



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:00 PM UTC

PDB ID : 2HPQ / pdb_00002hpq
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

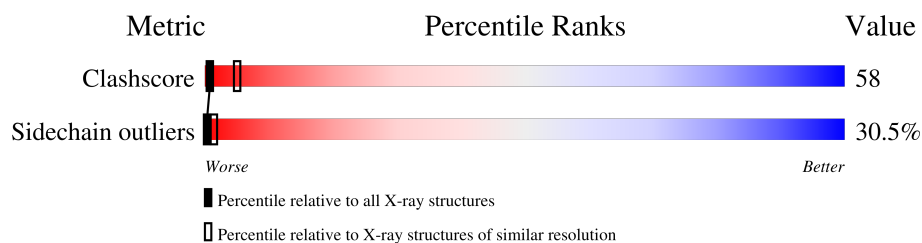
1 Overall quality at a glance

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)
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 3029 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 (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	30	Total	C	N	O	S	9	0	0
			240	150	39	50	1			

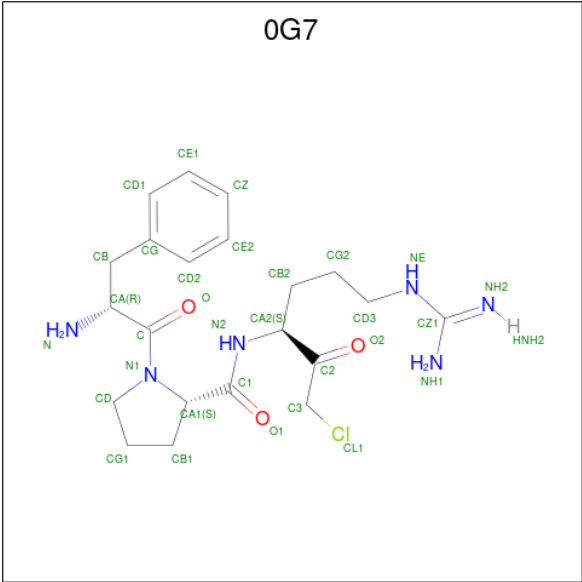
- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	251	Total	C	N	O	S	38	0	0
			2029	1294	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	46	0	0
			608	379	107	116	6			

- 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.

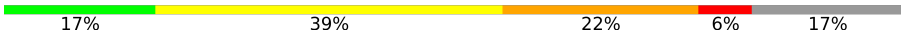
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	19	Total	O	0	0
			19	19		
5	H	79	Total	O	0	0
			79	79		
5	P	24	Total	O	0	0
			24	24		

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.

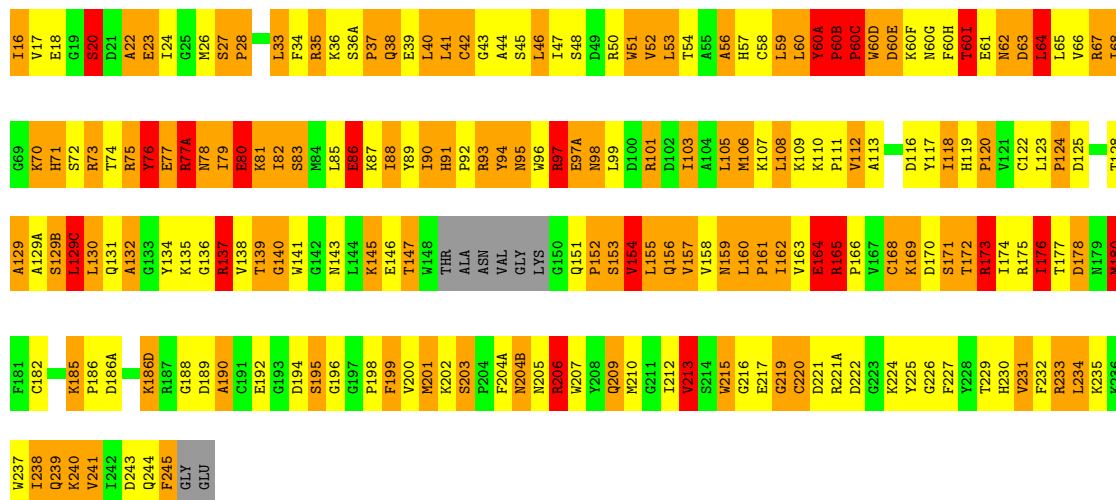
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 

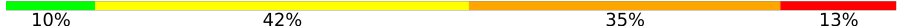


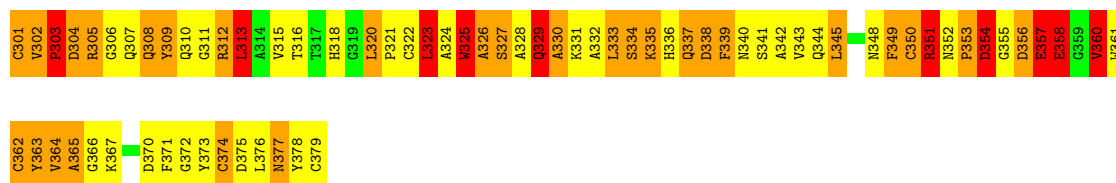
• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 



• Molecule 3: Prothrombin

Chain P: 



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	123.60Å 123.60Å 101.10Å 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}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3029	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	1.24	1/242 (0.4%)	2.49	21/322 (6.5%)
2	H	1.32	2/2081 (0.1%)	2.79	231/2811 (8.2%)
3	P	1.37	3/624 (0.5%)	2.60	59/848 (7.0%)
All	All	1.32	6/2947 (0.2%)	2.72	311/3981 (7.8%)

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
3	P	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	374	CYS	CA-C	-13.16	1.36	1.52
3	P	374	CYS	N-CA	6.29	1.53	1.45
2	H	172	THR	CA-CB	5.77	1.63	1.53
1	L	14(K)	ILE	C-O	5.48	1.30	1.24
3	P	360	VAL	C-N	-5.31	1.28	1.33
2	H	217	GLU	N-CA	5.08	1.52	1.46

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	NE-CZ-NH2	13.95	131.76	119.20
3	P	338	ASP	CA-CB-CG	-12.21	100.39	112.60
2	H	27	SER	O-C-N	12.08	131.44	121.17
2	H	180	MET	O-C-N	12.00	136.89	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	379	CYS	N-CA-CB	11.49	130.04	110.50
3	P	335	LYS	N-CA-C	11.28	124.91	111.82
2	H	57	HIS	CA-CB-CG	11.17	124.97	113.80
2	H	164	GLU	CB-CG-CD	11.12	131.50	112.60
2	H	91	HIS	CA-CB-CG	-11.10	102.70	113.80
2	H	93	ARG	NE-CZ-NH1	-10.97	110.53	121.50
2	H	154	VAL	CA-C-O	10.95	130.07	121.09
2	H	172	THR	N-CA-C	10.53	123.97	108.60
2	H	151	GLN	OE1-CD-NE2	10.38	132.98	122.60
2	H	161	PRO	CB-CA-C	-10.32	96.36	110.60
2	H	101	ARG	NE-CZ-NH2	-10.14	110.07	119.20
2	H	71	HIS	CA-CB-CG	-10.00	103.80	113.80
2	H	158	VAL	CA-C-O	-9.98	110.70	121.28
2	H	40	LEU	CA-C-O	-9.93	109.50	120.92
2	H	160	LEU	O-C-N	9.82	131.10	121.57
2	H	229	THR	CA-C-O	-9.78	110.21	121.16
2	H	204(A)	PHE	N-CA-C	9.68	122.84	111.71
2	H	68	ILE	CA-C-O	-9.61	109.69	120.84
2	H	122	CYS	CA-C-O	-9.57	110.03	120.36
2	H	77(A)	ARG	NE-CZ-NH1	9.54	131.04	121.50
2	H	190	ALA	N-CA-C	-9.54	96.76	110.59
2	H	153	SER	CA-C-N	9.53	132.78	122.11
2	H	153	SER	C-N-CA	9.53	132.78	122.11
2	H	50	ARG	O-C-N	9.38	131.86	122.19
2	H	78	ASN	CA-C-O	-9.34	108.57	119.59
2	H	77(A)	ARG	NH1-CZ-NH2	-9.31	107.19	119.30
3	P	374	CYS	O-C-N	9.29	133.79	123.10
3	P	323	LEU	CB-CA-C	9.28	124.84	109.53
2	H	28	PRO	N-CA-CB	9.16	112.31	103.51
2	H	77	GLU	CB-CG-CD	9.14	128.13	112.60
3	P	320	LEU	N-CA-C	-9.03	97.86	110.31
2	H	20	SER	N-CA-C	8.92	120.02	108.34
3	P	375	ASP	N-CA-C	8.91	124.06	108.56
2	H	201	MET	CA-C-O	-8.58	110.30	120.60
3	P	321	PRO	CA-C-O	-8.51	111.27	121.48
2	H	205	ASN	OD1-CG-ND2	8.47	131.07	122.60
2	H	170	ASP	N-CA-C	-8.45	101.97	113.30
2	H	70	LYS	O-C-N	-8.34	113.54	122.96
3	P	323	LEU	N-CA-C	-8.33	95.96	109.96
3	P	374	CYS	CB-CA-C	8.32	123.57	109.50
2	H	186(A)	ASP	CA-CB-CG	-8.30	104.30	112.60
2	H	58	CYS	N-CA-C	-8.24	102.68	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	NE-CZ-NH1	-8.19	113.31	121.50
3	P	351	ARG	CA-CB-CG	8.18	130.46	114.10
2	H	173	ARG	NE-CZ-NH2	-8.12	111.89	119.20
2	H	213	VAL	CB-CA-C	8.13	120.21	111.35
2	H	70	LYS	N-CA-C	8.06	122.40	110.48
2	H	63	ASP	O-C-N	8.03	132.15	122.27
2	H	60(I)	THR	CA-CB-OG1	-8.00	97.60	109.60
3	P	356	ASP	CA-CB-CG	-7.88	104.72	112.60
2	H	59	LEU	N-CA-CB	-7.86	100.13	110.59
2	H	28	PRO	CA-C-O	-7.84	108.03	119.00
3	P	362	CYS	CA-C-O	-7.82	112.38	121.06
2	H	212	ILE	CA-C-O	-7.81	111.01	121.32
2	H	154	VAL	CB-CA-C	-7.80	100.40	111.40
2	H	40	LEU	O-C-N	7.77	132.17	123.16
2	H	123	LEU	N-CA-C	-7.77	99.96	109.83
2	H	222	ASP	CA-CB-CG	-7.75	104.85	112.60
2	H	172	THR	CA-CB-OG1	-7.69	98.06	109.60
2	H	118	ILE	N-CA-C	7.67	120.13	107.24
2	H	70	LYS	CA-C-O	7.63	130.25	121.47
2	H	168	CYS	O-C-N	7.61	129.91	122.07
2	H	143	ASN	O-C-N	7.60	132.70	122.59
2	H	216	GLY	CA-C-O	-7.60	113.26	122.15
2	H	153	SER	CA-CB-OG	-7.60	95.91	111.10
3	P	321	PRO	CB-CA-C	-7.54	100.22	110.85
2	H	65	LEU	CA-C-O	-7.51	112.34	121.06
2	H	78	ASN	OD1-CG-ND2	7.46	130.06	122.60
2	H	77(A)	ARG	N-CA-CB	7.45	123.07	110.49
2	H	16	ILE	CA-C-O	-7.43	108.17	120.80
2	H	165	ARG	CD-NE-CZ	7.41	134.78	124.40
2	H	129(C)	LEU	N-CA-C	7.39	122.47	113.38
2	H	140	GLY	CA-C-N	7.39	133.75	122.37
2	H	140	GLY	C-N-CA	7.39	133.75	122.37
2	H	206	ARG	CD-NE-CZ	-7.36	114.10	124.40
2	H	56	ALA	O-C-N	7.28	131.23	122.27
2	H	163	VAL	CA-C-N	7.26	131.14	120.90
2	H	163	VAL	C-N-CA	7.26	131.14	120.90
2	H	159	ASN	N-CA-CB	7.25	121.96	110.65
2	H	186(D)	LYS	N-CA-CB	7.25	122.80	111.56
2	H	64	LEU	N-CA-C	7.22	121.21	110.52
2	H	28	PRO	O-C-N	7.21	132.11	122.30
2	H	220	CYS	N-CA-CB	7.14	121.86	110.86
2	H	65	LEU	N-CA-CB	-7.14	98.25	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ARG	NE-CZ-NH1	7.13	128.63	121.50
3	P	325	TRP	O-C-N	7.12	132.05	122.59
2	H	151	GLN	CG-CD-NE2	-7.10	105.75	116.40
3	P	364	VAL	CA-C-O	7.09	129.64	120.78
2	H	152	PRO	CA-C-N	7.08	135.22	122.06
2	H	152	PRO	C-N-CA	7.08	135.22	122.06
3	P	332	ALA	CA-C-O	7.03	128.18	120.80
2	H	146	GLU	N-CA-CB	6.97	120.41	109.82
1	L	1(A)	ASP	N-CA-C	-6.92	104.71	113.02
2	H	151	GLN	CA-C-O	6.89	127.47	120.03
2	H	137	ARG	CA-C-O	6.86	127.51	120.24
2	H	64	LEU	N-CA-CB	-6.86	99.49	110.46
2	H	185	LYS	N-CA-C	-6.86	100.33	110.20
2	H	229	THR	O-C-N	6.82	131.21	122.89
2	H	42	CYS	CB-CA-C	-6.79	98.09	112.82
2	H	23	GLU	N-CA-C	-6.78	102.08	110.41
2	H	200	VAL	O-C-N	6.78	130.49	122.36
3	P	339	PHE	CA-C-O	6.74	128.70	121.16
2	H	160	LEU	CA-C-O	-6.72	112.41	120.41
3	P	339	PHE	CB-CA-C	6.72	121.14	109.65
2	H	203	SER	N-CA-C	6.71	119.36	109.50
2	H	176	ILE	N-CA-CB	6.67	117.99	110.72
1	L	13	GLU	CA-C-N	-6.65	110.34	121.39
1	L	13	GLU	C-N-CA	-6.65	110.34	121.39
2	H	80	GLU	O-C-N	-6.60	115.50	122.96
1	L	8	GLU	CA-CB-CG	6.59	127.28	114.10
2	H	129(C)	LEU	N-CA-CB	-6.55	100.76	110.53
2	H	118	ILE	CB-CA-C	-6.55	102.94	110.73
2	H	97	ARG	N-CA-CB	6.54	120.27	110.53
2	H	113	ALA	CA-C-O	-6.53	113.75	120.54
2	H	42	CYS	O-C-N	6.53	130.32	122.75
3	P	321	PRO	O-C-N	6.52	131.28	123.06
2	H	18	GLU	N-CA-C	6.51	120.63	111.52
1	L	5	PRO	CA-C-N	-6.51	111.85	122.65
1	L	5	PRO	C-N-CA	-6.51	111.85	122.65
2	H	118	ILE	CA-C-O	-6.51	113.93	120.31
2	H	216	GLY	CA-C-N	-6.50	113.95	123.05
2	H	216	GLY	C-N-CA	-6.50	113.95	123.05
2	H	37	PRO	O-C-N	6.49	133.43	121.10
2	H	129(A)	ALA	N-CA-C	6.47	118.42	111.36
3	P	323	LEU	CA-C-N	6.47	133.91	121.54
3	P	323	LEU	C-N-CA	6.47	133.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(C)	GLU	CB-CA-C	-6.47	97.54	110.42
2	H	27	SER	CA-C-O	-6.45	113.73	121.22
2	H	162	ILE	CA-C-N	6.44	131.17	123.19
2	H	162	ILE	C-N-CA	6.44	131.17	123.19
2	H	42	CYS	CA-C-N	-6.43	115.60	122.67
2	H	42	CYS	C-N-CA	-6.43	115.60	122.67
2	H	52	VAL	N-CA-CB	-6.43	101.67	112.47
3	P	336	HIS	O-C-N	6.40	130.54	122.22
2	H	145	LYS	O-C-N	6.39	130.69	123.27
3	P	303	PRO	O-C-N	-6.39	114.01	122.64
2	H	231	VAL	N-CA-CB	6.34	119.17	110.54
3	P	320	LEU	N-CA-CB	6.33	120.56	110.11
2	H	79	ILE	CB-CA-C	6.33	117.11	110.91
2	H	60(A)	TYR	O-C-N	6.33	133.12	121.10
2	H	60(A)	TYR	CA-C-O	-6.31	111.51	120.16
2	H	165	ARG	NH1-CZ-NH2	-6.31	111.09	119.30
2	H	46	LEU	CB-CA-C	-6.30	100.70	110.78
2	H	137	ARG	CB-CA-C	6.29	120.20	110.14
2	H	86	GLU	CB-CA-C	6.29	119.08	109.34
3	P	375	ASP	N-CA-CB	-6.26	102.12	110.57
2	H	156	GLN	CA-C-O	-6.24	113.87	120.80
3	P	353	PRO	O-C-N	6.21	130.56	122.24
2	H	152	PRO	N-CA-C	-6.21	101.51	111.38
2	H	51	TRP	N-CA-C	6.20	119.51	109.40
2	H	220	CYS	CB-CA-C	-6.19	103.75	111.43
2	H	77	GLU	CG-CD-OE1	6.18	132.61	118.40
2	H	77(A)	ARG	CG-CD-NE	6.18	125.59	112.00
2	H	82	ILE	CA-C-O	-6.17	113.23	120.75
2	H	77(A)	ARG	CA-C-O	-6.16	111.70	120.51
2	H	86	GLU	N-CA-CB	-6.16	101.47	110.40
2	H	124	PRO	CA-C-O	-6.11	114.41	121.86
2	H	93	ARG	O-C-N	6.10	130.06	122.19
3	P	337	GLN	OE1-CD-NE2	6.09	128.69	122.60
2	H	165	ARG	NE-CZ-NH1	6.09	127.59	121.50
2	H	41	LEU	O-C-N	6.08	130.30	122.03
3	P	374	CYS	CA-C-O	-6.08	114.10	121.28
3	P	318	HIS	O-C-N	6.06	129.57	122.24
2	H	53	LEU	CB-CA-C	6.05	120.64	109.70
3	P	313	LEU	N-CA-C	-6.01	101.65	110.42
2	H	106	MET	CA-C-N	-5.98	114.82	122.77
2	H	106	MET	C-N-CA	-5.98	114.82	122.77
2	H	219	GLY	N-CA-C	-5.98	101.37	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	PHE	O-C-N	5.94	129.93	123.10
2	H	204(A)	PHE	CB-CA-C	-5.93	99.66	110.63
2	H	168	CYS	CA-C-N	5.88	130.00	120.60
2	H	168	CYS	C-N-CA	5.88	130.00	120.60
3	P	304	ASP	CA-CB-CG	5.85	118.45	112.60
2	H	192	GLU	CB-CG-CD	5.84	122.52	112.60
2	H	178	ASP	CA-CB-CG	5.83	118.43	112.60
2	H	209	GLN	CA-C-O	-5.83	113.72	120.49
2	H	171	SER	N-CA-C	-5.82	105.08	111.82
1	L	14(I)	SER	N-CA-C	-5.81	105.29	112.38
2	H	129(B)	SER	O-C-N	5.81	131.99	122.70
3	P	350	CYS	CB-CA-C	5.81	119.58	109.65
3	P	360	VAL	O-C-N	5.80	129.72	122.59
2	H	77(A)	ARG	CA-C-N	-5.80	113.56	122.60
2	H	77(A)	ARG	C-N-CA	-5.80	113.56	122.60
2	H	153	SER	N-CA-CB	-5.79	101.37	110.46
2	H	66	VAL	CA-C-O	-5.76	113.92	120.67
3	P	313	LEU	CA-C-O	-5.75	115.20	120.95
3	P	333	LEU	N-CA-C	-5.75	104.70	110.97
2	H	83	SER	CA-C-O	-5.73	114.75	121.46
1	L	14(G)	LEU	CA-C-O	-5.73	114.81	120.82
2	H	122	CYS	CA-CB-SG	5.72	127.56	114.40
2	H	160	LEU	CA-C-N	5.70	125.89	120.31
2	H	160	LEU	C-N-CA	5.70	125.89	120.31
2	H	230	HIS	CA-CB-CG	-5.70	108.10	113.80
2	H	206	ARG	NE-CZ-NH2	5.69	124.32	119.20
3	P	330	ALA	N-CA-C	-5.69	106.42	113.19
2	H	201	MET	O-C-N	5.65	130.16	123.33
2	H	199	PHE	N-CA-C	-5.64	96.50	107.62
3	P	329	GLN	CA-C-O	-5.64	113.00	119.60
2	H	185	LYS	CB-CA-C	-5.64	99.08	109.51
3	P	304	ASP	O-C-N	5.64	130.09	122.59
2	H	163	VAL	N-CA-C	5.63	116.06	108.17
2	H	198	PRO	CA-C-O	-5.62	115.00	121.86
3	P	357	GLU	CA-CB-CG	5.61	125.33	114.10
2	H	90	ILE	N-CA-CB	5.61	117.77	111.21
3	P	357	GLU	O-C-N	5.61	130.05	122.59
2	H	60(B)	PRO	N-CA-C	5.61	117.54	110.70
2	H	71	HIS	CA-C-N	5.60	128.66	120.71
2	H	71	HIS	C-N-CA	5.60	128.66	120.71
2	H	132	ALA	CB-CA-C	5.59	118.22	109.84
1	L	2	GLY	CA-C-N	5.58	130.78	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2	GLY	C-N-CA	5.58	130.78	122.86
2	H	200	VAL	CA-C-O	-5.57	115.69	121.93
2	H	205	ASN	N-CA-C	5.56	119.35	112.24
2	H	60(C)	PRO	CB-CA-C	5.55	121.53	112.26
2	H	112	VAL	O-C-N	5.54	129.00	122.69
2	H	140	GLY	CA-C-O	-5.54	116.23	121.60
2	H	93	ARG	CD-NE-CZ	-5.51	116.69	124.40
2	H	103	ILE	CA-C-O	-5.50	114.90	121.28
2	H	227	PHE	CA-C-O	-5.50	114.79	121.28
2	H	129	ALA	CA-C-O	5.48	128.35	120.51
2	H	194	ASP	O-C-N	5.47	129.35	122.23
3	P	312	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	H	50	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	H	233	ARG	NE-CZ-NH2	5.45	124.11	119.20
3	P	301	CYS	CB-CA-C	-5.44	99.76	110.10
2	H	172	THR	OG1-CB-CG2	5.43	120.17	109.30
2	H	230	HIS	CB-CA-C	5.42	120.21	111.05
2	H	105	LEU	CA-C-O	-5.42	114.51	120.36
3	P	354	ASP	N-CA-C	5.42	122.33	110.80
2	H	122	CYS	CA-C-N	5.40	128.15	120.49
2	H	122	CYS	C-N-CA	5.40	128.15	120.49
2	H	98	ASN	CA-CB-CG	-5.39	107.21	112.60
3	P	305	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	H	231	VAL	O-C-N	5.36	127.06	121.87
1	L	1(B)	ALA	N-CA-C	-5.35	99.41	110.80
3	P	363	TYR	N-CA-C	-5.35	103.83	110.41
2	H	154	VAL	N-CA-CB	5.35	119.78	110.96
3	P	365	ALA	O-C-N	5.35	129.70	122.59
2	H	216	GLY	N-CA-C	-5.35	104.47	111.37
1	L	4	ARG	CD-NE-CZ	-5.33	116.93	124.40
3	P	358	GLU	O-C-N	5.33	129.68	122.59
2	H	157	VAL	CA-C-O	-5.33	114.43	120.67
2	H	180	MET	CA-C-O	-5.32	115.03	120.99
2	H	164	GLU	CB-CA-C	-5.32	101.14	109.70
2	H	53	LEU	N-CA-CB	-5.30	101.63	110.80
2	H	189	ASP	O-C-N	5.30	129.09	123.42
1	L	14(K)	ILE	N-CA-C	5.30	116.07	110.72
3	P	360	VAL	N-CA-C	-5.30	102.24	109.55
2	H	38	GLN	N-CA-C	-5.29	101.53	109.15
2	H	189	ASP	CA-CB-CG	5.28	117.88	112.60
3	P	338	ASP	N-CA-C	5.28	122.04	110.80
2	H	120	PRO	CB-CA-C	-5.27	103.09	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	151	GLN	CA-CB-CG	-5.27	103.56	114.10
1	L	10	LYS	N-CA-C	-5.26	106.91	113.38
3	P	315	VAL	O-C-N	5.26	129.14	122.57
2	H	204(B)	ASN	N-CA-CB	-5.26	102.70	111.06
1	L	14(G)	LEU	CB-CA-C	5.25	119.13	110.88
3	P	329	GLN	N-CA-CB	5.25	118.21	110.33
2	H	60(I)	THR	CA-CB-CG2	5.25	119.42	110.50
2	H	80	GLU	CA-C-N	5.25	130.40	123.05
2	H	80	GLU	C-N-CA	5.25	130.40	123.05
2	H	204(B)	ASN	CB-CA-C	5.21	117.16	109.29
2	H	195	SER	CA-CB-OG	-5.21	100.68	111.10
1	L	1(A)	ASP	CA-CB-CG	-5.21	107.39	112.60
2	H	67	ARG	CA-C-O	-5.21	114.93	120.40
2	H	95	ASN	OD1-CG-ND2	5.21	127.81	122.60
2	H	129(B)	SER	CA-C-O	-5.20	113.18	119.27
3	P	349	PHE	CB-CA-C	-5.20	100.73	109.83
3	P	326	ALA	O-C-N	5.20	128.65	122.26
2	H	77	GLU	N-CA-CB	-5.19	101.72	110.49
2	H	134	TYR	CB-CG-CD1	5.19	128.59	120.80
2	H	238	ILE	CA-C-N	-5.19	112.57	122.53
2	H	238	ILE	C-N-CA	-5.19	112.57	122.53
1	L	1	CYS	CA-C-N	5.19	131.58	121.41
1	L	1	CYS	C-N-CA	5.19	131.58	121.41
2	H	235	LYS	CB-CA-C	-5.19	102.51	110.81
2	H	215	TRP	CA-C-O	-5.18	115.80	121.14
3	P	339	PHE	CA-C-N	5.17	128.69	121.24
3	P	339	PHE	C-N-CA	5.17	128.69	121.24
3	P	352	ASN	N-CA-CB	-5.17	102.82	110.99
2	H	155	LEU	CA-C-O	-5.17	115.33	120.96
2	H	81	LYS	CB-CG-CD	5.16	123.17	111.30
2	H	60(C)	PRO	N-CA-C	-5.15	106.34	113.81
2	H	22	ALA	CA-C-O	-5.15	115.39	121.16
1	L	14(H)	GLU	CB-CG-CD	5.14	121.34	112.60
3	P	304	ASP	CB-CA-C	5.13	120.63	110.42
2	H	22	ALA	N-CA-C	-5.12	102.71	110.28
2	H	117	TYR	N-CA-CB	-5.11	102.43	110.46
2	H	161	PRO	CA-C-O	-5.10	115.79	122.12
2	H	18	GLU	CB-CG-CD	5.10	121.27	112.60
2	H	147	THR	O-C-N	5.10	129.38	123.41
2	H	162	ILE	CA-CB-CG2	5.09	119.16	110.50
2	H	37	PRO	CA-C-N	-5.09	113.72	121.66
2	H	37	PRO	C-N-CA	-5.09	113.72	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	194	ASP	CA-CB-CG	-5.08	107.52	112.60
3	P	337	GLN	O-C-N	5.07	128.81	122.43
2	H	219	GLY	CA-C-N	5.06	128.41	121.33
2	H	219	GLY	C-N-CA	5.06	128.41	121.33
2	H	80	GLU	CB-CG-CD	5.05	121.19	112.60
2	H	156	GLN	CB-CG-CD	5.05	121.19	112.60
2	H	239	GLN	N-CA-CB	5.05	118.15	110.42
2	H	186(D)	LYS	N-CA-C	-5.05	101.07	108.79
1	L	14	ASP	N-CA-CB	5.03	117.94	110.29
2	H	76	TYR	CA-C-O	-5.02	115.70	120.92
2	H	44	ALA	CA-C-O	-5.02	115.94	121.31
2	H	111	PRO	O-C-N	5.01	128.97	122.91
2	H	140	GLY	O-C-N	5.00	129.50	123.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	303	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	240	0	236	22	0
2	H	2029	0	2002	205	0
3	P	608	0	553	101	0
4	H	30	0	28	12	0
5	H	79	0	0	2	0
5	L	19	0	0	0	0
5	P	24	0	0	1	0
All	All	3029	0	2819	317	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 58.

All (317) 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:169:LYS:NZ	2:H:169:LYS:HB3	1.65	1.10
3:P:333:LEU:HD21	3:P:366:GLY:O	1.49	1.10
2:H:35:ARG:HG3	2:H:35:ARG:HH11	1.17	1.08
3:P:333:LEU:HD12	3:P:363:TYR:CD1	1.89	1.08
1:L:3:LEU:HD13	2:H:206:ARG:HG3	1.35	1.07
3:P:309:TYR:CD2	3:P:376:LEU:HD21	1.89	1.07
2:H:169:LYS:HB3	2:H:169:LYS:HZ3	1.20	1.03
2:H:42:CYS:HB3	2:H:195:SER:O	1.57	1.01
2:H:195:SER:CB	4:H:1:OG7:C3	2.42	0.98
2:H:195:SER:OG	4:H:1:OG7:C2	2.12	0.97
3:P:365:ALA:HB3	3:P:370:ASP:HB3	1.44	0.95
3:P:310:GLN:HA	3:P:351:ARG:HH12	1.29	0.94
2:H:203:SER:HB3	2:H:204(B):ASN:HD22	1.33	0.92
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.51	0.91
3:P:309:TYR:CE2	3:P:376:LEU:HD21	2.05	0.90
3:P:358:GLU:HA	3:P:358:GLU:OE1	1.68	0.90
2:H:76:TYR:CE1	2:H:77(A):ARG:HA	2.08	0.89
2:H:195:SER:OG	4:H:1:OG7:C3	2.21	0.88
3:P:350:CYS:HB3	3:P:360:VAL:HG23	1.57	0.86
2:H:206:ARG:NH1	2:H:206:ARG:HG2	1.87	0.86
2:H:76:TYR:HE1	2:H:77(A):ARG:HA	1.38	0.86
2:H:128:THR:HG22	2:H:210:MET:HE1	1.57	0.85
3:P:324:ALA:O	3:P:327:SER:HB2	1.77	0.85
3:P:324:ALA:O	3:P:327:SER:N	2.09	0.84
3:P:339:PHE:CG	3:P:353:PRO:HB2	2.13	0.84
2:H:23:GLU:HG3	2:H:26:MET:HE3	1.58	0.83
2:H:86:GLU:HB3	2:H:107:LYS:O	1.77	0.83
3:P:350:CYS:HB3	3:P:360:VAL:CG2	2.07	0.83
2:H:68:ILE:HG22	2:H:118:ILE:HD13	1.62	0.82
2:H:195:SER:CB	4:H:1:OG7:C2	2.57	0.82
2:H:60(I):THR:C	2:H:62:ASN:H	1.87	0.81
3:P:313:LEU:HD23	3:P:376:LEU:HD12	1.63	0.81
3:P:345:LEU:HD11	3:P:353:PRO:HG3	1.61	0.81
2:H:86:GLU:HG2	2:H:107:LYS:HD3	1.61	0.80
2:H:35:ARG:HH11	2:H:35:ARG:CG	1.95	0.80
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.16	0.80
2:H:35:ARG:HG3	2:H:35:ARG:NH1	1.92	0.78
3:P:313:LEU:HD23	3:P:376:LEU:CD1	2.14	0.77
3:P:365:ALA:HB3	3:P:370:ASP:CB	2.14	0.77
3:P:309:TYR:OH	3:P:313:LEU:HB2	1.84	0.76
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.68	0.76
2:H:206:ARG:HH11	2:H:206:ARG:CG	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:TYR:CE1	2:H:96:TRP:HB3	2.20	0.76
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.68	0.74
2:H:68:ILE:HG22	2:H:118:ILE:CD1	2.18	0.73
3:P:302:VAL:O	3:P:378:TYR:HA	1.88	0.73
2:H:232:PHE:O	2:H:234:LEU:N	2.22	0.73
2:H:168:CYS:O	2:H:171:SER:HB3	1.89	0.73
3:P:310:GLN:HA	3:P:351:ARG:NH1	2.03	0.72
3:P:330:ALA:O	3:P:334:SER:HB2	1.88	0.72
2:H:97(A):GLU:OE2	2:H:175:ARG:NH1	2.22	0.72
2:H:68:ILE:CG2	2:H:118:ILE:HD13	2.19	0.72
2:H:60(B):PRO:O	2:H:60(E):ASP:N	2.19	0.72
2:H:195:SER:HB2	4:H:1:OG7:O2	1.89	0.72
2:H:201:MET:HE3	2:H:210:MET:HG3	1.72	0.71
2:H:35:ARG:NE	5:H:463:HOH:O	2.23	0.71
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.73	0.70
2:H:171:SER:O	2:H:224:LYS:HE2	1.91	0.70
2:H:130:LEU:C	2:H:131:GLN:HG2	2.16	0.70
3:P:333:LEU:CD1	3:P:363:TYR:CD1	2.72	0.70
2:H:60(I):THR:O	2:H:62:ASN:N	2.24	0.70
2:H:169:LYS:NZ	2:H:169:LYS:CB	2.49	0.70
2:H:177:THR:HG23	2:H:180:MET:HE3	1.71	0.70
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.25	0.69
3:P:356:ASP:OD2	3:P:373:TYR:OH	2.11	0.68
1:L:10:LYS:HB2	1:L:12:LEU:HD12	1.76	0.68
2:H:237:TRP:O	2:H:241:VAL:HG12	1.92	0.68
3:P:303:PRO:O	3:P:305:ARG:N	2.25	0.68
2:H:204(B):ASN:OD1	2:H:206:ARG:HD3	1.92	0.68
2:H:60(B):PRO:HG2	2:H:96:TRP:CH2	2.29	0.67
2:H:195:SER:HB2	4:H:1:OG7:C2	2.23	0.67
2:H:233:ARG:C	2:H:234:LEU:HD23	2.19	0.67
3:P:301:CYS:HB2	3:P:377:ASN:O	1.94	0.67
2:H:232:PHE:C	2:H:234:LEU:H	2.01	0.67
2:H:195:SER:HB2	4:H:1:OG7:C3	2.23	0.67
3:P:335:LYS:NZ	5:P:551:HOH:O	2.27	0.67
2:H:60(I):THR:C	2:H:62:ASN:N	2.54	0.66
2:H:22:ALA:HB3	2:H:155:LEU:HB3	1.77	0.65
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.79	0.65
3:P:304:ASP:O	3:P:307:GLN:HB2	1.97	0.65
3:P:361:TRP:HA	3:P:372:GLY:O	1.97	0.64
2:H:169:LYS:HB3	2:H:169:LYS:HZ2	1.58	0.64
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:LYS:HE3	2:H:72:SER:O	1.97	0.64
3:P:312:ARG:HA	3:P:349:PHE:CD1	2.32	0.64
3:P:309:TYR:CD2	3:P:376:LEU:CD2	2.74	0.64
3:P:309:TYR:CZ	3:P:311:GLY:HA3	2.31	0.64
3:P:360:VAL:CG2	3:P:374:CYS:HB2	2.28	0.64
3:P:354:ASP:HB3	3:P:356:ASP:H	1.63	0.63
1:L:14:ASP:CG	2:H:137:ARG:HH22	2.07	0.62
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	1.99	0.62
1:L:14:ASP:H	1:L:14(C):GLU:HG3	1.63	0.62
2:H:41:LEU:HD11	2:H:64:LEU:HD11	1.81	0.62
3:P:349:PHE:HB2	3:P:351:ARG:HE	1.65	0.62
2:H:80:GLU:OE2	2:H:82:ILE:HD13	1.99	0.62
2:H:232:PHE:C	2:H:234:LEU:N	2.57	0.61
3:P:329:GLN:H	3:P:329:GLN:HE21	1.48	0.61
1:L:7:PHE:O	1:L:8:GLU:C	2.42	0.61
3:P:312:ARG:O	3:P:313:LEU:C	2.43	0.61
3:P:329:GLN:H	3:P:329:GLN:NE2	1.97	0.61
2:H:91:HIS:CE1	2:H:92:PRO:HD2	2.35	0.61
3:P:309:TYR:HD2	3:P:376:LEU:HD21	1.58	0.60
2:H:33:LEU:HD21	2:H:106:MET:CE	2.32	0.59
1:L:6:LEU:HD11	2:H:116:ASP:HB3	1.85	0.59
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.85	0.59
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.18	0.58
3:P:323:LEU:CD2	3:P:363:TYR:HB2	2.32	0.58
2:H:60:LEU:C	2:H:60:LEU:HD12	2.29	0.58
3:P:303:PRO:O	3:P:304:ASP:C	2.46	0.58
2:H:20:SER:O	2:H:156:GLN:HA	2.04	0.58
1:L:14(B):THR:O	1:L:14(C):GLU:C	2.47	0.57
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.39	0.57
3:P:311:GLY:O	3:P:349:PHE:CD2	2.58	0.56
3:P:316:THR:N	3:P:320:LEU:O	2.38	0.56
2:H:61:GLU:HG3	2:H:88:ILE:HG13	1.88	0.56
2:H:128:THR:O	2:H:129(C):LEU:HB2	2.05	0.56
2:H:36:LYS:O	2:H:38:GLN:HG2	2.06	0.56
2:H:174:ILE:HD12	2:H:215:TRP:CZ3	2.41	0.56
2:H:130:LEU:O	2:H:131:GLN:HG2	2.06	0.56
2:H:96:TRP:CE3	2:H:96:TRP:C	2.84	0.56
2:H:219:GLY:HA3	2:H:221(A):ARG:HG3	1.88	0.56
3:P:350:CYS:HB3	3:P:360:VAL:HG21	1.85	0.56
2:H:51:TRP:CH2	2:H:245:PHE:O	2.59	0.55
2:H:34:PHE:HZ	2:H:38:GLN:HB3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:LYS:HG2	2:H:176:ILE:HG12	1.88	0.55
3:P:311:GLY:N	3:P:351:ARG:HH22	2.04	0.55
2:H:85:LEU:HD22	2:H:106:MET:CB	2.29	0.55
2:H:95:ASN:ND2	2:H:97(A):GLU:HB2	2.21	0.55
2:H:128:THR:HG22	2:H:210:MET:CE	2.33	0.55
2:H:91:HIS:HB2	2:H:103:ILE:CG2	2.37	0.55
2:H:36:LYS:HB2	2:H:63:ASP:O	2.08	0.54
3:P:325:TRP:CE3	3:P:325:TRP:HA	2.41	0.54
2:H:17:VAL:O	2:H:188:GLY:HA2	2.08	0.54
1:L:14(B):THR:O	1:L:14(D):ARG:N	2.41	0.53
2:H:60:LEU:HD12	2:H:60(B):PRO:HD3	1.90	0.53
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.23	0.53
1:L:14(B):THR:OG1	2:H:137:ARG:NH1	2.41	0.53
2:H:60(B):PRO:O	2:H:60(C):PRO:C	2.50	0.53
2:H:91:HIS:CE1	2:H:93:ARG:H	2.25	0.53
3:P:340:ASN:C	3:P:342:ALA:H	2.17	0.53
2:H:54:THR:HG21	2:H:106:MET:HE3	1.89	0.53
2:H:139:THR:HG22	2:H:155:LEU:HD11	1.91	0.53
3:P:360:VAL:HG22	3:P:374:CYS:HB2	1.90	0.53
2:H:36(A):SER:HA	2:H:37:PRO:C	2.33	0.53
2:H:206:ARG:HG2	2:H:206:ARG:HH11	1.57	0.53
3:P:356:ASP:CG	3:P:373:TYR:OH	2.52	0.52
2:H:91:HIS:HB2	2:H:103:ILE:HG22	1.90	0.52
2:H:169:LYS:CG	2:H:176:ILE:HG12	2.40	0.52
3:P:329:GLN:C	3:P:331:LYS:H	2.16	0.52
2:H:33:LEU:HD21	2:H:106:MET:SD	2.50	0.52
3:P:325:TRP:NE1	3:P:349:PHE:O	2.43	0.52
2:H:60:LEU:CD1	2:H:60(B):PRO:HD3	2.40	0.52
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.08	0.52
3:P:361:TRP:O	3:P:362:CYS:HB3	2.10	0.52
2:H:60(I):THR:HG22	2:H:62:ASN:HB2	1.92	0.52
3:P:335:LYS:O	3:P:335:LYS:HG3	2.10	0.52
2:H:51:TRP:CZ2	2:H:245:PHE:O	2.63	0.52
2:H:96:TRP:O	2:H:96:TRP:HE3	1.92	0.52
3:P:313:LEU:HD23	3:P:376:LEU:HD11	1.91	0.51
2:H:60:LEU:HD12	2:H:60(A):TYR:N	2.26	0.51
1:L:14:ASP:CG	2:H:137:ARG:NH2	2.69	0.51
2:H:97:ARG:NH2	3:P:370:ASP:OD1	2.44	0.51
3:P:356:ASP:CG	3:P:373:TYR:HH	2.17	0.51
1:L:14:ASP:N	1:L:14(C):GLU:HG3	2.25	0.50
3:P:329:GLN:C	3:P:331:LYS:N	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:N	2:H:166:PRO:HD2	2.27	0.50
2:H:203:SER:CB	2:H:204(B):ASN:HD22	2.16	0.50
3:P:306:GLY:C	3:P:308:GLN:H	2.19	0.50
2:H:165:ARG:HG2	2:H:176:ILE:HD11	1.92	0.50
2:H:41:LEU:HD11	2:H:64:LEU:CD1	2.42	0.50
2:H:98:ASN:OD1	2:H:98:ASN:C	2.50	0.50
2:H:71:HIS:CD2	2:H:154:VAL:HG11	2.46	0.50
3:P:327:SER:HB3	3:P:330:ALA:H	1.75	0.50
3:P:324:ALA:O	3:P:327:SER:CB	2.55	0.49
2:H:86:GLU:HG2	2:H:107:LYS:CD	2.37	0.49
2:H:169:LYS:HE3	5:H:545:HOH:O	2.11	0.49
3:P:310:GLN:CA	3:P:351:ARG:HH12	2.14	0.49
3:P:329:GLN:HE21	3:P:329:GLN:N	2.09	0.49
2:H:118:ILE:HG22	2:H:118:ILE:O	2.12	0.49
2:H:135:LYS:HA	2:H:161:PRO:HA	1.95	0.49
3:P:367:LYS:O	3:P:370:ASP:HB2	2.13	0.49
2:H:85:LEU:CD2	2:H:106:MET:HB3	2.34	0.49
2:H:129:ALA:O	2:H:130:LEU:HB2	2.13	0.49
2:H:86:GLU:N	2:H:107:LYS:O	2.43	0.48
2:H:33:LEU:CD1	2:H:64:LEU:HG	2.43	0.48
2:H:177:THR:HB	3:P:357:GLU:OE2	2.13	0.48
3:P:328:ALA:HB3	3:P:329:GLN:HE21	1.79	0.48
3:P:334:SER:OG	3:P:339:PHE:CE2	2.64	0.48
3:P:360:VAL:O	3:P:373:TYR:HD1	1.97	0.48
2:H:35:ARG:HB2	2:H:41:LEU:HD21	1.94	0.48
2:H:59:LEU:HD11	2:H:106:MET:HE3	1.96	0.48
3:P:311:GLY:H	3:P:351:ARG:HH22	1.62	0.48
3:P:355:GLY:O	3:P:356:ASP:C	2.56	0.48
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.76	0.47
3:P:309:TYR:CE2	3:P:376:LEU:HD11	2.49	0.47
3:P:354:ASP:OD2	3:P:361:TRP:CZ2	2.67	0.47
2:H:93:ARG:HD2	3:P:361:TRP:CH2	2.50	0.47
3:P:305:ARG:C	3:P:307:GLN:N	2.72	0.47
2:H:91:HIS:CG	2:H:92:PRO:HD2	2.48	0.47
2:H:185:LYS:HB3	2:H:186:PRO:HD2	1.96	0.47
2:H:56:ALA:HB2	2:H:103:ILE:O	2.15	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.50	0.47
2:H:202:LYS:HD2	2:H:207:TRP:CE2	2.49	0.47
3:P:339:PHE:HA	3:P:353:PRO:O	2.14	0.47
2:H:215:TRP:CE3	4:H:1:OG7:HD2	2.49	0.47
3:P:365:ALA:HB3	3:P:370:ASP:CG	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:LEU:HD11	2:H:106:MET:CE	2.45	0.47
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.50	0.46
2:H:124:PRO:HD3	2:H:209:GLN:O	2.16	0.46
2:H:86:GLU:CG	2:H:107:LYS:HD3	2.39	0.46
1:L:10:LYS:CB	1:L:12:LEU:HD12	2.44	0.46
2:H:237:TRP:O	2:H:241:VAL:CG1	2.63	0.46
2:H:99:LEU:HD12	2:H:215:TRP:HB3	1.97	0.46
3:P:301:CYS:HB2	3:P:302:VAL:H	1.27	0.46
3:P:309:TYR:CD1	3:P:309:TYR:C	2.93	0.46
2:H:93:ARG:HH11	2:H:93:ARG:HD3	1.28	0.46
1:L:4:ARG:HE	1:L:7:PHE:HB2	1.81	0.46
2:H:60(B):PRO:C	2:H:60(E):ASP:H	2.18	0.46
2:H:195:SER:HA	2:H:213:VAL:HB	1.97	0.46
2:H:125:ASP:OD1	2:H:128:THR:N	2.32	0.46
3:P:303:PRO:HB2	3:P:304:ASP:H	1.38	0.46
3:P:316:THR:HB	3:P:320:LEU:H	1.80	0.46
2:H:60(D):TRP:O	2:H:60(E):ASP:C	2.59	0.45
2:H:186(D):LYS:HB3	2:H:186(D):LYS:HE2	1.77	0.45
3:P:309:TYR:O	3:P:351:ARG:NH1	2.49	0.45
1:L:6:LEU:CD1	2:H:116:ASP:HB3	2.46	0.45
2:H:16:ILE:HD11	2:H:139:THR:C	2.41	0.45
2:H:61:GLU:HG3	2:H:88:ILE:CG1	2.46	0.45
2:H:138:VAL:HG11	2:H:190:ALA:HB2	1.97	0.45
3:P:344:GLN:O	3:P:351:ARG:HD3	2.17	0.45
3:P:324:ALA:C	3:P:326:ALA:N	2.72	0.45
2:H:99:LEU:CD1	2:H:215:TRP:HB3	2.47	0.45
2:H:74:THR:HG22	2:H:75:ARG:N	2.32	0.45
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.75	0.44
2:H:220:CYS:O	2:H:221:ASP:HB3	2.16	0.44
2:H:68:ILE:HD13	2:H:112:VAL:HG11	1.99	0.44
2:H:178:ASP:N	3:P:357:GLU:OE2	2.47	0.44
2:H:73:ARG:HG3	2:H:141:TRP:HB3	1.99	0.44
2:H:182:CYS:HA	2:H:226:GLY:O	2.17	0.44
1:L:14:ASP:OD2	1:L:14(C):GLU:HG2	2.16	0.44
3:P:305:ARG:O	3:P:307:GLN:N	2.50	0.44
3:P:350:CYS:CB	3:P:360:VAL:HG21	2.48	0.44
2:H:56:ALA:O	2:H:59:LEU:HB2	2.18	0.44
2:H:56:ALA:CB	2:H:90:ILE:HG23	2.47	0.44
2:H:172:THR:OG1	2:H:173:ARG:N	2.51	0.44
2:H:95:ASN:O	2:H:99:LEU:N	2.51	0.43
2:H:85:LEU:CD2	2:H:106:MET:CB	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:312:ARG:HA	3:P:349:PHE:CG	2.53	0.43
2:H:33:LEU:HD12	2:H:41:LEU:HD12	2.00	0.43
2:H:195:SER:OG	4:H:1:OG7:CB2	2.67	0.43
3:P:324:ALA:C	3:P:326:ALA:H	2.26	0.43
3:P:333:LEU:HB2	3:P:363:TYR:CE1	2.53	0.43
2:H:23:GLU:HB2	2:H:26:MET:HB2	1.98	0.43
2:H:204(B):ASN:HD21	2:H:206:ARG:H	1.66	0.43
3:P:334:SER:OG	3:P:339:PHE:HE2	2.01	0.43
2:H:52:VAL:CG2	2:H:108:LEU:HD21	2.48	0.43
2:H:60(B):PRO:CD	2:H:60(C):PRO:HD2	2.49	0.43
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ3	2.54	0.43
2:H:155:LEU:HD12	2:H:155:LEU:HA	1.83	0.43
2:H:165:ARG:N	2:H:166:PRO:CD	2.82	0.43
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ2	2.53	0.43
2:H:152:PRO:HB2	2:H:154:VAL:O	2.19	0.43
2:H:59:LEU:HD21	2:H:106:MET:CE	2.49	0.42
2:H:239:GLN:C	2:H:241:VAL:N	2.75	0.42
3:P:358:GLU:HB3	3:P:373:TYR:CE1	2.54	0.42
2:H:28:PRO:HB2	2:H:119:HIS:H	1.83	0.42
2:H:71:HIS:CD2	2:H:154:VAL:CG1	3.01	0.42
2:H:76:TYR:CD1	2:H:77(A):ARG:HA	2.53	0.42
2:H:239:GLN:O	2:H:240:LYS:C	2.59	0.42
3:P:310:GLN:HA	3:P:351:ARG:HH22	1.84	0.42
3:P:325:TRP:CD2	3:P:345:LEU:HG	2.54	0.42
2:H:89:TYR:HB2	2:H:105:LEU:HB2	2.01	0.42
2:H:43:GLY:O	2:H:196:GLY:HA3	2.19	0.42
2:H:52:VAL:HG23	2:H:108:LEU:HD21	2.01	0.42
2:H:60(I):THR:CG2	2:H:62:ASN:HB2	2.49	0.42
2:H:75:ARG:HH11	2:H:75:ARG:HD3	1.53	0.42
2:H:80:GLU:OE2	2:H:82:ILE:CD1	2.67	0.42
2:H:47:ILE:HG21	2:H:53:LEU:HD22	2.01	0.42
3:P:339:PHE:CD1	3:P:353:PRO:HB2	2.52	0.42
2:H:195:SER:CB	4:H:1:OG7:O2	2.57	0.42
1:L:3:LEU:HD12	1:L:8:GLU:HG2	2.01	0.42
2:H:89:TYR:HB2	2:H:105:LEU:CB	2.49	0.42
2:H:16:ILE:HD11	2:H:140:GLY:N	2.35	0.42
3:P:322:CYS:SG	3:P:350:CYS:SG	3.18	0.41
2:H:215:TRP:CD2	4:H:1:OG7:HD2	2.55	0.41
1:L:3:LEU:HB3	1:L:9:LYS:HE3	2.02	0.41
2:H:86:GLU:HB2	2:H:109:LYS:HA	2.02	0.41
2:H:171:SER:HB2	2:H:225:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:323:LEU:HD23	3:P:363:TYR:HB2	2.00	0.41
3:P:361:TRP:HB3	3:P:373:TYR:CD1	2.56	0.41
1:L:14(K):ILE:H	1:L:14(K):ILE:HG12	1.75	0.41
1:L:14(G):LEU:HD13	1:L:14(G):LEU:HA	1.92	0.41
2:H:46:LEU:O	2:H:120:PRO:HA	2.21	0.41
2:H:51:TRP:CZ3	2:H:107:LYS:HB2	2.54	0.41
3:P:340:ASN:C	3:P:342:ALA:N	2.77	0.41
2:H:96:TRP:C	2:H:96:TRP:HE3	2.25	0.41
2:H:131:GLN:O	2:H:132:ALA:C	2.63	0.41
3:P:313:LEU:O	3:P:349:PHE:HA	2.20	0.41
2:H:185:LYS:HA	2:H:185:LYS:HD3	1.81	0.41
2:H:195:SER:OG	4:H:1:0G7:CA2	2.69	0.41
3:P:324:ALA:O	3:P:326:ALA:N	2.53	0.41
2:H:86:GLU:CB	2:H:107:LYS:O	2.59	0.41
2:H:164:GLU:H	2:H:164:GLU:CD	2.29	0.41
3:P:301:CYS:SG	3:P:302:VAL:N	2.90	0.41
2:H:130:LEU:CD2	2:H:162:ILE:HD13	2.42	0.41
3:P:365:ALA:HB1	3:P:366:GLY:H	1.50	0.41
3:P:302:VAL:CB	3:P:376:LEU:HD23	2.50	0.40
2:H:60:LEU:O	2:H:60:LEU:HG	2.20	0.40
2:H:98:ASN:O	2:H:99:LEU:HB2	2.21	0.40
2:H:237:TRP:O	2:H:238:ILE:C	2.64	0.40
3:P:361:TRP:CE3	3:P:362:CYS:N	2.89	0.40
2:H:51:TRP:HH2	2:H:245:PHE:O	2.02	0.40
2:H:60(B):PRO:CD	2:H:60(C):PRO:CD	3.00	0.40
2:H:78:ASN:HD22	2:H:78:ASN:HA	1.46	0.40
2:H:220:CYS:O	2:H:221:ASP:CB	2.69	0.40
2:H:60:LEU:HG	2:H:94:TYR:HE2	1.85	0.40
2:H:76:TYR:CD1	2:H:76:TYR:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	26/31 (84%)	21 (81%)	5 (19%)	1	7
2	H	219/225 (97%)	153 (70%)	66 (30%)	0	1
3	P	63/63 (100%)	40 (64%)	23 (36%)	0	1
All	All	308/319 (97%)	214 (70%)	94 (30%)	0	1

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

Mol	Chain	Res	Type
1	L	3	LEU
1	L	8	GLU
1	L	9	LYS
1	L	10	LYS
1	L	11	SER
2	H	20	SER
2	H	24	ILE
2	H	27	SER
2	H	33	LEU
2	H	35	ARG
2	H	39	GLU
2	H	40	LEU
2	H	45	SER
2	H	48	SER
2	H	60	LEU
2	H	60(A)	TYR
2	H	60(B)	PRO
2	H	60(C)	PRO
2	H	60(D)	TRP
2	H	60(E)	ASP
2	H	60(F)	LYS
2	H	60(G)	ASN
2	H	60(H)	PHE
2	H	60(I)	THR
2	H	62	ASN
2	H	64	LEU

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Mol	Chain	Res	Type
2	H	67	ARG
2	H	73	ARG
2	H	75	ARG
2	H	76	TYR
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	86	GLU
2	H	88	ILE
2	H	94	TYR
2	H	97	ARG
2	H	97(A)	GLU
2	H	101	ARG
2	H	108	LEU
2	H	110	LYS
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	137	ARG
2	H	139	THR
2	H	145	LYS
2	H	147	THR
2	H	153	SER
2	H	154	VAL
2	H	157	VAL
2	H	159	ASN
2	H	160	LEU
2	H	164	GLU
2	H	165	ARG
2	H	169	LYS
2	H	173	ARG
2	H	176	ILE
2	H	180	MET
2	H	206	ARG
2	H	213	VAL
2	H	231	VAL
2	H	234	LEU
2	H	240	LYS
2	H	241	VAL

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Mol	Chain	Res	Type
2	H	243	ASP
2	H	244	GLN
2	H	245	PHE
3	P	302	VAL
3	P	308	GLN
3	P	309	TYR
3	P	313	LEU
3	P	323	LEU
3	P	325	TRP
3	P	327	SER
3	P	329	GLN
3	P	334	SER
3	P	337	GLN
3	P	338	ASP
3	P	341	SER
3	P	343	VAL
3	P	345	LEU
3	P	348	ASN
3	P	351	ARG
3	P	354	ASP
3	P	357	GLU
3	P	358	GLU
3	P	360	VAL
3	P	364	VAL
3	P	371	PHE
3	P	377	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	156	GLN
2	H	204(B)	ASN
3	P	318	HIS
3	P	329	GLN
3	P	336	HIS
3	P	340	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	0G7	H	1	-	30,31,32	2.06	1 (3%)	36,41,42	2.27	13 (36%)

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	-	-	8/31/41/43	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	-10.40	1.24	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G7	O-C-N1	5.89	131.96	121.38
4	H	1	0G7	NH1-CZ1-NE	5.39	131.51	119.27
4	H	1	0G7	CB-CA-C	-4.17	98.28	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	0G7	O1-C1-CA1	-3.64	111.91	120.69
4	H	1	0G7	NE-CZ1-NH2	-3.60	114.50	120.67
4	H	1	0G7	O1-C1-N2	3.49	129.21	122.96
4	H	1	0G7	CB1-CA1-N1	2.94	107.33	103.02
4	H	1	0G7	O-C-CA	-2.90	114.26	119.61
4	H	1	0G7	CG2-CB2-CA2	2.61	121.82	113.80
4	H	1	0G7	CA-C-N1	-2.53	113.72	118.74
4	H	1	0G7	CB1-CG1-CD	2.23	111.10	104.90
4	H	1	0G7	C1-CA1-N1	-2.16	106.61	112.50
4	H	1	0G7	NH1-CZ1-NH2	-2.14	113.99	120.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

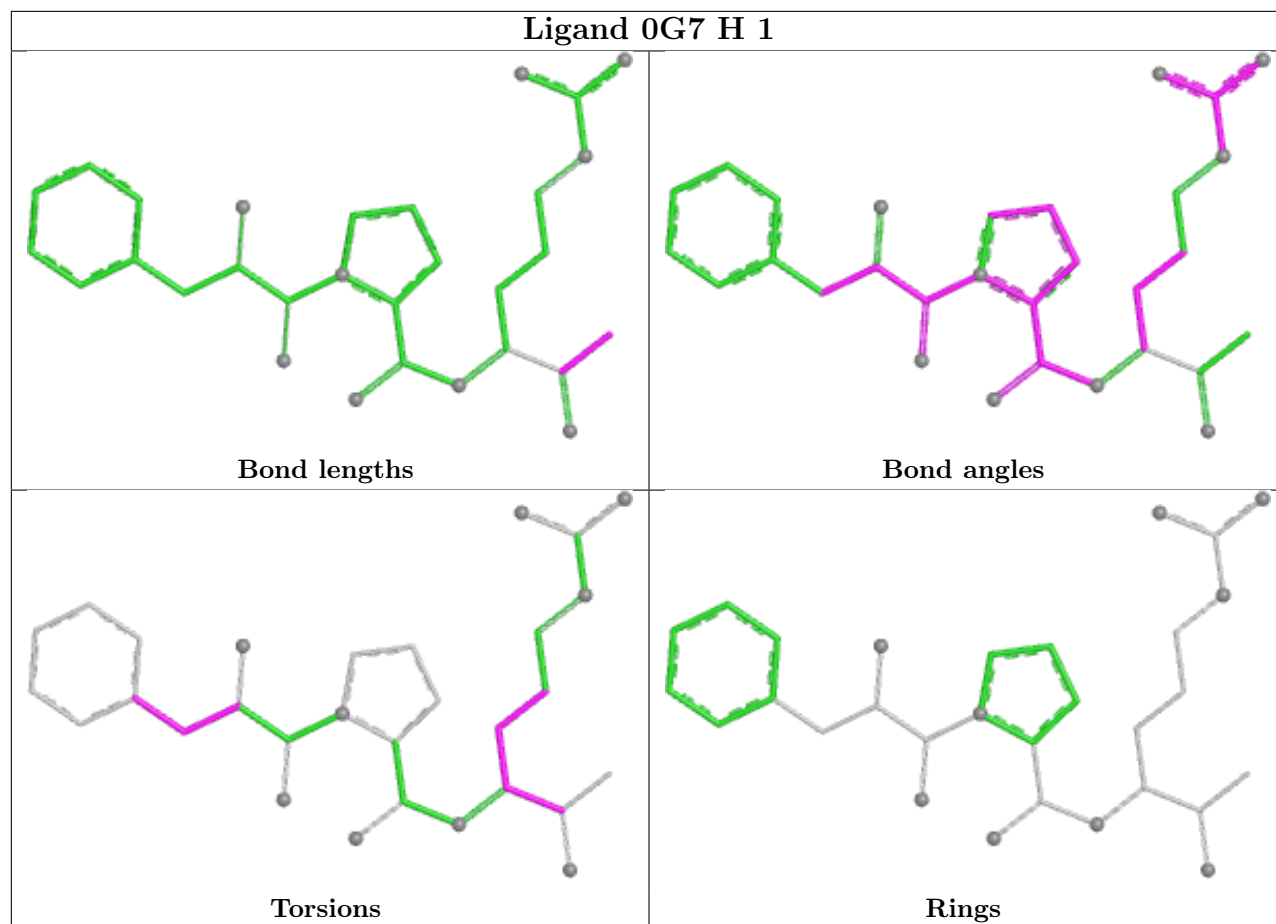
Mol	Chain	Res	Type	Atoms
4	H	1	0G7	C3-C2-CA2-N2
4	H	1	0G7	C2-CA2-CB2-CG2
4	H	1	0G7	N2-CA2-CB2-CG2
4	H	1	0G7	C-CA-CB-CG
4	H	1	0G7	CA-CB-CG-CD2
4	H	1	0G7	CA-CB-CG-CD1
4	H	1	0G7	CA2-CB2-CG2-CD3
4	H	1	0G7	O2-C2-CA2-N2

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	0G7	12	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.