



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:14 AM UTC

PDB ID : 1A2C / pdb_00001a2c
Title : Structure of thrombin inhibited by AERUGINOSIN298-A from a BLUE-GREEN ALGA
Authors : Rios-Steiner, J.L.; Murakami, M.; Tulinsky, A.
Deposited on : 1997-12-26
Resolution : 2.10 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

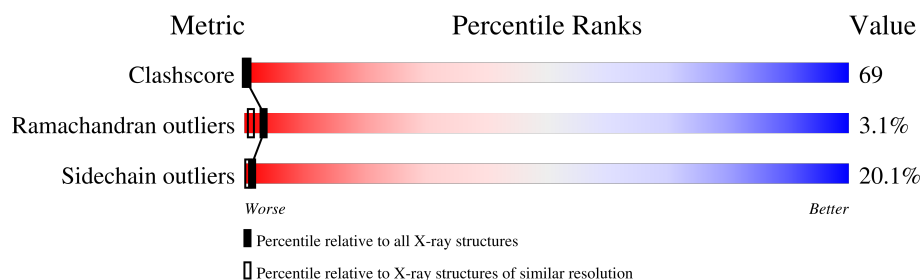
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

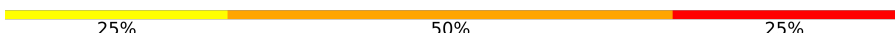
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	12	
4	J	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TYS	I	363	-	-	X	-
4	OAR	J	4	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2629 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	L	36	Total	C	N	O	S	0	0	0
			281	174	45	61	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2039	1299	360	366	14			

- Molecule 3 is a protein called Hirudin variant-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			89	56	10	22	1			

- Molecule 4 is a protein called Aeruginosin 298-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	4	Total	C	N	O	0	0	0
			43	30	6	7			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	138	Total 138	O 138	0	0
6	I	6	Total 6	O 6	0	0
6	J	6	Total 6	O 6	0	0

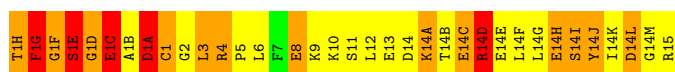
3 Residue-property plots

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.

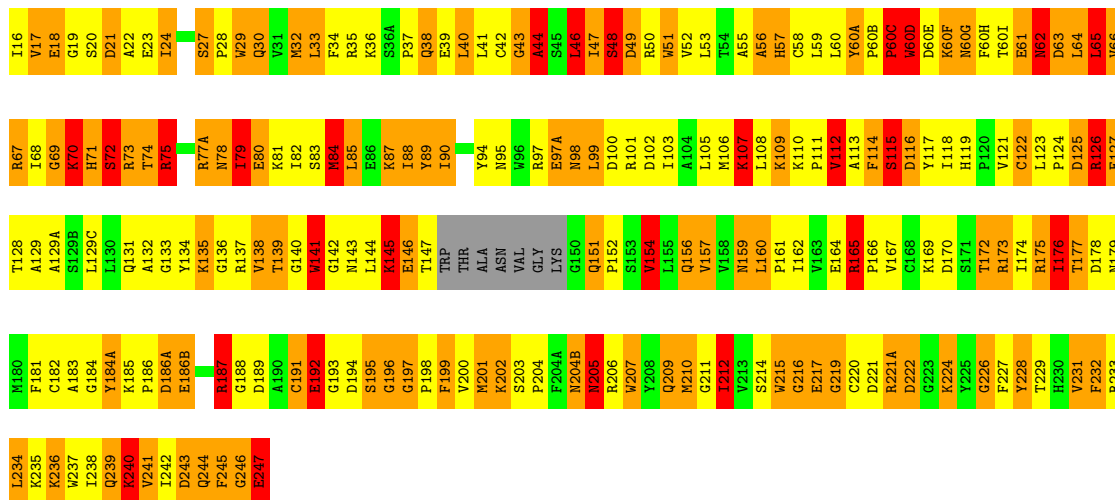
- Molecule 1: Thrombin light chain

Chain L: 



- Molecule 2: Thrombin heavy chain

Chain H: 



- Molecule 3: Hirudin variant-2

Chain I: 



- Molecule 4: Aeruginosin 298-A

Chain J: 



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	71.97Å 72.48Å 72.24Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	70.0 (7.00-2.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.150 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2629	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: OAR, 34H, NA, PRJ, 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	L	1.92	2/284 (0.7%)	2.76	25/377 (6.6%)
2	H	1.45	12/2091 (0.6%)	2.88	242/2823 (8.6%)
3	I	0.98	0/73	3.11	7/96 (7.3%)
4	J	0.54	0/7	3.42	1/8 (12.5%)
All	All	1.50	14/2455 (0.6%)	2.87	275/3304 (8.3%)

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	L	0	3
2	H	0	21
All	All	0	24

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14(L)	ASP	C-N	23.18	1.74	1.33
2	H	216	GLY	C-N	11.88	1.49	1.33
1	L	14(J)	TYR	C-N	-9.23	1.12	1.34
2	H	172	THR	C-O	5.98	1.31	1.23
2	H	187	ARG	C-N	5.82	1.40	1.33
2	H	207	TRP	NE1-CE2	-5.49	1.31	1.37
2	H	237	TRP	NE1-CE2	-5.45	1.31	1.37
2	H	141	TRP	NE1-CE2	-5.42	1.31	1.37
2	H	51	TRP	NE1-CE2	-5.40	1.31	1.37
2	H	29	TRP	NE1-CE2	-5.39	1.31	1.37
2	H	55	ALA	N-CA	5.27	1.52	1.46
2	H	215	TRP	NE1-CE2	-5.27	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	97(A)	GLU	C-N	5.17	1.41	1.33
2	H	199	PHE	CA-C	5.03	1.58	1.52

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(L)	ASP	O-C-N	-15.15	97.45	123.20
2	H	60(D)	TRP	N-CA-C	-13.83	95.72	112.59
2	H	62	ASN	OD1-CG-ND2	12.38	134.98	122.60
2	H	143	ASN	CA-C-O	-11.99	107.96	121.15
2	H	116	ASP	CA-CB-CG	11.87	124.47	112.60
2	H	243	ASP	CA-CB-CG	11.86	124.46	112.60
2	H	137	ARG	CA-C-O	-11.86	106.37	120.60
1	L	10	LYS	O-C-N	11.21	134.44	122.23
3	I	362	GLU	CB-CG-CD	10.96	131.24	112.60
2	H	98	ASN	OD1-CG-ND2	10.92	133.52	122.60
1	L	1(G)	PHE	CA-CB-CG	-10.87	102.94	113.80
2	H	141	TRP	O-C-N	-10.87	109.30	122.34
1	L	14(L)	ASP	CA-C-N	-10.62	94.96	116.20
2	H	175	ARG	CA-C-N	10.59	136.27	121.66
2	H	175	ARG	C-N-CA	10.59	136.27	121.66
2	H	135	LYS	CA-C-N	10.34	134.04	122.67
2	H	135	LYS	C-N-CA	10.34	134.04	122.67
1	L	1(A)	ASP	CA-CB-CG	-10.23	102.37	112.60
2	H	126	ARG	NE-CZ-NH2	10.18	128.36	119.20
2	H	132	ALA	O-C-N	10.06	135.24	122.87
2	H	204(B)	ASN	OD1-CG-ND2	9.74	132.34	122.60
3	I	359	ILE	O-C-N	9.63	132.07	121.10
2	H	128	THR	CA-C-N	9.61	132.93	120.44
2	H	128	THR	C-N-CA	9.61	132.93	120.44
2	H	77(A)	ARG	CA-C-O	-9.57	106.82	120.51
2	H	233	ARG	CD-NE-CZ	9.56	137.78	124.40
2	H	243	ASP	CA-C-O	9.49	130.61	120.55
2	H	157	VAL	CA-C-O	-9.45	111.45	121.19
2	H	65	LEU	CA-C-O	-9.33	110.52	121.44
2	H	137	ARG	O-C-N	9.30	134.59	123.33
2	H	79	ILE	CB-CA-C	9.13	120.11	111.44
1	L	13	GLU	CA-C-O	-8.99	110.67	121.28
2	H	177	THR	CA-C-N	8.95	133.45	120.38
2	H	177	THR	C-N-CA	8.95	133.45	120.38
2	H	199	PHE	O-C-N	-8.95	112.71	123.27
2	H	176	ILE	CA-CB-CG2	8.94	125.69	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	18	GLU	CB-CG-CD	8.84	127.63	112.60
1	L	2	GLY	N-CA-C	8.81	127.98	115.30
2	H	97	ARG	NE-CZ-NH2	8.78	127.11	119.20
2	H	143	ASN	O-C-N	8.73	133.62	122.97
2	H	60(E)	ASP	CA-CB-CG	-8.66	103.94	112.60
2	H	165	ARG	CA-CB-CG	8.63	131.37	114.10
2	H	60(E)	ASP	N-CA-CB	-8.58	99.65	112.78
2	H	97	ARG	CD-NE-CZ	-8.55	112.43	124.40
2	H	55	ALA	CA-C-O	-8.45	111.70	121.16
2	H	64	LEU	N-CA-C	8.37	123.07	109.85
2	H	74	THR	CA-CB-OG1	-8.30	97.14	109.60
2	H	200	VAL	CA-C-O	8.29	130.07	121.28
2	H	24	ILE	CA-C-N	8.28	137.64	121.41
2	H	24	ILE	C-N-CA	8.28	137.64	121.41
2	H	40	LEU	CA-C-O	-8.26	111.00	120.58
1	L	12	LEU	CA-C-O	-8.19	112.03	120.71
2	H	206	ARG	NE-CZ-NH1	8.07	129.57	121.50
2	H	38	GLN	O-C-N	7.97	133.19	122.59
4	J	2	LEU	CB-CA-C	7.97	125.24	110.10
2	H	176	ILE	N-CA-CB	-7.96	101.85	110.53
2	H	186(A)	ASP	N-CA-C	-7.92	102.72	111.36
2	H	212	ILE	O-C-N	-7.87	114.92	123.18
2	H	159	ASN	CA-C-O	-7.86	111.81	120.38
3	I	358	GLU	CB-CG-CD	7.85	125.95	112.60
2	H	117	TYR	CA-C-N	7.81	133.60	123.13
2	H	117	TYR	C-N-CA	7.81	133.60	123.13
2	H	178	ASP	CA-CB-CG	-7.77	104.83	112.60
2	H	142	GLY	CA-C-O	7.72	131.40	122.76
2	H	33	LEU	N-CA-CB	-7.71	97.30	109.87
2	H	89	TYR	CA-C-O	-7.66	112.12	120.24
1	L	14(J)	TYR	N-CA-C	-7.65	102.80	113.20
2	H	129	ALA	CA-C-O	7.63	128.84	120.82
2	H	60(G)	ASN	CA-CB-CG	-7.57	105.03	112.60
2	H	173	ARG	CD-NE-CZ	-7.51	113.89	124.40
2	H	73	ARG	NH1-CZ-NH2	-7.49	109.56	119.30
2	H	82	ILE	CA-C-O	-7.49	112.55	120.57
2	H	222	ASP	CA-CB-CG	-7.48	105.12	112.60
2	H	63	ASP	O-C-N	7.47	132.51	122.49
2	H	17	VAL	O-C-N	-7.46	115.34	123.18
2	H	115	SER	CA-C-O	-7.46	113.18	120.94
1	L	13	GLU	CB-CA-C	-7.46	96.90	109.50
2	H	232	PHE	CA-CB-CG	-7.45	106.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60(E)	ASP	N-CA-C	7.44	122.09	113.38
2	H	17	VAL	CA-C-O	7.42	128.34	120.48
2	H	160	LEU	O-C-N	-7.41	115.43	121.80
2	H	27	SER	N-CA-CB	-7.35	101.23	110.79
2	H	105	LEU	O-C-N	7.33	132.02	123.30
2	H	154	VAL	N-CA-CB	-7.31	100.18	112.47
1	L	4	ARG	NE-CZ-NH2	7.29	125.76	119.20
3	I	359	ILE	CA-C-N	7.28	127.55	119.90
3	I	359	ILE	C-N-CA	7.28	127.55	119.90
2	H	144	LEU	CA-C-O	-7.25	110.79	119.27
2	H	68	ILE	O-C-N	-7.25	115.35	123.18
2	H	216	GLY	O-C-N	7.24	128.77	123.27
2	H	232	PHE	O-C-N	-7.24	114.62	122.07
2	H	97	ARG	NE-CZ-NH1	-7.24	114.27	121.50
2	H	173	ARG	NE-CZ-NH2	7.23	125.71	119.20
2	H	216	GLY	CA-C-O	-7.23	114.55	121.06
2	H	60(D)	TRP	CA-C-O	-7.14	111.52	119.95
2	H	206	ARG	NE-CZ-NH2	-7.08	112.83	119.20
2	H	49	ASP	CA-CB-CG	-7.06	105.54	112.60
1	L	14(H)	GLU	CA-C-O	-7.03	110.98	119.49
1	L	11	SER	CB-CA-C	7.00	121.15	111.63
2	H	228	TYR	CA-C-O	-6.97	112.23	120.60
2	H	60(A)	TYR	CA-CB-CG	-6.96	101.38	113.90
2	H	79	ILE	CA-C-O	-6.93	114.08	120.73
2	H	179	ASN	CB-CG-ND2	6.91	126.76	116.40
2	H	122	CYS	CA-C-O	-6.90	113.08	121.36
2	H	132	ALA	CA-C-O	-6.89	113.61	121.19
2	H	175	ARG	CA-C-O	6.87	128.46	120.49
2	H	72	SER	CA-C-O	-6.84	113.50	121.16
2	H	139	THR	O-C-N	6.83	131.04	123.33
2	H	139	THR	CA-CB-OG1	-6.83	99.36	109.60
2	H	78	ASN	CA-CB-CG	6.82	119.42	112.60
2	H	73	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	L	14(J)	TYR	CA-C-N	-6.81	102.22	117.20
2	H	60(F)	LYS	CA-C-O	6.78	128.03	120.43
2	H	200	VAL	CA-CB-CG1	6.77	121.90	110.40
2	H	231	VAL	CA-C-O	-6.76	114.24	121.27
2	H	30	GLN	CA-CB-CG	6.76	127.62	114.10
1	L	14(A)	LYS	CA-C-O	-6.70	111.38	119.49
2	H	143	ASN	CB-CG-ND2	-6.69	106.36	116.40
2	H	165	ARG	CD-NE-CZ	-6.66	115.07	124.40
2	H	157	VAL	O-C-N	6.66	130.33	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	137	ARG	NE-CZ-NH1	-6.63	114.87	121.50
2	H	169	LYS	CA-C-N	6.63	133.32	120.99
2	H	169	LYS	C-N-CA	6.63	133.32	120.99
2	H	129(A)	ALA	CA-C-O	-6.59	113.43	120.42
2	H	186(A)	ASP	CA-CB-CG	6.57	119.17	112.60
2	H	145	LYS	N-CA-CB	6.57	121.74	111.56
2	H	66	VAL	CA-C-O	-6.55	113.25	120.72
2	H	186(A)	ASP	CA-C-O	-6.53	113.50	120.42
2	H	80	GLU	CA-C-O	-6.53	113.53	121.36
2	H	186	PRO	N-CA-C	-6.52	105.36	113.84
2	H	204(B)	ASN	CB-CG-ND2	-6.51	106.63	116.40
1	L	4	ARG	NH1-CZ-NH2	-6.50	110.85	119.30
2	H	167	VAL	CA-C-O	6.50	127.71	120.95
2	H	181	PHE	CA-C-O	-6.49	114.07	121.40
2	H	173	ARG	N-CA-CB	6.48	120.39	110.61
2	H	183	ALA	CA-C-N	6.45	131.62	121.62
2	H	183	ALA	C-N-CA	6.45	131.62	121.62
2	H	67	ARG	CA-C-O	-6.37	113.32	120.32
2	H	38	GLN	OE1-CD-NE2	6.36	128.96	122.60
2	H	78	ASN	CB-CG-ND2	6.34	125.92	116.40
2	H	48	SER	CA-C-O	-6.33	111.45	120.51
2	H	71	HIS	CA-C-O	6.31	129.53	120.51
1	L	4	ARG	O-C-N	6.29	128.09	121.42
2	H	187	ARG	CA-C-N	-6.24	111.78	122.01
2	H	187	ARG	C-N-CA	-6.24	111.78	122.01
2	H	196	GLY	CA-C-O	6.24	125.90	119.10
2	H	212	ILE	CA-CB-CG1	6.23	121.00	110.40
2	H	116	ASP	O-C-N	6.22	131.52	122.43
2	H	174	ILE	CA-C-N	-6.22	112.70	121.72
2	H	174	ILE	C-N-CA	-6.22	112.70	121.72
2	H	237	TRP	N-CA-C	-6.22	104.42	111.14
2	H	75	ARG	CA-CB-CG	-6.21	101.68	114.10
2	H	113	ALA	O-C-N	6.17	131.05	123.21
2	H	162	ILE	N-CA-CB	6.14	118.68	110.26
2	H	69	GLY	O-C-N	6.13	129.30	122.50
2	H	112	VAL	CB-CA-C	-6.12	102.81	111.38
2	H	137	ARG	NE-CZ-NH2	6.12	124.71	119.20
2	H	146	GLU	CA-C-O	6.11	127.05	120.20
2	H	186(B)	GLU	CG-CD-OE2	6.11	132.45	118.40
2	H	125	ASP	O-C-N	-6.11	116.08	123.10
2	H	146	GLU	N-CA-C	6.10	119.56	111.75
2	H	201	MET	CA-CB-CG	-6.10	101.89	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	77(A)	ARG	CD-NE-CZ	-6.09	115.88	124.40
1	L	1(C)	GLU	N-CA-C	6.08	123.76	110.80
2	H	32	MET	CA-C-O	-6.07	113.87	120.36
2	H	173	ARG	O-C-N	6.05	129.56	122.24
2	H	64	LEU	N-CA-CB	-6.03	101.43	111.20
2	H	144	LEU	O-C-N	6.00	130.68	122.46
2	H	205	ASN	N-CA-CB	-6.00	103.61	112.78
2	H	46	LEU	O-C-N	5.97	130.03	123.22
2	H	46	LEU	CA-C-O	-5.97	113.79	120.54
1	L	8	GLU	O-C-N	5.96	128.23	122.03
2	H	196	GLY	O-C-N	-5.96	114.61	122.42
3	I	359	ILE	CA-C-O	-5.96	111.97	119.95
2	H	84	MET	N-CA-C	-5.93	101.22	110.42
2	H	226	GLY	N-CA-C	-5.92	104.08	112.37
2	H	146	GLU	CA-C-N	5.92	132.35	121.70
2	H	146	GLU	C-N-CA	5.92	132.35	121.70
2	H	114	PHE	CA-C-O	-5.90	115.16	121.94
2	H	221(A)	ARG	NE-CZ-NH1	-5.89	115.61	121.50
2	H	60(D)	TRP	N-CA-CB	5.89	120.34	110.92
2	H	19	GLY	CA-C-O	-5.87	116.13	121.47
2	H	84	MET	O-C-N	5.87	129.66	123.03
2	H	38	GLN	CA-C-O	-5.87	112.12	120.51
2	H	240	LYS	CA-C-O	-5.87	114.61	121.07
2	H	191	CYS	N-CA-C	-5.86	99.24	108.14
2	H	224	LYS	CB-CA-C	5.84	120.23	109.71
2	H	101	ARG	NE-CZ-NH2	-5.82	113.97	119.20
2	H	156	GLN	OE1-CD-NE2	5.80	128.40	122.60
2	H	186(B)	GLU	CG-CD-OE1	-5.79	105.09	118.40
2	H	74	THR	N-CA-CB	-5.78	102.63	110.67
2	H	177	THR	CA-CB-OG1	-5.77	100.94	109.60
2	H	67	ARG	CB-CG-CD	-5.76	98.05	111.30
2	H	125	ASP	CA-CB-CG	-5.72	106.88	112.60
2	H	227	PHE	CA-CB-CG	-5.72	108.08	113.80
2	H	129(C)	LEU	O-C-N	5.69	130.67	122.13
2	H	70	LYS	CA-C-O	-5.68	115.11	121.81
2	H	126	ARG	CG-CD-NE	5.68	124.50	112.00
2	H	220	CYS	CA-C-O	5.67	127.16	120.69
2	H	209	GLN	CA-C-O	5.65	126.63	120.58
2	H	88	ILE	N-CA-CB	5.64	119.75	111.52
2	H	220	CYS	O-C-N	-5.63	116.45	123.04
1	L	14(C)	GLU	CB-CA-C	-5.62	99.25	110.42
2	H	172	THR	N-CA-CB	-5.62	101.83	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	175	ARG	O-C-N	-5.62	116.11	123.02
2	H	162	ILE	N-CA-C	-5.61	101.58	109.21
2	H	146	GLU	OE1-CD-OE2	5.60	136.33	122.90
2	H	246	GLY	N-CA-C	5.58	126.41	113.18
2	H	33	LEU	CB-CA-C	5.57	119.42	110.29
2	H	210	MET	CA-CB-CG	-5.57	102.97	114.10
2	H	197	GLY	N-CA-C	-5.53	105.54	112.23
2	H	98	ASN	CB-CG-ND2	-5.53	108.11	116.40
2	H	133	GLY	O-C-N	5.51	129.87	122.70
2	H	221(A)	ARG	CA-C-O	5.51	127.34	121.05
2	H	170	ASP	CA-CB-CG	-5.51	107.09	112.60
2	H	75	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	H	186	PRO	O-C-N	5.50	131.50	122.70
2	H	95	ASN	CA-C-N	-5.47	111.56	121.14
2	H	95	ASN	C-N-CA	-5.47	111.56	121.14
2	H	57	HIS	CA-CB-CG	-5.46	108.34	113.80
2	H	29	TRP	CA-C-N	5.46	129.10	121.24
2	H	29	TRP	C-N-CA	5.46	129.10	121.24
2	H	98	ASN	CA-C-O	-5.46	113.34	119.95
2	H	138	VAL	CA-CB-CG1	5.46	119.67	110.40
2	H	161	PRO	CA-C-N	5.45	129.89	121.71
2	H	161	PRO	C-N-CA	5.45	129.89	121.71
2	H	58	CYS	CA-C-O	5.45	126.25	120.10
2	H	236	LYS	CB-CG-CD	5.42	123.77	111.30
1	L	14(D)	ARG	NE-CZ-NH2	5.41	124.07	119.20
3	I	355	ASP	CB-CA-C	5.39	120.34	110.10
2	H	109	LYS	CA-CB-CG	-5.38	103.33	114.10
1	L	8	GLU	CA-C-O	-5.36	115.38	121.00
2	H	244	GLN	CB-CG-CD	-5.35	103.50	112.60
2	H	40	LEU	O-C-N	5.34	129.68	122.96
2	H	186(B)	GLU	O-C-N	-5.33	114.13	123.20
2	H	212	ILE	CA-CB-CG2	-5.33	101.44	110.50
2	H	160	LEU	CA-C-O	5.33	126.48	120.46
2	H	193	GLY	CA-C-N	5.31	129.71	120.68
2	H	193	GLY	C-N-CA	5.31	129.71	120.68
2	H	62	ASN	CB-CG-OD1	-5.31	110.18	120.80
2	H	89	TYR	O-C-N	5.30	129.47	123.27
1	L	1(G)	PHE	CA-C-O	5.28	128.06	120.51
2	H	177	THR	CA-CB-CG2	5.25	119.42	110.50
2	H	114	PHE	CA-C-N	-5.25	113.34	122.84
2	H	114	PHE	C-N-CA	-5.25	113.34	122.84
2	H	126	ARG	NH1-CZ-NH2	-5.24	112.49	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	MET	O-C-N	5.24	129.68	123.24
2	H	56	ALA	O-C-N	-5.22	115.85	122.27
2	H	157	VAL	N-CA-CB	-5.22	101.71	111.62
2	H	126	ARG	CA-C-O	-5.21	113.06	120.51
2	H	60(C)	PRO	CB-CA-C	-5.21	104.08	112.21
2	H	211	GLY	O-C-N	-5.21	118.79	123.37
2	H	52	VAL	CA-C-O	-5.20	114.85	120.67
2	H	140	GLY	O-C-N	5.16	129.40	122.70
2	H	202	LYS	CA-C-O	-5.16	114.84	120.36
2	H	236	LYS	CA-C-O	5.16	126.01	120.55
2	H	108	LEU	CA-C-O	-5.15	115.95	121.56
2	H	176	ILE	O-C-N	-5.15	117.09	122.81
2	H	169	LYS	CB-CA-C	-5.14	102.21	110.74
1	L	11	SER	CA-C-O	5.12	127.33	120.98
2	H	47	ILE	O-C-N	-5.12	116.51	122.09
2	H	90	ILE	CA-C-O	-5.12	114.98	121.48
2	H	82	ILE	N-CA-CB	-5.11	104.86	110.99
2	H	141	TRP	CA-C-N	5.11	130.57	121.48
2	H	141	TRP	C-N-CA	5.11	130.57	121.48
2	H	247	GLU	CB-CG-CD	5.11	121.28	112.60
2	H	71	HIS	O-C-N	-5.11	115.80	122.59
2	H	184(A)	TYR	O-C-N	-5.10	117.35	123.06
2	H	98	ASN	N-CA-C	5.08	119.01	112.41
2	H	192	GLU	CB-CA-C	-5.08	100.31	110.42
2	H	156	GLN	O-C-N	5.05	129.61	123.10
2	H	198	PRO	CB-CA-C	-5.05	102.28	110.21
2	H	237	TRP	O-C-N	5.03	127.52	122.09
2	H	21	ASP	N-CA-CB	5.02	117.74	109.95
1	L	14(I)	SER	CA-CB-OG	5.00	121.10	111.10

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	107	LYS	Mainchain
2	H	134	TYR	Mainchain
2	H	141	TRP	Mainchain
2	H	151	GLN	Mainchain
2	H	164	GLU	Mainchain
2	H	172	THR	Mainchain
2	H	192	GLU	Mainchain
2	H	196	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	H	197	GLY	Mainchain
2	H	212	ILE	Mainchain
2	H	29	TRP	Mainchain
2	H	43	GLY	Mainchain
2	H	44	ALA	Mainchain
2	H	47	ILE	Mainchain
2	H	60(C)	PRO	Mainchain
2	H	60(D)	TRP	Mainchain
2	H	65	LEU	Mainchain
2	H	72	SER	Mainchain
2	H	75	ARG	Sidechain
2	H	79	ILE	Mainchain
2	H	99	LEU	Mainchain
1	L	14(D)	ARG	Mainchain
1	L	3	LEU	Mainchain
1	L	5	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	281	0	265	80	2
2	H	2039	0	2010	260	2
3	I	89	0	67	20	0
4	J	43	0	44	24	0
5	H	1	0	0	0	0
6	H	138	0	0	13	0
6	I	6	0	0	1	0
6	J	6	0	0	1	0
6	L	26	0	0	0	0
All	All	2629	0	2386	336	2

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 69.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(C):GLU:CG	1:L:1(B):ALA:H	1.21	1.46
1:L:14(L):ASP:C	1:L:14(M):GLY:N	1.74	1.42
2:H:201:MET:CE	2:H:210:MET:HG3	1.55	1.33
1:L:1(C):GLU:HG3	1:L:1(B):ALA:N	1.33	1.18
1:L:1(E):SER:HA	2:H:123:LEU:O	1.43	1.14
1:L:14(D):ARG:HD3	1:L:14(E):GLU:N	1.62	1.13
2:H:195:SER:CB	4:J:4:OAR:HC2	1.79	1.13
2:H:195:SER:HB2	4:J:4:OAR:C	1.80	1.10
2:H:50:ARG:HG3	2:H:247:GLU:CG	1.81	1.09
2:H:201:MET:HE3	2:H:210:MET:CG	1.81	1.09
2:H:110:LYS:HG3	2:H:111:PRO:HD2	1.23	1.08
1:L:14(D):ARG:HH11	1:L:14(E):GLU:HB2	0.91	1.08
1:L:14(D):ARG:NH1	1:L:14(E):GLU:HB2	1.69	1.07
1:L:14(D):ARG:HD3	1:L:14(E):GLU:H	0.94	1.06
2:H:69:GLY:O	2:H:79:ILE:HD11	1.55	1.05
2:H:50:ARG:HG3	2:H:247:GLU:HG3	1.32	1.05
2:H:195:SER:HB2	4:J:4:OAR:HC2	1.33	1.03
1:L:14(D):ARG:CD	1:L:14(E):GLU:H	1.72	1.01
2:H:17:VAL:O	2:H:188:GLY:HA2	1.61	1.01
2:H:50:ARG:HG3	2:H:247:GLU:CD	1.86	1.00
2:H:201:MET:CE	2:H:210:MET:CG	2.38	1.00
1:L:1(H):THR:O	2:H:123:LEU:HD12	1.64	0.97
2:H:21:ASP:HB3	2:H:154:VAL:CG1	1.97	0.95
2:H:50:ARG:HH21	2:H:107:LYS:CD	1.80	0.94
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	1.67	0.94
2:H:50:ARG:CG	2:H:247:GLU:HG3	1.98	0.93
1:L:14(A):LYS:HE2	2:H:23:GLU:OE2	1.70	0.92
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.50	0.91
1:L:1(C):GLU:HB3	1:L:1:CYS:HB3	1.53	0.91
2:H:75:ARG:HD3	3:I:357:GLU:OE1	1.70	0.90
2:H:201:MET:HE3	2:H:210:MET:HG3	0.90	0.89
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.78	0.89
2:H:50:ARG:HH21	2:H:107:LYS:CE	1.87	0.88
2:H:103:ILE:HG21	2:H:234:LEU:HD12	1.55	0.87
3:I:360:PRO:HG2	3:I:363:TYS:CD2	2.05	0.87
1:L:14(D):ARG:CD	1:L:14(E):GLU:N	2.34	0.86
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.00	0.86
2:H:49:ASP:O	2:H:112:VAL:HG23	1.75	0.85
2:H:110:LYS:HG3	2:H:111:PRO:CD	2.06	0.85
3:I:360:PRO:HG2	3:I:363:TYS:HD2	1.57	0.85
2:H:65:LEU:HD11	2:H:84:MET:HE2	1.59	0.85
2:H:22:ALA:HB2	2:H:157:VAL:CG1	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:PRO:O	2:H:235:LYS:NZ	2.09	0.84
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	1.92	0.84
2:H:242:ILE:O	2:H:246:GLY:HA3	1.79	0.83
1:L:1(G):PHE:CD2	1:L:1(F):GLY:N	2.46	0.83
1:L:14(L):ASP:CA	1:L:14(M):GLY:N	2.41	0.83
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.61	0.83
2:H:60(I):THR:HG23	2:H:63:ASP:CG	2.05	0.82
1:L:14(D):ARG:HH11	1:L:14(E):GLU:CB	1.84	0.82
2:H:60(D):TRP:CZ2	4:J:3:PRJ:H13	2.15	0.82
1:L:1(C):GLU:CG	1:L:1(B):ALA:N	2.04	0.81
2:H:191:CYS:O	2:H:194:ASP:HB2	1.79	0.81
2:H:195:SER:OG	4:J:4:OAR:HC2	1.79	0.81
2:H:65:LEU:CD1	2:H:84:MET:HE2	2.11	0.81
2:H:50:ARG:CB	2:H:247:GLU:HG3	2.11	0.80
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.45	0.80
2:H:87:LYS:HE3	2:H:88:ILE:H	1.46	0.80
2:H:219:GLY:N	4:J:1:34H:O4	2.13	0.80
1:L:14(G):LEU:O	1:L:14(L):ASP:HA	1.81	0.79
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.17	0.79
2:H:35:ARG:O	2:H:38:GLN:HA	1.83	0.79
2:H:217:GLU:HB2	2:H:224:LYS:HD3	1.62	0.79
2:H:36:LYS:O	2:H:38:GLN:HG3	1.83	0.79
2:H:103:ILE:HG21	2:H:234:LEU:CD1	2.13	0.79
2:H:21:ASP:HB3	2:H:154:VAL:HG11	1.64	0.78
2:H:50:ARG:HH21	2:H:107:LYS:HE3	1.47	0.78
2:H:56:ALA:CB	2:H:90:ILE:HG23	2.14	0.78
2:H:107:LYS:HB2	2:H:107:LYS:NZ	1.99	0.77
2:H:67:ARG:HD3	2:H:70:LYS:HD2	1.67	0.77
2:H:156:GLN:C	2:H:157:VAL:HG13	2.08	0.76
2:H:78:ASN:N	6:H:453:HOH:O	1.95	0.76
2:H:22:ALA:HB2	2:H:157:VAL:HG11	1.67	0.75
2:H:217:GLU:HG3	2:H:224:LYS:HD3	1.69	0.75
2:H:240:LYS:O	2:H:244:GLN:HB2	1.86	0.74
2:H:67:ARG:CD	2:H:70:LYS:HD2	2.17	0.74
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.88	0.74
1:L:1(E):SER:CA	2:H:123:LEU:O	2.30	0.73
2:H:65:LEU:HD11	2:H:84:MET:CE	2.18	0.73
2:H:217:GLU:OE1	4:J:2:LEU:HD21	1.88	0.73
1:L:1(A):ASP:OD2	1:L:9:LYS:HE3	1.88	0.73
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.54	0.73
2:H:32:MET:HG3	2:H:40:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:TYR:CE2	2:H:245:PHE:CE1	2.77	0.73
4:J:4:OAR:HG3	6:J:462:HOH:O	1.87	0.73
1:L:1(E):SER:H	2:H:235:LYS:HZ1	1.36	0.72
2:H:69:GLY:O	2:H:79:ILE:CD1	2.36	0.72
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.48	0.71
2:H:37:PRO:O	2:H:39:GLU:HG2	1.90	0.71
2:H:184(A):TYR:O	6:H:503:HOH:O	2.09	0.71
1:L:1(D):GLY:CA	6:H:529:HOH:O	2.39	0.71
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.44	0.70
2:H:165:ARG:N	2:H:166:PRO:HD2	2.05	0.70
1:L:1(D):GLY:HA3	6:H:529:HOH:O	1.91	0.70
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.22	0.70
2:H:217:GLU:HG3	2:H:224:LYS:CE	2.22	0.70
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.21	0.70
2:H:156:GLN:C	2:H:157:VAL:CG1	2.64	0.70
1:L:1(G):PHE:CD1	1:L:1(G):PHE:N	2.59	0.70
1:L:1(G):PHE:O	1:L:1(F):GLY:C	2.35	0.70
1:L:8:GLU:OE2	2:H:202:LYS:HE3	1.90	0.70
2:H:50:ARG:HB2	2:H:247:GLU:HG3	1.73	0.69
2:H:217:GLU:CG	2:H:224:LYS:HD3	2.22	0.69
2:H:74:THR:O	6:H:615:HOH:O	2.10	0.69
2:H:217:GLU:HG3	2:H:224:LYS:HE3	1.73	0.69
1:L:1(C):GLU:HG3	1:L:1(B):ALA:H	0.53	0.69
1:L:14(D):ARG:CG	1:L:14(E):GLU:N	2.55	0.69
2:H:60(D):TRP:CH2	4:J:3:PRJ:H13	2.26	0.69
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.93	0.69
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.15	0.69
3:I:360:PRO:HG2	3:I:363:TYS:CE2	2.23	0.69
2:H:107:LYS:O	2:H:107:LYS:HG3	1.94	0.68
1:L:14(D):ARG:NH1	1:L:14(E):GLU:CB	2.51	0.68
2:H:221(A):ARG:HH22	4:J:1:34H:H5	1.58	0.68
2:H:98:ASN:ND2	2:H:175:ARG:O	2.18	0.68
2:H:221(A):ARG:NH2	4:J:1:34H:H5	2.07	0.68
1:L:1(H):THR:O	2:H:123:LEU:CD1	2.40	0.68
2:H:50:ARG:NH2	2:H:107:LYS:CD	2.54	0.68
3:I:355:ASP:HB3	6:I:553:HOH:O	1.92	0.68
2:H:201:MET:HE3	2:H:210:MET:HE3	1.74	0.67
1:L:1(H):THR:HB	1:L:1(G):PHE:CD1	2.29	0.67
1:L:14(L):ASP:O	1:L:14(M):GLY:N	2.27	0.67
2:H:217:GLU:CB	2:H:224:LYS:HD3	2.25	0.66
2:H:79:ILE:HD11	6:H:500:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60(I):THR:HG23	2:H:63:ASP:OD1	1.95	0.66
2:H:60(A):TYR:CE2	4:J:3:PRJ:H12	2.31	0.66
2:H:147:THR:HG22	6:H:521:HOH:O	1.96	0.65
3:I:357:GLU:HG2	3:I:358:GLU:N	2.10	0.65
4:J:2:LEU:HD23	4:J:2:LEU:N	2.12	0.65
1:L:14(B):THR:O	1:L:14(D):ARG:HD3	1.97	0.65
2:H:182:CYS:HA	2:H:226:GLY:O	1.96	0.65
2:H:56:ALA:HB1	2:H:90:ILE:HG23	1.77	0.65
2:H:56:ALA:HB2	2:H:90:ILE:HG23	1.78	0.65
2:H:125:ASP:O	2:H:126:ARG:C	2.40	0.64
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.12	0.64
1:L:4:ARG:NH2	1:L:14(C):GLU:OE2	2.31	0.64
2:H:59:LEU:HD22	2:H:88:ILE:HD13	1.80	0.64
2:H:49:ASP:OD1	2:H:49:ASP:N	2.27	0.64
2:H:50:ARG:NH2	2:H:107:LYS:HE3	2.12	0.63
2:H:165:ARG:NH2	2:H:177:THR:O	2.32	0.63
2:H:50:ARG:NH2	2:H:107:LYS:HD2	2.14	0.63
1:L:14(G):LEU:O	1:L:14(L):ASP:CA	2.46	0.62
2:H:79:ILE:CD1	6:H:500:HOH:O	2.47	0.62
2:H:217:GLU:HG3	2:H:224:LYS:CD	2.28	0.62
3:I:361:GLU:C	3:I:363:TYS:N	2.52	0.62
1:L:1(D):GLY:N	2:H:123:LEU:H	1.97	0.62
1:L:1(G):PHE:HD2	1:L:1(F):GLY:N	1.97	0.61
1:L:3:LEU:O	2:H:119:HIS:CD2	2.54	0.61
2:H:30:GLN:OE1	2:H:139:THR:OG1	2.18	0.61
1:L:14(F):LEU:N	1:L:14(F):LEU:HD12	2.15	0.61
2:H:216:GLY:O	4:J:2:LEU:N	2.35	0.60
2:H:81:LYS:HE3	6:H:468:HOH:O	2.00	0.60
2:H:125:ASP:O	2:H:127:GLU:N	2.35	0.60
2:H:49:ASP:O	2:H:112:VAL:CG2	2.48	0.60
2:H:201:MET:HE3	2:H:210:MET:CE	2.31	0.60
2:H:201:MET:CE	2:H:210:MET:CB	2.80	0.60
2:H:115:SER:OG	2:H:116:ASP:N	2.30	0.60
3:I:360:PRO:O	3:I:363:TYS:N	2.35	0.60
2:H:165:ARG:HB2	2:H:166:PRO:CD	2.32	0.60
2:H:201:MET:HE2	2:H:210:MET:HG3	1.75	0.59
2:H:22:ALA:CB	2:H:157:VAL:HG11	2.32	0.58
4:J:2:LEU:N	4:J:2:LEU:CD2	2.65	0.58
2:H:217:GLU:O	2:H:219:GLY:O	2.21	0.58
1:L:1(C):GLU:HG3	1:L:1(B):ALA:CA	2.26	0.58
2:H:60(F):LYS:HD3	2:H:60(H):PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:SER:CB	4:J:4:OAR:C	2.54	0.58
2:H:242:ILE:O	2:H:246:GLY:CA	2.49	0.58
2:H:102:ASP:OD2	2:H:214:SER:OG	2.23	0.57
1:L:1(G):PHE:HD1	1:L:1(G):PHE:H	1.46	0.57
1:L:14(F):LEU:N	1:L:14(F):LEU:CD1	2.67	0.57
2:H:165:ARG:N	2:H:166:PRO:CD	2.68	0.57
2:H:219:GLY:H	4:J:1:34H:H4	1.47	0.57
2:H:107:LYS:HB2	2:H:107:LYS:HZ3	1.68	0.56
2:H:165:ARG:CB	2:H:166:PRO:HD3	2.31	0.56
2:H:217:GLU:HB2	2:H:224:LYS:CD	2.34	0.56
2:H:241:VAL:HB	2:H:245:PHE:CE1	2.41	0.56
1:L:14(A):LYS:CE	2:H:23:GLU:OE2	2.51	0.56
2:H:60:LEU:HD13	2:H:60(G):ASN:OD1	2.05	0.56
2:H:146:GLU:HG2	2:H:146:GLU:O	2.05	0.55
2:H:94:TYR:HE1	2:H:99:LEU:HD22	1.72	0.55
1:L:1(C):GLU:HG2	1:L:1(A):ASP:H	1.71	0.55
2:H:165:ARG:CB	2:H:166:PRO:CD	2.85	0.54
1:L:14(F):LEU:HD11	2:H:159:ASN:CG	2.33	0.54
2:H:51:TRP:CZ3	2:H:107:LYS:HB3	2.43	0.54
2:H:67:ARG:HD2	2:H:70:LYS:CD	2.37	0.54
2:H:67:ARG:HH11	2:H:70:LYS:HD2	1.71	0.54
2:H:110:LYS:CG	2:H:111:PRO:HD2	2.17	0.54
1:L:14(F):LEU:CD1	1:L:14(F):LEU:H	2.21	0.54
2:H:46:LEU:HD22	2:H:48:SER:O	2.07	0.54
2:H:135:LYS:HA	2:H:160:LEU:O	2.08	0.54
2:H:81:LYS:HD3	2:H:118:ILE:CD1	2.38	0.53
3:I:360:PRO:CG	3:I:363:TYS:HD2	2.36	0.53
1:L:14(B):THR:O	1:L:14(D):ARG:CD	2.57	0.53
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.91	0.53
2:H:38:GLN:NE2	3:I:359:ILE:HG23	2.23	0.53
2:H:103:ILE:CG2	2:H:234:LEU:HD12	2.32	0.53
2:H:242:ILE:O	2:H:246:GLY:N	2.41	0.53
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.09	0.53
1:L:1(C):GLU:HG3	1:L:1(B):ALA:CB	2.39	0.53
1:L:1(C):GLU:N	6:H:529:HOH:O	2.38	0.52
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.51	0.52
2:H:146:GLU:O	2:H:146:GLU:CG	2.58	0.52
1:L:14(B):THR:O	1:L:14(E):GLU:N	2.40	0.52
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.40	0.52
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.45	0.52
2:H:67:ARG:HD2	2:H:70:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:LYS:HE2	2:H:205:ASN:O	2.10	0.52
1:L:14(A):LYS:HE2	2:H:23:GLU:CG	2.40	0.51
2:H:204(B):ASN:ND2	2:H:204(B):ASN:N	2.54	0.51
2:H:42:CYS:HB3	2:H:195:SER:O	2.10	0.51
2:H:21:ASP:HB3	2:H:154:VAL:HG12	1.85	0.51
2:H:51:TRP:CH2	2:H:107:LYS:HB3	2.44	0.51
2:H:204(B):ASN:ND2	2:H:204(B):ASN:H	2.08	0.51
2:H:210:MET:O	2:H:231:VAL:HB	2.11	0.51
2:H:241:VAL:HA	2:H:244:GLN:HB2	1.93	0.51
3:I:360:PRO:O	3:I:363:TYS:HB3	2.10	0.51
3:I:357:GLU:CG	3:I:358:GLU:N	2.74	0.51
2:H:43:GLY:O	2:H:44:ALA:HB2	2.10	0.50
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.25	0.50
2:H:202:LYS:HD2	2:H:207:TRP:CE2	2.46	0.50
2:H:73:ARG:CZ	2:H:151:GLN:HB3	2.42	0.50
1:L:14:ASP:OD1	1:L:14:ASP:C	2.53	0.50
3:I:358:GLU:H	3:I:358:GLU:CD	2.20	0.50
1:L:14(M):GLY:O	1:L:15:ARG:OXT	2.30	0.49
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.47	0.49
2:H:139:THR:HG22	2:H:157:VAL:HG12	1.94	0.49
2:H:75:ARG:CD	3:I:357:GLU:OE1	2.50	0.49
2:H:184:GLY:O	6:H:464:HOH:O	2.20	0.49
1:L:1(C):GLU:HG2	1:L:1(A):ASP:N	2.27	0.49
1:L:14(C):GLU:O	1:L:14(D):ARG:C	2.56	0.49
2:H:176:ILE:HD11	2:H:215:TRP:CH2	2.48	0.49
3:I:363:TYS:O1	3:I:363:TYS:HE2	2.13	0.48
2:H:60(I):THR:O	2:H:63:ASP:HB2	2.14	0.48
3:I:360:PRO:HG2	3:I:363:TYS:HE2	1.96	0.48
2:H:60(A):TYR:C	2:H:60(C):PRO:CD	2.80	0.48
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.48	0.48
4:J:2:LEU:CB	4:J:3:PRJ:HD2	2.43	0.48
2:H:22:ALA:HB2	2:H:157:VAL:HG13	1.93	0.48
1:L:14(M):GLY:C	1:L:15:ARG:OXT	2.56	0.48
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.49	0.48
1:L:14(D):ARG:NH1	1:L:14(E):GLU:CG	2.77	0.48
2:H:60(B):PRO:CD	2:H:60(C):PRO:CD	2.92	0.48
1:L:14(D):ARG:HG2	1:L:14(E):GLU:N	2.26	0.47
2:H:21:ASP:CB	2:H:154:VAL:CG1	2.83	0.47
2:H:100:ASP:OD1	2:H:177:THR:OG1	2.26	0.47
2:H:189:ASP:OD1	4:J:4:OAR:NH1	2.45	0.47
1:L:14(A):LYS:HE2	2:H:23:GLU:CD	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ALA:HB1	2:H:90:ILE:CG2	2.43	0.47
2:H:235:LYS:O	2:H:239:GLN:N	2.44	0.47
1:L:1(E):SER:H	2:H:235:LYS:NZ	2.08	0.47
2:H:195:SER:HB2	4:J:4:OAR:HC1	1.85	0.47
2:H:36:LYS:HG3	2:H:65:LEU:HD22	1.96	0.47
2:H:62:ASN:C	2:H:62:ASN:HD22	2.23	0.47
2:H:65:LEU:HD12	2:H:84:MET:HE2	1.95	0.47
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.96	0.47
2:H:50:ARG:CG	2:H:247:GLU:CD	2.73	0.47
2:H:81:LYS:NZ	2:H:118:ILE:HD12	2.29	0.47
2:H:60(G):ASN:ND2	6:H:550:HOH:O	2.48	0.47
2:H:21:ASP:CB	2:H:154:VAL:HG11	2.42	0.46
2:H:191:CYS:O	2:H:192:GLU:C	2.57	0.46
2:H:74:THR:HB	3:I:356:PHE:HA	1.96	0.46
2:H:100:ASP:CG	2:H:177:THR:HG21	2.40	0.46
1:L:14(B):THR:HB	1:L:14(D):ARG:NH1	2.30	0.46
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.12	0.46
2:H:131:GLN:HE21	2:H:131:GLN:HB3	1.49	0.46
1:L:1(A):ASP:OD2	1:L:9:LYS:CE	2.61	0.46
2:H:89:TYR:CZ	2:H:245:PHE:CE1	3.04	0.46
2:H:70:LYS:NZ	2:H:80:GLU:OE1	2.45	0.46
2:H:41:LEU:HD13	2:H:60(H):PHE:CE2	2.51	0.46
2:H:73:ARG:NE	2:H:152:PRO:O	2.32	0.46
1:L:1(G):PHE:CD2	1:L:1(G):PHE:C	2.94	0.46
2:H:34:PHE:HE2	2:H:38:GLN:HG2	1.81	0.45
2:H:60(B):PRO:CD	2:H:60(C):PRO:HD2	2.46	0.45
2:H:124:PRO:C	2:H:235:LYS:HZ2	2.12	0.45
2:H:77(A):ARG:HG3	2:H:77(A):ARG:O	2.17	0.45
2:H:103:ILE:HD12	2:H:212:ILE:HD12	1.97	0.45
1:L:1(A):ASP:O	2:H:119:HIS:NE2	2.42	0.45
2:H:49:ASP:HB2	2:H:112:VAL:O	2.16	0.45
4:J:1:34H:C8	4:J:2:LEU:CD2	2.95	0.45
2:H:38:GLN:NE2	3:I:359:ILE:CG2	2.80	0.45
2:H:204(B):ASN:HD22	2:H:204(B):ASN:N	2.03	0.45
2:H:216:GLY:O	4:J:2:LEU:CA	2.65	0.45
2:H:32:MET:HB2	2:H:141:TRP:CZ3	2.51	0.45
1:L:14(K):ILE:O	1:L:14(L):ASP:HB2	2.16	0.44
3:I:363:TYS:CE2	3:I:363:TYS:O1	2.65	0.44
1:L:14(A):LYS:HE2	2:H:23:GLU:HG3	2.00	0.44
2:H:17:VAL:O	2:H:18:GLU:HB2	2.17	0.44
4:J:2:LEU:HB3	4:J:3:PRJ:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(B):THR:O	1:L:14(C):GLU:C	2.61	0.44
2:H:217:GLU:C	2:H:219:GLY:O	2.61	0.44
2:H:57:HIS:CE1	2:H:195:SER:OG	2.71	0.44
2:H:64:LEU:O	6:H:460:HOH:O	2.21	0.44
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.44	0.44
2:H:89:TYR:CE2	2:H:245:PHE:CZ	3.06	0.43
2:H:125:ASP:OD1	2:H:127:GLU:HG2	2.18	0.43
2:H:61:GLU:H	2:H:61:GLU:HG2	1.26	0.43
2:H:103:ILE:CG2	2:H:234:LEU:CD1	2.92	0.43
2:H:85:LEU:HD13	2:H:106:MET:CE	2.36	0.43
2:H:173:ARG:HH11	2:H:173:ARG:HD2	1.52	0.43
2:H:107:LYS:HB2	2:H:107:LYS:HZ2	1.82	0.43
2:H:165:ARG:HH11	2:H:165:ARG:HD2	1.50	0.43
2:H:32:MET:CG	2:H:40:LEU:HD13	2.47	0.43
2:H:185:LYS:C	2:H:186(A):ASP:N	2.76	0.43
2:H:16:ILE:N	2:H:194:ASP:OD2	2.52	0.42
1:L:14(A):LYS:HG3	2:H:23:GLU:CD	2.42	0.42
2:H:61:GLU:OE1	2:H:88:ILE:N	2.53	0.42
2:H:212:ILE:O	2:H:228:TYR:HB3	2.18	0.42
2:H:77(A):ARG:O	2:H:77(A):ARG:CG	2.67	0.42
2:H:201:MET:CE	2:H:210:MET:HE3	2.45	0.42
2:H:103:ILE:HD11	2:H:238:ILE:HD11	2.00	0.42
2:H:38:GLN:OE1	3:I:364:LEU:HD11	2.20	0.42
1:L:14(J):TYR:HD2	2:H:204:PRO:HG3	1.85	0.41
2:H:67:ARG:HD2	2:H:70:LYS:HD3	2.00	0.41
2:H:232:PHE:C	2:H:234:LEU:N	2.78	0.41
2:H:61:GLU:OE1	2:H:87:LYS:CA	2.64	0.41
2:H:70:LYS:CE	2:H:72:SER:O	2.68	0.41
2:H:77(A):ARG:HH11	2:H:77(A):ARG:HD2	1.50	0.41
2:H:187:ARG:HD3	2:H:221:ASP:OD2	2.21	0.41
2:H:60:LEU:HA	2:H:60(F):LYS:O	2.20	0.41
2:H:73:ARG:NE	2:H:151:GLN:HB3	2.35	0.41
2:H:97(A):GLU:OE1	2:H:175:ARG:NH2	2.52	0.41
2:H:121:VAL:HG11	2:H:209:GLN:HB2	2.02	0.41
2:H:185:LYS:O	2:H:186(B):GLU:N	2.53	0.41
2:H:98:ASN:OD1	2:H:98:ASN:N	2.47	0.41
1:L:1(H):THR:HB	1:L:1(G):PHE:CE1	2.55	0.41
1:L:1(D):GLY:H	2:H:123:LEU:H	1.66	0.41
2:H:49:ASP:HB3	2:H:114:PHE:HZ	1.81	0.41
2:H:53:LEU:HD11	2:H:103:ILE:HG13	2.02	0.41
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:HD3	2:H:111:PRO:HD3	2.03	0.41
2:H:195:SER:OG	4:J:4:OAR:C	2.60	0.41
2:H:56:ALA:CB	2:H:90:ILE:CG2	2.93	0.40
2:H:145:LYS:HZ3	2:H:145:LYS:HG2	1.76	0.40
1:L:14(J):TYR:N	1:L:14(J):TYR:CD1	2.87	0.40
2:H:35:ARG:HB3	2:H:39:GLU:HG3	2.04	0.40
2:H:21:ASP:CB	2:H:154:VAL:HG12	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(L):ASP:C	2:H:173:ARG:NH2[4_556]	1.86	0.34
1:L:14(L):ASP:O	2:H:173:ARG:NH2[4_556]	2.09	0.11

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	L	34/36 (94%)	19 (56%)	10 (29%)	5 (15%)	0	0
2	H	248/259 (96%)	223 (90%)	21 (8%)	4 (2%)	7	4
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	289/307 (94%)	249 (86%)	31 (11%)	9 (3%)	3	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(G)	PHE
1	L	1(F)	GLY
1	L	1(D)	GLY
2	H	219	GLY

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Mol	Chain	Res	Type
1	L	1(E)	SER
1	L	1(C)	GLU
2	H	192	GLU
2	H	126	ARG
2	H	44	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	30/31 (97%)	23 (77%)	7 (23%)	1	0
2	H	220/225 (98%)	179 (81%)	41 (19%)	1	1
3	I	8/10 (80%)	5 (62%)	3 (38%)	0	0
4	J	1/1 (100%)	0	1 (100%)	0	0
All	All	259/267 (97%)	207 (80%)	52 (20%)	1	0

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(H)	THR
1	L	1(G)	PHE
1	L	1(E)	SER
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	1	CYS
1	L	6	LEU
2	H	20	SER
2	H	24	ILE
2	H	27	SER
2	H	33	LEU
2	H	46	LEU
2	H	48	SER
2	H	61	GLU
2	H	62	ASN
2	H	65	LEU

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Mol	Chain	Res	Type
2	H	66	VAL
2	H	70	LYS
2	H	79	ILE
2	H	83	SER
2	H	84	MET
2	H	85	LEU
2	H	87	LYS
2	H	107	LYS
2	H	109	LYS
2	H	112	VAL
2	H	115	SER
2	H	127	GLU
2	H	138	VAL
2	H	145	LYS
2	H	154	VAL
2	H	165	ARG
2	H	176	ILE
2	H	187	ARG
2	H	192	GLU
2	H	195	SER
2	H	205	ASN
2	H	217	GLU
2	H	222	ASP
2	H	229	THR
2	H	234	LEU
2	H	236	LYS
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
2	H	245	PHE
2	H	247	GLU
3	I	358	GLU
3	I	359	ILE
3	I	362	GLU
4	J	2	LEU

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	62	ASN
2	H	131	GLN

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Mol	Chain	Res	Type
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN
2	H	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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	PRJ	J	3	4	12,13,14	2.65	5 (41%)	11,18,20	2.61	7 (63%)
3	TYS	I	363	3	15,16,17	1.79	2 (13%)	15,22,24	2.12	5 (33%)
4	OAR	J	4	4	10,10,10	1.31	0	9,11,11	2.78	4 (44%)

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	PRJ	J	3	4	-	0/0/23/25	0/2/2/2
3	TYS	I	363	3	-	3/10/11/13	0/1/1/1
4	OAR	J	4	4	-	1/9/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	PRJ	C14-CD	6.12	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	363	TYS	OH-S	5.51	1.69	1.58
4	J	3	PRJ	CA-N	-3.56	1.42	1.48
4	J	3	PRJ	C14-C13	3.55	1.58	1.52
3	I	363	TYS	OH-CZ	-3.26	1.37	1.42
4	J	3	PRJ	CD-N	-2.86	1.43	1.48
4	J	3	PRJ	C12-C11	2.67	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	4	OAR	CB-CA-C	-5.98	104.06	112.25
3	I	363	TYS	OH-S-O2	-5.39	91.14	107.56
4	J	3	PRJ	CB-CG-CD	-4.62	94.27	100.75
4	J	4	OAR	CG-CB-CA	-3.95	95.62	116.12
4	J	3	PRJ	C11-CG-CD	3.57	121.57	113.66
4	J	3	PRJ	C14-C13-C12	3.33	114.67	110.62
3	I	363	TYS	O2-S-O1	3.09	124.16	112.24
4	J	3	PRJ	O-C-CA	-2.96	117.16	124.77
4	J	4	OAR	CB-CG-CD	-2.90	103.72	112.07
4	J	3	PRJ	C11-C12-C13	-2.74	107.14	111.53
3	I	363	TYS	CD1-CE1-CZ	-2.36	117.03	119.73
3	I	363	TYS	OH-CZ-CE2	-2.31	114.17	118.70
3	I	363	TYS	CE2-CZ-CE1	2.18	123.34	120.16
4	J	3	PRJ	CG-CB-CA	2.07	107.75	104.16
4	J	4	OAR	CB-CA-N	2.02	115.31	109.16
4	J	3	PRJ	O2-C13-C14	2.01	113.85	109.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	363	TYS	O-C-CA-CB
4	J	4	OAR	NE-CD-CG-CB
3	I	363	TYS	CA-CB-CG-CD1
3	I	363	TYS	CA-CB-CG-CD2

There are no ring outliers.

3 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	3	PRJ	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	363	TYS	10	0
4	J	4	OAR	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	14(L):ASP	C	14(M):GLY	N	1.74
1	L	14(J):TYR	C	14(K):ILE	N	1.12

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.