



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 03:16 pm GMT

PDB ID : 1A2C  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

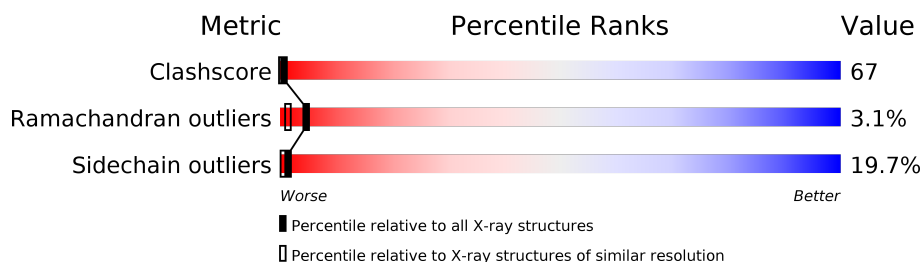
# 1 Overall quality at a glance

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	122078	5107 (2.10-2.10)
Ramachandran outliers	120005	5057 (2.10-2.10)
Sidechain outliers	119972	5058 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 (three-letter code: 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

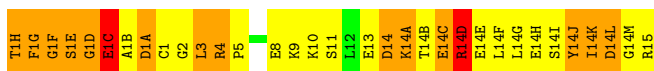
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

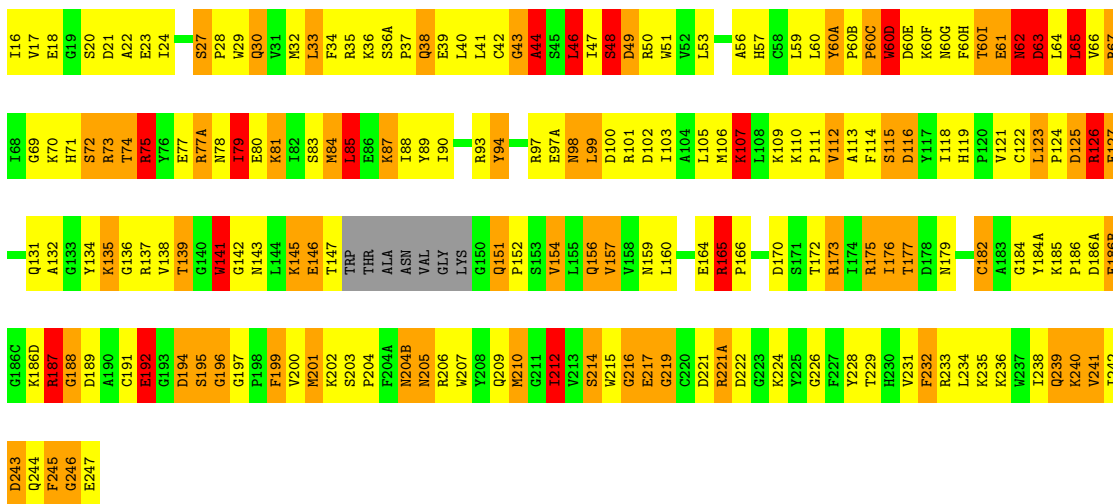
#### • Molecule 1: Thrombin light chain

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: NA, TYS, 34H, OAR, PRJ

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	1.85	2/284 (0.7%)	2.66	18/377 (4.8%)
2	H	1.16	1/2091 (0.0%)	2.39	109/2823 (3.9%)
3	I	1.00	0/73	2.41	4/96 (4.2%)
4	J	0.53	0/7	3.36	1/8 (12.5%)
All	All	1.25	3/2455 (0.1%)	2.43	132/3304 (4.0%)

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 (3) 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
1	L	14(J)	TYR	C-N	-9.23	1.12	1.34
2	H	216	GLY	C-N	6.85	1.49	1.34

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	206	ARG	NE-CZ-NH1	18.54	129.57	120.30
2	H	126	ARG	NE-CZ-NH2	16.13	128.36	120.30
1	L	14(L)	ASP	O-C-N	-15.15	97.45	123.20
2	H	206	ARG	NE-CZ-NH2	-14.95	112.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	ARG	NE-CZ-NH2	13.61	127.11	120.30
2	H	101	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	L	1(A)	ASP	CB-CG-OD1	-12.53	107.02	118.30
2	H	243	ASP	CB-CG-OD1	12.27	129.34	118.30
2	H	194	ASP	CB-CG-OD1	-12.10	107.41	118.30
2	H	97	ARG	NE-CZ-NH1	-12.07	114.27	120.30
1	L	1(A)	ASP	CB-CG-OD2	11.53	128.67	118.30
1	L	4	ARG	NE-CZ-NH2	10.93	125.76	120.30
2	H	137	ARG	NE-CZ-NH1	-10.87	114.87	120.30
2	H	146	GLU	OE1-CD-OE2	10.86	136.33	123.30
2	H	173	ARG	NE-CZ-NH2	10.82	125.71	120.30
1	L	14(L)	ASP	CA-C-N	-10.62	94.96	116.20
2	H	194	ASP	CB-CG-OD2	10.14	127.42	118.30
2	H	233	ARG	CD-NE-CZ	10.13	137.78	123.60
1	L	14	ASP	CB-CG-OD1	-10.11	109.20	118.30
2	H	73	ARG	NE-CZ-NH2	10.06	125.33	120.30
2	H	221(A)	ARG	NE-CZ-NH1	-9.38	115.61	120.30
2	H	73	ARG	NH1-CZ-NH2	-8.95	109.56	119.40
2	H	73	ARG	NE-CZ-NH1	8.93	124.76	120.30
2	H	49	ASP	CB-CG-OD1	-8.86	110.33	118.30
2	H	137	ARG	NE-CZ-NH2	8.82	124.71	120.30
2	H	60(E)	ASP	CB-CG-OD1	-8.66	110.51	118.30
1	L	14	ASP	CB-CG-OD2	8.62	126.05	118.30
2	H	141	TRP	O-C-N	-8.18	109.30	123.20
2	H	165	ARG	CA-CB-CG	8.17	131.37	113.40
2	H	97	ARG	CD-NE-CZ	-7.98	112.43	123.60
4	J	2	LEU	CB-CA-C	7.92	125.24	110.20
1	L	4	ARG	NH1-CZ-NH2	-7.78	110.85	119.40
2	H	75	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	L	14(D)	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	H	137	ARG	O-C-N	7.43	134.59	122.70
2	H	176	ILE	CA-CB-CG2	7.40	125.69	110.90
2	H	49	ASP	CB-CG-OD2	7.35	124.92	118.30
1	L	10	LYS	O-C-N	7.34	134.44	122.70
2	H	200	VAL	CA-CB-CG1	7.33	121.90	110.90
2	H	123	LEU	CA-CB-CG	7.33	132.15	115.30
2	H	24	ILE	C-N-CA	7.30	137.64	122.30
2	H	125	ASP	CB-CG-OD2	7.17	124.76	118.30
2	H	132	ALA	O-C-N	7.08	135.24	123.20
2	H	186(B)	GLU	CG-CD-OE2	7.08	132.45	118.30
2	H	173	ARG	CD-NE-CZ	-6.94	113.89	123.60
2	H	94	TYR	CB-CG-CD2	-6.84	116.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	143	ASN	O-C-N	6.82	133.62	122.70
1	L	14(J)	TYR	CA-C-N	-6.81	102.22	117.20
1	L	13	GLU	CB-CA-C	-6.75	96.90	110.40
2	H	201	MET	CA-CB-CG	-6.71	101.89	113.30
2	H	186(B)	GLU	CG-CD-OE1	-6.60	105.09	118.30
2	H	38	GLN	O-C-N	6.56	133.19	122.70
2	H	33	LEU	N-CA-CB	-6.55	97.30	110.40
2	H	137	ARG	CA-C-O	-6.54	106.37	120.10
2	H	173	ARG	NE-CZ-NH1	-6.47	117.06	120.30
2	H	30	GLN	CA-CB-CG	6.46	127.62	113.40
2	H	60(A)	TYR	CA-CB-CG	-6.33	101.38	113.40
2	H	77(A)	ARG	CA-C-O	-6.32	106.82	120.10
3	I	362	GLU	CB-CG-CD	6.31	131.24	114.20
2	H	126	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
2	H	199	PHE	O-C-N	-6.25	112.71	122.70
2	H	145	LYS	N-CA-CB	6.19	121.74	110.60
2	H	27	SER	N-CA-CB	-6.18	101.23	110.50
2	H	77(A)	ARG	NE-CZ-NH1	-6.14	117.23	120.30
2	H	63	ASP	O-C-N	6.13	132.51	122.70
2	H	210	MET	CG-SD-CE	-6.11	90.43	100.20
2	H	165	ARG	CD-NE-CZ	-6.09	115.07	123.60
2	H	60(E)	ASP	N-CA-CB	-6.09	99.65	110.60
2	H	210	MET	CA-CB-CG	-6.08	102.97	113.30
2	H	126	ARG	CG-CD-NE	6.05	124.50	111.80
2	H	142	GLY	CA-C-O	6.00	131.40	120.60
1	L	2	GLY	N-CA-C	5.95	127.98	113.10
2	H	138	VAL	CA-CB-CG1	5.85	119.67	110.90
2	H	175	ARG	C-N-CA	5.83	136.27	121.70
2	H	105	LEU	O-C-N	5.82	132.02	122.70
1	L	11	SER	CB-CA-C	5.82	121.15	110.10
2	H	233	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	H	143	ASN	CA-C-O	-5.78	107.96	120.10
3	I	359	ILE	O-C-N	5.78	132.07	121.10
1	L	10	LYS	CD-CE-NZ	-5.76	98.45	111.70
3	I	362	GLU	CG-CD-OE1	5.73	129.76	118.30
2	H	62	ASN	CB-CG-OD1	-5.71	110.18	121.60
2	H	44	ALA	CB-CA-C	5.71	118.66	110.10
2	H	62	ASN	OD1-CG-ND2	5.69	134.98	121.90
2	H	60(D)	TRP	N-CA-C	-5.66	95.72	111.00
2	H	74	THR	CA-CB-OG1	-5.65	97.14	109.00
2	H	93	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	H	165	ARG	NE-CZ-NH1	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	LYS	C-N-CA	5.59	134.04	122.30
1	L	14(C)	GLU	CB-CA-C	-5.58	99.25	110.40
2	H	77(A)	ARG	CD-NE-CZ	-5.51	115.88	123.60
2	H	116	ASP	O-C-N	5.51	131.52	122.70
2	H	60(A)	TYR	CB-CG-CD1	-5.51	117.69	121.00
2	H	186	PRO	O-C-N	5.50	131.50	122.70
2	H	200	VAL	CG1-CB-CG2	-5.45	102.17	110.90
2	H	46	LEU	CA-CB-CG	5.45	127.83	115.30
2	H	173	ARG	N-CA-CB	5.44	120.39	110.60
2	H	187	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	H	60(D)	TRP	N-CA-CB	5.41	120.34	110.60
2	H	170	ASP	CB-CG-OD2	5.40	123.16	118.30
2	H	243	ASP	CA-C-N	-5.37	105.39	117.20
2	H	156	GLN	CG-CD-OE1	-5.34	110.92	121.60
2	H	186(B)	GLU	O-C-N	-5.33	114.13	123.20
2	H	75	ARG	CA-CB-CG	-5.33	101.68	113.40
2	H	179	ASN	CB-CG-OD1	-5.32	110.96	121.60
2	H	246	GLY	N-CA-C	5.32	126.41	113.10
2	H	46	LEU	CB-CG-CD2	5.30	120.02	111.00
2	H	157	VAL	CA-CB-CG2	5.26	118.79	110.90
2	H	212	ILE	CA-CB-CG1	5.26	121.00	111.00
2	H	48	SER	CB-CA-C	5.23	120.04	110.10
2	H	85	LEU	CA-C-N	-5.22	105.72	117.20
2	H	113	ALA	O-C-N	5.22	131.05	122.70
2	H	67	ARG	CB-CG-CD	-5.21	98.05	111.60
2	H	77	GLU	CG-CD-OE2	5.19	128.68	118.30
2	H	154	VAL	N-CA-CB	-5.14	100.18	111.50
3	I	357	GLU	CG-CD-OE2	-5.14	108.02	118.30
2	H	154	VAL	CA-CB-CG1	5.11	118.57	110.90
2	H	139	THR	CA-C-N	-5.10	105.99	116.20
2	H	196	GLY	O-C-N	-5.05	114.61	123.20
2	H	232	PHE	O-C-N	-5.05	114.62	122.70
2	H	98	ASN	OD1-CG-ND2	5.05	133.52	121.90
2	H	123	LEU	CB-CG-CD2	-5.05	102.41	111.00
2	H	77(A)	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	H	192	GLU	CB-CA-C	-5.04	100.31	110.40
2	H	116	ASP	CA-CB-CG	5.03	124.47	113.40
2	H	243	ASP	CA-CB-CG	5.03	124.46	113.40
2	H	177	THR	CA-CB-CG2	5.02	119.42	112.40
1	L	4	ARG	CG-CD-NE	5.02	122.33	111.80
1	L	1(A)	ASP	CA-CB-CG	-5.01	102.37	113.40
2	H	187	ARG	C-N-CA	-5.01	111.78	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	GLY	N-CA-C	-5.00	100.59	113.10
2	H	243	ASP	CA-C-O	5.00	130.61	120.10

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
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	78	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2039	0	2010	251	2
3	I	89	0	67	20	0
4	J	43	0	45	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	2387	326	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 67.

All (326) 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	1.37
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	1.20
1:L:1(E):SER:HA	2:H:123:LEU:O	1.43	1.14
2:H:195:SER:CB	4:J:4:OAR:HC2	1.79	1.13
1:L:14(D):ARG:HD3	1:L:14(E):GLU:N	1.62	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: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:201:MET:HE3	2:H:210:MET:CG	1.91	1.01
2:H:17:VAL:O	2:H:188:GLY:HA2	1.61	1.01
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:50:ARG:HG3	2:H:247:GLU:CD	1.86	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:MET:HE3	2:H:210:MET:HG3	0.95	0.93
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
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: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:110:LYS:HG3	2:H:111:PRO:CD	2.06	0.85
2:H:49:ASP:O	2:H:112:VAL:HG23	1.75	0.85
3:I:360:PRO:HG2	3:I:363:TYS:HD2	1.57	0.85
2:H:22:ALA:HB2	2:H:157:VAL:CG1	2.08	0.84
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:204(B):ASN:C	2:H:204(B):ASN:HD22	1.78	0.83
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
1:L:14(D):ARG:HH11	1:L:14(E):GLU:CB	1.84	0.82
2:H:60(A):TYR:C	2:H:60(C):PRO:HD2	2.00	0.82
2:H:60(D):TRP:CZ2	4:J:3:PRJ:H13	2.15	0.82
2:H:191:CYS:O	2:H:194:ASP:HB2	1.79	0.81
1:L:1(C):GLU:CG	1:L:1(B):ALA:N	2.04	0.81
2:H:195:SER:OG	4:J:4:OAR:HC2	1.79	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:103:ILE:HG21	2:H:234:LEU:CD1	2.13	0.79
2:H:36:LYS:O	2:H:38:GLN:HG3	1.83	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:60(I):THR:HG23	2:H:63:ASP:CG	2.05	0.77
2:H:107:LYS:NZ	2:H:107:LYS:HB2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:ARG:HD3	2:H:70:LYS:HD2	1.67	0.77
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
2:H:201:MET:HE1	2:H:210:MET:HG3	1.68	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
2:H:156:GLN:C	2:H:157:VAL:HG13	2.08	0.73
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
2:H:69:GLY:O	2:H:79:ILE:CD1	2.36	0.72
2:H:37:PRO:O	2:H:39:GLU:HG2	1.90	0.71
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.44	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
2:H:165:ARG:N	2:H:166:PRO:HD2	2.05	0.70
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.22	0.70
1:L:1(D):GLY:HA3	6:H:529:HOH:O	1.91	0.70
2:H:217:GLU:HG3	2:H:224:LYS:CE	2.22	0.70
1:L:1(G):PHE:CD1	1:L:1(G):PHE:N	2.59	0.70
1:L:8:GLU:OE2	2:H:202:LYS:HE3	1.90	0.70
2:H:217:GLU:CG	2:H:224:LYS:HD3	2.22	0.69
2:H:50:ARG:HB2	2:H:247:GLU:HG3	1.73	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
2:H:60(D):TRP:CH2	4:J:3:PRJ:H13	2.26	0.69
1:L:14(D):ARG:CG	1:L:14(E):GLU:N	2.55	0.69
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.93	0.69
1:L:1(C):GLU:HG3	1:L:1(B):ALA:H	0.53	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
2:H:221(A):ARG:HH22	4:J:1:34H:H5	1.58	0.68
1:L:14(D):ARG:NH1	1:L:14(E):GLU:CB	2.51	0.68
2:H:98:ASN:ND2	2:H:175:ARG:O	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:LEU:HD13	2:H:106:MET:HE2	1.77	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:156:GLN:C	2:H:157:VAL:CG1	2.64	0.66
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
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
2:H:204(B):ASN:C	2:H:204(B):ASN:ND2	2.48	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:1(G):PHE:O	1:L:1(F):GLY:C	2.35	0.65
2:H:182:CYS:HA	2:H:226:GLY:O	1.96	0.65
1:L:14(B):THR:O	1:L:14(D):ARG:HD3	1.97	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:203:SER:HB3	2:H:204(B):ASN:ND2	2.12	0.64
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.15	0.64
2:H:59:LEU:HD22	2:H:88:ILE:HD13	1.80	0.64
1:L:4:ARG:NH2	1:L:14(C):GLU:OE2	2.31	0.64
2:H:49:ASP:N	2:H:49:ASP:OD1	2.27	0.64
2:H:201:MET:HE1	2:H:210:MET:CG	2.25	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
2:H:217:GLU:HG3	2:H:224:LYS:CD	2.28	0.62
2:H:79:ILE:CD1	6:H:500:HOH:O	2.47	0.62
1:L:14(G):LEU:O	1:L:14(L):ASP:CA	2.46	0.62
1:L:1(D):GLY:N	2:H:123:LEU:H	1.97	0.62
2:H:30:GLN:OE1	2:H:139:THR:OG1	2.18	0.61
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
1:L:14(F):LEU:HD12	1:L:14(F):LEU:N	2.15	0.61
2:H:216:GLY:O	4:J:2:LEU:N	2.35	0.60
2:H:125:ASP:O	2:H:127:GLU:N	2.35	0.60
2:H:81:LYS:HE3	6:H:468:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:361:GLU:C	3:I:363:TYS:N	2.52	0.60
2:H:49:ASP:O	2:H:112:VAL:CG2	2.48	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
2:H:125:ASP:O	2:H:126:ARG:C	2.40	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:65:LEU:HD11	2:H:84:MET:HE1	1.84	0.60
2:H:22:ALA:CB	2:H:157:VAL:HG11	2.32	0.58
4:J:2:LEU:CD2	4:J:2:LEU:N	2.65	0.58
2:H:107:LYS:HZ2	2:H:107:LYS:HB2	1.66	0.58
2:H:217:GLU:O	2:H:219:GLY:O	2.21	0.58
2:H:195:SER:CB	4:J:4:OAR:C	2.54	0.58
2:H:60(F):LYS:HD3	2:H:60(H):PHE:CE2	2.38	0.58
1:L:1(C):GLU:HG3	1:L:1(B):ALA:CA	2.26	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:H	1:L:1(G):PHE:HD1	1.46	0.57
2:H:165:ARG:N	2:H:166:PRO:CD	2.68	0.57
1:L:14(F):LEU:CD1	1:L:14(F):LEU:N	2.67	0.57
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
2:H:165:ARG:CB	2:H:166:PRO:HD3	2.31	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:85:LEU:HD13	2:H:106:MET:CE	2.36	0.55
2:H:146:GLU:HG2	2:H:146:GLU:O	2.05	0.55
1:L:1(E):SER:H	2:H:235:LYS:HZ1	1.53	0.55
2:H:94:TYR:HE1	2:H:99:LEU:HD22	1.72	0.55
2:H:201:MET:HB2	2:H:210:MET:HE2	1.88	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
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:H	1:L:14(F):LEU:CD1	2.21	0.54
2:H:135:LYS:HA	2:H:160:LEU:O	2.08	0.54
2:H:46:LEU:HD22	2:H:48:SER:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(B):THR:O	1:L:14(D):ARG:CD	2.57	0.53
2:H:103:ILE:CG2	2:H:234:LEU:HD12	2.32	0.53
2:H:38:GLN:NE2	3:I:359:ILE:HG23	2.23	0.53
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.91	0.53
2:H:242:ILE:O	2:H:246:GLY:N	2.41	0.53
2:H:65:LEU:HD11	2:H:84:MET:HE2	1.87	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(E):SER:H	2:H:235:LYS:NZ	2.08	0.52
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:CG	2:H:146:GLU:O	2.58	0.52
1:L:14(B):THR:O	1:L:14(E):GLU:N	2.40	0.52
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.45	0.52
1:L:4:ARG:HG2	2:H:28:PRO:CG	2.40	0.52
2:H:202:LYS:HE2	2:H:205:ASN:O	2.10	0.52
2:H:67:ARG:HD2	2:H:70:LYS:HD2	1.92	0.52
2:H:204(B):ASN:N	2:H:204(B):ASN:ND2	2.54	0.51
1:L:14(A):LYS:HE2	2:H:23:GLU:CG	2.40	0.51
2:H:195:SER:HG	4:J:4:OAR:HC2	1.76	0.51
2:H:42:CYS:HB3	2:H:195:SER:O	2.10	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:21:ASP:HB3	2:H:154:VAL:HG12	1.85	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
2:H:43:GLY:O	2:H:44:ALA:HB2	2.10	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
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
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.47	0.49
1:L:14(F):LEU:HD11	2:H:159:ASN:CG	2.33	0.49
1:L:14(M):GLY:O	1:L:15:ARG:OXT	2.30	0.49
2:H:139:THR:HG22	2:H:157:VAL:HG12	1.94	0.49
2:H:184:GLY:O	6:H:464:HOH:O	2.20	0.49
2:H:75:ARG:CD	3:I:357:GLU:OE1	2.50	0.49
2:H:176:ILE:HD11	2:H:215:TRP:CH2	2.48	0.49
1:L:1(C):GLU:HG2	1:L:1(A):ASP:N	2.27	0.49
3:I:363:TYS:O1	3:I:363:TYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.49	0.48
2:H:60(B):PRO:CD	2:H:60(C):PRO:CD	2.92	0.48
1:L:14(D):ARG:NH1	1:L:14(E):GLU:CG	2.77	0.48
2:H:65:LEU:CD1	2:H:84:MET:HE2	2.44	0.47
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:189:ASP:OD1	4:J:4:OAR:NH1	2.45	0.47
2:H:235:LYS:O	2:H:239:GLN:N	2.44	0.47
2:H:56:ALA:HB1	2:H:90:ILE:CG2	2.43	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:85:LEU:HD22	2:H:106:MET:HB3	1.96	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:74:THR:HB	3:I:356:PHE:HA	1.96	0.46
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.12	0.46
1:L:14(B):THR:HB	1:L:14(D):ARG:NH1	2.30	0.46
2:H:131:GLN:HB3	2:H:131:GLN:HE21	1.49	0.46
1:L:14:ASP:C	1:L:14:ASP:OD1	2.53	0.46
2:H:89:TYR:CZ	2:H:245:PHE:CE1	3.04	0.46
1:L:1(A):ASP:OD2	1:L:9:LYS:CE	2.61	0.46
2:H:70:LYS:NZ	2:H:80:GLU:OE1	2.45	0.46
2:H:73:ARG:NE	2:H:152:PRO:O	2.32	0.46
2:H:41:LEU:HD13	2:H:60(H):PHE:CE2	2.51	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: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
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
1:L:1(A):ASP:O	2:H:119:HIS:NE2	2.42	0.45
2:H:204(B):ASN:N	2:H:204(B):ASN:HD22	2.03	0.45
2:H:216:GLY:O	4:J:2:LEU:CA	2.65	0.45
2:H:38:GLN:NE2	3:I:359:ILE:CG2	2.80	0.45
2:H:32:MET:HB2	2:H:141:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:363:TYS:CE2	3:I:363:TYS:O1	2.65	0.44
1:L:14(K):ILE:O	1:L:14(L):ASP:HB2	2.16	0.44
2:H:17:VAL:O	2:H:18:GLU:HB2	2.17	0.44
1:L:14(A):LYS:HE2	2:H:23:GLU:HG3	2.00	0.44
4:J:2:LEU:HB3	4:J:3:PRJ:HD2	2.00	0.44
3:I:358:GLU:CD	3:I:358:GLU:H	2.20	0.44
2:H:57:HIS:CE1	2:H:195:SER:OG	2.71	0.44
1:L:14(C):GLU:O	1:L:14(D):ARG:C	2.56	0.44
2:H:64:LEU:O	6:H:460:HOH:O	2.21	0.44
2:H:70:LYS:HB3	2:H:70:LYS:HE3	1.44	0.44
2:H:125:ASP:OD1	2:H:127:GLU:HG2	2.18	0.43
2:H:89:TYR:CE2	2:H:245:PHE:CZ	3.06	0.43
2:H:103:ILE:CG2	2:H:234:LEU:CD1	2.92	0.43
2:H:61:GLU:HG2	2:H:61:GLU:H	1.26	0.43
2:H:173:ARG:HH11	2:H:173:ARG:HD2	1.52	0.43
1:L:14(M):GLY:C	1:L:15:ARG:OXT	2.56	0.43
2:H:165:ARG:HD2	2:H:165:ARG:HH11	1.50	0.43
2:H:32:MET:CG	2:H:40:LEU:HD13	2.47	0.43
2:H:16:ILE:N	2:H:194:ASP:OD2	2.52	0.42
1:L:14(A):LYS:HE2	2:H:23:GLU:CD	2.37	0.42
2:H:212:ILE:O	2:H:228:TYR:HB3	2.18	0.42
2:H:61:GLU:OE1	2:H:88:ILE:N	2.53	0.42
2:H:62:ASN:HD22	2:H:62:ASN:C	2.23	0.42
2:H:77(A):ARG:O	2:H:77(A):ARG:CG	2.67	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
2:H:191:CYS:O	2:H:192:GLU:C	2.57	0.42
2:H:100:ASP:CG	2:H:177:THR:HG21	2.40	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:65:LEU:CD1	2:H:84:MET:CE	2.92	0.41
2:H:187:ARG:HD3	2:H:221:ASP:OD2	2.21	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:73:ARG:NE	2:H:151:GLN:HB3	2.35	0.41
2:H:60:LEU:HA	2:H:60(F):LYS:O	2.20	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:N	2:H:98:ASN:OD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(G):PHE:C	1:L:1(G):PHE:CD2	2.94	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
1:L:1(D):GLY:H	2:H:123:LEU:H	1.66	0.41
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.56	0.41
1:L:1(H):THR:HB	1:L:1(G):PHE:CE1	2.55	0.41
2:H:195:SER:OG	4:J:4:OAR:C	2.60	0.41
2:H:50:ARG:HD3	2:H:111:PRO:HD3	2.03	0.41
2:H:56:ALA:CB	2:H:90:ILE:CG2	2.93	0.40
2:H:85:LEU:CD1	2:H:106:MET:CE	2.99	0.40
2:H:35:ARG:HB3	2:H:39:GLU:HG3	2.04	0.40
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.52	0.40
1:L:14(J):TYR:N	1:L:14(J):TYR:CD1	2.87	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	34/36 (94%)	19 (56%)	10 (29%)	5 (15%)	0	0
2	H	248/259 (96%)	223 (90%)	21 (8%)	4 (2%)	11	5
3	I	7/12 (58%)	7 (100%)	0	0	100	100
All	All	289/307 (94%)	249 (86%)	31 (11%)	9 (3%)	4	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
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%)	25 (83%)	5 (17%)	2	1
2	H	220/225 (98%)	177 (80%)	43 (20%)	1	0
3	I	8/10 (80%)	6 (75%)	2 (25%)	0	0
4	J	1/1 (100%)	0	1 (100%)	0	0
All	All	259/267 (97%)	208 (80%)	51 (20%)	1	0

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(H)	THR
1	L	1(C)	GLU
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(K)	ILE
2	H	20	SER
2	H	27	SER
2	H	33	LEU
2	H	36(A)	SER
2	H	46	LEU
2	H	48	SER

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Mol	Chain	Res	Type
2	H	60(I)	THR
2	H	61	GLU
2	H	62	ASN
2	H	63	ASP
2	H	65	LEU
2	H	66	VAL
2	H	79	ILE
2	H	81	LYS
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	145	LYS
2	H	165	ARG
2	H	182	CYS
2	H	186(A)	ASP
2	H	186(D)	LYS
2	H	187	ARG
2	H	192	GLU
2	H	195	SER
2	H	204(B)	ASN
2	H	205	ASN
2	H	214	SER
2	H	217	GLU
2	H	222	ASP
2	H	229	THR
2	H	236	LYS
2	H	239	GLN
2	H	240	LYS
2	H	241	VAL
2	H	243	ASP
2	H	245	PHE
3	I	358	GLU
3	I	359	ILE
4	J	2	LEU

Some 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
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
3	TYS	I	363	3	15,16,17	1.23	2 (13%)	19,22,24	2.34	7 (36%)
4	PRJ	J	3	4	12,13,14	2.64	6 (50%)	12,18,20	2.82	6 (50%)
4	OAR	J	4	4	10,10,10	1.26	0	8,11,11	2.32	3 (37%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	PRJ	CA-C	-4.20	1.44	1.50
3	I	363	TYS	OH-CZ	-3.27	1.37	1.42
4	J	3	PRJ	CD-N	-2.95	1.43	1.48
4	J	3	PRJ	CG-CD	2.22	1.56	1.53
3	I	363	TYS	CA-C	2.41	1.53	1.50
4	J	3	PRJ	C11-C12	2.54	1.59	1.52
4	J	3	PRJ	C14-C13	3.41	1.58	1.51
4	J	3	PRJ	C14-CD	5.58	1.62	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	PRJ	CB-CG-CD	-6.11	94.27	100.59
3	I	363	TYS	OH-S-O2	-5.70	91.14	107.50
4	J	4	OAR	CG-CB-CA	-5.07	95.62	115.29
3	I	363	TYS	CB-CA-C	-4.59	102.56	111.41
3	I	363	TYS	O-C-CA	-3.55	115.21	124.96
4	J	3	PRJ	O-C-CA	-3.40	117.16	125.09
4	J	4	OAR	CB-CG-CD	-2.74	103.72	112.06
4	J	3	PRJ	C11-C12-C13	-2.58	107.14	111.58
3	I	363	TYS	OH-CZ-CE2	-2.37	114.17	118.69
3	I	363	TYS	CD1-CE1-CZ	-2.19	117.03	119.73
4	J	3	PRJ	O2-C13-C12	2.03	115.03	110.14
3	I	363	TYS	CE2-CZ-CE1	2.03	123.34	120.18
4	J	4	OAR	CB-CA-N1	2.14	115.31	109.00
3	I	363	TYS	O2-S-O1	2.76	124.16	112.25
4	J	3	PRJ	C11-CG-CD	3.34	121.57	113.84
4	J	3	PRJ	C14-C13-C12	3.37	114.67	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	363	TYS	10	0
4	J	3	PRJ	5	0
4	J	4	OAR	10	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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.