



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:13 PM UTC

PDB ID : 1NY2 / pdb_00001ny2
Title : Human alpha thrombin inhibited by RPPGF and hirugen
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Deposited on : 2003-02-11
Resolution : 2.30 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**
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

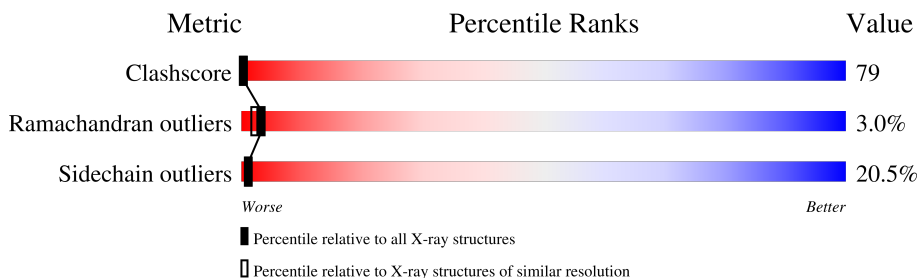
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	1	36	8% 31% 50% 11%
2	2	259	13% 43% 34% 10%
3	3	10	30% 10% 40% 20%
4	4	5	20% 20% 20% 20% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2554 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 thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called thrombin Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	259	Total	C	N	O	S	0	0	0
			2093	1334	370	375	14			

- Molecule 3 is a protein called Hirugen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	S	0	0	0
			94	59	10	24	1			

- Molecule 4 is a protein called Inhibitor peptide RPPGF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	4	Total	C	N	O	0	0	0
			29	18	7	4			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1	3	Total	O	0	0
			3	3		
5	2	44	Total	O	0	0
			44	44		
5	3	4	Total	O	0	0
			4	4		

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: thrombin light chain

Chain 1: 

T1H F1G G1F E18 S1E G1D E1C A1B D1A C1 G2 G25 L3 R4 P5 L6 F7 E8 K9 K10 S11 L12 E13 D14 K14A T14B E14C R14D E14E L14F L14G E14H S14I Y14J T14K D14L G14M R15

- Molecule 2: thrombin Heavy chain

Chain 2: 

I16 V17 E18 G19 D21 A22 E23 T24 G25 M26 S27 P28 W29 Q30 V31 M32 K33 F34 R35 K36 S36A P37 Q38 I39 E39 L40 L41 C42 S45 L46 T47 S48 D49 R50 A51 W52 L53 T54 A55 A56 H57 C58 L59 L60 Y60A P60B P60C W60D D60E K60F M60G F60H T60I E61 N62 D63 L64 L65 V66

R67 I68 G69 K70 S71 D72 R73 T74 T75 Y76 E77 R77A W78 I79 E80 K81 V81 I82 S83 M84 L85 E86 K87 S88 Y89 Q88 H91 P92 R93 Y94 N95 N96 R97A S97A N98 L99 P100 D100 W101 R101 D102 I103 A104 L105 M106 K107 L108 K109 K110 P111 P112 A113 V114 F114 C115 S115 D116 Y117 I118 T119 H119 P120 V121 C122 L123 P124

D125 R126 E127 T128 A129 A129A S129B L129C L130 Q131 Y134 K135 G136 R137 V138 T139 G140 W141 G142 N143 L144 K145 E146 T147 W148 T149 A149A M149B V149C G149D K149E G150 Q151 P152 S153 V154 L155 Q156 V157 V158 M159 I162 V163 E164 R165 P166 V167 C168 K169 D170 S171 T172 T173 I174 R175 T176 D178

N179 M180 F181 C182 W183 G184 Y184A K185 D186A E186B G186C K186D R187 G188 D189 A190 C191 E192 G193 S195 L196 G197 P198 F199 V200 M201 K202 S203 P204 F204A N204B N205 R206 W207 Y208 Q209 M210 G211 I212 V213 S214 W215 G216 E217 G219 C220 D221 R221A K224 Y225 G226 F227 Y228 T229 H230 V231 F232

R233 L234 K235 K236 W237 I238 P239 Q239 K240 V241 I242 Q244 F245 G246 E247

- Molecule 3: Hirugen

Chain 3: 

D55 F56 E57 E58 I59 P60 E61 E62 Y63 L64

- Molecule 4: Inhibitor peptide RPPGF

Chain 4: 

R350 P351 P352 G353 PHE

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.15Å 104.97Å 45.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2554	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: TYS

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	1	1.23	0/290	2.61	25/384 (6.5%)
2	2	1.49	9/2148 (0.4%)	2.96	227/2903 (7.8%)
3	3	1.07	0/78	2.38	3/103 (2.9%)
4	4	1.70	0/30	3.03	2/40 (5.0%)
All	All	1.45	9/2546 (0.4%)	2.90	257/3430 (7.5%)

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	2	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	75	ARG	NE-CZ	7.31	1.41	1.33
2	2	75	ARG	CD-NE	-6.73	1.36	1.46
2	2	65	LEU	CA-C	6.28	1.60	1.52
2	2	206	ARG	CD-NE	-5.67	1.38	1.46
2	2	48	SER	N-CA	5.64	1.54	1.46
2	2	73	ARG	CD-NE	5.46	1.53	1.46
2	2	112	VAL	CA-C	5.32	1.59	1.52
2	2	211	GLY	N-CA	5.12	1.50	1.45
2	2	106	MET	CG-SD	5.04	1.93	1.80

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	75	ARG	CD-NE-CZ	30.10	166.53	124.40
2	2	206	ARG	CD-NE-CZ	25.26	159.76	124.40
2	2	175	ARG	CD-NE-CZ	19.96	152.35	124.40
2	2	75	ARG	CG-CD-NE	17.66	150.85	112.00
2	2	77(A)	ARG	CD-NE-CZ	13.86	143.80	124.40
2	2	187	ARG	CD-NE-CZ	13.74	143.64	124.40
2	2	73	ARG	NE-CZ-NH1	-13.11	108.39	121.50
2	2	73	ARG	CD-NE-CZ	-12.87	106.39	124.40
2	2	135	LYS	CA-C-N	12.73	136.44	122.69
2	2	135	LYS	C-N-CA	12.73	136.44	122.69
2	2	26	MET	CA-C-N	12.50	136.60	122.85
2	2	26	MET	C-N-CA	12.50	136.60	122.85
4	4	380	ARG	CD-NE-CZ	12.48	141.88	124.40
2	2	149(B)	ASN	CA-CB-CG	11.92	124.52	112.60
2	2	91	HIS	O-C-N	11.48	130.79	121.38
2	2	154	VAL	N-CA-CB	-11.21	99.57	112.34
2	2	77	GLU	CB-CG-CD	11.17	131.59	112.60
2	2	192	GLU	CB-CA-C	11.02	125.38	110.06
2	2	116	ASP	CA-CB-CG	10.81	123.41	112.60
2	2	206	ARG	NE-CZ-NH2	10.66	128.79	119.20
2	2	91	HIS	CA-CB-CG	-10.61	103.19	113.80
2	2	166	PRO	O-C-N	10.48	133.50	122.18
2	2	112	VAL	N-CA-CB	10.09	124.48	110.56
2	2	54	THR	CA-C-O	-10.05	110.48	121.33
1	1	1(C)	GLU	CA-CB-CG	9.68	133.46	114.10
2	2	117	TYR	CA-C-N	9.55	136.54	122.98
2	2	117	TYR	C-N-CA	9.55	136.54	122.98
2	2	84	MET	CA-C-O	9.47	130.71	120.38
2	2	156	GLN	OE1-CD-NE2	9.47	132.07	122.60
2	2	18	GLU	CA-C-N	9.42	132.91	122.55
2	2	18	GLU	C-N-CA	9.42	132.91	122.55
2	2	73	ARG	CA-C-N	9.15	133.07	120.63
2	2	73	ARG	C-N-CA	9.15	133.07	120.63
2	2	112	VAL	CA-C-N	9.12	134.95	121.72
2	2	112	VAL	C-N-CA	9.12	134.95	121.72
2	2	149	THR	N-CA-CB	9.05	123.68	110.20
2	2	164	GLU	O-C-N	8.76	133.29	123.04
2	2	76	TYR	CA-C-N	8.64	135.54	122.23
2	2	76	TYR	C-N-CA	8.64	135.54	122.23
2	2	60(D)	TRP	N-CA-C	-8.64	102.28	113.17
2	2	137	ARG	CD-NE-CZ	8.56	136.38	124.40
2	2	203	SER	O-C-N	8.49	129.16	121.35
3	3	64	LEU	CA-C-O	-8.34	106.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	229	THR	N-CA-CB	8.33	123.27	109.60
2	2	186(D)	LYS	CB-CA-C	8.29	126.72	110.30
2	2	175	ARG	NE-CZ-NH1	8.24	129.74	121.50
2	2	112	VAL	O-C-N	8.17	132.30	122.83
2	2	35	ARG	CD-NE-CZ	-8.10	113.06	124.40
2	2	48	SER	CA-CB-OG	8.08	127.26	111.10
2	2	147	THR	CB-CA-C	8.02	122.42	109.90
2	2	95	ASN	N-CA-CB	8.01	126.82	110.64
2	2	103	ILE	CA-C-O	7.97	129.16	120.64
2	2	179	ASN	CA-CB-CG	-7.87	104.73	112.60
2	2	73	ARG	NE-CZ-NH2	7.85	126.26	119.20
2	2	30	GLN	N-CA-CB	7.83	121.64	109.83
2	2	212	ILE	CA-C-O	-7.79	111.84	120.72
2	2	75	ARG	NE-CZ-NH2	-7.74	112.23	119.20
2	2	237	TRP	N-CA-C	-7.73	102.93	111.36
2	2	80	GLU	CA-C-N	7.63	134.20	123.07
2	2	80	GLU	C-N-CA	7.63	134.20	123.07
2	2	60(H)	PHE	CA-CB-CG	-7.62	106.18	113.80
2	2	239	GLN	CA-C-N	7.61	130.33	120.44
2	2	239	GLN	C-N-CA	7.61	130.33	120.44
1	1	1(A)	ASP	CA-CB-CG	7.57	120.17	112.60
1	1	13	GLU	CA-CB-CG	7.57	129.23	114.10
2	2	98	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	1	14(L)	ASP	N-CA-C	7.56	120.01	108.52
1	1	14	ASP	CA-CB-CG	7.52	120.12	112.60
1	1	13	GLU	CA-C-O	-7.52	112.67	121.16
2	2	71	HIS	N-CA-C	-7.51	102.94	112.93
2	2	163	VAL	CB-CA-C	7.47	121.84	111.38
2	2	33	LEU	CA-C-O	7.46	128.90	120.84
2	2	125	ASP	CB-CA-C	7.45	122.10	109.80
2	2	196	GLY	CA-C-N	7.41	133.51	121.87
2	2	196	GLY	C-N-CA	7.41	133.51	121.87
2	2	28	PRO	CA-C-N	7.40	135.82	122.06
2	2	28	PRO	C-N-CA	7.40	135.82	122.06
2	2	93	ARG	CD-NE-CZ	7.29	134.60	124.40
2	2	97	ARG	CD-NE-CZ	7.28	134.59	124.40
2	2	21	ASP	CA-C-O	-7.27	113.64	121.56
1	1	7	PHE	O-C-N	7.18	132.14	122.59
2	2	138	VAL	CB-CA-C	7.18	121.44	110.96
2	2	56	ALA	O-C-N	-7.16	114.64	122.09
2	2	39	GLU	N-CA-C	7.16	119.75	108.79
2	2	35	ARG	NH1-CZ-NH2	7.14	128.58	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	156	GLN	CB-CG-CD	-7.10	100.54	112.60
2	2	60(G)	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	1	14(L)	ASP	CA-CB-CG	-7.06	105.54	112.60
2	2	41	LEU	CB-CA-C	7.06	123.48	110.56
2	2	237	TRP	O-C-N	7.04	130.17	122.15
2	2	123	LEU	O-C-N	7.03	133.12	121.59
2	2	74	THR	N-CA-C	6.97	118.77	111.03
2	2	149(B)	ASN	CB-CA-C	6.94	121.16	109.84
2	2	165	ARG	O-C-N	6.92	129.28	121.32
2	2	176	ILE	CA-CB-CG2	6.92	122.27	110.50
2	2	77(A)	ARG	NE-CZ-NH2	6.92	125.43	119.20
2	2	60(D)	TRP	O-C-N	6.91	133.75	122.70
1	1	3	LEU	O-C-N	6.88	133.42	122.96
2	2	234	LEU	N-CA-CB	-6.88	100.52	110.56
2	2	35	ARG	NE-CZ-NH1	-6.87	114.63	121.50
2	2	205	ASN	N-CA-C	6.84	121.57	113.23
2	2	153	SER	O-C-N	6.83	129.47	122.09
1	1	1(F)	GLY	N-CA-C	-6.79	97.08	113.18
2	2	163	VAL	CA-C-N	6.79	131.21	121.50
2	2	163	VAL	C-N-CA	6.79	131.21	121.50
2	2	31	VAL	CA-C-O	-6.78	113.08	120.67
2	2	87	LYS	CA-C-O	6.73	128.35	120.14
1	1	1(C)	GLU	CB-CG-CD	6.70	123.99	112.60
2	2	205	ASN	N-CA-CB	-6.68	101.88	112.63
2	2	21	ASP	O-C-N	6.68	130.74	122.86
2	2	247	GLU	N-CA-CB	6.67	121.84	110.50
2	2	221(A)	ARG	CG-CD-NE	6.67	126.66	112.00
1	1	14(E)	GLU	CA-CB-CG	6.66	127.42	114.10
2	2	74	THR	OG1-CB-CG2	6.66	122.61	109.30
2	2	65	LEU	N-CA-CB	6.65	123.47	111.37
2	2	42	CYS	O-C-N	6.60	130.31	122.72
1	1	1(F)	GLY	O-C-N	6.60	133.25	122.70
2	2	149(E)	LYS	CB-CA-C	6.56	120.55	109.80
1	1	14(G)	LEU	CB-CA-C	6.54	121.03	110.96
2	2	60(I)	THR	CB-CA-C	6.52	120.66	109.51
2	2	187	ARG	NE-CZ-NH2	6.48	125.03	119.20
2	2	224	LYS	CA-C-O	-6.44	113.77	121.56
2	2	157	VAL	CA-C-O	-6.43	113.54	120.36
1	1	14(J)	TYR	N-CA-C	-6.41	104.48	113.20
2	2	54	THR	O-C-N	6.40	130.54	123.25
2	2	77(A)	ARG	O-C-N	6.38	131.07	122.59
2	2	47	ILE	CB-CA-C	6.37	118.81	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	83	SER	N-CA-C	6.37	120.07	109.95
2	2	219	GLY	N-CA-C	-6.34	100.76	112.62
2	2	62	ASN	CA-C-N	6.33	131.29	120.72
2	2	62	ASN	C-N-CA	6.33	131.29	120.72
2	2	27	SER	CB-CA-C	-6.31	102.00	111.27
2	2	127	GLU	CB-CG-CD	6.28	123.28	112.60
2	2	59	LEU	N-CA-CB	-6.27	101.31	110.40
2	2	52	VAL	CA-C-N	6.27	130.46	121.50
2	2	52	VAL	C-N-CA	6.27	130.46	121.50
2	2	185	LYS	N-CA-CB	6.26	119.26	110.11
2	2	98	ASN	CA-CB-CG	6.24	118.84	112.60
2	2	99	LEU	CA-C-O	-6.22	114.25	122.03
2	2	231	VAL	CA-CB-CG1	6.21	120.96	110.40
2	2	34	PHE	CB-CA-C	6.19	119.96	109.75
2	2	175	ARG	NH1-CZ-NH2	-6.16	111.29	119.30
2	2	220	CYS	N-CA-CB	6.16	121.15	110.81
2	2	91	HIS	CA-C-O	-6.12	114.57	119.71
2	2	56	ALA	CA-C-O	6.11	127.44	120.90
2	2	235	LYS	N-CA-C	6.09	118.89	111.82
2	2	97(A)	GLU	CB-CG-CD	6.09	122.94	112.60
2	2	228	TYR	N-CA-CB	-6.08	100.91	110.69
2	2	93	ARG	CA-C-N	6.07	129.38	120.82
2	2	93	ARG	C-N-CA	6.07	129.38	120.82
1	1	10	LYS	CA-CB-CG	-6.06	101.98	114.10
2	2	216	GLY	CA-C-N	6.06	131.56	122.47
2	2	216	GLY	C-N-CA	6.06	131.56	122.47
2	2	230	HIS	CA-C-N	6.05	128.41	120.60
2	2	230	HIS	C-N-CA	6.05	128.41	120.60
2	2	69	GLY	CA-C-O	6.01	126.56	119.46
2	2	154	VAL	O-C-N	-5.96	117.14	122.69
2	2	204(B)	ASN	CB-CG-ND2	5.96	125.33	116.40
2	2	190	ALA	N-CA-C	-5.95	101.14	110.36
2	2	28	PRO	O-C-N	-5.92	115.01	122.17
2	2	237	TRP	N-CA-CB	5.90	118.89	110.16
2	2	204	PRO	C-N-CA	5.89	136.43	121.70
2	2	95	ASN	CA-CB-CG	5.88	118.48	112.60
2	2	180	MET	CA-C-N	5.88	131.51	121.87
2	2	180	MET	C-N-CA	5.88	131.51	121.87
2	2	65	LEU	N-CA-C	-5.88	100.22	109.50
1	1	14(L)	ASP	CA-C-O	5.88	127.33	120.75
2	2	156	GLN	CG-CD-NE2	-5.87	107.60	116.40
2	2	184(A)	TYR	N-CA-CB	5.85	118.72	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	176	ILE	CB-CG1-CD1	-5.85	101.52	113.80
1	1	12	LEU	CB-CA-C	5.84	119.90	109.38
2	2	203	SER	CA-C-O	-5.84	115.00	119.32
2	2	214	SER	O-C-N	5.83	130.34	122.59
2	2	123	LEU	N-CA-C	-5.81	101.20	109.62
2	2	221(A)	ARG	CD-NE-CZ	5.79	132.51	124.40
2	2	129(B)	SER	CB-CA-C	-5.79	101.80	110.88
1	1	13	GLU	N-CA-C	-5.76	100.79	109.95
2	2	65	LEU	O-C-N	5.76	130.33	123.24
2	2	162	ILE	N-CA-CB	-5.73	103.26	110.31
2	2	212	ILE	O-C-N	5.73	128.98	123.14
2	2	182	CYS	CA-CB-SG	5.72	127.56	114.40
2	2	91	HIS	CB-CA-C	-5.66	100.84	109.50
2	2	60(G)	ASN	N-CA-CB	5.66	120.05	110.49
2	2	91	HIS	N-CA-CB	5.65	119.29	109.57
2	2	46	LEU	O-C-N	5.65	129.71	122.93
2	2	129(B)	SER	CA-C-O	-5.65	114.89	120.82
1	1	14(D)	ARG	CD-NE-CZ	-5.62	116.53	124.40
2	2	116	ASP	O-C-N	5.61	129.95	122.43
2	2	158	VAL	CA-CB-CG1	5.61	119.93	110.40
2	2	163	VAL	O-C-N	-5.59	115.66	122.36
2	2	65	LEU	CA-CB-CG	5.57	135.81	116.30
2	2	69	GLY	CA-C-N	5.57	130.94	122.65
2	2	69	GLY	C-N-CA	5.57	130.94	122.65
2	2	94	TYR	CA-C-O	-5.56	114.58	120.92
2	2	85	LEU	O-C-N	5.55	129.76	122.93
1	1	14	ASP	CA-C-O	-5.55	115.40	121.89
2	2	75	ARG	N-CA-CB	5.54	119.86	110.49
2	2	24	ILE	N-CA-CB	5.53	117.54	110.13
2	2	31	VAL	CB-CA-C	5.52	119.00	110.50
2	2	126	ARG	CA-C-O	5.52	126.38	120.20
2	2	83	SER	CA-C-O	5.52	127.39	121.16
1	1	14(K)	ILE	O-C-N	5.51	131.52	122.70
2	2	143	ASN	CA-CB-CG	5.50	118.10	112.60
2	2	80	GLU	N-CA-CB	5.46	119.31	110.41
2	2	33	LEU	CB-CA-C	5.45	120.46	111.31
2	2	30	GLN	CA-C-N	-5.44	115.38	122.94
2	2	30	GLN	C-N-CA	-5.44	115.38	122.94
3	3	57	GLU	CG-CD-OE2	-5.44	105.90	118.40
2	2	74	THR	N-CA-CB	-5.40	102.15	109.98
4	4	380	ARG	NE-CZ-NH1	5.37	126.87	121.50
2	2	167	VAL	N-CA-CB	-5.36	104.28	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	196	GLY	CA-C-O	5.34	125.32	119.55
2	2	149(D)	GLY	N-CA-C	-5.32	106.71	112.08
2	2	143	ASN	N-CA-CB	5.31	118.13	109.69
2	2	134	TYR	O-C-N	5.30	129.26	123.01
2	2	186(D)	LYS	CA-C-O	-5.29	115.45	121.58
2	2	100	ASP	CB-CA-C	5.27	118.93	110.29
2	2	181	PHE	CA-CB-CG	5.26	119.06	113.80
2	2	82	ILE	N-CA-CB	5.26	117.36	111.21
2	2	54	THR	CA-CB-CG2	5.25	119.43	110.50
2	2	97	ARG	CA-C-O	-5.25	113.01	120.51
2	2	233	ARG	N-CA-CB	5.24	118.42	110.14
1	1	1(A)	ASP	N-CA-C	-5.24	104.48	111.87
2	2	47	ILE	N-CA-C	-5.22	107.74	113.43
2	2	82	ILE	O-C-N	5.21	129.85	122.97
2	2	49	ASP	CB-CG-OD1	5.21	130.38	118.40
2	2	202	LYS	O-C-N	5.20	129.15	123.27
2	2	76	TYR	CA-CB-CG	-5.19	104.55	113.90
2	2	162	ILE	CB-CA-C	5.19	119.06	111.33
2	2	242	ILE	O-C-N	5.15	126.93	121.89
1	1	14(B)	THR	N-CA-C	5.14	119.12	111.87
2	2	164	GLU	N-CA-CB	5.14	117.92	109.95
2	2	158	VAL	CB-CA-C	5.14	118.41	110.50
2	2	118	ILE	O-C-N	5.13	128.52	123.18
2	2	56	ALA	N-CA-C	5.13	117.27	111.11
2	2	181	PHE	N-CA-CB	5.11	119.64	111.56
2	2	60	LEU	N-CA-C	5.11	116.64	107.80
2	2	241	VAL	CB-CA-C	5.11	118.46	111.87
2	2	217	GLU	CA-C-O	5.10	127.36	120.47
2	2	125	ASP	CA-C-O	-5.06	115.48	121.66
2	2	231	VAL	O-C-N	5.05	127.00	121.94
2	2	49	ASP	N-CA-C	-5.04	106.64	112.89
2	2	149(B)	ASN	N-CA-CB	5.04	117.76	109.95
3	3	58	GLU	CB-CG-CD	5.04	121.17	112.60
2	2	110	LYS	O-C-N	5.04	124.93	121.71
2	2	206	ARG	NE-CZ-NH1	-5.04	116.47	121.50
2	2	75	ARG	CB-CA-C	-5.03	100.41	110.42
2	2	17	VAL	N-CA-C	5.03	116.51	108.87
2	2	243	ASP	CA-CB-CG	5.02	117.62	112.60
1	1	11	SER	N-CA-CB	5.02	119.92	112.30
2	2	25	GLY	O-C-N	5.02	127.33	122.41
2	2	70	LYS	O-C-N	5.02	129.06	123.19
2	2	226	GLY	O-C-N	5.01	130.18	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	120	PRO	O-C-N	-5.01	116.81	123.13
2	2	219	GLY	O-C-N	5.01	127.67	122.91
2	2	221(A)	ARG	CB-CG-CD	5.01	122.82	111.30
2	2	90	ILE	N-CA-C	5.00	116.47	108.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	192	GLU	Mainchain
2	2	233	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	287	0	278	71	0
2	2	2093	0	2064	342	0
3	3	94	0	74	6	0
4	4	29	0	29	5	0
5	1	3	0	0	1	0
5	2	44	0	0	10	0
5	3	4	0	0	0	0
All	All	2554	0	2445	391	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 79.

All (391) 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)
2:2:195:SER:HG	4:4:380:ARG:N	1.27	1.29
2:2:165:ARG:HB2	2:2:166:PRO:HD3	1.27	1.17
2:2:81:LYS:HD2	2:2:118:ILE:CD1	1.77	1.15
2:2:81:LYS:HD2	2:2:118:ILE:HD12	1.20	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:149(E):LYS:HE3	2:2:150:GLY:H	1.11	1.07
1:1:1(G):PHE:H	1:1:1(D):GLY:HA2	1.13	1.06
2:2:35:ARG:HG3	2:2:41:LEU:HD11	1.39	1.04
2:2:81:LYS:HE2	2:2:113:ALA:HB3	1.40	1.03
2:2:236:LYS:HD3	2:2:239:GLN:NE2	1.73	1.02
2:2:165:ARG:O	2:2:169:LYS:HG2	1.59	1.02
2:2:81:LYS:CD	2:2:118:ILE:HD12	1.91	1.01
2:2:56:ALA:HA	2:2:104:ALA:HB2	1.44	0.99
1:1:1(H):THR:HG23	2:2:242:ILE:HG21	1.44	0.99
2:2:122:CYS:HB2	2:2:208:TYR:CD1	1.97	0.98
2:2:236:LYS:HD3	2:2:239:GLN:HE21	1.27	0.97
2:2:23:GLU:HB2	2:2:26:MET:HG3	1.48	0.96
2:2:216:GLY:O	4:4:382:PRO:HA	1.65	0.96
2:2:36:LYS:HZ2	2:2:65:LEU:HD22	1.34	0.92
1:1:1(G):PHE:N	1:1:1(D):GLY:HA2	1.85	0.91
2:2:66:VAL:CG1	2:2:68:ILE:HD11	2.02	0.90
2:2:73:ARG:HH12	2:2:151:GLN:HB2	1.38	0.89
1:1:1(F):GLY:N	2:2:235:LYS:HZ1	1.70	0.89
2:2:165:ARG:HD3	2:2:169:LYS:CE	2.02	0.89
2:2:241:VAL:O	2:2:245:PHE:HB2	1.73	0.88
2:2:84:MET:HE3	2:2:109:LYS:HE3	1.54	0.88
2:2:46:LEU:HD22	2:2:48:SER:O	1.73	0.88
2:2:237:TRP:O	2:2:241:VAL:HG13	1.72	0.87
1:1:14(J):TYR:O	1:1:14(K):ILE:HB	1.71	0.87
2:2:21:ASP:HB3	2:2:154:VAL:HG11	1.56	0.86
2:2:36(A):SER:HA	2:2:37:PRO:C	2.01	0.85
2:2:195:SER:OG	4:4:380:ARG:N	2.08	0.85
1:1:1(G):PHE:O	1:1:1(D):GLY:N	2.10	0.84
2:2:237:TRP:O	2:2:241:VAL:CG1	2.26	0.83
2:2:35:ARG:HB3	2:2:39:GLU:HG3	1.60	0.82
2:2:60(B):PRO:HG2	2:2:96:TRP:CE2	2.14	0.82
1:1:1(H):THR:CG2	2:2:242:ILE:HG21	2.10	0.82
2:2:149(E):LYS:HE3	2:2:150:GLY:N	1.93	0.82
2:2:96:TRP:CZ2	2:2:97:ARG:CZ	2.66	0.79
2:2:81:LYS:CD	2:2:118:ILE:CD1	2.55	0.79
2:2:211:GLY:HA2	2:2:229:THR:O	1.84	0.78
2:2:165:ARG:CB	2:2:166:PRO:HD3	2.09	0.78
1:1:14(I):SER:C	1:1:14(K):ILE:H	1.94	0.76
2:2:28:PRO:HB2	2:2:119:HIS:HB3	1.68	0.76
2:2:35:ARG:HD2	2:2:39:GLU:OE1	1.84	0.76
2:2:16:ILE:HD13	2:2:190:ALA:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:35:ARG:CG	2:2:41:LEU:HD11	2.15	0.75
2:2:60(A):TYR:CZ	2:2:60(C):PRO:HG2	2.21	0.75
2:2:195:SER:HA	2:2:213:VAL:HB	1.68	0.75
2:2:73:ARG:NH1	2:2:151:GLN:HB2	2.01	0.75
2:2:165:ARG:HB2	2:2:166:PRO:CD	2.11	0.75
2:2:79:ILE:CD1	5:2:406:HOH:O	2.35	0.74
2:2:235:LYS:O	2:2:239:GLN:HG3	1.87	0.74
2:2:136:GLY:HA3	2:2:199:PHE:CZ	2.22	0.74
2:2:129(C):LEU:CD2	2:2:204(A):PHE:HE2	1.99	0.74
1:1:10:LYS:HE3	1:1:12:LEU:HD12	1.69	0.74
2:2:81:LYS:CE	2:2:113:ALA:HB3	2.18	0.74
2:2:137:ARG:HD3	2:2:159:ASN:OD1	1.87	0.74
2:2:73:ARG:HG3	2:2:141:TRP:HB3	1.70	0.73
2:2:16:ILE:HD12	2:2:158:VAL:HG12	1.70	0.73
1:1:10:LYS:HE3	1:1:12:LEU:CD1	2.18	0.73
2:2:181:PHE:CZ	2:2:211:GLY:HA3	2.23	0.73
2:2:59:LEU:HD12	2:2:104:ALA:HB1	1.69	0.73
2:2:36:LYS:HZ2	2:2:65:LEU:CD2	2.01	0.72
2:2:66:VAL:HG12	2:2:68:ILE:HD11	1.70	0.72
1:1:1(H):THR:H2	1:1:1(D):GLY:CA	2.03	0.72
2:2:139:THR:HG22	2:2:157:VAL:HG12	1.70	0.72
2:2:144:LEU:HD21	2:2:152:PRO:HB3	1.70	0.72
2:2:75:ARG:H	2:2:75:ARG:HD3	1.55	0.72
2:2:169:LYS:HZ2	2:2:176:ILE:CG2	2.03	0.72
1:1:1(G):PHE:HA	2:2:235:LYS:HZ3	1.54	0.71
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.19	0.71
2:2:36:LYS:NZ	2:2:65:LEU:HD22	2.04	0.71
2:2:184(A):TYR:CE2	2:2:186(D):LYS:HD3	2.25	0.71
2:2:84:MET:HE3	2:2:109:LYS:CE	2.20	0.71
1:1:6:LEU:HD23	2:2:24:ILE:HG22	1.72	0.71
2:2:69:GLY:O	2:2:79:ILE:HD11	1.91	0.71
2:2:67:ARG:HG2	2:2:82:ILE:HG12	1.72	0.70
1:1:14(E):GLU:HG2	2:2:159:ASN:HD22	1.55	0.70
1:1:10:LYS:HB3	1:1:12:LEU:CD1	2.22	0.70
2:2:79:ILE:HD11	5:2:406:HOH:O	1.90	0.70
2:2:169:LYS:HZ2	2:2:176:ILE:HG22	1.56	0.70
2:2:164:GLU:OE1	2:2:164:GLU:N	2.19	0.69
2:2:236:LYS:CD	2:2:239:GLN:HE21	2.02	0.69
1:1:14(J):TYR:O	1:1:14(K):ILE:CB	2.40	0.69
2:2:28:PRO:HG2	2:2:29:TRP:CZ3	2.26	0.69
2:2:28:PRO:HG2	2:2:29:TRP:CE3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:129(C):LEU:HD23	2:2:204(A):PHE:HE2	1.57	0.69
2:2:55:ALA:H	2:2:196:GLY:HA2	1.56	0.69
2:2:169:LYS:NZ	2:2:176:ILE:HG21	2.08	0.68
1:1:4:ARG:HG2	2:2:28:PRO:CD	2.23	0.68
2:2:21:ASP:HB3	2:2:154:VAL:CG1	2.23	0.68
2:2:60(I):THR:O	2:2:64:LEU:HD11	1.94	0.68
2:2:201:MET:HG3	2:2:210:MET:HG3	1.76	0.68
1:1:1(F):GLY:N	2:2:235:LYS:NZ	2.43	0.67
2:2:181:PHE:HZ	2:2:211:GLY:HA3	1.59	0.67
2:2:181:PHE:CD1	2:2:228:TYR:HB2	2.30	0.67
2:2:23:GLU:HB2	2:2:26:MET:CG	2.22	0.67
2:2:59:LEU:HD12	2:2:104:ALA:CB	2.23	0.67
2:2:83:SER:HB3	2:2:108:LEU:HD22	1.75	0.67
2:2:17:VAL:O	2:2:188:GLY:HA2	1.94	0.67
2:2:165:ARG:HD3	2:2:169:LYS:HE2	1.75	0.67
2:2:17:VAL:HG13	2:2:144:LEU:O	1.95	0.67
2:2:46:LEU:CD2	2:2:48:SER:O	2.41	0.67
1:1:13:GLU:OE2	1:1:14(D):ARG:HG3	1.94	0.66
1:1:4:ARG:HG2	2:2:28:PRO:HG3	1.77	0.66
2:2:148:TRP:HB3	2:2:149(B):ASN:CG	2.20	0.66
2:2:172:THR:CG2	2:2:176:ILE:HD11	2.25	0.66
2:2:75:ARG:HD3	2:2:75:ARG:N	2.08	0.66
2:2:165:ARG:O	2:2:169:LYS:N	2.26	0.65
2:2:54:THR:HG23	2:2:104:ALA:HB3	1.77	0.65
2:2:176:ILE:HD12	5:2:453:HOH:O	1.96	0.65
2:2:172:THR:HG23	2:2:176:ILE:HD11	1.79	0.64
1:1:14:ASP:CG	2:2:26:MET:HE2	2.22	0.64
2:2:229:THR:HG23	5:2:434:HOH:O	1.98	0.64
2:2:47:ILE:HD13	2:2:53:LEU:HD13	1.80	0.64
2:2:144:LEU:HG	2:2:150:GLY:O	1.98	0.63
2:2:164:GLU:H	2:2:164:GLU:CD	2.06	0.63
1:1:1(H):THR:H2	1:1:1(D):GLY:HA3	1.61	0.63
1:1:1(H):THR:N	1:1:1(D):GLY:CA	2.61	0.63
2:2:182:CYS:HA	2:2:226:GLY:O	1.99	0.62
2:2:221(A):ARG:HG3	5:2:416:HOH:O	1.98	0.62
2:2:181:PHE:CE1	2:2:228:TYR:HB2	2.35	0.62
2:2:165:ARG:NH2	2:2:178:ASP:HA	2.15	0.62
2:2:230:HIS:CD2	2:2:233:ARG:NH1	2.67	0.62
2:2:169:LYS:NZ	2:2:176:ILE:CG2	2.61	0.62
2:2:165:ARG:HB3	2:2:169:LYS:HE2	1.82	0.61
1:1:5:PRO:N	1:1:9:LYS:HD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:93:ARG:O	2:2:101:ARG:NH1	2.34	0.60
1:1:1(H):THR:HG23	2:2:242:ILE:CG2	2.24	0.60
1:1:1(C):GLU:HG2	2:2:120:PRO:HG2	1.84	0.60
2:2:16:ILE:N	2:2:143:ASN:O	2.35	0.60
2:2:16:ILE:N	2:2:194:ASP:OD1	2.35	0.60
2:2:174:ILE:N	2:2:174:ILE:HD13	2.16	0.60
2:2:134:TYR:HD1	2:2:134:TYR:N	1.99	0.59
1:1:1(H):THR:N	1:1:1(D):GLY:HA3	2.17	0.59
1:1:1(C):GLU:HG2	2:2:120:PRO:CG	2.33	0.59
2:2:61:GLU:O	2:2:64:LEU:HD12	2.00	0.59
2:2:129(C):LEU:CD2	2:2:204(A):PHE:CE2	2.84	0.59
2:2:183:ALA:HB3	2:2:228:TYR:CE1	2.37	0.59
2:2:165:ARG:C	2:2:169:LYS:HG2	2.28	0.59
2:2:167:VAL:HA	5:2:440:HOH:O	2.03	0.59
2:2:35:ARG:HB2	2:2:41:LEU:HG	1.84	0.59
2:2:96:TRP:CE3	2:2:97:ARG:HA	2.38	0.59
2:2:236:LYS:CD	2:2:239:GLN:NE2	2.59	0.59
1:1:14(D):ARG:O	1:1:14(H):GLU:HG3	2.03	0.59
2:2:32:MET:HB3	2:2:67:ARG:HB2	1.85	0.58
2:2:129(A):ALA:O	2:2:131:GLN:OE1	2.21	0.58
1:1:14(K):ILE:HD12	5:1:421:HOH:O	2.03	0.58
2:2:180:MET:HA	2:2:228:TYR:O	2.03	0.58
2:2:181:PHE:CE1	2:2:228:TYR:CB	2.85	0.58
1:1:1(G):PHE:HA	2:2:235:LYS:NZ	2.18	0.58
2:2:169:LYS:HZ3	2:2:176:ILE:HG21	1.68	0.58
2:2:86:GLU:HB2	2:2:109:LYS:HA	1.84	0.58
2:2:165:ARG:O	2:2:168:CYS:HB2	2.03	0.58
2:2:36(A):SER:CA	2:2:37:PRO:C	2.74	0.58
1:1:5:PRO:HA	1:1:9:LYS:HB2	1.85	0.58
2:2:122:CYS:HB2	2:2:208:TYR:CE1	2.39	0.58
1:1:7:PHE:O	1:1:11:SER:N	2.36	0.57
2:2:197:GLY:O	2:2:213:VAL:HG23	2.04	0.57
2:2:219:GLY:HA3	2:2:221(A):ARG:HD3	1.84	0.57
2:2:47:ILE:CD1	2:2:53:LEU:HD13	2.34	0.57
1:1:1(G):PHE:C	2:2:235:LYS:NZ	2.63	0.57
2:2:33:LEU:O	2:2:41:LEU:N	2.23	0.57
2:2:134:TYR:N	2:2:134:TYR:CD1	2.69	0.57
2:2:146:GLU:OE2	2:2:221(A):ARG:CD	2.53	0.57
1:1:1(F):GLY:H	2:2:235:LYS:HZ1	1.50	0.57
2:2:81:LYS:HE2	2:2:113:ALA:CB	2.27	0.57
2:2:96:TRP:HZ2	2:2:97:ARG:CZ	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:174:ILE:N	2:2:174:ILE:CD1	2.67	0.57
2:2:96:TRP:CG	2:2:97:ARG:H	2.22	0.57
2:2:96:TRP:CG	2:2:97:ARG:N	2.72	0.57
2:2:61:GLU:OE2	2:2:87:LYS:HD3	2.04	0.56
2:2:122:CYS:CB	2:2:208:TYR:CD1	2.81	0.56
2:2:50:ARG:HH11	2:2:107:LYS:HD3	1.70	0.56
2:2:171:SER:O	2:2:224:LYS:NZ	2.37	0.56
2:2:83:SER:CB	2:2:108:LEU:HD22	2.35	0.56
1:1:6:LEU:CD2	2:2:24:ILE:HG22	2.35	0.56
2:2:96:TRP:C	2:2:97(A):GLU:H	2.14	0.56
1:1:1(H):THR:H2	1:1:1(D):GLY:HA2	1.68	0.55
2:2:185:LYS:HB3	2:2:186:PRO:HD2	1.87	0.55
2:2:123:LEU:HB3	2:2:235:LYS:HE2	1.86	0.55
2:2:185:LYS:O	2:2:186(B):GLU:HB2	2.06	0.55
2:2:59:LEU:CD1	2:2:104:ALA:HB1	2.35	0.55
3:3:60:PRO:C	3:3:62:GLU:H	2.14	0.55
2:2:129(C):LEU:HD23	2:2:204(A):PHE:CE2	2.41	0.55
2:2:165:ARG:HD3	2:2:169:LYS:HE3	1.87	0.55
1:1:10:LYS:HB3	1:1:12:LEU:HD12	1.88	0.55
2:2:234:LEU:O	2:2:238:ILE:HG13	2.06	0.55
1:1:1(D):GLY:O	1:1:1(C):GLU:O	2.25	0.54
1:1:3:LEU:O	1:1:9:LYS:HE3	2.07	0.54
1:1:7:PHE:CE2	1:1:14:ASP:HB3	2.41	0.54
2:2:59:LEU:HD22	2:2:88:ILE:HD13	1.89	0.54
2:2:200:VAL:HG12	2:2:209:GLN:HA	1.88	0.54
4:4:380:ARG:N	4:4:381:PRO:HD3	2.21	0.54
2:2:125:ASP:OD1	2:2:125:ASP:N	2.41	0.54
2:2:60(B):PRO:HG2	2:2:96:TRP:CZ2	2.42	0.54
2:2:144:LEU:HD11	2:2:151:GLN:C	2.33	0.54
2:2:148:TRP:CE2	2:2:149(A):ALA:HB3	2.43	0.54
2:2:170:ASP:HB2	5:2:440:HOH:O	2.07	0.54
1:1:1(A):ASP:OD1	1:1:3:LEU:HD12	2.07	0.54
2:2:54:THR:CG2	2:2:104:ALA:HB3	2.38	0.54
2:2:64:LEU:HD12	2:2:64:LEU:H	1.72	0.54
2:2:60(I):THR:O	2:2:64:LEU:CD1	2.56	0.53
2:2:103:ILE:HG13	2:2:212:ILE:CD1	2.38	0.53
2:2:191:CYS:N	2:2:194:ASP:OD1	2.41	0.53
2:2:23:GLU:O	2:2:26:MET:HB2	2.09	0.53
2:2:60(F):LYS:O	2:2:60(G):ASN:HB2	2.09	0.53
2:2:146:GLU:OE2	2:2:221(A):ARG:HD3	2.09	0.53
2:2:151:GLN:N	2:2:151:GLN:CD	2.64	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:178:ASP:O	2:2:233:ARG:NH1	2.42	0.53
2:2:96:TRP:CD2	2:2:97:ARG:N	2.76	0.53
2:2:129(C):LEU:HD21	2:2:204(A):PHE:CE2	2.44	0.53
2:2:136:GLY:O	2:2:159:ASN:HA	2.08	0.53
2:2:165:ARG:HH11	2:2:169:LYS:NZ	2.06	0.53
2:2:69:GLY:O	2:2:79:ILE:CD1	2.57	0.53
2:2:185:LYS:HG2	2:2:225:TYR:OH	2.08	0.53
2:2:105:LEU:HD13	2:2:241:VAL:CG2	2.39	0.53
2:2:204:PRO:HG2	2:2:204(A):PHE:CE1	2.43	0.53
2:2:235:LYS:O	2:2:239:GLN:CG	2.57	0.53
2:2:137:ARG:CD	2:2:159:ASN:OD1	2.55	0.53
2:2:122:CYS:CB	2:2:208:TYR:CE1	2.92	0.52
2:2:165:ARG:HH22	2:2:178:ASP:HA	1.74	0.52
2:2:214:SER:HB3	2:2:215:TRP:CD1	2.45	0.52
2:2:167:VAL:HG22	5:2:463:HOH:O	2.08	0.52
1:1:1:CYS:O	1:1:3:LEU:HG	2.09	0.52
1:1:5:PRO:CA	1:1:9:LYS:HD2	2.40	0.52
2:2:195:SER:CB	4:4:380:ARG:N	2.72	0.52
2:2:94:TYR:HA	2:2:100:ASP:O	2.09	0.52
2:2:127:GLU:OE2	2:2:127:GLU:N	2.41	0.52
1:1:14:ASP:OD1	2:2:137:ARG:NH1	2.39	0.52
2:2:139:THR:CG2	2:2:157:VAL:HG12	2.37	0.52
2:2:35:ARG:HD3	2:2:37:PRO:O	2.10	0.51
2:2:91:HIS:CE1	2:2:101:ARG:HD3	2.46	0.51
2:2:48:SER:HB3	2:2:51:TRP:H	1.75	0.51
2:2:148:TRP:HD1	2:2:149(B):ASN:HB3	1.76	0.51
2:2:200:VAL:HA	2:2:208:TYR:O	2.11	0.51
2:2:135:LYS:HE2	2:2:184(A):TYR:OH	2.10	0.51
1:1:1(G):PHE:CE2	1:1:1(D):GLY:O	2.63	0.51
2:2:21:ASP:OD1	2:2:154:VAL:HB	2.10	0.51
2:2:18:GLU:HG3	2:2:187:ARG:HB3	1.93	0.51
2:2:214:SER:HB2	2:2:227:PHE:O	2.11	0.51
2:2:81:LYS:HD3	2:2:112:VAL:CG1	2.41	0.51
2:2:69:GLY:O	2:2:79:ILE:CG1	2.59	0.51
2:2:89:TYR:HB2	2:2:105:LEU:HB2	1.93	0.51
2:2:103:ILE:HG13	2:2:212:ILE:HD11	1.93	0.50
2:2:146:GLU:OE2	2:2:221(A):ARG:HD2	2.12	0.50
2:2:195:SER:HA	2:2:213:VAL:CB	2.39	0.50
1:1:2:GLY:HA2	2:2:29:TRP:CZ3	2.46	0.50
1:1:5:PRO:HA	1:1:9:LYS:CD	2.42	0.50
2:2:36(A):SER:HA	2:2:38:GLN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:50:ARG:NH1	2:2:86:GLU:OE1	2.44	0.50
2:2:148:TRP:HB3	2:2:149(B):ASN:OD1	2.10	0.50
2:2:140:GLY:C	2:2:155:LEU:HD12	2.36	0.50
2:2:20:SER:O	2:2:157:VAL:HG22	2.12	0.50
2:2:21:ASP:OD1	2:2:154:VAL:CG1	2.60	0.50
2:2:203:SER:OG	2:2:204(A):PHE:HB2	2.12	0.50
2:2:60(B):PRO:HB2	2:2:60(C):PRO:HD3	1.93	0.49
2:2:181:PHE:CZ	2:2:228:TYR:HB3	2.46	0.49
1:1:1(G):PHE:O	1:1:1(E):SER:N	2.44	0.49
2:2:88:ILE:HG12	2:2:106:MET:HE2	1.93	0.49
2:2:169:LYS:HA	2:2:176:ILE:CD1	2.42	0.49
2:2:178:ASP:OD1	2:2:233:ARG:NH2	2.45	0.49
2:2:144:LEU:HD21	2:2:152:PRO:CB	2.40	0.49
2:2:201:MET:HG3	2:2:210:MET:CG	2.42	0.49
3:3:59:ILE:HD11	3:3:64:LEU:HD13	1.95	0.49
2:2:165:ARG:N	2:2:166:PRO:CD	2.76	0.49
2:2:148:TRP:HA	2:2:148:TRP:HE3	1.77	0.49
2:2:169:LYS:HA	2:2:176:ILE:HD13	1.94	0.48
2:2:35:ARG:HB2	2:2:41:LEU:CG	2.43	0.48
2:2:100:ASP:OD1	2:2:179:ASN:HB2	2.13	0.48
2:2:50:ARG:NH1	2:2:107:LYS:HD3	2.27	0.48
1:1:14(I):SER:C	1:1:14(K):ILE:N	2.62	0.48
2:2:35:ARG:CD	2:2:39:GLU:OE1	2.58	0.48
2:2:96:TRP:CZ2	2:2:97:ARG:NH1	2.81	0.48
2:2:164:GLU:HB3	2:2:166:PRO:HD2	1.95	0.48
2:2:181:PHE:O	2:2:227:PHE:HA	2.14	0.48
2:2:108:LEU:O	2:2:109:LYS:C	2.56	0.48
2:2:192:GLU:H	2:2:192:GLU:HG3	1.39	0.48
2:2:164:GLU:O	2:2:167:VAL:HB	2.14	0.48
2:2:112:VAL:HG12	2:2:113:ALA:N	2.29	0.47
2:2:235:LYS:HA	2:2:238:ILE:HD12	1.96	0.47
2:2:105:LEU:HD13	2:2:241:VAL:HG21	1.96	0.47
2:2:126:ARG:HB2	2:2:232:PHE:CZ	2.50	0.47
2:2:136:GLY:HA3	2:2:199:PHE:CE2	2.50	0.47
2:2:124:PRO:HD3	2:2:209:GLN:O	2.14	0.47
2:2:130:LEU:HG	2:2:210:MET:HE2	1.96	0.47
2:2:201:MET:CG	2:2:210:MET:HG3	2.44	0.47
2:2:36:LYS:HE2	2:2:62:ASN:O	2.14	0.47
2:2:219:GLY:HA3	2:2:221(A):ARG:CG	2.44	0.47
2:2:60(B):PRO:N	2:2:60(C):PRO:CD	2.77	0.47
1:1:10:LYS:O	1:1:12:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:35:ARG:CB	2:2:41:LEU:HD11	2.44	0.46
1:1:1(H):THR:N	1:1:1(D):GLY:HA2	2.29	0.46
1:1:14:ASP:OD2	2:2:26:MET:HE2	2.14	0.46
2:2:162:ILE:HD12	2:2:201:MET:CE	2.46	0.46
2:2:166:PRO:O	2:2:170:ASP:CG	2.58	0.46
2:2:182:CYS:HB3	2:2:227:PHE:CE2	2.50	0.46
2:2:60(G):ASN:ND2	5:2:402:HOH:O	2.49	0.46
2:2:149(E):LYS:HD2	2:2:149(E):LYS:HA	1.75	0.46
1:1:1(A):ASP:O	2:2:119:HIS:NE2	2.49	0.46
2:2:59:LEU:HD11	2:2:106:MET:HE1	1.97	0.46
2:2:73:ARG:HD3	2:2:152:PRO:O	2.15	0.46
1:1:14(B):THR:HG23	2:2:137:ARG:NH2	2.31	0.46
2:2:184(A):TYR:CZ	2:2:186(D):LYS:HD3	2.51	0.46
2:2:23:GLU:HB2	2:2:26:MET:HB2	1.97	0.46
2:2:69:GLY:O	2:2:79:ILE:HG13	2.16	0.45
2:2:70:LYS:HB3	2:2:70:LYS:HE3	1.33	0.45
1:1:10:LYS:HE3	1:1:12:LEU:HD11	1.98	0.45
2:2:81:LYS:HE2	2:2:113:ALA:O	2.17	0.45
2:2:18:GLU:HB2	2:2:188:GLY:HA2	1.99	0.45
1:1:1(G):PHE:CA	2:2:235:LYS:NZ	2.79	0.45
2:2:29:TRP:CG	2:2:121:VAL:HB	2.52	0.45
1:1:1(G):PHE:C	2:2:235:LYS:HZ3	2.24	0.45
2:2:56:ALA:O	2:2:59:LEU:HB2	2.17	0.45
2:2:181:PHE:HZ	2:2:211:GLY:CA	2.28	0.45
2:2:21:ASP:OD1	2:2:154:VAL:HG12	2.17	0.45
2:2:70:LYS:HD2	2:2:80:GLU:OE2	2.16	0.45
2:2:178:ASP:O	2:2:233:ARG:HD2	2.17	0.45
1:1:14(C):GLU:O	1:1:14(F):LEU:HB2	2.17	0.45
2:2:35:ARG:CB	2:2:39:GLU:HG3	2.42	0.45
2:2:96:TRP:CE3	2:2:97:ARG:CA	2.99	0.45
2:2:114:PHE:CZ	2:2:120:PRO:HD3	2.52	0.45
2:2:165:ARG:HH11	2:2:169:LYS:HZ2	1.66	0.44
1:1:1(C):GLU:HG2	2:2:120:PRO:HG3	1.99	0.44
2:2:204:PRO:HD2	2:2:204(A):PHE:CE2	2.52	0.44
2:2:35:ARG:HD3	2:2:39:GLU:HG3	1.98	0.44
1:1:5:PRO:O	1:1:7:PHE:N	2.50	0.44
2:2:21:ASP:CB	2:2:154:VAL:HG11	2.37	0.44
2:2:148:TRP:HA	2:2:148:TRP:CE3	2.52	0.44
3:3:57:GLU:HG2	3:3:58:GLU:O	2.17	0.44
1:1:14(G):LEU:O	1:1:14(H):GLU:C	2.61	0.44
2:2:96:TRP:C	2:2:97(A):GLU:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:214:SER:HB3	2:2:215:TRP:HD1	1.83	0.44
1:1:4:ARG:HE	1:1:4:ARG:HB2	1.66	0.44
2:2:35:ARG:O	2:2:38:GLN:HA	2.18	0.44
2:2:198:PRO:HA	2:2:209:GLN:HE21	1.83	0.44
2:2:230:HIS:NE2	2:2:233:ARG:NH1	2.66	0.44
2:2:35:ARG:HD2	2:2:35:ARG:HH11	1.29	0.43
2:2:64:LEU:HD12	2:2:64:LEU:N	2.32	0.43
2:2:183:ALA:HB3	2:2:228:TYR:HE1	1.83	0.43
2:2:65:LEU:HD11	3:3:63:TYS:O	2.18	0.43
2:2:162:ILE:HD12	2:2:201:MET:HE1	2.00	0.43
1:1:1(G):PHE:CA	2:2:235:LYS:HZ3	2.25	0.43
2:2:126:ARG:HA	2:2:232:PHE:CZ	2.53	0.43
2:2:36:LYS:NZ	2:2:64:LEU:O	2.50	0.43
2:2:203:SER:OG	2:2:204(A):PHE:CD2	2.71	0.43
3:3:60:PRO:C	3:3:62:GLU:N	2.75	0.43
1:1:4:ARG:HG2	2:2:28:PRO:HD2	1.99	0.43
2:2:46:LEU:O	2:2:120:PRO:HA	2.19	0.42
2:2:51:TRP:NE1	2:2:247:GLU:O	2.52	0.42
2:2:66:VAL:HG13	2:2:68:ILE:HD11	1.95	0.42
1:1:1(G):PHE:N	1:1:1(G):PHE:CD2	2.80	0.42
2:2:66:VAL:HG12	2:2:83:SER:HB2	2.01	0.42
2:2:23:GLU:HB2	2:2:26:MET:CB	2.50	0.42
2:2:29:TRP:CD2	2:2:121:VAL:HB	2.54	0.42
2:2:51:TRP:CD1	2:2:247:GLU:O	2.72	0.42
2:2:126:ARG:N	2:2:127:GLU:OE2	2.53	0.42
2:2:60(B):PRO:C	2:2:60(E):ASP:H	2.28	0.42
2:2:96:TRP:CE3	2:2:97:ARG:N	2.88	0.42
2:2:65:LEU:HG	2:2:82:ILE:CG2	2.49	0.41
2:2:191:CYS:O	2:2:192:GLU:C	2.61	0.41
2:2:199:PHE:HD2	2:2:210:MET:HB2	1.84	0.41
1:1:5:PRO:C	1:1:7:PHE:H	2.28	0.41
2:2:165:ARG:HD3	2:2:169:LYS:NZ	2.34	0.41
2:2:91:HIS:HB3	2:2:94:TYR:HB2	2.01	0.41
2:2:95:ASN:N	2:2:100:ASP:O	2.52	0.41
2:2:106:MET:HE2	2:2:106:MET:HB3	1.25	0.41
2:2:181:PHE:HE2	2:2:230:HIS:HA	1.86	0.41
2:2:181:PHE:CZ	2:2:211:GLY:CA	2.98	0.41
2:2:198:PRO:HA	2:2:209:GLN:NE2	2.35	0.41
1:1:14(I):SER:O	1:1:14(K):ILE:N	2.52	0.41
2:2:21:ASP:CB	2:2:154:VAL:CG1	2.97	0.41
2:2:81:LYS:NZ	2:2:118:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:185:LYS:NZ	2:2:185:LYS:HB2	2.34	0.41
2:2:203:SER:OG	2:2:204(A):PHE:HD2	2.03	0.41
1:1:1(G):PHE:O	1:1:1(F):GLY:C	2.62	0.41
2:2:29:TRP:O	2:2:45:SER:HA	2.21	0.41
2:2:36:LYS:HZ3	2:2:36:LYS:HG3	1.54	0.41
2:2:73:ARG:NH1	2:2:151:GLN:CB	2.76	0.41
2:2:85:LEU:HD12	2:2:88:ILE:HD11	2.03	0.41
2:2:96:TRP:O	2:2:97(A):GLU:N	2.53	0.41
2:2:126:ARG:HB2	2:2:232:PHE:HZ	1.85	0.41
2:2:181:PHE:CZ	2:2:228:TYR:CB	3.04	0.41
2:2:236:LYS:HD3	2:2:239:GLN:HE22	1.73	0.41
2:2:236:LYS:O	2:2:240:LYS:HB2	2.21	0.41
2:2:60(H):PHE:HB3	2:2:64:LEU:HD21	2.02	0.40
2:2:60(I):THR:O	2:2:61:GLU:C	2.64	0.40
2:2:175:ARG:HG3	5:2:456:HOH:O	2.20	0.40
1:1:14(L):ASP:HB3	1:1:15:ARG:HG3	2.03	0.40
2:2:81:LYS:CD	2:2:118:ILE:HD13	2.48	0.40
3:3:58:GLU:H	3:3:58:GLU:CD	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	34/36 (94%)	22 (65%)	6 (18%)	6 (18%)	0	0
2	2	257/259 (99%)	235 (91%)	19 (7%)	3 (1%)	10	12
3	3	7/10 (70%)	5 (71%)	2 (29%)	0	100	100
4	4	2/5 (40%)	2 (100%)	0	0	100	100
All	All	300/310 (97%)	264 (88%)	27 (9%)	9 (3%)	3	2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	1(D)	GLY
1	1	1(C)	GLU
1	1	14(K)	ILE
2	2	97	ARG
1	1	1(B)	ALA
2	2	77(A)	ARG
2	2	60(G)	ASN
1	1	1(F)	GLY
1	1	5	PRO

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	1	31/31 (100%)	27 (87%)	4 (13%)	4	4
2	2	225/225 (100%)	180 (80%)	45 (20%)	1	1
3	3	9/9 (100%)	5 (56%)	4 (44%)	0	0
4	4	3/4 (75%)	1 (33%)	2 (67%)	0	0
All	All	268/269 (100%)	213 (80%)	55 (20%)	1	1

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	6	LEU
1	1	9	LYS
1	1	10	LYS
1	1	15	ARG
2	2	17	VAL
2	2	24	ILE
2	2	26	MET
2	2	30	GLN
2	2	33	LEU
2	2	39	GLU
2	2	46	LEU
2	2	53	LEU
2	2	57	HIS

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Mol	Chain	Res	Type
2	2	61	GLU
2	2	62	ASN
2	2	64	LEU
2	2	66	VAL
2	2	70	LYS
2	2	75	ARG
2	2	79	ILE
2	2	81	LYS
2	2	90	ILE
2	2	106	MET
2	2	109	LYS
2	2	125	ASP
2	2	126	ARG
2	2	128	THR
2	2	129(B)	SER
2	2	129(C)	LEU
2	2	130	LEU
2	2	134	TYR
2	2	138	VAL
2	2	148	TRP
2	2	151	GLN
2	2	153	SER
2	2	154	VAL
2	2	164	GLU
2	2	170	ASP
2	2	174	ILE
2	2	182	CYS
2	2	185	LYS
2	2	192	GLU
2	2	195	SER
2	2	214	SER
2	2	239	GLN
2	2	241	VAL
2	2	242	ILE
2	2	244	GLN
2	2	247	GLU
3	3	58	GLU
3	3	59	ILE
3	3	62	GLU
3	3	64	LEU
4	4	380	ARG
4	4	382	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	30	GLN
2	2	60(G)	ASN
2	2	131	GLN
2	2	204(B)	ASN
2	2	239	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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
3	TYS	3	63	3	15,16,17	1.47	2 (13%)	15,22,24	1.68	3 (20%)

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
3	TYS	3	63	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	63	TYS	OH-S	3.52	1.65	1.58
3	3	63	TYS	OH-CZ	-3.28	1.37	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	63	TYS	CD1-CE1-CZ	-3.39	115.86	119.73
3	3	63	TYS	CB-CG-CD1	-2.90	115.52	120.90
3	3	63	TYS	CE2-CZ-CE1	2.41	123.68	120.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	63	TYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.