Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:30 pm BST

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

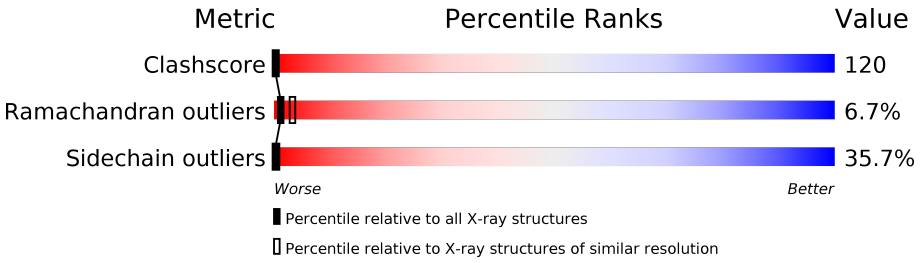
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	15	100%
2	L	36	14% 39% 33% 14%
3	H	259	8% 47% 31% 12% •

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	0G7	H	1	-	-	X	-

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
			Total	C	N	O	P			
1	D	15	315	150	57	94	14	0	0	0

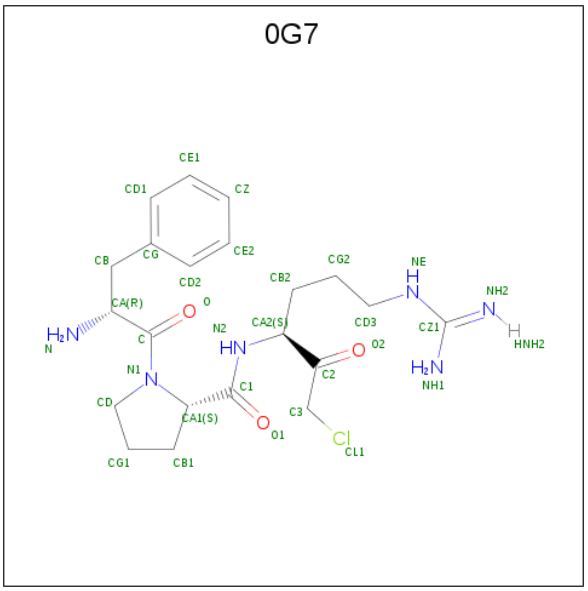
- Molecule 2 is a protein called ALPHA-Thrombin light chain.

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

- Molecule 3 is a protein called ALPHA-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-[(3S)-6-carbamimidamido-1-chloro-2-oxohexan-3-yl]-L-prolinamide (three-letter code: 0G7) (formula: $C_{21}H_{31}ClN_6O_3$).



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

- Molecule 5 is water.

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

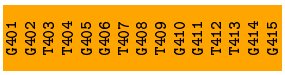
3 Residue-property plots (i)

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

Note EDS was not executed.

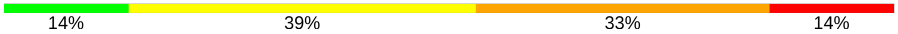
- Molecule 1: DNA 5'-D(*GP*GP*TP*TP*GP*GP*TP*GP*TP*GP*GP*TP*TP*GP*G)-3'

Chain D:



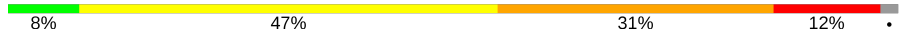
- Molecule 2: ALPHA-Thrombin light chain

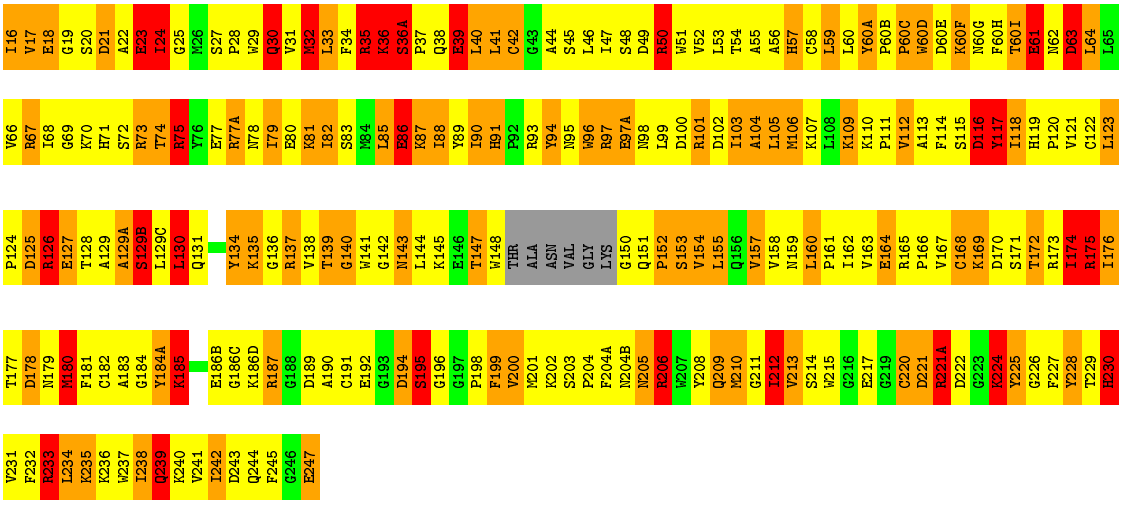
Chain L:



- Molecule 3: ALPHA-Thrombin heavy chain

Chain H:





4 Data and refinement statistics (i)

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	2.32	17/353 (4.8%)	5.35	121/547 (22.1%)
2	L	1.37	1/290 (0.3%)	2.37	14/384 (3.6%)
3	H	1.13	1/2107 (0.0%)	2.23	91/2846 (3.2%)
All	All	1.36	19/2750 (0.7%)	2.91	226/3777 (6.0%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	407	DT	C3'-C2'	9.18	1.63	1.52
1	D	404	DT	C4'-O4'	7.73	1.52	1.45
2	L	1(F)	GLY	C-N	7.53	1.51	1.34
1	D	401	DG	O4'-C1'	6.92	1.50	1.42
1	D	413	DT	O4'-C1'	6.77	1.50	1.42
1	D	408	DG	O4'-C1'	6.67	1.50	1.42
1	D	402	DG	O4'-C1'	6.40	1.50	1.42
1	D	405	DG	P-O5'	6.30	1.66	1.59
1	D	412	DT	C4-O4	5.97	1.28	1.23
1	D	404	DT	C3'-C2'	5.86	1.59	1.52
3	H	247	GLU	C-OXT	5.76	1.34	1.23
1	D	409	DT	C4-O4	5.73	1.28	1.23
1	D	404	DT	C2-O2	5.71	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	412	DT	C2'-C1'	5.70	1.58	1.52
1	D	404	DT	N1-C2	5.66	1.42	1.38
1	D	410	DG	O3'-P	5.54	1.67	1.61
1	D	404	DT	O4'-C1'	5.48	1.48	1.42
1	D	403	DT	C4-O4	5.45	1.28	1.23
1	D	407	DT	C4-O4	5.16	1.27	1.23

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	406	DG	O4'-C1'-N9	33.65	131.56	108.00
3	H	101	ARG	NE-CZ-NH1	29.38	134.99	120.30
1	D	412	DT	O4'-C1'-N1	26.15	126.31	108.00
1	D	412	DT	P-O3'-C3'	24.52	149.12	119.70
1	D	404	DT	O4'-C1'-N1	22.93	124.05	108.00
1	D	411	DG	O4'-C1'-N9	20.91	122.64	108.00
1	D	410	DG	O4'-C1'-N9	20.16	122.11	108.00
1	D	402	DG	P-O3'-C3'	19.87	143.54	119.70
1	D	405	DG	P-O3'-C3'	19.18	142.71	119.70
1	D	404	DT	P-O3'-C3'	18.48	141.87	119.70
1	D	407	DT	O4'-C1'-N1	-18.43	95.10	108.00
1	D	410	DG	O4'-C4'-C3'	-18.22	95.07	106.00
1	D	404	DT	O4'-C4'-C3'	-18.12	95.13	106.00
1	D	403	DT	OP1-P-OP2	-17.02	94.07	119.60
1	D	403	DT	O4'-C1'-N1	15.74	119.02	108.00
1	D	410	DG	C1'-O4'-C4'	-15.11	95.00	110.10
1	D	404	DT	C1'-O4'-C4'	-14.57	95.53	110.10
3	H	126	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	D	404	DT	P-O5'-C5'	13.17	141.97	120.90
1	D	411	DG	P-O3'-C3'	13.03	135.33	119.70
1	D	413	DT	O4'-C1'-N1	12.72	116.90	108.00
1	D	407	DT	C3'-C2'-C1'	-12.48	87.52	102.50
1	D	407	DT	C4'-C3'-C2'	-12.32	92.02	103.10
1	D	412	DT	P-O5'-C5'	11.85	139.87	120.90
1	D	402	DG	C1'-O4'-C4'	-11.64	98.46	110.10
1	D	413	DT	N3-C4-O4	-11.27	113.14	119.90
2	L	4	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	D	406	DG	P-O5'-C5'	10.89	138.32	120.90
3	H	75	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	D	404	DT	O5'-P-OP1	10.71	123.56	110.70
1	D	413	DT	P-O5'-C5'	10.71	138.04	120.90
3	H	97	ARG	NE-CZ-NH1	10.54	125.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	4	ARG	NE-CZ-NH2	10.43	125.52	120.30
1	D	409	DT	P-O3'-C3'	10.39	132.17	119.70
3	H	137	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	D	411	DG	O4'-C1'-C2'	-10.30	97.66	105.90
1	D	404	DT	C5'-C4'-C3'	10.13	132.34	114.10
1	D	402	DG	O4'-C4'-C3'	-10.12	99.93	106.00
1	D	403	DT	O3'-P-O5'	10.00	123.01	104.00
1	D	408	DG	P-O3'-C3'	9.99	131.69	119.70
3	H	101	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	D	407	DT	C1'-O4'-C4'	-9.96	100.14	110.10
1	D	413	DT	OP1-P-OP2	-9.78	104.93	119.60
2	L	10	LYS	C-N-CA	9.66	145.85	121.70
1	D	409	DT	C2-N3-C4	-9.45	121.53	127.20
1	D	412	DT	OP1-P-OP2	-9.39	105.51	119.60
1	D	404	DT	C2-N3-C4	-9.04	121.78	127.20
1	D	413	DT	C2-N3-C4	-9.03	121.78	127.20
3	H	129(B)	SER	N-CA-CB	-8.98	97.02	110.50
3	H	101	ARG	NH1-CZ-NH2	-8.95	109.55	119.40
3	H	60(E)	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	D	403	DT	C2-N3-C4	-8.87	121.88	127.20
3	H	86	GLU	CA-CB-CG	8.84	132.85	113.40
1	D	409	DT	OP1-P-OP2	-8.83	106.35	119.60
1	D	413	DT	O4'-C1'-C2'	-8.75	98.90	105.90
1	D	406	DG	OP1-P-OP2	-8.75	106.47	119.60
1	D	407	DT	N3-C4-C5	8.65	120.39	115.20
1	D	414	DG	C5-C6-N1	8.65	115.83	111.50
1	D	409	DT	O5'-P-OP2	8.64	121.06	110.70
3	H	196	GLY	C-N-CA	8.62	140.39	122.30
3	H	233	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	L	14(D)	ARG	NE-CZ-NH2	8.57	124.58	120.30
3	H	96	TRP	CA-CB-CG	8.54	129.92	113.70
3	H	135	LYS	C-N-CA	8.48	140.11	122.30
1	D	404	DT	O5'-P-OP2	-8.35	98.18	105.70
1	D	405	DG	O5'-P-OP1	-8.27	98.26	105.70
1	D	410	DG	OP1-P-OP2	-8.19	107.31	119.60
1	D	409	DT	N1-C2-N3	8.16	119.50	114.60
1	D	414	DG	OP1-P-OP2	-8.14	107.39	119.60
3	H	50	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	D	415	DG	O4'-C1'-N9	8.06	113.64	108.00
1	D	407	DT	N1-C1'-C2'	-7.98	97.44	112.60
1	D	413	DT	N1-C2-N3	7.96	119.38	114.60
1	D	404	DT	C4'-C3'-O3'	7.94	129.56	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	412	DT	C2-N3-C4	-7.94	122.44	127.20
3	H	101	ARG	CD-NE-CZ	7.94	134.72	123.60
1	D	403	DT	C4'-C3'-O3'	7.92	129.50	109.70
3	H	77(A)	ARG	NE-CZ-NH2	7.89	124.24	120.30
3	H	127	GLU	OE1-CD-OE2	7.86	132.74	123.30
1	D	404	DT	C6-N1-C2	-7.86	117.37	121.30
2	L	4	ARG	CD-NE-CZ	-7.79	112.69	123.60
1	D	406	DG	N1-C6-O6	-7.78	115.23	119.90
3	H	126	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	L	14(D)	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	D	404	DT	N3-C4-C5	7.57	119.75	115.20
1	D	403	DT	N1-C2-N3	7.50	119.10	114.60
1	D	407	DT	O5'-P-OP1	7.49	119.68	110.70
2	L	14(D)	ARG	NH1-CZ-NH2	-7.48	111.17	119.40
3	H	243	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	D	407	DT	C2-N3-C4	-7.47	122.72	127.20
3	H	187	ARG	NE-CZ-NH2	7.42	124.01	120.30
3	H	30	GLN	O-C-N	7.42	134.56	122.70
1	D	404	DT	N1-C2-N3	7.40	119.04	114.60
3	H	116	ASP	O-C-N	-7.37	110.92	122.70
1	D	412	DT	N3-C4-C5	7.36	119.62	115.20
3	H	39	GLU	OE1-CD-OE2	7.33	132.09	123.30
1	D	407	DT	C6-N1-C2	7.31	124.95	121.30
1	D	413	DT	O4'-C4'-C3'	-7.26	101.59	104.50
1	D	412	DT	O5'-P-OP1	7.24	119.38	110.70
1	D	408	DG	C1'-O4'-C4'	-7.20	102.90	110.10
1	D	402	DG	P-O5'-C5'	-7.10	109.54	120.90
3	H	67	ARG	NE-CZ-NH1	7.09	123.84	120.30
3	H	50	ARG	CD-NE-CZ	-7.06	113.72	123.60
3	H	73	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	410	DG	C8-N9-C4	-7.04	103.58	106.40
3	H	221(A)	ARG	NE-CZ-NH2	6.96	123.78	120.30
3	H	97	ARG	CD-NE-CZ	6.87	133.22	123.60
1	D	407	DT	C4'-C3'-O3'	6.86	126.85	109.70
2	L	14	ASP	CB-CG-OD1	-6.85	112.13	118.30
3	H	125	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	401	DG	C5'-C4'-O4'	6.71	122.06	109.30
1	D	403	DT	C6-N1-C2	-6.69	117.95	121.30
3	H	105	LEU	O-C-N	-6.66	112.04	122.70
1	D	414	DG	C6-N1-C2	-6.66	121.10	125.10
3	H	123	LEU	CB-CA-C	6.65	122.84	110.20
3	H	60(F)	LYS	N-CA-CB	6.63	122.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	402	DG	C4'-C3'-C2'	-6.57	97.19	103.10
3	H	97(A)	GLU	OE1-CD-OE2	-6.57	115.41	123.30
2	L	14(C)	GLU	O-C-N	6.56	133.19	122.70
3	H	60(F)	LYS	O-C-N	6.47	133.04	122.70
2	L	14(J)	TYR	CA-C-O	-6.45	106.56	120.10
3	H	75	ARG	CD-NE-CZ	6.43	132.60	123.60
3	H	36(A)	SER	CB-CA-C	-6.42	97.90	110.10
1	D	403	DT	P-O3'-C3'	-6.40	112.02	119.70
3	H	97	ARG	NH1-CZ-NH2	-6.38	112.39	119.40
1	D	408	DG	O5'-P-OP1	6.37	118.35	110.70
1	D	406	DG	N9-C1'-C2'	-6.36	100.52	112.60
1	D	407	DT	N3-C4-O4	-6.33	116.10	119.90
1	D	410	DG	N9-C4-C5	6.31	107.92	105.40
1	D	403	DT	N3-C4-C5	6.30	118.98	115.20
3	H	67	ARG	NE-CZ-NH2	-6.29	117.15	120.30
3	H	36	LYS	O-C-N	-6.28	112.65	122.70
3	H	89	TYR	CA-CB-CG	6.27	125.32	113.40
1	D	415	DG	N1-C6-O6	-6.27	116.14	119.90
1	D	404	DT	N3-C2-O2	-6.27	118.54	122.30
1	D	413	DT	C6-N1-C2	-6.26	118.17	121.30
3	H	206	ARG	NE-CZ-NH2	6.23	123.42	120.30
3	H	185	LYS	CB-CA-C	6.22	122.83	110.40
3	H	60(D)	TRP	CA-CB-CG	6.20	125.49	113.70
2	L	14	ASP	CA-C-N	-6.19	103.59	117.20
1	D	413	DT	N3-C4-C5	6.18	118.91	115.20
3	H	225	TYR	CB-CA-C	6.17	122.75	110.40
3	H	175	ARG	NE-CZ-NH1	6.17	123.38	120.30
3	H	137	ARG	CD-NE-CZ	6.14	132.20	123.60
1	D	410	DG	N1-C6-O6	-6.13	116.22	119.90
1	D	404	DT	OP2-P-O3'	6.13	118.68	105.20
3	H	129(A)	ALA	C-N-CA	6.10	136.95	121.70
3	H	102	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	403	DT	O5'-P-OP2	6.03	117.94	110.70
1	D	403	DT	O4'-C1'-C2'	-6.00	101.10	105.90
1	D	409	DT	N3-C2-O2	-5.96	118.72	122.30
3	H	17	VAL	CA-CB-CG1	5.95	119.82	110.90
1	D	413	DT	C1'-O4'-C4'	-5.94	104.16	110.10
1	D	405	DG	O4'-C1'-N9	5.94	112.16	108.00
1	D	404	DT	C4'-C3'-C2'	-5.93	97.76	103.10
1	D	410	DG	O5'-P-OP1	5.85	117.72	110.70
3	H	50	ARG	NE-CZ-NH2	5.84	123.22	120.30
3	H	127	GLU	CG-CD-OE2	-5.84	106.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	409	DT	C6-N1-C2	-5.83	118.38	121.30
1	D	403	DT	O5'-C5'-C4'	5.83	125.58	111.00
1	D	405	DG	C5-C6-N1	5.83	114.41	111.50
3	H	131	GLN	O-C-N	5.81	132.00	122.70
1	D	407	DT	C5'-C4'-C3'	5.79	124.53	114.10
1	D	401	DG	O5'-C5'-C4'	5.75	125.36	111.00
3	H	210	MET	CB-CA-C	5.70	121.79	110.40
1	D	405	DG	P-O5'-C5'	-5.69	111.79	120.90
3	H	60(A)	TYR	CB-CG-CD2	5.69	124.41	121.00
1	D	404	DT	O4'-C1'-C2'	-5.67	101.36	105.90
3	H	36	LYS	C-N-CA	5.66	135.84	121.70
1	D	411	DG	C5-C6-N1	5.64	114.32	111.50
3	H	30	GLN	N-CA-CB	5.63	120.74	110.60
3	H	40	LEU	CA-C-O	-5.63	108.28	120.10
3	H	35	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	H	212	ILE	O-C-N	5.62	131.69	122.70
1	D	405	DG	C5-C6-O6	-5.62	125.23	128.60
1	D	411	DG	O3'-P-O5'	5.61	114.67	104.00
1	D	406	DG	N9-C4-C5	5.59	107.64	105.40
3	H	226	GLY	CA-C-O	-5.59	110.53	120.60
1	D	409	DT	N3-C4-C5	5.59	118.55	115.20
3	H	168	CYS	N-CA-CB	-5.59	100.54	110.60
1	D	409	DT	O4'-C1'-C2'	-5.58	101.43	105.90
3	H	73	ARG	CA-C-N	-5.58	104.92	117.20
2	L	4	ARG	N-CA-C	5.58	126.06	111.00
3	H	154	VAL	CA-C-N	-5.56	104.96	117.20
1	D	413	DT	P-O3'-C3'	5.56	126.37	119.70
3	H	185	LYS	CB-CG-CD	5.54	126.02	111.60
1	D	407	DT	C5-C6-N1	-5.52	120.39	123.70
3	H	184(A)	TYR	CB-CG-CD1	-5.52	117.69	121.00
3	H	32	MET	CG-SD-CE	5.51	109.01	100.20
1	D	404	DT	N3-C4-O4	-5.49	116.61	119.90
1	D	411	DG	C1'-O4'-C4'	-5.49	104.61	110.10
1	D	405	DG	C5'-C4'-C3'	5.49	123.97	114.10
3	H	194	ASP	CB-CG-OD1	-5.39	113.45	118.30
3	H	152	PRO	O-C-N	5.38	131.31	122.70
1	D	404	DT	OP1-P-OP2	-5.36	111.56	119.60
3	H	157	VAL	O-C-N	5.33	131.23	122.70
3	H	239	GLN	N-CA-CB	5.32	120.18	110.60
3	H	126	ARG	CA-CB-CG	5.31	125.09	113.40
3	H	73	ARG	CB-CA-C	-5.30	99.79	110.40
3	H	24	ILE	CB-CG1-CD1	5.29	128.73	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	192	GLU	C-N-CA	5.29	133.41	122.30
3	H	116	ASP	CA-C-N	5.26	128.77	117.20
2	L	14(L)	ASP	CA-C-N	-5.25	105.71	116.20
3	H	224	LYS	N-CA-CB	5.24	120.03	110.60
3	H	97(A)	GLU	CG-CD-OE1	5.22	128.74	118.30
1	D	408	DG	N9-C1'-C2'	5.22	122.51	112.60
1	D	411	DG	N9-C1'-C2'	-5.19	102.74	112.60
3	H	36(A)	SER	CA-CB-OG	5.19	125.22	111.20
1	D	414	DG	O5'-P-OP1	5.18	116.92	110.70
3	H	140	GLY	C-N-CA	5.18	134.64	121.70
1	D	412	DT	C4'-C3'-O3'	5.17	122.64	112.30
3	H	137	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
3	H	195	SER	CA-C-N	-5.15	105.89	116.20
3	H	243	ASP	CA-C-N	-5.15	105.86	117.20
3	H	109	LYS	CD-CE-NZ	5.15	123.54	111.70
3	H	23	GLU	CA-CB-CG	5.14	124.71	113.40
1	D	403	DT	OP1-P-O3'	-5.12	93.93	105.20
3	H	39	GLU	CG-CD-OE2	-5.12	108.06	118.30
3	H	104	ALA	C-N-CA	5.12	134.50	121.70
3	H	105	LEU	CA-C-N	5.12	128.47	117.20
1	D	401	DG	N9-C1'-C2'	5.12	122.32	112.60
2	L	14(C)	GLU	CA-C-N	-5.10	105.98	117.20
3	H	175	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	402	DG	O5'-C5'-C4'	-5.08	98.31	111.00
3	H	180	MET	C-N-CA	5.05	134.33	121.70
3	H	75	ARG	CG-CD-NE	5.03	122.36	111.80

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
2	L	14(K)	ILE	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	315	0	173	107	0
2	L	287	0	277	76	0
3	H	2053	0	2016	517	0
4	H	30	0	27	21	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	2493	620	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 120.

All (620) 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:C6	1:D:407:DT:H3'	1.41	1.44
1:D:408:DG:H8	3:H:75:ARG:CD	1.34	1.41
1:D:407:DT:C3'	1:D:407:DT:C6	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
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
1:D:408:DG:C8	3:H:75:ARG:HB2	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:7:PHE:HE1	2:L:12:LEU:HD22	1.17	1.01
1:D:407:DT:C4'	1:D:407:DT:C6	2.40	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:N3	1:D:405:DG:H2'	1.75	0.98
3:H:41:LEU:HD12	3:H:41:LEU:N	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:NH1	2:L:15:ARG:HA	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
3:H:162:ILE:HD11	3:H:201:MET:HE3	1.52	0.91
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
3:H:99:LEU:CD1	3:H:215:TRP:HB3	2.00	0.90
3:H:50:ARG:HD3	3:H:247:GLU:HB3	1.52	0.90
1:D:407:DT:H3	3:H:77:GLU:HG2	1.33	0.90
1:D:402:DG:N2	1:D:405:DG:N7	2.19	0.90
2:L:1(A):ASP:O	2:L:1(A):ASP:OD1	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:0G7: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:212:ILE:O	3:H:228:TYR:HB3	1.76	0.84
3:H:157:VAL:O	3:H:157:VAL:HG23	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:1:0G7: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
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:177:THR:HG22	3:H:179:ASN:H	1.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1(F):GLY:HA2	3:H:123:LEU:O	1.80	0.81
1:D:407:DT:C5	1:D:407:DT:H3'	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
3:H:58:CYS:C	3:H:59:LEU:HD12	2.02	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:190:ALA:CB	3:H:213:VAL:HG11	2.12	0.79
3:H:46:LEU:O	3:H:121:VAL:HG12	1.83	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
3:H:60(A):TYR:C	3:H:60(C):PRO:HD2	2.05	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:110:LYS:HB3	3:H:111:PRO:CD	2.15	0.77
3:H:68:ILE:CG2	3:H:118:ILE:CG2	2.60	0.77
3:H:46:LEU:HD21	3:H:114:PHE:CE1	2.20	0.77
3:H:85:LEU:HD23	3:H:85:LEU:O	1.83	0.77
1:D:408:DG:N7	3:H:75:ARG:HD2	1.96	0.77
3:H:21:ASP:OD1	3:H:154:VAL:CG2	2.31	0.76
2:L:14(J):TYR:HD1	3:H:134:TYR:CD2	2.03	0.76
3:H:183:ALA:HB3	3:H:228:TYR:CE1	2.19	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
3:H:25:GLY:HA2	5:H:506:HOH:O	1.86	0.76
1:D:407:DT:H6	1:D:407:DT:C5'	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:98:ASN:ND2	3:H:175:ARG:O	2.20	0.74
3:H:41:LEU:H	3:H:41:LEU:CD1	2.01	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
3:H:181:PHE:CE1	3:H:230:HIS:HA	2.15	0.73
1:D:408:DG:H5'	3:H:75:ARG:NH2	2.04	0.73
3:H:204(B):ASN:ND2	3:H:206:ARG:HG3	2.03	0.73
3:H:35:ARG:HE	3:H:36:LYS:N	1.86	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:195:SER:OG	4:H:1:0G7:C3	2.37	0.72
3:H:60(I):THR:O	3:H:64:LEU:HD12	1.89	0.72
1:D:408:DG:O4'	3:H:75:ARG:NE	2.23	0.72
3:H:213:VAL:HG13	3:H:228:TYR:CD2	2.24	0.72
1:D:409:DT:C5'	3:H:77(A):ARG:HB3	2.20	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
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
3:H:122:CYS:O	3:H:208:TYR:HA	1.91	0.71
3:H:54:THR:HG22	3:H:55:ALA:N	2.06	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
3:H:77:GLU:O	3:H:77(A):ARG:C	2.29	0.71
2:L:3:LEU:HD22	3:H:206:ARG:HH11	1.55	0.71
2:L:14(J):TYR:O	2:L:14(K):ILE:C	2.29	0.70
3:H:211:GLY:HA2	3:H:231:VAL:CG2	2.20	0.70
3:H:67:ARG:NH2	3:H:80:GLU:OE2	2.24	0.70
3:H:128:THR:O	3:H:129(C):LEU:CB	2.40	0.70
2:L:1(G):PHE:CD1	3:H:239:GLN:HB2	2.27	0.70
2:L:1(A):ASP:CG	2:L:1(A):ASP:O	2.29	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:95:ASN:HD21	3:H:97(A):GLU:CB	2.04	0.70
3:H:129:ALA:HA	3:H:210:MET:CE	2.21	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: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:211:GLY:CA	3:H:231:VAL:CG2	2.71	0.69
3:H:47:ILE:HD13	3:H:53:LEU:HD23	1.74	0.69
1:D:406:DG:C8	1:D:409:DT:OP2	2.47	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:189:ASP:CG	4:H:1:0G7:NH2	2.47	0.68
1:D:407:DT:H73	3:H:24:ILE:HG22	1.75	0.68
3:H:31:VAL:HG13	3:H:66:VAL:HG23	1.75	0.67
3:H:60(A):TYR:CE2	4:H:1:0G7: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: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:172:THR:HG23	3:H:174:ILE:HG13	1.76	0.67
3:H:67:ARG:HG2	3:H:82:ILE:HG12	1.77	0.67
3:H:144:LEU:C	3:H:145:LYS:HG2	2.12	0.67
3:H:189:ASP:OD2	4:H:1:0G7: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
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: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:61:GLU:C	3:H:85:LEU:HD21	2.16	0.65
3:H:177:THR:CG2	3:H:179:ASN:HB2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	3:H:159:ASN:ND2	2.58	0.65
3:H:17:VAL:HG22	3:H:144:LEU:C	2.17	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
3:H:22:ALA:HB2	3:H:157:VAL:CG1	2.28	0.64
1:D:406:DG:N2	3:H:75:ARG:NH2	2.45	0.64
2:L:14(F):LEU:C	2:L:14(H):GLU:H	1.98	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: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:41:LEU:H	3:H:41:LEU:HD12	1.58	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
3:H:99:LEU:HD12	3:H:215:TRP:HB3	1.80	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
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:129:ALA:HA	3:H:210:MET:HE1	1.81	0.63
3:H:177:THR:HG22	3:H:179:ASN:HB2	1.81	0.63
3:H:17:VAL:O	3:H:18:GLU:C	2.34	0.63
3:H:162:ILE:CD1	3:H:201:MET:HE3	2.28	0.63
3:H:232:PHE:C	3:H:234:LEU:H	2.00	0.63
3:H:56:ALA:HB2	3:H:90:ILE:HG22	1.81	0.63
1:D:403:DT:H2'	1:D:403:DT:O2	1.98	0.63
2:L:7:PHE:CD1	2:L:12:LEU:HB3	2.34	0.63
3:H:214:SER:OG	3:H:229:THR:HG23	1.99	0.63
1:D:407:DT:O2	3:H:77:GLU:HG3	1.98	0.63
2:L:8:GLU:O	2:L:10:LYS:N	2.32	0.62
3:H:115:SER:O	3:H:118:ILE:HD13	1.96	0.62
3:H:130:LEU:O	3:H:130:LEU:HD12	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:HG23	2.19	0.62
3:H:190:ALA:H	4:H:1:0G7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14(F):LEU:HD11	3:H:159:ASN:HD22	1.63	0.62
3:H:150:GLY:N	3:H:151:GLN:NE2	2.47	0.62
3:H:33:LEU:HD12	3:H:42:CYS:SG	2.40	0.62
2:L:8:GLU:C	2:L:10:LYS:H	2.04	0.62
3:H:123:LEU:HG	3:H:235:LYS:HD3	1.82	0.61
3:H:16:ILE:HG12	3:H:158:VAL:HG12	1.82	0.61
3:H:73:ARG:HH12	3:H:74:THR:HG23	1.61	0.61
3:H:195:SER:HG	4:H:1:0G7:C3	2.12	0.61
3:H:91:HIS:HB3	3:H:103:ILE:CG2	2.30	0.61
3:H:60:LEU:C	3:H:60:LEU:HD23	2.20	0.61
1:D:409:DT:H5'	3:H:77(A):ARG:HB3	1.81	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
2:L:14(F):LEU:C	2:L:14(H):GLU:N	2.54	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:144:LEU:HD12	3:H:150:GLY:C	2.21	0.60
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:O2	1:D:403:DT:H2"	2.00	0.60
3:H:211:GLY:HA2	3:H:229:THR:O	2.00	0.60
2:L:6:LEU:HD12	3:H:24:ILE:HB	1.82	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
3:H:186(B):GLU:O	3:H:186(D):LYS:N	2.35	0.60
3:H:28:PRO:HB2	3:H:119:HIS:HB3	1.84	0.60
3:H:190:ALA:HB3	3:H:213:VAL:HG11	1.84	0.59
3:H:137:ARG:O	3:H:137:ARG:HG3	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
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
2:L:13:GLU:OE2	2:L:14(D):ARG:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:DT:C2	3:H:77:GLU:HG2	2.38	0.59
3:H:162:ILE:CD1	3:H:201:MET:CE	2.80	0.59
3:H:234:LEU:O	3:H:238:ILE:HD12	2.03	0.58
3:H:142:GLY:O	3:H:143:ASN:C	2.42	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:91:HIS:C	3:H:91:HIS:CD2	2.77	0.58
3:H:232:PHE:O	3:H:235:LYS:N	2.20	0.58
3:H:30:GLN:HE22	3:H:139:THR:C	2.04	0.58
1:D:411:DG:H21	1:D:412:DT:H2'	1.69	0.58
3:H:129:ALA:HA	3:H:210:MET:HE3	1.86	0.58
3:H:49:ASP:O	3:H:111:PRO:HA	2.04	0.57
3:H:56:ALA:CB	3:H:90:ILE:CG2	2.82	0.57
3:H:56:ALA:HB1	3:H:90:ILE:CG2	2.34	0.57
3:H:21:ASP:CG	3:H:154:VAL:CG2	2.73	0.57
3:H:234:LEU:O	3:H:238:ILE:CD1	2.52	0.57
3:H:35:ARG:HH22	3:H:36:LYS:HG2	1.69	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: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:57:HIS:NE2	4:H:1:0G7:C3	2.68	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
3:H:91:HIS:HB2	3:H:237:TRP:CD2	2.39	0.56
1:D:409:DT:P	1:D:409:DT:O4'	2.64	0.56
2:L:14(J):TYR:CD1	3:H:134:TYR:HD2	2.21	0.56
3:H:209:GLN:O	3:H:231:VAL:HB	2.06	0.56
3:H:172:THR:CG2	3:H:174:ILE:CG1	2.82	0.55
3:H:163:VAL:HB	3:H:182:CYS:SG	2.46	0.55
3:H:160:LEU:CD2	3:H:184(A):TYR:CE1	2.83	0.55
3:H:61:GLU:OE2	3:H:88:ILE:HD13	2.05	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
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
2:L:1(F):GLY:C	2:L:1(D):GLY:N	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:CYS:C	3:H:122:CYS:SG	2.84	0.55
3:H:144:LEU:HD21	3:H:152:PRO:CG	2.35	0.55
3:H:123:LEU:CD2	3:H:235:LYS:HD3	2.36	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:221:ASP:O	3:H:221(A):ARG:C	2.44	0.55
3:H:234:LEU:HD23	3:H:237:TRP:CB	2.26	0.55
3:H:56:ALA:CB	3:H:90:ILE:HG22	2.36	0.55
3:H:126:ARG:O	3:H:129(A):ALA:HB2	2.06	0.55
3:H:31:VAL:HG13	3:H:66:VAL:HG22	1.87	0.55
2:L:4:ARG:HG2	3:H:28:PRO:CG	2.37	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: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
3:H:206:ARG:HB2	3:H:208:TYR:HE1	1.72	0.54
2:L:4:ARG:HG2	3:H:28:PRO:HG2	1.90	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
1:D:411:DG:N3	1:D:412:DT:H2'	2.23	0.53
3:H:177:THR:HG22	3:H:179:ASN:CB	2.38	0.53
3:H:51:TRP:NE1	3:H:242:ILE:HG23	2.22	0.53
3:H:31:VAL:CB	3:H:44:ALA:O	2.57	0.53
2:L:8:GLU:C	2:L:10:LYS:N	2.61	0.53
2:L:14:ASP:N	2:L:14(C):GLU:OE1	2.36	0.53
2:L:1(G):PHE:HA	3:H:235:LYS:NZ	2.24	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
3:H:22:ALA:HB3	3:H:155:LEU:HG	1.91	0.52
2:L:1(H):THR:HG22	2:L:1(G):PHE:N	2.06	0.52
2:L:1(F):GLY:CA	3:H:123:LEU:O	2.56	0.52
3:H:18:GLU:HA	3:H:18:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14(A):LYS:HG3	3:H:23:GLU:OE1	2.09	0.52
3:H:33:LEU:HB2	3:H:42:CYS:O	2.09	0.52
3:H:206:ARG:HB2	3:H:208:TYR:CE1	2.44	0.52
3:H:35:ARG:NH2	3:H:36:LYS:H	2.06	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:165:ARG:N	3:H:166:PRO:HD2	2.25	0.52
3:H:34:PHE:HA	3:H:39:GLU:O	2.10	0.52
3:H:232:PHE:O	3:H:234:LEU:N	2.42	0.52
2:L:14:ASP:O	2:L:14(A):LYS:C	2.47	0.52
3:H:159:ASN:C	3:H:160:LEU:HG	2.29	0.51
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
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
2:L:14(I):SER:HB3	3:H:135:LYS:HG3	1.91	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:177:THR:C	3:H:179:ASN:H	2.13	0.51
3:H:212:ILE:O	3:H:228:TYR:CB	2.52	0.51
3:H:150:GLY:C	3:H:151:GLN:NE2	2.64	0.51
3:H:35:ARG:HD2	3:H:60(H):PHE:CZ	2.46	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
2:L:8:GLU:OE1	2:L:14(C):GLU:OE2	2.29	0.51
1:D:404:DT:C4	1:D:411:DG:C5	2.99	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
2:L:14:ASP:OD1	2:L:14(C):GLU:OE1	2.29	0.50
3:H:234:LEU:C	3:H:236:LYS:N	2.64	0.50
2:L:6:LEU:HD21	3:H:116:ASP:HB3	1.93	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:22:ALA:CB	3:H:155:LEU:HG	2.41	0.50
1:D:410:DG:C4'	3:H:77(A):ARG:HH12	2.19	0.50
3:H:169:LYS:C	3:H:171:SER:H	2.15	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
3:H:49:ASP:HA	3:H:114:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14(F):LEU:HD12	2:L:14(F):LEU:N	2.26	0.50
3:H:238:ILE:H	3:H:238:ILE:HD12	1.77	0.49
3:H:60(H):PHE:HB3	3:H:64:LEU:HD11	1.94	0.49
3:H:160:LEU:CD2	3:H:184(A):TYR:HE1	2.20	0.49
3:H:51:TRP:CZ2	3:H:245:PHE:O	2.65	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
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:136:GLY:HA3	3:H:199:PHE:HE1	1.76	0.49
3:H:212:ILE:C	3:H:228:TYR:HB3	2.31	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
3:H:98:ASN:O	3:H:99:LEU:C	2.52	0.48
3:H:45:SER:O	3:H:47:ILE:CG2	2.62	0.48
1:D:407:DT:C2	3:H:77:GLU:CG	2.96	0.48
3:H:28:PRO:HB2	3:H:119:HIS:CB	2.43	0.48
3:H:57:HIS:CD2	3:H:57:HIS:C	2.86	0.48
3:H:214:SER:HB2	3:H:227:PHE:O	2.14	0.48
3:H:172:THR:HG22	3:H:174:ILE:HB	1.94	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:35:ARG:HE	3:H:35:ARG:CA	2.27	0.48
3:H:228:TYR:N	3:H:228:TYR:CD1	2.82	0.47
3:H:29:TRP:O	3:H:45:SER:HA	2.14	0.47
2:L:1:CYS:O	3:H:206:ARG:HD2	2.14	0.47
1:D:414:DG:N3	1:D:414:DG:O4'	2.46	0.47
3:H:212:ILE:O	3:H:228:TYR:HA	2.15	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:167:VAL:HG12	3:H:225:TYR:CE2	2.49	0.47
3:H:69:GLY:O	3:H:79:ILE:HG22	2.13	0.47
1:D:407:DT:C1'	1:D:409:DT:H3	2.22	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
3:H:147:THR:HG23	3:H:148:TRP:N	2.28	0.47
1:D:409:DT:H5'	3:H:77(A):ARG:HD3	1.97	0.47
3:H:114:PHE:CZ	3:H:120:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:177:THR:HG21	3:H:179:ASN:HB2	1.97	0.47
2:L:1(G):PHE:O	3:H:123:LEU:HB3	2.15	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
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: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:O2	1:D:413:DT:O4'	2.30	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:1:0G7:HD3	2.45	0.46
3:H:163:VAL:N	3:H:182:CYS:O	2.41	0.46
3:H:33:LEU:HB3	3:H:42:CYS:H	1.79	0.46
3:H:184:GLY:CA	5:H:562:HOH:O	2.63	0.46
3:H:135:LYS:HA	3:H:161:PRO:HA	1.97	0.46
3:H:191:CYS:HA	4:H:1:0G7:HD3	1.96	0.46
2:L:14:ASP:OD2	3:H:137:ARG:NH2	2.43	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
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:OP1	1:D:409:DT:O4'	2.34	0.45
3:H:159:ASN:O	3:H:184(A):TYR:OH	2.24	0.45
3:H:199:PHE:C	3:H:199:PHE:CD1	2.89	0.45
2:L:14(J):TYR:CE1	3:H:134:TYR:CD2	3.04	0.45
3:H:31:VAL:HB	3:H:44:ALA:C	2.37	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
3:H:144:LEU:O	3:H:145:LYS:HG2	2.16	0.45
3:H:215:TRP:HA	4:H:1:0G7:HB2A	1.99	0.45
2:L:14(E):GLU:HG3	2:L:14(F):LEU:HD12	1.97	0.45
3:H:203:SER:C	3:H:204(A):PHE:H	2.19	0.45
3:H:210:MET:C	3:H:231:VAL:HG23	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:32:MET:CE	3:H:40:LEU:HD13	2.47	0.45
3:H:128:THR:O	3:H:129(C):LEU:CG	2.65	0.45
3:H:73:ARG:HD3	3:H:152:PRO:O	2.17	0.45
3:H:31:VAL:N	3:H:44:ALA:O	2.47	0.45
3:H:186(B):GLU:C	3:H:186(D):LYS:H	2.20	0.44
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:181:PHE:HZ	3:H:210:MET:O	2.00	0.44
3:H:51:TRP:CD2	3:H:242:ILE:HG23	2.52	0.44
3:H:199:PHE:C	3:H:199:PHE:HD1	2.20	0.44
3:H:31:VAL:CG1	3:H:32:MET:H	2.30	0.44
3:H:60:LEU:C	3:H:60:LEU:CD2	2.84	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:HA	3:H:129(C):LEU:HD23	1.72	0.44
3:H:233:ARG:O	3:H:233:ARG:HG3	2.16	0.44
3:H:116:ASP:O	3:H:117:TYR:CG	2.71	0.44
3:H:68:ILE:HG22	3:H:118:ILE:CG2	2.33	0.44
3:H:77:GLU:HG2	3:H:79:ILE:HB	1.99	0.44
3:H:61:GLU:OE2	3:H:87:LYS:HE3	2.17	0.44
3:H:69:GLY:HA3	3:H:118:ILE:HG13	2.00	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:1:0G7:NH1	2.65	0.44
2:L:1(G):PHE:HA	3:H:235:LYS:HZ3	1.82	0.44
3:H:22:ALA:N	3:H:155:LEU:O	2.48	0.43
3:H:158:VAL:CG2	3:H:160:LEU:HD11	2.47	0.43
3:H:73:ARG:CG	3:H:73:ARG:O	2.59	0.43
1:D:404:DT:O4	1:D:412:DT:C3'	2.63	0.43
3:H:112:VAL:HG23	3:H:113:ALA:O	2.18	0.43
3:H:54:THR:CG2	3:H:55:ALA:N	2.70	0.43
3:H:123:LEU:CG	3:H:235:LYS:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:215:TRP:CE3	4:H:1:0G7:HD2	2.54	0.43
3:H:162:ILE:CD1	3:H:201:MET:HE1	2.48	0.43
3:H:46:LEU:C	3:H:47:ILE:CG2	2.86	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:91:HIS:O	3:H:94:TYR:HB3	2.19	0.43
2:L:15:ARG:HH11	2:L:15:ARG:CA	2.12	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: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:203:SER:C	3:H:204(A):PHE:N	2.72	0.42
3:H:180:MET:HE1	3:H:215:TRP:HE1	1.84	0.42
3:H:118:ILE:N	3:H:118:ILE:CD1	2.77	0.42
3:H:190:ALA:O	4:H:1:0G7:NH1	2.52	0.42
3:H:209:GLN:NE2	3:H:212:ILE:HG12	2.34	0.42
3:H:45:SER:OG	3:H:53:LEU:HG	2.19	0.42
1:D:409:DT:OP1	1:D:409:DT:O2	2.37	0.42
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
2:L:1(H):THR:CG2	2:L:1(G):PHE:CD1	3.02	0.42
3:H:25:GLY:C	3:H:27:SER:N	2.72	0.42
3:H:41:LEU:CD2	3:H:64:LEU:HD23	2.49	0.42
2:L:14(F):LEU:O	2:L:14(I):SER:N	2.33	0.42
1:D:407:DT:C1'	1:D:409:DT:C2	2.90	0.42
3:H:106:MET:HE2	3:H:106:MET:HB2	1.70	0.42
3:H:98:ASN:HD21	3:H:175:ARG:HH11	1.68	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:60(I):THR:C	3:H:64:LEU:HD12	2.39	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
3:H:209:GLN:HE22	3:H:212:ILE:HG12	1.86	0.41
1:D:408:DG:H4'	3:H:77:GLU:HG3	2.00	0.41
3:H:16:ILE:CG2	3:H:158:VAL:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:190:ALA:C	4:H:1:0G7:NH1	2.74	0.41
3:H:163:VAL:HG12	3:H:168:CYS:SG	2.61	0.41
3:H:124:PRO:HA	3:H:208:TYR:HD2	1.85	0.41
3:H:189:ASP:OD2	3:H:220:CYS:HA	2.21	0.41
3:H:233:ARG:HD3	3:H:233:ARG:HA	1.98	0.41
3:H:51:TRP:NE1	3:H:242:ILE:CG2	2.83	0.41
3:H:81:LYS:HZ3	3:H:115:SER:HB3	1.86	0.41
3:H:177:THR:C	3:H:179:ASN:N	2.74	0.41
3:H:24:ILE:CD1	3:H:24:ILE:H	2.32	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
2:L:3:LEU:HD22	3:H:206:ARG:NH1	2.30	0.41
3:H:230:HIS:C	3:H:232:PHE:H	2.25	0.40
3:H:94:TYR:HA	3:H:100:ASP:O	2.21	0.40
3:H:139:THR:HG22	3:H:157:VAL:HG12	2.02	0.40
3:H:172:THR:CG2	3:H:174:ILE:CB	3.00	0.40
3:H:163:VAL:O	3:H:182:CYS:SG	2.79	0.40
3:H:195:SER:HG	4:H:1:0G7:C2	2.35	0.40
3:H:221:ASP:O	3:H:222:ASP:N	2.55	0.40
3:H:41:LEU:HD21	3:H:64:LEU:HD23	2.03	0.40
3:H:105:LEU:C	3:H:106:MET:HG3	2.42	0.40
2:L:3:LEU:HA	2:L:3:LEU:HD12	1.84	0.40
2:L:8:GLU:HG3	3:H:202:LYS:NZ	2.37	0.40
3:H:61:GLU:CD	3:H:87:LYS:HD3	2.41	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%)	2 6
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 (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	31/31 (100%)	21 (68%)	10 (32%)	0 0
3	H	221/225 (98%)	141 (64%)	80 (36%)	0 0
All	All	252/256 (98%)	162 (64%)	90 (36%)	0 0

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	1(G)	PHE
2	L	1(A)	ASP
2	L	10	LYS
2	L	12	LEU
2	L	14(A)	LYS
2	L	14(C)	GLU
2	L	14(E)	GLU
2	L	14(G)	LEU
2	L	14(K)	ILE
2	L	15	ARG
3	H	16	ILE
3	H	18	GLU
3	H	23	GLU
3	H	24	ILE
3	H	30	GLN
3	H	32	MET
3	H	33	LEU
3	H	35	ARG
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	60(C)	PRO
3	H	60(G)	ASN
3	H	60(I)	THR
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
3	H	85	LEU
3	H	86	GLU
3	H	87	LYS
3	H	88	ILE
3	H	90	ILE

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Mol	Chain	Res	Type
3	H	91	HIS
3	H	94	TYR
3	H	97	ARG
3	H	103	ILE
3	H	106	MET
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	130	LEU
3	H	134	TYR
3	H	138	VAL
3	H	139	THR
3	H	147	THR
3	H	153	SER
3	H	155	LEU
3	H	160	LEU
3	H	164	GLU
3	H	169	LYS
3	H	170	ASP
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	187	ARG
3	H	199	PHE
3	H	205	ASN
3	H	206	ARG
3	H	209	GLN
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

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Mol	Chain	Res	Type
3	H	230	HIS
3	H	234	LEU
3	H	235	LYS
3	H	239	GLN
3	H	240	LYS
3	H	242	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	31,31,32	2.25	3 (9%)	36,41,42	2.13	10 (27%)

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	-10.80	1.22	1.49
4	H	1	0G7	O1-C1	4.19	1.31	1.23
4	H	1	0G7	C1-N2	-2.83	1.27	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	0G7	CA1-C1-N2	7.32	132.90	116.58
4	H	1	0G7	O1-C1-N2	-4.37	114.84	122.93
4	H	1	0G7	CG-CB-CA	4.24	122.94	114.13
4	H	1	0G7	C1-CA1-N1	3.41	121.94	112.56
4	H	1	0G7	O1-C1-CA1	-3.37	112.23	120.63
4	H	1	0G7	CB-CA-C	2.77	115.90	109.27
4	H	1	0G7	CB2-CA2-N2	2.65	116.24	110.88
4	H	1	0G7	CG2-CB2-CA2	2.23	120.82	113.92
4	H	1	0G7	CB1-CA1-C1	2.22	115.95	111.22
4	H	1	0G7	CB2-CG2-CD3	2.16	118.52	112.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

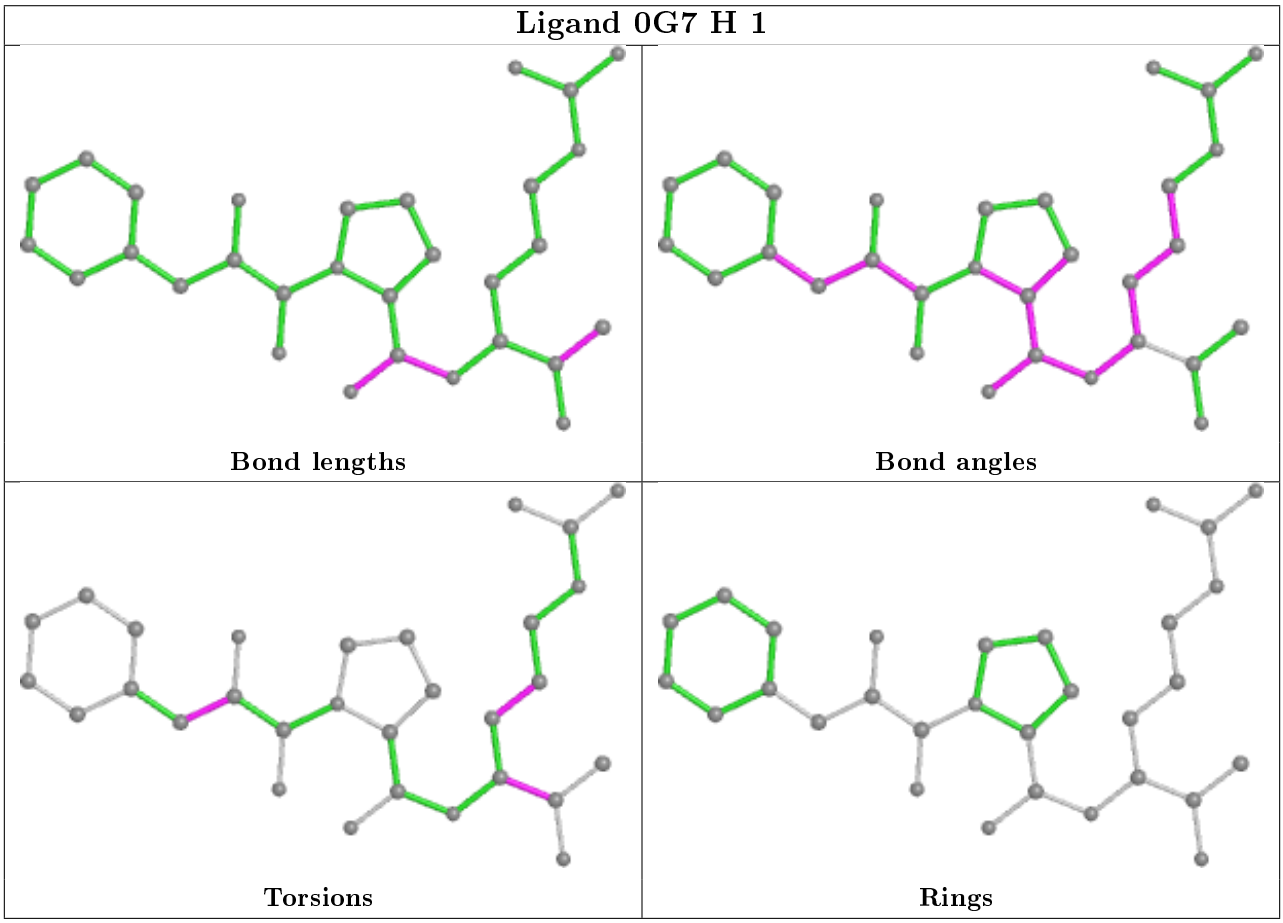
Mol	Chain	Res	Type	Atoms
4	H	1	0G7	C-CA-CB-CG
4	H	1	0G7	CA2-CB2-CG2-CD3
4	H	1	0G7	N-CA-CB-CG
4	H	1	0G7	C3-C2-CA2-CB2
4	H	1	0G7	O2-C2-CA2-CB2

There are no ring outliers.

1 monomer is involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	0G7	21	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 then 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.