



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 2HPP / pdb_00002hpp
Title : Structures of the noncovalent complexes of human and bovine prothrombin fragment 2 with human ppack-thrombin
Authors : Tulinsky, A.; Padmanabhan, K.
Deposited on : 1993-04-28
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

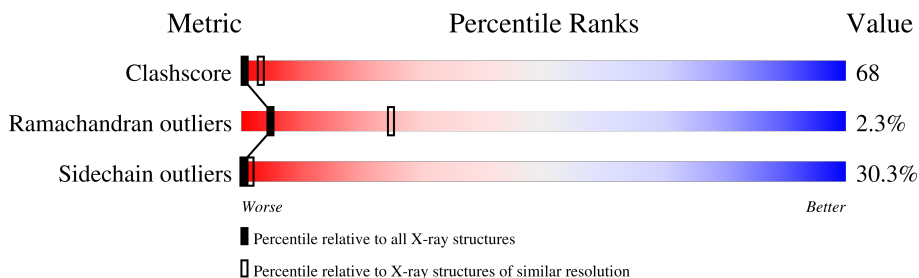
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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	L	36	
2	H	259	
3	P	79	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3031 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 protein called ALPHA-THROMBIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	30	Total	C	N	O	S	0	0	0
			243	151	39	52	1			

- Molecule 2 is a protein called ALPHA-THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	0	0	0
			2022	1287	359	362	14			

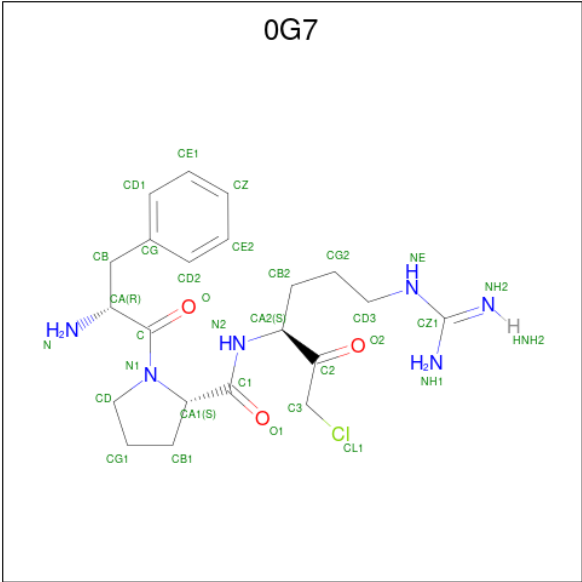
- Molecule 3 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	79	Total	C	N	O	S	0	0	0
			617	378	109	124	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	375	ASN	ASP	conflict	UNP P00735

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	14	Total	O	0	0
			14	14		
5	H	79	Total	O	0	0
			79	79		
5	P	26	Total	O	0	0
			26	26		

3 Residue-property plots

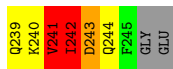
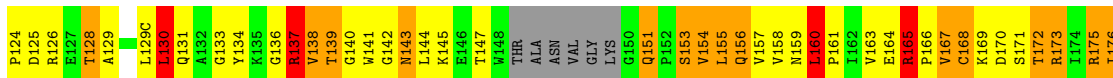
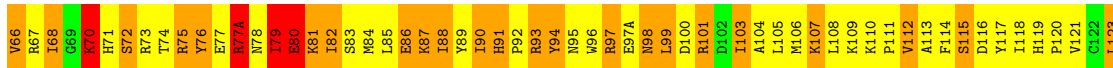
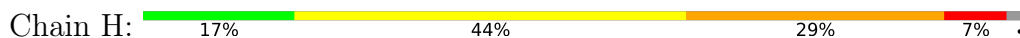
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ALPHA-THROMBIN LIGHT CHAIN



- Molecule 2: ALPHA-THROMBIN HEAVY CHAIN



- Molecule 3: Prothrombin



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.70Å 122.70Å 103.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.98	0/245	2.64	21/326 (6.4%)
2	H	1.11	2/2073 (0.1%)	2.58	175/2800 (6.2%)
3	P	1.25	2/632 (0.3%)	2.53	59/858 (6.9%)
All	All	1.13	4/2950 (0.1%)	2.57	255/3984 (6.4%)

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
2	H	0	1
3	P	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	359	GLY	C-N	16.25	1.56	1.33
2	H	90	ILE	CA-CB	6.28	1.62	1.54
2	H	215	TRP	NE1-CE2	-5.46	1.31	1.37
3	P	361	TRP	NE1-CE2	-5.28	1.31	1.37

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	91	HIS	CA-CB-CG	-12.87	100.93	113.80
2	H	33	LEU	CA-C-N	12.44	139.32	122.77
2	H	33	LEU	C-N-CA	12.44	139.32	122.77
2	H	182	CYS	CA-C-O	-11.84	107.26	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	160	LEU	O-C-N	10.91	131.18	121.80
2	H	170	ASP	CA-CB-CG	10.75	123.35	112.60
2	H	123	LEU	CB-CA-C	10.69	123.54	108.68
2	H	233	ARG	NE-CZ-NH2	10.42	128.58	119.20
2	H	182	CYS	O-C-N	10.27	135.88	123.24
2	H	136	GLY	CA-C-O	-9.88	112.48	121.47
1	L	1(A)	ASP	CA-CB-CG	-9.88	102.72	112.60
2	H	110	LYS	O-C-N	9.88	130.18	121.39
1	L	10	LYS	N-CA-C	-9.86	101.25	113.38
2	H	161	PRO	CA-C-O	-9.57	110.25	122.12
2	H	76	TYR	N-CA-C	-9.42	94.06	108.67
2	H	27	SER	O-C-N	9.34	129.11	121.17
2	H	77(A)	ARG	O-C-N	-8.98	112.60	122.12
2	H	182	CYS	N-CA-C	-8.94	95.38	109.50
2	H	181	PHE	CA-CB-CG	8.91	122.71	113.80
2	H	101	ARG	NE-CZ-NH1	8.86	130.36	121.50
2	H	155	LEU	CA-C-O	-8.82	111.54	121.07
3	P	373	TYR	O-C-N	8.75	133.41	122.65
2	H	143	ASN	O-C-N	8.73	133.61	122.87
2	H	116	ASP	O-C-N	8.67	132.36	122.22
2	H	34	PHE	CA-CB-CG	-8.63	105.17	113.80
3	P	335	LYS	CA-C-O	-8.59	111.36	120.55
2	H	23	GLU	CA-C-O	-8.58	112.18	121.88
2	H	239	GLN	N-CA-CB	8.51	123.40	110.30
2	H	172	THR	CA-C-N	8.41	134.98	120.68
2	H	172	THR	C-N-CA	8.41	134.98	120.68
2	H	186(A)	ASP	CA-CB-CG	-8.38	104.22	112.60
3	P	309	TYR	N-CA-CB	8.34	123.27	109.60
2	H	231	VAL	N-CA-CB	8.33	121.87	110.54
3	P	304	ASP	CA-CB-CG	8.30	120.90	112.60
2	H	216	GLY	CA-C-O	-8.24	113.29	121.86
2	H	184(A)	TYR	CA-C-O	-8.14	111.59	121.36
3	P	366	ASP	CA-CB-CG	-8.14	104.46	112.60
2	H	243	ASP	CA-CB-CG	8.09	120.69	112.60
1	L	14(G)	LEU	CA-C-O	-8.09	111.85	120.42
3	P	330	ALA	N-CA-C	-8.00	103.33	113.72
2	H	184(A)	TYR	O-C-N	7.96	131.97	123.06
3	P	348	ASN	CA-CB-CG	-7.75	104.85	112.60
2	H	82	ILE	CA-C-O	-7.67	111.84	120.74
3	P	340	ASN	CA-C-O	7.67	125.95	119.66
3	P	346	ALA	N-CA-C	7.66	120.54	108.67
2	H	172	THR	N-CA-C	7.63	118.68	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	99	LEU	N-CA-CB	-7.61	100.64	112.13
2	H	142	GLY	O-C-N	7.58	130.40	122.59
3	P	359	GLY	O-C-N	7.58	132.64	124.15
2	H	33	LEU	CB-CA-C	7.58	123.96	111.23
2	H	125	ASP	CA-C-O	-7.51	112.49	121.66
2	H	117	TYR	CA-C-O	-7.48	110.81	119.56
2	H	165	ARG	CD-NE-CZ	7.47	134.86	124.40
2	H	209	GLN	O-C-N	7.47	132.85	122.77
2	H	198	PRO	N-CA-C	7.43	122.85	111.19
2	H	175	ARG	CD-NE-CZ	-7.41	114.02	124.40
2	H	23	GLU	CA-C-N	-7.39	114.03	123.19
2	H	23	GLU	C-N-CA	-7.39	114.03	123.19
1	L	14(G)	LEU	O-C-N	7.38	134.51	122.70
2	H	33	LEU	CA-C-O	7.38	129.87	120.57
2	H	153	SER	N-CA-CB	-7.37	99.82	110.65
2	H	163	VAL	CA-C-O	-7.34	113.71	121.93
2	H	65	LEU	CB-CA-C	7.33	123.57	110.16
2	H	128	THR	CA-C-N	7.28	130.37	120.54
2	H	128	THR	C-N-CA	7.28	130.37	120.54
2	H	209	GLN	N-CA-CB	7.26	121.50	109.60
2	H	76	TYR	CA-C-O	-7.22	112.44	120.60
2	H	93	ARG	NE-CZ-NH1	-7.20	114.30	121.50
3	P	339	PHE	CA-CB-CG	7.18	120.98	113.80
3	P	357	GLU	O-C-N	7.18	130.62	122.22
2	H	98	ASN	CA-CB-CG	-7.16	105.44	112.60
2	H	159	ASN	OD1-CG-ND2	-7.05	115.55	122.60
3	P	375	ASN	N-CA-C	7.05	121.20	108.17
1	L	14(D)	ARG	N-CA-C	7.03	118.94	111.28
2	H	93	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	L	1	CYS	O-C-N	6.96	131.84	122.59
3	P	354	ASP	O-C-N	6.95	130.31	122.11
2	H	136	GLY	N-CA-C	-6.95	101.56	111.42
2	H	51	TRP	CA-C-N	6.92	132.03	123.10
2	H	51	TRP	C-N-CA	6.92	132.03	123.10
1	L	10	LYS	CA-C-O	6.89	127.01	119.15
1	L	13	GLU	CB-CG-CD	6.85	124.25	112.60
2	H	210	MET	N-CA-C	-6.83	105.08	113.41
3	P	309	TYR	N-CA-C	-6.81	99.35	109.15
2	H	68	ILE	N-CA-C	6.81	118.40	108.53
3	P	314	ALA	O-C-N	6.76	128.14	121.85
3	P	369	GLY	N-CA-C	-6.75	106.66	114.69
3	P	305	ARG	NE-CZ-NH2	6.75	125.27	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	242	ILE	O-C-N	6.71	129.12	121.94
2	H	198	PRO	CB-CA-C	-6.70	102.30	111.21
3	P	306	GLY	O-C-N	6.68	128.95	122.41
3	P	323	LEU	CB-CA-C	6.64	120.70	109.75
2	H	115	SER	CA-C-O	-6.62	111.04	120.51
2	H	237	TRP	N-CA-C	-6.62	104.07	111.28
1	L	14	ASP	N-CA-C	-6.61	101.19	110.50
3	P	350	CYS	O-C-N	6.59	131.13	122.95
1	L	14(H)	GLU	CB-CA-C	-6.56	98.49	110.63
2	H	77(A)	ARG	N-CA-C	6.55	119.25	111.33
2	H	209	GLN	CA-C-O	-6.49	112.89	120.62
2	H	230	HIS	CA-C-O	-6.49	113.98	120.98
3	P	321	ARG	N-CA-C	6.47	119.27	108.73
2	H	156	GLN	N-CA-CB	-6.46	101.36	111.05
2	H	140	GLY	CA-C-O	-6.45	114.66	121.56
3	P	327	SER	N-CA-C	-6.42	97.13	110.80
2	H	50	ARG	N-CA-CB	-6.41	102.47	111.00
2	H	77(A)	ARG	CA-C-N	-6.41	112.61	122.60
2	H	77(A)	ARG	C-N-CA	-6.41	112.61	122.60
2	H	129(C)	LEU	CA-C-N	-6.40	112.56	122.16
2	H	129(C)	LEU	C-N-CA	-6.40	112.56	122.16
3	P	344	PRO	CB-CA-C	-6.40	103.62	111.11
1	L	1(C)	GLU	N-CA-C	6.39	118.86	108.63
2	H	142	GLY	CA-C-O	-6.39	114.63	122.75
3	P	343	VAL	O-C-N	6.33	128.32	121.10
3	P	315	VAL	O-C-N	6.32	129.54	123.03
2	H	40	LEU	CA-C-O	-6.29	113.43	120.54
2	H	233	ARG	NH1-CZ-NH2	-6.29	111.13	119.30
1	L	3	LEU	CA-C-O	-6.28	108.57	120.69
2	H	209	GLN	CB-CA-C	-6.27	101.14	110.67
2	H	99	LEU	CA-C-N	6.26	129.71	120.95
2	H	99	LEU	C-N-CA	6.26	129.71	120.95
3	P	376	LEU	N-CA-CB	6.26	120.32	110.87
2	H	201	MET	CA-C-O	-6.25	113.47	120.66
3	P	359	GLY	CA-C-N	-6.24	112.57	121.50
3	P	359	GLY	C-N-CA	-6.24	112.57	121.50
2	H	175	ARG	NE-CZ-NH1	-6.24	115.26	121.50
2	H	138	VAL	CB-CA-C	6.23	120.09	111.49
2	H	199	PHE	CA-CB-CG	6.22	120.02	113.80
2	H	219	GLY	N-CA-C	-6.22	100.78	111.47
2	H	153	SER	N-CA-C	-6.21	105.64	113.72
2	H	178	ASP	CA-C-O	-6.21	113.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	47	ILE	CA-C-O	6.21	125.16	119.20
2	H	80	GLU	CA-CB-CG	6.17	126.43	114.10
2	H	215	TRP	CB-CA-C	-6.16	105.57	114.87
2	H	161	PRO	CB-CA-C	-6.14	102.13	110.60
2	H	130	LEU	CB-CA-C	6.12	121.58	112.03
2	H	210	MET	O-C-N	6.11	131.03	122.36
2	H	212	ILE	CA-C-O	-6.11	113.89	120.36
2	H	22	ALA	N-CA-C	-6.09	102.06	110.35
2	H	195	SER	N-CA-C	6.09	118.88	110.35
2	H	197	GLY	O-C-N	6.07	127.84	121.77
2	H	23	GLU	N-CA-C	-6.05	102.01	110.35
2	H	113	ALA	O-C-N	6.04	130.24	123.05
2	H	220	CYS	O-C-N	6.01	130.58	122.59
2	H	239	GLN	OE1-CD-NE2	6.01	128.61	122.60
3	P	371	PHE	CA-CB-CG	-6.00	107.80	113.80
2	H	30	GLN	OE1-CD-NE2	6.00	128.60	122.60
2	H	176	ILE	CB-CA-C	6.00	119.86	111.34
2	H	151	GLN	CB-CA-C	5.99	117.50	109.42
2	H	233	ARG	CD-NE-CZ	5.98	132.77	124.40
2	H	231	VAL	O-C-N	5.96	127.65	121.87
3	P	342	ALA	N-CA-C	-5.94	98.14	110.80
3	P	349	PHE	CB-CA-C	-5.93	99.51	109.53
2	H	159	ASN	CA-CB-CG	5.91	118.51	112.60
2	H	18	GLU	CB-CG-CD	5.89	122.62	112.60
2	H	112	VAL	O-C-N	5.87	129.38	122.69
3	P	325	TRP	O-C-N	5.85	130.37	122.59
1	L	14(C)	GLU	CB-CG-CD	-5.84	102.67	112.60
2	H	147	THR	N-CA-C	5.84	117.90	108.32
3	P	363	TYR	CA-C-O	-5.82	115.08	121.89
2	H	76	TYR	O-C-N	5.81	130.38	122.82
2	H	101	ARG	CD-NE-CZ	5.80	132.51	124.40
2	H	241	VAL	O-C-N	5.76	129.44	121.84
2	H	243	ASP	N-CA-C	-5.75	106.30	113.15
2	H	226	GLY	N-CA-C	-5.75	100.97	111.25
3	P	335	LYS	N-CA-C	5.74	118.40	111.40
2	H	125	ASP	N-CA-C	-5.73	101.53	110.42
2	H	77(A)	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	H	25	GLY	N-CA-C	-5.72	107.36	115.43
1	L	4	ARG	CD-NE-CZ	-5.72	116.39	124.40
1	L	14(H)	GLU	N-CA-C	-5.71	105.14	111.71
2	H	172	THR	CA-CB-OG1	-5.70	101.05	109.60
2	H	178	ASP	O-C-N	5.69	128.88	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	167	VAL	O-C-N	5.68	127.38	121.87
2	H	167	VAL	N-CA-CB	5.68	118.26	110.54
2	H	215	TRP	O-C-N	5.68	127.37	123.11
2	H	186(D)	LYS	N-CA-CB	5.67	122.07	111.52
2	H	27	SER	N-CA-CB	5.66	118.11	111.09
2	H	181	PHE	CA-C-N	-5.63	113.84	122.62
2	H	181	PHE	C-N-CA	-5.63	113.84	122.62
2	H	40	LEU	O-C-N	5.62	129.63	123.22
2	H	205	ASN	CA-CB-CG	-5.62	106.98	112.60
2	H	239	GLN	CB-CG-CD	-5.62	103.05	112.60
2	H	210	MET	CA-C-O	-5.58	113.10	119.41
3	P	373	TYR	CA-C-O	-5.58	115.52	121.94
2	H	160	LEU	CB-CA-C	5.58	117.51	108.87
3	P	351	ARG	CA-C-O	-5.57	115.49	121.45
3	P	336	ASP	CA-CB-CG	-5.56	107.04	112.60
2	H	201	MET	O-C-N	5.51	130.00	123.27
2	H	123	LEU	CA-C-O	5.51	125.31	120.19
2	H	179	ASN	O-C-N	5.50	129.99	121.63
2	H	227	PHE	CB-CA-C	5.48	118.76	109.50
2	H	66	VAL	CA-CB-CG2	5.47	119.69	110.40
3	P	376	LEU	N-CA-C	-5.46	101.82	109.69
2	H	113	ALA	CA-C-O	-5.46	114.87	120.54
3	P	327	SER	CA-C-O	-5.46	112.71	120.51
1	L	1	CYS	CA-C-N	5.43	132.05	121.41
1	L	1	CYS	C-N-CA	5.43	132.05	121.41
2	H	68	ILE	O-C-N	-5.42	117.62	123.14
2	H	20	SER	N-CA-CB	-5.41	101.46	111.53
2	H	133	GLY	CA-C-O	5.41	124.27	119.56
2	H	168	CYS	CA-C-N	5.40	127.83	120.54
2	H	168	CYS	C-N-CA	5.40	127.83	120.54
3	P	342	ALA	O-C-N	5.40	129.77	122.59
3	P	321	ARG	NE-CZ-NH2	5.38	124.05	119.20
3	P	334	SER	N-CA-C	5.35	119.07	112.54
2	H	131	GLN	OE1-CD-NE2	5.33	127.93	122.60
3	P	342	ALA	N-CA-CB	5.32	119.49	110.49
3	P	310	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	H	125	ASP	O-C-N	5.32	129.04	123.03
3	P	312	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	H	172	THR	CA-CB-CG2	5.32	119.54	110.50
2	H	243	ASP	CB-CA-C	5.31	120.19	110.36
2	H	54	THR	CA-CB-OG1	-5.31	101.64	109.60
2	H	137	ARG	CA-CB-CG	5.30	124.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	160	LEU	CA-C-O	-5.30	114.47	120.46
2	H	161	PRO	O-C-N	5.29	129.60	123.14
2	H	120	PRO	CB-CA-C	-5.29	104.05	110.98
2	H	47	ILE	CB-CA-C	5.29	118.77	110.95
3	P	346	ALA	N-CA-CB	-5.29	101.48	109.94
2	H	70	LYS	CA-CB-CG	5.28	124.65	114.10
2	H	34	PHE	CA-C-O	-5.28	114.72	120.36
2	H	28	PRO	O-C-N	5.27	129.47	122.30
2	H	35	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	L	14(C)	GLU	CA-C-O	-5.25	113.00	120.51
3	P	308	GLU	CA-C-N	-5.23	113.50	121.66
3	P	308	GLU	C-N-CA	-5.23	113.50	121.66
2	H	156	GLN	CA-CB-CG	-5.23	103.65	114.10
3	P	368	PRO	CA-C-O	5.23	127.02	121.32
3	P	330	ALA	O-C-N	5.21	128.76	122.35
3	P	356	ASP	CA-C-N	5.21	127.78	120.28
3	P	356	ASP	C-N-CA	5.21	127.78	120.28
2	H	25	GLY	O-C-N	5.20	128.53	122.45
2	H	79	ILE	O-C-N	5.18	129.05	122.57
2	H	119	HIS	CA-C-N	5.18	125.08	119.85
2	H	119	HIS	C-N-CA	5.18	125.08	119.85
1	L	14	ASP	CB-CA-C	5.17	119.06	109.54
3	P	351	ARG	O-C-N	5.17	129.05	123.10
3	P	367	GLN	CB-CA-C	5.17	117.00	109.08
2	H	187	ARG	O-C-N	5.17	129.47	122.96
2	H	60	LEU	N-CA-CB	-5.16	101.87	110.80
3	P	340	ASN	N-CA-C	5.16	116.17	109.72
3	P	337	GLN	OE1-CD-NE2	5.11	127.70	122.60
2	H	225	TYR	CA-C-O	-5.08	115.68	121.68
1	L	14(D)	ARG	CA-CB-CG	-5.08	103.95	114.10
3	P	364	VAL	CB-CA-C	5.07	119.60	111.29
3	P	333	LEU	N-CA-CB	-5.06	102.47	110.06
2	H	53	LEU	CA-C-O	-5.05	115.36	120.71
1	L	7	PHE	CA-CB-CG	-5.04	108.76	113.80
2	H	32	MET	O-C-N	5.04	129.30	123.30
2	H	239	GLN	CA-C-N	-5.03	113.54	120.28
2	H	239	GLN	C-N-CA	-5.03	113.54	120.28
2	H	136	GLY	O-C-N	5.03	127.82	123.95
2	H	30	GLN	CB-CG-CD	-5.01	104.08	112.60
2	H	93	ARG	CA-C-N	5.00	130.28	122.17
2	H	93	ARG	C-N-CA	5.00	130.28	122.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	97	ARG	Sidechain
3	P	310	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	L	243	0	238	35	0
2	H	2022	0	1991	224	0
3	P	617	0	553	149	0
4	H	30	0	28	10	0
5	H	79	0	0	11	0
5	L	14	0	0	0	0
5	P	26	0	0	1	0
All	All	3031	0	2810	387	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 68.

All (387) 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)
2:H:57:HIS:NE2	4:H:1:OG7:C3	1.71	1.48
1:L:1(C):GLU:CD	5:H:454:HOH:O	1.68	1.25
3:P:343:VAL:HG11	3:P:353:PRO:HA	1.21	1.16
2:H:59:LEU:HD13	2:H:88:ILE:HD13	1.28	1.15
2:H:50:ARG:HH21	2:H:107:LYS:HE3	1.15	1.11
1:L:1(C):GLU:CG	5:H:454:HOH:O	1.89	1.08
2:H:124:PRO:HG3	2:H:210:MET:HE2	1.25	1.07
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.36	1.06
3:P:304:ASP:O	3:P:306:GLY:N	1.89	1.05
3:P:304:ASP:HB3	3:P:307:ARG:HB2	1.39	1.05
2:H:241:VAL:HA	2:H:244:GLN:HE21	1.17	1.04
3:P:342:ALA:O	3:P:344:PRO:HD3	1.61	1.01
3:P:340:ASN:C	3:P:340:ASN:HD22	1.68	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:315:VAL:HG12	3:P:320:SER:O	1.63	0.99
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.46	0.98
2:H:178:ASP:HB3	2:H:233:ARG:HH21	1.29	0.97
2:H:57:HIS:CE1	4:H:1:OG7:C3	2.48	0.96
2:H:68:ILE:HG22	2:H:118:ILE:HG12	1.48	0.94
2:H:70:LYS:HE3	2:H:72:SER:O	1.68	0.93
3:P:340:ASN:C	3:P:340:ASN:ND2	2.25	0.90
2:H:165:ARG:HG2	2:H:165:ARG:HH11	1.37	0.88
3:P:345:LEU:HD11	3:P:353:PRO:HG3	1.53	0.88
2:H:60(I):THR:O	2:H:62:ASN:N	2.07	0.88
3:P:309:TYR:OH	3:P:313:LEU:HB2	1.72	0.88
2:H:195:SER:OG	4:H:1:OG7:C2	2.22	0.87
2:H:169:LYS:HE3	5:H:438:HOH:O	1.75	0.85
3:P:326:SER:C	3:P:327:SER:O	2.02	0.85
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.10	0.85
3:P:316:THR:OG1	3:P:372:GLU:HB3	1.77	0.84
3:P:343:VAL:CG1	3:P:353:PRO:HA	2.07	0.83
2:H:201:MET:HG3	2:H:210:MET:HG3	1.57	0.83
3:P:316:THR:OG1	3:P:372:GLU:CB	2.26	0.83
2:H:241:VAL:O	2:H:244:GLN:HB3	1.78	0.83
3:P:316:THR:HG21	3:P:320:SER:HB2	1.58	0.83
2:H:241:VAL:HA	2:H:244:GLN:NE2	1.93	0.82
3:P:326:SER:O	3:P:327:SER:O	1.96	0.82
2:H:178:ASP:CB	2:H:233:ARG:HH21	1.93	0.81
1:L:11:SER:C	1:L:12:LEU:HD13	2.05	0.81
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.13	0.81
2:H:235:LYS:HA	2:H:238:ILE:HD12	1.60	0.81
2:H:204(B):ASN:ND2	2:H:206:ARG:HG2	1.94	0.81
2:H:240:LYS:O	2:H:244:GLN:HB2	1.82	0.80
2:H:100:ASP:O	2:H:101:ARG:HB2	1.82	0.79
2:H:204(B):ASN:HD21	2:H:206:ARG:CG	1.95	0.78
2:H:139:THR:HG23	2:H:157:VAL:HG12	1.65	0.78
3:P:316:THR:HG22	3:P:320:SER:O	1.82	0.78
2:H:237:TRP:O	2:H:241:VAL:HG13	1.84	0.78
2:H:59:LEU:HD13	2:H:88:ILE:CD1	2.11	0.78
1:L:11:SER:O	1:L:12:LEU:HD13	1.84	0.78
2:H:124:PRO:HG3	2:H:210:MET:CE	2.10	0.78
2:H:208:TYR:CB	2:H:210:MET:HE3	2.14	0.77
2:H:204(B):ASN:ND2	2:H:206:ARG:CG	2.48	0.77
1:L:10:LYS:CB	1:L:12:LEU:HD22	2.14	0.77
1:L:10:LYS:HB2	1:L:12:LEU:HD22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:LYS:HD3	3:P:336:ASP:O	1.83	0.77
2:H:204(B):ASN:O	2:H:205:ASN:HB2	1.83	0.77
3:P:305:ARG:NH1	3:P:358:GLU:O	2.17	0.76
2:H:50:ARG:HH21	2:H:107:LYS:CE	1.97	0.76
2:H:215:TRP:C	4:H:1:0G7:HD3	2.11	0.76
3:P:316:THR:CG2	3:P:320:SER:HB2	2.15	0.76
2:H:36(A):SER:HA	2:H:37:PRO:C	2.10	0.76
2:H:60(I):THR:C	2:H:62:ASN:H	1.92	0.76
2:H:168:CYS:O	2:H:171:SER:HB3	1.86	0.76
1:L:14:ASP:CG	1:L:14(C):GLU:HG2	2.11	0.75
3:P:302:VAL:HG23	3:P:377:ASN:O	1.86	0.74
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.68	0.74
3:P:312:ARG:HB3	5:P:505:HOH:O	1.88	0.74
2:H:105:LEU:HD12	2:H:241:VAL:HG21	1.68	0.74
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.70	0.73
3:P:316:THR:HG21	3:P:320:SER:CB	2.19	0.73
1:L:10:LYS:CB	1:L:12:LEU:CD2	2.67	0.73
3:P:313:LEU:HD12	3:P:315:VAL:H	1.52	0.72
3:P:311:GLY:O	3:P:351:ARG:NH2	2.22	0.72
3:P:310:ARG:HA	3:P:351:ARG:CZ	2.19	0.72
3:P:312:ARG:HG3	3:P:312:ARG:O	1.90	0.71
3:P:323:LEU:HD23	3:P:363:TYR:HB2	1.72	0.71
2:H:35:ARG:HG2	2:H:39:GLU:HG3	1.72	0.71
3:P:348:ASN:C	3:P:348:ASN:ND2	2.46	0.71
2:H:52:VAL:CG2	2:H:108:LEU:HD21	2.20	0.71
3:P:325:TRP:CE3	3:P:345:LEU:CD2	2.73	0.71
2:H:124:PRO:CG	2:H:210:MET:HE2	2.14	0.70
4:H:1:0G7:H29	4:H:1:0G7:CD1	2.21	0.70
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ3	2.27	0.70
3:P:325:TRP:CE3	3:P:345:LEU:HD21	2.27	0.70
2:H:93:ARG:HD3	3:P:337:GLN:OE1	1.91	0.70
2:H:52:VAL:HG23	2:H:108:LEU:HD21	1.74	0.69
1:L:10:LYS:HB2	1:L:12:LEU:CD2	2.21	0.69
2:H:50:ARG:HE	2:H:107:LYS:HD3	1.58	0.69
2:H:158:VAL:HG22	2:H:160:LEU:HD21	1.73	0.69
3:P:367:GLN:HB2	3:P:370:ASP:OD2	1.93	0.68
3:P:312:ARG:O	3:P:312:ARG:CG	2.41	0.68
2:H:224:LYS:O	5:H:402:HOH:O	2.09	0.68
3:P:322:CYS:HG	3:P:362:CYS:HG	0.69	0.68
2:H:33:LEU:HD12	2:H:42:CYS:HB2	1.76	0.68
2:H:215:TRP:CE3	2:H:216:GLY:HA2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:LEU:HD11	2:H:106:MET:HE3	1.73	0.68
2:H:50:ARG:NH2	2:H:107:LYS:HE3	1.99	0.67
3:P:325:TRP:CD2	3:P:345:LEU:CD2	2.78	0.67
3:P:323:LEU:HD23	3:P:363:TYR:CB	2.25	0.67
2:H:240:LYS:HD3	3:P:336:ASP:C	2.20	0.66
3:P:342:ALA:O	3:P:344:PRO:CD	2.41	0.66
2:H:124:PRO:HB3	2:H:210:MET:CE	2.24	0.66
3:P:325:TRP:CD2	3:P:345:LEU:HD23	2.31	0.66
3:P:316:THR:HG22	3:P:320:SER:C	2.21	0.66
3:P:326:SER:O	3:P:327:SER:C	2.38	0.65
1:L:10:LYS:HB3	1:L:12:LEU:CD2	2.26	0.65
3:P:316:THR:CG2	3:P:320:SER:CB	2.73	0.65
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.26	0.65
3:P:330:ALA:O	3:P:334:SER:HB2	1.97	0.65
2:H:241:VAL:CA	2:H:244:GLN:HE21	2.04	0.64
2:H:35:ARG:HD3	2:H:37:PRO:O	1.98	0.64
2:H:215:TRP:HB2	4:H:1:OG7:O	1.97	0.64
3:P:359:GLY:O	3:P:361:TRP:HD1	1.81	0.64
2:H:35:ARG:HG2	2:H:41:LEU:HD21	1.80	0.64
2:H:32:MET:HE2	2:H:141:TRP:CE3	2.32	0.64
3:P:356:ASP:OD2	3:P:373:TYR:OH	2.10	0.64
2:H:230:HIS:HB3	2:H:233:ARG:HB2	1.79	0.63
2:H:195:SER:OG	4:H:1:OG7:C3	2.46	0.63
2:H:60:LEU:HD23	2:H:94:TYR:CE2	2.33	0.63
2:H:215:TRP:CE3	2:H:216:GLY:CA	2.81	0.63
2:H:215:TRP:CE3	2:H:216:GLY:N	2.68	0.62
3:P:316:THR:OG1	3:P:372:GLU:OE1	2.16	0.62
2:H:67:ARG:HG2	2:H:82:ILE:HD13	1.80	0.61
3:P:340:ASN:ND2	3:P:341:PRO:N	2.47	0.61
3:P:346:ALA:HB1	3:P:349:PHE:CD2	2.34	0.61
2:H:242:ILE:C	2:H:244:GLN:H	2.07	0.61
1:L:7:PHE:O	1:L:11:SER:N	2.34	0.61
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.36	0.61
3:P:308:GLU:O	3:P:310:ARG:CG	2.49	0.60
3:P:313:LEU:HD12	3:P:314:ALA:N	2.16	0.60
3:P:340:ASN:O	3:P:343:VAL:HG12	2.02	0.60
2:H:70:LYS:CE	2:H:72:SER:O	2.47	0.59
3:P:315:VAL:CG1	3:P:320:SER:O	2.47	0.59
3:P:348:ASN:HD22	3:P:348:ASN:H	1.50	0.59
3:P:375:ASN:C	3:P:376:LEU:HD13	2.25	0.59
1:L:14(B):THR:O	1:L:14(C):GLU:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:ASP:HB3	2:H:233:ARG:NH2	2.08	0.59
2:H:36:LYS:HE2	2:H:62:ASN:O	2.03	0.59
2:H:232:PHE:O	2:H:235:LYS:HB2	2.02	0.59
3:P:309:TYR:CD1	3:P:309:TYR:C	2.80	0.59
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.49	0.59
3:P:343:VAL:O	3:P:343:VAL:HG13	2.01	0.59
3:P:302:VAL:O	3:P:378:TYR:HA	2.01	0.58
3:P:348:ASN:HD22	3:P:348:ASN:N	2.01	0.58
3:P:367:GLN:O	3:P:370:ASP:HB2	2.04	0.58
3:P:322:CYS:HG	3:P:362:CYS:CB	2.15	0.58
3:P:325:TRP:CE3	3:P:345:LEU:HD23	2.37	0.58
3:P:377:ASN:HD22	3:P:378:TYR:N	2.02	0.58
2:H:129:ALA:O	2:H:130:LEU:HB2	2.03	0.58
2:H:240:LYS:HE2	3:P:336:ASP:HA	1.85	0.58
2:H:54:THR:OG1	2:H:55:ALA:N	2.37	0.58
2:H:204(B):ASN:HD22	2:H:206:ARG:HG2	1.65	0.58
3:P:377:ASN:ND2	3:P:378:TYR:O	2.37	0.58
2:H:32:MET:HE3	2:H:141:TRP:CZ3	2.39	0.57
2:H:78:ASN:C	2:H:79:ILE:HD13	2.29	0.57
2:H:79:ILE:HD13	2:H:79:ILE:N	2.18	0.57
2:H:240:LYS:CE	3:P:336:ASP:HA	2.34	0.57
2:H:60(I):THR:C	2:H:62:ASN:N	2.57	0.57
2:H:172:THR:OG1	2:H:173:ARG:N	2.37	0.57
2:H:35:ARG:HB3	2:H:41:LEU:HD11	1.85	0.57
1:L:12:LEU:HD13	1:L:12:LEU:N	2.16	0.57
3:P:306:GLY:C	3:P:308:GLU:H	2.12	0.57
3:P:315:VAL:HG12	3:P:320:SER:C	2.29	0.57
3:P:358:GLU:HA	3:P:358:GLU:OE1	2.04	0.57
2:H:91:HIS:CE1	2:H:92:PRO:HD2	2.40	0.56
2:H:60(B):PRO:HG2	2:H:96:TRP:CH2	2.40	0.56
3:P:305:ARG:HB2	3:P:307:ARG:HH11	1.71	0.56
2:H:32:MET:HE2	2:H:141:TRP:CD2	2.41	0.56
3:P:323:LEU:CD2	3:P:363:TYR:HB3	2.34	0.56
2:H:215:TRP:HA	4:H:1:OG7:HB2A	1.87	0.56
3:P:309:TYR:CZ	3:P:311:GLY:HA3	2.41	0.56
2:H:35:ARG:CG	2:H:39:GLU:HG3	2.35	0.56
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.41	0.56
3:P:309:TYR:OH	3:P:313:LEU:CB	2.52	0.56
1:L:3:LEU:HG	2:H:206:ARG:HD3	1.87	0.55
2:H:93:ARG:O	2:H:101:ARG:HD2	2.05	0.55
3:P:308:GLU:O	3:P:310:ARG:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:345:LEU:HD11	3:P:353:PRO:CG	2.34	0.55
3:P:323:LEU:CD2	3:P:363:TYR:CB	2.84	0.55
2:H:240:LYS:HD3	3:P:336:ASP:CA	2.37	0.55
3:P:366:ASP:OD1	3:P:366:ASP:N	2.40	0.55
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.22	0.55
3:P:331:LYS:HD2	3:P:331:LYS:O	2.07	0.55
2:H:32:MET:CE	2:H:141:TRP:CE3	2.90	0.54
3:P:322:CYS:SG	3:P:362:CYS:CB	2.95	0.54
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.22	0.54
2:H:134:TYR:N	2:H:134:TYR:CD1	2.72	0.54
1:L:14:ASP:OD2	1:L:14(C):GLU:HG2	2.08	0.54
2:H:165:ARG:NH2	2:H:178:ASP:OD1	2.40	0.54
2:H:60:LEU:HD23	2:H:94:TYR:HE2	1.72	0.54
3:P:324:ALA:O	3:P:327:SER:N	2.22	0.54
2:H:76:TYR:HE2	2:H:77(A):ARG:HE	1.55	0.53
2:H:130:LEU:HD11	2:H:210:MET:HB3	1.91	0.53
2:H:139:THR:CG2	2:H:157:VAL:HG12	2.36	0.53
2:H:155:LEU:C	2:H:156:GLN:HG2	2.34	0.53
3:P:308:GLU:O	3:P:310:ARG:HG3	2.08	0.53
3:P:311:GLY:N	3:P:351:ARG:NH2	2.56	0.53
1:L:14:ASP:H	1:L:14(C):GLU:CG	2.21	0.53
3:P:365:ALA:HB3	3:P:370:ASP:HB3	1.91	0.53
2:H:17:VAL:HG22	2:H:144:LEU:C	2.33	0.53
2:H:60(D):TRP:HE3	2:H:60(F):LYS:HE3	1.74	0.53
2:H:81:LYS:CD	2:H:118:ILE:HD13	2.38	0.53
2:H:177:THR:HB	3:P:357:GLU:OE2	2.08	0.53
2:H:204(B):ASN:HD21	2:H:206:ARG:CB	2.21	0.53
2:H:50:ARG:HH11	2:H:111:PRO:HD3	1.73	0.53
2:H:124:PRO:CB	2:H:210:MET:HE1	2.31	0.53
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.91	0.53
2:H:32:MET:HE3	2:H:141:TRP:CH2	2.44	0.53
2:H:35:ARG:HB3	2:H:41:LEU:HD21	1.91	0.53
2:H:94:TYR:CD1	2:H:94:TYR:C	2.87	0.53
3:P:310:ARG:C	3:P:351:ARG:NH2	2.67	0.52
3:P:313:LEU:CD1	3:P:314:ALA:H	2.22	0.52
2:H:45:SER:O	2:H:52:VAL:HA	2.10	0.52
3:P:304:ASP:C	3:P:306:GLY:N	2.67	0.52
2:H:51:TRP:CE2	2:H:242:ILE:HG12	2.45	0.52
1:L:1(C):GLU:HG3	5:H:454:HOH:O	1.79	0.52
3:P:313:LEU:CD1	3:P:314:ALA:N	2.73	0.51
3:P:348:ASN:C	3:P:348:ASN:HD22	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.73	0.51
2:H:61:GLU:HG2	2:H:87:LYS:CA	2.40	0.51
3:P:316:THR:HG22	3:P:320:SER:CA	2.41	0.51
3:P:346:ALA:CB	3:P:349:PHE:CD2	2.94	0.51
2:H:182:CYS:SG	2:H:225:TYR:HB2	2.50	0.51
2:H:134:TYR:N	2:H:134:TYR:HD1	2.08	0.51
3:P:310:ARG:HA	3:P:351:ARG:NH1	2.25	0.51
2:H:95:ASN:ND2	2:H:97(A):GLU:HB2	2.26	0.50
2:H:236:LYS:O	2:H:240:LYS:N	2.37	0.50
2:H:124:PRO:CG	2:H:210:MET:CE	2.84	0.50
2:H:240:LYS:HD3	3:P:336:ASP:HA	1.93	0.50
2:H:191:CYS:O	2:H:194:ASP:HB2	2.11	0.50
2:H:200:VAL:HG12	2:H:209:GLN:HA	1.93	0.50
3:P:325:TRP:HZ3	3:P:363:TYR:HE2	1.60	0.50
1:L:14(G):LEU:HD11	2:H:202:LYS:HD3	1.93	0.50
2:H:165:ARG:HG2	2:H:165:ARG:NH1	2.10	0.50
2:H:240:LYS:CD	3:P:336:ASP:HA	2.41	0.50
3:P:306:GLY:C	3:P:308:GLU:N	2.68	0.49
3:P:325:TRP:CG	3:P:345:LEU:HD23	2.47	0.49
2:H:208:TYR:O	2:H:210:MET:HG2	2.11	0.49
3:P:362:CYS:SG	3:P:363:TYR:O	2.70	0.49
2:H:52:VAL:HG21	2:H:108:LEU:HD21	1.94	0.49
2:H:86:GLU:HB3	2:H:107:LYS:O	2.12	0.49
2:H:195:SER:C	2:H:197:GLY:H	2.19	0.49
3:P:360:ALA:O	3:P:374:CYS:N	2.45	0.49
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.37	0.49
3:P:325:TRP:HZ3	3:P:363:TYR:CE2	2.31	0.49
1:L:14(B):THR:C	1:L:14(D):ARG:N	2.69	0.49
2:H:32:MET:HB3	2:H:67:ARG:HB2	1.95	0.49
2:H:158:VAL:HG22	2:H:160:LEU:CD2	2.42	0.49
3:P:328:GLU:O	3:P:328:GLU:HG2	2.13	0.49
1:L:14(D):ARG:O	1:L:14(H):GLU:HG2	2.13	0.49
3:P:316:THR:CG2	3:P:320:SER:H	2.26	0.49
2:H:32:MET:CE	2:H:141:TRP:CD2	2.96	0.48
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.48	0.48
2:H:68:ILE:HG22	2:H:118:ILE:CG1	2.34	0.48
2:H:94:TYR:O	2:H:94:TYR:CG	2.66	0.48
3:P:316:THR:HG1	3:P:372:GLU:CD	2.19	0.48
2:H:98:ASN:OD1	2:H:98:ASN:C	2.54	0.48
3:P:305:ARG:O	3:P:352:ASN:ND2	2.46	0.48
2:H:200:VAL:CG2	5:H:540:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ARG:NH2	3:P:370:ASP:OD1	2.46	0.48
3:P:371:PHE:CD1	3:P:372:GLU:N	2.81	0.48
2:H:22:ALA:CB	2:H:155:LEU:HD23	2.44	0.48
2:H:165:ARG:N	2:H:166:PRO:HD2	2.28	0.48
1:L:14:ASP:CG	2:H:137:ARG:HH22	2.22	0.48
2:H:175:ARG:NH2	3:P:358:GLU:HB2	2.29	0.48
2:H:107:LYS:C	2:H:107:LYS:HD2	2.38	0.48
2:H:124:PRO:CB	2:H:210:MET:CE	2.91	0.48
3:P:313:LEU:HB3	3:P:350:CYS:HB2	1.96	0.48
2:H:165:ARG:HH21	2:H:178:ASP:HA	1.78	0.48
3:P:302:VAL:N	3:P:377:ASN:O	2.46	0.48
2:H:35:ARG:CG	2:H:41:LEU:HD21	2.43	0.47
2:H:56:ALA:HB2	2:H:103:ILE:O	2.12	0.47
2:H:60(D):TRP:HE3	2:H:60(F):LYS:CE	2.27	0.47
2:H:60(B):PRO:HG2	2:H:96:TRP:CE3	2.49	0.47
3:P:354:ASP:HB3	3:P:356:ASP:H	1.78	0.47
2:H:182:CYS:SG	2:H:225:TYR:CB	3.02	0.47
2:H:201:MET:HE3	2:H:210:MET:SD	2.55	0.47
2:H:215:TRP:HE3	2:H:216:GLY:CA	2.26	0.47
2:H:59:LEU:HD11	2:H:106:MET:CE	2.43	0.47
2:H:164:GLU:C	2:H:166:PRO:HD2	2.40	0.47
2:H:164:GLU:O	2:H:167:VAL:N	2.48	0.47
2:H:175:ARG:HH11	2:H:175:ARG:HD3	1.37	0.47
2:H:70:LYS:HG2	2:H:80:GLU:OE1	2.15	0.47
3:P:355:GLY:O	3:P:356:ASP:C	2.57	0.47
1:L:1(C):GLU:OE1	5:H:454:HOH:O	2.04	0.47
2:H:67:ARG:HG2	2:H:82:ILE:CD1	2.45	0.46
3:P:316:THR:OG1	3:P:372:GLU:HB2	2.13	0.46
3:P:325:TRP:N	3:P:347:GLU:O	2.44	0.46
2:H:221(A):ARG:HB2	2:H:224:LYS:HG3	1.97	0.46
2:H:154:VAL:O	2:H:156:GLN:HG2	2.14	0.46
2:H:195:SER:OG	4:H:1:OG7:O2	2.31	0.46
2:H:242:ILE:C	2:H:244:GLN:N	2.71	0.46
3:P:309:TYR:HD1	3:P:309:TYR:O	1.98	0.46
2:H:115:SER:OG	2:H:118:ILE:HD12	2.16	0.46
2:H:242:ILE:HG22	2:H:243:ASP:N	2.30	0.46
1:L:4:ARG:HD3	2:H:26:MET:O	2.16	0.46
2:H:98:ASN:O	2:H:99:LEU:CB	2.62	0.46
3:P:343:VAL:HG11	3:P:353:PRO:CA	2.16	0.46
3:P:358:GLU:OE1	3:P:358:GLU:CA	2.62	0.46
1:L:1(C):GLU:HG3	1:L:1:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:HIS:HA	2:H:60:LEU:O	2.16	0.46
2:H:94:TYR:HE1	2:H:99:LEU:HD12	1.81	0.46
3:P:312:ARG:HA	3:P:349:PHE:CD1	2.51	0.46
2:H:43:GLY:O	2:H:44:ALA:HB2	2.16	0.46
3:P:315:VAL:C	3:P:316:THR:O	2.59	0.45
3:P:332:ALA:O	3:P:335:LYS:HD2	2.15	0.45
2:H:240:LYS:NZ	3:P:337:GLN:O	2.49	0.45
2:H:91:HIS:ND1	2:H:91:HIS:C	2.75	0.45
2:H:236:LYS:HD3	3:P:338:ASP:CB	2.37	0.45
3:P:316:THR:OG1	3:P:372:GLU:CD	2.58	0.45
2:H:215:TRP:HE3	2:H:216:GLY:N	2.14	0.45
2:H:89:TYR:O	2:H:104:ALA:HA	2.16	0.45
2:H:103:ILE:HG23	2:H:237:TRP:CZ3	2.52	0.45
3:P:316:THR:CG2	3:P:320:SER:CA	2.95	0.45
1:L:7:PHE:O	1:L:8:GLU:C	2.60	0.45
1:L:14:ASP:O	1:L:14(C):GLU:HG3	2.17	0.45
2:H:91:HIS:HB2	2:H:103:ILE:HG22	1.99	0.45
1:L:12:LEU:HD12	1:L:12:LEU:HA	1.73	0.44
3:P:352:ASN:HD22	3:P:359:GLY:C	2.25	0.44
2:H:35:ARG:HG2	2:H:41:LEU:CD2	2.47	0.44
3:P:313:LEU:HD23	3:P:376:LEU:CD1	2.47	0.44
3:P:331:LYS:HD2	3:P:331:LYS:HA	1.58	0.44
2:H:98:ASN:ND2	2:H:175:ARG:NH1	2.66	0.44
1:L:1(C):GLU:HB2	5:H:454:HOH:O	2.08	0.44
2:H:68:ILE:HD12	2:H:112:VAL:HG11	1.99	0.44
2:H:158:VAL:CG2	2:H:160:LEU:HD21	2.44	0.44
3:P:304:ASP:C	3:P:306:GLY:H	2.21	0.44
3:P:376:LEU:HD13	3:P:376:LEU:N	2.32	0.44
2:H:60(H):PHE:CG	2:H:64:LEU:HD21	2.53	0.44
3:P:337:GLN:HB3	3:P:339:PHE:CE1	2.53	0.43
3:P:347:GLU:HB2	3:P:348:ASN:H	1.29	0.43
2:H:200:VAL:HG21	5:H:540:HOH:O	2.18	0.43
2:H:17:VAL:O	2:H:18:GLU:HB2	2.17	0.43
3:P:316:THR:HG23	3:P:320:SER:H	1.82	0.43
2:H:74:THR:OG1	2:H:75:ARG:N	2.52	0.43
2:H:235:LYS:O	2:H:238:ILE:HB	2.18	0.43
2:H:60(D):TRP:O	2:H:60(E):ASP:C	2.61	0.43
2:H:50:ARG:HG2	5:H:429:HOH:O	2.19	0.43
1:L:14(K):ILE:H	1:L:14(K):ILE:HG12	1.72	0.43
2:H:71:HIS:CE1	2:H:154:VAL:CG1	3.01	0.43
3:P:324:ALA:O	3:P:326:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:HG22	2:H:144:LEU:O	2.18	0.43
2:H:31:VAL:CG1	2:H:32:MET:N	2.82	0.42
2:H:81:LYS:HD2	2:H:118:ILE:HD13	2.01	0.42
3:P:324:ALA:C	3:P:326:SER:N	2.74	0.42
3:P:340:ASN:HA	3:P:341:PRO:HD3	1.57	0.42
2:H:215:TRP:CE2	2:H:227:PHE:HB2	2.54	0.42
2:H:123:LEU:HA	2:H:124:PRO:HD3	1.95	0.42
3:P:361:TRP:CD1	3:P:361:TRP:N	2.87	0.42
3:P:378:TYR:N	3:P:378:TYR:CD1	2.86	0.42
2:H:60:LEU:HD23	2:H:94:TYR:CD2	2.53	0.42
3:P:313:LEU:CD1	3:P:315:VAL:H	2.26	0.42
2:H:32:MET:CG	2:H:40:LEU:HD12	2.49	0.42
3:P:313:LEU:HD23	3:P:376:LEU:HD11	2.00	0.42
3:P:353:PRO:HD2	3:P:361:TRP:CZ2	2.54	0.42
2:H:16:ILE:HG12	2:H:194:ASP:OD2	2.19	0.42
2:H:38:GLN:CD	5:H:415:HOH:O	2.62	0.42
3:P:377:ASN:HD22	3:P:377:ASN:C	2.28	0.42
2:H:92:PRO:HG2	3:P:337:GLN:NE2	2.35	0.41
2:H:195:SER:HA	2:H:213:VAL:CG1	2.50	0.41
3:P:309:TYR:CD1	3:P:309:TYR:O	2.73	0.41
2:H:91:HIS:ND1	2:H:92:PRO:CD	2.83	0.41
1:L:14:ASP:HB2	2:H:26:MET:HE3	2.02	0.41
2:H:36(A):SER:CA	2:H:37:PRO:C	2.86	0.41
2:H:100:ASP:O	2:H:101:ARG:CB	2.57	0.41
3:P:302:VAL:HG21	3:P:376:LEU:CB	2.51	0.41
1:L:14:ASP:N	1:L:14(C):GLU:CG	2.83	0.41
2:H:34:PHE:HB3	2:H:65:LEU:HD23	2.03	0.41
2:H:97(A):GLU:HB3	2:H:98:ASN:H	1.47	0.41
3:P:301:CYS:SG	3:P:302:VAL:N	2.92	0.41
2:H:91:HIS:ND1	2:H:92:PRO:N	2.68	0.41
2:H:215:TRP:HB2	2:H:216:GLY:H	1.56	0.41
3:P:335:LYS:HG2	3:P:336:ASP:N	2.32	0.41
1:L:1(C):GLU:HB2	2:H:47:ILE:O	2.21	0.41
2:H:156:GLN:C	2:H:157:VAL:HG13	2.45	0.41
3:P:303:PRO:HB2	3:P:304:ASP:H	1.51	0.41
3:P:322:CYS:HA	3:P:362:CYS:SG	2.60	0.41
2:H:60(D):TRP:CE3	2:H:60(F):LYS:HE3	2.55	0.40
3:P:351:ARG:C	3:P:353:PRO:HD3	2.46	0.40
1:L:14:ASP:CG	2:H:137:ARG:NH2	2.77	0.40
2:H:51:TRP:NE1	2:H:242:ILE:HG12	2.36	0.40
3:P:309:TYR:OH	3:P:313:LEU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:ARG:HE	2:H:35:ARG:HB2	1.72	0.40
2:H:50:ARG:NH1	2:H:111:PRO:HD3	2.36	0.40
2:H:81:LYS:HD2	2:H:118:ILE:CD1	2.52	0.40
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.85	0.40
2:H:215:TRP:CB	4:H:1:0G7:O	2.66	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	
1	L	28/36 (78%)	20 (71%)	6 (21%)	2 (7%)	1	6
2	H	247/259 (95%)	213 (86%)	32 (13%)	2 (1%)	16	45
3	P	77/79 (98%)	58 (75%)	15 (20%)	4 (5%)	1	11
All	All	352/374 (94%)	291 (83%)	53 (15%)	8 (2%)	5	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	61	GLU
3	P	303	PRO
3	P	305	ARG
3	P	327	SER
1	L	1(B)	ALA
1	L	14(A)	LYS
3	P	347	GLU
2	H	213	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	27/31 (87%)	23 (85%)	4 (15%)	3	13
2	H	218/225 (97%)	155 (71%)	63 (29%)	0	2
3	P	65/65 (100%)	38 (58%)	27 (42%)	0	0
All	All	310/321 (97%)	216 (70%)	94 (30%)	0	1

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
1	L	10	LYS
1	L	11	SER
1	L	12	LEU
2	H	16	ILE
2	H	20	SER
2	H	21	ASP
2	H	24	ILE
2	H	27	SER
2	H	33	LEU
2	H	34	PHE
2	H	35	ARG
2	H	36	LYS
2	H	36(A)	SER
2	H	40	LEU
2	H	41	LEU
2	H	45	SER
2	H	48	SER
2	H	50	ARG
2	H	53	LEU
2	H	62	ASN
2	H	63	ASP
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	70	LYS

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Mol	Chain	Res	Type
2	H	72	SER
2	H	73	ARG
2	H	75	ARG
2	H	77	GLU
2	H	77(A)	ARG
2	H	79	ILE
2	H	80	GLU
2	H	81	LYS
2	H	83	SER
2	H	84	MET
2	H	86	GLU
2	H	87	LYS
2	H	88	ILE
2	H	90	ILE
2	H	94	TYR
2	H	103	ILE
2	H	107	LYS
2	H	109	LYS
2	H	121	VAL
2	H	126	ARG
2	H	128	THR
2	H	130	LEU
2	H	137	ARG
2	H	138	VAL
2	H	139	THR
2	H	143	ASN
2	H	145	LYS
2	H	151	GLN
2	H	153	SER
2	H	154	VAL
2	H	160	LEU
2	H	165	ARG
2	H	173	ARG
2	H	176	ILE
2	H	177	THR
2	H	187	ARG
2	H	210	MET
2	H	224	LYS
2	H	235	LYS
2	H	241	VAL
2	H	242	ILE
3	P	301	CYS

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Mol	Chain	Res	Type
3	P	302	VAL
3	P	304	ASP
3	P	308	GLU
3	P	309	TYR
3	P	312	ARG
3	P	313	LEU
3	P	315	VAL
3	P	317	THR
3	P	320	SER
3	P	323	LEU
3	P	329	GLN
3	P	331	LYS
3	P	334	SER
3	P	335	LYS
3	P	337	GLN
3	P	338	ASP
3	P	340	ASN
3	P	345	LEU
3	P	347	GLU
3	P	348	ASN
3	P	351	ARG
3	P	357	GLU
3	P	362	CYS
3	P	364	VAL
3	P	375	ASN
3	P	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	151	GLN
2	H	156	GLN
2	H	204(B)	ASN
2	H	244	GLN
3	P	329	GLN
3	P	340	ASN
3	P	348	ASN
3	P	375	ASN
3	P	377	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	0G7	H	1	-	30,31,32	1.87	1 (3%)	36,41,42	1.49	6 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0G7	H	1	-	-	7/31/41/43	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	0G7	C3-C2	-9.51	1.26	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G7	O1-C1-N2	3.69	129.56	122.96
4	H	1	0G7	C1-CA1-N1	-3.11	104.01	112.50
4	H	1	0G7	CA-C-N1	-2.98	112.83	118.74
4	H	1	0G7	O-C-N1	2.60	126.06	121.38
4	H	1	0G7	CB1-CA1-N1	2.45	106.61	103.02
4	H	1	0G7	CG2-CD3-NE	2.18	118.31	112.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

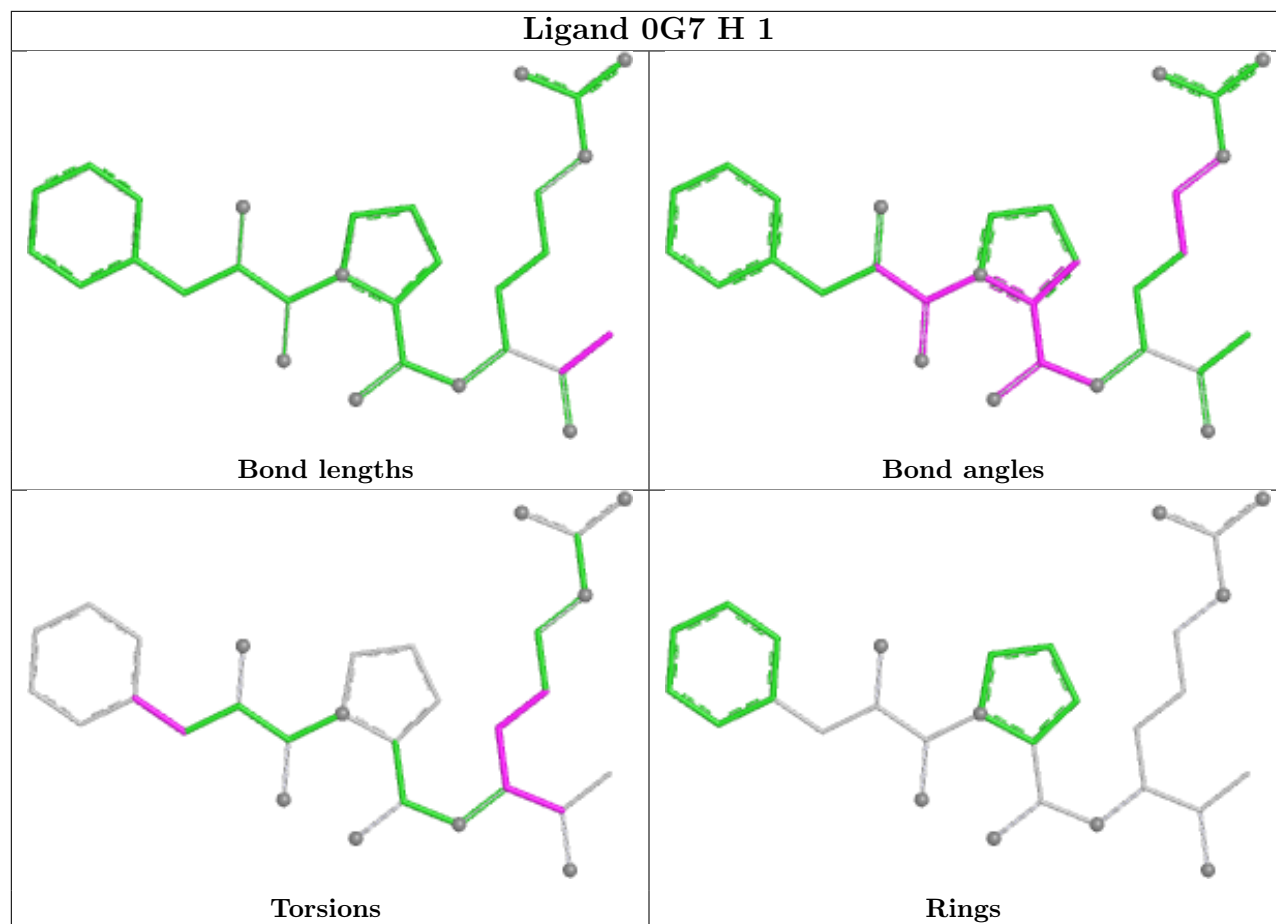
Mol	Chain	Res	Type	Atoms
4	H	1	0G7	C3-C2-CA2-N2
4	H	1	0G7	N2-CA2-CB2-CG2
4	H	1	0G7	C2-CA2-CB2-CG2
4	H	1	0G7	CA2-CB2-CG2-CD3
4	H	1	0G7	CA-CB-CG-CD1
4	H	1	0G7	CA-CB-CG-CD2
4	H	1	0G7	O2-C2-CA2-N2

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	0G7	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.