



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:37 AM UTC

PDB ID : 1HAO / pdb_00001hao
Title : COMPLEX OF HUMAN ALPHA-THROMBIN WITH A 15MER OLIGONUCLEOTIDE GGTTGGTGTGGTTGG (BASED ON NMR MODEL OF DNA)
Authors : Tulinsky, A.; Padmanabhan, K.
Deposited on : 1995-10-03
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

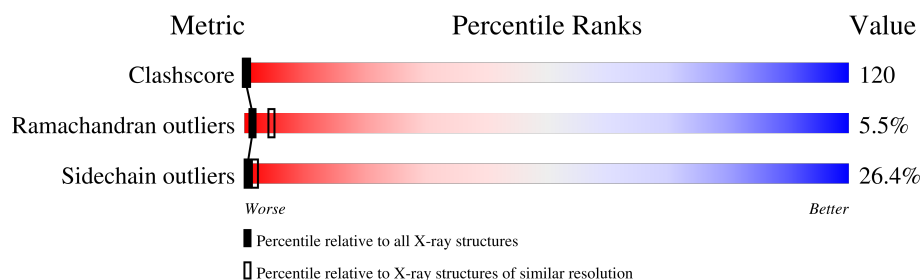
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	15	93% 7%
2	L	36	6% 28% 31% 11% 25%
3	H	259	6% 34% 43% 15% .

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

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2769 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			

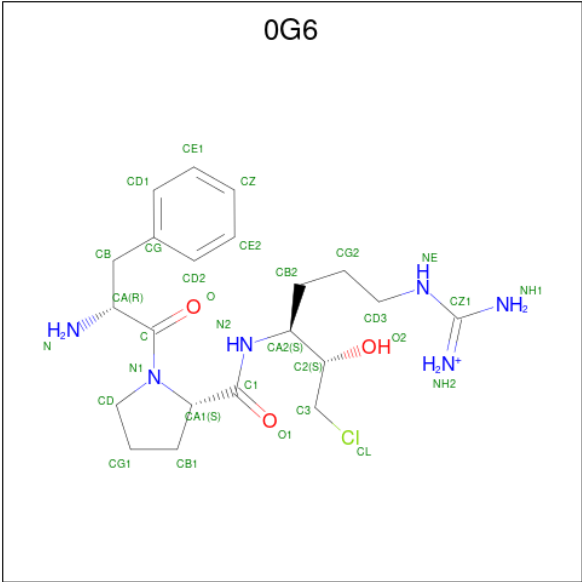
- Molecule 2 is a protein called ALPHA-THROMBIN light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	27	Total	C	N	O	S	0	0	0
			222	140	36	45	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-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



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

- Molecule 5 is water.

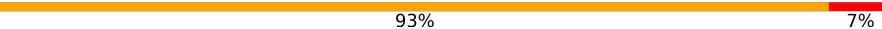
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	19	Total	O	0	0
			19	19		
5	L	11	Total	O	0	0
			11	11		
5	H	119	Total	O	0	0
			119	119		

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.

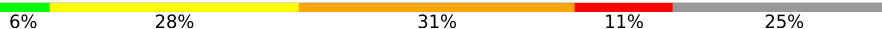
Note EDS was not executed.

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

Chain D: 

G401
G402
T403
T404
G405
G406
T407
G408
T409
G410
G411
T412
T413
G414
G415

- Molecule 2: ALPHA-THROMBIN light chain

Chain L: 

THR
PHE
GLY
SER
GLY
GLY
A1B
D1A
C1
G2
L3
R4
P5
L6
F7
E8
K9
K10
S11
L12
E13
D14
K14A
T14B
E14C
R14D
E14E
L14F
L14G
S14I
Y14J
I14K
ASP
GLY
ARG

- Molecule 3: ALPHA-THROMBIN heavy chain

Chain H: 

I16
V17
E18
G19
S20
D21
A22
E23
I24
G25
R26
S27
P28
K29
Q30
V31
M32
L33
K34
R35
K36
S36A
P37
Q38
Q39
E39
L40
L41
C42
L44F
L44G
A44
S45
S45
L46
I47
S48
D49
R50
W51
V52
L53
T54
A55
A56
H57
C58
L59
L60
Y60A
P60B
P60C
W60D
D60E
K60F
N60G
F60H
T60I
E61
N62
D63
L64
L65

V66
R67
I68
G69
H70
K71
S72
R73
T74
R75
Y76
E77
R77A
W78
I79
E80
K81
I82
S83
M84
L85
E86
K87
I88
Y89
I90
H91
P92
R93
Y94
A94
N95
W96
R97
E97A
N98
L99
D100
R101
D102
L103
A104
L105
M106
K107
L108
K109
K110
P111
V112
A113
F114
S115
D116
Y117
I118
H119
P120
V121
C122
L123

P124
D125
E126
E127
I128
A129
A129A
S129B
L129C
L130
Q131
Y132
G133
Y134
K135
G136
R137
V138
T139
G140
W141
G142
N143
L144
K145
E146
T147
THR
ALA
ASN
VAL
GLY
LYS
G150
Q151
P152
S153
V154
L155
Q156
V157
V158
N159
L160
P161
V162
V163
E164
R165
P166
V167
C168
K169
D170
S171
T172
R173
I174
R175

I176
I177
D178
M179
M180
F181
C182
A183
G184
Y184A
K185
Y241
I242
D243
E186B
G186D
R187
G188
D189
A190
C191
E192
G193
D194
S195
G196
G197
P198
F199
V200
M201
K202
S203
P204
F204A
N204B
N205
R206
W207
Y208
Q209
M210
G211
I212
V213
S214
W215
G216
C220
D221
R221A
D222
G223
K224
F227
Y228
T229
H230

V231
F232
R233
L234
K235
K236
W237
I238
Q239
K240
Y241
I242
D243
Q244
F245
G246
E247

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	58.28Å 77.61Å 100.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	68.0 (10.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLIN, PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2769	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0G6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.98	0/353	2.75	34/547 (6.2%)
2	L	1.13	0/224	2.91	26/298 (8.7%)
3	H	1.34	10/2107 (0.5%)	2.96	250/2846 (8.8%)
All	All	1.29	10/2684 (0.4%)	2.93	310/3691 (8.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
3	H	0	3
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	44	ALA	C-N	-11.36	1.17	1.33
3	H	60(D)	TRP	C-N	-6.71	1.18	1.34
3	H	181	PHE	C-N	6.62	1.42	1.33
3	H	161	PRO	C-N	-6.40	1.25	1.33
3	H	138	VAL	C-N	6.05	1.41	1.33
3	H	148	TRP	NE1-CE2	-5.68	1.31	1.37
3	H	19	GLY	N-CA	5.51	1.48	1.44
3	H	215	TRP	C-N	-5.40	1.28	1.33
3	H	145	LYS	C-N	-5.21	1.26	1.33
3	H	100	ASP	N-CA	5.05	1.52	1.46

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	410	DG	P-O3'-C3'	19.29	149.13	120.20
3	H	135	LYS	CA-C-N	19.07	141.00	121.35
3	H	135	LYS	C-N-CA	19.07	141.00	121.35
3	H	62	ASN	CA-CB-CG	17.76	130.36	112.60
1	D	409	DT	P-O3'-C3'	14.02	141.24	120.20
3	H	209	GLN	OE1-CD-NE2	13.33	135.93	122.60
1	D	414	DG	O5'-C5'-C4'	-12.93	91.41	110.80
3	H	160	LEU	O-C-N	12.90	131.04	121.88
3	H	184	GLY	N-CA-C	12.80	131.81	110.56
3	H	140	GLY	N-CA-C	12.78	126.33	111.63
1	D	409	DT	O5'-C5'-C4'	-12.38	92.23	110.80
3	H	194	ASP	N-CA-C	12.06	124.51	111.36
3	H	119	HIS	O-C-N	11.91	131.13	121.84
3	H	199	PHE	CA-CB-CG	11.62	125.42	113.80
3	H	27	SER	O-C-N	11.52	129.60	121.19
1	D	414	DG	P-O5'-C5'	11.18	136.77	120.00
3	H	62	ASN	CA-C-N	11.17	136.36	120.28
3	H	62	ASN	C-N-CA	11.17	136.36	120.28
1	D	408	DG	P-O3'-C3'	-11.10	103.55	120.20
3	H	187	ARG	NE-CZ-NH2	10.98	129.08	119.20
3	H	18	GLU	CB-CG-CD	10.82	131.00	112.60
3	H	221	ASP	CA-CB-CG	10.56	123.16	112.60
3	H	40	LEU	CA-C-O	-10.41	108.94	120.92
3	H	207	TRP	CA-C-O	-10.05	109.75	121.11
3	H	33	LEU	CA-C-O	-10.02	109.40	120.92
3	H	200	VAL	N-CA-C	9.88	120.82	110.05
3	H	222	ASP	CA-CB-CG	9.79	122.39	112.60
3	H	151	GLN	N-CA-CB	9.78	121.37	111.10
3	H	205	ASN	N-CA-CB	-9.77	96.90	112.63
3	H	91	HIS	O-C-N	9.76	131.76	121.42
3	H	40	LEU	O-C-N	9.73	134.45	123.16
3	H	211	GLY	CA-C-N	9.71	136.21	122.23
3	H	211	GLY	C-N-CA	9.71	136.21	122.23
3	H	157	VAL	O-C-N	9.63	133.58	123.18
3	H	62	ASN	CA-C-O	9.59	131.07	121.00
3	H	196	GLY	CA-C-O	9.55	129.51	119.10
2	L	10	LYS	CA-C-O	9.49	131.74	120.53
3	H	46	LEU	CB-CA-C	9.34	125.12	109.80
3	H	126	ARG	CD-NE-CZ	9.32	137.45	124.40
3	H	74	THR	CB-CA-C	-9.32	96.57	111.39
3	H	27	SER	CA-C-O	-9.26	112.64	121.34
3	H	22	ALA	N-CA-C	-9.20	96.86	110.48
3	H	247	GLU	N-CA-CB	9.20	126.13	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	CYS	CA-C-N	9.18	139.41	121.41
2	L	1	CYS	C-N-CA	9.18	139.41	121.41
3	H	216	GLY	N-CA-C	-9.05	102.26	111.85
1	D	415	DG	P-O5'-C5'	9.01	133.52	120.00
3	H	156	GLN	OE1-CD-NE2	8.92	131.52	122.60
3	H	17	VAL	CA-C-N	8.81	135.21	122.35
3	H	17	VAL	C-N-CA	8.81	135.21	122.35
3	H	153	SER	N-CA-C	-8.74	102.63	113.38
3	H	74	THR	N-CA-C	8.68	124.49	111.04
3	H	194	ASP	CA-CB-CG	-8.62	103.98	112.60
2	L	14(E)	GLU	N-CA-C	-8.62	101.84	111.07
3	H	238	ILE	CA-C-O	-8.60	112.11	121.05
3	H	55	ALA	CA-C-O	-8.47	111.72	121.72
3	H	139	THR	N-CA-C	8.45	122.25	108.99
3	H	247	GLU	CB-CG-CD	8.42	126.91	112.60
3	H	215	TRP	CA-C-N	8.36	134.19	122.57
3	H	215	TRP	C-N-CA	8.36	134.19	122.57
3	H	173	ARG	N-CA-C	-8.35	103.25	113.19
3	H	81	LYS	CA-C-N	8.32	133.55	122.90
3	H	81	LYS	C-N-CA	8.32	133.55	122.90
3	H	172	THR	CA-CB-OG1	-8.27	97.20	109.60
3	H	26	MET	CA-C-O	8.25	129.53	119.79
3	H	127	GLU	CB-CG-CD	8.10	126.36	112.60
3	H	204(B)	ASN	CA-CB-CG	-8.09	104.51	112.60
3	H	170	ASP	CB-CA-C	8.07	124.78	110.81
3	H	63	ASP	CA-CB-CG	8.05	120.65	112.60
3	H	206	ARG	N-CA-C	-8.04	97.89	110.36
3	H	194	ASP	CA-C-N	8.03	136.87	121.54
3	H	194	ASP	C-N-CA	8.03	136.87	121.54
1	D	414	DG	C2'-C3'-O3'	7.97	123.46	111.50
3	H	111	PRO	N-CA-C	7.94	123.69	111.15
2	L	1	CYS	N-CA-C	-7.89	100.40	110.19
3	H	184	GLY	CA-C-O	7.89	130.00	121.56
2	L	14(B)	THR	CA-CB-OG1	-7.88	97.77	109.60
3	H	106	MET	O-C-N	7.88	133.07	122.59
3	H	67	ARG	CA-C-O	7.84	128.80	120.33
3	H	118	ILE	CA-C-O	7.75	129.73	120.66
1	D	405	DG	P-O5'-C5'	7.73	131.59	120.00
3	H	238	ILE	N-CA-CB	7.72	120.12	110.47
2	L	14(B)	THR	N-CA-CB	-7.71	100.64	110.90
1	D	412	DT	P-O5'-C5'	-7.65	108.52	120.00
3	H	84	MET	O-C-N	7.62	132.88	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	151	GLN	OE1-CD-NE2	7.59	130.19	122.60
3	H	133	GLY	O-C-N	7.54	130.50	122.65
3	H	34	PHE	CB-CA-C	7.54	120.89	110.34
3	H	122	CYS	O-C-N	7.54	131.86	123.04
3	H	61	GLU	CB-CG-CD	7.52	125.38	112.60
3	H	78	ASN	CB-CA-C	7.50	122.61	110.09
3	H	198	PRO	CB-CA-C	-7.49	99.92	110.63
3	H	119	HIS	CA-CB-CG	-7.48	106.32	113.80
3	H	169	LYS	N-CA-C	7.46	119.41	111.28
3	H	246	GLY	O-C-N	7.43	131.06	123.11
2	L	3	LEU	O-C-N	7.38	132.74	123.14
3	H	23	GLU	CA-CB-CG	7.38	128.85	114.10
1	D	412	DT	N1-C1'-C2'	-7.37	102.44	113.50
3	H	18	GLU	N-CA-CB	7.35	124.01	112.46
1	D	403	DT	O3'-P-O5'	7.34	115.01	104.00
3	H	77	GLU	CA-CB-CG	-7.34	99.43	114.10
3	H	151	GLN	O-C-N	7.32	128.37	121.71
3	H	243	ASP	CA-CB-CG	7.31	119.91	112.60
3	H	60(D)	TRP	CB-CA-C	-7.29	99.14	110.37
3	H	238	ILE	O-C-N	7.28	129.03	121.89
1	D	412	DT	O5'-C5'-C4'	-7.27	99.89	110.80
1	D	409	DT	C5'-C4'-O4'	-7.27	98.50	109.40
2	L	4	ARG	CA-C-O	7.23	126.19	119.76
3	H	184(A)	TYR	CA-C-O	-7.23	112.38	120.54
3	H	199	PHE	CB-CA-C	-7.16	101.10	111.70
3	H	230	HIS	CA-CB-CG	7.15	120.95	113.80
1	D	404	DT	O5'-C5'-C4'	-7.15	100.08	110.80
3	H	95	ASN	N-CA-C	7.14	118.60	108.54
3	H	245	PHE	CA-CB-CG	7.13	120.93	113.80
3	H	39	GLU	CA-CB-CG	7.11	128.31	114.10
3	H	210	MET	CA-C-O	7.09	130.91	120.42
3	H	127	GLU	CB-CA-C	7.06	121.89	110.95
3	H	106	MET	N-CA-C	-7.04	95.81	110.80
3	H	82	ILE	N-CA-C	7.04	118.26	107.99
3	H	222	ASP	CB-CA-C	6.98	121.58	109.65
3	H	129(A)	ALA	N-CA-CB	-6.98	99.55	109.94
3	H	61	GLU	N-CA-CB	-6.97	98.70	110.49
3	H	206	ARG	CA-C-O	-6.93	113.43	121.82
3	H	158	VAL	CA-C-O	-6.93	113.94	121.28
2	L	14(F)	LEU	CA-C-O	-6.92	113.56	120.82
3	H	199	PHE	N-CA-CB	6.90	123.02	110.60
3	H	187	ARG	N-CA-C	6.85	119.56	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	94	TYR	CA-C-O	-6.81	113.53	120.96
3	H	204(B)	ASN	CA-C-N	-6.80	113.06	123.47
3	H	204(B)	ASN	C-N-CA	-6.80	113.06	123.47
3	H	127	GLU	CA-CB-CG	6.78	127.67	114.10
3	H	191	CYS	N-CA-CB	-6.78	99.55	111.49
1	D	411	DG	C3'-C2'-C1'	-6.77	91.45	101.60
3	H	29	TRP	CA-CB-CG	6.75	126.42	113.60
3	H	20	SER	CA-CB-OG	-6.72	97.66	111.10
3	H	33	LEU	CA-C-N	-6.71	110.72	121.58
3	H	33	LEU	C-N-CA	-6.71	110.72	121.58
3	H	105	LEU	N-CA-C	-6.71	100.03	109.69
3	H	222	ASP	N-CA-C	-6.68	100.39	110.28
1	D	405	DG	N9-C1'-C2'	6.66	123.49	113.50
1	D	401	DG	P-O3'-C3'	6.62	130.13	120.20
2	L	14(I)	SER	N-CA-CB	-6.61	100.36	110.07
3	H	50	ARG	NE-CZ-NH1	-6.56	114.94	121.50
3	H	204	PRO	N-CA-C	-6.54	99.00	112.47
3	H	94	TYR	CB-CA-C	6.54	119.65	109.84
3	H	206	ARG	O-C-N	6.53	130.30	122.20
3	H	191	CYS	N-CA-C	6.51	117.06	107.88
3	H	161	PRO	CB-CA-C	-6.49	100.86	111.56
3	H	66	VAL	O-C-N	6.48	130.20	123.20
3	H	116	ASP	CA-CB-CG	-6.47	106.13	112.60
3	H	159	ASN	OD1-CG-ND2	-6.42	116.18	122.60
3	H	237	TRP	N-CA-C	-6.40	104.39	111.36
3	H	155	LEU	CA-C-O	-6.38	114.01	120.96
3	H	82	ILE	N-CA-CB	-6.36	103.76	111.21
3	H	187	ARG	NE-CZ-NH1	-6.34	115.16	121.50
3	H	161	PRO	CA-C-N	6.34	129.94	120.69
3	H	161	PRO	C-N-CA	6.34	129.94	120.69
2	L	7	PHE	CA-CB-CG	-6.32	107.48	113.80
3	H	193	GLY	CA-C-N	6.32	129.26	120.29
3	H	193	GLY	C-N-CA	6.32	129.26	120.29
3	H	77	GLU	CG-CD-OE1	-6.27	103.99	118.40
3	H	60(H)	PHE	O-C-N	6.26	132.72	122.70
3	H	102	ASP	CA-C-N	-6.25	114.25	122.94
3	H	102	ASP	C-N-CA	-6.25	114.25	122.94
3	H	117	TYR	CA-C-N	6.25	131.61	123.11
3	H	117	TYR	C-N-CA	6.25	131.61	123.11
3	H	52	VAL	CA-C-N	6.24	130.96	122.84
3	H	52	VAL	C-N-CA	6.24	130.96	122.84
2	L	14(F)	LEU	N-CA-C	6.20	117.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	197	GLY	O-C-N	6.18	127.95	121.77
3	H	209	GLN	CG-CD-NE2	-6.18	107.14	116.40
3	H	208	TYR	N-CA-C	6.17	119.24	109.50
3	H	203	SER	O-C-N	6.15	126.78	121.30
3	H	177	THR	CB-CA-C	-6.13	100.30	114.41
3	H	199	PHE	O-C-N	6.11	131.08	122.83
3	H	73	ARG	O-C-N	6.08	129.08	122.15
3	H	204(B)	ASN	N-CA-C	-6.06	105.43	114.64
1	D	408	DG	P-O5'-C5'	-6.06	110.92	120.00
3	H	221(A)	ARG	CA-C-N	-6.04	112.29	120.87
3	H	221(A)	ARG	C-N-CA	-6.04	112.29	120.87
3	H	30	GLN	CA-C-N	6.00	132.24	122.69
3	H	30	GLN	C-N-CA	6.00	132.24	122.69
3	H	215	TRP	N-CA-C	-6.00	99.96	108.23
3	H	35	ARG	CA-C-O	-5.98	114.61	121.07
3	H	80	GLU	CA-CB-CG	5.97	126.05	114.10
3	H	170	ASP	N-CA-C	-5.95	106.27	112.93
3	H	38	GLN	CA-CB-CG	5.94	125.99	114.10
3	H	235	LYS	N-CA-CB	5.94	118.92	110.13
2	L	14(I)	SER	CA-C-O	5.93	127.02	120.80
3	H	119	HIS	CA-C-O	-5.91	113.22	119.13
1	D	410	DG	P-O5'-C5'	-5.90	111.15	120.00
3	H	206	ARG	NE-CZ-NH2	5.89	124.50	119.20
3	H	123	LEU	CB-CA-C	5.88	117.16	108.87
3	H	55	ALA	CB-CA-C	5.85	120.07	109.83
3	H	151	GLN	CB-CG-CD	-5.83	102.69	112.60
3	H	158	VAL	O-C-N	5.81	129.63	123.00
3	H	184(A)	TYR	N-CA-C	-5.81	99.82	109.46
2	L	14(G)	LEU	CB-CA-C	5.79	121.47	109.95
2	L	14(B)	THR	N-CA-C	5.78	121.77	114.31
3	H	235	LYS	O-C-N	5.78	129.16	122.17
3	H	230	HIS	N-CA-CB	5.78	120.25	110.49
3	H	26	MET	CA-C-N	5.77	127.74	122.37
3	H	26	MET	C-N-CA	5.77	127.74	122.37
3	H	41	LEU	CB-CA-C	5.76	118.28	109.34
3	H	131	GLN	CA-C-N	5.76	130.42	121.26
3	H	131	GLN	C-N-CA	5.76	130.42	121.26
1	D	409	DT	O4'-C1'-N1	5.76	117.04	108.40
3	H	98	ASN	CA-CB-CG	-5.76	106.84	112.60
3	H	157	VAL	CA-C-O	-5.76	113.93	120.67
1	D	411	DG	O4'-C1'-N9	5.75	117.03	108.40
3	H	91	HIS	CA-CB-CG	5.74	119.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	156	GLN	CA-CB-CG	-5.74	102.63	114.10
3	H	62	ASN	OD1-CG-ND2	-5.73	116.87	122.60
3	H	212	ILE	N-CA-CB	5.73	122.52	111.62
3	H	31	VAL	CA-C-O	-5.73	114.63	121.28
3	H	60(I)	THR	O-C-N	5.71	129.89	123.27
3	H	133	GLY	N-CA-C	-5.71	106.83	114.25
3	H	23	GLU	N-CA-CB	5.70	119.92	110.63
1	D	405	DG	C5'-C4'-O4'	5.70	117.95	109.40
3	H	186	PRO	CA-C-N	-5.68	104.69	117.20
3	H	205	ASN	CA-CB-CG	5.68	118.28	112.60
3	H	232	PHE	CA-CB-CG	-5.68	108.12	113.80
3	H	50	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	L	10	LYS	CA-CB-CG	5.64	125.39	114.10
1	D	401	DG	O5'-C5'-C4'	-5.64	102.34	110.80
1	D	415	DG	O4'-C1'-C2'	-5.64	97.94	106.40
3	H	95	ASN	CB-CA-C	-5.62	103.38	111.70
3	H	21	ASP	CA-CB-CG	-5.62	106.98	112.60
3	H	229	THR	CA-CB-CG2	5.62	120.06	110.50
3	H	177	THR	N-CA-C	5.62	115.82	108.07
3	H	113	ALA	CA-C-N	-5.62	110.78	122.07
3	H	113	ALA	C-N-CA	-5.62	110.78	122.07
3	H	60(D)	TRP	CA-CB-CG	5.57	124.17	113.60
3	H	230	HIS	O-C-N	5.56	129.98	122.59
3	H	98	ASN	CB-CA-C	-5.54	100.87	109.80
3	H	234	LEU	CA-C-O	-5.54	111.56	120.65
3	H	146	GLU	O-C-N	5.54	129.95	122.59
3	H	77(A)	ARG	CA-C-N	-5.53	113.41	122.54
3	H	77(A)	ARG	C-N-CA	-5.53	113.41	122.54
2	L	2	GLY	N-CA-C	5.53	126.28	113.18
3	H	211	GLY	CA-C-O	5.51	128.45	122.33
3	H	216	GLY	CA-C-O	5.50	126.79	122.33
3	H	70	LYS	CA-C-N	5.50	132.05	121.54
3	H	70	LYS	C-N-CA	5.50	132.05	121.54
1	D	408	DG	C4'-C3'-C2'	-5.50	94.16	102.40
3	H	169	LYS	CA-C-O	-5.49	114.73	120.55
3	H	65	LEU	CA-CB-CG	5.46	135.40	116.30
2	L	14(E)	GLU	CB-CG-CD	5.45	121.87	112.60
2	L	4	ARG	CD-NE-CZ	5.45	132.03	124.40
3	H	86	GLU	N-CA-C	-5.45	106.69	113.55
3	H	169	LYS	CA-C-N	-5.44	113.62	122.65
3	H	169	LYS	C-N-CA	-5.44	113.62	122.65
3	H	56	ALA	CA-C-O	5.43	126.36	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	156	GLN	O-C-N	5.41	129.98	123.16
1	D	406	DG	P-O3'-C3'	-5.40	112.10	120.20
3	H	160	LEU	CA-C-O	-5.38	114.73	120.28
3	H	238	ILE	CA-C-N	-5.37	112.65	122.38
3	H	238	ILE	C-N-CA	-5.37	112.65	122.38
3	H	208	TYR	O-C-N	-5.37	116.63	123.24
1	D	409	DT	C4'-C3'-O3'	5.36	118.04	110.00
3	H	198	PRO	O-C-N	5.34	129.86	123.13
3	H	182	CYS	N-CA-CB	5.34	119.01	110.46
3	H	156	GLN	CA-C-N	5.34	130.43	123.06
3	H	156	GLN	C-N-CA	5.34	130.43	123.06
3	H	60(H)	PHE	CA-C-N	-5.34	105.45	117.20
3	H	55	ALA	N-CA-C	-5.33	102.63	110.52
3	H	18	GLU	CA-C-O	-5.32	114.39	120.98
3	H	230	HIS	ND1-CE1-NE2	5.32	113.72	108.40
3	H	68	ILE	O-C-N	5.31	128.56	122.93
3	H	137	ARG	NH1-CZ-NH2	-5.31	112.40	119.30
3	H	232	PHE	CB-CA-C	-5.28	102.52	110.92
3	H	165	ARG	CA-C-N	5.28	126.44	119.84
3	H	165	ARG	C-N-CA	5.28	126.44	119.84
3	H	54	THR	CA-CB-CG2	5.27	119.46	110.50
3	H	199	PHE	CA-C-O	-5.26	110.54	120.96
2	L	14(B)	THR	OG1-CB-CG2	5.25	119.81	109.30
3	H	213	VAL	CA-C-O	-5.25	114.86	120.85
3	H	122	CYS	CA-C-O	-5.25	114.71	120.69
3	H	157	VAL	CB-CA-C	-5.23	102.82	110.62
3	H	79	ILE	CA-C-N	5.23	128.27	120.90
3	H	79	ILE	C-N-CA	5.23	128.27	120.90
3	H	73	ARG	CA-C-N	5.22	128.73	120.89
3	H	73	ARG	C-N-CA	5.22	128.73	120.89
3	H	60(G)	ASN	CA-CB-CG	-5.21	107.39	112.60
3	H	209	GLN	O-C-N	-5.21	116.68	122.93
1	D	411	DG	P-O3'-C3'	-5.19	112.42	120.20
2	L	13	GLU	CA-CB-CG	5.19	124.48	114.10
3	H	128	THR	CB-CA-C	-5.17	101.88	110.68
3	H	109	LYS	CA-C-O	-5.16	115.58	121.00
3	H	60(D)	TRP	CB-CG-CD2	-5.16	119.58	126.80
3	H	156	GLN	CG-CD-NE2	-5.16	108.67	116.40
3	H	50	ARG	CA-C-O	-5.15	113.14	120.51
1	D	407	DT	P-O3'-C3'	-5.15	112.48	120.20
1	D	413	DT	P-O3'-C3'	-5.14	112.49	120.20
3	H	156	GLN	CA-C-O	-5.13	115.36	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	40	LEU	N-CA-C	-5.13	101.35	109.96
2	L	14(C)	GLU	C-N-CA	5.11	134.47	121.70
1	D	405	DG	C1'-O4'-C4'	-5.10	102.06	109.70
2	L	4	ARG	NE-CZ-NH1	5.10	126.60	121.50
3	H	93	ARG	CA-CB-CG	-5.10	103.91	114.10
1	D	405	DG	O5'-P-OP2	5.09	123.28	108.00
3	H	159	ASN	CA-CB-CG	-5.09	107.51	112.60
2	L	4	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
3	H	241	VAL	O-C-N	5.07	128.91	122.57
1	D	406	DG	C4'-C3'-O3'	5.07	117.60	110.00
3	H	221(A)	ARG	N-CA-C	-5.06	102.99	110.48
3	H	185	LYS	N-CA-CB	5.03	116.74	110.04
3	H	129(C)	LEU	CB-CA-C	5.02	119.75	110.56
3	H	137	ARG	CB-CA-C	5.01	118.19	110.62
2	L	8	GLU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	402	DG	Sidechain
1	D	405	DG	Sidechain
3	H	181	PHE	Mainchain
3	H	247	GLU	Sidechain
3	H	77(A)	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	315	0	173	62	0
2	L	222	0	225	57	0
3	H	2053	0	2018	502	0
4	H	30	0	30	19	0
5	D	19	0	0	1	0
5	H	119	0	0	23	0
5	L	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2769	0	2446	601	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 (601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:144:LEU:HD21	3:H:152:PRO:CD	1.58	1.31
3:H:195:SER:CB	4:H:297:OG6:C3	2.09	1.29
3:H:84:MET:SD	3:H:109:LYS:HE3	1.79	1.20
3:H:17:VAL:O	3:H:188:GLY:HA2	1.40	1.20
3:H:144:LEU:CD2	3:H:152:PRO:HD3	1.71	1.20
3:H:195:SER:HB2	4:H:297:OG6:C3	1.69	1.19
3:H:81:LYS:HD3	3:H:118:ILE:CD1	1.71	1.19
3:H:60:LEU:HD23	3:H:94:TYR:HE2	1.09	1.17
3:H:89:TYR:HD2	5:H:567:HOH:O	1.21	1.17
3:H:91:HIS:CE1	3:H:101:ARG:HD3	1.79	1.16
2:L:3:LEU:HD23	3:H:206:ARG:HA	1.28	1.14
3:H:91:HIS:CE1	3:H:101:ARG:CD	2.31	1.14
2:L:14(J):TYR:C	2:L:14(K):ILE:HG13	1.72	1.11
3:H:24:ILE:HD13	3:H:24:ILE:N	1.61	1.11
3:H:60:LEU:HD23	3:H:94:TYR:CE2	1.86	1.11
3:H:172:THR:CG2	3:H:176:ILE:HD11	1.79	1.10
3:H:50:ARG:HD2	3:H:111:PRO:HD3	1.23	1.10
3:H:33:LEU:HD12	3:H:42:CYS:HB2	1.30	1.10
1:D:408:DG:O5'	1:D:408:DG:C2'	2.00	1.09
3:H:50:ARG:HD3	3:H:247:GLU:HG3	1.27	1.09
1:D:408:DG:O5'	1:D:408:DG:H2'	1.15	1.09
3:H:58:CYS:C	3:H:60(F):LYS:HD3	1.78	1.09
3:H:124:PRO:HB3	3:H:210:MET:HE1	1.26	1.09
3:H:172:THR:HG21	3:H:176:ILE:HD11	1.31	1.09
3:H:72:SER:HB3	3:H:77:GLU:OE2	1.52	1.08
3:H:32:MET:HE2	3:H:40:LEU:HD13	1.37	1.07
3:H:195:SER:OG	4:H:297:OG6:C3	2.00	1.07
1:D:406:DG:N2	1:D:410:DG:N7	2.01	1.07
3:H:234:LEU:O	3:H:238:ILE:HG13	1.55	1.06
3:H:140:GLY:HA2	3:H:155:LEU:HD12	1.38	1.06
1:D:413:DT:O2	3:H:77(A):ARG:HD3	1.54	1.05
1:D:401:DG:H2''	1:D:402:DG:H5'	1.06	1.05
3:H:60(B):PRO:HG2	3:H:96:TRP:CD2	1.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:ARG:NE	3:H:37:PRO:HD2	1.72	1.04
3:H:81:LYS:HD3	3:H:118:ILE:HD11	1.04	1.03
3:H:32:MET:HE2	3:H:40:LEU:CD1	1.88	1.03
3:H:165:ARG:HB3	3:H:166:PRO:HD3	1.36	1.03
3:H:201:MET:SD	3:H:210:MET:HG3	2.01	1.01
3:H:50:ARG:HD3	3:H:247:GLU:CG	1.89	1.01
3:H:70:LYS:HE3	3:H:80:GLU:OE1	1.61	1.01
3:H:60(B):PRO:HG2	3:H:96:TRP:CE2	1.96	1.00
3:H:34:PHE:CD1	3:H:65:LEU:HD23	1.97	1.00
1:D:401:DG:C2'	1:D:402:DG:H5'	1.93	0.99
3:H:26:MET:HE2	3:H:137:ARG:NH1	1.77	0.98
1:D:411:DG:H2'	1:D:411:DG:O5'	1.62	0.98
1:D:403:DT:C5'	1:D:404:DT:OP2	2.12	0.97
3:H:140:GLY:CA	5:H:579:HOH:O	2.13	0.96
1:D:410:DG:H2'	1:D:410:DG:N3	1.77	0.96
1:D:402:DG:C4	1:D:404:DT:H72	2.00	0.96
3:H:240:LYS:O	3:H:244:GLN:HG2	1.64	0.96
3:H:91:HIS:HE1	3:H:101:ARG:CD	1.76	0.95
3:H:183:ALA:HB3	3:H:228:TYR:HE2	1.31	0.94
3:H:97(A):GLU:HG3	5:H:542:HOH:O	1.66	0.94
3:H:91:HIS:CE1	3:H:101:ARG:HD2	2.01	0.94
1:D:412:DT:O2	3:H:79:ILE:HG21	1.69	0.92
3:H:230:HIS:HB3	3:H:233:ARG:HB2	1.51	0.92
3:H:51:TRP:HE1	3:H:247:GLU:H	1.15	0.92
3:H:175:ARG:HD2	3:H:175:ARG:O	1.70	0.92
3:H:140:GLY:HA2	3:H:155:LEU:CD1	2.00	0.91
1:D:406:DG:H4'	1:D:407:DT:OP1	1.68	0.91
3:H:73:ARG:HG3	3:H:141:TRP:HB3	1.52	0.91
3:H:24:ILE:HD13	3:H:24:ILE:H	1.28	0.91
3:H:41:LEU:HD11	3:H:64:LEU:HD21	1.53	0.90
3:H:73:ARG:HD3	3:H:152:PRO:O	1.71	0.90
3:H:204(B):ASN:HD22	3:H:205:ASN:N	1.70	0.89
3:H:51:TRP:HZ2	3:H:246:GLY:HA2	1.37	0.89
3:H:127:GLU:O	3:H:129(A):ALA:HB3	1.73	0.89
1:D:406:DG:C4'	1:D:407:DT:OP1	2.22	0.88
3:H:240:LYS:O	3:H:244:GLN:CG	2.22	0.87
3:H:50:ARG:CD	3:H:247:GLU:HG3	2.04	0.87
3:H:79:ILE:HD12	3:H:117:TYR:CD2	2.09	0.87
1:D:401:DG:H2''	1:D:402:DG:C5'	2.00	0.87
3:H:57:HIS:O	3:H:60(F):LYS:HD2	1.76	0.86
3:H:81:LYS:CD	3:H:118:ILE:HD11	2.00	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:ARG:HD2	3:H:111:PRO:CD	2.06	0.86
3:H:221(A):ARG:HB2	3:H:224:LYS:HG3	1.57	0.86
3:H:41:LEU:HD21	3:H:64:LEU:HD21	1.59	0.85
3:H:164:GLU:OE2	3:H:185:LYS:HE2	1.75	0.85
3:H:91:HIS:HE1	3:H:101:ARG:HD2	1.37	0.84
3:H:34:PHE:CE1	3:H:65:LEU:HD23	2.11	0.84
2:L:14(J):TYR:O	2:L:14(K):ILE:HG13	1.77	0.84
3:H:85:LEU:HD22	3:H:106:MET:HE2	1.57	0.84
3:H:144:LEU:N	3:H:144:LEU:HD23	1.91	0.84
3:H:204(B):ASN:HD22	3:H:204(B):ASN:C	1.85	0.84
3:H:32:MET:HG3	3:H:40:LEU:HD12	1.58	0.84
3:H:175:ARG:HD2	3:H:175:ARG:C	2.00	0.84
3:H:228:TYR:OH	5:H:654:HOH:O	1.96	0.83
1:D:403:DT:H5'	1:D:404:DT:OP2	1.76	0.83
3:H:123:LEU:HD23	3:H:124:PRO:HD2	1.60	0.83
3:H:165:ARG:CB	3:H:166:PRO:HD3	2.09	0.82
3:H:24:ILE:N	3:H:24:ILE:CD1	2.38	0.82
3:H:123:LEU:CD2	3:H:124:PRO:HD2	2.09	0.82
3:H:33:LEU:HD13	3:H:41:LEU:CD1	2.10	0.81
3:H:141:TRP:CZ2	3:H:155:LEU:HD13	2.15	0.81
1:D:406:DG:C5'	1:D:407:DT:OP1	2.29	0.81
3:H:165:ARG:HD3	3:H:165:ARG:C	2.04	0.81
1:D:406:DG:H5''	1:D:407:DT:OP1	1.80	0.81
3:H:84:MET:O	3:H:109:LYS:N	2.14	0.81
3:H:114:PHE:CZ	3:H:120:PRO:HG3	2.15	0.81
3:H:185:LYS:HB3	3:H:186:PRO:CD	2.11	0.81
2:L:1(A):ASP:OD1	2:L:1(A):ASP:O	1.99	0.80
3:H:221(A):ARG:HB2	3:H:224:LYS:CG	2.12	0.80
3:H:51:TRP:CZ2	3:H:246:GLY:HA2	2.16	0.80
3:H:60(A):TYR:H	3:H:60(F):LYS:HB3	1.45	0.80
3:H:97:ARG:NH2	5:H:550:HOH:O	2.06	0.79
3:H:204(B):ASN:O	3:H:205:ASN:HB3	1.82	0.79
3:H:58:CYS:O	3:H:60(F):LYS:HD3	1.83	0.78
3:H:144:LEU:HD21	3:H:152:PRO:HD3	0.82	0.78
3:H:165:ARG:HB3	3:H:166:PRO:CD	2.13	0.78
3:H:185:LYS:HB3	3:H:186:PRO:HD2	1.65	0.78
3:H:195:SER:OG	4:H:297:OG6:CA2	2.31	0.78
2:L:14(B):THR:O	2:L:14(C):GLU:C	2.26	0.78
3:H:35:ARG:CD	3:H:37:PRO:HD2	2.14	0.78
3:H:35:ARG:HD3	3:H:37:PRO:N	1.99	0.78
3:H:105:LEU:C	3:H:106:MET:HG3	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:DG:N3	1:D:404:DT:H72	2.00	0.77
1:D:401:DG:N1	1:D:406:DG:O6	2.16	0.77
3:H:180:MET:HE2	3:H:215:TRP:HE1	1.49	0.77
2:L:4:ARG:O	2:L:9:LYS:HB2	1.85	0.77
2:L:6:LEU:HD11	3:H:116:ASP:CB	2.14	0.77
3:H:195:SER:CB	4:H:297:OG6:C2	2.51	0.77
1:D:413:DT:O2	3:H:77(A):ARG:CD	2.31	0.77
3:H:210:MET:O	3:H:231:VAL:HG23	1.85	0.76
3:H:50:ARG:NH2	3:H:107:LYS:HE2	1.98	0.76
1:D:402:DG:H2''	1:D:404:DT:OP2	1.86	0.76
3:H:230:HIS:CG	3:H:233:ARG:HB2	2.20	0.76
3:H:122:CYS:HB2	3:H:207:TRP:O	1.85	0.76
3:H:184(A):TYR:CE1	3:H:186(D):LYS:HD3	2.20	0.76
2:L:3:LEU:CD2	3:H:206:ARG:HA	2.14	0.75
3:H:230:HIS:CB	3:H:233:ARG:HB2	2.16	0.75
3:H:44:ALA:HB1	3:H:52:VAL:CG1	2.17	0.75
3:H:124:PRO:CB	3:H:210:MET:HE1	2.12	0.75
3:H:17:VAL:O	3:H:188:GLY:CA	2.30	0.75
2:L:6:LEU:HD11	3:H:116:ASP:HB3	1.67	0.74
3:H:76:TYR:CD1	3:H:76:TYR:O	2.41	0.74
3:H:89:TYR:CD2	5:H:567:HOH:O	2.08	0.74
3:H:35:ARG:HE	3:H:37:PRO:HD2	1.53	0.73
3:H:98:ASN:O	3:H:99:LEU:HB2	1.86	0.72
3:H:41:LEU:HD11	3:H:64:LEU:CD2	2.19	0.72
3:H:144:LEU:HD21	3:H:152:PRO:CG	2.20	0.72
3:H:157:VAL:CG2	3:H:157:VAL:O	2.36	0.72
3:H:162:ILE:HD11	3:H:199:PHE:HE2	1.55	0.71
3:H:122:CYS:HB3	3:H:208:TYR:CE1	2.26	0.71
3:H:210:MET:HE2	3:H:210:MET:HA	1.73	0.71
3:H:34:PHE:HD1	3:H:65:LEU:HD23	1.51	0.71
3:H:130:LEU:HD21	3:H:210:MET:HB3	1.71	0.71
3:H:212:ILE:O	3:H:228:TYR:HA	1.90	0.71
1:D:403:DT:H5''	1:D:404:DT:OP2	1.91	0.71
3:H:41:LEU:HD21	3:H:64:LEU:CD2	2.20	0.71
3:H:84:MET:SD	3:H:109:LYS:CE	2.71	0.71
3:H:115:SER:O	3:H:117:TYR:N	2.23	0.71
1:D:408:DG:H2'	1:D:408:DG:P	2.30	0.70
3:H:70:LYS:CE	3:H:80:GLU:OE1	2.38	0.70
3:H:183:ALA:HB3	3:H:228:TYR:CE2	2.19	0.70
3:H:221(A):ARG:CB	3:H:224:LYS:HG3	2.22	0.70
3:H:32:MET:CE	3:H:40:LEU:CD1	2.68	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:TRP:HE1	3:H:247:GLU:N	1.89	0.70
2:L:14:ASP:OD1	2:L:14(C):GLU:N	2.21	0.70
3:H:33:LEU:HD13	3:H:41:LEU:HD12	1.73	0.70
3:H:148:TRP:N	3:H:148:TRP:CE3	2.60	0.70
3:H:112:VAL:O	3:H:112:VAL:HG23	1.92	0.70
3:H:150:GLY:O	3:H:151:GLN:HG3	1.91	0.70
3:H:224:LYS:O	5:H:529:HOH:O	2.10	0.69
3:H:140:GLY:HA3	5:H:579:HOH:O	1.82	0.69
3:H:57:HIS:CE1	4:H:297:OG6:C3	2.76	0.69
1:D:410:DG:N3	1:D:410:DG:C2'	2.54	0.69
3:H:124:PRO:HG3	3:H:210:MET:HE2	1.76	0.69
3:H:90:ILE:HG21	3:H:94:TYR:CD2	2.28	0.68
1:D:403:DT:H4'	1:D:404:DT:OP1	1.93	0.68
3:H:24:ILE:H	3:H:24:ILE:CD1	1.92	0.68
3:H:163:VAL:HG23	3:H:184:GLY:H	1.57	0.68
3:H:72:SER:CB	3:H:77:GLU:OE2	2.38	0.68
3:H:124:PRO:HB3	3:H:210:MET:CE	2.16	0.68
3:H:32:MET:HE2	3:H:40:LEU:HD12	1.74	0.68
3:H:79:ILE:HG12	3:H:80:GLU:N	2.07	0.68
3:H:161:PRO:HG2	3:H:184:GLY:O	1.93	0.68
2:L:14:ASP:H	2:L:14(C):GLU:HG3	1.57	0.67
3:H:122:CYS:HB3	3:H:208:TYR:CD1	2.28	0.67
3:H:212:ILE:O	3:H:228:TYR:HB3	1.94	0.67
3:H:158:VAL:HG22	3:H:160:LEU:HG	1.75	0.67
3:H:162:ILE:HD11	3:H:199:PHE:CE2	2.29	0.67
3:H:20:SER:O	3:H:156:GLN:HA	1.94	0.67
3:H:215:TRP:HB2	4:H:297:OG6:HD1	1.76	0.67
3:H:60(A):TYR:C	3:H:60(C):PRO:HD2	2.20	0.67
3:H:26:MET:SD	3:H:157:VAL:HG11	2.35	0.66
3:H:177:THR:OG1	3:H:178:ASP:N	2.20	0.66
2:L:14:ASP:CG	2:L:14(C):GLU:HG2	2.20	0.66
3:H:24:ILE:HG12	5:H:607:HOH:O	1.94	0.66
3:H:99:LEU:HD22	4:H:297:OG6:HE1	1.75	0.66
3:H:50:ARG:HH21	3:H:107:LYS:HE2	1.59	0.66
3:H:89:TYR:CE2	3:H:245:PHE:CE1	2.83	0.66
3:H:81:LYS:CD	3:H:118:ILE:CD1	2.63	0.66
3:H:81:LYS:NZ	3:H:113:ALA:HB3	2.11	0.66
3:H:79:ILE:HD12	3:H:117:TYR:CG	2.31	0.66
3:H:204(B):ASN:O	3:H:205:ASN:CB	2.44	0.65
3:H:33:LEU:HB3	3:H:41:LEU:HD12	1.78	0.65
3:H:215:TRP:HB2	4:H:297:OG6:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:LEU:HD23	2:L:13:GLU:H	1.61	0.65
3:H:35:ARG:HD3	3:H:36(A):SER:C	2.21	0.65
3:H:35:ARG:HD3	3:H:37:PRO:CD	2.27	0.65
3:H:60(B):PRO:CG	3:H:96:TRP:CE2	2.78	0.65
3:H:165:ARG:HD3	3:H:165:ARG:O	1.95	0.65
3:H:199:PHE:O	3:H:199:PHE:CD2	2.50	0.65
3:H:148:TRP:N	3:H:148:TRP:HE3	1.96	0.64
3:H:185:LYS:H	3:H:186(B):GLU:HG3	1.61	0.64
2:L:3:LEU:HD23	3:H:206:ARG:CA	2.17	0.64
3:H:230:HIS:HB3	3:H:233:ARG:CB	2.26	0.64
2:L:14(C):GLU:O	2:L:14(F):LEU:HB2	1.98	0.64
3:H:157:VAL:O	3:H:157:VAL:HG22	1.97	0.64
2:L:8:GLU:OE1	3:H:202:LYS:NZ	2.27	0.64
3:H:180:MET:HE2	3:H:215:TRP:NE1	2.11	0.64
1:D:402:DG:C4	1:D:404:DT:C7	2.78	0.64
3:H:44:ALA:HB1	3:H:52:VAL:HG12	1.79	0.64
3:H:140:GLY:CA	3:H:155:LEU:HD12	2.23	0.63
2:L:4:ARG:NH1	2:L:14:ASP:OD2	2.26	0.63
3:H:195:SER:HA	3:H:213:VAL:HB	1.79	0.63
3:H:237:TRP:O	3:H:241:VAL:HG13	1.98	0.63
3:H:123:LEU:HD23	3:H:124:PRO:CD	2.27	0.63
3:H:212:ILE:O	3:H:228:TYR:CB	2.47	0.63
1:D:411:DG:O5'	1:D:411:DG:C2'	2.35	0.63
3:H:195:SER:OG	4:H:297:OG6:CB2	2.47	0.63
3:H:235:LYS:O	3:H:238:ILE:HB	1.99	0.63
1:D:414:DG:H5''	1:D:414:DG:N3	2.14	0.63
3:H:98:ASN:O	3:H:99:LEU:CB	2.46	0.63
1:D:401:DG:C6	1:D:406:DG:O6	2.51	0.63
1:D:412:DT:O4'	3:H:24:ILE:HG21	1.99	0.63
2:L:4:ARG:H	2:L:8:GLU:HG2	1.64	0.62
3:H:32:MET:CE	3:H:40:LEU:HD13	2.23	0.62
3:H:165:ARG:CB	3:H:166:PRO:CD	2.74	0.62
2:L:6:LEU:HD11	3:H:116:ASP:CG	2.24	0.62
2:L:7:PHE:CE1	2:L:14:ASP:HA	2.34	0.62
3:H:34:PHE:CE1	3:H:65:LEU:CD2	2.81	0.62
2:L:7:PHE:HE1	2:L:14:ASP:HA	1.62	0.62
3:H:115:SER:C	3:H:117:TYR:N	2.55	0.62
3:H:172:THR:OG1	3:H:174:ILE:N	2.23	0.62
3:H:53:LEU:HD11	3:H:103:ILE:HD11	1.81	0.62
3:H:95:ASN:HD21	3:H:97(A):GLU:HB2	1.64	0.62
3:H:203:SER:OG	3:H:204(A):PHE:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:70:LYS:HE2	3:H:77:GLU:HG3	1.82	0.62
1:D:402:DG:C6	1:D:404:DT:C4	2.88	0.62
3:H:60(A):TYR:CZ	3:H:60(C):PRO:HG2	2.35	0.61
2:L:7:PHE:CE1	2:L:14:ASP:CA	2.83	0.61
3:H:35:ARG:N	3:H:39:GLU:O	2.33	0.61
3:H:42:CYS:HB3	3:H:195:SER:O	2.01	0.61
3:H:165:ARG:N	3:H:166:PRO:HD2	2.15	0.61
1:D:401:DG:O6	1:D:406:DG:O6	2.18	0.61
3:H:97:ARG:HD3	5:H:544:HOH:O	1.99	0.61
3:H:212:ILE:O	3:H:228:TYR:CA	2.48	0.61
3:H:215:TRP:CB	4:H:297:OG6:O	2.49	0.60
1:D:409:DT:H1'	1:D:410:DG:C2	2.36	0.60
1:D:414:DG:H2''	1:D:415:DG:O4'	2.01	0.60
3:H:60(A):TYR:N	3:H:60(F):LYS:HB3	2.14	0.60
1:D:406:DG:H2'	1:D:408:DG:C8	2.36	0.60
3:H:33:LEU:HD22	3:H:64:LEU:HD22	1.83	0.60
3:H:191:CYS:O	3:H:192:GLU:C	2.44	0.60
3:H:69:GLY:O	3:H:79:ILE:HD11	2.01	0.60
3:H:161:PRO:HD3	3:H:184(A):TYR:CZ	2.37	0.60
3:H:178:ASP:HB3	3:H:233:ARG:NH1	2.17	0.60
3:H:28:PRO:HB2	3:H:119:HIS:CB	2.31	0.60
3:H:183:ALA:CB	3:H:228:TYR:HE2	2.10	0.60
3:H:191:CYS:N	3:H:194:ASP:OD2	2.35	0.60
3:H:235:LYS:O	3:H:239:GLN:N	2.34	0.59
3:H:224:LYS:HE2	5:H:512:HOH:O	2.02	0.59
3:H:124:PRO:HG3	3:H:210:MET:CE	2.32	0.59
3:H:50:ARG:HD3	3:H:247:GLU:HG2	1.80	0.59
3:H:143:ASN:HB3	3:H:145:LYS:O	2.03	0.59
2:L:14(J):TYR:O	2:L:14(K):ILE:CG1	2.49	0.59
3:H:144:LEU:CD2	3:H:144:LEU:N	2.62	0.59
3:H:162:ILE:CG1	3:H:199:PHE:HZ	2.16	0.59
2:L:5:PRO:HA	2:L:9:LYS:CB	2.33	0.59
3:H:56:ALA:C	3:H:58:CYS:H	2.10	0.59
3:H:141:TRP:CE2	3:H:155:LEU:HD13	2.38	0.59
3:H:221(A):ARG:HG2	3:H:221(A):ARG:HH11	1.68	0.59
3:H:61:GLU:HG2	3:H:88:ILE:HD12	1.85	0.58
3:H:115:SER:O	3:H:116:ASP:C	2.46	0.58
2:L:5:PRO:HA	2:L:9:LYS:HB2	1.84	0.58
3:H:16:ILE:HG13	3:H:156:GLN:O	2.03	0.58
3:H:103:ILE:HG13	3:H:104:ALA:N	2.18	0.58
3:H:199:PHE:O	3:H:199:PHE:CG	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:ARG:C	3:H:126:ARG:CD	2.75	0.58
2:L:7:PHE:O	2:L:12:LEU:O	2.20	0.58
3:H:79:ILE:CG1	3:H:80:GLU:N	2.66	0.58
3:H:124:PRO:HG3	3:H:209:GLN:O	2.04	0.58
2:L:14:ASP:N	2:L:14(C):GLU:HG3	2.19	0.57
3:H:181:PHE:CE2	3:H:211:GLY:CA	2.87	0.57
3:H:200:VAL:HG21	5:H:503:HOH:O	2.03	0.57
3:H:201:MET:O	3:H:208:TYR:N	2.33	0.57
3:H:73:ARG:NH1	3:H:151:GLN:HB2	2.19	0.57
3:H:126:ARG:HD2	3:H:126:ARG:O	2.04	0.57
3:H:142:GLY:O	3:H:144:LEU:HD23	2.04	0.57
3:H:175:ARG:C	3:H:175:ARG:CD	2.74	0.57
3:H:185:LYS:CB	3:H:186:PRO:HD2	2.34	0.57
2:L:3:LEU:HD11	5:L:531:HOH:O	2.04	0.57
3:H:16:ILE:HB	3:H:156:GLN:HB2	1.85	0.57
3:H:61:GLU:HA	3:H:85:LEU:HD12	1.87	0.57
3:H:152:PRO:HB2	3:H:154:VAL:O	2.03	0.57
3:H:191:CYS:H	3:H:194:ASP:HB2	1.69	0.57
1:D:413:DT:O4	3:H:75:ARG:NH2	2.33	0.57
3:H:59:LEU:O	3:H:60(G):ASN:HA	2.04	0.57
3:H:143:ASN:C	3:H:144:LEU:HD23	2.29	0.57
2:L:7:PHE:HE1	2:L:14:ASP:CA	2.16	0.57
3:H:197:GLY:O	3:H:213:VAL:HG23	2.05	0.57
3:H:60(B):PRO:N	3:H:60(C):PRO:CD	2.68	0.57
1:D:402:DG:C4	1:D:404:DT:C5	2.93	0.57
3:H:50:ARG:CG	3:H:247:GLU:HG3	2.34	0.57
3:H:181:PHE:HE2	3:H:211:GLY:HA2	1.69	0.57
3:H:240:LYS:O	3:H:240:LYS:HG2	2.04	0.57
3:H:81:LYS:HD3	3:H:118:ILE:HD12	1.80	0.56
3:H:60:LEU:HA	3:H:60(F):LYS:O	2.06	0.56
2:L:12:LEU:HD23	2:L:13:GLU:N	2.19	0.56
3:H:58:CYS:CA	3:H:60(F):LYS:HD3	2.35	0.56
3:H:189:ASP:CG	4:H:297:OG6:HH22	2.13	0.56
3:H:123:LEU:HD22	3:H:124:PRO:HD2	1.85	0.56
1:D:414:DG:H1'	1:D:415:DG:H5'	1.86	0.56
3:H:34:PHE:HB2	3:H:40:LEU:HA	1.88	0.56
3:H:101:ARG:HB3	3:H:234:LEU:HD11	1.86	0.56
3:H:191:CYS:H	3:H:194:ASP:CB	2.18	0.56
3:H:240:LYS:HE2	3:H:244:GLN:HG3	1.88	0.56
3:H:184(A):TYR:CZ	3:H:186(D):LYS:HD3	2.41	0.55
1:D:413:DT:C4'	1:D:414:DG:OP1	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:76:TYR:HE2	3:H:82:ILE:CD1	2.19	0.55
3:H:164:GLU:C	3:H:166:PRO:HD2	2.31	0.55
3:H:23:GLU:O	3:H:24:ILE:C	2.49	0.55
2:L:3:LEU:CD1	5:L:531:HOH:O	2.55	0.55
3:H:29:TRP:HA	3:H:46:LEU:HD12	1.88	0.55
3:H:203:SER:C	3:H:204(A):PHE:H	2.14	0.55
3:H:211:GLY:HA2	3:H:229:THR:O	2.06	0.55
2:L:4:ARG:NE	2:L:8:GLU:OE2	2.38	0.54
1:D:405:DG:H2''	1:D:406:DG:O4'	2.07	0.54
1:D:408:DG:O5'	1:D:408:DG:H8	1.90	0.54
3:H:72:SER:N	3:H:77:GLU:OE2	2.38	0.54
3:H:105:LEU:O	3:H:106:MET:HG3	2.07	0.54
2:L:14(C):GLU:N	3:H:137:ARG:NH2	2.56	0.54
3:H:57:HIS:CD2	4:H:297:OG6:HB31	2.42	0.54
1:D:409:DT:H4'	1:D:410:DG:H5'	1.89	0.54
3:H:200:VAL:CG2	5:H:503:HOH:O	2.55	0.54
3:H:54:THR:HG22	3:H:106:MET:SD	2.48	0.54
3:H:81:LYS:HZ3	3:H:113:ALA:HB3	1.71	0.54
3:H:107:LYS:CG	3:H:107:LYS:O	2.56	0.54
3:H:140:GLY:HA2	5:H:579:HOH:O	1.94	0.54
3:H:191:CYS:O	3:H:194:ASP:HB2	2.08	0.53
1:D:402:DG:C5	1:D:404:DT:C5	2.97	0.53
3:H:159:ASN:O	3:H:184(A):TYR:HE2	1.90	0.53
3:H:181:PHE:CE2	3:H:211:GLY:HA2	2.43	0.53
3:H:35:ARG:CD	3:H:37:PRO:CD	2.82	0.53
3:H:68:ILE:CD1	3:H:83:SER:OG	2.57	0.53
3:H:80:GLU:C	3:H:81:LYS:HG3	2.32	0.53
3:H:215:TRP:HA	4:H:297:OG6:O	2.09	0.53
3:H:185:LYS:CB	3:H:186:PRO:CD	2.72	0.53
3:H:130:LEU:HD21	3:H:210:MET:SD	2.49	0.53
3:H:162:ILE:HD12	3:H:201:MET:HE1	1.90	0.53
3:H:56:ALA:O	3:H:58:CYS:N	2.41	0.53
3:H:99:LEU:HD22	4:H:297:OG6:CE1	2.39	0.53
3:H:165:ARG:N	3:H:166:PRO:CD	2.71	0.53
3:H:212:ILE:H	3:H:228:TYR:HB3	1.73	0.52
3:H:53:LEU:HD13	3:H:105:LEU:CD2	2.40	0.52
3:H:99:LEU:O	3:H:102:ASP:HB2	2.09	0.52
1:D:412:DT:O2	3:H:79:ILE:CG2	2.50	0.52
3:H:141:TRP:N	5:H:579:HOH:O	1.77	0.52
3:H:16:ILE:HG12	3:H:140:GLY:O	2.09	0.52
3:H:34:PHE:HE1	3:H:65:LEU:CD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:89:TYR:HB3	5:H:567:HOH:O	2.09	0.52
3:H:32:MET:HB2	3:H:141:TRP:CZ3	2.44	0.52
3:H:204(B):ASN:ND2	3:H:204(B):ASN:H	2.07	0.52
3:H:235:LYS:O	3:H:238:ILE:N	2.43	0.52
3:H:240:LYS:O	3:H:244:GLN:HG3	2.08	0.52
3:H:33:LEU:CD1	3:H:42:CYS:HB2	2.21	0.52
1:D:408:DG:O5'	1:D:408:DG:C8	2.62	0.52
2:L:1(A):ASP:O	2:L:1(A):ASP:CG	2.53	0.52
3:H:204(B):ASN:ND2	3:H:204(B):ASN:N	2.52	0.52
3:H:41:LEU:CD1	3:H:64:LEU:HD21	2.32	0.52
3:H:68:ILE:O	3:H:81:LYS:N	2.33	0.52
3:H:28:PRO:HB2	3:H:119:HIS:HB3	1.90	0.51
3:H:60(F):LYS:HG3	3:H:60(H):PHE:CE1	2.46	0.51
3:H:91:HIS:HD2	3:H:237:TRP:CD2	2.28	0.51
3:H:128:THR:O	3:H:129(C):LEU:HB2	2.10	0.51
3:H:190:ALA:O	3:H:191:CYS:HB2	2.09	0.51
3:H:243:ASP:OD1	3:H:243:ASP:O	2.29	0.51
3:H:76:TYR:HE2	3:H:82:ILE:HD12	1.76	0.51
2:L:14:ASP:H	2:L:14(C):GLU:CG	2.23	0.51
1:D:402:DG:H1'	1:D:404:DT:H72	1.91	0.51
3:H:41:LEU:CD2	3:H:64:LEU:HD21	2.36	0.51
3:H:172:THR:HG21	3:H:215:TRP:HH2	1.74	0.51
3:H:195:SER:OG	4:H:297:OG6:HB22	2.10	0.51
2:L:4:ARG:NH2	2:L:7:PHE:HB3	2.26	0.51
2:L:7:PHE:HE1	2:L:13:GLU:C	2.18	0.51
3:H:84:MET:O	3:H:109:LYS:HB2	2.10	0.51
3:H:50:ARG:NH2	3:H:109:LYS:O	2.44	0.51
3:H:172:THR:HG21	3:H:176:ILE:CD1	2.21	0.51
3:H:66:VAL:HG11	3:H:108:LEU:HD21	1.93	0.50
3:H:60(I):THR:O	3:H:63:ASP:N	2.43	0.50
3:H:176:ILE:HD12	3:H:227:PHE:CE2	2.46	0.50
3:H:143:ASN:ND2	3:H:192:GLU:HB3	2.26	0.50
3:H:130:LEU:O	3:H:131:GLN:HG3	2.12	0.50
3:H:221(A):ARG:CB	3:H:224:LYS:CG	2.85	0.50
2:L:5:PRO:C	2:L:6:LEU:HD12	2.36	0.50
3:H:72:SER:H	3:H:77:GLU:CD	2.19	0.50
3:H:153:SER:HB3	5:H:647:HOH:O	2.11	0.50
1:D:402:DG:H2''	1:D:403:DT:H5''	1.94	0.50
3:H:49:ASP:O	3:H:111:PRO:HA	2.11	0.50
3:H:91:HIS:HD2	3:H:237:TRP:CE2	2.30	0.50
3:H:115:SER:C	3:H:117:TYR:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:ARG:HB2	3:H:247:GLU:CB	2.42	0.50
3:H:84:MET:HG3	3:H:109:LYS:HB3	1.94	0.50
3:H:159:ASN:O	3:H:184(A):TYR:CE2	2.65	0.50
3:H:59:LEU:HD22	3:H:88:ILE:HG21	1.93	0.49
3:H:169:LYS:C	3:H:171:SER:H	2.16	0.49
3:H:183:ALA:CB	3:H:228:TYR:CE2	2.92	0.49
2:L:7:PHE:CE1	2:L:14:ASP:N	2.80	0.49
2:L:7:PHE:CE1	2:L:13:GLU:C	2.90	0.49
3:H:49:ASP:OD2	3:H:111:PRO:HB3	2.12	0.49
3:H:166:PRO:O	3:H:169:LYS:HB2	2.13	0.49
3:H:191:CYS:H	3:H:194:ASP:CG	2.20	0.49
3:H:59:LEU:C	3:H:60(F):LYS:HG2	2.38	0.49
3:H:60(I):THR:C	3:H:62:ASN:N	2.67	0.49
3:H:185:LYS:HB3	3:H:186:PRO:HD3	1.92	0.49
3:H:83:SER:HB2	3:H:108:LEU:HD22	1.95	0.49
2:L:14:ASP:OD2	2:L:14(C):GLU:HG2	2.13	0.49
3:H:59:LEU:HD22	3:H:88:ILE:CG2	2.42	0.49
3:H:95:ASN:ND2	3:H:97(A):GLU:HB2	2.28	0.49
3:H:147:THR:HA	3:H:148:TRP:CE3	2.48	0.49
3:H:162:ILE:CG1	3:H:199:PHE:CZ	2.96	0.49
3:H:179:ASN:N	3:H:179:ASN:ND2	2.61	0.49
1:D:402:DG:N9	1:D:404:DT:H72	2.28	0.48
3:H:35:ARG:HD3	3:H:37:PRO:HD2	1.87	0.48
3:H:125:ASP:O	3:H:126:ARG:C	2.56	0.48
3:H:60(A):TYR:CE2	3:H:60(C):PRO:HG2	2.48	0.48
3:H:116:ASP:CG	5:H:559:HOH:O	2.56	0.48
3:H:222:ASP:O	3:H:224:LYS:HG2	2.13	0.48
3:H:47:ILE:O	3:H:48:SER:HB3	2.12	0.48
3:H:60(B):PRO:N	3:H:60(C):PRO:HD2	2.27	0.48
3:H:163:VAL:HG23	3:H:184:GLY:N	2.24	0.48
2:L:7:PHE:CE1	2:L:14:ASP:HB3	2.49	0.48
3:H:151:GLN:HG2	5:H:581:HOH:O	2.14	0.48
3:H:26:MET:HE2	3:H:137:ARG:CZ	2.41	0.48
3:H:117:TYR:N	3:H:117:TYR:CD1	2.81	0.48
3:H:47:ILE:HD13	3:H:53:LEU:HD22	1.95	0.48
3:H:89:TYR:CE2	3:H:245:PHE:CZ	3.01	0.48
3:H:105:LEU:O	3:H:106:MET:CG	2.62	0.48
3:H:116:ASP:OD2	5:H:559:HOH:O	2.19	0.48
3:H:131:GLN:O	3:H:134:TYR:HB2	2.14	0.48
3:H:85:LEU:HD22	3:H:106:MET:CE	2.37	0.48
3:H:162:ILE:HG13	3:H:199:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:DG:C5	1:D:404:DT:C4	3.01	0.47
1:D:403:DT:C4'	1:D:404:DT:OP2	2.61	0.47
3:H:73:ARG:HH11	3:H:151:GLN:HB2	1.79	0.47
3:H:32:MET:CE	3:H:40:LEU:HD12	2.42	0.47
3:H:215:TRP:CB	4:H:297:OG6:HD1	2.44	0.47
3:H:179:ASN:HB3	3:H:234:LEU:HD21	1.96	0.47
3:H:122:CYS:O	3:H:208:TYR:HA	2.14	0.47
3:H:172:THR:C	3:H:174:ILE:N	2.72	0.47
3:H:181:PHE:HE2	3:H:211:GLY:CA	2.27	0.47
3:H:47:ILE:HD12	3:H:123:LEU:HD11	1.96	0.47
2:L:14(J):TYR:CD2	3:H:204:PRO:HG3	2.50	0.47
3:H:60(I):THR:O	3:H:62:ASN:N	2.48	0.47
3:H:144:LEU:HG	3:H:151:GLN:HA	1.97	0.47
3:H:160:LEU:HD23	3:H:184(A):TYR:CE2	2.49	0.47
3:H:60(I):THR:O	3:H:63:ASP:HB2	2.15	0.47
3:H:137:ARG:O	3:H:200:VAL:HG22	2.15	0.47
3:H:60:LEU:HD23	3:H:94:TYR:CD2	2.44	0.47
1:D:402:DG:C2'	1:D:404:DT:OP2	2.61	0.47
3:H:23:GLU:O	3:H:26:MET:HB2	2.14	0.46
3:H:29:TRP:O	3:H:31:VAL:CG2	2.63	0.46
3:H:110:LYS:HB2	3:H:111:PRO:HD2	1.96	0.46
3:H:241:VAL:HA	3:H:244:GLN:HB2	1.97	0.46
3:H:48:SER:C	3:H:50:ARG:H	2.23	0.46
3:H:147:THR:C	3:H:148:TRP:HE3	2.23	0.46
3:H:167:VAL:O	3:H:168:CYS:C	2.59	0.46
3:H:204(B):ASN:C	3:H:204(B):ASN:ND2	2.60	0.46
3:H:236:LYS:HA	3:H:239:GLN:OE1	2.15	0.46
2:L:14(A):LYS:HB3	2:L:14(A):LYS:HE2	1.42	0.46
3:H:93:ARG:O	3:H:94:TYR:C	2.58	0.46
3:H:163:VAL:CG1	3:H:167:VAL:HG12	2.46	0.46
3:H:203:SER:OG	3:H:204(A):PHE:CB	2.64	0.46
3:H:54:THR:CG2	3:H:106:MET:SD	3.04	0.46
3:H:78:ASN:HD22	3:H:78:ASN:HA	1.35	0.46
3:H:87:LYS:O	3:H:106:MET:HA	2.15	0.46
1:D:401:DG:C2	1:D:405:DG:N2	2.84	0.46
2:L:14(J):TYR:HD2	3:H:204:PRO:HG3	1.80	0.46
3:H:98:ASN:O	3:H:180:MET:HE1	2.16	0.46
3:H:56:ALA:C	3:H:58:CYS:N	2.68	0.45
2:L:12:LEU:CD2	2:L:13:GLU:N	2.80	0.45
2:L:13:GLU:OE2	2:L:14(D):ARG:NH2	2.49	0.45
3:H:50:ARG:CZ	3:H:109:LYS:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:53:LEU:HD13	3:H:105:LEU:HD23	1.97	0.45
3:H:107:LYS:O	3:H:107:LYS:HG3	2.17	0.45
3:H:142:GLY:O	3:H:144:LEU:CD2	2.64	0.45
3:H:204(B):ASN:ND2	3:H:206:ARG:H	2.14	0.45
1:D:404:DT:O2	1:D:404:DT:C2'	2.62	0.45
3:H:51:TRP:CE2	3:H:242:ILE:HG23	2.51	0.45
3:H:114:PHE:CZ	3:H:120:PRO:CG	2.94	0.45
3:H:53:LEU:HD11	3:H:103:ILE:CD1	2.45	0.45
2:L:4:ARG:NH2	2:L:8:GLU:OE2	2.49	0.45
3:H:47:ILE:HD12	3:H:123:LEU:CD1	2.47	0.45
3:H:57:HIS:O	3:H:57:HIS:CD2	2.70	0.45
3:H:57:HIS:CE1	3:H:195:SER:HB3	2.51	0.45
3:H:85:LEU:CD2	3:H:106:MET:HE2	2.39	0.45
3:H:36:LYS:O	3:H:38:GLN:HB2	2.16	0.45
3:H:48:SER:C	3:H:50:ARG:N	2.75	0.45
3:H:50:ARG:NH2	3:H:86:GLU:OE1	2.50	0.45
3:H:50:ARG:CB	3:H:247:GLU:HB2	2.47	0.45
1:D:402:DG:C8	1:D:404:DT:C6	3.05	0.45
1:D:402:DG:C1'	1:D:404:DT:H72	2.47	0.45
2:L:14(E):GLU:OE1	3:H:159:ASN:HB2	2.15	0.45
3:H:31:VAL:HB	3:H:44:ALA:HB3	1.99	0.45
3:H:164:GLU:H	3:H:164:GLU:HG3	1.44	0.45
3:H:34:PHE:O	3:H:65:LEU:HB3	2.17	0.44
3:H:140:GLY:HA2	3:H:155:LEU:HD11	1.94	0.44
3:H:146:GLU:HG2	3:H:147:THR:HG22	1.98	0.44
3:H:160:LEU:HD23	3:H:184(A):TYR:HE2	1.82	0.44
3:H:181:PHE:CZ	3:H:211:GLY:HA3	2.51	0.44
3:H:237:TRP:O	3:H:238:ILE:C	2.60	0.44
3:H:123:LEU:HD23	3:H:123:LEU:HA	1.68	0.44
3:H:221(A):ARG:HD2	3:H:224:LYS:HG3	1.99	0.44
3:H:57:HIS:CE1	4:H:297:OG6:H1	2.35	0.44
3:H:184(A):TYR:OH	3:H:186(D):LYS:HE2	2.17	0.44
3:H:36(A):SER:HA	3:H:37:PRO:C	2.41	0.44
3:H:44:ALA:CB	3:H:52:VAL:CG1	2.90	0.44
3:H:49:ASP:OD2	3:H:247:GLU:OE1	2.34	0.44
3:H:191:CYS:O	3:H:193:GLY:N	2.50	0.44
3:H:112:VAL:O	3:H:112:VAL:CG2	2.64	0.44
3:H:141:TRP:CE3	5:H:579:HOH:O	2.57	0.44
3:H:125:ASP:OD2	3:H:128:THR:OG1	2.35	0.44
3:H:47:ILE:HD13	3:H:47:ILE:HG21	1.75	0.44
3:H:50:ARG:CB	3:H:247:GLU:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:200:VAL:HA	3:H:208:TYR:O	2.17	0.44
2:L:12:LEU:HD22	2:L:13:GLU:O	2.17	0.44
3:H:36(A):SER:HA	3:H:38:GLN:N	2.33	0.44
3:H:172:THR:HG22	3:H:176:ILE:HD11	1.88	0.44
3:H:98:ASN:OD1	3:H:98:ASN:N	2.50	0.44
3:H:144:LEU:HG	3:H:151:GLN:CA	2.48	0.44
3:H:210:MET:C	3:H:231:VAL:HG23	2.41	0.44
1:D:409:DT:H6	1:D:409:DT:H2'	1.51	0.43
3:H:121:VAL:HG22	3:H:122:CYS:N	2.33	0.43
2:L:1(A):ASP:HA	3:H:206:ARG:HH21	1.82	0.43
3:H:105:LEU:C	3:H:106:MET:CG	2.85	0.43
3:H:154:VAL:O	3:H:156:GLN:OE1	2.35	0.43
3:H:220:CYS:O	3:H:221:ASP:HB3	2.18	0.43
2:L:4:ARG:N	2:L:8:GLU:HG2	2.31	0.43
3:H:38:GLN:HB2	3:H:38:GLN:HE21	1.43	0.43
3:H:43:GLY:O	3:H:196:GLY:HA3	2.18	0.43
2:L:5:PRO:CA	2:L:9:LYS:HB2	2.48	0.43
3:H:93:ARG:HA	3:H:93:ARG:HD2	1.73	0.43
3:H:129(C):LEU:HD23	3:H:129(C):LEU:HA	1.64	0.43
2:L:14:ASP:OD1	3:H:137:ARG:NH2	2.38	0.43
3:H:143:ASN:CG	3:H:148:TRP:CH2	2.97	0.43
3:H:16:ILE:CB	3:H:156:GLN:HB2	2.48	0.42
3:H:119:HIS:HA	3:H:120:PRO:HD3	1.80	0.42
3:H:90:ILE:HG22	3:H:91:HIS:N	2.34	0.42
3:H:181:PHE:CZ	3:H:211:GLY:CA	3.02	0.42
3:H:71:HIS:O	3:H:72:SER:C	2.61	0.42
3:H:141:TRP:CD2	5:H:579:HOH:O	2.71	0.42
3:H:144:LEU:HD21	3:H:152:PRO:HG3	1.98	0.42
3:H:16:ILE:HG13	3:H:156:GLN:HB2	2.02	0.42
3:H:210:MET:HE2	3:H:210:MET:CA	2.46	0.42
1:D:410:DG:H1'	1:D:411:DG:H5'	2.01	0.42
3:H:185:LYS:N	3:H:186(B):GLU:HG3	2.33	0.42
3:H:126:ARG:CD	3:H:126:ARG:O	2.67	0.42
1:D:407:DT:C4'	1:D:408:DG:OP2	2.68	0.42
3:H:57:HIS:CD2	3:H:57:HIS:C	2.96	0.42
3:H:96:TRP:CZ3	3:H:97:ARG:HG2	2.55	0.42
3:H:33:LEU:HD12	3:H:42:CYS:CB	2.23	0.41
3:H:88:ILE:HA	3:H:106:MET:HA	2.02	0.41
3:H:235:LYS:O	3:H:238:ILE:CA	2.67	0.41
2:L:3:LEU:HD21	3:H:206:ARG:HG2	2.01	0.41
3:H:60(I):THR:C	3:H:62:ASN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60(B):PRO:HG2	3:H:96:TRP:CE3	2.49	0.41
3:H:68:ILE:HD11	3:H:83:SER:OG	2.20	0.41
1:D:413:DT:H4'	1:D:414:DG:OP1	2.20	0.41
3:H:76:TYR:CD1	3:H:76:TYR:C	2.97	0.41
3:H:76:TYR:O	3:H:77(A):ARG:N	2.53	0.41
3:H:50:ARG:HB2	3:H:247:GLU:HG3	2.03	0.41
3:H:53:LEU:CD1	3:H:105:LEU:HD23	2.51	0.41
3:H:53:LEU:HD13	3:H:105:LEU:HD21	2.03	0.41
3:H:36:LYS:O	3:H:38:GLN:CA	2.69	0.41
3:H:42:CYS:HB3	3:H:43:GLY:H	1.67	0.41
3:H:81:LYS:HZ1	3:H:113:ALA:HB3	1.84	0.41
3:H:126:ARG:C	3:H:126:ARG:HD2	2.43	0.41
3:H:213:VAL:HG23	3:H:213:VAL:H	1.67	0.41
3:H:77:GLU:HB2	3:H:80:GLU:HB3	2.03	0.41
3:H:125:ASP:C	3:H:127:GLU:N	2.79	0.41
3:H:126:ARG:HA	3:H:232:PHE:CZ	2.56	0.41
3:H:144:LEU:CD2	3:H:152:PRO:HG3	2.51	0.41
3:H:144:LEU:HD11	3:H:152:PRO:N	2.36	0.41
3:H:160:LEU:HA	3:H:184(A):TYR:CE2	2.56	0.41
1:D:405:DG:H2''	1:D:406:DG:O5'	2.21	0.41
1:D:412:DT:H71	5:D:629:HOH:O	2.21	0.41
2:L:14(D):ARG:HA	2:L:14(D):ARG:HD3	1.84	0.41
3:H:212:ILE:HG22	3:H:213:VAL:N	2.36	0.40
3:H:60(D):TRP:CH2	4:H:297:OG6:HG3	2.56	0.40
3:H:76:TYR:CE2	3:H:82:ILE:HD11	2.57	0.40
2:L:14(C):GLU:HB2	2:L:14(D):ARG:H	1.62	0.40
3:H:16:ILE:CG1	3:H:156:GLN:HB2	2.51	0.40
3:H:49:ASP:HA	3:H:112:VAL:HG22	2.02	0.40
3:H:125:ASP:OD1	3:H:127:GLU:HB3	2.21	0.40
3:H:60(F):LYS:HG3	3:H:60(H):PHE:HE1	1.84	0.40
3:H:97:ARG:HB3	5:H:544:HOH:O	2.21	0.40
1:D:402:DG:H1'	1:D:404:DT:C7	2.51	0.40
3:H:125:ASP:O	3:H:127:GLU:N	2.54	0.40
3:H:158:VAL:CG2	3:H:160:LEU:HD21	2.51	0.40
3:H:161:PRO:HD3	3:H:184(A):TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	25/36 (69%)	19 (76%)	3 (12%)	3 (12%)	0	1
3	H	249/259 (96%)	192 (77%)	45 (18%)	12 (5%)	2	6
All	All	274/295 (93%)	211 (77%)	48 (18%)	15 (6%)	1	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	2	GLY
3	H	38	GLN
3	H	77	GLU
2	L	14(D)	ARG
3	H	49	ASP
3	H	57	HIS
3	H	61	GLU
3	H	116	ASP
3	H	99	LEU
3	H	126	ARG
2	L	14(C)	GLU
3	H	77(A)	ARG
3	H	244	GLN
3	H	93	ARG
3	H	146	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	25/31 (81%)	17 (68%)	8 (32%)	0	1
3	H	221/225 (98%)	164 (74%)	57 (26%)	0	2
All	All	246/256 (96%)	181 (74%)	65 (26%)	0	2

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	1(A)	ASP
2	L	1	CYS
2	L	3	LEU
2	L	8	GLU
2	L	10	LYS
2	L	11	SER
2	L	12	LEU
2	L	13	GLU
3	H	16	ILE
3	H	18	GLU
3	H	20	SER
3	H	23	GLU
3	H	24	ILE
3	H	26	MET
3	H	29	TRP
3	H	32	MET
3	H	34	PHE
3	H	35	ARG
3	H	38	GLN
3	H	40	LEU
3	H	46	LEU
3	H	61	GLU
3	H	68	ILE
3	H	72	SER
3	H	74	THR
3	H	75	ARG
3	H	78	ASN
3	H	79	ILE
3	H	80	GLU
3	H	83	SER
3	H	84	MET
3	H	86	GLU
3	H	87	LYS
3	H	99	LEU
3	H	103	ILE

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Mol	Chain	Res	Type
3	H	106	MET
3	H	110	LYS
3	H	126	ARG
3	H	135	LYS
3	H	137	ARG
3	H	139	THR
3	H	144	LEU
3	H	148	TRP
3	H	154	VAL
3	H	157	VAL
3	H	158	VAL
3	H	165	ARG
3	H	167	VAL
3	H	169	LYS
3	H	171	SER
3	H	173	ARG
3	H	175	ARG
3	H	177	THR
3	H	180	MET
3	H	203	SER
3	H	222	ASP
3	H	224	LYS
3	H	233	ARG
3	H	234	LEU
3	H	235	LYS
3	H	239	GLN
3	H	240	LYS
3	H	241	VAL
3	H	242	ILE
3	H	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	38	GLN
3	H	57	HIS
3	H	71	HIS
3	H	78	ASN
3	H	91	HIS
3	H	95	ASN
3	H	179	ASN
3	H	204(B)	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 oligosaccharides 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	0G6	H	297	3	30,31,32	2.25	2 (6%)	37,41,42	1.87	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	0G6	H	297	3	1/1/8/10	7/31/41/43	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	297	0G6	C3-C2	-9.72	1.24	1.51
4	H	297	0G6	O2-C2	-6.35	1.26	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	297	0G6	NE-CZ1-NH2	-4.19	113.49	120.67
4	H	297	0G6	C1-CA1-N1	-3.87	101.93	112.50
4	H	297	0G6	O2-C2-C3	3.83	121.14	109.68
4	H	297	0G6	CA2-N2-C1	-3.77	116.69	123.25
4	H	297	0G6	CG2-CB2-CA2	-3.29	107.67	113.94
4	H	297	0G6	CB2-CA2-N2	3.05	114.25	110.30
4	H	297	0G6	NH1-CZ1-NE	2.91	125.87	119.27
4	H	297	0G6	CB1-CA1-N1	2.56	106.78	103.02
4	H	297	0G6	C2-CA2-N2	2.45	115.35	110.90
4	H	297	0G6	CB2-CG2-CD3	2.10	118.13	112.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	297	0G6	C2

All (7) torsion outliers are listed below:

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

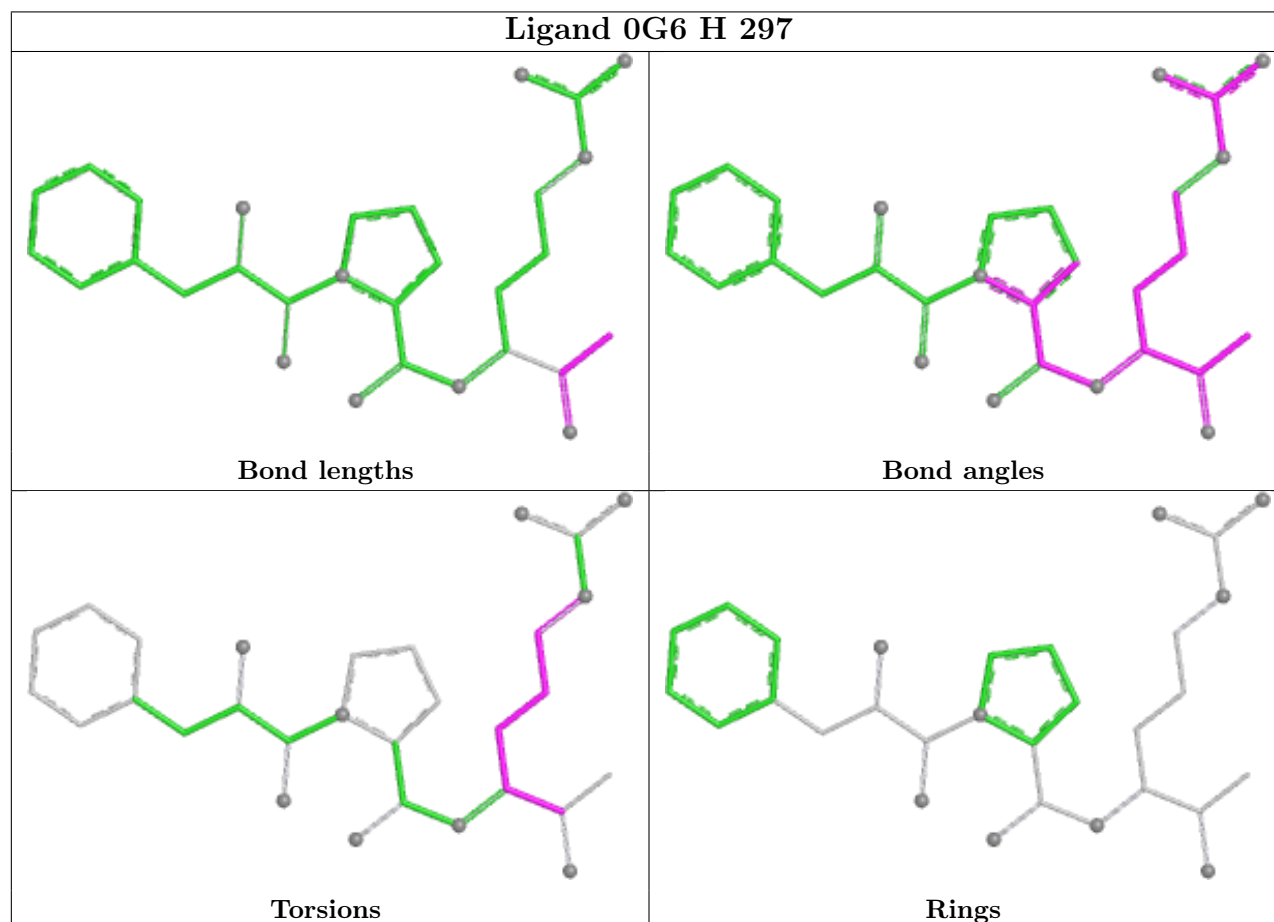
There are no ring outliers.

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	297	0G6	19	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	60(D):TRP	C	60(E):ASP	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	44:ALA	C	45:SER	N	1.17

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.