
4	H	1	0G7	C-CA-CB-CG
4	H	1	0G7	C3-C2-CA2-CB2
4	H	1	0G7	CA2-CB2-CG2-CD3
4	H	1	0G7	O2-C2-CA2-CB2
4	H	1	0G7	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	0G7	20	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.