



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:45 am GMT

PDB ID : 4TWH  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) mutant F16'S  
Authors : Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.  
Deposited on : 2014-06-30  
Resolution : 3.60 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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

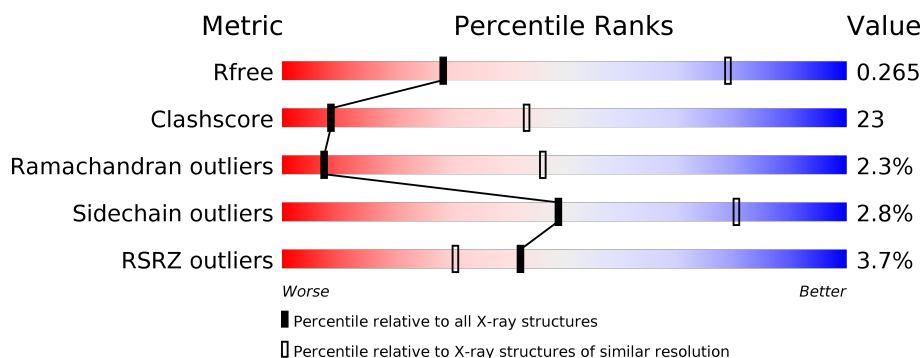
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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.

Mol	Chain	Length	Quality of chain
1	A	307	<div> <div>3%</div> <div>63%</div> <div>34%</div> <div>.</div> </div>
1	B	307	<div> <div>3%</div> <div>57%</div> <div>39%</div> <div>..</div> </div>
1	C	307	<div> <div>3%</div> <div>58%</div> <div>39%</div> <div>.</div> </div>
1	D	307	<div> <div>3%</div> <div>56%</div> <div>39%</div> <div>.</div> </div>
1	E	307	<div> <div>4%</div> <div>54%</div> <div>43%</div> <div>..</div> </div>
1	F	307	<div> <div>4%</div> <div>59%</div> <div>38%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	307	<div><div></div><div>4%</div><div>56%</div><div>40%</div><div></div></div>
1	H	307	<div><div></div><div>7%</div><div>61%</div><div>36%</div><div></div></div>
1	I	307	<div><div></div><div>3%</div><div>64%</div><div>29%</div><div>6%</div><div></div></div>
1	J	307	<div><div></div><div>3%</div><div>57%</div><div>37%</div><div>5%</div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24970 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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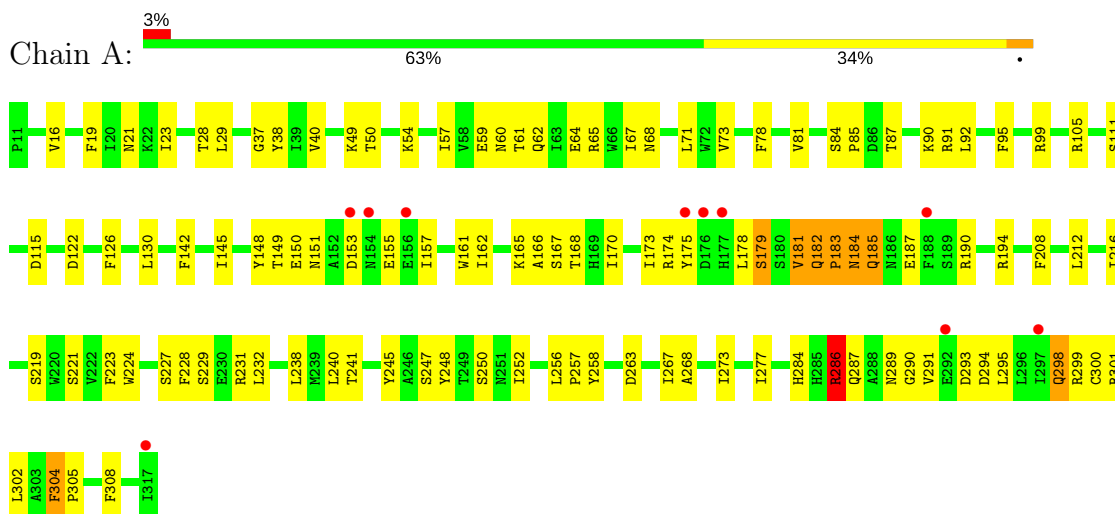
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Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

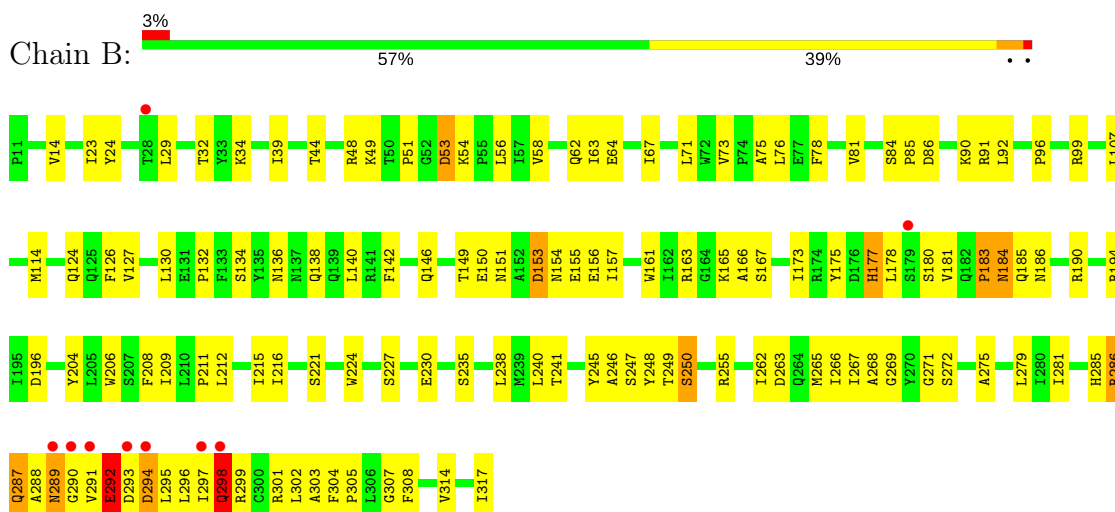
### 3 Residue-property plots

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.

#### • Molecule 1: Cys-loop ligand-gated ion channel

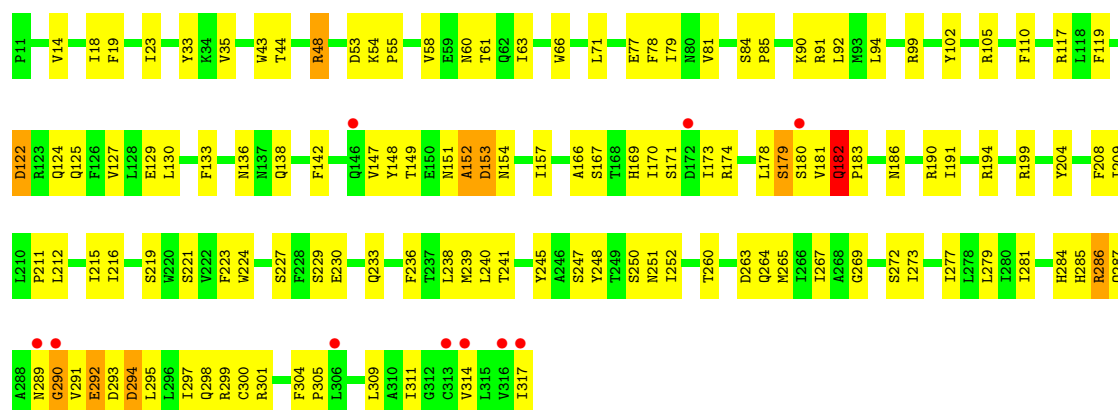


#### • Molecule 1: Cys-loop ligand-gated ion channel

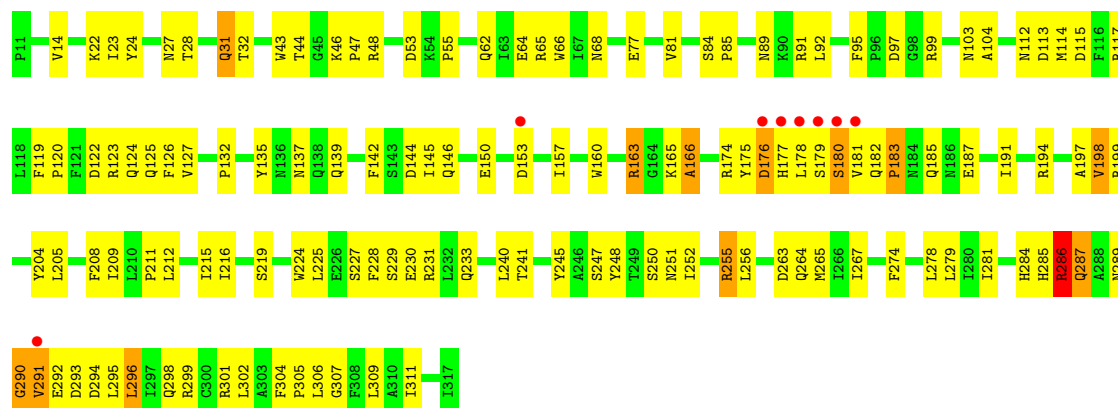


#### • Molecule 1: Cys-loop ligand-gated ion channel

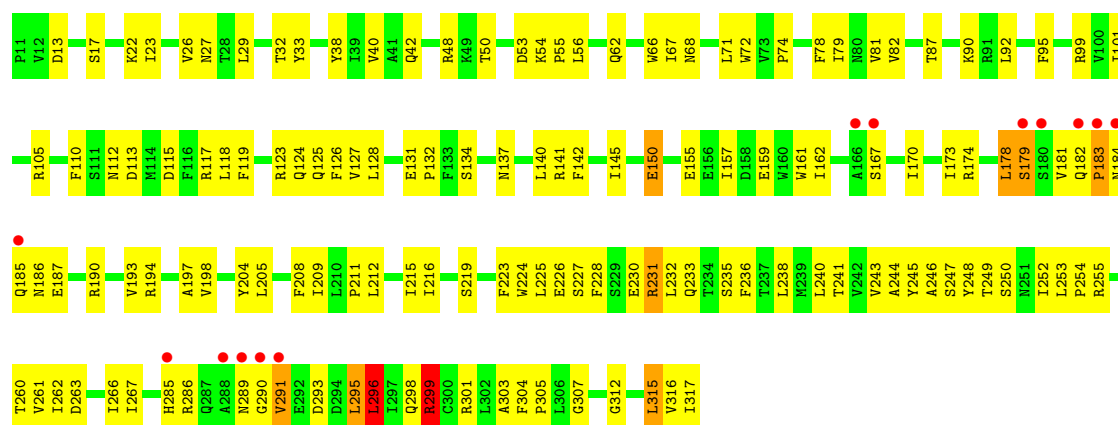




• Molecule 1: Cys-loop ligand-gated ion channel

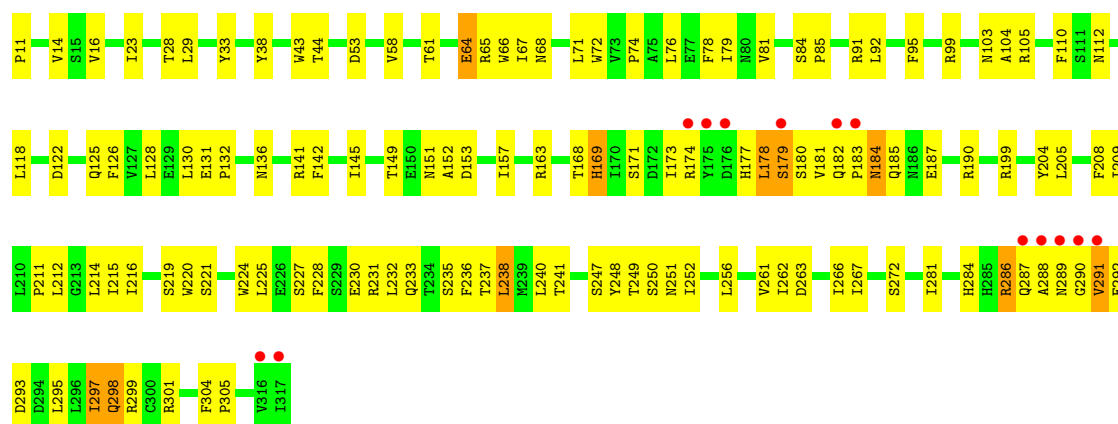


• Molecule 1: Cys-loop ligand-gated ion channel

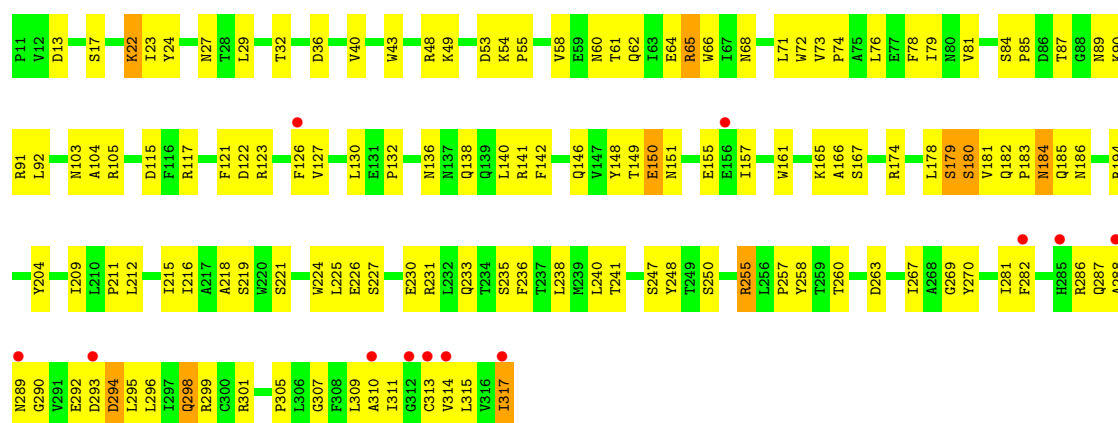


• Molecule 1: Cys-loop ligand-gated ion channel

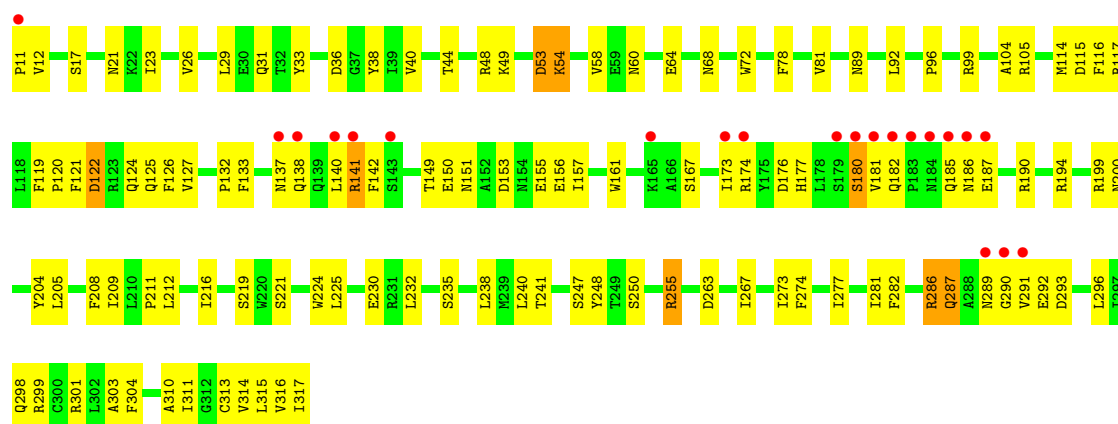




• Molecule 1: Cys-loop ligand-gated ion channel



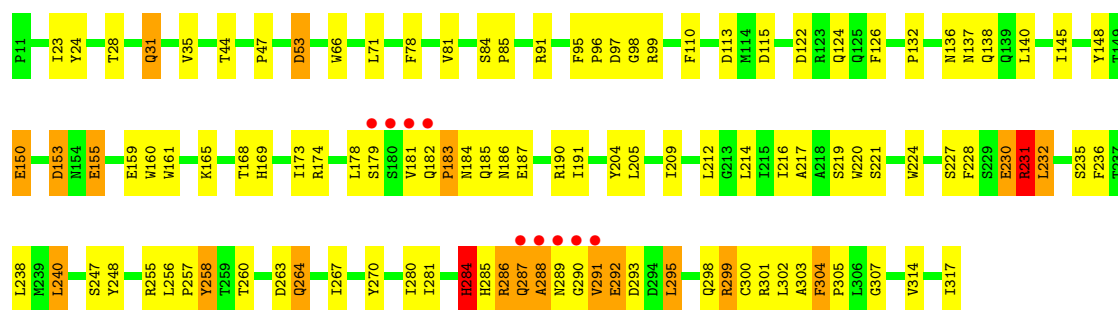
• Molecule 1: Cys-loop ligand-gated ion channel



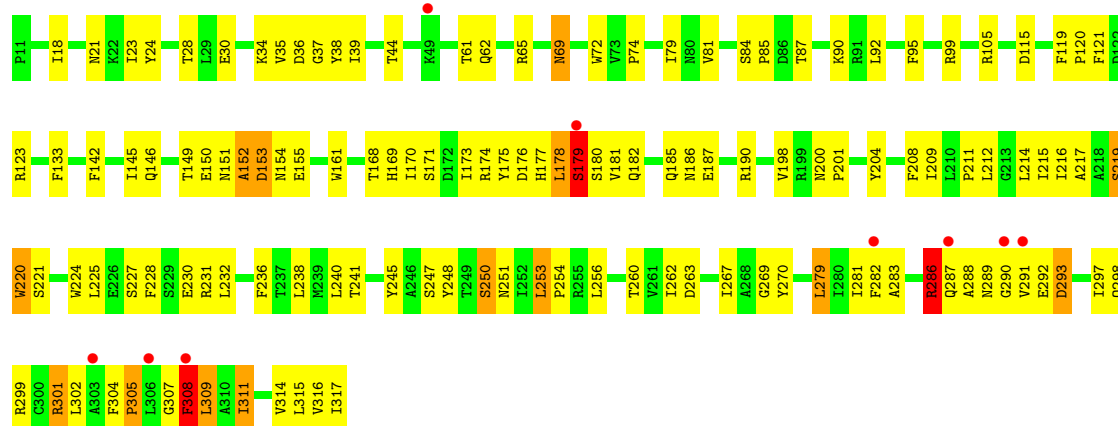
• Molecule 1: Cys-loop ligand-gated ion channel







• Molecule 1: Cys-loop ligand-gated ion channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.90Å 264.97Å 111.33Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	48.62 – 3.60 48.62 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.62-3.60) 90.3 (48.62-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.220 , 0.263 0.223 , 0.265	Depositor DCC
$R_{free}$ test set	3359 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	24970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.44	0/2564	0.77	2/3495 (0.1%)
1	B	0.48	1/2564 (0.0%)	0.82	5/3495 (0.1%)
1	C	0.42	0/2564	0.75	1/3495 (0.0%)
1	D	0.46	0/2564	0.81	4/3495 (0.1%)
1	E	0.44	0/2564	0.79	5/3495 (0.1%)
1	F	0.39	0/2564	0.72	3/3495 (0.1%)
1	G	0.41	0/2564	0.72	1/3495 (0.0%)
1	H	0.40	0/2564	0.73	1/3495 (0.0%)
1	I	0.50	1/2564 (0.0%)	0.82	7/3495 (0.2%)
1	J	0.47	0/2564	0.83	6/3495 (0.2%)
All	All	0.44	2/25640 (0.0%)	0.78	35/34950 (0.1%)

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	2
1	B	0	4
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	2
1	I	0	3
1	J	0	5
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	258	TYR	CD1-CE1	-6.01	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	GLU	CG-CD	-5.18	1.44	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	LEU	CA-CB-CG	7.19	131.84	115.30
1	D	198	VAL	CB-CA-C	-6.94	98.21	111.40
1	B	293	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	293	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	J	308	PHE	CB-CA-C	-6.23	97.93	110.40
1	E	62	GLN	CA-CB-CG	6.23	127.11	113.40
1	E	296	LEU	CA-CB-CG	6.14	129.42	115.30
1	J	279	LEU	CA-CB-CG	6.11	129.35	115.30
1	I	231	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	G	315	LEU	CB-CG-CD2	6.01	121.22	111.00
1	J	309	LEU	CA-CB-CG	5.86	128.78	115.30
1	I	284	HIS	CB-CA-C	-5.74	98.91	110.40
1	D	163	ARG	CG-CD-NE	5.73	123.84	111.80
1	D	286	ARG	C-N-CA	-5.71	107.44	121.70
1	E	178	LEU	CA-CB-CG	5.68	128.37	115.30
1	F	238	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	290	GLY	N-CA-C	-5.63	99.02	113.10
1	I	287	GLN	CA-CB-CG	5.58	125.67	113.40
1	D	296	LEU	CA-CB-CG	5.50	127.95	115.30
1	J	115	ASP	CB-CG-OD1	5.49	123.24	118.30
1	I	231	ARG	CA-C-N	-5.43	105.24	117.20
1	B	285	HIS	N-CA-C	5.43	125.66	111.00
1	I	231	ARG	N-CA-C	5.42	125.64	111.00
1	H	296	LEU	CA-CB-CG	5.36	127.62	115.30
1	J	253	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	I	232	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	J	308	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	298	GLN	CA-CB-CG	5.20	124.83	113.40
1	E	299	ARG	CG-CD-NE	5.16	122.64	111.80
1	F	286	ARG	CA-CB-CG	-5.11	102.16	113.40
1	I	295	LEU	CA-CB-CG	-5.10	103.57	115.30
1	E	179	SER	N-CA-C	-5.08	97.29	111.00
1	C	294	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	179	SER	N-CA-C	-5.04	97.40	111.00
1	B	294	ASP	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	VAL	Peptide
1	A	286	ARG	Peptide
1	B	177	HIS	Peptide
1	B	286	ARG	Peptide
1	B	288	ALA	Peptide
1	B	298	GLN	Peptide
1	C	286	ARG	Peptide
1	D	285	HIS	Peptide
1	E	181	VAL	Peptide
1	E	286	ARG	Peptide
1	F	177	HIS	Peptide
1	F	179	SER	Peptide
1	F	288	ALA	Peptide
1	G	178	LEU	Peptide
1	G	182	GLN	Peptide
1	I	153	ASP	Peptide
1	I	230	GLU	Peptide
1	I	286	ARG	Peptide
1	J	178	LEU	Peptide
1	J	182	GLN	Peptide
1	J	219	SER	Peptide
1	J	286	ARG	Peptide
1	J	308	PHE	Peptide

## 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	2497	0	2468	125	0
1	B	2497	0	2468	136	0
1	C	2497	0	2468	141	0
1	D	2497	0	2468	140	0
1	E	2497	0	2468	121	0
1	F	2497	0	2468	116	0
1	G	2497	0	2468	112	0
1	H	2497	0	2468	105	0
1	I	2497	0	2468	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2497	0	2468	140	0
All	All	24970	0	24680	1130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1130) 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:C:299:ARG:NH1	1:C:299:ARG:O	1.82	1.13
1:C:286:ARG:NH1	1:C:294:ASP:OD2	1.90	1.04
1:F:174:ARG:NH1	1:F:187:GLU:OE2	1.89	1.03
1:J:224:TRP:HE1	1:J:301:ARG:HG2	1.22	1.02
1:D:252:ILE:O	1:E:255:ARG:NH1	1.97	0.97
1:B:286:ARG:HG3	1:B:286:ARG:HH11	1.27	0.97
1:C:286:ARG:HH12	1:C:297:ILE:HD12	1.30	0.95
1:H:287:GLN:HB2	1:H:292:GLU:HB2	1.47	0.95
1:A:232:LEU:HD22	1:E:225:LEU:HD21	1.52	0.91
1:B:287:GLN:HG3	1:B:289:ASN:H	1.35	0.91
1:H:255:ARG:HG3	1:H:255:ARG:HH11	1.35	0.91
1:E:301:ARG:HG2	1:E:301:ARG:HH11	1.37	0.90
1:B:292:GLU:HG2	1:B:292:GLU:O	1.69	0.90
1:J:224:TRP:NE1	1:J:301:ARG:HG2	1.86	0.89
1:F:286:ARG:HH11	1:F:286:ARG:HG3	1.35	0.89
1:G:121:PHE:O	1:G:123:ARG:NH1	2.06	0.89
1:A:59:GLU:HG3	1:A:91:ARG:CZ	2.02	0.89
1:A:183:PRO:C	1:A:184:ASN:HD22	1.76	0.88
1:F:91:ARG:HH12	1:F:103:ASN:ND2	1.71	0.88
1:C:286:ARG:NH1	1:C:297:ILE:HD12	1.87	0.87
1:A:240:LEU:HD11	1:E:240:LEU:HD12	1.55	0.86
1:J:175:TYR:HB2	1:J:178:LEU:HD11	1.57	0.86
1:J:224:TRP:HE1	1:J:301:ARG:CG	1.88	0.86
1:A:181:VAL:HG13	1:A:185:GLN:HG3	1.57	0.85
1:F:76:LEU:HB3	1:F:130:LEU:HD21	1.56	0.85
1:D:286:ARG:HG3	1:D:286:ARG:O	1.74	0.85
1:J:287:GLN:HG3	1:J:289:ASN:H	1.39	0.84
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.57	0.84
1:B:298:GLN:HG3	1:B:299:ARG:N	1.92	0.83
1:A:231:ARG:HH22	1:A:298:GLN:HG2	1.44	0.83
1:J:288:ALA:H	1:J:289:ASN:HD22	1.27	0.83
1:C:223:PHE:O	1:C:301:ARG:NH1	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLU:OE2	1:C:229:SER:HB3	1.79	0.82
1:D:48:ARG:HG3	1:D:48:ARG:HH11	1.44	0.81
1:F:287:GLN:HB2	1:F:292:GLU:HB3	1.61	0.81
1:I:228:PHE:O	1:I:231:ARG:HB2	1.80	0.81
1:B:221:SER:HA	1:B:224:TRP:CZ3	2.17	0.80
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.62	0.80
1:I:159:GLU:HG3	1:I:160:TRP:CD1	2.17	0.80
1:B:286:ARG:HG3	1:B:286:ARG:NH1	1.85	0.79
1:A:219:SER:HA	1:A:238:LEU:HD23	1.64	0.79
1:C:122:ASP:HB3	1:C:124:GLN:HE22	1.48	0.79
1:B:167:SER:HB3	1:B:194:ARG:HB2	1.65	0.79
1:C:219:SER:HA	1:C:238:LEU:HD23	1.64	0.79
1:G:289:ASN:OD1	1:G:290:GLY:N	2.15	0.79
1:J:288:ALA:H	1:J:289:ASN:ND2	1.80	0.79
1:B:138:GLN:NE2	1:B:184:ASN:O	2.17	0.78
1:D:286:ARG:CZ	1:D:293:ASP:HA	2.14	0.78
1:B:163:ARG:HH11	1:B:163:ARG:HG2	1.50	0.77
1:D:250:SER:O	1:D:255:ARG:NH2	2.17	0.77
1:E:295:LEU:HA	1:E:298:GLN:HG2	1.66	0.77
1:C:63:ILE:HD13	1:C:90:LYS:HG3	1.66	0.76
1:G:219:SER:HA	1:G:238:LEU:HD23	1.66	0.76
1:C:251:ASN:HD21	1:D:251:ASN:HD22	1.34	0.76
1:I:238:LEU:HD21	1:J:236:PHE:CD2	2.21	0.76
1:A:99:ARG:HH21	1:B:180:SER:HB3	1.51	0.75
1:D:248:TYR:HE2	1:E:243:VAL:O	1.70	0.75
1:A:252:ILE:O	1:B:255:ARG:NH2	2.19	0.75
1:J:44:THR:HA	1:J:99:ARG:HA	1.67	0.75
1:G:287:GLN:OE1	1:G:289:ASN:N	2.20	0.75
1:J:287:GLN:CG	1:J:289:ASN:H	1.99	0.75
1:C:58:VAL:HG12	1:C:63:ILE:HG13	1.68	0.74
1:I:232:LEU:HA	1:I:235:SER:OG	1.86	0.74
1:B:299:ARG:C	1:B:301:ARG:H	1.87	0.74
1:C:63:ILE:HD13	1:C:90:LYS:NZ	2.01	0.74
1:G:294:ASP:C	1:G:296:LEU:H	1.91	0.74
1:C:179:SER:OG	1:C:180:SER:N	2.17	0.74
1:E:95:PHE:HB2	1:E:99:ARG:HB2	1.68	0.74
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.68	0.73
1:H:174:ARG:HG3	1:H:174:ARG:HH11	1.51	0.73
1:J:289:ASN:OD1	1:J:292:GLU:N	2.19	0.73
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.70	0.73
1:I:136:ASN:ND2	1:I:187:GLU:OE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:ARG:NH1	1:I:232:LEU:HD22	2.03	0.73
1:I:289:ASN:OD1	1:I:290:GLY:N	2.22	0.73
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.70	0.73
1:J:208:PHE:CE2	1:J:262:ILE:HG23	2.24	0.73
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.71	0.72
1:I:31:GLN:HE21	1:I:113:ASP:HA	1.51	0.72
1:A:223:PHE:O	1:A:301:ARG:NH2	2.21	0.72
1:E:223:PHE:C	1:E:301:ARG:HH12	1.92	0.72
1:D:287:GLN:NE2	1:D:289:ASN:OD1	2.22	0.72
1:G:248:TYR:HB2	1:H:247:SER:HB3	1.71	0.72
1:D:157:ILE:HD11	1:E:117:ARG:NH2	2.04	0.72
1:C:44:THR:HA	1:C:99:ARG:HA	1.71	0.72
1:H:287:GLN:HB2	1:H:292:GLU:CB	2.18	0.72
1:J:301:ARG:O	1:J:301:ARG:HD3	1.89	0.72
1:J:179:SER:OG	1:J:180:SER:N	2.20	0.71
1:C:90:LYS:HZ3	1:C:92:LEU:N	1.88	0.71
1:C:248:TYR:HB2	1:D:247:SER:HB3	1.70	0.71
1:A:59:GLU:HG3	1:A:91:ARG:NE	2.04	0.71
1:F:44:THR:HA	1:F:99:ARG:HA	1.72	0.71
1:H:219:SER:HA	1:H:238:LEU:HD22	1.71	0.71
1:I:314:VAL:O	1:I:317:ILE:HG22	1.90	0.71
1:H:248:TYR:HB2	1:I:247:SER:HB3	1.72	0.71
1:D:44:THR:HA	1:D:99:ARG:HA	1.72	0.71
1:A:174:ARG:HG2	1:A:187:GLU:HG2	1.70	0.71
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.72	0.71
1:G:87:THR:HG21	1:G:90:LYS:HE2	1.72	0.71
1:D:31:GLN:HE21	1:D:114:MET:H	1.39	0.70
1:J:174:ARG:HB2	1:J:187:GLU:HG2	1.72	0.70
1:D:289:ASN:CG	1:D:290:GLY:H	1.94	0.70
1:F:208:PHE:HE2	1:F:249:THR:HA	1.55	0.70
1:C:122:ASP:HB3	1:C:124:GLN:NE2	2.06	0.70
1:E:296:LEU:HA	1:E:299:ARG:HD2	1.74	0.70
1:J:289:ASN:CG	1:J:292:GLU:H	1.95	0.70
1:D:289:ASN:OD1	1:D:292:GLU:HG2	1.91	0.69
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.72	0.69
1:F:236:PHE:CD2	1:J:238:LEU:HD11	2.28	0.69
1:C:169:HIS:CE1	1:C:171:SER:HB3	2.27	0.69
1:D:64:GLU:O	1:D:68:ASN:ND2	2.25	0.69
1:F:91:ARG:HH12	1:F:103:ASN:HD22	1.39	0.69
1:A:61:THR:HG21	1:B:64:GLU:OE2	1.93	0.69
1:H:293:ASP:OD2	1:H:298:GLN:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:O	1:D:287:GLN:NE2	2.25	0.68
1:H:286:ARG:O	1:H:287:GLN:HB3	1.92	0.68
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.75	0.68
1:G:27:ASN:HB3	1:G:32:THR:HB	1.72	0.68
1:F:286:ARG:NH1	1:F:286:ARG:HG3	2.05	0.68
1:H:287:GLN:CD	1:H:292:GLU:H	1.96	0.68
1:A:111:SER:OG	1:E:22:LYS:NZ	2.27	0.68
1:G:212:LEU:O	1:G:216:ILE:HG12	1.93	0.68
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.23	0.68
1:J:253:LEU:HD21	1:J:262:ILE:HG21	1.76	0.68
1:A:182:GLN:N	1:A:182:GLN:OE1	2.26	0.68
1:H:225:LEU:HD22	1:H:230:GLU:CD	2.13	0.67
1:I:178:LEU:HD23	1:I:186:ASN:HB3	1.76	0.67
1:G:294:ASP:HB3	1:G:296:LEU:HG	1.76	0.67
1:I:299:ARG:C	1:I:301:ARG:H	1.97	0.67
1:C:223:PHE:C	1:C:301:ARG:HH12	1.97	0.67
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.76	0.67
1:I:44:THR:HA	1:I:99:ARG:HA	1.76	0.67
1:J:301:ARG:O	1:J:305:PRO:HG2	1.94	0.67
1:B:221:SER:HA	1:B:224:TRP:CE3	2.29	0.67
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.75	0.67
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.76	0.67
1:D:287:GLN:HG3	1:D:289:ASN:H	1.57	0.67
1:G:226:GLU:O	1:G:231:ARG:NH1	2.27	0.67
1:J:221:SER:HA	1:J:301:ARG:NH2	2.10	0.67
1:C:151:ASN:OD1	1:C:152:ALA:N	2.28	0.67
1:J:169:HIS:NE2	1:J:171:SER:HB3	2.09	0.67
1:I:219:SER:HA	1:I:238:LEU:HD13	1.77	0.67
1:I:264:GLN:HA	1:I:267:ILE:HG12	1.77	0.67
1:I:291:VAL:O	1:I:293:ASP:N	2.26	0.67
1:I:148:TYR:CE1	1:J:177:HIS:ND1	2.62	0.67
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.77	0.66
1:H:316:VAL:HG23	1:H:317:ILE:HD12	1.75	0.66
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.78	0.66
1:J:282:PHE:CZ	1:J:286:ARG:HD3	2.31	0.66
1:C:229:SER:O	1:C:233:GLN:HG2	1.95	0.66
1:E:295:LEU:O	1:E:299:ARG:HD2	1.96	0.66
1:F:287:GLN:HG2	1:F:289:ASN:H	1.59	0.66
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.76	0.66
1:C:63:ILE:HD13	1:C:90:LYS:HZ2	1.62	0.65
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:287:GLN:HE22	1:I:290:GLY:N	1.93	0.65
1:A:299:ARG:C	1:A:301:ARG:H	1.98	0.65
1:F:212:LEU:O	1:F:216:ILE:HG12	1.96	0.65
1:E:289:ASN:OD1	1:E:290:GLY:N	2.30	0.65
1:J:208:PHE:CZ	1:J:262:ILE:HG23	2.32	0.65
1:G:27:ASN:OD1	1:G:255:ARG:NH1	2.26	0.65
1:H:241:THR:HA	1:I:240:LEU:HD23	1.78	0.65
1:F:68:ASN:OD1	1:J:62:GLN:NE2	2.28	0.65
1:I:299:ARG:O	1:I:299:ARG:HG3	1.96	0.65
1:J:305:PRO:O	1:J:308:PHE:N	2.19	0.65
1:C:153:ASP:OD2	1:C:154:ASN:ND2	2.30	0.65
1:F:295:LEU:HA	1:F:298:GLN:HB2	1.79	0.64
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.12	0.64
1:C:294:ASP:OD1	1:C:294:ASP:N	2.28	0.64
1:E:299:ARG:C	1:E:301:ARG:H	2.00	0.64
1:D:65:ARG:NH1	1:E:68:ASN:O	2.30	0.64
1:J:176:ASP:HB2	1:J:177:HIS:CD2	2.33	0.64
1:J:221:SER:HA	1:J:301:ARG:HH22	1.62	0.64
1:D:211:PRO:O	1:D:215:ILE:HG12	1.98	0.64
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.78	0.64
1:B:54:LYS:H	1:B:54:LYS:HD2	1.63	0.64
1:D:286:ARG:HH12	1:D:298:GLN:HE21	1.45	0.64
1:G:219:SER:HA	1:G:238:LEU:CD2	2.27	0.63
1:H:235:SER:HA	1:H:238:LEU:HD12	1.80	0.63
1:H:38:TYR:CZ	1:H:105:ARG:HD2	2.33	0.63
1:I:231:ARG:CZ	1:I:232:LEU:HD13	2.28	0.63
1:C:63:ILE:CD1	1:C:90:LYS:NZ	2.60	0.63
1:C:251:ASN:ND2	1:D:251:ASN:HD22	1.96	0.63
1:H:167:SER:HB2	1:H:194:ARG:HB2	1.79	0.63
1:D:123:ARG:HH21	1:D:198:VAL:HG22	1.63	0.63
1:F:11:PRO:CA	1:F:141:ARG:HH12	2.11	0.63
1:F:11:PRO:CB	1:F:141:ARG:HH12	2.10	0.63
1:C:63:ILE:HG12	1:C:90:LYS:HZ1	1.64	0.63
1:C:90:LYS:HD2	1:C:91:ARG:N	2.14	0.63
1:B:241:THR:HA	1:C:240:LEU:HD23	1.80	0.63
1:A:184:ASN:N	1:A:184:ASN:HD22	1.95	0.63
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.81	0.63
1:D:212:LEU:O	1:D:216:ILE:HG12	1.99	0.63
1:A:19:PHE:CZ	1:B:178:LEU:HD11	2.33	0.63
1:H:44:THR:HA	1:H:99:ARG:HA	1.79	0.63
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:SER:OG	1:G:180:SER:N	2.29	0.63
1:D:248:TYR:OH	1:E:244:ALA:HA	1.99	0.62
1:F:91:ARG:NH1	1:F:103:ASN:HB3	2.13	0.62
1:J:123:ARG:HG3	1:J:198:VAL:HG22	1.79	0.62
1:B:298:GLN:HG3	1:B:299:ARG:CB	2.29	0.62
1:A:287:GLN:HG3	1:A:289:ASN:H	1.64	0.62
1:F:240:LEU:HD23	1:J:241:THR:HA	1.80	0.62
1:C:90:LYS:HD2	1:C:91:ARG:H	1.64	0.62
1:J:149:THR:O	1:J:151:ASN:N	2.31	0.62
1:B:177:HIS:CD2	1:B:178:LEU:HA	2.35	0.62
1:E:42:GLN:HB2	1:E:101:ILE:HG12	1.80	0.62
1:A:212:LEU:O	1:A:216:ILE:HG12	1.99	0.62
1:C:299:ARG:HH11	1:C:299:ARG:C	2.02	0.62
1:D:248:TYR:CE2	1:E:243:VAL:O	2.52	0.62
1:F:287:GLN:HG3	1:F:290:GLY:H	1.65	0.62
1:C:54:LYS:HD2	1:C:55:PRO:HD2	1.82	0.62
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.81	0.62
1:A:165:LYS:O	1:A:165:LYS:HG3	2.00	0.62
1:F:248:TYR:CD1	1:G:247:SER:HA	2.35	0.62
1:B:24:TYR:CE2	1:B:34:LYS:HD3	2.33	0.61
1:I:301:ARG:O	1:I:305:PRO:HG2	2.00	0.61
1:A:178:LEU:HB2	1:A:179:SER:O	1.99	0.61
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.82	0.61
1:C:311:ILE:O	1:C:314:VAL:HG22	2.00	0.61
1:J:24:TYR:CE2	1:J:34:LYS:HD3	2.35	0.61
1:G:293:ASP:O	1:G:295:LEU:N	2.34	0.61
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.82	0.61
1:I:286:ARG:O	1:I:292:GLU:HB3	1.99	0.61
1:D:286:ARG:NH2	1:D:293:ASP:OD1	2.33	0.61
1:F:252:ILE:HD11	1:G:250:SER:HB3	1.81	0.61
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.35	0.61
1:J:289:ASN:CG	1:J:290:GLY:H	2.02	0.61
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.36	0.61
1:C:169:HIS:ND1	1:C:171:SER:HB3	2.16	0.61
1:F:236:PHE:HD2	1:J:238:LEU:HD11	1.64	0.61
1:A:61:THR:HG21	1:B:64:GLU:CD	2.21	0.61
1:C:295:LEU:HA	1:C:298:GLN:HG2	1.81	0.61
1:A:95:PHE:HB2	1:A:99:ARG:HB3	1.81	0.61
1:C:289:ASN:OD1	1:C:290:GLY:N	2.27	0.61
1:I:216:ILE:O	1:I:219:SER:HB3	2.01	0.61
1:A:174:ARG:HD3	1:A:187:GLU:OE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH1	1:B:134:SER:HB2	2.16	0.60
1:E:225:LEU:HD13	1:E:230:GLU:HG2	1.83	0.60
1:E:208:PHE:O	1:E:245:TYR:OH	2.18	0.60
1:G:260:THR:H	1:G:263:ASP:HB2	1.64	0.60
1:I:289:ASN:OD1	1:I:291:VAL:N	2.32	0.60
1:I:295:LEU:CD2	1:I:298:GLN:HB2	2.32	0.60
1:C:90:LYS:HD3	1:C:102:TYR:CE1	2.36	0.60
1:E:301:ARG:HG2	1:E:301:ARG:NH1	2.12	0.60
1:B:76:LEU:HB3	1:B:130:LEU:HD21	1.82	0.60
1:I:178:LEU:CD2	1:I:186:ASN:HB3	2.31	0.60
1:J:232:LEU:HD23	1:J:236:PHE:HE1	1.66	0.60
1:B:208:PHE:HE2	1:B:249:THR:HA	1.67	0.60
1:C:241:THR:HA	1:D:240:LEU:HD23	1.82	0.60
1:B:153:ASP:CG	1:B:154:ASN:H	2.05	0.60
1:E:228:PHE:HA	1:E:231:ARG:HG3	1.83	0.60
1:J:23:ILE:HG12	1:J:35:VAL:HG22	1.83	0.60
1:C:63:ILE:HG21	1:C:90:LYS:HE3	1.83	0.60
1:I:204:TYR:O	1:I:209:ILE:HG12	2.02	0.60
1:B:149:THR:O	1:B:151:ASN:N	2.34	0.59
1:C:298:GLN:HG3	1:C:299:ARG:N	2.17	0.59
1:J:219:SER:HA	1:J:238:LEU:HD21	1.84	0.59
1:B:224:TRP:CD2	1:B:301:ARG:HD3	2.37	0.59
1:C:224:TRP:HA	1:C:301:ARG:NH1	2.17	0.59
1:G:127:VAL:HG22	1:G:194:ARG:HG2	1.83	0.59
1:I:159:GLU:HG3	1:I:160:TRP:HD1	1.67	0.59
1:C:124:GLN:OE1	1:C:124:GLN:N	2.34	0.59
1:G:288:ALA:N	1:G:292:GLU:OE2	2.30	0.59
1:I:155:GLU:HG2	1:I:161:TRP:CD1	2.37	0.59
1:J:291:VAL:O	1:J:293:ASP:N	2.35	0.59
1:B:127:VAL:HG22	1:B:194:ARG:HG2	1.84	0.59
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.84	0.59
1:I:260:THR:O	1:I:264:GLN:HG2	2.03	0.59
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.84	0.59
1:B:287:GLN:HG3	1:B:289:ASN:N	2.13	0.59
1:E:296:LEU:HA	1:E:299:ARG:CD	2.32	0.59
1:I:137:ASN:HA	1:I:140:LEU:O	2.03	0.59
1:F:11:PRO:C	1:F:141:ARG:HH12	2.06	0.59
1:D:123:ARG:NH2	1:D:198:VAL:HG22	2.16	0.59
1:J:220:TRP:CZ2	1:J:301:ARG:NH1	2.71	0.59
1:A:227:SER:O	1:A:231:ARG:HD2	2.03	0.59
1:A:300:CYS:HG	1:A:304:PHE:HE2	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HG12	1:G:183:PRO:HD2	1.83	0.59
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.83	0.59
1:B:296:LEU:HD23	1:B:298:GLN:HE22	1.68	0.58
1:D:31:GLN:HE21	1:D:113:ASP:HA	1.66	0.58
1:A:247:SER:HB3	1:E:248:TYR:HB2	1.83	0.58
1:F:287:GLN:HG2	1:F:289:ASN:N	2.17	0.58
1:J:228:PHE:HA	1:J:231:ARG:CZ	2.34	0.58
1:I:240:LEU:HD13	1:J:240:LEU:HD11	1.86	0.58
1:C:211:PRO:O	1:C:215:ILE:HG12	2.03	0.58
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.39	0.58
1:C:90:LYS:HD3	1:C:102:TYR:CZ	2.38	0.58
1:F:112:ASN:ND2	1:F:125:GLN:O	2.37	0.58
1:H:53:ASP:O	1:H:96:PRO:HG3	2.03	0.58
1:D:216:ILE:O	1:D:219:SER:HB3	2.04	0.58
1:D:248:TYR:N	1:D:248:TYR:HD1	2.00	0.58
1:G:314:VAL:O	1:G:317:ILE:HG12	2.04	0.58
1:H:33:TYR:OH	1:H:127:VAL:N	2.26	0.58
1:J:289:ASN:ND2	1:J:292:GLU:OE1	2.37	0.58
1:A:183:PRO:C	1:A:184:ASN:ND2	2.52	0.58
1:B:54:LYS:N	1:B:54:LYS:HD2	2.19	0.58
1:F:272:SER:HG	1:F:304:PHE:HZ	1.52	0.58
1:G:211:PRO:O	1:G:215:ILE:HG12	2.04	0.58
1:A:241:THR:HA	1:B:240:LEU:HD23	1.85	0.58
1:E:183:PRO:HD2	1:E:184:ASN:H	1.68	0.58
1:F:169:HIS:NE2	1:F:171:SER:HB3	2.19	0.58
1:A:142:PHE:HB3	1:A:170:ILE:HD13	1.85	0.57
1:D:123:ARG:HE	1:D:198:VAL:HG22	1.69	0.57
1:H:200:ASN:ND2	1:I:258:TYR:HE1	2.02	0.57
1:A:289:ASN:OD1	1:A:290:GLY:N	2.31	0.57
1:C:251:ASN:HD21	1:D:251:ASN:ND2	2.01	0.57
1:D:46:LYS:N	1:D:46:LYS:HD2	2.18	0.57
1:D:123:ARG:HH21	1:D:198:VAL:CG2	2.17	0.57
1:E:174:ARG:HA	1:E:186:ASN:O	2.04	0.57
1:C:208:PHE:O	1:C:245:TYR:OH	2.21	0.57
1:E:301:ARG:HH11	1:E:301:ARG:CG	2.14	0.57
1:G:204:TYR:O	1:G:209:ILE:HG12	2.04	0.57
1:H:157:ILE:C	1:I:258:TYR:OH	2.43	0.57
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.86	0.57
1:B:212:LEU:O	1:B:216:ILE:HG12	2.03	0.57
1:D:31:GLN:NE2	1:D:114:MET:H	2.03	0.57
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:CD1	1:C:90:LYS:HZ2	2.17	0.57
1:F:64:GLU:O	1:F:64:GLU:HG3	2.05	0.57
1:C:223:PHE:C	1:C:301:ARG:NH1	2.58	0.57
1:D:284:HIS:HA	1:D:286:ARG:CZ	2.35	0.57
1:H:176:ASP:OD1	1:H:177:HIS:N	2.38	0.57
1:A:224:TRP:HA	1:A:301:ARG:HH21	1.69	0.56
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.40	0.56
1:A:231:ARG:NH2	1:A:298:GLN:HG2	2.19	0.56
1:F:263:ASP:O	1:F:267:ILE:HG12	2.06	0.56
1:I:228:PHE:CE1	1:I:284:HIS:HB2	2.41	0.56
1:J:301:ARG:HD3	1:J:302:LEU:HD23	1.88	0.56
1:C:90:LYS:NZ	1:C:92:LEU:HG	2.20	0.56
1:G:299:ARG:C	1:G:301:ARG:H	2.06	0.56
1:A:295:LEU:HA	1:A:298:GLN:HG3	1.87	0.56
1:A:181:VAL:O	1:A:185:GLN:NE2	2.38	0.56
1:I:212:LEU:O	1:I:216:ILE:HG12	2.05	0.56
1:D:123:ARG:NE	1:D:198:VAL:HG22	2.21	0.56
1:I:257:PRO:HG2	1:I:258:TYR:CZ	2.41	0.56
1:C:149:THR:O	1:C:151:ASN:N	2.39	0.56
1:D:274:PHE:O	1:D:278:LEU:HD13	2.06	0.56
1:E:17:SER:HB2	1:E:40:VAL:HB	1.88	0.56
1:H:122:ASP:OD2	1:H:199:ARG:NE	2.33	0.56
1:A:148:TYR:HH	1:B:177:HIS:CE1	2.23	0.56
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.87	0.56
1:I:228:PHE:CZ	1:I:284:HIS:CD2	2.94	0.56
1:J:204:TYR:O	1:J:209:ILE:HG12	2.06	0.56
1:A:228:PHE:HA	1:A:231:ARG:HD3	1.87	0.56
1:C:212:LEU:O	1:C:216:ILE:HG12	2.06	0.56
1:D:263:ASP:O	1:D:267:ILE:HG12	2.05	0.56
1:F:251:ASN:HD22	1:J:251:ASN:ND2	2.04	0.56
1:G:294:ASP:C	1:G:296:LEU:N	2.58	0.56
1:H:216:ILE:O	1:H:219:SER:HB3	2.05	0.56
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.37	0.56
1:D:248:TYR:N	1:D:248:TYR:CD1	2.73	0.56
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.87	0.55
1:G:150:GLU:HG3	1:G:150:GLU:O	2.07	0.55
1:G:36:ASP:OD2	1:G:105:ARG:NH2	2.34	0.55
1:B:181:VAL:HG23	1:B:183:PRO:HD2	1.87	0.55
1:E:223:PHE:C	1:E:301:ARG:NH1	2.60	0.55
1:J:289:ASN:OD1	1:J:291:VAL:N	2.40	0.55
1:A:181:VAL:CG1	1:A:185:GLN:HG3	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:O	1:A:219:SER:HB3	2.07	0.55
1:A:148:TYR:OH	1:B:177:HIS:CE1	2.59	0.55
1:I:181:VAL:HG22	1:I:183:PRO:HD2	1.88	0.55
1:J:208:PHE:CE1	1:J:245:TYR:HE2	2.25	0.55
1:E:224:TRP:HA	1:E:301:ARG:NH1	2.21	0.55
1:G:91:ARG:HB3	1:G:103:ASN:HB3	1.89	0.55
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.88	0.55
1:B:298:GLN:HG3	1:B:299:ARG:HB2	1.88	0.55
1:B:71:LEU:HD22	1:B:73:VAL:HG22	1.89	0.55
1:J:279:LEU:HD11	1:J:304:PHE:CZ	2.42	0.55
1:A:19:PHE:CE1	1:B:178:LEU:HD11	2.42	0.55
1:B:44:THR:HA	1:B:99:ARG:HA	1.88	0.55
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.88	0.55
1:H:125:GLN:OE1	1:H:194:ARG:HD3	2.07	0.55
1:H:212:LEU:O	1:H:216:ILE:HG12	2.07	0.55
1:I:231:ARG:HH12	1:I:232:LEU:HD22	1.69	0.55
1:A:28:THR:HB	1:A:256:LEU:HD21	1.88	0.55
1:B:163:ARG:NH1	1:B:163:ARG:HG2	2.15	0.55
1:H:181:VAL:HG21	1:H:185:GLN:HB2	1.88	0.55
1:D:284:HIS:C	1:D:286:ARG:HG2	2.27	0.55
1:E:247:SER:HA	1:E:250:SER:HB2	1.88	0.55
1:E:247:SER:OG	1:E:248:TYR:N	2.39	0.55
1:J:279:LEU:HD11	1:J:304:PHE:CE2	2.41	0.55
1:D:286:ARG:NH1	1:D:298:GLN:HE21	2.04	0.54
1:H:255:ARG:HG3	1:H:255:ARG:NH1	2.13	0.54
1:I:286:ARG:HD3	1:I:287:GLN:H	1.72	0.54
1:D:174:ARG:NH1	1:D:187:GLU:OE2	2.40	0.54
1:E:212:LEU:O	1:E:216:ILE:HG12	2.06	0.54
1:J:28:THR:HB	1:J:256:LEU:HD21	1.88	0.54
1:D:174:ARG:CZ	1:D:187:GLU:HG2	2.36	0.54
1:E:263:ASP:O	1:E:267:ILE:HG12	2.08	0.54
1:G:136:ASN:HD21	1:G:185:GLN:HG3	1.72	0.54
1:H:180:SER:OG	1:H:180:SER:O	2.21	0.54
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.88	0.54
1:D:229:SER:O	1:D:233:GLN:HB2	2.07	0.54
1:J:231:ARG:NH2	1:J:298:GLN:HE22	2.05	0.54
1:B:81:VAL:HG21	1:B:85:PRO:HG3	1.89	0.54
1:G:289:ASN:HD21	1:G:292:GLU:HB3	1.71	0.54
1:J:179:SER:OG	1:J:181:VAL:N	2.39	0.54
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.89	0.54
1:D:183:PRO:HB2	1:D:185:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:HA	1:D:286:ARG:NE	2.22	0.54
1:F:178:LEU:HD11	1:F:181:VAL:O	2.08	0.54
1:I:122:ASP:N	1:I:122:ASP:OD1	2.41	0.54
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.42	0.54
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.88	0.54
1:I:295:LEU:HD22	1:I:298:GLN:HB2	1.90	0.54
1:I:53:ASP:O	1:I:96:PRO:HG3	2.08	0.54
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.89	0.54
1:D:286:ARG:HD2	1:D:292:GLU:C	2.28	0.53
1:E:178:LEU:HD21	1:E:185:GLN:O	2.08	0.53
1:E:174:ARG:HH12	1:E:187:GLU:CD	2.11	0.53
1:G:295:LEU:HA	1:G:298:GLN:HB2	1.91	0.53
1:G:305:PRO:O	1:G:309:LEU:HG	2.08	0.53
1:A:150:GLU:O	1:A:150:GLU:HG3	2.08	0.53
1:D:123:ARG:HG2	1:D:197:ALA:O	2.08	0.53
1:D:286:ARG:NH1	1:D:293:ASP:HA	2.24	0.53
1:H:174:ARG:HA	1:H:186:ASN:O	2.08	0.53
1:B:156:GLU:HG3	1:C:117:ARG:HH22	1.71	0.53
1:D:224:TRP:HD1	1:E:285:HIS:CD2	2.27	0.53
1:F:228:PHE:HA	1:F:231:ARG:NH1	2.22	0.53
1:F:78:PHE:HB3	1:F:81:VAL:HB	1.89	0.53
1:B:298:GLN:CG	1:B:299:ARG:N	2.69	0.53
1:D:176:ASP:HB2	1:D:177:HIS:CD2	2.44	0.53
1:D:181:VAL:HG21	1:D:185:GLN:O	2.09	0.53
1:I:228:PHE:CZ	1:I:231:ARG:NE	2.76	0.53
1:B:58:VAL:HG13	1:B:62:GLN:HB2	1.90	0.53
1:C:292:GLU:HG3	1:C:292:GLU:O	2.09	0.53
1:D:48:ARG:CG	1:D:48:ARG:HH11	2.17	0.53
1:I:228:PHE:CE1	1:I:231:ARG:NE	2.77	0.53
1:C:301:ARG:HH11	1:C:301:ARG:HG2	1.74	0.53
1:C:90:LYS:NZ	1:C:92:LEU:N	2.56	0.53
1:D:135:TYR:HD2	1:D:139:GLN:OE1	1.92	0.53
1:E:178:LEU:HB3	1:E:179:SER:O	2.08	0.53
1:E:66:TRP:CE3	1:E:71:LEU:HD12	2.44	0.53
1:G:241:THR:HA	1:H:240:LEU:HD23	1.89	0.53
1:J:224:TRP:CE2	1:J:301:ARG:HG2	2.44	0.53
1:A:293:ASP:HB2	1:A:295:LEU:HD12	1.91	0.53
1:D:27:ASN:HB3	1:D:32:THR:HB	1.91	0.53
1:I:228:PHE:CE2	1:I:284:HIS:CD2	2.97	0.53
1:I:47:PRO:HG3	1:I:97:ASP:O	2.09	0.53
1:J:174:ARG:HA	1:J:186:ASN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HA	1:A:238:LEU:CD2	2.37	0.52
1:C:18:ILE:HB	1:C:147:VAL:HG22	1.90	0.52
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.45	0.52
1:A:182:GLN:CD	1:A:183:PRO:HD3	2.30	0.52
1:B:114:MET:HA	1:B:124:GLN:HE22	1.74	0.52
1:B:153:ASP:OD1	1:B:154:ASN:N	2.33	0.52
1:G:136:ASN:ND2	1:G:185:GLN:HA	2.25	0.52
1:A:71:LEU:HD22	1:A:73:VAL:HG23	1.91	0.52
1:H:156:GLU:N	1:H:156:GLU:OE1	2.25	0.52
1:E:246:ALA:O	1:E:250:SER:N	2.40	0.52
1:G:294:ASP:O	1:G:296:LEU:N	2.43	0.52
1:A:263:ASP:O	1:A:267:ILE:HG12	2.09	0.52
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.44	0.52
1:A:62:GLN:NE2	1:B:67:ILE:HG22	2.25	0.52
1:C:301:ARG:O	1:C:305:PRO:HG2	2.10	0.52
1:E:117:ARG:O	1:E:260:THR:HA	2.09	0.52
1:J:299:ARG:C	1:J:301:ARG:H	2.13	0.52
1:B:301:ARG:NH1	1:B:302:LEU:HD12	2.24	0.52
1:D:144:ASP:OD2	1:D:146:GLN:NE2	2.43	0.52
1:A:284:HIS:HE1	1:E:226:GLU:OE2	1.93	0.52
1:J:153:ASP:OD1	1:J:154:ASN:N	2.33	0.52
1:A:91:ARG:NH1	1:B:134:SER:CB	2.73	0.52
1:C:63:ILE:CG1	1:C:90:LYS:HZ1	2.23	0.52
1:G:149:THR:HB	1:G:151:ASN:ND2	2.24	0.52
1:B:295:LEU:O	1:B:296:LEU:HG	2.10	0.52
1:B:272:SER:HG	1:B:304:PHE:HZ	1.58	0.52
1:H:122:ASP:HB3	1:H:124:GLN:HE21	1.75	0.52
1:H:225:LEU:HD22	1:H:230:GLU:OE2	2.10	0.52
1:E:246:ALA:O	1:E:249:THR:HB	2.09	0.52
1:D:241:THR:HA	1:E:240:LEU:HD23	1.91	0.51
1:F:289:ASN:HB2	1:F:292:GLU:HB2	1.92	0.51
1:E:211:PRO:O	1:E:215:ILE:HG12	2.09	0.51
1:D:62:GLN:HE21	1:E:67:ILE:HG22	1.75	0.51
1:H:287:GLN:NE2	1:H:290:GLY:C	2.64	0.51
1:I:95:PHE:HB2	1:I:99:ARG:HG2	1.92	0.51
1:A:185:GLN:N	1:A:185:GLN:OE1	2.40	0.51
1:A:208:PHE:O	1:A:245:TYR:OH	2.27	0.51
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.09	0.51
1:F:122:ASP:N	1:F:122:ASP:OD1	2.43	0.51
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.92	0.51
1:F:181:VAL:HG23	1:F:183:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:314:VAL:O	1:J:317:ILE:HG22	2.10	0.51
1:D:295:LEU:HD12	1:D:295:LEU:H	1.75	0.51
1:F:224:TRP:CD1	1:F:301:ARG:NH1	2.78	0.51
1:H:89:ASN:O	1:H:104:ALA:HA	2.11	0.51
1:J:212:LEU:O	1:J:216:ILE:HG12	2.11	0.51
1:B:48:ARG:O	1:B:96:PRO:HA	2.11	0.51
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.92	0.51
1:F:211:PRO:O	1:F:215:ILE:HG12	2.11	0.51
1:G:29:LEU:HD13	1:G:257:PRO:HD3	1.93	0.51
1:J:219:SER:HA	1:J:238:LEU:CD2	2.41	0.51
1:G:216:ILE:O	1:G:219:SER:HB3	2.11	0.51
1:J:311:ILE:O	1:J:314:VAL:HG22	2.11	0.51
1:A:149:THR:O	1:A:151:ASN:N	2.43	0.51
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.45	0.51
1:B:271:GLY:O	1:B:275:ALA:N	2.41	0.51
1:C:284:HIS:HD2	1:C:285:HIS:NE2	2.08	0.51
1:C:219:SER:HA	1:C:238:LEU:CD2	2.37	0.50
1:G:149:THR:O	1:G:151:ASN:N	2.43	0.50
1:G:65:ARG:HA	1:G:68:ASN:HD22	1.74	0.50
1:A:38:TYR:CZ	1:A:105:ARG:HD2	2.47	0.50
1:A:91:ARG:CD	1:B:134:SER:OG	2.60	0.50
1:F:28:THR:HB	1:F:256:LEU:HD21	1.93	0.50
1:G:54:LYS:HB3	1:G:55:PRO:HD2	1.93	0.50
1:I:66:TRP:HB3	1:I:71:LEU:HD13	1.94	0.50
1:B:296:LEU:HD23	1:B:298:GLN:NE2	2.25	0.50
1:H:225:LEU:HB3	1:H:230:GLU:HG2	1.93	0.50
1:J:153:ASP:CG	1:J:154:ASN:H	2.11	0.50
1:C:284:HIS:HD2	1:C:285:HIS:CD2	2.29	0.50
1:E:50:THR:HB	1:E:56:LEU:HB2	1.93	0.50
1:F:248:TYR:HD1	1:G:247:SER:HA	1.75	0.50
1:C:272:SER:HG	1:C:304:PHE:HZ	1.56	0.50
1:D:286:ARG:HD2	1:D:292:GLU:O	2.11	0.50
1:D:289:ASN:CG	1:D:290:GLY:N	2.63	0.50
1:C:129:GLU:HA	1:C:191:ILE:O	2.11	0.50
1:C:287:GLN:HG2	1:C:289:ASN:H	1.77	0.50
1:E:115:ASP:OD1	1:E:117:ARG:HG3	2.12	0.50
1:E:301:ARG:O	1:E:305:PRO:HG2	2.11	0.50
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.93	0.50
1:G:146:GLN:OE1	1:G:148:TYR:OH	2.30	0.50
1:A:155:GLU:OE2	1:A:161:TRP:HB3	2.11	0.50
1:B:173:ILE:HG12	1:B:190:ARG:CZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.46	0.50
1:H:174:ARG:HG3	1:H:174:ARG:NH1	2.24	0.50
1:H:299:ARG:HD3	1:H:299:ARG:O	2.11	0.50
1:A:229:SER:HA	1:E:230:GLU:OE2	2.12	0.50
1:C:264:GLN:HA	1:C:267:ILE:HG12	1.92	0.50
1:H:138:GLN:HA	1:H:141:ARG:CZ	2.42	0.50
1:H:287:GLN:CD	1:H:290:GLY:H	2.15	0.50
1:A:175:TYR:O	1:A:178:LEU:HD21	2.11	0.49
1:F:76:LEU:HB3	1:F:130:LEU:CD2	2.35	0.49
1:J:227:SER:HB3	1:J:230:GLU:HG3	1.94	0.49
1:C:167:SER:HB2	1:C:194:ARG:HB2	1.94	0.49
1:F:183:PRO:O	1:F:184:ASN:HB2	2.12	0.49
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.48	0.49
1:A:183:PRO:O	1:A:184:ASN:ND2	2.45	0.49
1:C:216:ILE:O	1:C:219:SER:HB3	2.11	0.49
1:D:205:LEU:O	1:D:209:ILE:HB	2.12	0.49
1:F:216:ILE:O	1:F:219:SER:HB3	2.12	0.49
1:G:155:GLU:HB3	1:G:161:TRP:NE1	2.26	0.49
1:D:289:ASN:CG	1:D:292:GLU:HG2	2.32	0.49
1:B:146:GLN:N	1:B:146:GLN:OE1	2.45	0.49
1:D:307:GLY:O	1:D:311:ILE:HD12	2.12	0.49
1:E:112:ASN:OD1	1:E:113:ASP:N	2.46	0.49
1:I:264:GLN:HA	1:I:267:ILE:CG1	2.42	0.49
1:J:311:ILE:HA	1:J:314:VAL:HG13	1.95	0.49
1:A:294:ASP:O	1:A:298:GLN:HG3	2.12	0.49
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.94	0.49
1:J:287:GLN:HG3	1:J:289:ASN:N	2.18	0.49
1:C:122:ASP:CG	1:C:199:ARG:HE	2.15	0.49
1:D:185:GLN:N	1:D:185:GLN:OE1	2.44	0.49
1:D:48:ARG:HG3	1:D:48:ARG:NH1	2.21	0.49
1:B:298:GLN:HG3	1:B:299:ARG:CA	2.43	0.49
1:D:290:GLY:O	1:D:291:VAL:HG13	2.12	0.49
1:H:26:VAL:HG22	1:H:33:TYR:HB3	1.95	0.49
1:B:246:ALA:O	1:B:250:SER:OG	2.30	0.49
1:B:297:ILE:O	1:B:299:ARG:N	2.46	0.49
1:D:123:ARG:CZ	1:D:198:VAL:HG22	2.43	0.49
1:G:76:LEU:HB3	1:G:130:LEU:HD21	1.94	0.49
1:A:302:LEU:C	1:A:305:PRO:HD2	2.34	0.49
1:A:57:ILE:HG22	1:A:91:ARG:NH2	2.27	0.49
1:C:33:TYR:CE2	1:C:110:PHE:HB2	2.48	0.49
1:G:282:PHE:O	1:G:286:ARG:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:TYR:CE1	1:J:250:SER:HB2	2.48	0.49
1:J:151:ASN:OD1	1:J:152:ALA:N	2.46	0.49
1:J:220:TRP:CE2	1:J:301:ARG:CZ	2.96	0.49
1:B:238:LEU:HD21	1:C:236:PHE:CE2	2.48	0.48
1:F:262:ILE:O	1:F:266:ILE:HG12	2.13	0.48
1:D:145:ILE:HD12	1:D:191:ILE:HG21	1.94	0.48
1:G:165:LYS:HG3	1:G:165:LYS:O	2.12	0.48
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.43	0.48
1:J:176:ASP:C	1:J:177:HIS:HD2	2.16	0.48
1:J:220:TRP:CE3	1:J:221:SER:HB3	2.48	0.48
1:B:287:GLN:HB2	1:B:292:GLU:OE1	2.13	0.48
1:D:227:SER:HB3	1:D:230:GLU:HG2	1.96	0.48
1:E:13:ASP:OD2	1:E:141:ARG:HD3	2.14	0.48
1:G:17:SER:HB2	1:G:40:VAL:HB	1.94	0.48
1:D:31:GLN:HE21	1:D:114:MET:N	2.09	0.48
1:F:145:ILE:HG23	1:F:168:THR:HG21	1.93	0.48
1:F:91:ARG:HH12	1:F:103:ASN:CG	2.16	0.48
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.95	0.48
1:C:212:LEU:HD12	1:C:265:MET:HB3	1.95	0.48
1:C:294:ASP:OD2	1:C:297:ILE:HD12	2.13	0.48
1:H:287:GLN:OE1	1:H:292:GLU:N	2.36	0.48
1:A:78:PHE:CE2	1:A:130:LEU:HD12	2.48	0.48
1:B:132:PRO:HD3	1:B:142:PHE:CE2	2.48	0.48
1:C:224:TRP:HA	1:C:301:ARG:HH12	1.76	0.48
1:F:204:TYR:O	1:F:209:ILE:HG12	2.13	0.48
1:F:241:THR:HA	1:G:240:LEU:HD23	1.95	0.48
1:H:204:TYR:O	1:H:208:PHE:HB2	2.13	0.48
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.48	0.48
1:G:48:ARG:HB2	1:G:48:ARG:NH1	2.28	0.48
1:J:283:ALA:HB1	1:J:298:GLN:HE21	1.78	0.48
1:C:204:TYR:O	1:C:209:ILE:HG12	2.14	0.48
1:E:223:PHE:O	1:E:301:ARG:NH1	2.21	0.48
1:E:29:LEU:HA	1:E:29:LEU:HD12	1.57	0.48
1:F:299:ARG:C	1:F:301:ARG:H	2.16	0.48
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.49	0.48
1:H:119:PHE:HA	1:H:122:ASP:OD1	2.13	0.48
1:A:19:PHE:O	1:A:37:GLY:HA3	2.14	0.48
1:C:90:LYS:HZ3	1:C:91:ARG:C	2.16	0.48
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.96	0.48
1:F:174:ARG:HB2	1:F:187:GLU:HG2	1.96	0.48
1:J:305:PRO:O	1:J:307:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:OD2	1:E:157:ILE:HD11	2.14	0.48
1:B:224:TRP:CZ2	1:B:301:ARG:CZ	2.97	0.48
1:B:248:TYR:HD1	1:C:247:SER:HA	1.78	0.48
1:F:65:ARG:HD2	1:G:68:ASN:OD1	2.14	0.48
1:H:137:ASN:HB3	1:H:187:GLU:O	2.13	0.48
1:H:248:TYR:HD1	1:I:247:SER:HA	1.78	0.48
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.49	0.47
1:G:218:ALA:HB2	1:H:274:PHE:CD1	2.50	0.47
1:H:11:PRO:HB3	1:H:141:ARG:CZ	2.44	0.47
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.97	0.47
1:J:95:PHE:HB2	1:J:99:ARG:HG2	1.96	0.47
1:B:235:SER:HA	1:B:238:LEU:HD12	1.95	0.47
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.80	0.47
1:C:60:ASN:O	1:C:63:ILE:HD12	2.14	0.47
1:D:175:TYR:O	1:D:178:LEU:HD21	2.15	0.47
1:E:295:LEU:HA	1:E:298:GLN:CG	2.39	0.47
1:J:227:SER:O	1:J:231:ARG:NH1	2.48	0.47
1:J:247:SER:HA	1:J:250:SER:HB3	1.97	0.47
1:B:165:LYS:HG3	1:B:165:LYS:O	2.14	0.47
1:G:181:VAL:HG12	1:G:183:PRO:CD	2.44	0.47
1:H:287:GLN:HE22	1:H:291:VAL:N	2.11	0.47
1:A:73:VAL:HG21	1:A:92:LEU:HD11	1.94	0.47
1:J:224:TRP:HE1	1:J:301:ARG:CD	2.26	0.47
1:D:62:GLN:HA	1:D:62:GLN:OE1	2.15	0.47
1:E:315:LEU:HG	1:E:316:VAL:N	2.29	0.47
1:F:235:SER:HA	1:F:238:LEU:HG	1.95	0.47
1:I:232:LEU:HA	1:I:235:SER:HG	1.75	0.47
1:A:228:PHE:HA	1:A:231:ARG:CD	2.45	0.47
1:B:53:ASP:H	1:B:54:LYS:HD2	1.79	0.47
1:B:51:PRO:HD2	1:B:56:LEU:HD13	1.97	0.47
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.96	0.47
1:D:299:ARG:C	1:D:301:ARG:H	2.16	0.47
1:G:29:LEU:HB2	1:G:255:ARG:HD2	1.96	0.47
1:H:287:GLN:HE22	1:H:290:GLY:C	2.18	0.47
1:B:78:PHE:HB3	1:B:81:VAL:HB	1.97	0.47
1:C:77:GLU:O	1:C:130:LEU:HD12	2.15	0.47
1:E:27:ASN:HB3	1:E:32:THR:HB	1.96	0.47
1:G:286:ARG:HD2	1:G:287:GLN:N	2.30	0.47
1:I:47:PRO:HB3	1:I:96:PRO:O	2.15	0.47
1:J:178:LEU:N	1:J:178:LEU:HD12	2.30	0.47
1:A:302:LEU:HA	1:A:305:PRO:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LEU:HD22	1:E:230:GLU:OE2	2.15	0.47
1:J:92:LEU:HA	1:J:92:LEU:HD23	1.78	0.47
1:A:65:ARG:HA	1:A:68:ASN:HD22	1.79	0.46
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.14	0.46
1:I:132:PRO:HG3	1:I:140:LEU:HD22	1.97	0.46
1:I:145:ILE:HD12	1:I:191:ILE:CG2	2.45	0.46
1:A:295:LEU:HA	1:A:298:GLN:CG	2.44	0.46
1:A:268:ALA:HB1	1:A:308:PHE:HE1	1.79	0.46
1:B:224:TRP:CD1	1:C:281:ILE:HG23	2.50	0.46
1:D:302:LEU:HD12	1:D:305:PRO:HG2	1.97	0.46
1:E:227:SER:O	1:E:231:ARG:HG2	2.15	0.46
1:A:289:ASN:CG	1:A:290:GLY:H	2.17	0.46
1:E:182:GLN:N	1:E:182:GLN:OE1	2.42	0.46
1:I:214:LEU:HD12	1:J:270:TYR:HB3	1.96	0.46
1:C:66:TRP:CE3	1:C:71:LEU:HD22	2.49	0.46
1:F:149:THR:O	1:F:151:ASN:N	2.46	0.46
1:A:64:GLU:OE2	1:A:67:ILE:HD12	2.16	0.46
1:C:294:ASP:OD2	1:C:297:ILE:HB	2.16	0.46
1:F:181:VAL:CG2	1:F:183:PRO:HD2	2.45	0.46
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.98	0.46
1:F:281:ILE:HG23	1:J:224:TRP:CZ3	2.50	0.46
1:F:248:TYR:HE1	1:G:250:SER:HG	1.61	0.46
1:A:87:THR:HG21	1:A:90:LYS:HE2	1.96	0.46
1:C:63:ILE:CD1	1:C:90:LYS:HG3	2.42	0.46
1:C:157:ILE:HD11	1:D:115:ASP:OD2	2.15	0.46
1:F:182:GLN:N	1:F:182:GLN:OE1	2.49	0.46
1:F:232:LEU:HD23	1:F:236:PHE:HE1	1.80	0.46
1:F:95:PHE:HB2	1:F:99:ARG:HG2	1.98	0.46
1:G:122:ASP:N	1:G:122:ASP:OD1	2.48	0.46
1:G:233:GLN:O	1:G:236:PHE:HB2	2.16	0.46
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.50	0.46
1:J:176:ASP:C	1:J:177:HIS:CD2	2.89	0.46
1:J:247:SER:O	1:J:250:SER:HB3	2.16	0.46
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.80	0.46
1:B:136:ASN:ND2	1:B:185:GLN:HA	2.31	0.46
1:B:208:PHE:O	1:B:245:TYR:OH	2.34	0.46
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.96	0.46
1:B:49:LYS:HD2	1:B:49:LYS:N	2.30	0.46
1:D:62:GLN:O	1:D:66:TRP:HD1	1.98	0.46
1:E:312:GLY:O	1:E:315:LEU:HD23	2.16	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ASP:CG	1:G:141:ARG:NH1	2.68	0.46
1:A:95:PHE:HB2	1:A:99:ARG:CB	2.43	0.46
1:B:211:PRO:O	1:B:215:ILE:HG12	2.15	0.46
1:A:250:SER:HG	1:E:248:TYR:HE1	1.62	0.46
1:I:231:ARG:HG2	1:I:280:ILE:HG21	1.98	0.46
1:F:233:GLN:HE21	1:J:230:GLU:HB3	1.80	0.46
1:H:225:LEU:CD2	1:I:231:ARG:NH1	2.79	0.46
1:I:84:SER:HA	1:I:85:PRO:HD3	1.67	0.46
1:B:48:ARG:HH11	1:B:48:ARG:HG2	1.80	0.46
1:C:248:TYR:O	1:C:252:ILE:HG12	2.16	0.46
1:D:295:LEU:CD1	1:D:295:LEU:H	2.29	0.46
1:D:97:ASP:OD2	1:D:99:ARG:NH1	2.49	0.46
1:E:291:VAL:O	1:E:293:ASP:N	2.49	0.46
1:G:29:LEU:CB	1:G:255:ARG:HD2	2.45	0.46
1:I:185:GLN:OE1	1:I:185:GLN:N	2.41	0.46
1:A:182:GLN:CG	1:A:183:PRO:HD3	2.45	0.45
1:D:48:ARG:CG	1:D:48:ARG:NH1	2.76	0.45
1:F:16:VAL:HG12	1:F:145:ILE:HD13	1.98	0.45
1:B:130:LEU:HD22	1:B:142:PHE:CZ	2.51	0.45
1:D:225:LEU:CD2	1:E:232:LEU:HD22	2.47	0.45
1:E:48:ARG:HB2	1:E:48:ARG:NH1	2.31	0.45
1:F:293:ASP:O	1:F:295:LEU:N	2.49	0.45
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.16	0.45
1:I:145:ILE:HD12	1:I:191:ILE:HG23	1.97	0.45
1:J:179:SER:OG	1:J:181:VAL:HG12	2.17	0.45
1:B:136:ASN:HD22	1:B:185:GLN:HA	1.81	0.45
1:E:142:PHE:HB3	1:E:170:ILE:HD13	1.97	0.45
1:I:28:THR:HB	1:I:256:LEU:HD21	1.98	0.45
1:J:65:ARG:O	1:J:69:ASN:ND2	2.49	0.45
1:C:19:PHE:CE2	1:C:148:TYR:CD2	3.05	0.45
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.88	0.45
1:E:262:ILE:O	1:E:266:ILE:HG12	2.17	0.45
1:F:179:SER:OG	1:F:180:SER:N	2.50	0.45
1:G:48:ARG:CZ	1:G:48:ARG:HB2	2.47	0.45
1:J:142:PHE:HB3	1:J:170:ILE:HD13	1.98	0.45
1:J:24:TYR:O	1:J:34:LYS:HG2	2.16	0.45
1:A:286:ARG:HD2	1:A:286:ARG:HA	1.50	0.45
1:C:178:LEU:HD23	1:C:181:VAL:O	2.16	0.45
1:C:58:VAL:O	1:C:63:ILE:HD11	2.16	0.45
1:E:241:THR:O	1:E:244:ALA:HB3	2.17	0.45
1:E:66:TRP:HE3	1:E:71:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ILE:HG22	1:J:62:GLN:NE2	2.31	0.45
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.79	0.45
1:G:29:LEU:HB3	1:G:255:ARG:HH11	1.81	0.45
1:J:177:HIS:CD2	1:J:177:HIS:N	2.84	0.45
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.82	0.45
1:B:291:VAL:O	1:B:291:VAL:HG22	2.16	0.45
1:C:174:ARG:HA	1:C:186:ASN:O	2.17	0.45
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.52	0.45
1:D:287:GLN:NE2	1:D:292:GLU:H	2.15	0.45
1:F:220:TRP:CD1	1:F:304:PHE:HE2	2.34	0.45
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.76	0.45
1:C:263:ASP:O	1:C:267:ILE:HG12	2.17	0.45
1:D:302:LEU:HA	1:D:302:LEU:HD12	1.60	0.45
1:G:132:PRO:HD3	1:G:142:PHE:CE2	2.51	0.45
1:H:224:TRP:CD1	1:H:301:ARG:NH1	2.84	0.45
1:J:146:GLN:OE1	1:J:146:GLN:N	2.50	0.45
1:J:175:TYR:HB2	1:J:178:LEU:CD1	2.39	0.45
1:J:24:TYR:OH	1:J:34:LYS:HE2	2.17	0.45
1:D:31:GLN:HG3	1:D:114:MET:HB2	1.98	0.45
1:F:110:PHE:CE2	1:F:128:LEU:HG	2.52	0.45
1:H:115:ASP:OD1	1:H:117:ARG:HG3	2.17	0.45
1:H:132:PRO:CG	1:H:140:LEU:HD22	2.47	0.45
1:I:299:ARG:C	1:I:301:ARG:N	2.69	0.45
1:B:86:ASP:HB3	1:B:107:LEU:HB3	1.97	0.45
1:B:84:SER:HA	1:B:85:PRO:HD3	1.75	0.45
1:C:81:VAL:HG21	1:C:85:PRO:HG3	1.98	0.45
1:D:123:ARG:NH2	1:D:163:ARG:HD3	2.32	0.45
1:D:23:ILE:HG21	1:D:126:PHE:CD1	2.52	0.45
1:A:284:HIS:CE1	1:E:226:GLU:OE2	2.69	0.45
1:E:253:LEU:HB3	1:E:254:PRO:HD2	1.99	0.45
1:G:136:ASN:ND2	1:G:185:GLN:HG3	2.30	0.45
1:G:13:ASP:CG	1:G:141:ARG:HH11	2.17	0.45
1:H:157:ILE:HD11	1:I:115:ASP:OD2	2.17	0.45
1:I:287:GLN:HE22	1:I:290:GLY:CA	2.30	0.45
1:I:248:TYR:CD1	1:J:247:SER:HA	2.52	0.45
1:J:291:VAL:HG12	1:J:291:VAL:O	2.17	0.45
1:B:263:ASP:O	1:B:267:ILE:HG12	2.17	0.45
1:C:317:ILE:HD12	1:C:317:ILE:HA	1.78	0.45
1:D:289:ASN:ND2	1:D:291:VAL:H	2.13	0.45
1:E:81:VAL:HA	1:E:110:PHE:HA	1.97	0.45
1:H:122:ASP:OD1	1:H:122:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:ASP:CB	1:J:177:HIS:CD2	3.00	0.45
1:A:16:VAL:HA	1:A:40:VAL:O	2.17	0.44
1:E:216:ILE:O	1:E:219:SER:HB3	2.18	0.44
1:E:223:PHE:CE1	1:E:304:PHE:HD2	2.35	0.44
1:H:140:LEU:C	1:H:141:ARG:HD3	2.37	0.44
1:A:78:PHE:O	1:A:81:VAL:HG12	2.18	0.44
1:B:173:ILE:HD13	1:B:190:ARG:CB	2.45	0.44
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.62	0.44
1:B:204:TYR:O	1:B:209:ILE:HG12	2.17	0.44
1:C:277:ILE:HG22	1:C:281:ILE:HD12	2.00	0.44
1:C:63:ILE:CD1	1:C:90:LYS:HZ1	2.29	0.44
1:D:264:GLN:HA	1:D:267:ILE:HG12	1.99	0.44
1:G:136:ASN:HD22	1:G:185:GLN:HA	1.82	0.44
1:I:295:LEU:HA	1:I:295:LEU:HD23	1.56	0.44
1:I:78:PHE:O	1:I:81:VAL:HG12	2.16	0.44
1:J:24:TYR:CZ	1:J:34:LYS:HE2	2.52	0.44
1:J:21:ASN:ND2	1:J:37:GLY:HA2	2.33	0.44
1:A:91:ARG:HD3	1:B:134:SER:OG	2.18	0.44
1:B:216:ILE:HD12	1:B:269:GLY:HA2	1.99	0.44
1:D:299:ARG:HG2	1:D:299:ARG:O	2.18	0.44
1:E:132:PRO:HG2	1:E:140:LEU:HD22	2.00	0.44
1:E:123:ARG:CZ	1:E:198:VAL:HG22	2.47	0.44
1:E:299:ARG:C	1:E:301:ARG:N	2.69	0.44
1:F:122:ASP:CG	1:F:199:ARG:HE	2.20	0.44
1:I:115:ASP:O	1:I:124:GLN:NE2	2.45	0.44
1:I:224:TRP:CZ2	1:I:301:ARG:HB3	2.52	0.44
1:A:21:ASN:ND2	1:A:37:GLY:HA2	2.32	0.44
1:E:224:TRP:HA	1:E:301:ARG:CZ	2.47	0.44
1:C:304:PHE:HB3	1:C:305:PRO:HD3	1.99	0.44
1:E:295:LEU:HA	1:E:298:GLN:HE21	1.83	0.44
1:G:22:LYS:HG3	1:G:24:TYR:HD1	1.83	0.44
1:G:66:TRP:CE3	1:G:71:LEU:HD12	2.53	0.44
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.17	0.44
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.66	0.44
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.86	0.44
1:J:288:ALA:N	1:J:289:ASN:ND2	2.57	0.44
1:C:291:VAL:O	1:C:293:ASP:N	2.50	0.44
1:C:58:VAL:HB	1:C:92:LEU:HB2	2.00	0.44
1:D:294:ASP:N	1:D:298:GLN:HE22	2.15	0.44
1:D:84:SER:HA	1:D:85:PRO:HD3	1.62	0.44
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:PHE:HZ	1:E:204:TYR:CZ	2.36	0.44
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.86	0.44
1:H:21:ASN:ND2	1:H:36:ASP:OD2	2.35	0.44
1:J:208:PHE:HE1	1:J:245:TYR:HE2	1.66	0.44
1:J:220:TRP:CE2	1:J:301:ARG:NH1	2.85	0.44
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.53	0.44
1:E:247:SER:HA	1:E:250:SER:CB	2.48	0.44
1:G:307:GLY:O	1:G:311:ILE:HG13	2.18	0.44
1:H:282:PHE:CZ	1:H:286:ARG:HD2	2.52	0.44
1:I:228:PHE:O	1:I:231:ARG:CB	2.59	0.44
1:J:200:ASN:HA	1:J:201:PRO:HD3	1.84	0.44
1:J:216:ILE:HD12	1:J:269:GLY:HA2	1.99	0.44
1:F:64:GLU:OE2	1:J:61:THR:HG21	2.18	0.44
1:A:151:ASN:ND2	1:A:162:ILE:HG21	2.33	0.44
1:A:145:ILE:HG23	1:A:168:THR:HG21	2.00	0.44
1:B:185:GLN:OE1	1:B:185:GLN:N	2.50	0.44
1:B:298:GLN:NE2	1:B:299:ARG:HB2	2.33	0.44
1:C:182:GLN:H	1:C:183:PRO:CD	2.30	0.44
1:D:28:THR:HB	1:D:256:LEU:CD2	2.47	0.44
1:C:61:THR:HG21	1:D:64:GLU:HG3	2.00	0.44
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.52	0.44
1:E:235:SER:HA	1:E:238:LEU:HD12	1.98	0.44
1:D:224:TRP:CD1	1:E:285:HIS:CD2	3.05	0.44
1:E:299:ARG:HA	1:E:301:ARG:HG3	2.00	0.44
1:F:227:SER:HB3	1:F:230:GLU:CG	2.48	0.44
1:F:291:VAL:O	1:F:293:ASP:N	2.51	0.44
1:C:279:LEU:HD13	1:C:300:CYS:SG	2.58	0.44
1:D:112:ASN:ND2	1:D:125:GLN:O	2.51	0.44
1:D:208:PHE:O	1:D:245:TYR:OH	2.35	0.44
1:H:225:LEU:HD23	1:I:231:ARG:NH1	2.33	0.44
1:I:231:ARG:HG2	1:I:280:ILE:CG2	2.48	0.44
1:J:214:LEU:HA	1:J:217:ALA:HB3	2.00	0.44
1:J:21:ASN:HB2	1:J:36:ASP:O	2.18	0.44
1:B:48:ARG:NH1	1:B:48:ARG:HG2	2.33	0.43
1:A:59:GLU:OE2	1:B:75:ALA:HB3	2.17	0.43
1:C:122:ASP:OD2	1:C:199:ARG:NE	2.36	0.43
1:C:182:GLN:H	1:C:183:PRO:HD3	1.83	0.43
1:D:137:ASN:HB3	1:D:187:GLU:O	2.18	0.43
1:F:61:THR:HG21	1:G:64:GLU:CD	2.38	0.43
1:H:310:ALA:O	1:H:314:VAL:HG23	2.17	0.43
1:B:287:GLN:HB2	1:B:292:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TRP:CG	1:C:281:ILE:HG12	2.52	0.43
1:E:162:ILE:HD13	1:E:197:ALA:HB2	2.00	0.43
1:F:130:LEU:HD23	1:F:131:GLU:N	2.33	0.43
1:F:29:LEU:HA	1:F:29:LEU:HD12	1.86	0.43
1:H:287:GLN:HE22	1:H:291:VAL:CA	2.31	0.43
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.53	0.43
1:C:273:ILE:O	1:C:277:ILE:HG12	2.19	0.43
1:C:84:SER:HA	1:C:85:PRO:HD3	1.87	0.43
1:F:287:GLN:HG3	1:F:290:GLY:N	2.30	0.43
1:F:297:ILE:HD13	1:F:297:ILE:HA	1.58	0.43
1:I:221:SER:HB2	1:J:281:ILE:HD11	1.99	0.43
1:B:153:ASP:CG	1:B:154:ASN:N	2.70	0.43
1:C:58:VAL:O	1:C:91:ARG:HA	2.19	0.43
1:E:183:PRO:CD	1:E:184:ASN:H	2.32	0.43
1:F:287:GLN:CG	1:F:290:GLY:H	2.30	0.43
1:G:89:ASN:HB2	1:H:133:PHE:CE1	2.54	0.43
1:G:91:ARG:N	1:G:103:ASN:O	2.51	0.43
1:I:35:VAL:HB	1:I:110:PHE:CE1	2.53	0.43
1:J:185:GLN:OE1	1:J:185:GLN:N	2.52	0.43
1:C:289:ASN:CG	1:C:290:GLY:H	2.14	0.43
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.53	0.43
1:I:285:HIS:O	1:I:285:HIS:ND1	2.51	0.43
1:A:84:SER:HA	1:A:85:PRO:HD3	1.87	0.43
1:C:90:LYS:NZ	1:C:91:ARG:C	2.72	0.43
1:F:118:LEU:HA	1:F:261:VAL:HG23	2.01	0.43
1:G:235:SER:HA	1:G:238:LEU:HD13	2.00	0.43
1:H:255:ARG:CG	1:H:255:ARG:HH11	2.15	0.43
1:A:59:GLU:OE2	1:B:75:ALA:CB	2.66	0.43
1:C:216:ILE:HD12	1:C:269:GLY:HA2	1.99	0.43
1:C:299:ARG:C	1:C:301:ARG:H	2.21	0.43
1:D:123:ARG:CZ	1:D:163:ARG:HD3	2.49	0.43
1:D:160:TRP:HA	1:D:198:VAL:O	2.18	0.43
1:A:81:VAL:O	1:E:105:ARG:NH2	2.51	0.43
1:E:233:GLN:O	1:E:236:PHE:HB2	2.18	0.43
1:H:287:GLN:HG3	1:H:289:ASN:H	1.84	0.43
1:A:59:GLU:OE2	1:A:91:ARG:NH1	2.51	0.43
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.54	0.43
1:C:142:PHE:HB3	1:C:170:ILE:HD13	2.00	0.43
1:D:123:ARG:NH2	1:D:163:ARG:HG3	2.34	0.43
1:E:54:LYS:HB3	1:E:55:PRO:HD2	2.01	0.43
1:F:33:TYR:CE2	1:F:110:PHE:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:GLN:CB	1:F:292:GLU:HB3	2.41	0.43
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.54	0.43
1:F:14:VAL:HG22	1:F:43:TRP:HB3	2.01	0.43
1:J:145:ILE:O	1:J:168:THR:HG21	2.19	0.43
1:J:178:LEU:HB3	1:J:179:SER:H	1.56	0.43
1:A:145:ILE:HG22	1:A:170:ILE:HD11	2.01	0.43
1:B:301:ARG:O	1:B:305:PRO:HG2	2.19	0.43
1:D:31:GLN:NE2	1:D:113:ASP:HA	2.33	0.43
1:D:22:LYS:HE3	1:D:24:TYR:CG	2.53	0.43
1:E:289:ASN:OD1	1:E:291:VAL:N	2.50	0.43
1:E:301:ARG:NH1	1:E:301:ARG:CG	2.77	0.43
1:B:14:VAL:HG21	1:B:140:LEU:HD21	2.01	0.43
1:C:230:GLU:HB3	1:D:233:GLN:NE2	2.34	0.43
1:D:287:GLN:HA	1:D:287:GLN:NE2	2.33	0.43
1:E:157:ILE:HA	1:E:157:ILE:HD13	1.79	0.43
1:F:228:PHE:HA	1:F:231:ARG:CZ	2.48	0.43
1:G:61:THR:HG21	1:H:64:GLU:HG3	2.00	0.43
1:A:289:ASN:ND2	1:A:291:VAL:HG12	2.34	0.42
1:D:91:ARG:HD2	1:E:134:SER:HB3	2.00	0.42
1:F:103:ASN:OD1	1:F:104:ALA:N	2.52	0.42
1:F:58:VAL:HB	1:F:92:LEU:HB2	2.01	0.42
1:G:225:LEU:HD21	1:H:232:LEU:HD22	2.02	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.69	0.42
1:H:17:SER:HB2	1:H:40:VAL:HB	2.00	0.42
1:J:289:ASN:ND2	1:J:292:GLU:CD	2.73	0.42
1:A:185:GLN:N	1:A:185:GLN:CD	2.73	0.42
1:A:289:ASN:CG	1:A:290:GLY:N	2.72	0.42
1:B:268:ALA:HB1	1:B:308:PHE:HZ	1.84	0.42
1:D:296:LEU:HD13	1:D:299:ARG:HD3	2.00	0.42
1:F:136:ASN:ND2	1:F:185:GLN:HB3	2.33	0.42
1:G:89:ASN:O	1:G:104:ALA:HA	2.19	0.42
1:I:231:ARG:NH1	1:I:232:LEU:HD13	2.34	0.42
1:I:248:TYR:HD1	1:J:247:SER:HA	1.84	0.42
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.54	0.42
1:A:50:THR:OG1	1:A:54:LYS:O	2.26	0.42
1:D:137:ASN:ND2	1:D:187:GLU:OE1	2.47	0.42
1:G:227:SER:HB3	1:G:230:GLU:HG3	2.02	0.42
1:H:138:GLN:HA	1:H:141:ARG:NH2	2.34	0.42
1:H:49:LYS:HA	1:H:49:LYS:HE3	2.01	0.42
1:H:12:VAL:HG11	1:H:72:TRP:HZ3	1.84	0.42
1:I:78:PHE:CD2	1:I:110:PHE:CE2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:LEU:HA	1:I:238:LEU:HD23	1.73	0.42
1:I:260:THR:N	1:I:263:ASP:HB2	2.34	0.42
1:B:298:GLN:CD	1:B:299:ARG:HD2	2.40	0.42
1:B:296:LEU:HA	1:B:298:GLN:HG2	2.00	0.42
1:B:298:GLN:HB2	1:B:299:ARG:HG3	2.00	0.42
1:C:23:ILE:HG12	1:C:35:VAL:HG22	2.00	0.42
1:D:304:PHE:HB3	1:D:305:PRO:HD3	2.02	0.42
1:E:125:GLN:OE1	1:E:194:ARG:HD3	2.18	0.42
1:G:260:THR:N	1:G:263:ASP:HB2	2.32	0.42
1:I:136:ASN:N	1:I:136:ASN:OD1	2.53	0.42
1:I:47:PRO:HA	1:I:98:GLY:HA2	2.02	0.42
1:J:28:THR:HG21	1:J:254:PRO:HB2	2.00	0.42
1:A:59:GLU:CG	1:A:91:ARG:CZ	2.87	0.42
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.87	0.42
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.83	0.42
1:E:303:ALA:O	1:E:307:GLY:N	2.48	0.42
1:F:220:TRP:CD1	1:F:304:PHE:CE2	3.07	0.42
1:F:232:LEU:CD2	1:F:236:PHE:HE1	2.33	0.42
1:H:48:ARG:O	1:H:96:PRO:HA	2.20	0.42
1:J:151:ASN:O	1:J:152:ALA:HB2	2.20	0.42
1:J:279:LEU:HD22	1:J:297:ILE:HD11	2.01	0.42
1:A:91:ARG:HD2	1:B:134:SER:OG	2.19	0.42
1:D:81:VAL:HG21	1:D:85:PRO:HG3	2.02	0.42
1:E:174:ARG:NH1	1:E:187:GLU:CG	2.82	0.42
1:F:228:PHE:CZ	1:F:232:LEU:HD13	2.53	0.42
1:H:120:PRO:HD2	1:H:121:PHE:CE1	2.55	0.42
1:C:136:ASN:OD1	1:C:138:GLN:HB2	2.20	0.42
1:C:19:PHE:CE2	1:C:148:TYR:HD2	2.37	0.42
1:C:90:LYS:CE	1:C:92:LEU:HG	2.50	0.42
1:F:301:ARG:O	1:F:305:PRO:HG2	2.20	0.42
1:H:114:MET:HB3	1:H:116:PHE:CZ	2.55	0.42
1:H:287:GLN:OE1	1:H:292:GLU:HB2	2.18	0.42
1:H:78:PHE:O	1:H:81:VAL:HG12	2.20	0.42
1:I:228:PHE:CE1	1:I:284:HIS:CG	3.07	0.42
1:I:289:ASN:ND2	1:I:291:VAL:HG22	2.34	0.42
1:B:301:ARG:NH1	1:B:301:ARG:O	2.53	0.42
1:D:157:ILE:N	1:D:157:ILE:HD12	2.35	0.42
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.85	0.42
1:D:306:LEU:HA	1:D:309:LEU:HB2	2.02	0.42
1:F:299:ARG:HG2	1:F:301:ARG:NE	2.34	0.42
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:TYR:HE2	1:J:30:GLU:OE2	2.02	0.42
1:J:87:THR:HG21	1:J:90:LYS:HE2	2.02	0.42
1:B:196:ASP:OD2	1:I:165:LYS:CE	2.67	0.42
1:E:137:ASN:HB3	1:E:187:GLU:O	2.20	0.42
1:I:302:LEU:C	1:I:305:PRO:HD2	2.39	0.42
1:A:182:GLN:HG2	1:A:183:PRO:HD3	2.02	0.42
1:A:273:ILE:O	1:A:277:ILE:HG12	2.20	0.42
1:C:78:PHE:O	1:C:81:VAL:HG12	2.19	0.42
1:D:286:ARG:O	1:D:287:GLN:CD	2.57	0.42
1:D:89:ASN:O	1:D:104:ALA:HA	2.20	0.42
1:E:78:PHE:O	1:E:81:VAL:HG12	2.20	0.42
1:F:76:LEU:CB	1:F:130:LEU:HD21	2.40	0.42
1:F:66:TRP:HB3	1:F:71:LEU:HD23	2.02	0.42
1:G:132:PRO:CG	1:G:140:LEU:HD22	2.50	0.42
1:G:58:VAL:HB	1:G:92:LEU:HB2	2.02	0.42
1:H:263:ASP:O	1:H:267:ILE:HG12	2.19	0.42
1:I:145:ILE:CG2	1:I:168:THR:HG21	2.49	0.42
1:I:264:GLN:HG2	1:I:264:GLN:H	1.61	0.42
1:J:293:ASP:CG	1:J:298:GLN:NE2	2.73	0.42
1:F:64:GLU:CD	1:J:61:THR:HG21	2.41	0.42
1:A:167:SER:HB3	1:A:194:ARG:HB2	2.01	0.41
1:B:286:ARG:N	1:B:292:GLU:OE2	2.52	0.41
1:C:122:ASP:HB3	1:C:124:GLN:CD	2.40	0.41
1:C:239:MET:HA	1:C:273:ILE:HD13	2.00	0.41
1:D:119:PHE:CG	1:D:120:PRO:HA	2.55	0.41
1:D:132:PRO:HD3	1:D:142:PHE:CE2	2.55	0.41
1:D:179:SER:HB3	1:D:180:SER:H	1.66	0.41
1:D:122:ASP:CG	1:D:199:ARG:HE	2.23	0.41
1:F:78:PHE:O	1:F:81:VAL:HG12	2.20	0.41
1:F:91:ARG:NH1	1:F:103:ASN:CB	2.82	0.41
1:F:214:LEU:HD12	1:G:270:TYR:HB3	2.00	0.41
1:J:260:THR:H	1:J:263:ASP:HB2	1.85	0.41
1:B:314:VAL:O	1:B:317:ILE:HB	2.20	0.41
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.55	0.41
1:G:221:SER:HB2	1:H:281:ILE:CD1	2.48	0.41
1:A:300:CYS:SG	1:A:304:PHE:HE2	2.43	0.41
1:B:183:PRO:HB2	1:B:184:ASN:H	1.62	0.41
1:B:262:ILE:O	1:B:266:ILE:HG12	2.21	0.41
1:F:237:THR:O	1:F:240:LEU:HB3	2.21	0.41
1:G:216:ILE:HD12	1:G:269:GLY:HA2	2.01	0.41
1:H:185:GLN:OE1	1:H:185:GLN:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.76	0.41
1:J:72:TRP:CZ2	1:J:74:PRO:HB3	2.54	0.41
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.85	0.41
1:A:64:GLU:O	1:A:68:ASN:ND2	2.53	0.41
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.83	0.41
1:D:91:ARG:N	1:D:103:ASN:O	2.53	0.41
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.55	0.41
1:E:137:ASN:OD1	1:E:137:ASN:N	2.53	0.41
1:F:132:PRO:HD3	1:F:142:PHE:CE2	2.55	0.41
1:F:299:ARG:HA	1:F:301:ARG:HG3	2.02	0.41
1:G:138:GLN:HG2	1:G:138:GLN:H	1.67	0.41
1:G:224:TRP:CH2	1:G:301:ARG:HB3	2.55	0.41
1:G:310:ALA:O	1:G:314:VAL:HG23	2.19	0.41
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.87	0.41
1:I:304:PHE:HA	1:I:307:GLY:HA3	2.03	0.41
1:J:38:TYR:CZ	1:J:105:ARG:HD2	2.55	0.41
1:J:227:SER:C	1:J:231:ARG:NH1	2.74	0.41
1:A:257:PRO:HB3	1:E:159:GLU:CB	2.50	0.41
1:A:28:THR:HB	1:A:256:LEU:CD2	2.50	0.41
1:B:303:ALA:O	1:B:307:GLY:N	2.52	0.41
1:B:91:ARG:HB2	1:C:133:PHE:CE2	2.55	0.41
1:F:247:SER:HB3	1:J:248:TYR:HB2	2.03	0.41
1:H:174:ARG:CG	1:H:174:ARG:NH1	2.83	0.41
1:H:176:ASP:N	1:H:176:ASP:OD1	2.53	0.41
1:H:311:ILE:O	1:H:315:LEU:HD13	2.19	0.41
1:I:224:TRP:CE2	1:I:301:ARG:HD3	2.55	0.41
1:D:165:LYS:O	1:D:166:ALA:HB3	2.20	0.41
1:G:43:TRP:CH2	1:G:74:PRO:HD2	2.56	0.41
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.21	0.41
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.68	0.41
1:C:204:TYR:O	1:C:208:PHE:HB2	2.21	0.41
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.20	0.41
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.56	0.41
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.56	0.41
1:G:62:GLN:O	1:G:66:TRP:HD1	2.03	0.41
1:H:238:LEU:HD21	1:I:236:PHE:CE2	2.56	0.41
1:H:273:ILE:O	1:H:277:ILE:HG12	2.21	0.41
1:I:138:GLN:HG3	1:I:187:GLU:OE1	2.21	0.41
1:I:231:ARG:HD3	1:I:231:ARG:HH11	1.62	0.41
1:J:18:ILE:HD13	1:J:39:ILE:HG22	2.03	0.41
1:A:248:TYR:HD1	1:B:250:SER:HG	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:HE2	1:C:102:TYR:CD1	2.56	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.85	0.41
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.88	0.41
1:I:173:ILE:HD13	1:I:190:ARG:HB3	2.02	0.41
1:J:304:PHE:HD1	1:J:304:PHE:N	2.19	0.41
1:B:297:ILE:C	1:B:299:ARG:H	2.24	0.41
1:B:206:TRP:O	1:C:267:ILE:HD12	2.21	0.41
1:D:112:ASN:OD1	1:D:113:ASP:N	2.54	0.41
1:F:81:VAL:HG21	1:F:85:PRO:HG3	2.01	0.41
1:F:84:SER:HA	1:F:85:PRO:HD3	1.84	0.41
1:G:117:ARG:HD3	1:G:117:ARG:HH11	1.74	0.41
1:G:71:LEU:HD22	1:G:73:VAL:CG2	2.50	0.41
1:H:54:LYS:HB3	1:H:54:LYS:HE2	1.91	0.41
1:I:288:ALA:HB3	1:I:292:GLU:OE2	2.21	0.41
1:I:78:PHE:CD2	1:I:110:PHE:CZ	3.09	0.41
1:B:63:ILE:HD12	1:B:90:LYS:HB2	2.03	0.41
1:D:293:ASP:C	1:D:298:GLN:HE22	2.24	0.41
1:F:151:ASN:O	1:F:152:ALA:HB2	2.20	0.41
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.89	0.41
1:H:287:GLN:NE2	1:H:292:GLU:H	2.19	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.02	0.41
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.86	0.41
1:G:13:ASP:OD1	1:G:141:ARG:HD3	2.20	0.41
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.90	0.41
1:J:120:PRO:HD2	1:J:121:PHE:CE1	2.55	0.41
1:J:263:ASP:O	1:J:267:ILE:HG12	2.21	0.41
1:A:240:LEU:HD11	1:E:240:LEU:CD1	2.40	0.40
1:A:295:LEU:HA	1:A:298:GLN:CD	2.41	0.40
1:B:24:TYR:OH	1:B:34:LYS:HE2	2.20	0.40
1:C:79:ILE:HA	1:C:79:ILE:HD13	1.88	0.40
1:D:204:TYR:O	1:D:209:ILE:HG12	2.21	0.40
1:D:228:PHE:HA	1:D:231:ARG:NH1	2.36	0.40
1:F:118:LEU:HD12	1:F:122:ASP:HA	2.03	0.40
1:F:157:ILE:HA	1:F:157:ILE:HD13	1.74	0.40
1:F:205:LEU:HD23	1:F:205:LEU:HA	1.94	0.40
1:G:263:ASP:O	1:G:267:ILE:HG12	2.22	0.40
1:J:211:PRO:O	1:J:215:ILE:HG12	2.21	0.40
1:J:301:ARG:O	1:J:301:ARG:CD	2.64	0.40
1:A:122:ASP:N	1:A:122:ASP:OD1	2.53	0.40
1:B:287:GLN:CG	1:B:289:ASN:H	2.20	0.40
1:C:125:GLN:OE1	1:C:194:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LEU:HA	1:C:279:LEU:HD23	1.80	0.40
1:C:66:TRP:HE3	1:C:71:LEU:HD22	1.86	0.40
1:D:117:ARG:HD3	1:D:117:ARG:HH11	1.74	0.40
1:D:212:LEU:HD12	1:D:265:MET:HB3	2.04	0.40
1:F:157:ILE:HD11	1:G:115:ASP:OD2	2.22	0.40
1:H:313:CYS:O	1:H:316:VAL:HG22	2.21	0.40
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.91	0.40
1:A:184:ASN:N	1:A:184:ASN:ND2	2.68	0.40
1:A:59:GLU:HA	1:A:91:ARG:HG2	2.03	0.40
1:B:175:TYR:O	1:B:186:ASN:HB2	2.22	0.40
1:C:48:ARG:HH12	1:C:94:LEU:HB3	1.86	0.40
1:G:174:ARG:HA	1:G:186:ASN:O	2.20	0.40
1:H:132:PRO:HD3	1:H:142:PHE:CE2	2.57	0.40
1:H:149:THR:C	1:H:151:ASN:H	2.25	0.40
1:B:71:LEU:HD22	1:B:73:VAL:CG2	2.50	0.40
1:C:119:PHE:HA	1:C:122:ASP:OD1	2.22	0.40
1:D:46:LYS:HA	1:D:47:PRO:HD3	1.93	0.40
1:E:304:PHE:HB3	1:E:305:PRO:HD3	2.03	0.40
1:F:286:ARG:NH1	1:F:286:ARG:CG	2.76	0.40
1:G:78:PHE:HB3	1:G:81:VAL:HB	2.03	0.40
1:H:211:PRO:HB3	1:I:270:TYR:CD1	2.56	0.40
1:J:119:PHE:CD2	1:J:262:ILE:HD12	2.57	0.40
1:J:289:ASN:HD22	1:J:292:GLU:CD	2.25	0.40
1:J:84:SER:HA	1:J:85:PRO:HD3	1.75	0.40
1:A:250:SER:HB3	1:E:252:ILE:HG13	2.03	0.40
1:B:292:GLU:O	1:B:294:ASP:N	2.54	0.40
1:C:151:ASN:O	1:C:152:ALA:HB2	2.22	0.40
1:C:90:LYS:HZ3	1:C:92:LEU:CA	2.35	0.40
1:D:123:ARG:NH2	1:D:198:VAL:CG2	2.81	0.40
1:E:87:THR:HG21	1:E:90:LYS:HE2	2.04	0.40
1:H:31:GLN:HG2	1:H:114:MET:HB2	2.04	0.40
1:I:174:ARG:HG3	1:I:174:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	274 (90%)	24 (8%)	7 (2%)	7	46
1	B	305/307 (99%)	272 (89%)	27 (9%)	6 (2%)	9	49
1	C	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	7	46
1	D	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	5	40
1	E	305/307 (99%)	280 (92%)	22 (7%)	3 (1%)	18	62
1	F	305/307 (99%)	277 (91%)	25 (8%)	3 (1%)	18	62
1	G	305/307 (99%)	278 (91%)	19 (6%)	8 (3%)	6	43
1	H	305/307 (99%)	277 (91%)	19 (6%)	9 (3%)	5	40
1	I	305/307 (99%)	276 (90%)	18 (6%)	11 (4%)	4	36
1	J	305/307 (99%)	271 (89%)	27 (9%)	7 (2%)	7	46
All	All	3050/3070 (99%)	2756 (90%)	224 (7%)	70 (2%)	7	46

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	185	GLN
1	B	166	ALA
1	B	183	PRO
1	B	298	GLN
1	C	166	ALA
1	C	182	GLN
1	D	180	SER
1	D	291	VAL
1	F	153	ASP
1	F	184	ASN
1	G	166	ALA
1	G	179	SER
1	H	287	GLN
1	I	153	ASP
1	I	179	SER
1	I	288	ALA
1	I	292	GLU
1	J	179	SER
1	J	220	TRP

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Mol	Chain	Res	Type
1	J	308	PHE
1	B	150	GLU
1	C	122	ASP
1	C	152	ALA
1	C	153	ASP
1	C	290	GLY
1	D	183	PRO
1	E	150	GLU
1	G	184	ASN
1	G	294	ASP
1	H	150	GLU
1	A	60	ASN
1	A	153	ASP
1	B	53	ASP
1	D	286	ARG
1	D	290	GLY
1	E	53	ASP
1	G	150	GLU
1	H	180	SER
1	C	53	ASP
1	D	150	GLU
1	D	166	ALA
1	I	150	GLU
1	I	184	ASN
1	I	231	ARG
1	J	150	GLU
1	J	152	ALA
1	A	304	PHE
1	B	153	ASP
1	G	53	ASP
1	G	60	ASN
1	G	180	SER
1	H	53	ASP
1	H	60	ASN
1	H	303	ALA
1	I	53	ASP
1	A	166	ALA
1	D	53	ASP
1	E	183	PRO
1	F	53	ASP
1	H	153	ASP
1	H	304	PHE

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Mol	Chain	Res	Type
1	I	304	PHE
1	J	153	ASP
1	J	305	PRO
1	H	182	GLN
1	D	182	GLN
1	I	183	PRO
1	I	182	GLN
1	A	182	GLN

### 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	274/274 (100%)	271 (99%)	3 (1%)	78	91
1	B	274/274 (100%)	267 (97%)	7 (3%)	51	81
1	C	274/274 (100%)	268 (98%)	6 (2%)	57	84
1	D	274/274 (100%)	267 (97%)	7 (3%)	51	81
1	E	274/274 (100%)	263 (96%)	11 (4%)	36	73
1	F	274/274 (100%)	266 (97%)	8 (3%)	48	80
1	G	274/274 (100%)	266 (97%)	8 (3%)	48	80
1	H	274/274 (100%)	268 (98%)	6 (2%)	57	84
1	I	274/274 (100%)	264 (96%)	10 (4%)	40	75
1	J	274/274 (100%)	264 (96%)	10 (4%)	40	75
All	All	2740/2740 (100%)	2664 (97%)	76 (3%)	49	80

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	184	ASN
1	A	286	ARG
1	B	32	THR
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	250	SER
1	B	279	LEU
1	B	287	GLN
1	B	289	ASN
1	B	292	GLU
1	C	48	ARG
1	C	179	SER
1	C	182	GLN
1	C	250	SER
1	C	292	GLU
1	C	309	LEU
1	D	31	GLN
1	D	124	GLN
1	D	153	ASP
1	D	176	ASP
1	D	255	ARG
1	D	286	ARG
1	D	287	GLN
1	E	82	VAL
1	E	124	GLN
1	E	145	ILE
1	E	150	GLU
1	E	231	ARG
1	E	291	VAL
1	E	295	LEU
1	E	296	LEU
1	E	299	ARG
1	E	315	LEU
1	E	317	ILE
1	F	64	GLU
1	F	163	ARG
1	F	169	HIS
1	F	250	SER
1	F	284	HIS
1	F	291	VAL
1	F	297	ILE
1	F	298	GLN
1	G	22	LYS
1	G	49	LYS
1	G	65	ARG
1	G	184	ASN
1	G	255	ARG

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Mol	Chain	Res	Type
1	G	298	GLN
1	G	313	CYS
1	G	317	ILE
1	H	54	LYS
1	H	122	ASP
1	H	141	ARG
1	H	250	SER
1	H	255	ARG
1	H	286	ARG
1	I	31	GLN
1	I	150	GLU
1	I	155	GLU
1	I	169	HIS
1	I	240	LEU
1	I	255	ARG
1	I	264	GLN
1	I	284	HIS
1	I	291	VAL
1	I	299	ARG
1	J	69	ASN
1	J	179	SER
1	J	250	SER
1	J	286	ARG
1	J	293	ASP
1	J	301	ARG
1	J	309	LEU
1	J	311	ILE
1	J	315	LEU
1	J	316	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	184	ASN
1	A	285	HIS
1	B	124	GLN
1	B	298	GLN
1	C	62	GLN
1	D	31	GLN
1	D	68	ASN
1	D	251	ASN

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Mol	Chain	Res	Type
1	D	285	HIS
1	D	287	GLN
1	D	298	GLN
1	E	233	GLN
1	E	285	HIS
1	E	298	GLN
1	F	233	GLN
1	F	284	HIS
1	G	136	ASN
1	H	124	GLN
1	H	182	GLN
1	H	289	ASN
1	H	298	GLN
1	I	31	GLN
1	I	89	ASN
1	I	284	HIS
1	I	287	GLN
1	J	69	ASN
1	J	182	GLN
1	J	251	ASN
1	J	298	GLN

### 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 [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	307/307 (100%)	-0.26	10 (3%)	47	35	69, 114, 205, 266	0
1	B	307/307 (100%)	-0.17	9 (2%)	52	38	67, 100, 210, 287	0
1	C	307/307 (100%)	-0.17	10 (3%)	47	35	64, 99, 199, 276	0
1	D	307/307 (100%)	-0.16	8 (2%)	56	42	71, 102, 210, 290	0
1	E	307/307 (100%)	-0.12	13 (4%)	37	26	70, 109, 203, 258	0
1	F	307/307 (100%)	-0.16	13 (4%)	37	26	70, 110, 211, 306	0
1	G	307/307 (100%)	-0.09	12 (3%)	40	29	70, 101, 201, 258	0
1	H	307/307 (100%)	-0.09	21 (6%)	18	13	67, 108, 206, 301	0
1	I	307/307 (100%)	-0.25	9 (2%)	52	38	62, 103, 206, 335	0
1	J	307/307 (100%)	-0.27	9 (2%)	52	38	75, 111, 230, 307	0
All	All	3070/3070 (100%)	-0.17	114 (3%)	42	31	62, 106, 209, 335	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	288	ALA	10.5
1	D	180	SER	8.1
1	H	184	ASN	6.8
1	D	179	SER	6.2
1	E	290	GLY	5.9
1	F	287	GLN	5.6
1	C	317	ILE	5.5
1	I	182	GLN	5.5
1	H	185	GLN	4.8
1	E	180	SER	4.7
1	I	180	SER	4.7
1	A	176	ASP	4.6
1	C	289	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	176	ASP	4.4
1	C	314	VAL	4.4
1	C	313	CYS	4.3
1	J	290	GLY	4.3
1	H	180	SER	4.2
1	I	179	SER	4.2
1	D	177	HIS	3.9
1	D	178	LEU	3.8
1	I	290	GLY	3.8
1	E	291	VAL	3.7
1	A	175	TYR	3.6
1	G	288	ALA	3.6
1	F	183	PRO	3.6
1	E	285	HIS	3.6
1	E	182	GLN	3.6
1	C	316	VAL	3.6
1	H	141	ARG	3.5
1	E	185	GLN	3.5
1	B	179	SER	3.5
1	F	317	ILE	3.4
1	E	179	SER	3.4
1	F	182	GLN	3.4
1	G	313	CYS	3.3
1	H	183	PRO	3.3
1	C	172	ASP	3.3
1	F	289	ASN	3.2
1	F	175	TYR	3.2
1	B	293	ASP	3.1
1	G	285	HIS	3.1
1	A	153	ASP	3.1
1	B	294	ASP	3.0
1	E	183	PRO	3.0
1	E	289	ASN	3.0
1	C	290	GLY	3.0
1	H	291	VAL	2.9
1	I	291	VAL	2.9
1	H	174	ARG	2.9
1	H	165	LYS	2.9
1	J	306	LEU	2.9
1	E	167	SER	2.8
1	E	184	ASN	2.8
1	H	186	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	288	ALA	2.8
1	H	179	SER	2.8
1	G	314	VAL	2.7
1	A	317	ILE	2.7
1	B	297	ILE	2.7
1	A	156	GLU	2.6
1	H	290	GLY	2.6
1	C	180	SER	2.6
1	D	291	VAL	2.6
1	H	181	VAL	2.6
1	A	188	PHE	2.6
1	D	181	VAL	2.6
1	J	49	LYS	2.5
1	A	297	ILE	2.5
1	B	291	VAL	2.5
1	H	138	GLN	2.5
1	J	303	ALA	2.5
1	F	290	GLY	2.5
1	H	187	GLU	2.4
1	I	288	ALA	2.4
1	H	11	PRO	2.4
1	G	126	PHE	2.4
1	G	156	GLU	2.4
1	D	176	ASP	2.4
1	I	289	ASN	2.4
1	A	177	HIS	2.4
1	E	166	ALA	2.4
1	H	182	GLN	2.4
1	G	312	GLY	2.3
1	H	140	LEU	2.3
1	A	154	ASN	2.3
1	J	179	SER	2.3
1	B	298	GLN	2.2
1	B	290	GLY	2.2
1	G	317	ILE	2.2
1	D	153	ASP	2.2
1	G	293	ASP	2.2
1	G	289	ASN	2.2
1	G	282	PHE	2.2
1	J	291	VAL	2.2
1	H	137	ASN	2.1
1	H	143	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	174	ARG	2.1
1	G	310	ALA	2.1
1	F	291	VAL	2.1
1	J	308	PHE	2.1
1	H	289	ASN	2.1
1	J	287	GLN	2.1
1	C	306	LEU	2.1
1	B	28	THR	2.1
1	H	173	ILE	2.1
1	C	146	GLN	2.1
1	B	289	ASN	2.1
1	J	282	PHE	2.1
1	I	181	VAL	2.0
1	I	287	GLN	2.0
1	F	316	VAL	2.0
1	A	292	GLU	2.0
1	F	179	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.