



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:50 am BST

PDB ID : 2HPP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

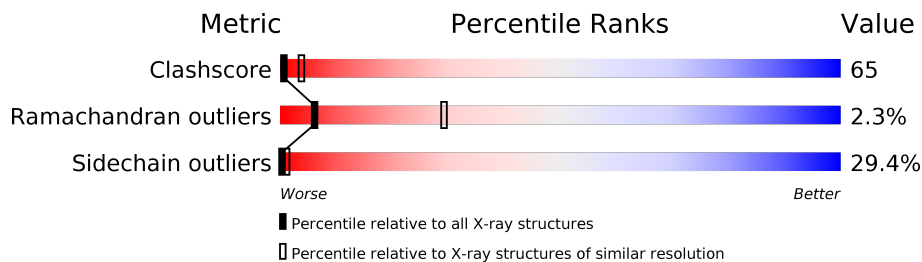
1 Overall quality at a glance i

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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	P	79	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	L	30	243	151	39	52	1	0	0	0

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

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

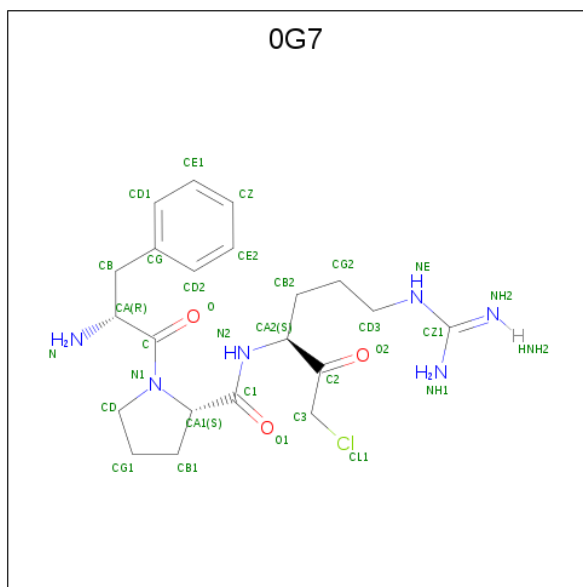
- Molecule 3 is a protein called Prothrombin.

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

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 (three-letter code: 0G7) (formula: C₂₁H₃₁ClN₆O₃).



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

- 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 i

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

Note EDS was not executed.

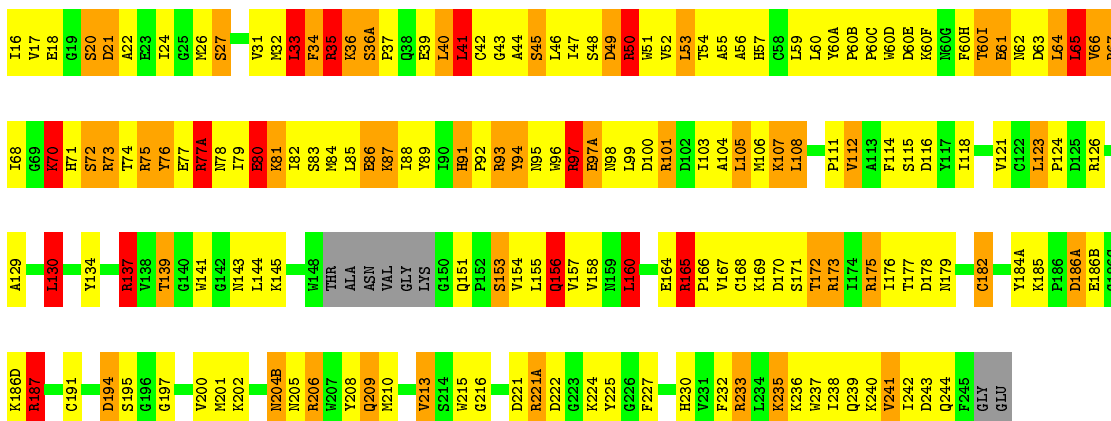
• Molecule 1: ALPHA-THROMBIN LIGHT CHAIN

Chain L: 



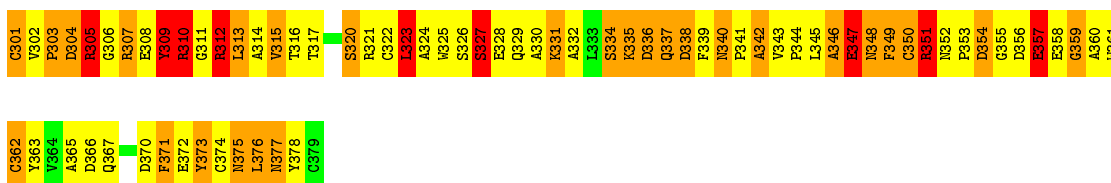
• Molecule 2: ALPHA-THROMBIN HEAVY CHAIN

Chain H: 



• Molecule 3: Prothrombin

Chain P: 



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.95	0/245	2.29	10/326 (3.1%)
2	H	0.91	0/2073	2.11	74/2800 (2.6%)
3	P	0.99	1/632 (0.2%)	2.06	19/858 (2.2%)
All	All	0.93	1/2950 (0.0%)	2.11	103/3984 (2.6%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	359	GLY	C-N	9.72	1.56	1.34

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ARG	NE-CZ-NH1	20.12	130.36	120.30
2	H	233	ARG	NE-CZ-NH2	16.56	128.58	120.30
2	H	93	ARG	NE-CZ-NH1	-12.00	114.30	120.30
2	H	93	ARG	NE-CZ-NH2	10.42	125.51	120.30
2	H	194	ASP	CB-CG-OD2	10.24	127.52	118.30
2	H	101	ARG	NE-CZ-NH2	-10.18	115.21	120.30
2	H	175	ARG	NE-CZ-NH1	-10.07	115.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	305	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	L	14(D)	ARG	NE-CZ-NH1	9.78	125.19	120.30
2	H	21	ASP	CB-CG-OD1	9.28	126.66	118.30
2	H	97	ARG	NE-CZ-NH1	8.81	124.71	120.30
2	H	170	ASP	CB-CG-OD1	8.64	126.08	118.30
2	H	187	ARG	NE-CZ-NH2	-8.57	116.01	120.30
2	H	137	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	L	14(D)	ARG	NE-CZ-NH2	-8.37	116.12	120.30
2	H	182	CYS	O-C-N	8.23	135.88	122.70
2	H	77(A)	ARG	NE-CZ-NH2	8.11	124.36	120.30
2	H	165	ARG	CD-NE-CZ	8.05	134.86	123.60
2	H	233	ARG	NH1-CZ-NH2	-7.52	111.13	119.40
3	P	321	ARG	NE-CZ-NH2	7.49	124.05	120.30
2	H	91	HIS	CA-CB-CG	-7.45	100.93	113.60
1	L	14(G)	LEU	O-C-N	7.38	134.51	122.70
3	P	310	ARG	NE-CZ-NH2	7.38	123.99	120.30
3	P	312	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	H	35	ARG	NE-CZ-NH2	7.27	123.93	120.30
2	H	206	ARG	NE-CZ-NH1	7.24	123.92	120.30
2	H	33	LEU	CB-CA-C	7.24	123.96	110.20
2	H	73	ARG	NE-CZ-NH1	7.24	123.92	120.30
2	H	153	SER	N-CA-CB	-7.12	99.82	110.50
2	H	239	GLN	N-CA-CB	7.11	123.40	110.60
2	H	33	LEU	C-N-CA	7.05	139.32	121.70
3	P	309	TYR	N-CA-CB	7.04	123.27	110.60
2	H	65	LEU	CB-CA-C	7.04	123.57	110.20
2	H	123	LEU	CB-CA-C	7.02	123.54	110.20
2	H	175	ARG	CD-NE-CZ	-6.84	114.02	123.60
2	H	143	ASN	O-C-N	6.82	133.61	122.70
3	P	342	ALA	N-CA-CB	6.71	119.49	110.10
3	P	373	TYR	O-C-N	6.69	133.41	122.70
2	H	41	LEU	CA-CB-CG	6.55	130.38	115.30
2	H	233	ARG	CD-NE-CZ	6.55	132.77	123.60
2	H	49	ASP	CB-CG-OD2	6.53	124.18	118.30
2	H	50	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	H	186(A)	ASP	CB-CG-OD1	-6.48	112.47	118.30
2	H	186(D)	LYS	N-CA-CB	6.37	122.07	110.60
2	H	101	ARG	CD-NE-CZ	6.37	132.51	123.60
2	H	209	GLN	O-C-N	6.34	132.85	122.70
2	H	21	ASP	CB-CG-OD2	-6.31	112.62	118.30
2	H	77(A)	ARG	O-C-N	-6.31	112.60	122.70
2	H	67	ARG	NE-CZ-NH1	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	76	TYR	N-CA-C	-6.27	94.06	111.00
3	P	359	GLY	O-C-N	6.21	132.64	122.70
2	H	116	ASP	CB-CG-OD1	-6.19	112.73	118.30
3	P	346	ALA	N-CA-CB	-6.16	101.48	110.10
2	H	182	CYS	CA-C-O	-6.12	107.26	120.10
3	P	357	GLU	OE1-CD-OE2	-6.06	116.03	123.30
2	H	209	GLN	N-CA-CB	6.06	121.50	110.60
2	H	116	ASP	O-C-N	6.04	132.36	122.70
2	H	20	SER	N-CA-CB	-6.03	101.46	110.50
2	H	194	ASP	CB-CG-OD1	-6.03	112.88	118.30
2	H	130	LEU	CB-CA-C	5.99	121.58	110.20
1	L	14(H)	GLU	CB-CA-C	-5.96	98.49	110.40
2	H	80	GLU	CA-CB-CG	5.92	126.43	113.40
3	P	307	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	H	66	VAL	CA-CB-CG2	5.86	119.69	110.90
2	H	165	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	H	184(A)	TYR	O-C-N	5.80	131.97	122.70
2	H	182	CYS	N-CA-C	-5.79	95.38	111.00
2	H	46	LEU	CA-CB-CG	5.77	128.56	115.30
2	H	175	ARG	NH1-CZ-NH2	5.76	125.74	119.40
2	H	221(A)	ARG	NE-CZ-NH1	-5.73	117.43	120.30
2	H	108	LEU	CA-CB-CG	5.64	128.28	115.30
2	H	221	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	H	105	LEU	CA-CB-CG	5.61	128.21	115.30
2	H	186(B)	GLU	OE1-CD-OE2	5.57	129.98	123.30
3	P	359	GLY	CA-C-N	-5.55	105.00	117.20
3	P	323	LEU	CB-CA-C	5.53	120.70	110.20
3	P	336	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	L	3	LEU	CA-C-O	-5.49	108.57	120.10
3	P	349	PHE	CB-CA-C	-5.45	99.51	110.40
1	L	14(J)	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	H	112	VAL	CA-C-N	-5.43	105.25	117.20
1	L	14(J)	TYR	CB-CG-CD2	5.37	124.22	121.00
1	L	1(A)	ASP	CB-CG-OD1	-5.36	113.47	118.30
3	P	323	LEU	CA-CB-CG	5.33	127.55	115.30
2	H	172	THR	C-N-CA	5.31	134.98	121.70
2	H	160	LEU	O-C-N	5.31	131.18	121.10
3	P	350	CYS	O-C-N	5.27	131.13	122.70
2	H	67	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
2	H	67	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	H	184(A)	TYR	CB-CG-CD2	-5.21	117.88	121.00
2	H	50	ARG	NH1-CZ-NH2	-5.20	113.69	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	53	LEU	CA-CB-CG	5.15	127.14	115.30
1	L	4	ARG	CD-NE-CZ	-5.15	116.39	123.60
2	H	184(A)	TYR	CB-CG-CD1	5.15	124.09	121.00
3	P	327	SER	N-CA-C	-5.14	97.13	111.00
2	H	137	ARG	CA-CB-CG	5.13	124.70	113.40
2	H	156	GLN	N-CA-CB	-5.13	101.36	110.60
2	H	70	LYS	CA-CB-CG	5.12	124.65	113.40
2	H	172	THR	CA-CB-CG2	5.10	119.54	112.40
3	P	351	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	L	1	CYS	O-C-N	5.08	131.84	123.20
2	H	27	SER	N-CA-CB	5.07	118.11	110.50
2	H	33	LEU	CA-CB-CG	5.04	126.89	115.30

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	32	0
2	H	2022	0	1991	216	0
3	P	617	0	553	140	0
4	H	30	0	28	9	0
5	H	79	0	0	10	0
5	L	14	0	0	0	0
5	P	26	0	0	1	0
All	All	3031	0	2810	369	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 65.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
1:L:1(C):GLU:CG	5:H:454:HOH:O	1.89	1.14
2:H:50:ARG:HH21	2:H:107:LYS:HE3	1.15	1.11
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
2:H:124:PRO:HG3	2:H:210:MET:HE1	1.40	1.03
3:P:342:ALA:O	3:P:344:PRO:HD3	1.61	1.01
3:P:315:VAL:HG12	3:P:320:SER:O	1.63	0.99
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
3:P:340:ASN:C	3:P:340:ASN:HD22	1.68	0.95
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
2:H:165:ARG:HH11	2:H:165:ARG:HG2	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:124:PRO:CG	2:H:210:MET:HE1	2.04	0.86
2:H:169:LYS:HE3	5:H:438:HOH:O	1.75	0.85
3:P:340:ASN:ND2	3:P:340:ASN:C	2.25	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:326:SER:C	3:P:327:SER:O	2.02	0.83
3:P:316:THR:HG21	3:P:320:SER:HB2	1.58	0.83
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.61	0.82
2:H:241:VAL:HA	2:H:244:GLN:NE2	1.93	0.82
2:H:124:PRO:HG3	2:H:210:MET:CE	2.10	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: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:32:MET:HE2	2:H:141:TRP:CE3	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:204(B):ASN:ND2	2:H:206:ARG:CG	2.48	0.77
2:H:124:PRO:CB	2:H:210:MET:HE1	2.13	0.77
1:L:10:LYS:CB	1:L:12:LEU:HD22	2.14	0.77
2:H:240:LYS:HD3	3:P:336:ASP:O	1.83	0.77
1:L:10:LYS:HB2	1:L:12:LEU:HD22	1.66	0.77
2:H:204(B):ASN:O	2:H:205:ASN:HB2	1.83	0.77
1:L:11:SER:C	1:L:12:LEU:HD13	2.05	0.76
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
3:P:316:THR:CG2	3:P:320:SER:HB2	2.15	0.76
2:H:168:CYS:O	2:H:171:SER:HB3	1.86	0.76
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
2:H:36(A):SER:HA	2:H:37:PRO:C	2.10	0.72
3:P:312:ARG:O	3:P:312:ARG:HG3	1.90	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:323:LEU:HD23	3:P:363:TYR:HB2	1.72	0.71
2:H:215:TRP:C	4:H:1:0G7:HD3	2.11	0.71
2:H:35:ARG:HG2	2:H:39:GLU:HG3	1.72	0.71
2:H:52:VAL:CG2	2:H:108:LEU:HD21	2.20	0.71
2:H:60(I):THR:C	2:H:62:ASN:H	1.92	0.71
3:P:325:TRP:CE3	3:P:345:LEU:CD2	2.73	0.71
4:H:1:0G7:H29	4:H:1:0G7:CD1	2.21	0.70
1:L:14:ASP:CG	1:L:14(C):GLU:HG2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:215:TRP:CE3	2:H:216:GLY:HA2	2.28	0.68
2:H:33:LEU:HD12	2:H:42:CYS:HB2	1.76	0.68
2:H:50:ARG:NH2	2:H:107:LYS:HE3	1.99	0.67
2:H:124:PRO:HB3	2:H:210:MET:CE	2.24	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
3:P:348:ASN:ND2	3:P:348:ASN:C	2.46	0.66
3:P:342:ALA:O	3:P:344:PRO:CD	2.41	0.66
3:P:325:TRP:CD2	3:P:345:LEU:HD23	2.31	0.66
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
3:P:322:CYS:HG	3:P:362:CYS:HG	0.64	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:215:TRP:CE3	2:H:216:GLY:CA	2.81	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:N	2.68	0.62
2:H:240:LYS:HD3	3:P:336:ASP:C	2.20	0.62
3:P:316:THR:OG1	3:P:372:GLU:OE1	2.16	0.62
2:H:208:TYR:HB3	2:H:210:MET:CE	2.29	0.61
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:208:TYR:HB3	2:H:210:MET:HE2	1.82	0.61
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.36	0.61
1:L:7:PHE:O	1:L:11:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:316:THR:HG22	3:P:320:SER:C	2.21	0.61
3:P:326:SER:O	3:P:327:SER:C	2.38	0.60
3:P:343:VAL:O	3:P:343:VAL:HG13	2.01	0.60
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
2:H:178:ASP:HB3	2:H:233:ARG:NH2	2.08	0.59
1:L:12:LEU:HD13	1:L:12:LEU:N	2.16	0.59
2:H:232:PHE:O	2:H:235:LYS:HB2	2.02	0.59
2:H:36:LYS:HE2	2:H:62:ASN:O	2.03	0.59
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.49	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: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:204(B):ASN:HD22	2:H:206:ARG:HG2	1.65	0.58
2:H:54:THR:OG1	2:H:55:ALA:N	2.37	0.58
3:P:377:ASN:ND2	3:P:378:TYR:O	2.37	0.58
2:H:240:LYS:CE	3:P:336:ASP:HA	2.34	0.57
2:H:79:ILE:HD13	2:H:79:ILE:N	2.18	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
3:P:358:GLU:HA	3:P:358:GLU:OE1	2.04	0.57
2:H:32:MET:HE2	2:H:141:TRP:CD2	2.39	0.57
2:H:242:ILE:C	2:H:244:GLN:H	2.07	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
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
3:P:375:ASN:C	3:P:376:LEU:HD13	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	3:P:366:ASP:OD1	2.40	0.55
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.22	0.55
1:L:14(B):THR:O	1:L:14(C):GLU:C	2.46	0.55
3:P:331:LYS:O	3:P:331:LYS:HD2	2.07	0.55
3:P:322:CYS:SG	3:P:362:CYS:CB	2.95	0.54
3:P:309:TYR:C	3:P:309:TYR:CD1	2.80	0.54
2:H:134:TYR:N	2:H:134:TYR:CD1	2.72	0.54
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.22	0.54
2:H:165:ARG:NH2	2:H:178:ASP:OD1	2.40	0.54
1:L:14:ASP:OD2	1:L:14(C):GLU:HG2	2.08	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:130:LEU:HD11	2:H:210:MET:HB3	1.91	0.53
2:H:76:TYR:HE2	2:H:77(A):ARG:HE	1.55	0.53
2:H:139:THR:CG2	2:H:157:VAL:HG12	2.36	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:60(D):TRP:HE3	2:H:60(F):LYS:HE3	1.74	0.53
2:H:204(B):ASN:HD21	2:H:206:ARG:CB	2.21	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:32:MET:CE	2:H:141:TRP:CE3	2.90	0.53
2:H:50:ARG:HH11	2:H:111:PRO:HD3	1.73	0.53
2:H:78:ASN:C	2:H:79:ILE:HD13	2.29	0.53
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.91	0.53
2:H:35:ARG:HB3	2:H:41:LEU:HD21	1.91	0.53
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
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:306:GLY:C	3:P:308:GLU:H	2.12	0.52
3:P:313:LEU:CD1	3:P:314:ALA:N	2.73	0.51
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:GLU:HG2	2:H:87:LYS:CA	2.40	0.51
3:P:315:VAL:HG12	3:P:320:SER:C	2.29	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:HD1	2:H:134:TYR:N	2.08	0.51
2:H:60(I):THR:C	2:H:62:ASN:N	2.57	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: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:NH1	2:H:165:ARG:HG2	2.10	0.50
2:H:240:LYS:CD	3:P:336:ASP:HA	2.41	0.50
2:H:59:LEU:HD11	2:H:106:MET:HE3	1.94	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
3:P:360:ALA:O	3:P:374:CYS:N	2.45	0.49
3:P:325:TRP:HZ3	3:P:363:TYR:CE2	2.31	0.49
2:H:158:VAL:HG22	2:H:160:LEU:CD2	2.42	0.49
2:H:32:MET:HB3	2:H:67:ARG:HB2	1.95	0.49
3:P:328:GLU:HG2	3:P:328:GLU:O	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:CG	2:H:94:TYR:O	2.66	0.48
3:P:310:ARG:C	3:P:351:ARG:NH2	2.67	0.48
2:H:17:VAL:HG22	2:H:144:LEU:C	2.33	0.48
2:H:155:LEU:C	2:H:156:GLN:HG2	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:94:TYR:CD1	2:H:94:TYR:C	2.87	0.48
3:P:358:GLU:CA	3:P:358:GLU:OE1	2.62	0.48
2:H:175:ARG:NH2	3:P:358:GLU:HB2	2.29	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:56:ALA:HB2	2:H:103:ILE:O	2.12	0.47
2:H:35:ARG:CG	2:H:41:LEU:HD21	2.43	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:59:LEU:HD11	2:H:106:MET:CE	2.43	0.47
2:H:215:TRP:HE3	2:H:216:GLY:CA	2.26	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
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
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
2:H:98:ASN:O	2:H:99:LEU:CB	2.62	0.46
1:L:4:ARG:HD3	2:H:26:MET:O	2.16	0.46
3:P:343:VAL:HG11	3:P:353:PRO:CA	2.16	0.46
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
1:L:1(C):GLU:HG3	1:L:1:CYS:HB3	1.97	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:306:GLY:C	3:P:308:GLU:N	2.68	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:98:ASN:C	2:H:98:ASN:OD1	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:236:LYS:HD3	3:P:338:ASP:CB	2.37	0.45
2:H:215:TRP:HE3	2:H:216:GLY:N	2.14	0.45
2:H:103:ILE:HG23	2:H:237:TRP:CZ3	2.52	0.45
2:H:89:TYR:O	2:H:104:ALA:HA	2.16	0.45
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.37	0.45
3:P:316:THR:CG2	3:P:320:SER:CA	2.95	0.45
2:H:91:HIS:HB2	2:H:103:ILE:HG22	1.99	0.45
1:L:14:ASP:O	1:L:14(C):GLU:HG3	2.17	0.45
1:L:12:LEU:HA	1:L:12:LEU:HD12	1.73	0.44
2:H:195:SER:C	2:H:197:GLY:H	2.19	0.44
2:H:35:ARG:HG2	2:H:41:LEU:CD2	2.47	0.44
1:L:14(B):THR:C	1:L:14(D):ARG:N	2.69	0.44
3:P:331:LYS:HA	3:P:331:LYS:HD2	1.58	0.44
3:P:313:LEU:HD23	3:P:376:LEU:CD1	2.47	0.44
2:H:208:TYR:HB3	2:H:210:MET:HE3	2.00	0.44
2:H:32:MET:HE3	2:H:141:TRP:CH2	2.52	0.44
2:H:98:ASN:ND2	2:H:175:ARG:NH1	2.66	0.44
2:H:98:ASN:N	2:H:98:ASN:OD1	2.47	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:376:LEU:N	3:P:376:LEU:HD13	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:107:LYS:C	2:H:107:LYS:HD2	2.38	0.43
2:H:235:LYS:O	2:H:238:ILE:HB	2.18	0.43
2:H:74:THR:OG1	2:H:75:ARG:N	2.52	0.43
1:L:14:ASP:CG	2:H:137:ARG:HH22	2.22	0.43
2:H:50:ARG:HG2	5:H:429:HOH:O	2.19	0.43
2:H:71:HIS:CE1	2:H:154:VAL:CG1	3.01	0.43
1:L:14(K):ILE:HG12	1:L:14(K):ILE:H	1.72	0.43
3:P:324:ALA:O	3:P:326:SER:N	2.51	0.43
2:H:17:VAL:HG22	2:H:144:LEU:O	2.18	0.43
2:H:81:LYS:HD2	2:H:118:ILE:HD13	2.01	0.42
2:H:31:VAL:CG1	2:H:32:MET:N	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:LEU:HA	2:H:124:PRO:HD3	1.95	0.42
3:P:361:TRP:N	3:P:361:TRP:CD1	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:164:GLU:C	2:H:166:PRO:HD2	2.40	0.42
2:H:32:MET:CG	2:H:40:LEU:HD12	2.49	0.42
3:P:353:PRO:HD2	3:P:361:TRP:CZ2	2.54	0.42
3:P:313:LEU:HD23	3:P:376:LEU:HD11	2.00	0.42
2:H:242:ILE:C	2:H:244:GLN:N	2.71	0.42
3:P:355:GLY:O	3:P:356:ASP:C	2.57	0.42
2:H:16:ILE:HG12	2:H:194:ASP:OD2	2.19	0.42
2:H:195:SER:HA	2:H:213:VAL:CG1	2.50	0.41
2:H:92:PRO:HG2	3:P:337:GLN:NE2	2.35	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
2:H:100:ASP:O	2:H:101:ARG:CB	2.57	0.41
2:H:36(A):SER:CA	2:H:37:PRO:C	2.86	0.41
3:P:302:VAL:HG21	3:P:376:LEU:CB	2.51	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
1:L:14:ASP:N	1:L:14(C):GLU:CG	2.83	0.41
3:P:301:CYS:SG	3:P:302:VAL:N	2.92	0.41
2:H:215:TRP:HB2	2:H:216:GLY:H	1.56	0.41
2:H:91:HIS:ND1	2:H:92:PRO:N	2.68	0.41
3:P:335:LYS:HG2	3:P:336:ASP:N	2.32	0.41
3:P:315:VAL:C	3:P:316:THR:O	2.59	0.41
1:L:1(C):GLU:HB2	2:H:47:ILE:O	2.21	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
2:H:91:HIS:C	2:H:91:HIS:ND1	2.75	0.40
3:P:316:THR:OG1	3:P:372:GLU:CD	2.58	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
2:H:50:ARG:NH1	2:H:111:PRO:HD3	2.36	0.40
2:H:204(B):ASN:HD21	2:H:206:ARG:HB2	1.85	0.40
2:H:35:ARG:HE	2:H:35:ARG:HB2	1.72	0.40
2:H:81:LYS:HD2	2:H:118:ILE:CD1	2.52	0.40
2:H:215:TRP:CB	4:H:1:OG7: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	7
2	H	247/259 (95%)	213 (86%)	32 (13%)	2 (1%)	19	51
3	P	77/79 (98%)	58 (75%)	15 (20%)	4 (5%)	2	13
All	All	352/374 (94%)	291 (83%)	53 (15%)	8 (2%)	6	29

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 [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	
1	L	27/31 (87%)	18 (67%)	9 (33%)	0	1
2	H	218/225 (97%)	162 (74%)	56 (26%)	0	2
3	P	65/65 (100%)	39 (60%)	26 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	310/321 (97%)	219 (71%)	91 (29%)	0 1

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LYS
1	L	11	SER
1	L	12	LEU
1	L	14(C)	GLU
1	L	14(G)	LEU
1	L	14(H)	GLU
1	L	14(I)	SER
1	L	14(J)	TYR
1	L	14(K)	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	60(E)	ASP
2	H	60(I)	THR
2	H	63	ASP
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	70	LYS
2	H	72	SER
2	H	73	ARG
2	H	75	ARG
2	H	77	GLU
2	H	77(A)	ARG
2	H	80	GLU

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Mol	Chain	Res	Type
2	H	81	LYS
2	H	83	SER
2	H	84	MET
2	H	86	GLU
2	H	87	LYS
2	H	94	TYR
2	H	97(A)	GLU
2	H	107	LYS
2	H	121	VAL
2	H	126	ARG
2	H	130	LEU
2	H	137	ARG
2	H	139	THR
2	H	145	LYS
2	H	151	GLN
2	H	153	SER
2	H	156	GLN
2	H	160	LEU
2	H	165	ARG
2	H	173	ARG
2	H	176	ILE
2	H	179	ASN
2	H	185	LYS
2	H	186(A)	ASP
2	H	187	ARG
2	H	204(B)	ASN
2	H	235	LYS
2	H	241	VAL
3	P	301	CYS
3	P	304	ASP
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

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Mol	Chain	Res	Type
3	P	338	ASP
3	P	340	ASN
3	P	347	GLU
3	P	348	ASN
3	P	351	ARG
3	P	354	ASP
3	P	357	GLU
3	P	362	CYS
3	P	371	PHE
3	P	375	ASN
3	P	376	LEU
3	P	377	ASN

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

Mol	Chain	Res	Type
2	H	78	ASN
2	H	151	GLN
2	H	204(B)	ASN
2	H	244	GLN
3	P	340	ASN
3	P	348	ASN
3	P	367	GLN
3	P	377	ASN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	0G7	H	1	2	31,31,32	1.76	1 (3%)	36,41,42	1.46	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	2	-	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	-9.11	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	3.58	129.56	122.93
4	H	1	0G7	CA-C-N1	-3.12	112.83	118.65
4	H	1	0G7	C1-CA1-N1	-3.10	104.01	112.56
4	H	1	0G7	O-C-N1	2.63	126.06	121.38
4	H	1	0G7	CB1-CA1-N1	2.41	106.61	103.03
4	H	1	0G7	CG2-CD3-NE	2.13	118.31	112.21

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

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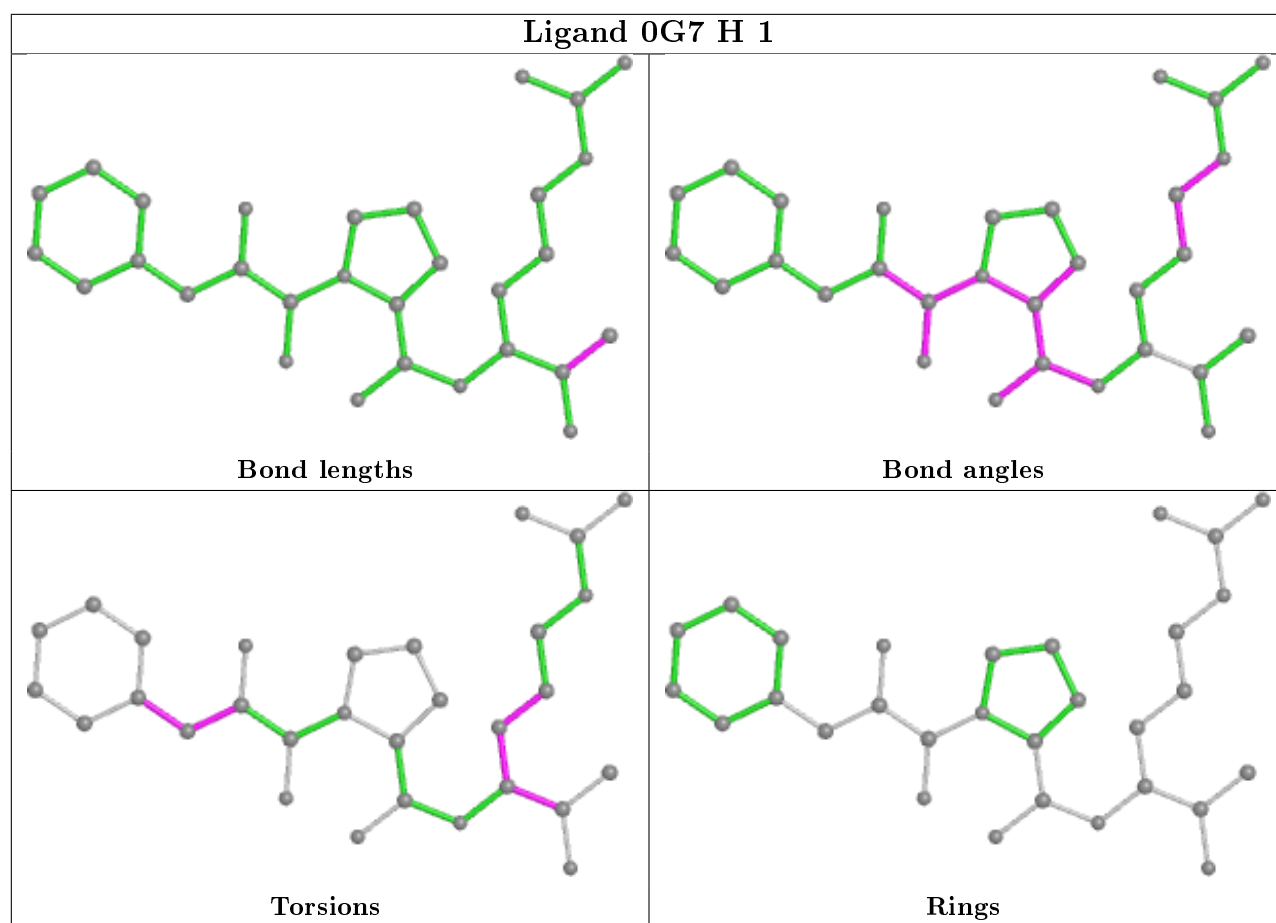
Mol	Chain	Res	Type	Atoms
4	H	1	0G7	N2-CA2-CB2-CG2
4	H	1	0G7	C2-CA2-CB2-CG2
4	H	1	0G7	CA2-CB2-CG2-CD3
4	H	1	0G7	CA-CB-CG-CD1
4	H	1	0G7	CA-CB-CG-CD2
4	H	1	0G7	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	0G7	9	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.