Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 01:04 PM EDT

PDB ID	:	2HPQ
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 (i) 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 (1)) were used in the production of this report:

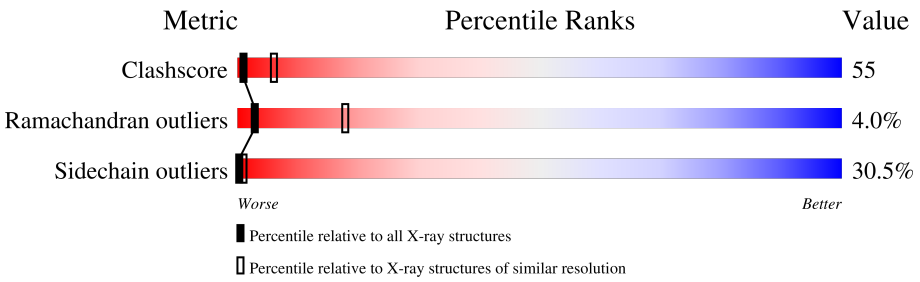
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	25% 33% 17% 8% 17%
2	H	259	26% 43% 22% 5% •
3	P	79	16% 41% 34% 9%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	L	30	240	150	39	50	1	9	0	0

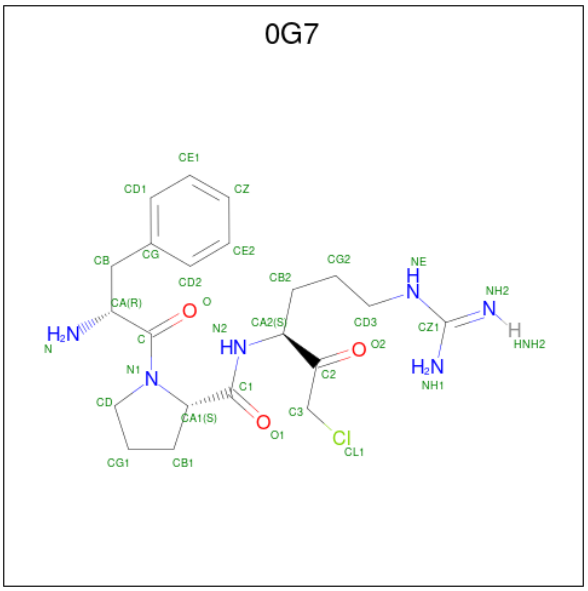
- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	251	2029	1294	359	362	14	38	0	0

- Molecule 3 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	P	79	608	379	107	116	6	46	0	0

- Molecule 4 is D-phenylalanyl-N-[(3S)-6-carbamimidamido-1-chloro-2-oxohexan-3-yl]-L-prolinamide (three-letter code: 0G7) (formula: $C_{21}H_{31}ClN_6O_3$).



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
			Total	O		
5	L	19	19	19	0	0
			Total	O		
5	H	79	79	79	0	0
			Total	O		
5	P	24	24	24	0	0

3 Residue-property plots (i)

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

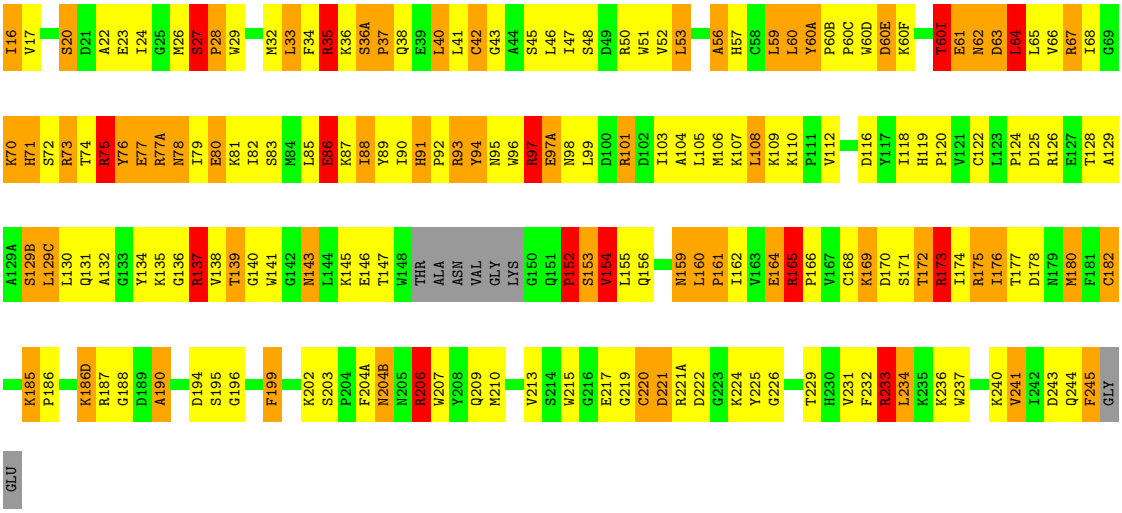
Note EDS was not executed.

• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L: 25% 33% 17% 8% 17%

• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H: 26% 43% 22% 5% •



• Molecule 3: Prothrombin

Chain P: 16% 41% 34% 9%

4 Data and refinement statistics (i)

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 (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	1.13	0/242	2.16	7/322 (2.2%)
2	H	1.06	0/2081	2.37	97/2811 (3.5%)
3	P	1.02	1/624 (0.2%)	2.15	25/848 (2.9%)
All	All	1.05	1/2947 (0.0%)	2.31	129/3981 (3.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	374	CYS	CA-C	-6.38	1.36	1.52

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	93	ARG	NE-CZ-NH2	22.91	131.76	120.30
2	H	77(A)	ARG	NE-CZ-NH1	21.48	131.04	120.30
2	H	101	ARG	NE-CZ-NH2	-20.45	110.07	120.30
2	H	93	ARG	NE-CZ-NH1	-19.54	110.53	120.30
2	H	173	ARG	NE-CZ-NH2	-16.82	111.89	120.30
2	H	101	ARG	NE-CZ-NH1	16.67	128.63	120.30
2	H	165	ARG	NE-CZ-NH1	14.57	127.59	120.30
2	H	206	ARG	NE-CZ-NH1	-13.98	113.31	120.30
2	H	134	TYR	CB-CG-CD1	12.64	128.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	77(A)	ARG	NH1-CZ-NH2	-11.10	107.19	119.40
2	H	175	ARG	NE-CZ-NH2	-10.98	114.81	120.30
3	P	379	CYS	N-CA-CB	10.80	130.04	110.60
3	P	351	ARG	NE-CZ-NH2	-10.23	115.19	120.30
2	H	194	ASP	CB-CG-OD2	9.72	127.05	118.30
2	H	222	ASP	CB-CG-OD1	-9.44	109.81	118.30
2	H	67	ARG	NE-CZ-NH1	9.28	124.94	120.30
3	P	373	TYR	CB-CG-CD1	-8.88	115.67	121.00
2	H	180	MET	O-C-N	8.87	136.89	122.70
1	L	1(A)	ASP	CB-CG-OD1	-8.86	110.33	118.30
2	H	170	ASP	CB-CG-OD2	8.21	125.69	118.30
2	H	206	ARG	NE-CZ-NH2	8.03	124.32	120.30
2	H	165	ARG	CD-NE-CZ	7.99	134.78	123.60
2	H	134	TYR	CB-CG-CD2	-7.91	116.25	121.00
3	P	351	ARG	CA-CB-CG	7.75	130.46	113.40
3	P	323	LEU	CB-CA-C	7.70	124.84	110.20
2	H	173	ARG	NE-CZ-NH1	7.67	124.14	120.30
3	P	312	ARG	NE-CZ-NH2	7.65	124.12	120.30
2	H	50	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	H	233	ARG	NE-CZ-NH2	7.61	124.11	120.30
2	H	165	ARG	NH1-CZ-NH2	-7.55	111.09	119.40
2	H	122	CYS	CA-CB-SG	7.53	127.56	114.00
2	H	28	PRO	N-CA-CB	7.51	112.31	103.30
3	P	305	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	H	221	ASP	CB-CG-OD2	-7.36	111.68	118.30
3	P	338	ASP	CB-CG-OD1	-7.25	111.77	118.30
2	H	77	GLU	CG-CD-OE1	7.16	132.61	118.30
2	H	77(A)	ARG	N-CA-CB	6.93	123.07	110.60
3	P	374	CYS	O-C-N	6.93	133.79	122.70
2	H	206	ARG	CD-NE-CZ	-6.78	114.10	123.60
2	H	186(D)	LYS	N-CA-CB	6.78	122.80	110.60
2	H	37	PRO	O-C-N	6.71	133.43	122.70
2	H	57	HIS	CA-CB-CG	6.69	124.97	113.60
1	L	4	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	L	14(F)	LEU	CA-CB-CG	6.64	130.57	115.30
3	P	374	CYS	CB-CA-C	6.58	123.57	110.40
2	H	77(A)	ARG	CG-CD-NE	6.57	125.59	111.80
2	H	97	ARG	NE-CZ-NH2	6.55	123.58	120.30
2	H	194	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	L	14(C)	GLU	CB-CA-C	-6.43	97.54	110.40
2	H	91	HIS	CA-CB-CG	-6.41	102.70	113.60
2	H	164	GLU	CB-CG-CD	6.41	131.50	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	35	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	H	187	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	H	60(A)	TYR	O-C-N	6.33	133.12	121.10
2	H	159	ASN	N-CA-CB	6.31	121.96	110.60
1	L	8	GLU	CA-CB-CG	6.31	127.28	113.40
2	H	222	ASP	CB-CG-OD2	6.30	123.97	118.30
2	H	161	PRO	CB-CA-C	-6.26	96.36	112.00
2	H	220	CYS	N-CA-CB	6.26	121.86	110.60
2	H	143	ASN	O-C-N	6.25	132.70	122.70
2	H	217	GLU	OE1-CD-OE2	6.24	130.79	123.30
2	H	42	CYS	CB-CA-C	-6.16	98.09	110.40
2	H	180	MET	CG-SD-CE	6.14	110.03	100.20
2	H	153	SER	N-CA-CB	-6.09	101.37	110.50
2	H	65	LEU	N-CA-CB	-6.08	98.25	110.40
2	H	32	MET	CG-SD-CE	6.03	109.85	100.20
2	H	154	VAL	CA-CB-CG2	-5.96	101.97	110.90
2	H	137	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	H	40	LEU	O-C-N	5.92	132.17	122.70
3	P	373	TYR	CB-CG-CD2	5.92	124.55	121.00
3	P	338	ASP	CA-CB-CG	-5.91	100.39	113.40
2	H	63	ASP	O-C-N	5.91	132.15	122.70
2	H	28	PRO	O-C-N	5.88	132.11	122.70
3	P	363	TYR	CB-CG-CD1	-5.85	117.49	121.00
3	P	325	TRP	O-C-N	5.85	132.05	122.70
2	H	129(B)	SER	O-C-N	5.81	131.99	122.70
2	H	154	VAL	CB-CA-C	-5.79	100.40	111.40
2	H	71	HIS	CA-CB-CG	-5.76	103.80	113.60
2	H	190	ALA	CB-CA-C	5.76	118.75	110.10
2	H	104	ALA	N-CA-CB	5.75	118.16	110.10
3	P	338	ASP	OD1-CG-OD2	5.75	134.22	123.30
2	H	70	LYS	O-C-N	-5.73	113.54	122.70
2	H	50	ARG	O-C-N	5.72	131.86	122.70
2	H	154	VAL	CG1-CB-CG2	5.71	120.03	110.90
2	H	16	ILE	CA-C-O	-5.68	108.17	120.10
2	H	153	SER	CA-CB-OG	-5.67	95.91	111.20
2	H	185	LYS	CB-CA-C	-5.66	99.08	110.40
2	H	60(A)	TYR	CB-CG-CD1	-5.62	117.63	121.00
3	P	323	LEU	CA-CB-CG	5.61	128.20	115.30
3	P	323	LEU	N-CA-C	-5.57	95.96	111.00
2	H	60(A)	TYR	CB-CG-CD2	5.55	124.33	121.00
2	H	65	LEU	CA-C-N	5.53	129.37	117.20
2	H	53	LEU	CB-CA-C	5.50	120.64	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	78	ASN	CA-C-O	-5.49	108.57	120.10
2	H	64	LEU	N-CA-CB	-5.46	99.49	110.40
2	H	146	GLU	N-CA-CB	5.45	120.41	110.60
2	H	27	SER	O-C-N	5.44	131.44	121.10
3	P	303	PRO	O-C-N	-5.43	114.01	122.70
2	H	60(I)	THR	CA-CB-OG1	-5.43	97.60	109.00
2	H	75	ARG	NE-CZ-NH1	-5.42	117.59	120.30
3	P	357	GLU	CA-CB-CG	5.42	125.33	113.40
2	H	132	ALA	CB-CA-C	5.41	118.22	110.10
2	H	152	PRO	C-N-CA	5.41	135.22	121.70
2	H	77(A)	ARG	CD-NE-CZ	5.40	131.16	123.60
2	H	199	PHE	N-CA-C	-5.37	96.50	111.00
3	P	339	PHE	CB-CA-C	5.37	121.14	110.40
2	H	97	ARG	N-CA-CB	5.37	120.27	110.60
2	H	204(A)	PHE	CB-CA-C	-5.37	99.66	110.40
3	P	321	PRO	O-C-N	5.36	131.28	122.70
2	H	56	ALA	O-C-N	5.33	131.23	122.70
3	P	301	CYS	CB-CA-C	-5.32	99.76	110.40
2	H	229	THR	O-C-N	5.32	131.21	122.70
2	H	126	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	H	190	ALA	N-CA-C	-5.28	96.76	111.00
2	H	160	LEU	O-C-N	5.26	131.10	121.10
1	L	4	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	H	66	VAL	CA-CB-CG1	5.24	118.76	110.90
2	H	172	THR	CA-CB-OG1	-5.21	98.06	109.00
2	H	77	GLU	CB-CG-CD	5.16	128.13	114.20
3	P	335	LYS	N-CA-C	5.15	124.91	111.00
2	H	59	LEU	N-CA-CB	-5.13	100.13	110.40
1	L	3	LEU	CB-CG-CD2	-5.13	102.28	111.00
3	P	304	ASP	CB-CA-C	5.11	120.63	110.40
2	H	217	GLU	CG-CD-OE2	-5.11	108.09	118.30
3	P	320	LEU	N-CA-CB	5.08	120.56	110.40
2	H	28	PRO	CA-C-O	-5.07	108.03	120.20
2	H	86	GLU	N-CA-CB	-5.07	101.47	110.60
2	H	40	LEU	CA-C-O	-5.05	109.50	120.10
2	H	60(I)	THR	CA-CB-CG2	5.02	119.42	112.40

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	240	0	236	22	0
2	H	2029	0	2002	195	0
3	P	608	0	553	98	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	304	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 55.

All (304) 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:42:CYS:HB3	2:H:195:SER:O	1.57	1.01
2:H:195:SER:CB	4:H:1:0G7:C3	2.42	0.98
2:H:195:SER:OG	4:H:1:0G7: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:1:0G7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:LYS:HB3	2:H:169:LYS:HZ2	1.36	0.86
3:P:324:ALA:O	3:P:327:SER:HB2	1.77	0.85
2:H:169:LYS:HB3	2:H:169:LYS:HZ3	1.42	0.84
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: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:1:0G7:C2	2.57	0.82
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
2:H:94:TYR:CE1	2:H:96:TRP:HB3	2.20	0.76
2:H:60(I):THR:C	2:H:62:ASN:H	1.87	0.75
2:H:68:ILE:HG22	2:H:118:ILE:CD1	2.18	0.73
2:H:59:LEU:HD11	2:H:106:MET:HE3	1.71	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
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.69	0.72
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:1:0G7:O2	1.89	0.72
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
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
1:L:14:ASP:OD2	2:H:137:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:0G7:C2	2.23	0.67
3:P:301:CYS:HB2	3:P:377:ASN:O	1.94	0.67
2:H:195:SER:HB2	4:H:1:0G7:C3	2.23	0.67
3:P:335:LYS:NZ	5:P:551:HOH:O	2.27	0.67
2:H:130:LEU:C	2:H:131:GLN:HG2	2.16	0.66
2:H:169:LYS:HZ2	2:H:169:LYS:CB	2.09	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:203:SER:HB3	2:H:204(B):ASN:ND2	2.09	0.64
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
2:H:233:ARG:C	2:H:234:LEU:HD23	2.19	0.63
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	1.99	0.62
2:H:232:PHE:C	2:H:234:LEU:H	2.01	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
3:P:329:GLN:H	3:P:329:GLN:HE21	1.48	0.61
2:H:60(I):THR:C	2:H:62:ASN:N	2.54	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
2:H:128:THR:HG22	2:H:210:MET:HE3	1.83	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:THR:HG22	2:H:210:MET:CE	2.33	0.58
1:L:14:ASP:CG	2:H:137:ARG:HH22	2.07	0.58
2:H:20:SER:O	2:H:156:GLN:HA	2.04	0.58
2:H:232:PHE:C	2:H:234:LEU:N	2.57	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
1:L:7:PHE:O	1:L:8:GLU:C	2.42	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
3:P:312:ARG:O	3:P:313:LEU:C	2.43	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: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
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: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:LEU:HD12	2:H:60:LEU:C	2.29	0.53
2:H:91:HIS:CE1	2:H:93:ARG:H	2.25	0.53
3:P:303:PRO:O	3:P:304:ASP:C	2.46	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:206:ARG:HG2	2:H:206:ARG:HH11	1.57	0.53
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
1:L:14(B):THR:O	1:L:14(C):GLU:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:97:ARG:NH2	3:P:370:ASP:OD1	2.44	0.51
1:L:14:ASP:N	1:L:14(C):GLU:HG3	2.25	0.50
2:H:96:TRP:CE3	2:H:96:TRP:C	2.84	0.50
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
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: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:60(B):PRO:O	2:H:60(C):PRO:C	2.50	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
3:P:340:ASN:C	3:P:342:ALA:H	2.17	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
2:H:36(A):SER:HA	2:H:37:PRO:C	2.33	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
3:P:311:GLY:H	3:P:351:ARG:HH22	1.62	0.48
3:P:329:GLN:C	3:P:331:LYS:H	2.16	0.48
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:329:GLN:C	3:P:331:LYS:N	2.67	0.47
3:P:339:PHE:HA	3:P:353:PRO:O	2.14	0.47
2:H:215:TRP:CE3	4:H:1:0G7:HD2	2.49	0.47
3:P:356:ASP:CG	3:P:373:TYR:OH	2.52	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
1:L:14:ASP:CG	2:H:137:ARG:NH2	2.69	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
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: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: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:220:CYS:O	2:H:221:ASP:HB3	2.16	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:306:GLY:C	3:P:308:GLN:H	2.19	0.45
3:P:344:GLN:O	3:P:351:ARG:HD3	2.17	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:98:ASN:OD1	2:H:98:ASN:C	2.50	0.45
2:H:130:LEU:HD23	2:H:130:LEU:HA	1.75	0.44
2:H:27:SER:HG	2:H:29:TRP:HE1	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:23:GLU:HG3	2:H:26:MET:CE	2.47	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
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:1:0G7:CB2	2.67	0.43
3:P:333:LEU:HB2	3:P:363:TYR:CE1	2.53	0.43
3:P:355:GLY:O	3:P:356:ASP:C	2.56	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
3:P:305:ARG:C	3:P:307:GLN:N	2.72	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
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
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
3:P:365:ALA:HB3	3:P:370:ASP:CG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:0G7:O2	2.57	0.42
3:P:301:CYS:SG	3:P:302:VAL:N	2.90	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:1:0G7: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
2:H:16:ILE:HD11	2:H:139:THR:C	2.41	0.41
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:309:TYR:CD1	3:P:309:TYR:C	2.93	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:60(D):TRP:O	2:H:60(E):ASP:C	2.59	0.41
2:H:86:GLU:CB	2:H:107:LYS:O	2.59	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
3:P:324:ALA:C	3:P:326:ALA:N	2.72	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
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

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%)	21 (75%)	5 (18%)	2 (7%)	1 7
2	H	247/259 (95%)	216 (87%)	28 (11%)	3 (1%)	13 42
3	P	77/79 (98%)	48 (62%)	20 (26%)	9 (12%)	0 2
All	All	352/374 (94%)	285 (81%)	53 (15%)	14 (4%)	3 18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(C)	GLU
2	H	61	GLU
2	H	233	ARG
3	P	303	PRO
3	P	304	ASP
3	P	325	TRP
3	P	347	GLU
3	P	356	ASP
1	L	14(A)	LYS
3	P	324	ALA
3	P	327	SER
2	H	143	ASN
3	P	306	GLY
3	P	316	THR

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	26/31 (84%)	17 (65%)	9 (35%)	0 1
2	H	219/225 (97%)	159 (73%)	60 (27%)	0 1
3	P	63/63 (100%)	38 (60%)	25 (40%)	0 0
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
1	L	14(G)	LEU
1	L	14(H)	GLU
1	L	14(I)	SER
1	L	14(K)	ILE
2	H	20	SER
2	H	24	ILE
2	H	27	SER
2	H	33	LEU
2	H	35	ARG
2	H	36(A)	SER
2	H	40	LEU
2	H	45	SER
2	H	48	SER
2	H	60	LEU
2	H	60(E)	ASP
2	H	60(F)	LYS
2	H	60(I)	THR
2	H	62	ASN
2	H	64	LEU
2	H	67	ARG
2	H	73	ARG
2	H	75	ARG
2	H	76	TYR
2	H	77	GLU
2	H	79	ILE
2	H	80	GLU
2	H	81	LYS
2	H	83	SER
2	H	86	GLU

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Mol	Chain	Res	Type
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	137	ARG
2	H	139	THR
2	H	145	LYS
2	H	147	THR
2	H	152	PRO
2	H	153	SER
2	H	154	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	182	CYS
2	H	204(B)	ASN
2	H	206	ARG
2	H	231	VAL
2	H	234	LEU
2	H	236	LYS
2	H	240	LYS
2	H	241	VAL
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	321	PRO
3	P	323	LEU
3	P	325	TRP

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Mol	Chain	Res	Type
3	P	327	SER
3	P	329	GLN
3	P	334	SER
3	P	337	GLN
3	P	338	ASP
3	P	340	ASN
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	371	PHE
3	P	375	ASP
3	P	377	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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	340	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 monosaccharides 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	2	31,31,32	1.95	1 (3%)	36,41,42	2.25	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	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	-9.96	1.24	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	0G7	O-C-N1	5.94	131.96	121.38
4	H	1	0G7	NH1-CZ1-NE	5.33	131.51	119.19
4	H	1	0G7	CB-CA-C	-4.59	98.28	109.27
4	H	1	0G7	NE-CZ1-NH2	-3.53	114.50	120.70
4	H	1	0G7	O1-C1-CA1	-3.50	111.91	120.63
4	H	1	0G7	O1-C1-N2	3.39	129.21	122.93
4	H	1	0G7	O-C-CA	-2.97	114.26	119.66
4	H	1	0G7	CB1-CA1-N1	2.89	107.33	103.03
4	H	1	0G7	CA-C-N1	-2.64	113.72	118.65
4	H	1	0G7	CG2-CB2-CA2	2.56	121.82	113.92
4	H	1	0G7	C1-CA1-N1	-2.16	106.61	112.56
4	H	1	0G7	CB1-CG1-CD	2.16	111.10	104.98
4	H	1	0G7	NH1-CZ1-NH2	-2.04	113.99	120.26

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	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

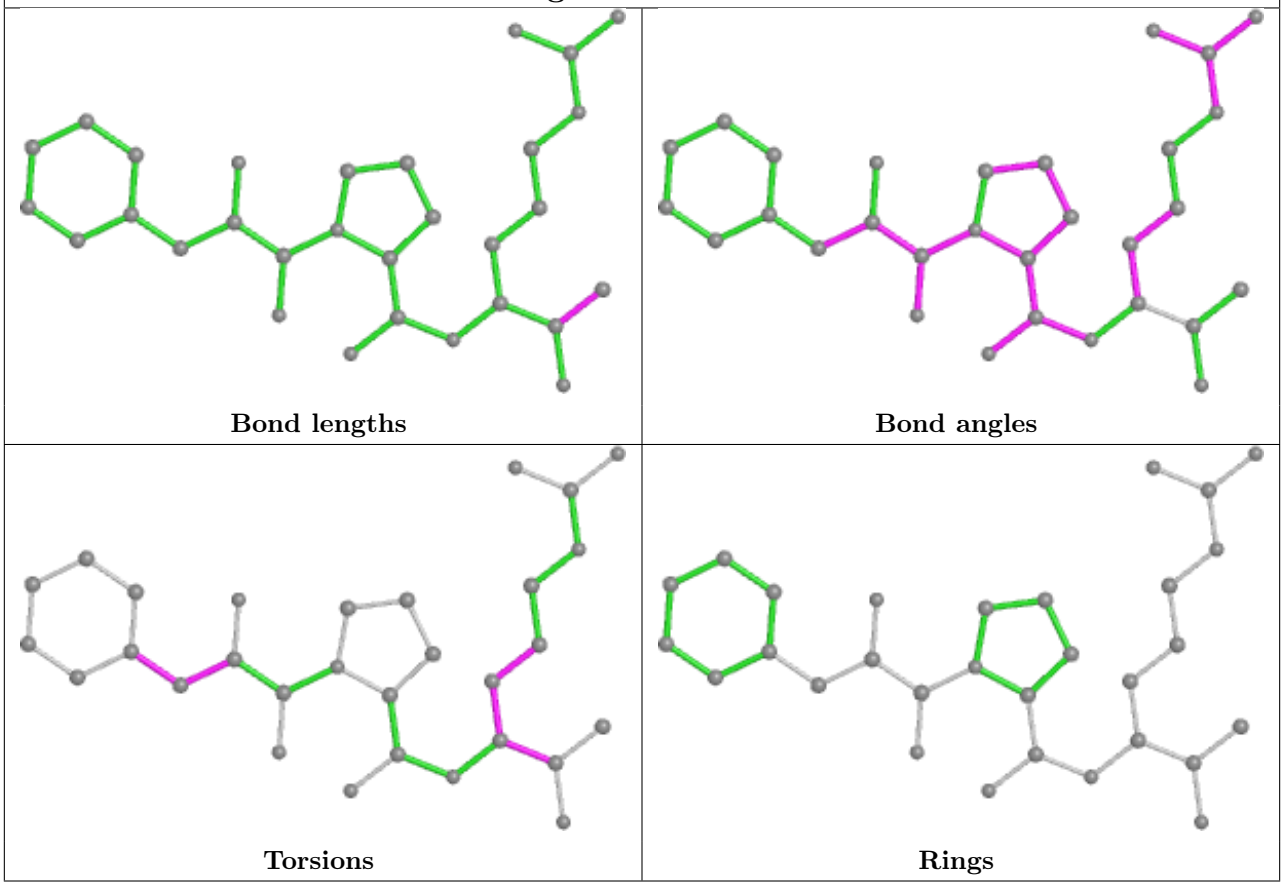
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 0G7 H 1



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.