



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 AM UTC

PDB ID : 1HAG / pdb_00001hag
Title : THE ISOMORPHOUS STRUCTURES OF PRETHROMBIN2, HIRUGEN-
AND PPACK-THROMBIN: CHANGES ACCOMPANYING ACTIVATION
AND EXOSITE BINDING TO THROMBIN
Authors : Tulinsky, A.; Vijayalakshmi, J.
Deposited on : 1994-06-27
Resolution : 2.00 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

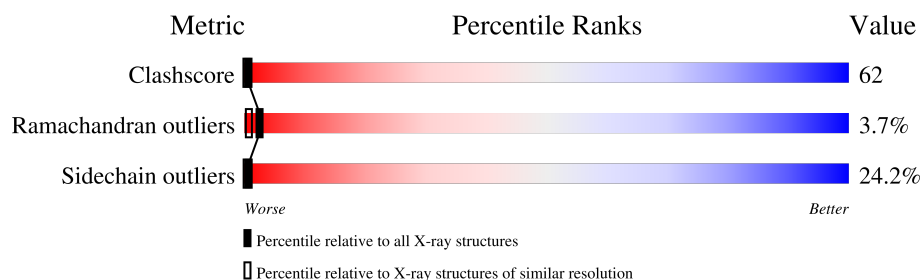
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	E	295	
2	I	10	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2690 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.

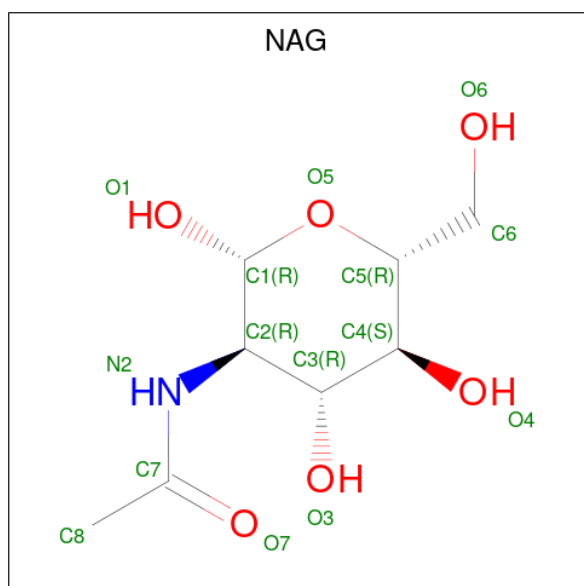
- Molecule 1 is a protein called PRETHROMBIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	295	Total	C	N	O	S	0	0	0
			2379	1511	418	435	15			

- Molecule 2 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	S	0	0	0
			95	59	10	25	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

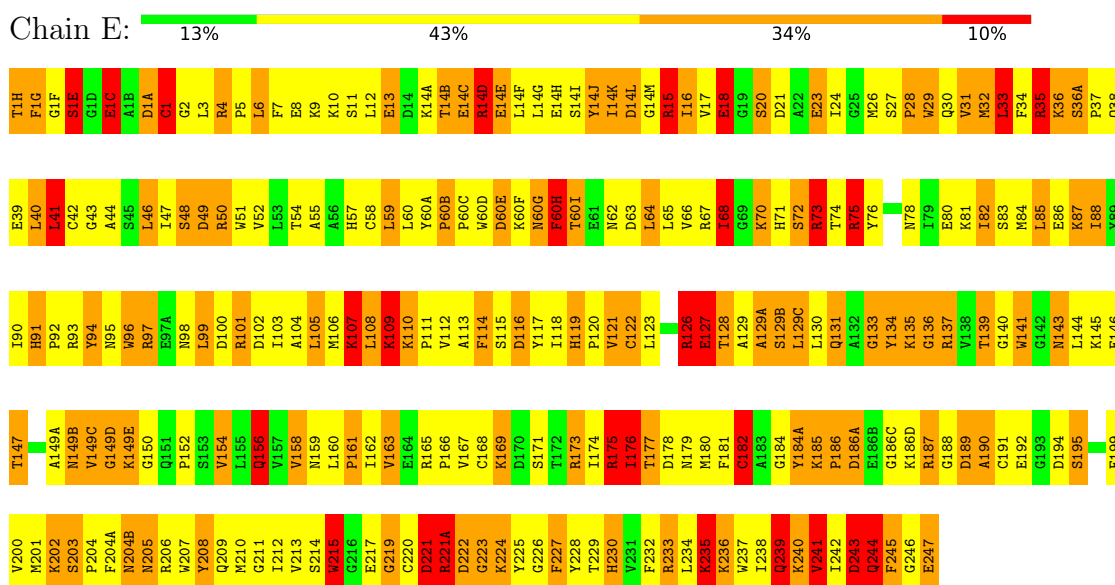
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	188	Total 188	O 188	0	0
4	I	14	Total 14	O 14	0	0

3 Residue-property plots

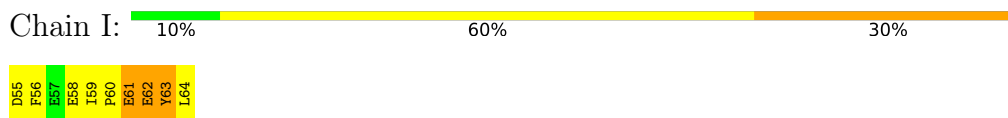
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PRETHROMBIN 2



• Molecule 2: HIRUGEN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.85Å 71.32Å 72.63Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	E	1.60	21/2438 (0.9%)	2.85	282/3290 (8.6%)
2	I	1.12	0/79	2.69	7/103 (6.8%)
All	All	1.59	21/2517 (0.8%)	2.84	289/3393 (8.5%)

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
1	E	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	TRP	C-N	-8.03	1.23	1.33
1	E	149(D)	GLY	N-CA	7.62	1.51	1.44
1	E	42	CYS	C-O	-7.22	1.16	1.24
1	E	122	CYS	N-CA	6.99	1.54	1.45
1	E	135	LYS	C-N	-6.59	1.27	1.33
1	E	47	ILE	C-N	-6.58	1.26	1.33
1	E	115	SER	C-N	-6.42	1.25	1.34
1	E	55	ALA	N-CA	6.34	1.54	1.46
1	E	147	THR	CA-CB	6.10	1.61	1.53
1	E	74	THR	CA-CB	5.97	1.62	1.54
1	E	201	MET	N-CA	5.92	1.53	1.45
1	E	46	LEU	C-N	-5.88	1.27	1.33
1	E	11	SER	C-N	5.82	1.41	1.33
1	E	208	TYR	CA-C	5.79	1.59	1.52
1	E	174	ILE	N-CA	5.67	1.53	1.46
1	E	232	PHE	C-O	5.59	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	33	LEU	CA-CB	-5.49	1.45	1.53
1	E	48	SER	CA-CB	-5.42	1.47	1.54
1	E	161	PRO	CA-CB	-5.20	1.48	1.54
1	E	33	LEU	CA-C	5.17	1.59	1.52
1	E	195	SER	C-O	5.07	1.29	1.23

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	243	ASP	CA-CB-CG	14.82	127.42	112.60
1	E	1(A)	ASP	CA-CB-CG	-14.29	98.31	112.60
1	E	75	ARG	NE-CZ-NH2	13.29	131.16	119.20
1	E	102	ASP	CA-CB-CG	12.37	124.97	112.60
1	E	186(A)	ASP	CA-CB-CG	12.24	124.84	112.60
1	E	233	ARG	NE-CZ-NH2	11.92	129.93	119.20
1	E	232	PHE	O-C-N	-11.60	110.02	122.09
1	E	187	ARG	CD-NE-CZ	11.56	140.59	124.40
1	E	117	TYR	CA-C-N	10.70	137.65	123.10
1	E	117	TYR	C-N-CA	10.70	137.65	123.10
1	E	179	ASN	CA-C-O	-10.38	105.67	120.51
1	E	205	ASN	CA-CB-CG	-10.33	102.27	112.60
1	E	14(I)	SER	N-CA-C	-10.31	99.47	113.18
1	E	67	ARG	NE-CZ-NH2	10.27	128.44	119.20
1	E	74	THR	N-CA-C	10.13	126.93	113.97
1	E	126	ARG	NE-CZ-NH1	-10.05	111.45	121.50
1	E	60(B)	PRO	CB-CA-C	9.94	123.04	110.92
1	E	18	GLU	CB-CG-CD	9.46	128.68	112.60
1	E	60(I)	THR	CA-CB-OG1	-9.44	95.44	109.60
1	E	126	ARG	CD-NE-CZ	-9.36	111.29	124.40
1	E	113	ALA	CA-C-O	-9.17	110.17	120.54
1	E	173	ARG	N-CA-C	-9.17	101.80	113.72
1	E	150	GLY	O-C-N	9.13	130.08	123.14
1	E	240	LYS	CA-C-O	-9.11	108.61	119.27
1	E	60(H)	PHE	CA-CB-CG	-9.08	104.72	113.80
1	E	13	GLU	CA-C-O	-9.07	110.73	120.80
1	E	176	ILE	CA-CB-CG2	9.06	125.90	110.50
1	E	4	ARG	NE-CZ-NH2	9.05	127.35	119.20
1	E	129	ALA	CB-CA-C	9.00	125.01	110.88
1	E	204(B)	ASN	OD1-CG-ND2	8.92	131.52	122.60
1	E	105	LEU	O-C-N	8.89	133.71	123.31
1	E	190	ALA	O-C-N	8.87	131.52	122.12
1	E	233	ARG	NE-CZ-NH1	-8.81	112.69	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	129(B)	SER	N-CA-C	8.78	122.00	111.82
1	E	8	GLU	O-C-N	8.77	131.56	122.09
2	I	61	GLU	CB-CG-CD	8.71	127.41	112.60
1	E	78	ASN	CB-CG-ND2	8.64	129.37	116.40
1	E	21	ASP	CA-CB-CG	8.55	121.15	112.60
1	E	13	GLU	CB-CA-C	-8.43	95.32	109.48
1	E	245	PHE	CA-C-N	8.41	134.91	122.64
1	E	245	PHE	C-N-CA	8.41	134.91	122.64
1	E	113	ALA	O-C-N	8.31	132.69	123.22
1	E	202	LYS	CA-C-O	-8.24	111.54	120.36
1	E	137	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	E	204(A)	PHE	CA-CB-CG	-8.10	105.70	113.80
1	E	129(A)	ALA	CA-C-O	-8.07	112.20	121.07
1	E	1(E)	SER	N-CA-C	-7.84	103.78	112.72
1	E	32	MET	CA-C-O	-7.72	112.05	120.24
1	E	118	ILE	N-CA-C	7.70	118.97	106.72
1	E	60(I)	THR	CB-CA-C	7.60	124.41	109.66
1	E	32	MET	O-C-N	7.60	132.16	123.27
1	E	176	ILE	N-CA-CB	7.59	118.81	110.53
1	E	33	LEU	CA-CB-CG	7.56	142.77	116.30
1	E	40	LEU	CA-C-O	-7.55	112.83	120.98
1	E	235	LYS	O-C-N	7.54	130.79	122.20
1	E	82	ILE	CA-C-O	-7.54	112.47	120.53
1	E	241	VAL	N-CA-CB	7.53	120.78	110.54
1	E	76	TYR	N-CA-C	-7.51	99.16	110.28
1	E	126	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	E	68	ILE	CB-CA-C	-7.50	100.40	110.98
1	E	60(I)	THR	CA-CB-CG2	7.50	123.25	110.50
1	E	128	THR	N-CA-C	-7.49	103.06	111.14
1	E	119	HIS	CA-C-N	7.37	127.29	119.85
1	E	119	HIS	C-N-CA	7.37	127.29	119.85
1	E	24	ILE	N-CA-C	-7.27	100.21	109.58
1	E	90	ILE	CA-C-O	-7.25	112.27	121.48
1	E	114	PHE	CA-CB-CG	-7.16	106.64	113.80
1	E	76	TYR	CA-C-O	-7.14	113.17	121.16
1	E	97	ARG	CA-C-O	-7.13	113.27	120.90
1	E	117	TYR	CA-C-O	-7.12	111.30	119.14
1	E	209	GLN	CA-C-O	-7.12	112.96	120.58
1	E	75	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	E	158	VAL	CA-C-N	7.07	132.18	122.77
1	E	158	VAL	C-N-CA	7.07	132.18	122.77
1	E	212	ILE	CA-C-O	-7.04	112.99	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	HIS	CA-CB-CG	7.03	120.83	113.80
1	E	144	LEU	N-CA-C	-7.03	104.68	113.18
1	E	23	GLU	CA-CB-CG	7.01	128.11	114.10
1	E	189	ASP	O-C-N	6.99	131.79	123.27
1	E	167	VAL	CA-C-O	-6.89	113.20	120.57
1	E	42	CYS	CA-C-N	6.89	130.43	121.13
1	E	42	CYS	C-N-CA	6.89	130.43	121.13
1	E	41	LEU	CA-C-O	-6.88	113.61	120.70
1	E	31	VAL	O-C-N	-6.86	115.63	122.76
1	E	14(B)	THR	N-CA-CB	-6.79	98.66	111.43
1	E	60(I)	THR	N-CA-CB	-6.79	100.20	111.20
1	E	154	VAL	N-CA-CB	-6.79	101.07	112.47
1	E	80	GLU	CG-CD-OE2	-6.77	102.82	118.40
1	E	204(B)	ASN	CA-C-O	-6.77	111.49	119.48
1	E	30	GLN	CA-C-N	6.71	132.11	122.45
1	E	30	GLN	C-N-CA	6.71	132.11	122.45
1	E	49	ASP	N-CA-C	-6.68	105.03	113.72
1	E	3	LEU	CA-C-O	6.67	127.41	120.40
1	E	137	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	E	145	LYS	CA-C-N	6.67	134.27	121.54
1	E	145	LYS	C-N-CA	6.67	134.27	121.54
1	E	202	LYS	CB-CA-C	-6.65	99.41	110.19
2	I	55	ASP	CB-CA-C	6.65	122.74	110.10
1	E	76	TYR	CB-CA-C	6.64	121.00	109.65
1	E	167	VAL	O-C-N	6.61	128.54	121.87
1	E	149(B)	ASN	N-CA-C	-6.59	102.63	110.41
1	E	161	PRO	CA-C-O	-6.56	113.91	121.98
1	E	70	LYS	N-CA-C	6.56	120.75	110.32
1	E	173	ARG	O-C-N	6.54	130.39	122.35
2	I	61	GLU	CA-CB-CG	6.53	127.16	114.10
1	E	91	HIS	CB-CA-C	6.51	119.81	109.52
1	E	75	ARG	CA-C-N	-6.51	111.63	120.87
1	E	75	ARG	C-N-CA	-6.51	111.63	120.87
1	E	154	VAL	CA-CB-CG1	6.48	121.42	110.40
1	E	202	LYS	O-C-N	6.46	130.59	123.22
1	E	135	LYS	CA-C-N	6.43	129.74	122.67
1	E	135	LYS	C-N-CA	6.43	129.74	122.67
1	E	49	ASP	O-C-N	6.38	130.20	122.35
1	E	75	ARG	CD-NE-CZ	-6.36	115.50	124.40
1	E	235	LYS	CA-C-O	-6.34	113.10	120.20
1	E	225	TYR	N-CA-CB	-6.34	101.21	111.22
1	E	149(E)	LYS	CA-C-N	-6.33	117.29	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149(E)	LYS	C-N-CA	-6.33	117.29	122.16
1	E	239	GLN	OE1-CD-NE2	6.32	128.92	122.60
1	E	163	VAL	CB-CA-C	6.32	121.12	110.95
1	E	1(C)	GLU	CA-C-O	6.32	128.10	120.27
1	E	94	TYR	CA-C-N	6.28	132.07	122.77
1	E	94	TYR	C-N-CA	6.28	132.07	122.77
1	E	126	ARG	CA-C-O	-6.27	114.19	120.90
1	E	105	LEU	CA-C-O	-6.26	113.37	120.32
1	E	128	THR	O-C-N	6.26	128.85	122.09
1	E	131	GLN	CB-CG-CD	-6.26	101.95	112.60
1	E	136	GLY	N-CA-C	-6.26	101.67	112.06
2	I	56	PHE	CA-CB-CG	-6.26	107.54	113.80
1	E	195	SER	N-CA-C	-6.25	101.17	110.23
1	E	68	ILE	CA-C-O	-6.23	113.61	120.84
1	E	171	SER	CA-C-O	6.22	125.85	118.69
1	E	88	ILE	N-CA-CB	6.21	119.98	111.41
1	E	241	VAL	N-CA-C	-6.21	104.29	110.62
1	E	100	ASP	CA-C-O	-6.21	114.21	121.16
1	E	156	GLN	CB-CG-CD	-6.20	102.05	112.60
1	E	99	LEU	CA-C-O	-6.20	113.30	120.98
1	E	120	PRO	CA-C-N	-6.18	113.74	122.34
1	E	120	PRO	C-N-CA	-6.18	113.74	122.34
1	E	28	PRO	N-CA-C	6.17	121.57	113.86
1	E	135	LYS	N-CA-CB	6.17	119.37	110.06
1	E	1(E)	SER	C-N-CA	6.16	135.24	122.30
1	E	60(E)	ASP	O-C-N	6.16	132.56	122.70
1	E	85	LEU	O-C-N	6.15	130.38	123.19
1	E	119	HIS	CA-C-O	-6.14	112.99	119.50
2	I	64	LEU	N-CA-CB	-6.10	100.12	110.50
1	E	67	ARG	NH1-CZ-NH2	-6.08	111.40	119.30
1	E	1(E)	SER	CA-C-O	6.07	127.00	119.78
1	E	27	SER	CA-C-N	6.04	125.66	119.56
1	E	27	SER	C-N-CA	6.04	125.66	119.56
1	E	115	SER	CA-C-N	6.03	129.48	120.31
1	E	115	SER	C-N-CA	6.03	129.48	120.31
1	E	123	LEU	N-CA-CB	6.03	118.43	110.29
1	E	121	VAL	CA-C-O	-6.02	115.19	121.93
1	E	204(B)	ASN	CA-C-N	6.02	133.90	123.91
1	E	204(B)	ASN	C-N-CA	6.02	133.90	123.91
1	E	14(C)	GLU	CA-C-O	-6.00	112.00	119.38
1	E	203	SER	CA-C-O	6.00	125.39	119.75
1	E	128	THR	N-CA-CB	5.97	118.73	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	187	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	E	243	ASP	CB-CG-OD1	5.96	132.11	118.40
1	E	177	THR	CA-CB-CG2	5.95	120.62	110.50
1	E	3	LEU	CB-CA-C	5.95	120.32	110.74
1	E	75	ARG	CB-CG-CD	5.94	124.96	111.30
1	E	30	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	E	35	ARG	O-C-N	5.92	129.94	123.13
1	E	85	LEU	CA-C-O	-5.91	114.24	120.80
1	E	182	CYS	CA-C-O	-5.90	114.21	121.11
1	E	209	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	E	169	LYS	CA-C-N	5.89	132.79	121.54
1	E	169	LYS	C-N-CA	5.89	132.79	121.54
1	E	175	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	E	136	GLY	CA-C-O	-5.87	115.19	121.88
1	E	176	ILE	CB-CA-C	5.86	118.77	111.15
1	E	186	PRO	N-CA-C	-5.86	100.40	112.47
1	E	100	ASP	O-C-N	5.83	130.01	122.89
1	E	235	LYS	N-CA-C	5.83	119.22	111.75
1	E	23	GLU	N-CA-CB	5.83	119.91	110.41
1	E	29	TRP	N-CA-C	-5.83	106.13	113.18
1	E	71	HIS	CA-C-O	5.82	125.80	119.40
1	E	14(D)	ARG	NE-CZ-NH2	-5.82	113.97	119.20
1	E	26	MET	CA-C-O	5.82	126.53	119.49
1	E	134	TYR	O-C-N	5.81	129.84	123.22
1	E	133	GLY	CA-C-N	5.80	130.37	122.19
1	E	133	GLY	C-N-CA	5.80	130.37	122.19
1	E	8	GLU	CA-C-O	-5.76	114.76	120.70
1	E	1	CYS	CA-C-N	5.76	131.94	120.77
1	E	1	CYS	C-N-CA	5.76	131.94	120.77
1	E	235	LYS	CA-CB-CG	-5.75	102.59	114.10
1	E	55	ALA	CB-CA-C	5.74	119.21	109.80
1	E	227	PHE	CA-CB-CG	-5.74	108.06	113.80
1	E	14(J)	TYR	N-CA-CB	5.73	119.15	110.45
1	E	97	ARG	CD-NE-CZ	5.73	132.42	124.40
1	E	232	PHE	CB-CA-C	5.72	119.97	110.81
1	E	149(D)	GLY	N-CA-C	-5.71	102.70	112.64
1	E	54	THR	CA-CB-OG1	-5.71	101.03	109.60
1	E	191	CYS	O-C-N	5.69	130.31	122.46
1	E	101	ARG	CD-NE-CZ	-5.68	116.44	124.40
1	E	115	SER	N-CA-C	-5.67	101.30	108.45
1	E	24	ILE	CA-C-N	5.66	132.51	121.41
1	E	24	ILE	C-N-CA	5.66	132.51	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	LEU	N-CA-CB	5.65	119.48	110.16
1	E	74	THR	N-CA-CB	-5.59	102.90	110.67
1	E	1(C)	GLU	C-N-CA	5.59	135.66	121.70
1	E	136	GLY	O-C-N	5.57	128.44	123.59
1	E	52	VAL	CA-C-N	5.56	130.68	123.00
1	E	52	VAL	C-N-CA	5.56	130.68	123.00
1	E	107	LYS	O-C-N	5.56	129.85	123.29
1	E	240	LYS	CA-C-N	-5.56	112.84	120.46
1	E	240	LYS	C-N-CA	-5.56	112.84	120.46
1	E	140	GLY	O-C-N	5.56	129.37	123.81
1	E	96	TRP	CB-CA-C	5.55	120.85	110.70
1	E	108	LEU	O-C-N	5.52	129.09	122.79
1	E	127	GLU	N-CA-C	5.52	118.22	111.82
1	E	58	CYS	O-C-N	5.50	129.03	122.27
1	E	107	LYS	N-CA-CB	5.49	119.19	110.57
1	E	195	SER	CA-C-O	-5.47	115.17	121.19
1	E	224	LYS	CB-CA-C	5.47	121.31	110.42
1	E	72	SER	CB-CA-C	5.47	118.79	109.72
1	E	46	LEU	CA-C-O	-5.46	114.31	120.43
1	E	14(K)	ILE	CB-CG1-CD1	-5.45	102.36	113.80
1	E	14(J)	TYR	CA-C-O	-5.44	115.39	121.81
1	E	141	TRP	CA-C-N	5.44	130.60	120.87
1	E	141	TRP	C-N-CA	5.44	130.60	120.87
1	E	104	ALA	N-CA-CB	5.43	121.63	111.53
1	E	222	ASP	CA-C-O	5.43	126.79	120.49
1	E	14(L)	ASP	CB-CA-C	5.40	121.17	110.42
1	E	33	LEU	N-CA-C	-5.40	100.50	109.46
1	E	58	CYS	CA-C-O	-5.40	113.76	119.97
1	E	158	VAL	CA-C-O	5.38	126.66	120.90
1	E	109	LYS	CA-CB-CG	5.37	124.85	114.10
2	I	64	LEU	CB-CA-C	5.37	120.30	110.10
1	E	33	LEU	O-C-N	5.35	129.32	123.22
1	E	194	ASP	O-C-N	5.35	130.19	123.23
1	E	222	ASP	CA-C-N	5.35	131.90	121.41
1	E	222	ASP	C-N-CA	5.35	131.90	121.41
1	E	163	VAL	CA-C-N	5.34	128.43	120.95
1	E	163	VAL	C-N-CA	5.34	128.43	120.95
1	E	208	TYR	CA-CB-CG	5.34	123.51	113.90
1	E	115	SER	CA-C-O	-5.33	115.66	121.14
1	E	200	VAL	CA-CB-CG1	5.33	119.45	110.40
1	E	9	LYS	CA-C-O	-5.32	113.05	119.49
1	E	99	LEU	N-CA-CB	-5.30	104.14	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	TYR	N-CA-C	5.29	117.85	109.50
1	E	1(C)	GLU	CA-CB-CG	5.27	124.65	114.10
1	E	91	HIS	O-C-N	-5.27	115.87	121.30
1	E	154	VAL	CB-CA-C	5.26	118.48	110.90
1	E	173	ARG	CA-C-N	-5.26	113.82	121.71
1	E	173	ARG	C-N-CA	-5.26	113.82	121.71
1	E	63	ASP	N-CA-CB	5.26	118.64	110.44
1	E	73	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	E	184(A)	TYR	CA-C-O	5.26	128.01	121.81
1	E	60(H)	PHE	N-CA-C	5.25	118.26	110.48
1	E	60(B)	PRO	N-CA-C	5.24	117.09	110.70
1	E	244	GLN	O-C-N	5.23	127.58	122.19
1	E	75	ARG	CG-CD-NE	5.22	123.49	112.00
1	E	134	TYR	CB-CA-C	-5.22	101.24	109.80
2	I	58	GLU	CG-CD-OE1	5.22	130.41	118.40
1	E	13	GLU	CA-CB-CG	5.21	124.53	114.10
1	E	184(A)	TYR	N-CA-C	-5.21	103.51	110.55
1	E	241	VAL	CA-C-O	-5.21	115.53	120.95
1	E	230	HIS	CA-C-O	-5.20	115.36	120.98
1	E	4	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	E	14(L)	ASP	C-N-CA	-5.18	111.42	122.30
1	E	184	GLY	O-C-N	5.18	130.98	122.70
1	E	14(I)	SER	CB-CA-C	5.17	119.33	110.23
1	E	43	GLY	N-CA-C	-5.17	104.80	113.02
1	E	2	GLY	N-CA-C	5.17	122.31	114.61
1	E	14(E)	GLU	CA-C-O	-5.16	115.14	120.92
1	E	80	GLU	CA-CB-CG	5.16	124.41	114.10
1	E	104	ALA	O-C-N	5.16	129.25	123.27
1	E	20	SER	CA-CB-OG	5.16	121.41	111.10
1	E	222	ASP	OD1-CG-OD2	5.15	135.26	122.90
1	E	139	THR	CA-C-O	-5.14	115.09	121.06
1	E	78	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	E	88	ILE	O-C-N	5.14	128.81	123.26
1	E	179	ASN	CA-CB-CG	-5.14	107.46	112.60
1	E	105	LEU	CA-C-N	-5.13	115.25	122.94
1	E	105	LEU	C-N-CA	-5.13	115.25	122.94
1	E	210	MET	CA-C-O	5.12	124.78	119.14
1	E	181	PHE	CB-CA-C	5.12	122.09	110.67
1	E	118	ILE	CB-CA-C	-5.10	105.15	111.32
1	E	204(B)	ASN	CB-CG-ND2	-5.09	108.77	116.40
1	E	24	ILE	N-CA-CB	5.09	118.07	110.13
1	E	60(E)	ASP	CA-CB-CG	-5.07	107.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173	ARG	N-CA-CB	5.07	118.11	110.65
1	E	63	ASP	O-C-N	5.05	129.38	122.46
1	E	72	SER	CA-C-O	5.03	126.72	121.19
1	E	116	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	126	ARG	Sidechain
1	E	14(D)	ARG	Sidechain
1	E	15	ARG	Sidechain
1	E	175	ARG	Sidechain
1	E	73	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	E	2379	0	2342	298	0
2	I	95	0	73	6	0
3	E	14	0	13	2	0
4	E	188	0	0	32	0
4	I	14	0	0	0	0
All	All	2690	0	2428	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 62.

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)
1:E:185:LYS:HE2	1:E:186(D):LYS:CE	1.63	1.28
1:E:14(K):ILE:CD1	1:E:161:PRO:HB3	1.62	1.27
1:E:75:ARG:NH1	1:E:75:ARG:CA	2.01	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:GLY:HA2	4:E:521:HOH:O	1.34	1.23
1:E:75:ARG:HH11	1:E:75:ARG:CB	1.59	1.15
1:E:75:ARG:NH1	1:E:75:ARG:HA	1.60	1.14
1:E:75:ARG:CA	1:E:75:ARG:HH11	1.58	1.13
1:E:14(K):ILE:HD11	1:E:161:PRO:HB3	1.13	1.13
1:E:185:LYS:CE	1:E:186(D):LYS:HE2	1.80	1.11
1:E:186:PRO:CB	1:E:223:GLY:HA3	1.80	1.10
1:E:14(D):ARG:H	1:E:14(D):ARG:HD2	0.97	1.07
1:E:110:LYS:HG3	1:E:111:PRO:HD2	1.36	1.06
1:E:245:PHE:O	4:E:556:HOH:O	1.72	1.06
1:E:185:LYS:HE2	1:E:186(D):LYS:HE2	1.05	1.05
1:E:186:PRO:HB3	1:E:223:GLY:HA3	1.09	1.05
1:E:35:ARG:HG3	1:E:41:LEU:HD11	1.38	1.03
1:E:186:PRO:HB3	1:E:223:GLY:CA	1.87	1.02
1:E:109:LYS:HE2	4:E:520:HOH:O	1.57	1.02
1:E:14(C):GLU:O	1:E:14(G):LEU:HD23	1.59	1.01
1:E:75:ARG:HH11	1:E:75:ARG:CG	1.63	0.99
1:E:149(E):LYS:O	1:E:149(E):LYS:HG2	1.56	0.99
1:E:18:GLU:HB3	1:E:187:ARG:HE	1.25	0.98
1:E:75:ARG:HA	1:E:75:ARG:HH12	1.18	0.97
1:E:130:LEU:CD1	1:E:230:HIS:CE1	2.47	0.97
1:E:204(B):ASN:C	1:E:204(B):ASN:HD22	1.67	0.96
1:E:14(D):ARG:HD2	1:E:14(D):ARG:N	1.76	0.95
1:E:185:LYS:HE2	1:E:186(D):LYS:NZ	1.83	0.93
1:E:49:ASP:O	1:E:112:VAL:HG12	1.67	0.93
1:E:14(B):THR:HG23	1:E:159:ASN:HD21	1.32	0.92
1:E:221:ASP:OD2	4:E:460:HOH:O	1.86	0.91
1:E:16:ILE:HD11	1:E:187:ARG:N	1.86	0.90
1:E:14(K):ILE:HD11	1:E:161:PRO:CB	1.99	0.90
1:E:186:PRO:HG3	1:E:223:GLY:C	1.96	0.90
1:E:186:PRO:HG3	1:E:223:GLY:O	1.73	0.88
1:E:14(B):THR:HG22	1:E:137:ARG:NH2	1.90	0.87
1:E:14(J):TYR:HD1	1:E:14(J):TYR:H	1.23	0.85
1:E:186(C):GLY:O	1:E:186(D):LYS:HE3	1.76	0.85
1:E:186(A):ASP:HB3	1:E:186(D):LYS:NZ	1.90	0.85
1:E:222:ASP:O	1:E:224:LYS:HG3	1.77	0.85
1:E:128:THR:HG22	1:E:129(C):LEU:HD12	1.57	0.84
1:E:14(D):ARG:H	1:E:14(D):ARG:CD	1.87	0.84
1:E:73:ARG:HG3	1:E:141:TRP:CD1	2.12	0.84
1:E:110:LYS:CG	1:E:111:PRO:HD2	2.07	0.83
1:E:72:SER:OG	1:E:75:ARG:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14(B):THR:HG22	1:E:137:ARG:HH21	1.44	0.82
1:E:241:VAL:O	1:E:245:PHE:HB2	1.78	0.82
1:E:204(B):ASN:C	1:E:204(B):ASN:ND2	2.36	0.82
1:E:14(A):LYS:HD3	4:E:585:HOH:O	1.78	0.81
1:E:98:ASN:O	1:E:99:LEU:HB2	1.80	0.81
1:E:103:ILE:HG21	1:E:234:LEU:HD13	1.61	0.81
1:E:130:LEU:HD11	1:E:230:HIS:CE1	2.15	0.80
1:E:192:GLU:OE2	4:E:474:HOH:O	1.98	0.79
1:E:188:GLY:CA	4:E:521:HOH:O	2.06	0.79
1:E:35:ARG:HG3	1:E:41:LEU:CD1	2.10	0.79
1:E:1(H):THR:HG23	1:E:1(H):THR:O	1.82	0.79
1:E:130:LEU:HD12	1:E:230:HIS:CE1	2.16	0.79
1:E:16:ILE:HD11	1:E:186(D):LYS:HA	1.63	0.78
1:E:84:MET:HE2	2:I:63:TYS:O	1.83	0.78
1:E:186(A):ASP:CB	1:E:186(D):LYS:HD3	2.14	0.78
1:E:75:ARG:NH1	1:E:75:ARG:N	2.32	0.78
1:E:130:LEU:HD12	1:E:230:HIS:HE1	1.48	0.77
1:E:16:ILE:HD11	1:E:186(D):LYS:CA	2.13	0.77
1:E:14(K):ILE:CD1	1:E:161:PRO:CB	2.56	0.77
1:E:189:ASP:O	1:E:192:GLU:HB2	1.83	0.77
1:E:128:THR:CG2	1:E:129(C):LEU:HD12	2.15	0.76
1:E:219:GLY:N	1:E:224:LYS:HE3	2.00	0.76
1:E:16:ILE:HD11	1:E:187:ARG:H	1.47	0.76
1:E:147:THR:OG1	1:E:149(A):ALA:HB3	1.86	0.76
1:E:35:ARG:CG	1:E:41:LEU:HD11	2.15	0.76
1:E:127:GLU:OE2	4:E:489:HOH:O	2.04	0.75
1:E:72:SER:OG	1:E:75:ARG:CG	2.35	0.74
1:E:239:GLN:HG3	4:E:436:HOH:O	1.85	0.74
1:E:97:ARG:HG3	4:E:419:HOH:O	1.89	0.72
1:E:36:LYS:O	1:E:38:GLN:HG3	1.89	0.71
1:E:103:ILE:CG2	1:E:234:LEU:HD13	2.21	0.71
1:E:64:LEU:O	4:E:449:HOH:O	2.09	0.71
1:E:204(B):ASN:HD22	1:E:205:ASN:N	1.87	0.71
1:E:49:ASP:HB3	1:E:114:PHE:CZ	2.26	0.71
1:E:14(K):ILE:HD12	1:E:161:PRO:HB3	1.71	0.70
1:E:94:TYR:HB2	1:E:101:ARG:O	1.92	0.70
1:E:185:LYS:CD	1:E:186(D):LYS:HE2	2.21	0.70
1:E:59:LEU:HD22	1:E:88:ILE:HD13	1.73	0.70
1:E:75:ARG:NH1	1:E:75:ARG:CB	2.39	0.69
1:E:75:ARG:NH1	1:E:75:ARG:CG	2.41	0.69
1:E:110:LYS:HG3	1:E:111:PRO:CD	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:GLU:HB3	1:E:187:ARG:NE	2.04	0.68
1:E:223:GLY:C	1:E:224:LYS:HG2	2.19	0.68
1:E:244:GLN:C	1:E:244:GLN:OE1	2.36	0.68
1:E:93:ARG:NH1	4:E:539:HOH:O	2.27	0.68
1:E:16:ILE:HD11	1:E:186(D):LYS:C	2.19	0.67
1:E:32:MET:CG	1:E:40:LEU:HD13	2.25	0.67
1:E:35:ARG:CG	1:E:41:LEU:CD1	2.72	0.67
1:E:35:ARG:O	1:E:38:GLN:HA	1.94	0.67
1:E:84:MET:O	1:E:109:LYS:HB2	1.94	0.67
1:E:18:GLU:HA	1:E:187:ARG:HB3	1.75	0.67
1:E:214:SER:HG	1:E:215:TRP:CD1	2.12	0.67
1:E:73:ARG:HG3	1:E:141:TRP:CG	2.30	0.67
1:E:14(E):GLU:O	1:E:14(H):GLU:HG3	1.94	0.66
1:E:59:LEU:HD13	1:E:88:ILE:HG21	1.75	0.66
1:E:147:THR:HG21	1:E:149(A):ALA:HB2	1.77	0.66
1:E:188:GLY:N	4:E:521:HOH:O	2.26	0.66
1:E:1(G):PHE:HD1	1:E:1(G):PHE:O	1.79	0.66
1:E:109:LYS:NZ	4:E:508:HOH:O	2.22	0.66
1:E:109:LYS:HD2	4:E:508:HOH:O	1.95	0.65
1:E:16:ILE:CD1	1:E:187:ARG:H	2.08	0.65
1:E:185:LYS:HD3	1:E:185:LYS:N	2.12	0.65
1:E:185:LYS:O	1:E:186(D):LYS:CG	2.44	0.65
1:E:14(D):ARG:O	1:E:14(G):LEU:HB2	1.96	0.65
1:E:5:PRO:HG3	4:E:523:HOH:O	1.96	0.65
1:E:175:ARG:HB3	4:E:410:HOH:O	1.96	0.64
1:E:126:ARG:O	1:E:126:ARG:HG3	1.96	0.64
1:E:185:LYS:O	1:E:186(D):LYS:HG2	1.97	0.64
1:E:186(A):ASP:HB3	1:E:186(D):LYS:HD3	1.78	0.64
1:E:215:TRP:CZ3	1:E:227:PHE:CG	2.85	0.64
1:E:129(A):ALA:O	4:E:602:HOH:O	2.15	0.64
1:E:235:LYS:HA	1:E:238:ILE:HD12	1.78	0.64
1:E:203:SER:HB3	1:E:204(B):ASN:ND2	2.13	0.63
1:E:143:ASN:O	1:E:146:GLU:HG3	1.98	0.63
1:E:203:SER:HB3	1:E:204(B):ASN:HD21	1.63	0.63
1:E:186(A):ASP:HB3	1:E:186(D):LYS:HZ2	1.63	0.63
1:E:165:ARG:HH22	1:E:177:THR:C	2.07	0.63
1:E:1(G):PHE:O	1:E:1(E):SER:N	2.31	0.63
1:E:85:LEU:HD12	4:E:449:HOH:O	1.98	0.62
1:E:186(A):ASP:CB	1:E:186(D):LYS:HZ3	2.12	0.62
1:E:35:ARG:HB2	1:E:41:LEU:CD1	2.29	0.62
1:E:185:LYS:HE2	1:E:186(D):LYS:HZ3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:GLY:H	1:E:224:LYS:HE3	1.63	0.62
1:E:4:ARG:HG2	1:E:28:PRO:CG	2.29	0.62
1:E:41:LEU:HD22	1:E:64:LEU:CD2	2.29	0.62
1:E:217:GLU:HB3	1:E:224:LYS:HB3	1.82	0.62
1:E:91:HIS:ND1	1:E:92:PRO:HD2	2.15	0.61
1:E:186:PRO:CG	1:E:223:GLY:O	2.48	0.61
1:E:158:VAL:HG21	1:E:188:GLY:HA2	1.82	0.61
1:E:224:LYS:HE2	4:E:497:HOH:O	2.00	0.61
1:E:75:ARG:HH11	1:E:75:ARG:N	1.95	0.61
1:E:14(B):THR:CG2	1:E:137:ARG:HH21	2.11	0.61
1:E:185:LYS:CD	1:E:185:LYS:N	2.60	0.60
1:E:186:PRO:CG	1:E:223:GLY:HA3	2.31	0.60
1:E:41:LEU:HD21	1:E:60(H):PHE:CE2	2.36	0.60
1:E:149(E):LYS:O	1:E:149(E):LYS:CG	2.37	0.60
1:E:186(C):GLY:C	1:E:186(D):LYS:HD2	2.27	0.60
1:E:14(J):TYR:N	1:E:14(J):TYR:CD1	2.70	0.60
1:E:185:LYS:CD	1:E:185:LYS:H	1.97	0.60
1:E:235:LYS:HG2	1:E:235:LYS:O	2.00	0.60
3:E:400:NAG:H4	4:E:560:HOH:O	2.02	0.60
1:E:75:ARG:HH11	1:E:75:ARG:HG2	1.63	0.59
1:E:14(F):LEU:HB3	4:E:406:HOH:O	2.03	0.59
1:E:14(M):GLY:O	1:E:15:ARG:C	2.47	0.58
1:E:84:MET:CE	2:I:63:TYS:O	2.52	0.58
1:E:186(D):LYS:HD2	1:E:186(D):LYS:N	2.19	0.58
1:E:32:MET:HG2	1:E:40:LEU:HD13	1.86	0.58
1:E:186(A):ASP:CB	1:E:186(D):LYS:NZ	2.64	0.58
1:E:186(A):ASP:HB3	1:E:186(D):LYS:HZ3	1.66	0.57
1:E:10:LYS:NZ	4:E:486:HOH:O	2.37	0.57
1:E:211:GLY:HA2	1:E:229:THR:O	2.04	0.57
1:E:176:ILE:HD12	1:E:180:MET:HB2	1.85	0.57
1:E:203:SER:HB2	1:E:208:TYR:HE1	1.70	0.57
1:E:41:LEU:HD22	1:E:64:LEU:HD22	1.86	0.56
1:E:247:GLU:O	1:E:247:GLU:HG3	2.04	0.56
1:E:70:LYS:HE3	1:E:72:SER:O	2.05	0.56
1:E:14(K):ILE:O	1:E:14(L):ASP:C	2.49	0.56
1:E:221:ASP:CG	1:E:221(A):ARG:N	2.64	0.56
1:E:1(H):THR:O	1:E:1(H):THR:CG2	2.51	0.56
1:E:217:GLU:CB	1:E:224:LYS:HB3	2.35	0.56
1:E:16:ILE:CD1	1:E:186(D):LYS:HA	2.33	0.56
1:E:35:ARG:HB3	1:E:39:GLU:HG2	1.88	0.56
1:E:215:TRP:CZ3	1:E:227:PHE:CD1	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:VAL:HG21	1:E:108:LEU:HD21	1.89	0.55
1:E:49:ASP:C	1:E:112:VAL:HG12	2.31	0.55
1:E:16:ILE:CD1	1:E:187:ARG:N	2.65	0.55
2:I:59:ILE:O	2:I:59:ILE:HG13	2.05	0.55
1:E:217:GLU:HB3	1:E:224:LYS:CB	2.36	0.55
1:E:185:LYS:CE	1:E:186(D):LYS:CE	2.55	0.54
1:E:14(G):LEU:N	1:E:14(G):LEU:HD22	2.22	0.54
1:E:135:LYS:HE2	1:E:184(A):TYR:OH	2.08	0.54
1:E:49:ASP:HB3	1:E:114:PHE:HZ	1.67	0.54
1:E:105:LEU:HD12	1:E:241:VAL:CG1	2.38	0.54
1:E:36(A):SER:HA	1:E:37:PRO:C	2.32	0.54
1:E:203:SER:N	1:E:206:ARG:O	2.38	0.54
1:E:182:CYS:HA	1:E:226:GLY:O	2.08	0.54
1:E:219:GLY:O	1:E:221:ASP:N	2.40	0.53
1:E:14(F):LEU:N	1:E:14(F):LEU:HD12	2.22	0.53
1:E:14(F):LEU:N	1:E:14(F):LEU:CD1	2.70	0.53
1:E:136:GLY:HA3	1:E:199:PHE:CZ	2.44	0.53
1:E:49:ASP:CB	1:E:114:PHE:CZ	2.92	0.53
1:E:158:VAL:HG21	1:E:188:GLY:CA	2.39	0.53
1:E:86:GLU:O	1:E:87:LYS:HG2	2.09	0.52
1:E:234:LEU:O	1:E:237:TRP:HB3	2.09	0.52
3:E:400:NAG:C4	4:E:560:HOH:O	2.57	0.52
1:E:186:PRO:HG3	1:E:223:GLY:CA	2.40	0.52
1:E:239:GLN:HA	4:E:436:HOH:O	2.08	0.52
1:E:35:ARG:CB	1:E:39:GLU:HG2	2.40	0.52
1:E:236:LYS:O	1:E:240:LYS:HG2	2.10	0.51
1:E:143:ASN:C	1:E:143:ASN:OD1	2.53	0.51
1:E:35:ARG:CB	1:E:41:LEU:CD1	2.88	0.51
1:E:59:LEU:HD22	1:E:88:ILE:CD1	2.38	0.51
1:E:241:VAL:O	1:E:245:PHE:CB	2.56	0.51
1:E:17:VAL:O	1:E:17:VAL:HG13	2.10	0.51
1:E:51:TRP:CZ3	1:E:107:LYS:HB3	2.45	0.51
1:E:186(A):ASP:CA	1:E:186(D):LYS:HD3	2.40	0.51
1:E:7:PHE:O	1:E:12:LEU:N	2.39	0.51
1:E:35:ARG:HB2	1:E:41:LEU:HD12	1.94	0.50
1:E:29:TRP:CG	1:E:121:VAL:HB	2.46	0.50
1:E:163:VAL:HG12	1:E:168:CYS:SG	2.50	0.50
1:E:5:PRO:HB3	4:E:555:HOH:O	2.10	0.50
1:E:139:THR:HA	1:E:156:GLN:O	2.12	0.50
1:E:204(B):ASN:ND2	1:E:206:ARG:H	2.10	0.50
1:E:217:GLU:CB	1:E:224:LYS:CB	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ASP:CG	1:E:221(A):ARG:H	2.20	0.50
1:E:14(K):ILE:HB	1:E:133:GLY:O	2.12	0.49
1:E:165:ARG:NH2	1:E:178:ASP:HA	2.27	0.49
1:E:18:GLU:CA	1:E:187:ARG:HB3	2.42	0.49
1:E:122:CYS:O	1:E:208:TYR:HA	2.11	0.49
1:E:242:ILE:HG22	1:E:243:ASP:N	2.26	0.49
1:E:6:LEU:HD11	1:E:116:ASP:CG	2.38	0.49
1:E:202:LYS:HE3	1:E:205:ASN:O	2.12	0.49
1:E:186(C):GLY:O	1:E:186(D):LYS:CE	2.56	0.49
1:E:14(D):ARG:O	1:E:14(G):LEU:N	2.46	0.49
1:E:14(H):GLU:HB2	1:E:14(J):TYR:O	2.12	0.49
1:E:135:LYS:HE2	1:E:184(A):TYR:CZ	2.48	0.49
1:E:66:VAL:HG21	1:E:108:LEU:CD2	2.42	0.49
1:E:217:GLU:C	1:E:224:LYS:HB2	2.37	0.48
1:E:186(A):ASP:HB3	1:E:186(D):LYS:CD	2.43	0.48
1:E:32:MET:HG3	1:E:40:LEU:HD13	1.95	0.48
1:E:72:SER:OG	1:E:75:ARG:HG2	2.12	0.48
2:I:60:PRO:C	2:I:62:GLU:N	2.72	0.48
1:E:14(J):TYR:HD1	1:E:14(J):TYR:N	1.99	0.47
1:E:91:HIS:CE1	1:E:93:ARG:HB2	2.48	0.47
1:E:235:LYS:O	1:E:235:LYS:CG	2.62	0.47
1:E:16:ILE:HG12	1:E:16:ILE:O	2.15	0.47
1:E:185:LYS:CE	1:E:186(D):LYS:NZ	2.67	0.47
1:E:1(C):GLU:HG3	1:E:1:CYS:HB3	1.97	0.47
1:E:185:LYS:O	1:E:186:PRO:C	2.57	0.47
1:E:105:LEU:HD12	1:E:241:VAL:HG11	1.96	0.47
1:E:186:PRO:CG	1:E:223:GLY:CA	2.94	0.46
1:E:1(G):PHE:C	1:E:1(E):SER:N	2.74	0.46
1:E:242:ILE:C	1:E:244:GLN:H	2.24	0.46
1:E:14(G):LEU:N	1:E:14(G):LEU:CD2	2.77	0.46
1:E:173:ARG:HB3	4:E:557:HOH:O	2.14	0.46
1:E:163:VAL:CG1	1:E:182:CYS:SG	3.04	0.45
1:E:135:LYS:HA	1:E:160:LEU:O	2.17	0.45
1:E:107:LYS:CD	1:E:246:GLY:HA2	2.47	0.45
1:E:96:TRP:O	1:E:97:ARG:C	2.59	0.45
1:E:185:LYS:HD3	1:E:186(D):LYS:HE2	1.97	0.45
1:E:1(G):PHE:C	1:E:1(E):SER:H	2.25	0.45
1:E:14(D):ARG:N	1:E:14(D):ARG:HH11	2.14	0.45
1:E:242:ILE:C	1:E:244:GLN:N	2.73	0.45
1:E:14(A):LYS:CE	4:E:585:HOH:O	2.64	0.44
1:E:129(C):LEU:HD21	1:E:204:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ASP:OD1	1:E:221(A):ARG:N	2.50	0.44
1:E:75:ARG:HG2	1:E:75:ARG:H	1.32	0.44
1:E:73:ARG:HD3	1:E:152:PRO:O	2.17	0.44
1:E:91:HIS:NE2	1:E:101:ARG:HD2	2.33	0.44
1:E:149(B):ASN:O	1:E:149(C):VAL:C	2.61	0.44
2:I:60:PRO:HB2	2:I:62:GLU:OE2	2.17	0.44
1:E:1(G):PHE:O	1:E:1(G):PHE:CD1	2.65	0.44
1:E:31:VAL:HG22	1:E:68:ILE:HD13	2.00	0.44
1:E:203:SER:HB2	1:E:208:TYR:CE1	2.52	0.43
1:E:50:ARG:HE	1:E:50:ARG:HB2	1.14	0.43
1:E:165:ARG:HB3	1:E:166:PRO:HD3	2.00	0.43
1:E:186(A):ASP:HB2	1:E:186(D):LYS:HD3	1.99	0.43
1:E:14(F):LEU:CD1	1:E:14(F):LEU:H	2.31	0.43
1:E:129(A):ALA:HA	4:E:493:HOH:O	2.19	0.43
1:E:29:TRP:CD2	1:E:121:VAL:HB	2.54	0.43
1:E:49:ASP:O	1:E:112:VAL:N	2.50	0.43
1:E:60(G):ASN:C	1:E:60(G):ASN:OD1	2.60	0.43
1:E:95:ASN:O	1:E:99:LEU:N	2.49	0.43
1:E:86:GLU:OE1	1:E:107:LYS:HD3	2.19	0.42
1:E:14(F):LEU:HD22	1:E:207:TRP:HH2	1.83	0.42
1:E:91:HIS:CG	1:E:92:PRO:HD2	2.53	0.42
1:E:130:LEU:O	1:E:131:GLN:HG3	2.19	0.42
1:E:17:VAL:O	1:E:17:VAL:CG1	2.67	0.42
2:I:60:PRO:C	2:I:62:GLU:H	2.27	0.42
1:E:107:LYS:HD2	1:E:246:GLY:HA2	2.02	0.42
1:E:163:VAL:HB	1:E:182:CYS:SG	2.60	0.42
1:E:175:ARG:NE	4:E:522:HOH:O	2.53	0.42
1:E:217:GLU:HA	1:E:217:GLU:OE1	2.20	0.42
1:E:66:VAL:O	1:E:82:ILE:HA	2.20	0.42
1:E:134:TYR:N	1:E:134:TYR:HD1	2.17	0.42
1:E:221(A):ARG:HD2	1:E:221(A):ARG:HA	1.92	0.42
1:E:34:PHE:CE2	1:E:38:GLN:HG2	2.55	0.41
1:E:165:ARG:O	1:E:169:LYS:HG3	2.20	0.41
1:E:86:GLU:CD	1:E:247:GLU:O	2.64	0.41
1:E:94:TYR:HE1	1:E:99:LEU:HD22	1.86	0.41
1:E:235:LYS:O	1:E:239:GLN:HB2	2.20	0.41
1:E:6:LEU:N	1:E:6:LEU:CD1	2.83	0.41
1:E:230:HIS:CD2	1:E:233:ARG:CG	3.03	0.41
1:E:237:TRP:HB2	4:E:427:HOH:O	2.19	0.41
1:E:14(E):GLU:OE2	1:E:135:LYS:HD2	2.20	0.41
1:E:103:ILE:HG21	1:E:234:LEU:CD1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LYS:HD3	1:E:239:GLN:HB3	2.01	0.41
1:E:190:ALA:C	1:E:192:GLU:H	2.26	0.41
1:E:1(G):PHE:HE1	1:E:243:ASP:HA	1.86	0.41
1:E:14(C):GLU:HG3	1:E:14(D):ARG:NH1	2.36	0.41
1:E:149(B):ASN:O	1:E:149(D):GLY:N	2.54	0.41
1:E:190:ALA:C	1:E:192:GLU:N	2.79	0.40
1:E:28:PRO:HB2	1:E:119:HIS:HB3	2.04	0.40
1:E:33:LEU:HD21	1:E:44:ALA:HB2	2.03	0.40
1:E:33:LEU:CD2	1:E:106:MET:HE1	2.52	0.40
1:E:105:LEU:HD12	1:E:241:VAL:HG13	2.02	0.40
1:E:128:THR:CG2	1:E:129(C):LEU:CD1	2.95	0.40
1:E:14(K):ILE:HD13	1:E:14(K):ILE:HG21	1.62	0.40
1:E:163:VAL:O	4:E:435:HOH:O	2.22	0.40
1:E:222:ASP:O	1:E:224:LYS:CG	2.61	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	E	293/295 (99%)	247 (84%)	35 (12%)	11 (4%)	2	1
2	I	7/10 (70%)	4 (57%)	3 (43%)	0	100	100
All	All	300/305 (98%)	251 (84%)	38 (13%)	11 (4%)	2	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1(F)	GLY
1	E	149(C)	VAL
1	E	223	GLY
1	E	18	GLU

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Mol	Chain	Res	Type
1	E	243	ASP
1	E	15	ARG
1	E	20	SER
1	E	221	ASP
1	E	221(A)	ARG
1	E	219	GLY
1	E	213	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	256/256 (100%)	194 (76%)	62 (24%)	1	0
2	I	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	265/265 (100%)	201 (76%)	64 (24%)	1	0

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1(H)	THR
1	E	1(G)	PHE
1	E	1(E)	SER
1	E	1(C)	GLU
1	E	1(A)	ASP
1	E	1	CYS
1	E	6	LEU
1	E	13	GLU
1	E	16	ILE
1	E	23	GLU
1	E	33	LEU
1	E	35	ARG
1	E	36	LYS
1	E	36(A)	SER
1	E	41	LEU
1	E	46	LEU

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Mol	Chain	Res	Type
1	E	48	SER
1	E	50	ARG
1	E	59	LEU
1	E	60	LEU
1	E	60(A)	TYR
1	E	60(B)	PRO
1	E	60(C)	PRO
1	E	60(D)	TRP
1	E	60(E)	ASP
1	E	60(F)	LYS
1	E	60(G)	ASN
1	E	60(H)	PHE
1	E	60(I)	THR
1	E	62	ASN
1	E	64	LEU
1	E	65	LEU
1	E	68	ILE
1	E	75	ARG
1	E	81	LYS
1	E	83	SER
1	E	87	LYS
1	E	107	LYS
1	E	109	LYS
1	E	110	LYS
1	E	127	GLU
1	E	129(B)	SER
1	E	129(C)	LEU
1	E	143	ASN
1	E	154	VAL
1	E	156	GLN
1	E	162	ILE
1	E	175	ARG
1	E	176	ILE
1	E	182	CYS
1	E	185	LYS
1	E	195	SER
1	E	215	TRP
1	E	220	CYS
1	E	221	ASP
1	E	221(A)	ARG
1	E	235	LYS
1	E	236	LYS

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Mol	Chain	Res	Type
1	E	239	GLN
1	E	241	VAL
1	E	244	GLN
1	E	247	GLU
2	I	61	GLU
2	I	62	GLU

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

Mol	Chain	Res	Type
1	E	38	GLN
1	E	156	GLN
1	E	159	ASN
1	E	204(B)	ASN
1	E	230	HIS

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	$\# Z > 2$
2	TYS	I	63	2	15,16,17	1.80	2 (13%)	15,22,24	1.75	6 (40%)

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
2	TYS	I	63	2	-	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)
2	I	63	TYS	OH-CZ	-4.81	1.34	1.42
2	I	63	TYS	OH-S	2.64	1.63	1.58

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	63	TYS	OH-S-O1	-2.73	99.24	107.56
2	I	63	TYS	O3-S-O2	2.53	117.42	108.56
2	I	63	TYS	O2-S-O1	-2.37	103.10	112.24
2	I	63	TYS	CE1-CD1-CG	-2.31	117.96	121.00
2	I	63	TYS	OH-CZ-CE1	2.19	123.00	118.70
2	I	63	TYS	CD2-CG-CD1	2.18	121.48	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	63	TYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	400	1	14,14,15	0.68	0	17,19,21	1.52	4 (23%)

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	NAG	E	400	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	400	NAG	O7-C7-C8	2.50	126.50	122.05
3	E	400	NAG	O6-C6-C5	-2.43	103.04	111.33
3	E	400	NAG	C2-N2-C7	-2.43	119.64	122.90
3	E	400	NAG	O5-C1-C2	-2.22	107.86	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	400	NAG	O7-C7-N2-C2
3	E	400	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	400	NAG	2	0

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.