



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:27 pm GMT

PDB ID : 2DFS  
Title : 3-D structure of Myosin-V inhibited state  
Authors : Liu, J.; Taylor, D.W.; Krementsova, E.B.; Trybus, K.M.; Taylor, K.A.  
Deposited on : 2006-03-03  
Resolution : 24.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29102

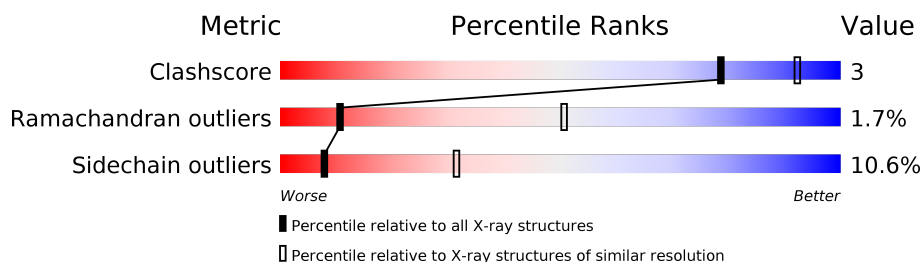
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 24.00 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	112137	1037 (15.00-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)

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	A	1080	
1	M	1080	
2	B	148	
2	C	148	
2	D	148	
2	E	148	
2	F	148	

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Mol	Chain	Length	Quality of chain
2	G	148	<div><div></div><div>61%25%5%•5%</div></div>
2	N	148	<div><div></div><div>57%29%6%•6%</div></div>
2	O	148	<div><div></div><div>72%19%•5%</div></div>
2	P	148	<div><div></div><div>76%14%••6%</div></div>
2	Q	148	<div><div></div><div>74%17%••5%</div></div>
2	R	148	<div><div></div><div>77%13%••6%</div></div>
2	S	148	<div><div></div><div>64%24%5%•5%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29614 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 Myosin-5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			8198	5219	1445	1486	48			
1	M	994	Total	C	N	O	S	0	0	0
			8198	5219	1445	1486	48			

- Molecule 2 is a protein called Calmodulin.

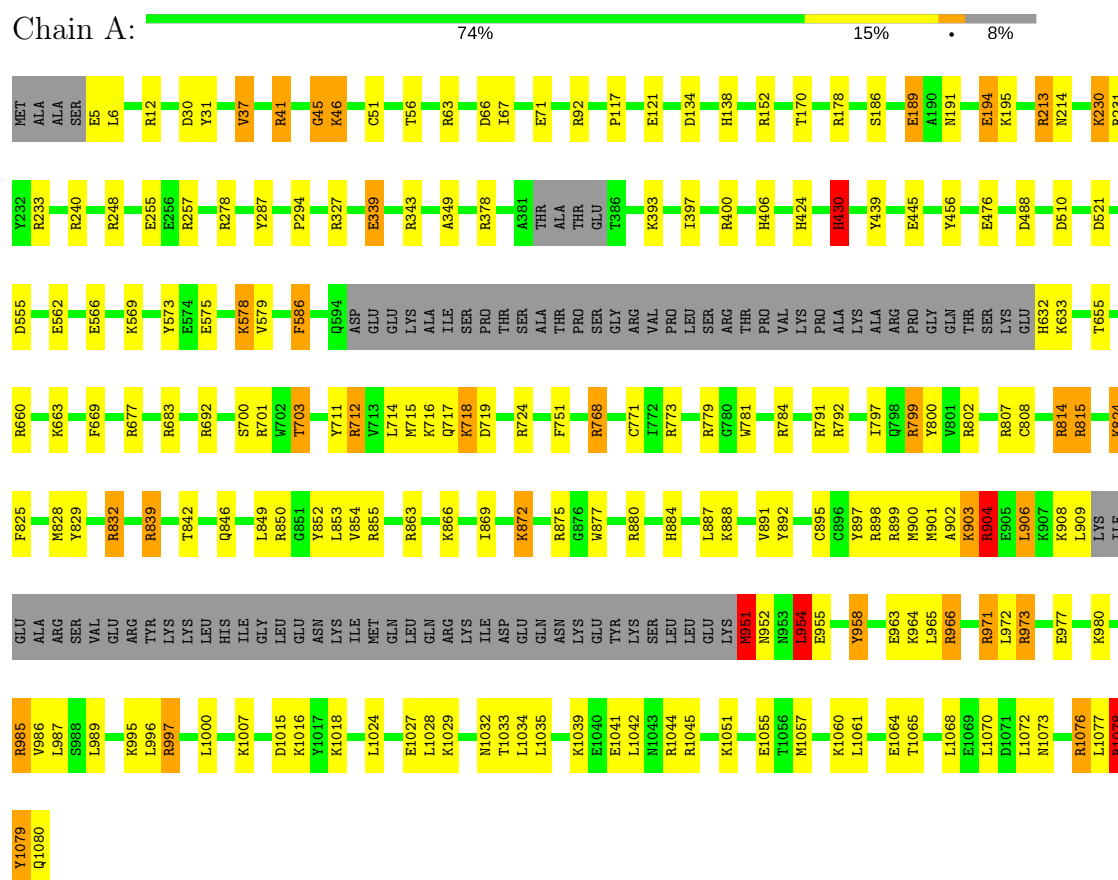
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	C	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			
2	D	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	E	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			
2	F	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	G	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			
2	N	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	O	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			
2	P	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	Q	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			
2	R	139	Total	C	N	O	S	0	0	0
			1093	671	177	236	9			
2	S	141	Total	C	N	O	S	0	0	0
			1110	682	180	239	9			

### 3 Residue-property plots

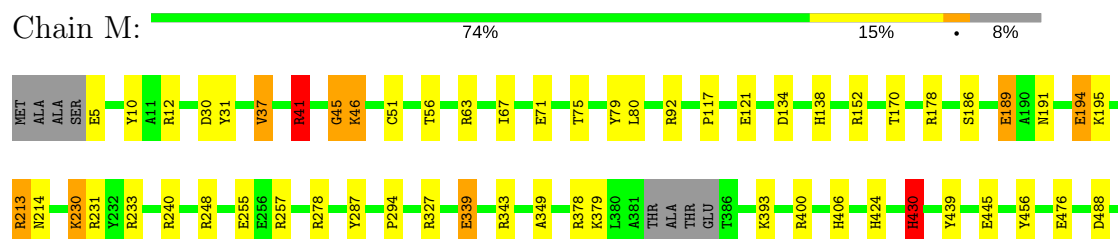
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

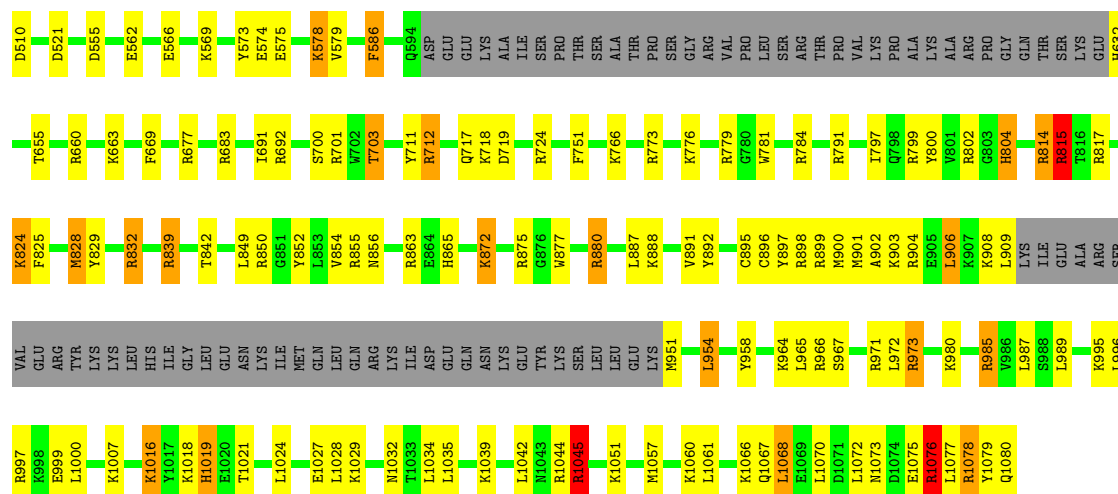
Note EDS was not executed.

#### • Molecule 1: Myosin-5A

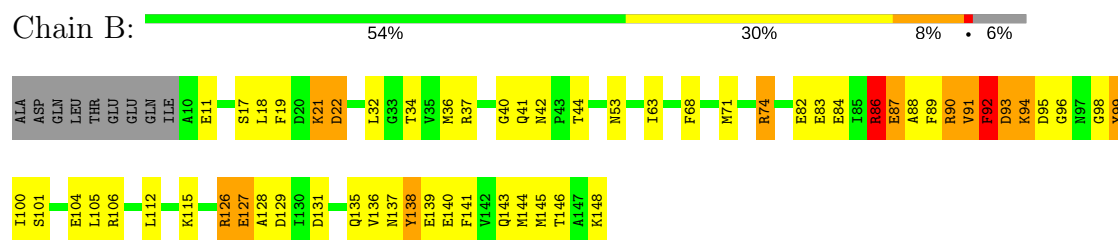


#### • Molecule 1: Myosin-5A

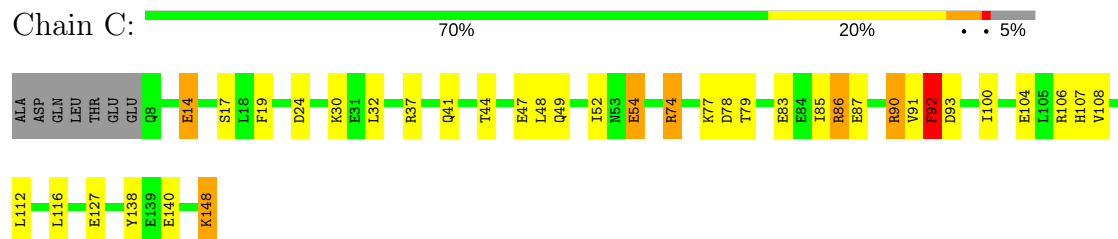




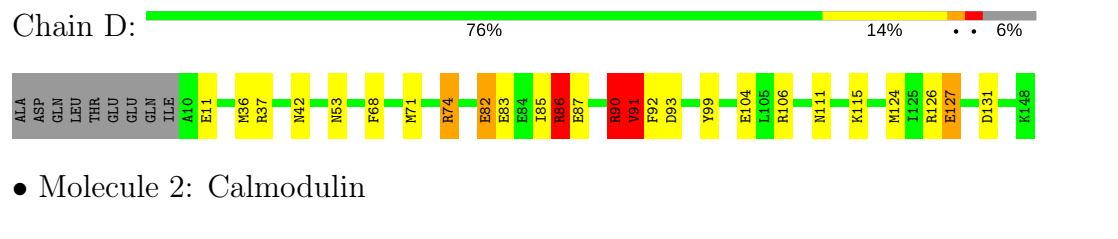
### • Molecule 2: Calmodulin



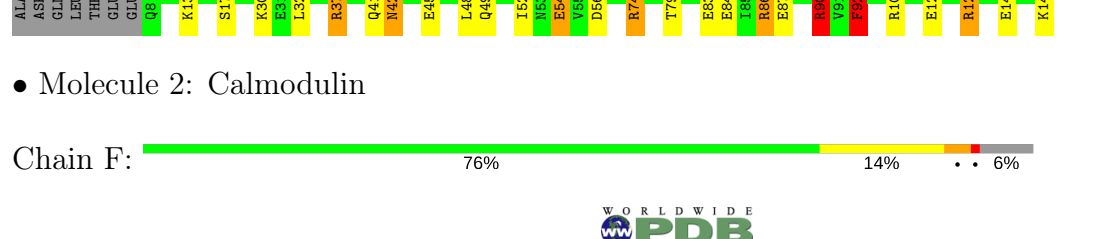
### • Molecule 2: Calmodulin



### • Molecule 2: Calmodulin



### • Molecule 2: Calmodulin

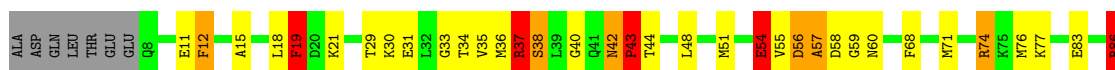




K148

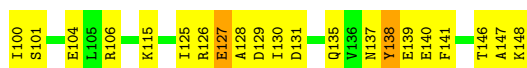
- Molecule 2: Calmodulin

Chain G: 61% 25% 5% • 5%



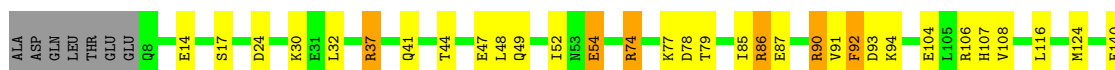
- Molecule 2: Calmodulin

Chain N: 57% 29% 6% • 6%



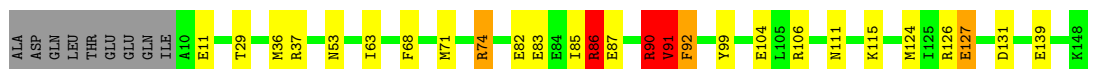
- Molecule 2: Calmodulin

Chain O: 72% 19% • 5%



- Molecule 2: Calmodulin

Chain P: 76% 14% • 6%



- Molecule 2: Calmodulin

Chain Q: 74% 17% • 5%



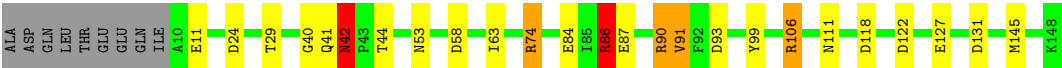
- Molecule 2: Calmodulin

Chain R: 

77%

13%

• • 6%



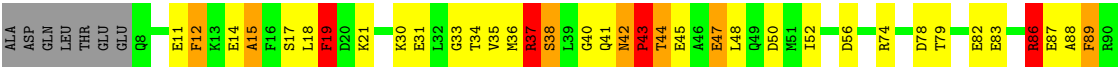
• Molecule 2: Calmodulin

Chain S: 

64%

24%

5% • 5%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	653.00Å 653.00Å 200.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 24.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-24.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	A	0.76	0/8359	1.25	76/11241 (0.7%)
1	M	0.76	0/8359	1.23	74/11241 (0.7%)
2	B	0.78	0/1105	1.39	12/1482 (0.8%)
2	C	0.75	0/1122	1.27	5/1505 (0.3%)
2	D	0.78	0/1105	1.38	15/1482 (1.0%)
2	E	0.74	0/1122	1.27	6/1505 (0.4%)
2	F	0.77	0/1105	1.33	6/1482 (0.4%)
2	G	0.83	0/1122	1.49	16/1505 (1.1%)
2	N	0.78	0/1105	1.35	11/1482 (0.7%)
2	O	0.75	0/1122	1.26	6/1505 (0.4%)
2	P	0.80	0/1105	1.35	13/1482 (0.9%)
2	Q	0.73	0/1122	1.26	6/1505 (0.4%)
2	R	0.77	0/1105	1.32	6/1482 (0.4%)
2	S	0.79	0/1122	1.41	15/1505 (1.0%)
All	All	0.77	0/30080	1.29	267/40404 (0.7%)

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	A	0	32
1	M	0	30
2	B	0	8
2	C	0	7
2	D	0	4
2	E	0	8
2	F	0	5
2	G	0	7
2	N	0	8
2	O	0	6
2	P	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Q	0	7
2	R	0	4
2	S	0	9
All	All	0	140

There are no bond length outliers.

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	997	ARG	NE-CZ-NH1	12.11	126.36	120.30
1	A	951	MET	CA-CB-CG	10.38	130.94	113.30
2	E	74	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	Q	74	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	M	1076	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	M	825	PHE	CB-CG-CD2	-9.94	113.84	120.80
1	M	850	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	825	PHE	CB-CG-CD2	-9.53	114.13	120.80
2	Q	90	ARG	NE-CZ-NH1	9.27	124.93	120.30
2	O	74	ARG	NE-CZ-NH1	9.21	124.91	120.30
2	S	37	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	A	958	TYR	CB-CG-CD1	9.13	126.48	121.00
2	F	106	ARG	NE-CZ-NH1	9.11	124.85	120.30
2	C	74	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	825	PHE	CB-CG-CD1	9.07	127.15	120.80
2	E	90	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	M	825	PHE	CB-CG-CD1	9.05	127.13	120.80
2	R	106	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	M	791	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	M	985	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	958	TYR	CB-CG-CD2	-8.56	115.87	121.00
2	F	74	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	248	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	985	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	M	784	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	M	248	ARG	NE-CZ-NH1	8.46	124.53	120.30
2	R	74	ARG	NE-CZ-NH1	8.41	124.50	120.30
2	C	92	PHE	CB-CG-CD1	8.33	126.63	120.80
2	B	83	GLU	CA-CB-CG	8.33	131.73	113.40
2	G	37	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	P	106	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	D	106	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	S	106	ARG	NE-CZ-NH1	8.15	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	106	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	C	106	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	791	ARG	NE-CZ-NH1	7.97	124.28	120.30
2	E	37	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	M	839	ARG	NE-CZ-NH1	7.93	124.26	120.30
2	B	106	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	784	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	M	287	TYR	CB-CG-CD2	-7.87	116.28	121.00
2	N	106	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	997	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	M	904	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	850	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	M	213	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	701	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	O	106	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	G	36	MET	CG-SD-CE	-7.62	88.01	100.20
1	A	951	MET	N-CA-CB	7.59	124.26	110.60
1	A	287	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	A	213	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	863	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	430	HIS	CA-CB-CG	7.48	126.31	113.60
1	M	430	HIS	CA-CB-CG	7.47	126.30	113.60
1	A	12	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	M	779	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	973	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	M	31	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	A	779	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	Q	37	ARG	NE-CZ-NH1	7.37	123.98	120.30
2	N	37	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	Q	106	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	B	37	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	E	106	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	573	TYR	CB-CG-CD1	-7.32	116.61	121.00
2	P	37	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	M	573	TYR	CB-CG-CD1	-7.29	116.62	121.00
1	A	839	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	G	57	ALA	N-CA-C	7.12	130.22	111.00
2	S	74	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	D	36	MET	CG-SD-CE	-7.07	88.89	100.20
1	M	287	TYR	CB-CG-CD1	7.05	125.23	121.00
1	M	1045	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	M	904	ARG	NE-CZ-NH2	-7.02	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	683	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	M	877	TRP	CB-CG-CD2	-6.95	117.56	126.60
1	M	683	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	M	257	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	G	126	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	P	36	MET	CG-SD-CE	-6.90	89.16	100.20
2	R	42	ASN	CA-C-N	6.89	136.40	117.10
1	M	573	TYR	CB-CG-CD2	6.86	125.12	121.00
1	M	779	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	G	86	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	287	TYR	CB-CG-CD1	6.78	125.07	121.00
2	D	83	GLU	CA-CB-CG	6.78	128.32	113.40
2	S	126	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	954	LEU	CB-CG-CD2	6.77	122.52	111.00
1	M	877	TRP	CB-CG-CD1	6.77	135.80	127.00
1	A	779	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	573	TYR	CB-CG-CD2	6.72	125.03	121.00
1	M	92	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	901	MET	CG-SD-CE	-6.68	89.52	100.20
1	A	768	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	973	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	877	TRP	CB-CG-CD2	-6.61	118.00	126.60
1	M	41	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	P	83	GLU	CA-CB-CG	6.58	127.87	113.40
2	D	86	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	31	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	S	86	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	724	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	G	54	GLU	CA-CB-CG	6.47	127.64	113.40
2	G	57	ALA	C-N-CA	6.47	137.87	121.70
1	A	92	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	877	TRP	CB-CG-CD1	6.45	135.39	127.00
1	M	701	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	231	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	M	231	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	M	973	ARG	NE-CZ-NH1	6.43	123.51	120.30
2	D	92	PHE	CB-CG-CD1	-6.42	116.30	120.80
2	D	37	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	S	83	GLU	CA-CB-CG	6.31	127.29	113.40
1	M	985	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	M	724	ARG	NE-CZ-NH1	6.24	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	985	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	M	850	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	M	31	TYR	CB-CG-CD1	6.21	124.72	121.00
2	D	92	PHE	CB-CG-CD2	6.13	125.09	120.80
1	M	1044	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	F	42	ASN	CA-C-N	6.11	134.19	117.10
2	D	126	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	M	12	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	F	90	ARG	C-N-CA	6.09	136.92	121.70
2	B	126	ARG	NE-CZ-NH2	-6.07	117.26	120.30
2	E	90	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	M	804	HIS	CA-CB-CG	6.07	123.92	113.60
1	A	669	PHE	CB-CG-CD2	-6.07	116.55	120.80
2	N	126	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	41	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	850	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	M	456	TYR	CB-CG-CD2	-6.04	117.38	121.00
2	N	36	MET	CG-SD-CE	-6.03	90.55	100.20
2	S	74	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	M	901	MET	CG-SD-CE	-6.02	90.57	100.20
1	M	660	ARG	NE-CZ-NH2	-6.01	117.30	120.30
2	R	90	ARG	C-N-CA	6.01	136.72	121.70
2	G	43	PRO	N-CA-C	6.00	127.70	112.10
1	A	951	MET	N-CA-C	6.00	127.20	111.00
2	B	86	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	660	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	M	828	MET	CG-SD-CE	5.99	109.78	100.20
2	Q	90	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	P	126	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	M	669	PHE	CB-CG-CD2	-5.98	116.61	120.80
2	O	93	ASP	N-CA-CB	-5.97	99.85	110.60
2	N	86	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	1044	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	456	TYR	CB-CG-CD2	-5.89	117.46	121.00
2	B	36	MET	CG-SD-CE	-5.89	90.77	100.20
2	S	36	MET	CG-SD-CE	-5.87	90.80	100.20
1	M	178	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	M	586	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	586	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	M	814	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	M	178	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	B	22	ASP	CB-CG-OD1	5.78	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	378	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	898	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	S	43	PRO	N-CA-C	5.77	127.11	112.10
1	A	909	LEU	N-CA-C	-5.74	95.51	111.00
2	S	15	ALA	N-CA-CB	-5.73	102.08	110.10
2	B	74	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	G	83	GLU	CA-CB-CG	5.72	125.98	113.40
2	R	93	ASP	N-CA-C	-5.71	95.57	111.00
2	F	93	ASP	N-CA-C	-5.70	95.61	111.00
2	S	144	MET	CG-SD-CE	-5.70	91.08	100.20
1	M	712	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	178	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	378	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	N	74	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	D	90	ARG	C-N-CA	5.67	135.88	121.70
2	G	37	ARG	CB-CG-CD	5.67	126.34	111.60
2	B	92	PHE	CB-CA-C	5.67	121.73	110.40
1	A	178	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	M	863	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	M	1045	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	863	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	M	815	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	N	92	PHE	CB-CA-C	5.62	121.64	110.40
1	A	669	PHE	CB-CG-CD1	5.62	124.73	120.80
1	M	63	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	M	278	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	S	126	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	P	86	ARG	NE-CZ-NH1	5.55	123.07	120.30
2	P	106	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	M	669	PHE	CB-CG-CD1	5.55	124.68	120.80
1	A	799	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	278	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	701	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	S	37	ARG	CB-CG-CD	5.51	125.93	111.60
2	D	93	ASP	N-CA-C	-5.50	96.16	111.00
1	M	909	LEU	N-CA-C	-5.49	96.19	111.00
2	D	74	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	63	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	712	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	P	90	ARG	C-N-CA	5.41	135.22	121.70
1	A	908	LYS	CA-CB-CG	5.41	125.29	113.40
2	G	56	ASP	O-C-N	-5.40	114.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	MET	CG-SD-CE	-5.39	91.58	100.20
2	G	126	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	Q	45	GLU	CA-CB-CG	-5.38	101.57	113.40
2	E	45	GLU	CA-CB-CG	-5.38	101.58	113.40
2	C	92	PHE	CB-CG-CD2	-5.37	117.04	120.80
2	P	68	PHE	CB-CG-CD2	-5.37	117.05	120.80
1	M	877	TRP	CA-CB-CG	5.36	123.89	113.70
2	O	37	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	M	832	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	G	91	VAL	N-CA-C	-5.33	96.60	111.00
1	A	1044	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	G	144	MET	CG-SD-CE	-5.33	91.67	100.20
2	F	86	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	N	71	MET	CG-SD-CE	-5.31	91.70	100.20
1	M	45	GLY	N-CA-C	5.30	126.36	113.10
1	M	79	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	M	400	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	904	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	400	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	M	278	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	P	127	GLU	CA-CB-CG	5.28	125.02	113.40
2	D	71	MET	CG-SD-CE	-5.28	91.76	100.20
1	M	231	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	P	71	MET	CG-SD-CE	-5.27	91.76	100.20
2	S	37	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	1079	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	815	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	966	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	231	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	31	TYR	CB-CG-CD1	5.25	124.15	121.00
2	D	106	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	278	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	M	779	ARG	CA-CB-CG	5.23	124.91	113.40
1	M	908	LYS	CA-CB-CG	5.22	124.89	113.40
2	P	74	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	M	1044	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	S	91	VAL	N-CA-C	-5.21	96.94	111.00
2	D	127	GLU	CA-CB-CG	5.21	124.85	113.40
1	M	973	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	703	THR	N-CA-CB	5.19	120.16	110.30
1	A	45	GLY	N-CA-C	5.18	126.04	113.10
2	R	127	GLU	CA-CB-CG	5.17	124.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	703	THR	N-CA-CB	5.16	120.11	110.30
1	A	832	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	B	68	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	A	792	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	M	41	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	P	68	PHE	CB-CG-CD1	5.14	124.40	120.80
2	D	68	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	A	814	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	G	54	GLU	O-C-N	-5.11	114.53	122.70
1	A	37	VAL	CG1-CB-CG2	5.10	119.06	110.90
2	B	44	THR	N-CA-CB	5.10	119.99	110.30
2	C	86	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	M	701	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	M	906	LEU	CB-CA-C	5.06	119.81	110.20
2	N	68	PHE	CB-CG-CD2	-5.06	117.26	120.80
2	O	106	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	M	586	PHE	CB-CG-CD1	5.04	124.32	120.80
1	A	1078	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	N	40	GLY	C-N-CA	5.03	134.28	121.70
1	M	37	VAL	CG1-CB-CG2	5.03	118.94	110.90
1	M	898	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	N	106	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	M	825	PHE	CB-CA-C	-5.02	100.36	110.40
2	O	86	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	ARG	Sidechain
1	A	1078	ARG	Sidechain
1	A	1079	TYR	Sidechain
1	A	152	ARG	Sidechain
1	A	191	ASN	Peptide
1	A	213	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	430	HIS	Sidechain
1	A	677	ARG	Sidechain
1	A	692	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	711	TYR	Sidechain
1	A	773	ARG	Sidechain
1	A	799	ARG	Sidechain
1	A	800	TYR	Sidechain
1	A	807	ARG	Sidechain
1	A	815	ARG	Sidechain
1	A	829	TYR	Sidechain
1	A	832	ARG	Sidechain
1	A	839	ARG	Sidechain
1	A	852	TYR	Sidechain
1	A	855	ARG	Sidechain
1	A	875	ARG	Sidechain
1	A	880	ARG	Sidechain
1	A	884	HIS	Sidechain
1	A	892	TYR	Sidechain
1	A	904	ARG	Sidechain
1	A	951	MET	Peptide
1	A	971	ARG	Sidechain
1	A	973	ARG	Sidechain
2	B	138	TYR	Sidechain
2	B	19	PHE	Peptide
2	B	74	ARG	Sidechain
2	B	82	GLU	Peptide
2	B	86	ARG	Sidechain
2	B	90	ARG	Sidechain,Peptide
2	B	99	TYR	Sidechain
2	C	19	PHE	Peptide
2	C	37	ARG	Sidechain
2	C	54	GLU	Peptide
2	C	74	ARG	Sidechain
2	C	86	ARG	Sidechain
2	C	90	ARG	Sidechain
2	C	92	PHE	Sidechain
2	D	74	ARG	Sidechain
2	D	86	ARG	Sidechain
2	D	90	ARG	Sidechain
2	D	99	TYR	Sidechain
2	E	126	ARG	Sidechain
2	E	42	ASN	Peptide
2	E	54	GLU	Peptide
2	E	74	ARG	Sidechain
2	E	86	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	90	ARG	Sidechain
2	E	92	PHE	Sidechain,Peptide
2	F	106	ARG	Sidechain
2	F	74	ARG	Sidechain
2	F	86	ARG	Sidechain
2	F	90	ARG	Sidechain
2	F	99	TYR	Sidechain
2	G	12	PHE	Sidechain
2	G	126	ARG	Sidechain
2	G	19	PHE	Sidechain
2	G	37	ARG	Sidechain
2	G	38	SER	Peptide
2	G	86	ARG	Sidechain
2	G	89	PHE	Sidechain
1	M	10	TYR	Sidechain
1	M	1045	ARG	Sidechain
1	M	1076	ARG	Sidechain
1	M	1078	ARG	Sidechain
1	M	1079	TYR	Sidechain
1	M	152	ARG	Sidechain
1	M	191	ASN	Peptide
1	M	213	ARG	Sidechain
1	M	233	ARG	Sidechain
1	M	240	ARG	Sidechain
1	M	327	ARG	Sidechain
1	M	41	ARG	Sidechain
1	M	430	HIS	Sidechain
1	M	677	ARG	Sidechain
1	M	692	ARG	Sidechain
1	M	711	TYR	Sidechain
1	M	773	ARG	Sidechain
1	M	799	ARG	Sidechain
1	M	800	TYR	Sidechain
1	M	815	ARG	Sidechain
1	M	817	ARG	Sidechain
1	M	829	TYR	Sidechain
1	M	832	ARG	Sidechain
1	M	839	ARG	Sidechain
1	M	852	TYR	Sidechain
1	M	855	ARG	Sidechain
1	M	875	ARG	Sidechain
1	M	880	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	892	TYR	Sidechain
1	M	973	ARG	Sidechain
2	N	138	TYR	Sidechain
2	N	19	PHE	Peptide
2	N	74	ARG	Sidechain
2	N	86	ARG	Sidechain
2	N	90	ARG	Sidechain,Peptide
2	N	91	VAL	Peptide
2	N	99	TYR	Sidechain
2	O	37	ARG	Sidechain
2	O	54	GLU	Peptide
2	O	74	ARG	Sidechain
2	O	86	ARG	Sidechain
2	O	90	ARG	Sidechain
2	O	92	PHE	Sidechain
2	P	74	ARG	Sidechain
2	P	86	ARG	Sidechain
2	P	90	ARG	Sidechain
2	P	92	PHE	Peptide
2	P	99	TYR	Sidechain
2	Q	126	ARG	Sidechain
2	Q	54	GLU	Peptide
2	Q	74	ARG	Sidechain
2	Q	86	ARG	Sidechain
2	Q	90	ARG	Sidechain
2	Q	91	VAL	Peptide
2	Q	92	PHE	Peptide
2	R	106	ARG	Sidechain
2	R	74	ARG	Sidechain
2	R	86	ARG	Sidechain
2	R	99	TYR	Sidechain
2	S	107	HIS	Sidechain
2	S	12	PHE	Sidechain
2	S	126	ARG	Sidechain
2	S	14	GLU	Peptide
2	S	19	PHE	Sidechain
2	S	37	ARG	Sidechain
2	S	38	SER	Peptide
2	S	86	ARG	Sidechain
2	S	89	PHE	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	A	8198	0	8280	64	72
1	M	8198	0	8280	64	56
2	B	1093	0	1027	10	371
2	C	1110	0	1046	15	0
2	D	1093	0	1027	2	0
2	E	1110	0	1046	7	0
2	F	1093	0	1027	3	0
2	G	1110	0	1046	50	0
2	N	1093	0	1027	9	387
2	O	1110	0	1046	14	0
2	P	1093	0	1027	3	0
2	Q	1110	0	1046	10	0
2	R	1093	0	1027	4	0
2	S	1110	0	1046	31	0
All	All	29614	0	28998	196	443

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 3.

All (196) 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:A:906:LEU:HD21	2:G:15:ALA:HB1	1.58	0.84
2:C:92:PHE:CE2	2:C:108:VAL:HG22	2.14	0.83
1:M:906:LEU:HD21	2:S:15:ALA:HB1	1.61	0.81
1:A:951:MET:HG3	2:G:59:GLY:H	1.46	0.81
1:A:906:LEU:CD2	2:G:15:ALA:HB1	2.17	0.74
1:M:899:ARG:HD3	2:S:37:ARG:HG2	1.74	0.69
1:A:899:ARG:HD3	2:G:37:ARG:HG2	1.74	0.68
1:M:902:ALA:HB3	2:S:37:ARG:CD	2.24	0.68
1:A:951:MET:N	2:G:58:ASP:H	1.92	0.67
2:G:54:GLU:HG3	2:G:56:ASP:H	1.59	0.67
1:M:872:LYS:HD3	2:R:44:THR:HA	1.78	0.66
2:O:92:PHE:CE2	2:O:108:VAL:HG22	2.32	0.65
1:A:951:MET:CA	2:G:58:ASP:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:89:PHE:CZ	2:S:108:VAL:HG21	2.34	0.63
1:A:902:ALA:HB3	2:G:37:ARG:CD	2.30	0.62
2:O:104:GLU:O	2:O:108:VAL:HG23	2.00	0.61
2:O:92:PHE:CZ	2:O:108:VAL:HG22	2.36	0.61
1:A:814:ARG:HH11	1:A:814:ARG:HG2	1.67	0.60
1:A:906:LEU:HB3	2:G:38:SER:CB	2.32	0.60
1:A:768:ARG:HA	2:B:112:LEU:HB3	1.83	0.59
1:M:906:LEU:HB3	2:S:38:SER:HB3	1.83	0.59
1:M:903:LYS:HA	2:S:38:SER:HA	1.85	0.59
2:C:104:GLU:O	2:C:108:VAL:HG23	2.03	0.58
1:M:906:LEU:HD22	2:S:38:SER:HB3	1.85	0.58
1:M:899:ARG:NE	2:S:37:ARG:HE	2.02	0.58
1:M:954:LEU:H	1:M:954:LEU:HD22	1.68	0.58
1:A:906:LEU:HD13	2:G:35:VAL:HG23	1.86	0.58
2:G:12:PHE:O	2:G:15:ALA:HB3	2.03	0.58
1:A:951:MET:HB3	2:G:56:ASP:HA	1.86	0.57
2:C:49:GLN:HA	2:C:52:ILE:HG22	1.87	0.57
2:O:49:GLN:HA	2:O:52:ILE:HG22	1.87	0.57
1:M:906:LEU:HB3	2:S:38:SER:CB	2.34	0.57
1:A:903:LYS:HA	2:G:38:SER:HA	1.87	0.56
1:M:230:LYS:HA	1:M:430:HIS:CD2	2.41	0.56
1:A:951:MET:HB3	2:G:56:ASP:CA	2.36	0.56
2:B:21:LYS:HA	2:C:92:PHE:CE2	2.41	0.56
1:M:906:LEU:HD13	2:S:35:VAL:HG23	1.88	0.56
2:G:89:PHE:CZ	2:G:108:VAL:HG21	2.41	0.56
2:Q:49:GLN:HA	2:Q:52:ILE:HG22	1.88	0.56
1:A:230:LYS:HA	1:A:430:HIS:CD2	2.41	0.56
2:E:49:GLN:HA	2:E:52:ILE:HG22	1.88	0.55
1:A:906:LEU:HB3	2:G:38:SER:HB3	1.88	0.55
1:M:906:LEU:CD2	2:S:15:ALA:HB1	2.34	0.55
2:S:37:ARG:HH22	2:S:45:GLU:CD	2.09	0.55
2:N:21:LYS:HA	2:O:92:PHE:CE2	2.43	0.54
2:S:41:GLN:HG2	2:S:79:THR:HG22	1.89	0.54
2:C:32:LEU:HD22	2:C:52:ILE:HD13	1.90	0.54
1:A:842:THR:CG2	2:E:90:ARG:HE	2.21	0.53
2:N:21:LYS:O	2:O:92:PHE:HA	2.09	0.53
2:G:51:MET:HG3	1:M:951:MET:HE2	1.91	0.53
1:A:189:GLU:CD	1:A:189:GLU:H	2.12	0.53
1:A:899:ARG:NE	2:G:37:ARG:HE	2.06	0.53
2:O:32:LEU:HD22	2:O:52:ILE:HD13	1.90	0.53
2:S:12:PHE:O	2:S:15:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:33:GLY:O	2:S:37:ARG:HG3	2.10	0.52
2:G:33:GLY:O	2:G:37:ARG:HG3	2.09	0.52
1:M:189:GLU:H	1:M:189:GLU:CD	2.12	0.52
1:M:814:ARG:HH11	1:M:814:ARG:HG2	1.73	0.52
1:A:906:LEU:HD22	2:G:38:SER:HB3	1.91	0.52
2:E:32:LEU:HD22	2:E:52:ILE:HD13	1.93	0.51
2:O:41:GLN:HG2	2:O:79:THR:HG22	1.92	0.51
1:A:903:LYS:HA	2:G:38:SER:CA	2.40	0.51
1:A:902:ALA:HB1	2:G:34:THR:HA	1.93	0.51
1:M:343:ARG:CZ	1:M:349:ALA:HB3	2.41	0.51
1:M:445:GLU:CD	1:M:445:GLU:H	2.13	0.51
2:Q:32:LEU:HD22	2:Q:52:ILE:HD13	1.93	0.51
2:G:55:VAL:HG22	2:G:55:VAL:O	2.11	0.51
1:A:445:GLU:H	1:A:445:GLU:CD	2.14	0.50
1:A:343:ARG:CZ	1:A:349:ALA:HB3	2.41	0.50
2:C:41:GLN:HG2	2:C:79:THR:HG22	1.93	0.50
1:M:899:ARG:CD	2:S:37:ARG:HG2	2.40	0.50
1:M:906:LEU:CD2	2:S:38:SER:HB3	2.42	0.50
1:M:903:LYS:HA	2:S:38:SER:CA	2.42	0.50
1:A:958:TYR:CZ	1:M:958:TYR:HB2	2.47	0.50
1:A:902:ALA:CB	2:G:34:THR:HA	2.42	0.49
2:B:94:LYS:NZ	2:B:94:LYS:HA	2.27	0.49
2:B:17:SER:O	2:C:112:LEU:HD21	2.12	0.49
1:A:899:ARG:CD	2:G:37:ARG:HG2	2.40	0.49
2:C:83:GLU:CD	2:C:148:LYS:HZ3	2.15	0.49
1:M:902:ALA:CB	2:S:34:THR:HA	2.43	0.49
1:M:872:LYS:HG3	2:R:42:ASN:O	2.13	0.49
2:F:84:GLU:CD	2:F:86:ARG:HH12	2.17	0.48
1:M:37:VAL:HG12	1:M:51:CYS:HA	1.95	0.48
1:A:578:LYS:HZ2	1:A:579:VAL:HA	1.79	0.48
2:P:90:ARG:HA	2:P:91:VAL:HG12	1.95	0.48
1:M:776:LYS:HZ3	2:N:44:THR:HG23	1.78	0.48
1:M:899:ARG:CB	2:S:42:ASN:HA	2.43	0.48
1:A:37:VAL:HG12	1:A:51:CYS:HA	1.96	0.48
2:B:90:ARG:HB3	2:B:92:PHE:H	1.78	0.48
2:N:90:ARG:HB3	2:N:92:PHE:H	1.79	0.48
2:E:41:GLN:HG2	2:E:79:THR:HG22	1.96	0.48
1:M:824:LYS:HZ2	1:M:824:LYS:HB3	1.77	0.47
1:M:902:ALA:HB1	2:S:34:THR:HA	1.96	0.47
1:M:815:ARG:HH21	2:P:92:PHE:HA	1.78	0.47
1:M:578:LYS:HZ2	1:M:579:VAL:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:19:PHE:CZ	2:S:31:GLU:HB3	2.49	0.47
1:A:872:LYS:HD2	1:A:872:LYS:HA	1.77	0.47
1:A:951:MET:HA	2:G:54:GLU:O	2.14	0.47
2:B:144:MET:O	2:B:148:LYS:HD2	2.14	0.47
2:R:84:GLU:CD	2:R:86:ARG:HH12	2.19	0.47
1:A:903:LYS:HA	2:G:38:SER:CB	2.45	0.47
2:Q:41:GLN:HG2	2:Q:79:THR:HG22	1.96	0.46
2:G:19:PHE:CZ	2:G:31:GLU:HB3	2.51	0.46
2:N:94:LYS:HA	2:N:94:LYS:NZ	2.29	0.46
1:A:339:GLU:CD	1:A:393:LYS:HZ1	2.18	0.46
1:A:951:MET:HB3	2:G:56:ASP:N	2.30	0.46
1:A:899:ARG:CZ	2:G:43:PRO:HB2	2.46	0.46
1:M:856:ASN:HD22	2:Q:127:GLU:CD	2.19	0.46
1:M:902:ALA:HB3	2:S:37:ARG:HD3	1.98	0.46
1:A:899:ARG:CB	2:G:42:ASN:HA	2.45	0.46
1:A:854:VAL:HG21	2:E:37:ARG:CB	2.46	0.46
1:M:842:THR:CG2	2:Q:90:ARG:HE	2.28	0.46
2:D:42:ASN:HB2	2:D:82:GLU:HB3	1.99	0.45
1:A:900:MET:HG3	1:A:904:ARG:HH21	1.81	0.45
2:G:107:HIS:CE1	2:G:111:ASN:HD22	2.34	0.45
2:G:51:MET:O	1:M:951:MET:HB3	2.17	0.45
2:N:22:ASP:HA	2:O:104:GLU:HG2	1.97	0.45
1:M:895:CYS:SG	2:S:44:THR:HG22	2.57	0.45
1:M:880:ARG:HH11	1:M:880:ARG:HG3	1.82	0.45
1:M:849:LEU:HD21	2:Q:124:MET:HB2	1.99	0.45
2:G:71:MET:HB3	1:M:951:MET:SD	2.57	0.45
1:M:824:LYS:CB	1:M:824:LYS:HZ2	2.30	0.44
2:C:92:PHE:CZ	2:C:108:VAL:HG22	2.51	0.44
1:A:952:ASN:H	2:G:59:GLY:N	2.15	0.44
2:C:92:PHE:O	2:C:100:ILE:HG22	2.17	0.44
2:D:90:ARG:HA	2:D:91:VAL:HG12	2.00	0.44
1:M:781:TRP:HE1	2:N:148:LYS:CB	2.30	0.44
1:M:854:VAL:HG21	2:Q:37:ARG:CB	2.47	0.44
1:A:194:GLU:CD	1:A:195:LYS:HZ2	2.21	0.44
1:A:899:ARG:HD3	2:G:37:ARG:CG	2.47	0.44
1:A:854:VAL:HG21	2:E:37:ARG:HB3	2.00	0.44
2:G:35:VAL:HG13	2:G:68:PHE:CE1	2.53	0.44
1:M:824:LYS:HA	1:M:824:LYS:HD2	1.75	0.44
1:M:854:VAL:HG21	2:Q:37:ARG:HB3	2.00	0.44
1:A:906:LEU:CG	2:G:15:ALA:HB1	2.47	0.44
1:M:888:LYS:HA	1:M:891:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:LEU:HG	1:M:691:ILE:HG23	2.01	0.43
1:A:824:LYS:HD2	1:A:824:LYS:HA	1.75	0.43
1:M:339:GLU:CD	1:M:393:LYS:HZ1	2.22	0.43
2:N:32:LEU:HD13	2:N:63:ILE:CD1	2.49	0.43
1:A:849:LEU:HD23	1:A:853:LEU:HG	2.01	0.43
1:A:955:GLU:CD	2:G:55:VAL:HG21	2.39	0.43
2:Q:47:GLU:CD	2:Q:75:LYS:HZ1	2.21	0.43
1:M:566:GLU:CD	1:M:569:LYS:HZ1	2.21	0.43
1:A:814:ARG:HH12	2:C:14:GLU:CD	2.23	0.42
1:M:802:ARG:HH11	2:O:116:LEU:HD22	1.84	0.42
1:M:896:CYS:HA	2:S:42:ASN:HB3	2.02	0.42
1:A:781:TRP:CD2	2:B:145:MET:O	2.73	0.42
1:A:866:LYS:HZ2	1:A:869:ILE:HG13	1.84	0.42
2:S:43:PRO:HB3	2:S:47:GLU:HG3	2.00	0.42
1:A:824:LYS:HB3	1:A:824:LYS:NZ	2.35	0.42
2:F:21:LYS:HA	2:G:107:HIS:CE1	2.55	0.42
2:S:88:ALA:HB3	2:S:142:VAL:HG11	2.02	0.42
1:A:802:ARG:HH11	2:C:116:LEU:HD22	1.85	0.41
2:F:29:THR:HG22	2:F:63:ILE:HG23	2.02	0.41
1:M:1016:LYS:HZ1	1:M:1019:HIS:CE1	2.36	0.41
1:M:379:LYS:NZ	1:M:574:GLU:OE1	2.46	0.41
2:C:100:ILE:HG23	2:C:138:TYR:CD2	2.55	0.41
1:M:194:GLU:CD	1:M:195:LYS:HZ2	2.23	0.41
2:O:77:LYS:NZ	2:O:78:ASP:OD1	2.48	0.41
2:C:77:LYS:NZ	2:C:78:ASP:OD1	2.48	0.41
2:E:123:GLU:HG3	2:E:126:ARG:HE	1.86	0.41
2:S:43:PRO:HG3	2:S:82:GLU:HG3	2.03	0.41
1:A:954:LEU:CD1	2:G:54:GLU:O	2.68	0.41
1:M:1068:LEU:HD13	1:M:1068:LEU:H	1.86	0.41
1:M:700:SER:HB2	1:M:751:PHE:HB2	2.02	0.41
1:M:804:HIS:CD2	2:O:145:MET:HA	2.55	0.41
2:R:29:THR:HG22	2:R:63:ILE:HG23	2.02	0.41
1:A:951:MET:HG2	2:G:56:ASP:C	2.41	0.41
2:G:107:HIS:HE1	2:G:111:ASN:HD22	1.67	0.41
2:B:32:LEU:HD13	2:B:63:ILE:CD1	2.51	0.41
1:M:776:LYS:HZ1	2:N:82:GLU:CD	2.22	0.41
1:M:804:HIS:CD2	2:O:124:MET:SD	3.14	0.41
1:A:393:LYS:HE3	1:A:397:ILE:HD11	2.03	0.41
1:A:824:LYS:HB3	1:A:824:LYS:HZ2	1.85	0.41
2:P:29:THR:HG22	2:P:63:ILE:HG23	2.03	0.41
1:M:899:ARG:HB3	2:S:42:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:LEU:CD1	2:G:35:VAL:HG23	2.51	0.41
1:M:903:LYS:HA	2:S:38:SER:CB	2.50	0.41
1:A:566:GLU:CD	1:A:569:LYS:HZ1	2.24	0.41
1:A:895:CYS:SG	2:G:44:THR:HG22	2.61	0.41
2:G:71:MET:CE	2:G:74:ARG:HH22	2.34	0.41
2:B:105:LEU:HD21	2:B:141:PHE:CE2	2.56	0.41
2:B:94:LYS:HZ3	2:B:94:LYS:HA	1.86	0.41
2:G:88:ALA:HB3	2:G:142:VAL:HG11	2.03	0.41
1:A:797:ILE:HG21	2:C:90:ARG:HH21	1.85	0.40
1:A:700:SER:HB2	1:A:751:PHE:HB2	2.03	0.40
1:A:902:ALA:HB3	2:G:37:ARG:CB	2.51	0.40
1:M:899:ARG:HD3	2:S:37:ARG:CG	2.47	0.40
1:A:888:LYS:HA	1:A:891:VAL:HG22	2.03	0.40
2:G:54:GLU:HB2	1:M:954:LEU:HD11	2.04	0.40
1:A:339:GLU:OE2	1:A:393:LYS:NZ	2.55	0.40
1:A:951:MET:N	2:G:57:ALA:H	2.20	0.40
1:M:339:GLU:OE2	1:M:393:LYS:NZ	2.55	0.40
1:M:797:ILE:HG21	2:O:90:ARG:HH21	1.86	0.40
2:Q:107:HIS:CD2	2:Q:107:HIS:C	2.94	0.40

All (443) 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)
2:B:99:TYR:CA	2:N:94:LYS:N[5_555]	0.37	1.83
2:B:99:TYR:CD1	2:N:94:LYS:CG[5_555]	0.39	1.81
2:B:92:PHE:CB	2:N:97:ASN:O[5_555]	0.41	1.79
2:B:129:ASP:CG	1:M:712:ARG:CB[5_555]	0.48	1.72
2:B:139:GLU:CB	2:N:90:ARG:CA[5_555]	0.50	1.70
2:B:91:VAL:O	2:N:99:TYR:CE2[5_555]	0.50	1.70
1:A:718:LYS:CB	2:N:127:GLU:CB[5_555]	0.54	1.66
2:B:86:ARG:CA	2:N:86:ARG:O[5_555]	0.54	1.66
2:B:129:ASP:OD2	1:M:712:ARG:CA[5_555]	0.57	1.63
2:B:89:PHE:CZ	2:N:140:GLU:CA[5_555]	0.58	1.62
2:B:138:TYR:CD1	2:N:138:TYR:OH[5_555]	0.59	1.61
2:B:98:GLY:CA	2:N:93:ASP:N[5_555]	0.63	1.57
2:B:96:GLY:O	2:N:104:GLU:CD[5_555]	0.63	1.57
1:A:717:GLN:CB	2:N:128:ALA:CA[5_555]	0.64	1.56
2:B:96:GLY:O	2:N:104:GLU:OE2[5_555]	0.66	1.54
1:A:718:LYS:N	2:N:127:GLU:C[5_555]	0.68	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ARG:CG	2:N:130:ILE:O[5_555]	0.70	1.50
1:A:718:LYS:CA	2:N:127:GLU:CA[5_555]	0.74	1.46
2:B:143:GLN:CB	2:N:89:PHE:CE1[5_555]	0.76	1.44
2:B:91:VAL:C	2:N:99:TYR:CE2[5_555]	0.76	1.44
2:B:100:ILE:CB	2:N:96:GLY:N[5_555]	0.77	1.43
1:A:717:GLN:C	2:N:127:GLU:C[5_555]	0.78	1.42
2:B:138:TYR:CE1	2:N:138:TYR:CZ[5_555]	0.79	1.41
2:B:143:GLN:CB	2:N:89:PHE:CD1[5_555]	0.80	1.40
2:B:129:ASP:CA	1:M:712:ARG:CG[5_555]	0.80	1.40
2:B:100:ILE:CB	2:N:96:GLY:CA[5_555]	0.81	1.39
2:B:137:ASN:CA	2:N:94:LYS:NZ[5_555]	0.82	1.38
2:B:100:ILE:CA	2:N:96:GLY:N[5_555]	0.83	1.37
2:B:89:PHE:CB	2:N:139:GLU:N[5_555]	0.83	1.37
2:B:138:TYR:CE1	2:N:138:TYR:OH[5_555]	0.86	1.34
2:B:94:LYS:CA	2:N:135:GLN:CD[5_555]	0.87	1.33
2:B:100:ILE:CA	2:N:95:ASP:C[5_555]	0.89	1.31
2:B:89:PHE:CB	2:N:138:TYR:C[5_555]	0.90	1.30
1:A:712:ARG:NE	2:N:130:ILE:CG2[5_555]	0.90	1.30
2:B:89:PHE:CA	2:N:139:GLU:N[5_555]	0.90	1.30
1:A:717:GLN:CG	2:N:128:ALA:CB[5_555]	0.92	1.28
2:B:94:LYS:C	2:N:135:GLN:CD[5_555]	0.92	1.28
2:B:128:ALA:N	1:M:712:ARG:NH2[5_555]	0.93	1.27
2:B:91:VAL:CG2	2:N:99:TYR:OH[5_555]	0.94	1.26
2:B:98:GLY:C	2:N:93:ASP:N[5_555]	0.95	1.25
2:B:129:ASP:CB	1:M:712:ARG:CG[5_555]	0.96	1.24
2:B:100:ILE:C	2:N:95:ASP:C[5_555]	0.97	1.23
2:B:92:PHE:CB	2:N:97:ASN:C[5_555]	1.00	1.20
2:B:129:ASP:OD2	1:M:712:ARG:N[5_555]	1.03	1.17
2:B:100:ILE:CG1	2:N:96:GLY:CA[5_555]	1.04	1.16
2:B:89:PHE:N	2:N:139:GLU:CA[5_555]	1.05	1.15
1:A:715:MET:N	2:N:129:ASP:OD2[5_555]	1.06	1.14
1:A:718:LYS:CA	2:N:127:GLU:CB[5_555]	1.07	1.13
2:B:139:GLU:OE1	2:N:90:ARG:CD[5_555]	1.08	1.12
2:B:126:ARG:O	1:M:717:GLN:NE2[5_555]	1.08	1.12
2:B:94:LYS:C	2:N:135:GLN:CG[5_555]	1.09	1.11
2:B:139:GLU:O	2:N:89:PHE:CB[5_555]	1.09	1.11
2:B:138:TYR:CE2	2:N:93:ASP:CB[5_555]	1.10	1.10
1:A:717:GLN:CA	2:N:128:ALA:CA[5_555]	1.11	1.09
1:A:717:GLN:C	2:N:128:ALA:N[5_555]	1.11	1.09
1:A:717:GLN:OE1	2:N:128:ALA:O[5_555]	1.11	1.09
2:B:135:GLN:OE1	2:N:95:ASP:CG[5_555]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LYS:O	2:N:135:GLN:CG[5_555]	1.12	1.08
2:B:127:GLU:OE1	1:M:717:GLN:CB[5_555]	1.12	1.08
2:B:89:PHE:CD2	2:N:140:GLU:N[5_555]	1.13	1.07
2:B:139:GLU:CB	2:N:90:ARG:N[5_555]	1.13	1.07
1:A:712:ARG:NH1	2:N:130:ILE:N[5_555]	1.14	1.06
2:B:99:TYR:CE1	2:N:94:LYS:CG[5_555]	1.15	1.05
1:A:717:GLN:CB	2:N:128:ALA:CB[5_555]	1.15	1.05
2:B:89:PHE:CE1	2:N:140:GLU:CA[5_555]	1.16	1.04
1:A:718:LYS:N	2:N:127:GLU:O[5_555]	1.17	1.03
2:B:143:GLN:CG	2:N:89:PHE:CD1[5_555]	1.18	1.02
2:B:100:ILE:CG2	2:N:97:ASN:N[5_555]	1.18	1.02
2:B:96:GLY:C	2:N:104:GLU:OE1[5_555]	1.18	1.02
2:B:92:PHE:CA	2:N:97:ASN:O[5_555]	1.19	1.01
2:B:127:GLU:OE1	1:M:717:GLN:CA[5_555]	1.19	1.01
2:B:98:GLY:O	2:N:92:PHE:O[5_555]	1.20	1.00
2:B:89:PHE:CG	2:N:140:GLU:N[5_555]	1.20	1.00
2:B:88:ALA:C	2:N:139:GLU:OE2[5_555]	1.20	1.00
2:B:135:GLN:NE2	2:N:95:ASP:OD1[5_555]	1.21	0.99
2:B:99:TYR:CD1	2:N:94:LYS:CB[5_555]	1.21	0.99
2:B:101:SER:N	2:N:95:ASP:O[5_555]	1.22	0.98
2:B:89:PHE:CA	2:N:139:GLU:CA[5_555]	1.22	0.98
2:B:129:ASP:CG	1:M:712:ARG:CA[5_555]	1.22	0.98
2:B:98:GLY:C	2:N:93:ASP:CA[5_555]	1.22	0.98
2:B:138:TYR:CE2	2:N:93:ASP:CG[5_555]	1.23	0.97
2:B:89:PHE:CE2	2:N:140:GLU:CB[5_555]	1.23	0.97
1:A:718:LYS:CB	2:N:127:GLU:CG[5_555]	1.24	0.96
2:B:139:GLU:CG	2:N:89:PHE:O[5_555]	1.24	0.96
2:B:86:ARG:O	2:N:87:GLU:CA[5_555]	1.24	0.96
2:B:128:ALA:CA	1:M:712:ARG:NH2[5_555]	1.25	0.95
2:B:94:LYS:N	2:N:135:GLN:OE1[5_555]	1.25	0.95
2:B:96:GLY:CA	2:N:104:GLU:OE1[5_555]	1.26	0.94
2:B:99:TYR:N	2:N:93:ASP:CA[5_555]	1.27	0.93
2:B:135:GLN:CD	2:N:95:ASP:OD1[5_555]	1.27	0.93
2:B:99:TYR:CE1	2:N:94:LYS:CD[5_555]	1.28	0.92
1:A:717:GLN:CA	2:N:128:ALA:C[5_555]	1.28	0.92
1:A:715:MET:CA	2:N:129:ASP:OD2[5_555]	1.28	0.92
2:B:127:GLU:CD	1:M:717:GLN:C[5_555]	1.29	0.91
1:A:717:GLN:C	2:N:127:GLU:O[5_555]	1.30	0.90
2:B:139:GLU:CA	2:N:90:ARG:N[5_555]	1.30	0.90
2:B:89:PHE:CE1	2:N:140:GLU:C[5_555]	1.31	0.89
2:B:129:ASP:OD1	1:M:712:ARG:CB[5_555]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASN:CA	2:N:94:LYS:CE[5_555]	1.32	0.88
2:B:137:ASN:N	2:N:94:LYS:NZ[5_555]	1.32	0.88
2:B:139:GLU:CG	2:N:89:PHE:C[5_555]	1.33	0.87
2:B:89:PHE:O	2:N:139:GLU:CB[5_555]	1.33	0.87
2:B:92:PHE:O	2:N:99:TYR:CD2[5_555]	1.34	0.86
2:B:129:ASP:CB	1:M:712:ARG:CB[5_555]	1.34	0.86
2:B:88:ALA:O	2:N:139:GLU:OE2[5_555]	1.35	0.85
2:B:96:GLY:C	2:N:104:GLU:CD[5_555]	1.35	0.85
2:B:89:PHE:CE2	2:N:140:GLU:CA[5_555]	1.35	0.85
2:B:100:ILE:C	2:N:95:ASP:O[5_555]	1.36	0.84
2:B:99:TYR:CA	2:N:93:ASP:C[5_555]	1.36	0.84
2:B:91:VAL:O	2:N:99:TYR:CZ[5_555]	1.36	0.84
2:B:98:GLY:CA	2:N:92:PHE:C[5_555]	1.37	0.83
2:B:89:PHE:CD1	2:N:139:GLU:C[5_555]	1.37	0.83
2:B:128:ALA:C	1:M:712:ARG:CZ[5_555]	1.37	0.83
2:B:93:ASP:O	2:N:99:TYR:CB[5_555]	1.37	0.83
2:B:138:TYR:OH	2:N:138:TYR:CE2[5_555]	1.37	0.83
2:B:88:ALA:CA	2:N:139:GLU:OE2[5_555]	1.38	0.82
1:A:712:ARG:CZ	2:N:130:ILE:CG2[5_555]	1.38	0.82
2:B:88:ALA:CB	2:N:139:GLU:OE2[5_555]	1.39	0.81
2:B:139:GLU:CG	2:N:90:ARG:N[5_555]	1.39	0.81
2:B:89:PHE:CG	2:N:139:GLU:C[5_555]	1.39	0.81
2:B:92:PHE:O	2:N:99:TYR:CG[5_555]	1.39	0.81
2:B:104:GLU:OE2	2:N:97:ASN:OD1[5_555]	1.40	0.80
2:B:98:GLY:C	2:N:92:PHE:C[5_555]	1.40	0.80
2:B:135:GLN:OE1	2:N:95:ASP:OD1[5_555]	1.40	0.80
2:B:94:LYS:CA	2:N:135:GLN:OE1[5_555]	1.41	0.79
2:B:139:GLU:CB	2:N:90:ARG:C[5_555]	1.42	0.78
1:A:712:ARG:CG	2:N:130:ILE:C[5_555]	1.43	0.77
2:B:100:ILE:N	2:N:95:ASP:N[5_555]	1.44	0.76
2:B:100:ILE:CG2	2:N:96:GLY:C[5_555]	1.44	0.76
1:A:717:GLN:CD	2:N:128:ALA:O[5_555]	1.44	0.76
2:B:90:ARG:O	2:N:137:ASN:CG[5_555]	1.45	0.75
2:B:138:TYR:CE2	2:N:93:ASP:OD2[5_555]	1.46	0.74
2:B:89:PHE:CD1	2:N:139:GLU:O[5_555]	1.46	0.74
2:B:91:VAL:C	2:N:99:TYR:CZ[5_555]	1.47	0.73
2:B:95:ASP:N	2:N:135:GLN:CD[5_555]	1.48	0.72
2:B:89:PHE:CE2	2:N:140:GLU:N[5_555]	1.49	0.71
2:B:137:ASN:ND2	2:N:91:VAL:CA[5_555]	1.49	0.71
2:B:94:LYS:CA	2:N:135:GLN:CG[5_555]	1.50	0.70
2:B:91:VAL:C	2:N:99:TYR:CD2[5_555]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:TYR:N	2:N:93:ASP:C[5_555]	1.50	0.70
2:B:89:PHE:CZ	2:N:140:GLU:CB[5_555]	1.51	0.69
2:B:137:ASN:CB	2:N:94:LYS:CE[5_555]	1.51	0.69
2:B:93:ASP:CG	2:N:99:TYR:O[5_555]	1.51	0.69
2:B:140:GLU:N	2:N:90:ARG:O[5_555]	1.52	0.68
2:B:100:ILE:C	2:N:95:ASP:CA[5_555]	1.53	0.67
2:B:127:GLU:CG	1:M:717:GLN:O[5_555]	1.53	0.67
2:B:143:GLN:NE2	2:N:89:PHE:CE2[5_555]	1.53	0.67
1:A:712:ARG:CZ	2:N:130:ILE:CB[5_555]	1.54	0.66
2:B:90:ARG:CB	2:N:98:GLY:O[5_555]	1.54	0.66
2:B:87:GLU:OE1	2:N:146:THR:OG1[5_555]	1.54	0.66
2:B:93:ASP:CB	2:N:99:TYR:O[5_555]	1.55	0.65
2:B:138:TYR:CZ	2:N:138:TYR:CE2[5_555]	1.55	0.65
2:B:139:GLU:CG	2:N:90:ARG:CA[5_555]	1.55	0.65
2:B:139:GLU:OE1	2:N:90:ARG:NE[5_555]	1.55	0.65
2:B:95:ASP:N	2:N:135:GLN:NE2[5_555]	1.55	0.65
2:B:99:TYR:CG	2:N:94:LYS:CG[5_555]	1.56	0.64
2:B:138:TYR:CD2	2:N:93:ASP:OD2[5_555]	1.56	0.64
1:A:712:ARG:CD	2:N:130:ILE:O[5_555]	1.56	0.64
2:B:137:ASN:OD1	2:N:91:VAL:N[5_555]	1.56	0.64
2:B:89:PHE:CD1	2:N:140:GLU:N[5_555]	1.56	0.64
2:B:91:VAL:CA	2:N:99:TYR:CZ[5_555]	1.56	0.64
1:A:717:GLN:O	2:N:127:GLU:C[5_555]	1.57	0.63
2:B:94:LYS:N	2:N:135:GLN:CD[5_555]	1.57	0.63
2:B:96:GLY:C	2:N:104:GLU:OE2[5_555]	1.57	0.63
2:B:143:GLN:CA	2:N:89:PHE:CD1[5_555]	1.57	0.63
2:B:99:TYR:C	2:N:94:LYS:N[5_555]	1.57	0.63
2:B:92:PHE:CG	2:N:97:ASN:O[5_555]	1.57	0.63
2:B:129:ASP:OD2	1:M:712:ARG:CB[5_555]	1.58	0.62
2:B:139:GLU:O	2:N:89:PHE:CG[5_555]	1.58	0.62
2:B:127:GLU:O	1:M:712:ARG:NH1[5_555]	1.58	0.62
2:B:92:PHE:O	2:N:99:TYR:CB[5_555]	1.58	0.62
2:B:93:ASP:O	2:N:99:TYR:C[5_555]	1.59	0.61
2:B:137:ASN:OD1	2:N:91:VAL:CA[5_555]	1.59	0.61
2:B:99:TYR:CB	2:N:94:LYS:N[5_555]	1.60	0.60
1:A:718:LYS:N	2:N:127:GLU:CA[5_555]	1.60	0.60
2:B:101:SER:N	2:N:95:ASP:C[5_555]	1.61	0.59
2:B:86:ARG:C	2:N:86:ARG:O[5_555]	1.61	0.59
2:B:143:GLN:CG	2:N:89:PHE:CE1[5_555]	1.62	0.58
1:A:718:LYS:CG	2:N:127:GLU:CG[5_555]	1.62	0.58
2:B:98:GLY:O	2:N:92:PHE:C[5_555]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:CG2	2:N:96:GLY:CA[5_555]	1.62	0.58
2:B:100:ILE:CA	2:N:95:ASP:CA[5_555]	1.62	0.58
2:B:96:GLY:O	2:N:104:GLU:OE1[5_555]	1.63	0.57
2:B:127:GLU:CD	1:M:717:GLN:CA[5_555]	1.63	0.57
2:B:90:ARG:O	2:N:137:ASN:CA[5_555]	1.64	0.56
2:B:90:ARG:CB	2:N:98:GLY:CA[5_555]	1.64	0.56
2:B:93:ASP:O	2:N:99:TYR:CA[5_555]	1.64	0.56
1:A:715:MET:O	2:N:129:ASP:CB[5_555]	1.64	0.56
2:B:93:ASP:N	2:N:97:ASN:CB[5_555]	1.64	0.56
2:B:88:ALA:CB	2:N:139:GLU:CD[5_555]	1.65	0.55
2:B:138:TYR:CE1	2:N:138:TYR:CE2[5_555]	1.66	0.54
1:A:712:ARG:CB	2:N:130:ILE:O[5_555]	1.66	0.54
2:B:138:TYR:CD2	2:N:93:ASP:CG[5_555]	1.66	0.54
2:B:137:ASN:CG	2:N:91:VAL:CA[5_555]	1.66	0.54
2:B:94:LYS:CE	2:N:99:TYR:CD1[5_555]	1.67	0.53
2:B:86:ARG:O	2:N:87:GLU:N[5_555]	1.67	0.53
1:A:717:GLN:CG	2:N:128:ALA:CA[5_555]	1.67	0.53
2:B:129:ASP:N	1:M:712:ARG:NE[5_555]	1.67	0.53
2:B:128:ALA:C	1:M:712:ARG:NH2[5_555]	1.67	0.53
2:B:127:GLU:CD	1:M:717:GLN:O[5_555]	1.67	0.53
2:B:99:TYR:CG	2:N:94:LYS:CB[5_555]	1.68	0.52
2:B:100:ILE:O	2:N:94:LYS:O[5_555]	1.68	0.52
2:B:92:PHE:N	2:N:99:TYR:CD2[5_555]	1.69	0.51
1:A:718:LYS:CA	2:N:127:GLU:C[5_555]	1.69	0.51
2:B:91:VAL:CA	2:N:99:TYR:CE1[5_555]	1.69	0.51
2:B:137:ASN:N	2:N:94:LYS:CE[5_555]	1.69	0.51
2:B:89:PHE:CB	2:N:138:TYR:O[5_555]	1.69	0.51
2:B:91:VAL:CB	2:N:99:TYR:OH[5_555]	1.69	0.51
2:B:98:GLY:C	2:N:92:PHE:O[5_555]	1.69	0.51
2:B:90:ARG:CB	2:N:98:GLY:C[5_555]	1.70	0.50
2:B:100:ILE:CB	2:N:96:GLY:C[5_555]	1.70	0.50
2:B:127:GLU:C	1:M:712:ARG:NH2[5_555]	1.70	0.50
2:B:127:GLU:OE1	1:M:717:GLN:C[5_555]	1.70	0.50
2:B:129:ASP:CA	1:M:712:ARG:CD[5_555]	1.71	0.49
1:A:717:GLN:CB	2:N:128:ALA:C[5_555]	1.71	0.49
2:B:128:ALA:CA	1:M:712:ARG:CZ[5_555]	1.71	0.49
2:B:91:VAL:O	2:N:99:TYR:CD2[5_555]	1.72	0.48
2:B:86:ARG:CA	2:N:86:ARG:C[5_555]	1.72	0.48
2:B:139:GLU:OE1	2:N:90:ARG:CG[5_555]	1.72	0.48
2:B:128:ALA:C	1:M:712:ARG:NE[5_555]	1.72	0.48
2:B:146:THR:OG1	2:N:87:GLU:CG[5_555]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ASP:N	1:M:712:ARG:CZ[5_555]	1.72	0.48
2:B:136:VAL:N	2:N:94:LYS:O[5_555]	1.73	0.47
2:B:86:ARG:NE	2:N:146:THR:CB[5_555]	1.73	0.47
1:A:715:MET:CB	2:N:129:ASP:OD1[5_555]	1.73	0.47
2:B:127:GLU:CD	1:M:717:GLN:CB[5_555]	1.73	0.47
2:B:99:TYR:N	2:N:94:LYS:N[5_555]	1.74	0.46
2:B:86:ARG:NE	2:N:146:THR:OG1[5_555]	1.74	0.46
2:B:138:TYR:CG	2:N:138:TYR:OH[5_555]	1.74	0.46
2:B:86:ARG:CB	2:N:86:ARG:O[5_555]	1.74	0.46
2:B:90:ARG:O	2:N:137:ASN:CB[5_555]	1.74	0.46
1:A:717:GLN:CA	2:N:129:ASP:N[5_555]	1.74	0.46
2:B:84:GLU:OE2	2:N:147:ALA:CB[5_555]	1.75	0.45
2:B:89:PHE:C	2:N:139:GLU:N[5_555]	1.75	0.45
2:B:100:ILE:CB	2:N:95:ASP:C[5_555]	1.75	0.45
2:B:91:VAL:N	2:N:98:GLY:O[5_555]	1.75	0.45
1:A:717:GLN:O	2:N:128:ALA:N[5_555]	1.75	0.45
2:B:98:GLY:N	2:N:93:ASP:N[5_555]	1.76	0.44
2:B:127:GLU:CB	1:M:717:GLN:O[5_555]	1.77	0.43
2:B:94:LYS:C	2:N:135:GLN:OE1[5_555]	1.77	0.43
2:B:143:GLN:CG	2:N:89:PHE:CG[5_555]	1.77	0.43
2:B:129:ASP:CG	1:M:712:ARG:CG[5_555]	1.77	0.43
2:B:89:PHE:CB	2:N:139:GLU:CA[5_555]	1.77	0.43
2:B:93:ASP:OD2	2:N:99:TYR:O[5_555]	1.78	0.42
2:B:127:GLU:O	1:M:712:ARG:CZ[5_555]	1.78	0.42
2:B:99:TYR:CD1	2:N:94:LYS:CD[5_555]	1.78	0.42
1:A:717:GLN:CA	2:N:128:ALA:N[5_555]	1.78	0.42
2:B:90:ARG:CA	2:N:98:GLY:O[5_555]	1.78	0.42
2:B:92:PHE:N	2:N:99:TYR:CE2[5_555]	1.79	0.41
2:B:100:ILE:CD1	2:N:96:GLY:CA[5_555]	1.79	0.41
2:B:100:ILE:N	2:N:96:GLY:N[5_555]	1.79	0.41
1:A:718:LYS:N	2:N:128:ALA:N[5_555]	1.80	0.40
2:B:89:PHE:CZ	2:N:140:GLU:N[5_555]	1.80	0.40
2:B:93:ASP:C	2:N:135:GLN:OE1[5_555]	1.80	0.40
2:B:99:TYR:CA	2:N:94:LYS:CA[5_555]	1.80	0.40
2:B:89:PHE:C	2:N:139:GLU:CB[5_555]	1.80	0.40
2:B:98:GLY:C	2:N:93:ASP:C[5_555]	1.80	0.40
2:B:90:ARG:C	2:N:98:GLY:O[5_555]	1.81	0.39
1:A:715:MET:CB	2:N:129:ASP:CG[5_555]	1.81	0.39
2:B:86:ARG:NH2	2:N:146:THR:OG1[5_555]	1.81	0.39
2:B:98:GLY:O	2:N:93:ASP:O[5_555]	1.82	0.38
2:B:89:PHE:CE1	2:N:140:GLU:O[5_555]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:N	2:N:94:LYS:C[5_555]	1.82	0.38
2:B:127:GLU:CD	1:M:717:GLN:CG[5_555]	1.83	0.37
2:B:98:GLY:O	2:N:93:ASP:C[5_555]	1.83	0.37
2:B:100:ILE:CG2	2:N:96:GLY:N[5_555]	1.83	0.37
2:B:93:ASP:C	2:N:99:TYR:CB[5_555]	1.83	0.37
2:B:89:PHE:N	2:N:139:GLU:CB[5_555]	1.83	0.37
2:B:99:TYR:O	2:N:93:ASP:OD1[5_555]	1.83	0.37
2:B:89:PHE:CE1	2:N:140:GLU:N[5_555]	1.83	0.37
2:B:135:GLN:OE1	2:N:95:ASP:CB[5_555]	1.84	0.36
2:B:91:VAL:CB	2:N:137:ASN:ND2[5_555]	1.84	0.36
2:B:139:GLU:OE1	2:N:90:ARG:CZ[5_555]	1.84	0.36
2:B:127:GLU:CG	1:M:717:GLN:CD[5_555]	1.84	0.36
2:B:143:GLN:NE2	2:N:89:PHE:CD2[5_555]	1.85	0.35
2:B:89:PHE:CA	2:N:138:TYR:C[5_555]	1.85	0.35
2:B:86:ARG:O	2:N:87:GLU:C[5_555]	1.86	0.34
2:B:135:GLN:OE1	2:N:95:ASP:OD2[5_555]	1.86	0.34
2:B:91:VAL:CG2	2:N:99:TYR:CZ[5_555]	1.86	0.34
2:B:94:LYS:C	2:N:135:GLN:NE2[5_555]	1.86	0.34
2:B:137:ASN:C	2:N:94:LYS:NZ[5_555]	1.87	0.33
1:A:712:ARG:NH1	2:N:130:ILE:CA[5_555]	1.87	0.33
1:A:712:ARG:NH2	2:N:130:ILE:CB[5_555]	1.87	0.33
2:B:86:ARG:N	2:N:86:ARG:O[5_555]	1.87	0.33
1:A:718:LYS:C	2:N:127:GLU:CA[5_555]	1.88	0.32
2:B:101:SER:N	2:N:95:ASP:CA[5_555]	1.88	0.32
2:B:127:GLU:CG	1:M:717:GLN:C[5_555]	1.88	0.32
2:B:92:PHE:C	2:N:99:TYR:CD2[5_555]	1.89	0.31
1:A:712:ARG:NH1	2:N:129:ASP:C[5_555]	1.89	0.31
2:B:89:PHE:CD1	2:N:140:GLU:C[5_555]	1.89	0.31
2:B:138:TYR:CZ	2:N:138:TYR:CZ[5_555]	1.90	0.30
2:B:99:TYR:N	2:N:93:ASP:N[5_555]	1.90	0.30
2:B:90:ARG:O	2:N:137:ASN:OD1[5_555]	1.91	0.29
2:B:88:ALA:C	2:N:139:GLU:CD[5_555]	1.91	0.29
2:B:100:ILE:CG1	2:N:96:GLY:N[5_555]	1.92	0.28
2:B:89:PHE:CZ	2:N:140:GLU:C[5_555]	1.92	0.28
1:A:715:MET:C	2:N:129:ASP:OD2[5_555]	1.92	0.28
2:B:89:PHE:CG	2:N:139:GLU:N[5_555]	1.92	0.28
2:B:138:TYR:CD1	2:N:138:TYR:CZ[5_555]	1.92	0.28
1:A:717:GLN:C	2:N:128:ALA:CA[5_555]	1.92	0.28
2:B:94:LYS:CB	2:N:135:GLN:CG[5_555]	1.92	0.28
1:A:712:ARG:NH2	2:N:130:ILE:CG2[5_555]	1.92	0.28
2:B:90:ARG:CG	2:N:98:GLY:CA[5_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ARG:C	1:M:717:GLN:NE2[5_555]	1.93	0.27
1:A:716:LYS:O	2:N:127:GLU:O[5_555]	1.93	0.27
2:B:127:GLU:CG	1:M:717:GLN:CA[5_555]	1.93	0.27
2:B:98:GLY:O	2:N:93:ASP:N[5_555]	1.93	0.27
2:B:91:VAL:CB	2:N:99:TYR:CZ[5_555]	1.94	0.26
2:B:136:VAL:C	2:N:94:LYS:NZ[5_555]	1.94	0.26
2:B:94:LYS:CA	2:N:135:GLN:NE2[5_555]	1.94	0.26
2:B:138:TYR:CZ	2:N:138:TYR:OH[5_555]	1.94	0.26
1:A:718:LYS:CG	2:N:127:GLU:CB[5_555]	1.94	0.26
2:B:139:GLU:OE1	2:N:90:ARG:NH1[5_555]	1.95	0.25
2:B:138:TYR:CD2	2:N:93:ASP:CB[5_555]	1.95	0.25
2:B:137:ASN:ND2	2:N:91:VAL:C[5_555]	1.95	0.25
1:A:717:GLN:N	2:N:129:ASP:N[5_555]	1.95	0.25
1:A:715:MET:CA	2:N:129:ASP:CG[5_555]	1.95	0.25
2:B:86:ARG:CZ	2:N:146:THR:OG1[5_555]	1.96	0.24
2:B:143:GLN:CB	2:N:89:PHE:CZ[5_555]	1.96	0.24
2:B:89:PHE:CD1	2:N:140:GLU:CA[5_555]	1.96	0.24
2:B:143:GLN:CD	2:N:89:PHE:CZ[5_555]	1.96	0.24
2:B:96:GLY:O	2:N:104:GLU:CG[5_555]	1.96	0.24
2:B:139:GLU:C	2:N:90:ARG:O[5_555]	1.96	0.24
2:B:94:LYS:CA	2:N:135:GLN:CB[5_555]	1.97	0.23
2:B:91:VAL:CG1	2:N:137:ASN:ND2[5_555]	1.97	0.23
2:B:135:GLN:OE1	2:N:95:ASP:N[5_555]	1.97	0.23
2:B:137:ASN:OD1	2:N:90:ARG:O[5_555]	1.97	0.23
2:B:99:TYR:C	2:N:95:ASP:N[5_555]	1.97	0.23
2:B:129:ASP:OD2	1:M:712:ARG:C[5_555]	1.97	0.23
2:B:99:TYR:CB	2:N:94:LYS:CB[5_555]	1.97	0.23
2:B:99:TYR:CB	2:N:94:LYS:CA[5_555]	1.97	0.23
2:B:89:PHE:CG	2:N:139:GLU:CA[5_555]	1.97	0.23
2:B:139:GLU:CB	2:N:90:ARG:CB[5_555]	1.97	0.23
2:B:95:ASP:O	2:N:101:SER:OG[5_555]	1.98	0.22
2:B:139:GLU:CD	2:N:89:PHE:C[5_555]	1.98	0.22
2:B:135:GLN:CD	2:N:95:ASP:CG[5_555]	1.98	0.22
2:B:92:PHE:CA	2:N:97:ASN:C[5_555]	1.98	0.22
2:B:129:ASP:C	1:M:712:ARG:CG[5_555]	1.99	0.21
2:B:100:ILE:CA	2:N:95:ASP:N[5_555]	1.99	0.21
2:B:139:GLU:O	2:N:89:PHE:CD2[5_555]	1.99	0.21
2:B:139:GLU:CA	2:N:90:ARG:CA[5_555]	1.99	0.21
2:B:94:LYS:N	2:N:135:GLN:NE2[5_555]	2.00	0.20
2:B:128:ALA:N	1:M:712:ARG:CZ[5_555]	2.00	0.20
2:B:143:GLN:CB	2:N:89:PHE:CG[5_555]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLY:O	2:N:93:ASP:CA[5_555]	2.00	0.20
2:B:90:ARG:NH1	2:N:139:GLU:OE1[5_555]	2.00	0.20
2:B:89:PHE:CE1	2:N:139:GLU:O[5_555]	2.00	0.20
1:A:717:GLN:OE1	2:N:128:ALA:C[5_555]	2.01	0.19
1:A:717:GLN:CB	2:N:128:ALA:N[5_555]	2.01	0.19
2:B:139:GLU:CD	2:N:90:ARG:N[5_555]	2.01	0.19
2:B:139:GLU:CD	2:N:90:ARG:CG[5_555]	2.01	0.19
2:B:92:PHE:CA	2:N:99:TYR:CD2[5_555]	2.02	0.18
2:B:128:ALA:O	1:M:712:ARG:NE[5_555]	2.02	0.18
2:B:138:TYR:OH	2:N:138:TYR:CD2[5_555]	2.02	0.18
2:B:100:ILE:CG2	2:N:93:ASP:OD1[5_555]	2.02	0.18
2:B:127:GLU:OE2	1:M:717:GLN:C[5_555]	2.02	0.18
2:B:137:ASN:OD1	2:N:90:ARG:C[5_555]	2.02	0.18
1:A:717:GLN:CA	2:N:127:GLU:O[5_555]	2.02	0.18
1:A:715:MET:CB	2:N:129:ASP:OD2[5_555]	2.02	0.18
2:B:89:PHE:CD2	2:N:137:ASN:OD1[5_555]	2.03	0.17
2:B:129:ASP:CB	1:M:712:ARG:CA[5_555]	2.03	0.17
2:B:135:GLN:OE1	2:N:95:ASP:CA[5_555]	2.03	0.17
2:B:127:GLU:OE2	1:M:717:GLN:O[5_555]	2.03	0.17
2:B:94:LYS:CB	2:N:135:GLN:CD[5_555]	2.03	0.17
2:B:100:ILE:C	2:N:96:GLY:N[5_555]	2.04	0.16
2:B:137:ASN:ND2	2:N:91:VAL:O[5_555]	2.04	0.16
2:B:129:ASP:N	1:M:712:ARG:CG[5_555]	2.04	0.16
2:B:139:GLU:CD	2:N:89:PHE:O[5_555]	2.05	0.15
2:B:95:ASP:N	2:N:135:GLN:OE1[5_555]	2.05	0.15
2:B:89:PHE:CA	2:N:139:GLU:CB[5_555]	2.05	0.15
2:B:129:ASP:N	1:M:712:ARG:NH1[5_555]	2.05	0.15
2:B:127:GLU:OE1	1:M:717:GLN:N[5_555]	2.06	0.14
2:B:95:ASP:OD2	2:N:135:GLN:NE2[5_555]	2.06	0.14
2:B:95:ASP:O	2:N:101:SER:CB[5_555]	2.06	0.14
2:B:129:ASP:CA	1:M:712:ARG:NE[5_555]	2.06	0.14
2:B:98:GLY:CA	2:N:93:ASP:CA[5_555]	2.06	0.14
2:B:139:GLU:CA	2:N:90:ARG:C[5_555]	2.06	0.14
1:A:718:LYS:C	2:N:127:GLU:CB[5_555]	2.07	0.13
2:B:88:ALA:CA	2:N:139:GLU:CD[5_555]	2.07	0.13
2:B:127:GLU:C	1:M:712:ARG:CZ[5_555]	2.07	0.13
2:B:99:TYR:C	2:N:93:ASP:C[5_555]	2.07	0.13
2:B:136:VAL:O	2:N:94:LYS:NZ[5_555]	2.07	0.13
2:B:92:PHE:N	2:N:97:ASN:O[5_555]	2.07	0.13
2:B:138:TYR:CE1	2:N:138:TYR:CE1[5_555]	2.07	0.13
2:B:100:ILE:CA	2:N:95:ASP:O[5_555]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:PHE:CD2	2:N:140:GLU:CA[5_555]	2.08	0.12
2:B:87:GLU:OE1	2:N:146:THR:CG2[5_555]	2.08	0.12
2:B:92:PHE:CB	2:N:98:GLY:N[5_555]	2.08	0.12
2:B:143:GLN:N	2:N:89:PHE:CD1[5_555]	2.09	0.11
2:B:104:GLU:CD	2:N:97:ASN:OD1[5_555]	2.09	0.11
2:B:129:ASP:OD1	1:M:712:ARG:CG[5_555]	2.09	0.11
1:A:718:LYS:CB	2:N:127:GLU:CA[5_555]	2.09	0.11
2:B:94:LYS:O	2:N:135:GLN:CD[5_555]	2.09	0.11
2:B:128:ALA:CA	1:M:712:ARG:NH1[5_555]	2.10	0.10
2:B:139:GLU:CB	2:N:90:ARG:O[5_555]	2.10	0.10
2:B:89:PHE:N	2:N:139:GLU:N[5_555]	2.10	0.10
1:A:717:GLN:NE2	2:N:125:ILE:O[5_555]	2.10	0.10
2:B:94:LYS:NZ	2:N:99:TYR:CD1[5_555]	2.10	0.10
1:A:712:ARG:NE	2:N:130:ILE:CB[5_555]	2.10	0.10
1:A:715:MET:O	2:N:129:ASP:OD2[5_555]	2.10	0.10
2:B:91:VAL:CA	2:N:99:TYR:CE2[5_555]	2.10	0.10
2:B:89:PHE:C	2:N:139:GLU:CA[5_555]	2.10	0.10
2:B:93:ASP:O	2:N:100:ILE:N[5_555]	2.11	0.09
2:B:96:GLY:N	2:N:104:GLU:OE1[5_555]	2.11	0.09
2:B:128:ALA:N	1:M:717:GLN:OE1[5_555]	2.11	0.09
1:A:712:ARG:NH1	2:N:130:ILE:CB[5_555]	2.12	0.08
1:A:718:LYS:CG	2:N:127:GLU:CD[5_555]	2.12	0.08
1:A:712:ARG:O	2:N:129:ASP:OD1[5_555]	2.12	0.08
2:B:139:GLU:CA	2:N:90:ARG:O[5_555]	2.12	0.08
2:B:88:ALA:O	2:N:139:GLU:CD[5_555]	2.12	0.08
1:A:718:LYS:CA	2:N:127:GLU:N[5_555]	2.12	0.08
2:B:86:ARG:CB	2:N:86:ARG:C[5_555]	2.12	0.08
2:B:100:ILE:O	2:N:95:ASP:C[5_555]	2.12	0.08
2:B:129:ASP:CB	1:M:712:ARG:C[5_555]	2.13	0.07
2:B:139:GLU:CD	2:N:90:ARG:NH1[5_555]	2.13	0.07
2:B:89:PHE:CD1	2:N:141:PHE:N[5_555]	2.13	0.07
2:B:128:ALA:O	1:M:712:ARG:NH2[5_555]	2.13	0.07
2:B:143:GLN:CD	2:N:89:PHE:CE2[5_555]	2.15	0.05
2:B:129:ASP:CB	1:M:712:ARG:CD[5_555]	2.15	0.05
2:B:143:GLN:CD	2:N:89:PHE:CE1[5_555]	2.15	0.05
2:B:89:PHE:CB	2:N:138:TYR:CA[5_555]	2.15	0.05
2:B:129:ASP:N	1:M:712:ARG:CD[5_555]	2.16	0.04
2:B:92:PHE:CB	2:N:97:ASN:CA[5_555]	2.16	0.04
1:A:715:MET:C	2:N:129:ASP:CB[5_555]	2.16	0.04
2:B:138:TYR:CZ	2:N:93:ASP:OD2[5_555]	2.16	0.04
1:A:717:GLN:CD	2:N:128:ALA:C[5_555]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:MET:C	2:N:129:ASP:CG[5_555]	2.17	0.03
2:B:99:TYR:CZ	2:N:94:LYS:CG[5_555]	2.17	0.03
1:A:717:GLN:CA	2:N:127:GLU:C[5_555]	2.17	0.03
2:B:139:GLU:OE2	2:N:89:PHE:C[5_555]	2.17	0.03
1:A:717:GLN:N	2:N:127:GLU:O[5_555]	2.18	0.02
2:B:139:GLU:CB	2:N:89:PHE:C[5_555]	2.18	0.02
2:B:86:ARG:O	2:N:86:ARG:C[5_555]	2.18	0.02
2:B:139:GLU:CD	2:N:90:ARG:CD[5_555]	2.18	0.02
1:A:714:LEU:C	2:N:129:ASP:OD2[5_555]	2.18	0.02
2:B:94:LYS:CB	2:N:135:GLN:CB[5_555]	2.18	0.02
1:A:718:LYS:N	2:N:127:GLU:CB[5_555]	2.18	0.02
2:B:89:PHE:CE1	2:N:139:GLU:C[5_555]	2.19	0.01
1:A:717:GLN:C	2:N:127:GLU:CA[5_555]	2.19	0.01
1:A:715:MET:O	2:N:129:ASP:CG[5_555]	2.19	0.01
2:B:138:TYR:CZ	2:N:93:ASP:CB[5_555]	2.19	0.01
2:B:139:GLU:C	2:N:89:PHE:CB[5_555]	2.19	0.01
2:B:139:GLU:OE2	2:N:90:ARG:N[5_555]	2.19	0.01

## 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	A	986/1080 (91%)	939 (95%)	39 (4%)	8 (1%)	22	67
1	M	986/1080 (91%)	942 (96%)	37 (4%)	7 (1%)	25	68
2	B	137/148 (93%)	123 (90%)	7 (5%)	7 (5%)	2	26
2	C	139/148 (94%)	129 (93%)	8 (6%)	2 (1%)	13	54
2	D	137/148 (93%)	124 (90%)	11 (8%)	2 (2%)	12	53
2	E	139/148 (94%)	129 (93%)	8 (6%)	2 (1%)	13	54
2	F	137/148 (93%)	124 (90%)	7 (5%)	6 (4%)	3	29
2	G	139/148 (94%)	128 (92%)	5 (4%)	6 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	137/148 (93%)	123 (90%)	8 (6%)	6 (4%)	3	29
2	O	139/148 (94%)	128 (92%)	10 (7%)	1 (1%)	25	68
2	P	137/148 (93%)	127 (93%)	8 (6%)	2 (2%)	12	53
2	Q	139/148 (94%)	128 (92%)	8 (6%)	3 (2%)	8	44
2	R	137/148 (93%)	123 (90%)	9 (7%)	5 (4%)	4	33
2	S	139/148 (94%)	129 (93%)	4 (3%)	6 (4%)	3	29
All	All	3628/3936 (92%)	3396 (94%)	169 (5%)	63 (2%)	11	50

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	SER
2	B	41	GLN
2	B	91	VAL
2	B	93	ASP
2	B	115	LYS
2	C	91	VAL
2	C	93	ASP
2	D	91	VAL
2	D	115	LYS
2	F	41	GLN
2	G	76	MET
2	G	92	PHE
1	M	186	SER
2	N	41	GLN
2	N	91	VAL
2	N	93	ASP
2	O	91	VAL
2	R	41	GLN
2	S	92	PHE
2	S	115	LYS
1	A	46	LYS
2	E	92	PHE
2	G	115	LYS
1	M	46	LYS
1	M	71	GLU
2	N	115	LYS
2	P	91	VAL
2	P	115	LYS
2	Q	92	PHE

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	439	TYR
2	B	92	PHE
2	F	44	THR
2	F	58	ASP
2	G	43	PRO
2	R	58	ASP
2	S	43	PRO
2	S	44	THR
1	A	45	GLY
1	A	294	PRO
2	F	42	ASN
1	M	294	PRO
2	Q	115	LYS
2	B	42	ASN
2	F	91	VAL
2	G	42	ASN
1	M	45	GLY
1	M	439	TYR
2	N	92	PHE
2	R	42	ASN
2	S	42	ASN
1	A	633	LYS
2	N	42	ASN
2	F	40	GLY
2	R	40	GLY
2	R	91	VAL
2	B	40	GLY
2	G	40	GLY
1	M	117	PRO
2	S	40	GLY
2	E	42	ASN
2	Q	42	ASN
1	A	117	PRO

### 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	A	886/961 (92%)	794 (90%)	92 (10%)	8	32
1	M	886/961 (92%)	798 (90%)	88 (10%)	9	34
2	B	118/126 (94%)	107 (91%)	11 (9%)	10	37
2	C	120/126 (95%)	106 (88%)	14 (12%)	6	27
2	D	118/126 (94%)	106 (90%)	12 (10%)	8	33
2	E	120/126 (95%)	107 (89%)	13 (11%)	7	31
2	F	118/126 (94%)	104 (88%)	14 (12%)	6	27
2	G	120/126 (95%)	105 (88%)	15 (12%)	5	26
2	N	118/126 (94%)	106 (90%)	12 (10%)	8	33
2	O	120/126 (95%)	106 (88%)	14 (12%)	6	27
2	P	118/126 (94%)	105 (89%)	13 (11%)	7	30
2	Q	120/126 (95%)	108 (90%)	12 (10%)	9	33
2	R	118/126 (94%)	106 (90%)	12 (10%)	8	33
2	S	120/126 (95%)	104 (87%)	16 (13%)	4	24
All	All	3200/3434 (93%)	2862 (89%)	338 (11%)	8	31

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6	LEU
1	A	30	ASP
1	A	46	LYS
1	A	56	THR
1	A	66	ASP
1	A	67	ILE
1	A	121	GLU
1	A	134	ASP
1	A	138	HIS
1	A	170	THR
1	A	189	GLU
1	A	194	GLU
1	A	214	ASN
1	A	230	LYS
1	A	255	GLU
1	A	339	GLU
1	A	406	HIS
1	A	424	HIS

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Mol	Chain	Res	Type
1	A	476	GLU
1	A	488	ASP
1	A	510	ASP
1	A	521	ASP
1	A	555	ASP
1	A	562	GLU
1	A	575	GLU
1	A	578	LYS
1	A	586	PHE
1	A	632	HIS
1	A	655	THR
1	A	663	LYS
1	A	703	THR
1	A	718	LYS
1	A	719	ASP
1	A	771	CYS
1	A	808	CYS
1	A	824	LYS
1	A	828	MET
1	A	846	GLN
1	A	872	LYS
1	A	887	LEU
1	A	897	TYR
1	A	903	LYS
1	A	906	LEU
1	A	954	LEU
1	A	963	GLU
1	A	964	LYS
1	A	965	LEU
1	A	966	ARG
1	A	971	ARG
1	A	972	LEU
1	A	977	GLU
1	A	980	LYS
1	A	985	ARG
1	A	986	VAL
1	A	987	LEU
1	A	989	LEU
1	A	995	LYS
1	A	996	LEU
1	A	997	ARG
1	A	1000	LEU

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Mol	Chain	Res	Type
1	A	1007	LYS
1	A	1015	ASP
1	A	1016	LYS
1	A	1018	LYS
1	A	1024	LEU
1	A	1027	GLU
1	A	1028	LEU
1	A	1029	LYS
1	A	1032	ASN
1	A	1033	THR
1	A	1034	LEU
1	A	1035	LEU
1	A	1039	LYS
1	A	1041	GLU
1	A	1042	LEU
1	A	1045	ARG
1	A	1051	LYS
1	A	1055	GLU
1	A	1057	MET
1	A	1060	LYS
1	A	1061	LEU
1	A	1064	GLU
1	A	1065	THR
1	A	1068	LEU
1	A	1070	LEU
1	A	1072	LEU
1	A	1073	ASN
1	A	1076	ARG
1	A	1077	LEU
1	A	1078	ARG
1	A	1080	GLN
2	B	11	GLU
2	B	18	LEU
2	B	21	LYS
2	B	22	ASP
2	B	34	THR
2	B	53	ASN
2	B	86	ARG
2	B	87	GLU
2	B	94	LYS
2	B	127	GLU
2	B	131	ASP

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Mol	Chain	Res	Type
2	C	14	GLU
2	C	17	SER
2	C	24	ASP
2	C	30	LYS
2	C	44	THR
2	C	47	GLU
2	C	48	LEU
2	C	54	GLU
2	C	85	ILE
2	C	87	GLU
2	C	107	HIS
2	C	127	GLU
2	C	140	GLU
2	C	148	LYS
2	D	11	GLU
2	D	53	ASN
2	D	82	GLU
2	D	85	ILE
2	D	86	ARG
2	D	87	GLU
2	D	91	VAL
2	D	104	GLU
2	D	111	ASN
2	D	124	MET
2	D	127	GLU
2	D	131	ASP
2	E	13	LYS
2	E	17	SER
2	E	30	LYS
2	E	48	LEU
2	E	54	GLU
2	E	56	ASP
2	E	83	GLU
2	E	84	GLU
2	E	86	ARG
2	E	87	GLU
2	E	92	PHE
2	E	140	GLU
2	E	148	LYS
2	F	11	GLU
2	F	24	ASP
2	F	53	ASN

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Mol	Chain	Res	Type
2	F	86	ARG
2	F	87	GLU
2	F	90	ARG
2	F	91	VAL
2	F	95	ASP
2	F	111	ASN
2	F	118	ASP
2	F	122	ASP
2	F	127	GLU
2	F	131	ASP
2	F	145	MET
2	G	11	GLU
2	G	18	LEU
2	G	19	PHE
2	G	21	LYS
2	G	29	THR
2	G	30	LYS
2	G	48	LEU
2	G	54	GLU
2	G	60	ASN
2	G	74	ARG
2	G	77	LYS
2	G	86	ARG
2	G	87	GLU
2	G	123	GLU
2	G	140	GLU
1	M	5	GLU
1	M	30	ASP
1	M	41	ARG
1	M	46	LYS
1	M	56	THR
1	M	67	ILE
1	M	75	THR
1	M	121	GLU
1	M	134	ASP
1	M	138	HIS
1	M	170	THR
1	M	189	GLU
1	M	194	GLU
1	M	214	ASN
1	M	230	LYS
1	M	255	GLU

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Mol	Chain	Res	Type
1	M	339	GLU
1	M	406	HIS
1	M	424	HIS
1	M	476	GLU
1	M	488	ASP
1	M	510	ASP
1	M	521	ASP
1	M	555	ASP
1	M	562	GLU
1	M	575	GLU
1	M	578	LYS
1	M	586	PHE
1	M	632	HIS
1	M	655	THR
1	M	663	LYS
1	M	703	THR
1	M	718	LYS
1	M	719	ASP
1	M	766	LYS
1	M	824	LYS
1	M	828	MET
1	M	865	HIS
1	M	872	LYS
1	M	887	LEU
1	M	897	TYR
1	M	900	MET
1	M	954	LEU
1	M	964	LYS
1	M	965	LEU
1	M	966	ARG
1	M	967	SER
1	M	971	ARG
1	M	972	LEU
1	M	980	LYS
1	M	985	ARG
1	M	987	LEU
1	M	989	LEU
1	M	995	LYS
1	M	996	LEU
1	M	997	ARG
1	M	999	GLU
1	M	1000	LEU

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Mol	Chain	Res	Type
1	M	1007	LYS
1	M	1016	LYS
1	M	1018	LYS
1	M	1019	HIS
1	M	1021	THR
1	M	1024	LEU
1	M	1027	GLU
1	M	1028	LEU
1	M	1029	LYS
1	M	1032	ASN
1	M	1034	LEU
1	M	1035	LEU
1	M	1039	LYS
1	M	1042	LEU
1	M	1045	ARG
1	M	1051	LYS
1	M	1057	MET
1	M	1060	LYS
1	M	1061	LEU
1	M	1066	LYS
1	M	1067	GLN
1	M	1068	LEU
1	M	1070	LEU
1	M	1072	LEU
1	M	1073	ASN
1	M	1075	GLU
1	M	1076	ARG
1	M	1077	LEU
1	M	1078	ARG
1	M	1080	GLN
2	N	11	GLU
2	N	18	LEU
2	N	21	LYS
2	N	24	ASP
2	N	34	THR
2	N	53	ASN
2	N	83	GLU
2	N	86	ARG
2	N	87	GLU
2	N	94	LYS
2	N	127	GLU
2	N	131	ASP

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Mol	Chain	Res	Type
2	O	14	GLU
2	O	17	SER
2	O	24	ASP
2	O	30	LYS
2	O	44	THR
2	O	47	GLU
2	O	48	LEU
2	O	54	GLU
2	O	85	ILE
2	O	87	GLU
2	O	94	LYS
2	O	107	HIS
2	O	140	GLU
2	O	148	LYS
2	P	11	GLU
2	P	53	ASN
2	P	82	GLU
2	P	85	ILE
2	P	86	ARG
2	P	87	GLU
2	P	91	VAL
2	P	104	GLU
2	P	111	ASN
2	P	124	MET
2	P	127	GLU
2	P	131	ASP
2	P	139	GLU
2	Q	13	LYS
2	Q	17	SER
2	Q	30	LYS
2	Q	48	LEU
2	Q	54	GLU
2	Q	83	GLU
2	Q	84	GLU
2	Q	86	ARG
2	Q	87	GLU
2	Q	92	PHE
2	Q	140	GLU
2	Q	148	LYS
2	R	11	GLU
2	R	24	ASP
2	R	53	ASN

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Mol	Chain	Res	Type
2	R	86	ARG
2	R	87	GLU
2	R	90	ARG
2	R	91	VAL
2	R	111	ASN
2	R	118	ASP
2	R	122	ASP
2	R	131	ASP
2	R	145	MET
2	S	11	GLU
2	S	17	SER
2	S	18	LEU
2	S	19	PHE
2	S	21	LYS
2	S	30	LYS
2	S	47	GLU
2	S	48	LEU
2	S	50	ASP
2	S	52	ILE
2	S	56	ASP
2	S	78	ASP
2	S	86	ARG
2	S	87	GLU
2	S	123	GLU
2	S	140	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	395	HIS
1	A	430	HIS
1	A	463	GLN
1	A	493	GLN
1	A	497	ASN
1	A	873	HIS
1	A	952	ASN
1	A	1080	GLN
2	B	107	HIS
2	D	107	HIS
2	E	107	HIS
2	G	107	HIS

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Mol	Chain	Res	Type
1	M	81	HIS
1	M	395	HIS
1	M	430	HIS
1	M	463	GLN
1	M	493	GLN
1	M	497	ASN
1	M	804	HIS
1	M	805	GLN
1	M	873	HIS
1	M	1067	GLN
1	M	1080	GLN
2	N	107	HIS
2	O	107	HIS
2	P	107	HIS
2	Q	107	HIS
2	S	107	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.