Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 04:31 PM EDT

PDB ID	:	1HAO
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.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

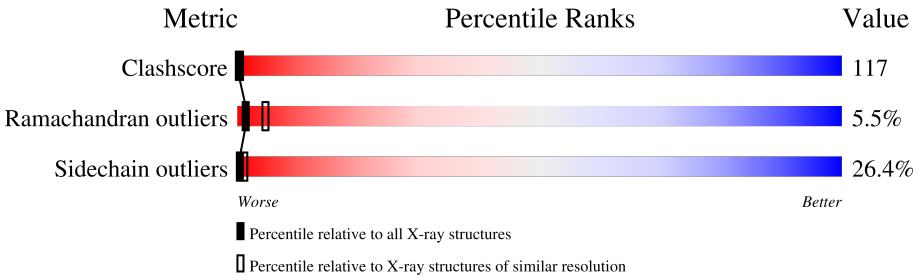
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	15	87% 13%
2	L	36	6% 25% 28% 17% 25%
3	H	259	10% 46% 32% 9% .

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	0G6	H	297	X	-	-	-

2 Entry composition (i)

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

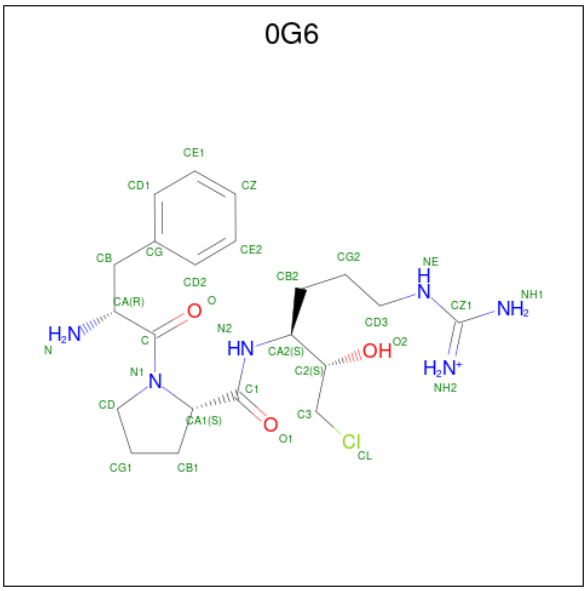
- Molecule 2 is a protein called ALPHA-THROMBIN light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	27	222	140	36	45	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-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



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	19	Total O 19 19	0	0
5	L	11	Total O 11 11	0	0
5	H	119	Total O 119 119	0	0

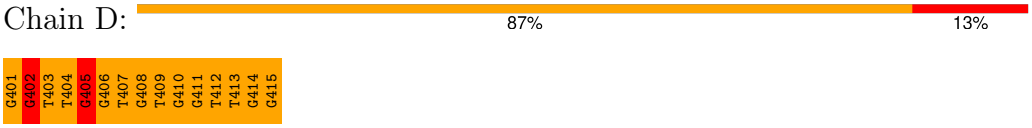
3 Residue-property plots (i)

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.

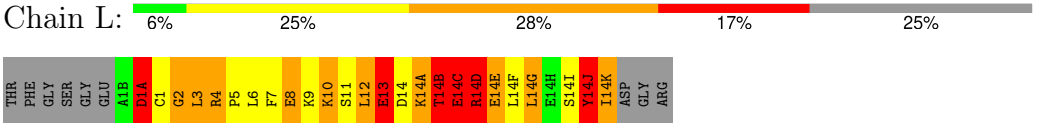
• Molecule 1: DNA 5'-D(*GP*GP*TP*TP*GP*GP*TP*GP*TP*GP*GP*TP*TP*GP*G)-3
'

Chain D:



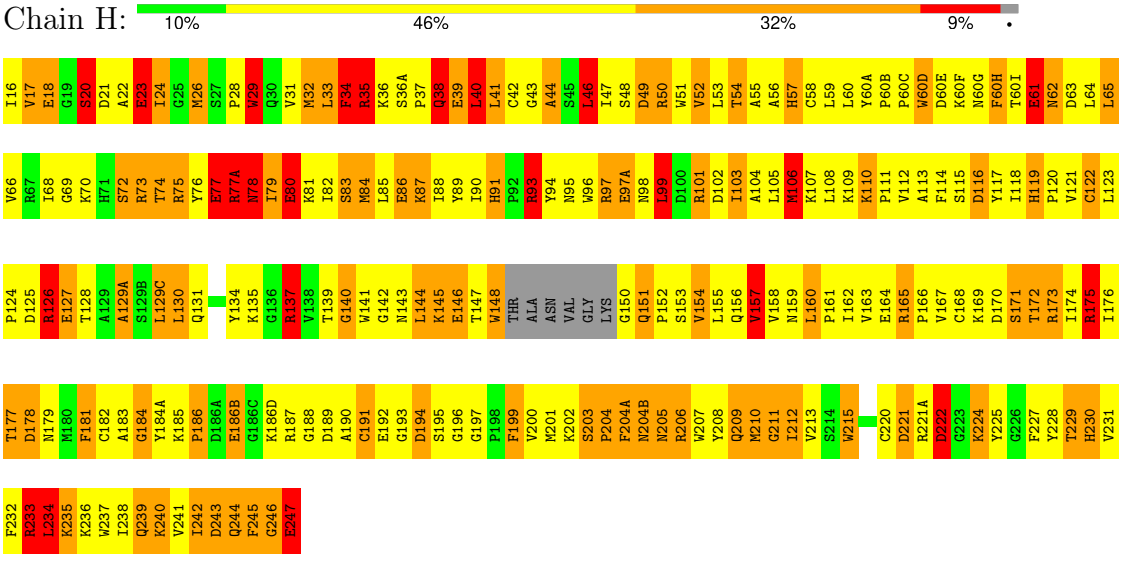
• Molecule 2: ALPHA-THROMBIN light chain

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	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

5.1 Standard geometry

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	1.77	4/353 (1.1%)	3.93	95/547 (17.4%)
2	L	0.97	0/224	2.60	24/298 (8.1%)
3	H	1.06	3/2107 (0.1%)	2.27	111/2846 (3.9%)
All	All	1.17	7/2684 (0.3%)	2.61	230/3691 (6.2%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	44	ALA	C-N	-7.03	1.17	1.34
3	H	60(D)	TRP	C-N	-6.71	1.18	1.34
1	D	415	DG	O4'-C1'	6.26	1.49	1.42
1	D	405	DG	O4'-C1'	6.09	1.49	1.42
1	D	403	DT	C4-O4	5.33	1.28	1.23
1	D	404	DT	C4-O4	5.25	1.27	1.23
3	H	60(D)	TRP	CD1-NE1	5.05	1.46	1.38

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	410	DG	P-O3'-C3'	24.52	149.13	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	409	DT	P-O3'-C3'	17.95	141.24	119.70
3	H	187	ARG	NE-CZ-NH2	17.57	129.08	120.30
1	D	408	DG	P-O3'-C3'	-13.46	103.55	119.70
1	D	409	DT	O4'-C1'-N1	12.92	117.04	108.00
1	D	411	DG	O4'-C1'-N9	12.90	117.03	108.00
2	L	4	ARG	NE-CZ-NH1	12.59	126.60	120.30
1	D	401	DG	O4'-C1'-N9	10.95	115.67	108.00
3	H	50	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	D	408	DG	O4'-C4'-C3'	-10.61	99.63	106.00
1	D	405	DG	O5'-P-OP2	10.48	123.28	110.70
3	H	194	ASP	CB-CG-OD1	-10.42	108.92	118.30
1	D	406	DG	O4'-C4'-C3'	-10.39	99.77	106.00
3	H	126	ARG	NE-CZ-NH1	10.37	125.48	120.30
3	H	187	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	D	414	DG	O4'-C4'-C3'	10.06	112.04	106.00
1	D	413	DT	O4'-C1'-N1	10.04	115.02	108.00
1	D	415	DG	O4'-C1'-C2'	-9.95	97.94	105.90
1	D	408	DG	C4'-C3'-C2'	-9.94	94.16	103.10
1	D	414	DG	P-O5'-C5'	9.92	136.77	120.90
3	H	126	ARG	CD-NE-CZ	9.89	137.45	123.60
1	D	407	DT	O4'-C1'-N1	9.77	114.84	108.00
1	D	410	DG	O4'-C1'-N9	9.75	114.83	108.00
1	D	403	DT	O5'-P-OP2	9.61	122.23	110.70
3	H	21	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	D	409	DT	C2-N3-C4	-9.47	121.52	127.20
3	H	173	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	411	DG	C3'-C2'-C1'	-9.21	91.45	102.50
3	H	137	ARG	NE-CZ-NH1	8.94	124.77	120.30
3	H	135	LYS	C-N-CA	8.90	141.00	122.30
1	D	412	DT	C2-N3-C4	-8.85	121.89	127.20
3	H	65	LEU	CA-CB-CG	8.74	135.40	115.30
3	H	77(A)	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	D	401	DG	P-O3'-C3'	8.69	130.13	119.70
1	D	402	DG	N1-C6-O6	-8.67	114.70	119.90
3	H	247	GLU	N-CA-CB	8.63	126.13	110.60
3	H	126	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	D	404	DT	C2-N3-C4	-8.61	122.04	127.20
3	H	206	ARG	NE-CZ-NH2	8.41	124.50	120.30
1	D	412	DT	N3-C4-C5	8.31	120.19	115.20
1	D	413	DT	C2-N3-C4	-8.31	122.21	127.20
1	D	411	DG	O4'-C4'-C3'	-8.28	101.03	106.00
2	L	1	CYS	C-N-CA	8.14	139.41	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	405	DG	C1'-O4'-C4'	-8.04	102.06	110.10
2	L	14(J)	TYR	CB-CG-CD1	8.04	125.83	121.00
1	D	407	DT	C2-N3-C4	-8.02	122.39	127.20
3	H	50	ARG	NE-CZ-NH2	8.01	124.30	120.30
1	D	415	DG	P-O5'-C5'	7.89	133.52	120.90
1	D	409	DT	O5'-P-OP2	7.88	120.16	110.70
3	H	46	LEU	CB-CA-C	7.85	125.12	110.20
1	D	414	DG	O5'-C5'-C4'	-7.84	91.41	111.00
1	D	412	DT	O4'-C1'-C2'	7.81	112.15	105.90
1	D	412	DT	P-O5'-C5'	-7.74	108.52	120.90
1	D	405	DG	O4'-C4'-C3'	-7.73	101.36	106.00
3	H	62	ASN	CA-CB-CG	7.71	130.36	113.40
2	L	14(C)	GLU	OE1-CD-OE2	7.69	132.53	123.30
1	D	415	DG	C1'-O4'-C4'	-7.66	102.44	110.10
3	H	205	ASN	N-CA-CB	-7.61	96.90	110.60
3	H	247	GLU	OE1-CD-OE2	-7.61	114.17	123.30
3	H	129(A)	ALA	N-CA-CB	-7.54	99.55	110.10
1	D	409	DT	O5'-C5'-C4'	-7.51	92.23	111.00
3	H	184	GLY	N-CA-C	7.49	131.81	113.10
3	H	18	GLU	N-CA-CB	7.45	124.01	110.60
3	H	173	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	D	404	DT	N3-C4-C5	7.39	119.64	115.20
1	D	405	DG	O4'-C1'-C2'	-7.39	99.98	105.90
1	D	404	DT	OP1-P-OP2	-7.37	108.55	119.60
1	D	406	DG	C4'-C3'-C2'	-7.35	96.49	103.10
3	H	40	LEU	O-C-N	7.34	134.45	122.70
3	H	77(A)	ARG	NE-CZ-NH2	-7.27	116.67	120.30
3	H	170	ASP	CB-CA-C	7.19	124.78	110.40
3	H	77	GLU	CG-CD-OE1	-7.16	103.99	118.30
1	D	406	DG	C1'-O4'-C4'	-7.06	103.04	110.10
3	H	23	GLU	CA-CB-CG	7.02	128.85	113.40
1	D	409	DT	OP1-P-OP2	-7.01	109.09	119.60
1	D	408	DG	C3'-C2'-C1'	-6.98	94.12	102.50
3	H	199	PHE	N-CA-CB	6.90	123.02	110.60
2	L	1(A)	ASP	CB-CG-OD2	-6.89	112.10	118.30
3	H	157	VAL	O-C-N	6.80	133.58	122.70
3	H	39	GLU	CA-CB-CG	6.78	128.31	113.40
3	H	35	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	L	14(I)	SER	N-CA-CB	-6.76	100.36	110.50
3	H	29	TRP	CA-CB-CG	6.69	126.42	113.70
1	D	405	DG	P-O5'-C5'	6.68	131.59	120.90
3	H	225	TYR	CB-CG-CD1	-6.66	117.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	402	DG	C5-C6-N1	6.65	114.83	111.50
3	H	55	ALA	CB-CA-C	6.65	120.07	110.10
1	D	413	DT	N3-C4-C5	6.63	119.18	115.20
3	H	61	GLU	N-CA-CB	-6.61	98.70	110.60
1	D	403	DT	OP1-P-OP2	-6.60	109.70	119.60
1	D	411	DG	OP1-P-OP2	-6.59	109.71	119.60
1	D	414	DG	C4'-C3'-C2'	-6.58	97.18	103.10
1	D	409	DT	C1'-O4'-C4'	-6.56	103.54	110.10
3	H	97	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	D	403	DT	C2-N3-C4	-6.54	123.28	127.20
1	D	409	DT	N1-C2-N3	6.53	118.52	114.60
3	H	127	GLU	CA-CB-CG	6.48	127.67	113.40
1	D	414	DG	OP1-P-O3'	6.48	119.46	105.20
3	H	106	MET	O-C-N	6.48	133.07	122.70
1	D	409	DT	C5-C4-O4	-6.40	120.42	124.90
2	L	3	LEU	CA-CB-CG	6.38	129.99	115.30
3	H	84	MET	O-C-N	6.36	132.88	122.70
3	H	137	ARG	NH1-CZ-NH2	-6.36	112.40	119.40
3	H	77	GLU	CA-CB-CG	-6.35	99.43	113.40
1	D	402	DG	C3'-C2'-C1'	-6.34	94.89	102.50
1	D	405	DG	OP1-P-OP2	-6.34	110.09	119.60
1	D	406	DG	P-O3'-C3'	-6.33	112.10	119.70
3	H	182	CYS	CA-CB-SG	6.31	125.36	114.00
1	D	409	DT	N3-C4-C5	6.31	118.98	115.20
1	D	407	DT	N3-C4-C5	6.29	118.97	115.20
2	L	3	LEU	O-C-N	6.27	132.74	122.70
3	H	60(H)	PHE	O-C-N	6.26	132.72	122.70
1	D	408	DG	P-O5'-C5'	-6.24	110.92	120.90
1	D	405	DG	N1-C2-N3	6.24	127.64	123.90
3	H	18	GLU	CB-CG-CD	6.22	131.00	114.20
1	D	401	DG	C8-N9-C4	-6.19	103.92	106.40
3	H	73	ARG	NE-CZ-NH2	6.19	123.39	120.30
3	H	35	ARG	NE-CZ-NH2	-6.15	117.23	120.30
3	H	191	CYS	N-CA-CB	-6.14	99.55	110.60
1	D	412	DT	OP1-P-OP2	-6.11	110.44	119.60
3	H	78	ASN	CB-CA-C	6.11	122.61	110.40
3	H	209	GLN	OE1-CD-NE2	6.10	135.93	121.90
2	L	4	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	D	410	DG	P-O5'-C5'	-6.09	111.15	120.90
1	D	411	DG	P-O3'-C3'	-6.07	112.42	119.70
3	H	194	ASP	C-N-CA	6.07	136.87	121.70
2	L	4	ARG	CD-NE-CZ	6.02	132.03	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	407	DT	P-O3'-C3'	-6.02	112.48	119.70
1	D	413	DT	P-O3'-C3'	-6.01	112.49	119.70
3	H	151	GLN	N-CA-CB	5.99	121.37	110.60
2	L	14(D)	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	L	1	CYS	CA-CB-SG	5.96	124.73	114.00
2	L	14(G)	LEU	CB-CA-C	5.93	121.47	110.20
1	D	401	DG	N9-C4-C5	5.91	107.77	105.40
1	D	415	DG	C5-C6-O6	-5.88	125.07	128.60
3	H	62	ASN	C-N-CA	5.86	136.36	121.70
1	D	415	DG	O4'-C1'-N9	-5.83	103.92	108.00
1	D	402	DG	C4'-C3'-C2'	-5.82	97.86	103.10
3	H	211	GLY	C-N-CA	5.80	136.21	121.70
1	D	403	DT	O3'-P-O5'	5.80	115.01	104.00
3	H	80	GLU	CA-CB-CG	5.75	126.05	113.40
3	H	127	GLU	CB-CA-C	5.75	121.89	110.40
1	D	405	DG	N9-C1'-C2'	5.73	123.49	112.60
3	H	122	CYS	O-C-N	5.73	131.86	122.70
3	H	38	GLN	CA-CB-CG	5.72	125.99	113.40
3	H	225	TYR	CB-CG-CD2	5.72	124.43	121.00
1	D	409	DT	C5'-C4'-O4'	-5.68	98.50	109.30
3	H	186	PRO	CA-C-N	-5.68	104.69	117.20
3	H	215	TRP	C-N-CA	5.66	134.19	122.30
3	H	101	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	D	404	DT	N3-C4-O4	-5.66	116.51	119.90
3	H	175	ARG	NE-CZ-NH2	5.65	123.13	120.30
2	L	14(E)	GLU	OE1-CD-OE2	-5.64	116.53	123.30
2	L	14(D)	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	408	DG	C5-C6-N1	5.63	114.31	111.50
3	H	60(D)	TRP	CB-CA-C	-5.63	99.14	110.40
3	H	106	MET	N-CA-C	-5.63	95.81	111.00
3	H	172	THR	CA-CB-OG1	-5.62	97.20	109.00
3	H	91	HIS	O-C-N	5.61	131.76	121.10
3	H	93	ARG	NE-CZ-NH1	-5.61	117.50	120.30
3	H	222	ASP	CB-CA-C	5.59	121.58	110.40
3	H	21	ASP	OD1-CG-OD2	5.57	133.88	123.30
3	H	74	THR	CB-CA-C	-5.57	96.57	111.60
3	H	77(A)	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	D	412	DT	N3-C4-O4	-5.56	116.57	119.90
2	L	10	LYS	CA-C-O	5.54	131.74	120.10
3	H	170	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	D	406	DG	C5-C6-N1	5.52	114.26	111.50
3	H	60(D)	TRP	CA-CB-CG	5.51	124.17	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	229	THR	CA-CB-CG2	5.47	120.06	112.40
2	L	14(J)	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	D	410	DG	O5'-P-OP2	5.46	117.25	110.70
2	L	10	LYS	CA-CB-CG	5.45	125.39	113.40
3	H	221	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	408	DG	C6-N1-C2	-5.44	121.84	125.10
1	D	415	DG	N3-C2-N2	-5.40	116.12	119.90
3	H	17	VAL	C-N-CA	5.40	135.21	121.70
3	H	60(D)	TRP	CB-CG-CD2	-5.40	119.58	126.60
3	H	204(A)	PHE	CB-CG-CD1	-5.40	117.02	120.80
3	H	52	VAL	CG1-CB-CG2	5.39	119.52	110.90
3	H	41	LEU	CA-CB-CG	5.38	127.69	115.30
1	D	412	DT	C5-C6-N1	-5.38	120.47	123.70
1	D	404	DT	C4-C5-C7	5.37	122.22	119.00
3	H	230	HIS	N-CA-CB	5.36	120.25	110.60
1	D	412	DT	N1-C1'-C2'	-5.35	102.44	112.60
2	L	14(B)	THR	CA-CB-OG1	-5.35	97.77	109.00
3	H	60(H)	PHE	CA-C-N	-5.34	105.45	117.20
3	H	233	ARG	NE-CZ-NH2	-5.33	117.63	120.30
3	H	61	GLU	CG-CD-OE1	5.33	128.96	118.30
1	D	403	DT	N3-C4-C5	5.32	118.39	115.20
1	D	410	DG	OP1-P-OP2	-5.32	111.62	119.60
1	D	413	DT	OP1-P-O3'	5.32	116.89	105.20
3	H	40	LEU	CA-C-O	-5.31	108.94	120.10
3	H	40	LEU	CA-CB-CG	5.31	127.51	115.30
3	H	140	GLY	N-CA-C	5.29	126.33	113.10
1	D	407	DT	N1-C2-N3	5.29	117.77	114.60
3	H	119	HIS	O-C-N	5.28	131.13	121.10
2	L	2	GLY	N-CA-C	5.27	126.28	113.10
3	H	34	PHE	CB-CA-C	5.25	120.89	110.40
2	L	14(B)	THR	CA-CB-CG2	-5.25	105.06	112.40
3	H	22	ALA	N-CA-C	-5.24	96.86	111.00
3	H	199	PHE	O-C-N	5.24	131.08	122.70
1	D	415	DG	OP1-P-OP2	-5.23	111.76	119.60
3	H	160	LEU	O-C-N	5.23	131.04	121.10
3	H	62	ASN	CA-C-O	5.22	131.07	120.10
3	H	246	GLY	O-C-N	5.22	131.06	122.70
3	H	184	GLY	CA-C-O	5.22	130.00	120.60
1	D	401	DG	C4-N9-C1'	5.20	133.26	126.50
3	H	234	LEU	CA-CB-CG	5.20	127.25	115.30
3	H	23	GLU	N-CA-CB	5.18	119.92	110.60
1	D	403	DT	P-O3'-C3'	-5.17	113.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	210	MET	CA-C-O	5.15	130.91	120.10
3	H	233	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	D	403	DT	C5-C4-O4	-5.11	121.32	124.90
2	L	14(C)	GLU	C-N-CA	5.11	134.47	121.70
1	D	414	DG	OP1-P-OP2	-5.11	111.94	119.60
1	D	408	DG	C1'-O4'-C4'	-5.10	105.00	110.10
1	D	412	DT	O5'-P-OP1	5.10	116.82	110.70
3	H	33	LEU	CA-C-O	-5.09	109.40	120.10
3	H	212	ILE	N-CA-CB	5.09	122.52	110.80
2	L	14(B)	THR	N-CA-CB	-5.08	100.64	110.30
3	H	54	THR	CA-CB-CG2	5.05	119.46	112.40
3	H	204	PRO	N-CA-C	-5.04	99.00	112.10
2	L	13	GLU	CA-CB-CG	5.04	124.48	113.40
3	H	129(C)	LEU	CB-CA-C	5.03	119.75	110.20
3	H	235	LYS	CA-C-N	-5.02	106.15	117.20
3	H	206	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
3	H	20	SER	CA-CB-OG	-5.01	97.66	111.20
3	H	194	ASP	N-CA-C	5.00	124.51	111.00
3	H	130	LEU	CB-CA-C	5.00	119.70	110.20

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 (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	59	0
2	L	222	0	224	57	0
3	H	2053	0	2017	492	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	30	0	30	19	0
5	D	19	0	0	0	0
5	H	119	0	0	23	0
5	L	11	0	0	2	0
All	All	2769	0	2444	588	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 117.

All (588) 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:297:0G6: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:297:0G6: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
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: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
2:L:14(J):TYR:C	2:L:14(K):ILE:HG13	1.72	1.08
3:H:195:SER:OG	4:H:297:0G6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:58:CYS:C	3:H:60(F):LYS:HD3	1.78	1.04
3:H:60(B):PRO:HG2	3:H:96:TRP:CD2	1.92	1.04
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: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
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
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
3:H:50:ARG:HD2	3:H:111:PRO:CD	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:LEU:N	3:H:144:LEU:HD23	1.91	0.84
3:H:32:MET:HG3	3:H:40:LEU:HD12	1.58	0.84
1:D:402:DG:H1'	1:D:404:DT:H73	1.59	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
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:124:PRO:HG3	3:H:210:MET:HE1	1.64	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:204(B):ASN:HD22	3:H:204(B):ASN:C	1.85	0.80
3:H:97:ARG:NH2	5:H:550:HOH:O	2.06	0.79
3:H:175:ARG:HD2	3:H:175:ARG:C	2.00	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:124:PRO:HB3	3:H:210:MET:HE3	1.64	0.78
3:H:195:SER:OG	4:H:297:0G6:CA2	2.31	0.78
3:H:35:ARG:CD	3:H:37:PRO:HD2	2.14	0.78
3:H:165:ARG:HD3	3:H:165:ARG:C	2.04	0.78
3:H:35:ARG:HD3	3:H:37:PRO:N	1.99	0.78
1:D:401:DG:N1	1:D:406:DG:O6	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:0G6: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:HB3	3:H:210:MET:CE	2.16	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
2:L:14(B):THR:O	2:L:14(C):GLU:C	2.26	0.73
3:H:35:ARG:HE	3:H:37:PRO:HD2	1.53	0.73
3:H:105:LEU:C	3:H:106:MET:HG3	2.09	0.73
3:H:98:ASN:O	3:H:99:LEU:HB2	1.86	0.72
3:H:32:MET:CE	3:H:40:LEU:CD1	2.68	0.72
3:H:157:VAL:CG2	3:H:157:VAL:O	2.36	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: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: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
3:H:32:MET:HE3	3:H:40:LEU:CD1	2.21	0.70
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:51:TRP:HE1	3:H:247:GLU:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:0G6:C3	2.76	0.69
1:D:410:DG:N3	1:D:410:DG:C2'	2.54	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:32:MET:HE2	3:H:40:LEU:HD13	1.73	0.68
3:H:72:SER:CB	3:H:77:GLU:OE2	2.38	0.68
3:H:32:MET:CE	3:H:40:LEU:HD13	2.23	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
3:H:177:THR:OG1	3:H:178:ASP:N	2.20	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
1:D:402:DG:C4	1:D:404:DT:C7	2.78	0.67
3:H:215:TRP:HB2	4:H:297:0G6:HD1	1.76	0.67
3:H:26:MET:SD	3:H:157:VAL:HG11	2.35	0.66
3:H:24:ILE:HG12	5:H:607:HOH:O	1.94	0.66
3:H:99:LEU:HD22	4:H:297:0G6: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:297:0G6:O	1.96	0.65
2:L:12:LEU:HD23	2:L:13:GLU:H	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:402:DG:N3	1:D:404:DT:H71	2.12	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: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:297:0G6: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:165:ARG:CB	3:H:166:PRO:CD	2.74	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: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:60(A):TYR:C	3:H:60(C):PRO:HD2	2.20	0.62
3:H:95:ASN:HD21	3:H:97(A):GLU:HB2	1.64	0.62
3:H:199:PHE:O	3:H:199:PHE:CG	2.50	0.62
3:H:203:SER:OG	3:H:204(A):PHE:HB2	1.99	0.62
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
2:L:14:ASP:CG	2:L:14(C):GLU:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:0G6: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:35:ARG:HD3	3:H:36(A):SER:C	2.21	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: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
3:H:85:LEU:HD22	3:H:106:MET:HE1	1.84	0.59
2:L:5:PRO:HA	2:L:9:LYS:CB	2.33	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:103:ILE:HG13	3:H:104:ALA:N	2.18	0.58
3:H:61:GLU:HG2	3:H:88:ILE:HD12	1.85	0.58
3:H:124:PRO:HG3	3:H:210:MET:CE	2.32	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
2:L:6:LEU:HD11	3:H:116:ASP:CG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:SER:C	3:H:117:TYR:N	2.55	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: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
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:26:MET:CE	3:H:137:ARG:NH1	2.68	0.56
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: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
3:H:191:CYS:O	3:H:192:GLU:C	2.44	0.55
1:D:413:DT:C4'	1:D:414:DG:OP1	2.53	0.55
3:H:76:TYR:HE2	3:H:82:ILE:CD1	2.19	0.55
3:H:85:LEU:HD22	3:H:106:MET:CE	2.37	0.55
3:H:124:PRO:CG	3:H:210:MET:HE1	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:175:ARG:C	3:H:175:ARG:CD	2.74	0.54
2:L:14(C):GLU:N	3:H:137:ARG:NH2	2.56	0.54
3:H:56:ALA:C	3:H:58:CYS:H	2.10	0.54
3:H:57:HIS:CD2	4:H:297:0G6: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:115:SER:O	3:H:116:ASP:C	2.46	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:126:ARG:C	3:H:126:ARG:CD	2.75	0.53
3:H:215:TRP:HA	4:H:297:0G6: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:56:ALA:O	3:H:58:CYS:N	2.41	0.53
3:H:99:LEU:HD22	4:H:297:0G6: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
3:H:143:ASN:C	3:H:144:LEU:HD23	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:DG:C1'	1:D:404:DT:H73	2.33	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
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:85:LEU:CD2	3:H:106:MET:HE1	2.39	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
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:297:0G6:HB22	2.10	0.51
2:L:4:ARG:NH2	2:L:7:PHE:HB3	2.26	0.51
3:H:84:MET:O	3:H:109:LYS:HB2	2.10	0.51
3:H:189:ASP:CG	4:H:297:0G6:HH22	2.13	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:164:GLU:C	3:H:166:PRO:HD2	2.31	0.50
3:H:23:GLU:O	3:H:24:ILE:C	2.49	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
3:H:124:PRO:HB3	3:H:210:MET:HE1	1.93	0.50
3:H:153:SER:HB3	5:H:647:HOH:O	2.11	0.50
3:H:203:SER:C	3:H:204(A):PHE:H	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:183:ALA:CB	3:H:228:TYR:CE2	2.92	0.49
1:D:402:DG:C4	1:D:404:DT:H71	2.46	0.49
2:L:7:PHE:CE1	2:L:14:ASP:N	2.80	0.49
3:H:49:ASP:OD2	3:H:111:PRO:HB3	2.12	0.49
3:H:60(B):PRO:N	3:H:60(C):PRO:HD2	2.27	0.49
3:H:166:PRO:O	3:H:169:LYS:HB2	2.13	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:32:MET:HE2	3:H:40:LEU:CD1	2.36	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
3:H:35:ARG:HD3	3:H:37:PRO:HD2	1.87	0.48
3:H:204(B):ASN:C	3:H:204(B):ASN:ND2	2.60	0.48
3:H:60(A):TYR:CE2	3:H:60(C):PRO:HG2	2.48	0.48
3:H:80:GLU:C	3:H:81:LYS:HG3	2.32	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:32:MET:CE	3:H:40:LEU:HD12	2.42	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: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:162:ILE:HG13	3:H:199:PHE:HZ	1.79	0.48
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:215:TRP:CB	4:H:297:0G6:HD1	2.44	0.47
3:H:60(I):THR:C	3:H:62:ASN:N	2.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1(A):ASP:O	2:L:1(A):ASP:CG	2.53	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:26:MET:HE2	3:H:137:ARG:NH1	2.30	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
2:L:7:PHE:HE1	2:L:13:GLU:C	2.18	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: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
2:L:5:PRO:C	2:L:6:LEU:HD12	2.36	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
3:H:53:LEU:HD13	3:H:105:LEU:HD23	1.97	0.45
3:H:72:SER:H	3:H:77:GLU:CD	2.19	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:169:LYS:C	3:H:171:SER:H	2.16	0.45
3:H:53:LEU:HD11	3:H:103:ILE:CD1	2.45	0.45
3:H:115:SER:C	3:H:117:TYR:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:LYS:O	3:H:38:GLN:HB2	2.16	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
2:L:7:PHE:CE1	2:L:13:GLU:C	2.90	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:191:CYS:H	3:H:194:ASP:CG	2.20	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:297:0G6:H1	2.35	0.44
3:H:59:LEU:C	3:H:60(F):LYS:HG2	2.38	0.44
3:H:184(A):TYR:OH	3:H:186(D):LYS:HE2	2.17	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:26:MET:HE1	3:H:137:ARG:CZ	2.48	0.44
3:H:124:PRO:CB	3:H:210:MET:HE1	2.47	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
3:H:125:ASP:O	3:H:126:ARG:C	2.56	0.44
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:ILE:CB	3:H:156:GLN:HB2	2.48	0.42
3:H:26:MET:HE1	3:H:137:ARG:NH1	2.34	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: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:116:ASP:CG	5:H:559:HOH:O	2.56	0.42
1:D:410:DG:H1'	1:D:411:DG:H5'	2.01	0.42
3:H:126:ARG:O	3:H:126:ARG:CD	2.67	0.42
3:H:185:LYS:N	3:H:186(B):GLU:HG3	2.33	0.42
3:H:56:ALA:C	3:H:58:CYS:N	2.68	0.42
1:D:407:DT:C4'	1:D:408:DG:OP2	2.68	0.42
3:H:103:ILE:CG1	3:H:104:ALA:N	2.82	0.42
3:H:96:TRP:CZ3	3:H:97:ARG:HG2	2.55	0.42
3:H:48:SER:C	3:H:50:ARG:H	2.23	0.41
3:H:124:PRO:CB	3:H:210:MET:CE	2.92	0.41
3:H:147:THR:C	3:H:148:TRP:HE3	2.23	0.41
3:H:167:VAL:O	3:H:168:CYS:C	2.59	0.41
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(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
3:H:93:ARG:O	3:H:94:TYR:C	2.58	0.41
1:D:413:DT:H4'	1:D:414:DG:OP1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:172:THR:C	3:H:174:ILE:N	2.72	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:213:VAL:HG23	3:H:213:VAL:H	1.67	0.41
3:H:36(A):SER:HA	3:H:37:PRO:C	2.41	0.41
3:H:77:GLU:HB2	3:H:80:GLU:HB3	2.03	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
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:297:0G6: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:48:SER:C	3:H:50:ARG:N	2.75	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
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%)	14 (56%)	11 (44%)	0 0
3	H	221/225 (98%)	167 (76%)	54 (24%)	0 2
All	All	246/256 (96%)	181 (74%)	65 (26%)	0 1

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

Mol	Chain	Res	Type
2	L	1(A)	ASP

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Mol	Chain	Res	Type
2	L	8	GLU
2	L	10	LYS
2	L	11	SER
2	L	12	LEU
2	L	13	GLU
2	L	14(A)	LYS
2	L	14(B)	THR
2	L	14(G)	LEU
2	L	14(J)	TYR
2	L	14(K)	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	60(E)	ASP
3	H	61	GLU
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	86	GLU
3	H	87	LYS
3	H	97(A)	GLU
3	H	99	LEU
3	H	103	ILE
3	H	106	MET
3	H	110	LYS
3	H	126	ARG
3	H	137	ARG
3	H	139	THR
3	H	144	LEU

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Mol	Chain	Res	Type
3	H	145	LYS
3	H	148	TRP
3	H	154	VAL
3	H	157	VAL
3	H	165	ARG
3	H	171	SER
3	H	173	ARG
3	H	175	ARG
3	H	177	THR
3	H	178	ASP
3	H	186(B)	GLU
3	H	203	SER
3	H	204(B)	ASN
3	H	222	ASP
3	H	224	LYS
3	H	233	ARG
3	H	234	LEU
3	H	239	GLN
3	H	240	LYS
3	H	242	ILE
3	H	243	ASP
3	H	245	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	38	GLN
3	H	57	HIS
3	H	62	ASN
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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	0G6	H	297	3	30,31,32	2.25	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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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.

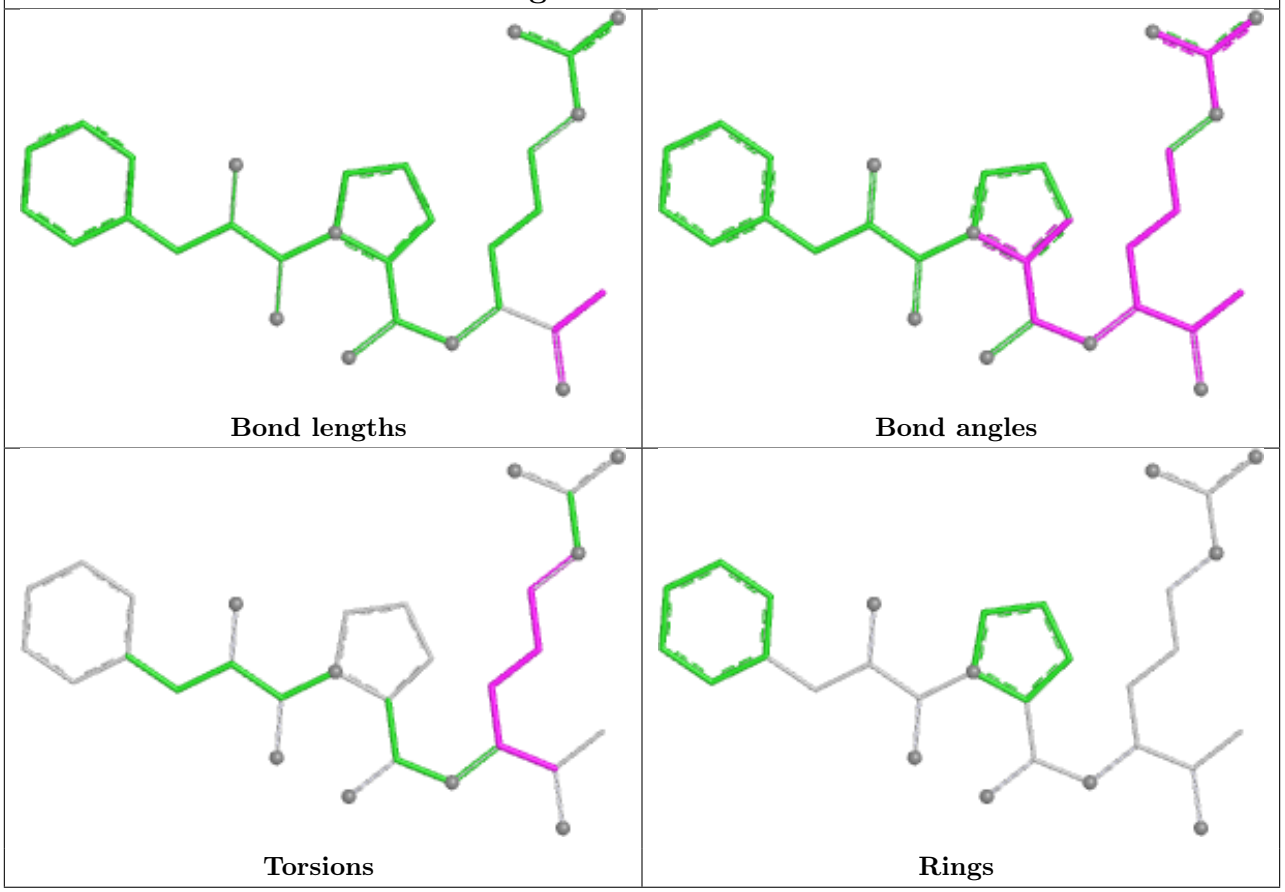
1 monomer is involved in 19 short contacts:

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 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.

Ligand 0G6 H 297



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
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.