



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 PM GMT

PDB ID : 3UQ5  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) mutant L240A F247L (L9A F16L) in the presence of 10 mM cysteamine  
Authors : Gonzalez-Gutierrez, G.; Lukk, T.; Agarwal, V.; Papke, D.; Nair, S.K.; Grosman, C.  
Deposited on : 2011-11-19  
Resolution : 4.20 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

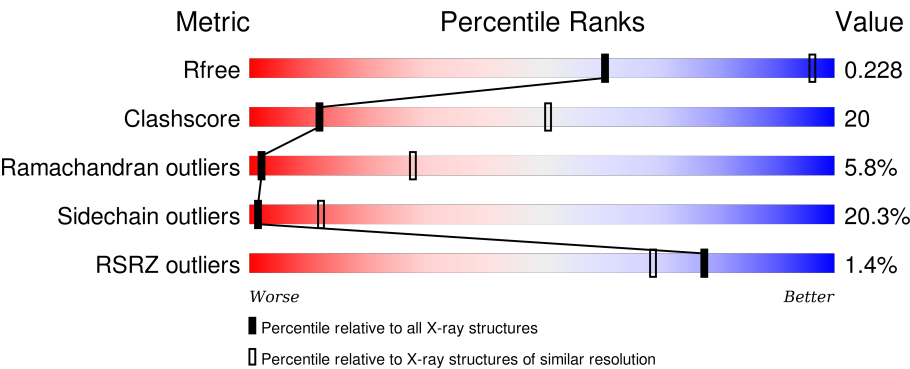
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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 <sub>free</sub>	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	324	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>46%37%11%• 5%</div></div>
1	B	324	<div><div></div><div></div><div></div><div></div><div></div></div> <div>43%40%12%5%</div>
1	C	324	<div><div>3%</div><div></div><div></div><div></div><div></div></div> <div>46%37%11%• 5%</div>
1	D	324	<div><div>%</div><div></div><div></div><div></div><div></div></div> <div>43%40%11%5%</div>
1	E	324	<div><div>2%</div><div></div><div></div><div></div><div></div></div> <div>45%39%11%5%</div>

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Mol	Chain	Length	Quality of chain
1	F	324	<div><div></div><div><div>%</div><div><div></div><div>45%</div><div>39%</div><div>11%</div><div>5%</div></div></div></div>
1	G	324	<div><div></div><div><div>2%</div><div><div></div><div>45%</div><div>39%</div><div>10%</div><div>5%</div></div></div></div>
1	H	324	<div><div></div><div><div>2%</div><div><div></div><div>45%</div><div>38%</div><div>12%</div><div>5%</div></div></div></div>
1	I	324	<div><div></div><div><div>2%</div><div><div></div><div>43%</div><div>39%</div><div>12%</div><div>5%</div></div></div></div>
1	J	324	<div><div></div><div><div>%</div><div><div></div><div>43%</div><div>40%</div><div>11%</div><div>5%</div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24991 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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2499	1627	416	450	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
A	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
A	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
A	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
B	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
B	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
B	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
B	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
C	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
C	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
C	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
D	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
D	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
D	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
D	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
E	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
E	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
E	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
E	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
F	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
F	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
F	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
F	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
G	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
G	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
G	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
G	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
H	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
H	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
H	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
H	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
I	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
I	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
I	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
I	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
J	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
J	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
J	240	ALA	LEU	ENGINEERED MUTATION	UNP E0SJQ4
J	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4

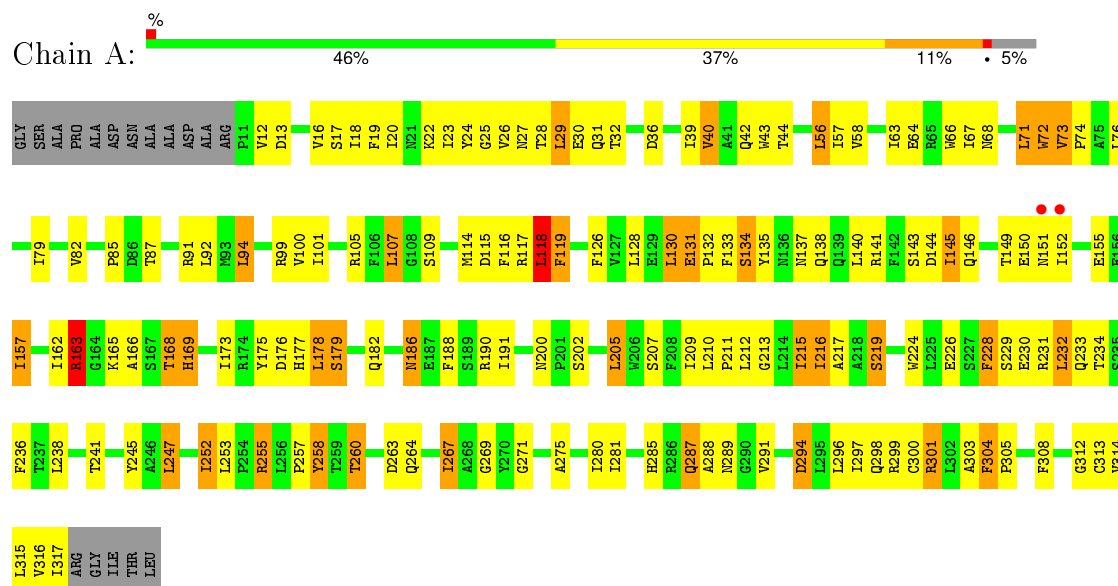
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Na 1 1	0	0

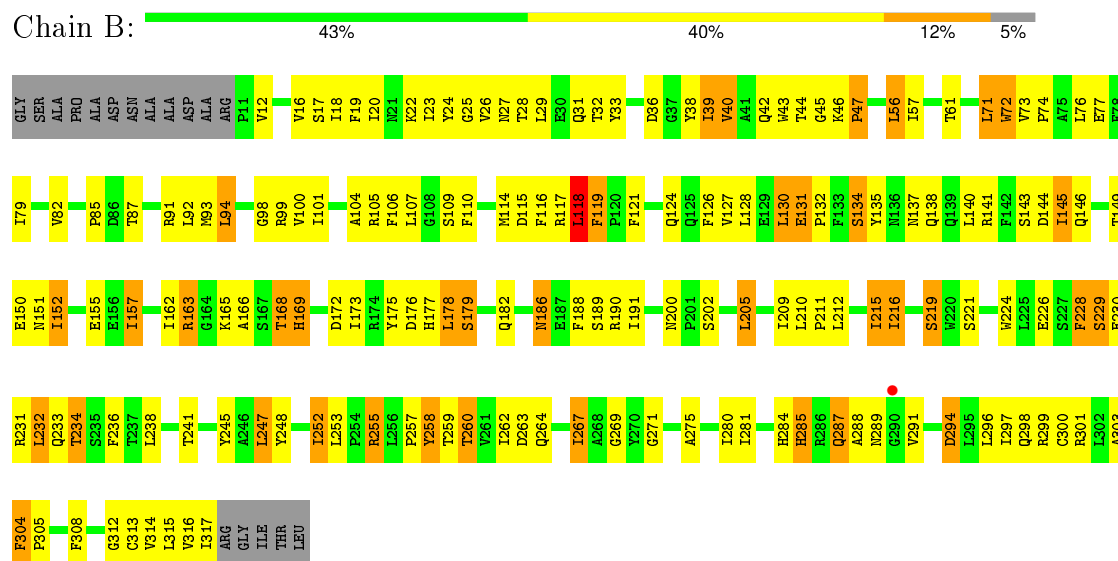
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

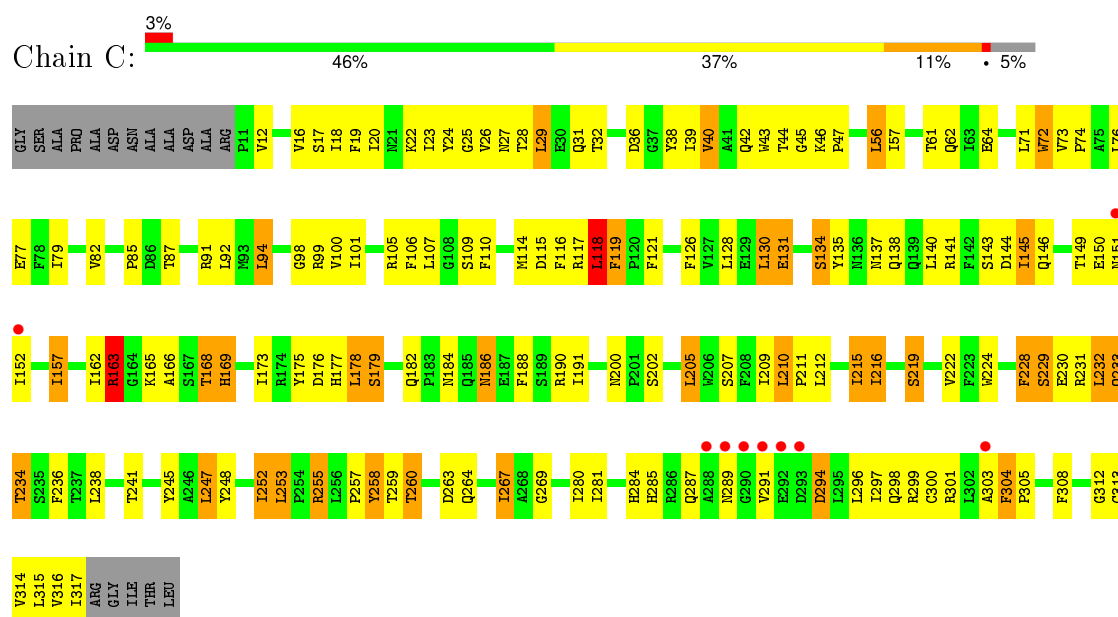
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



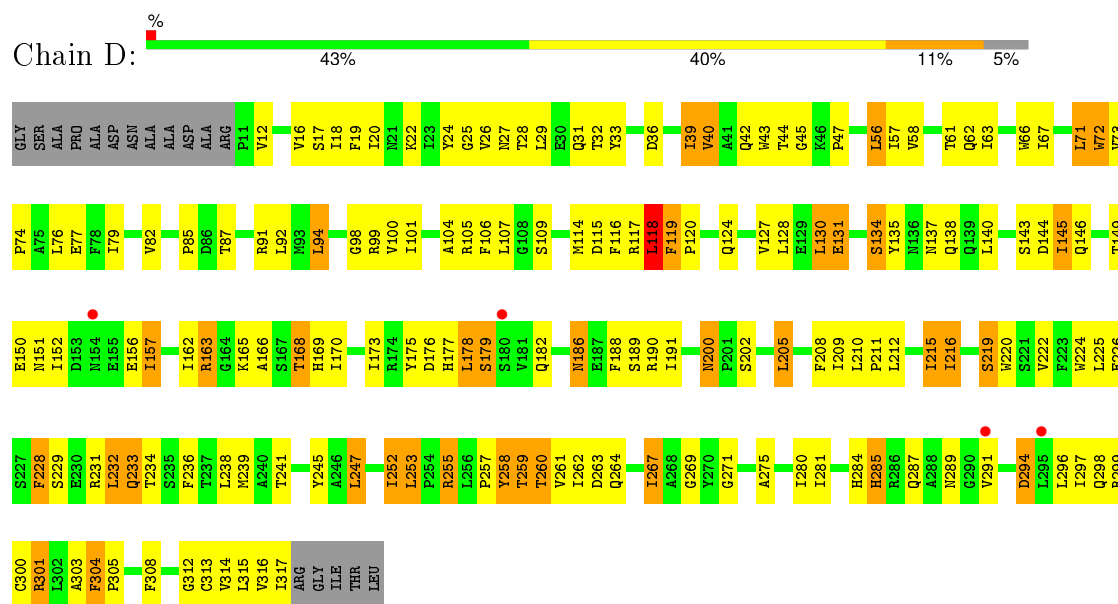
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



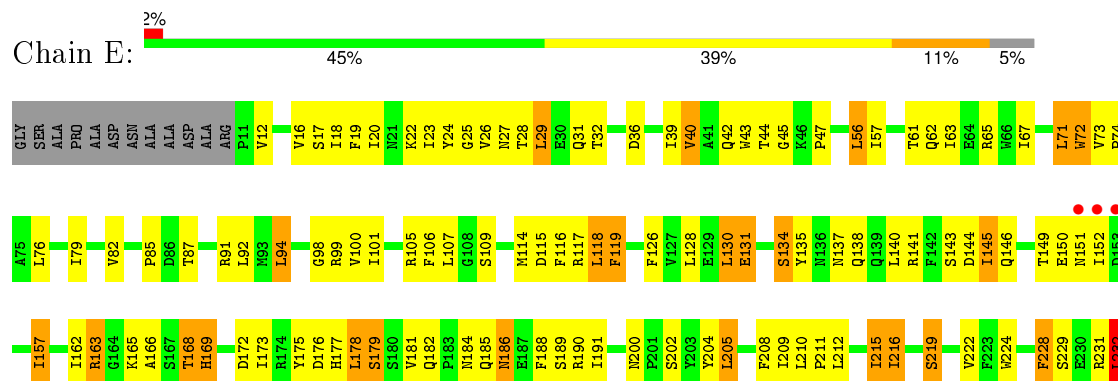
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

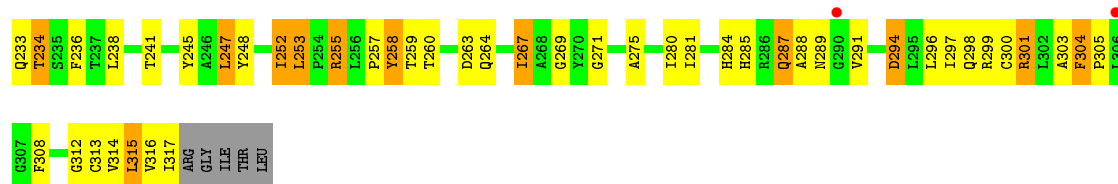


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

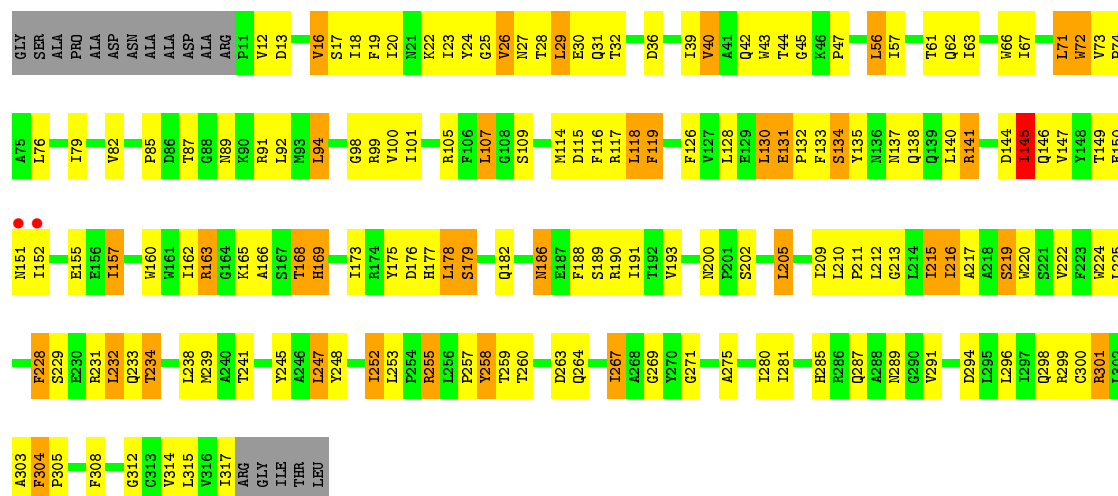


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

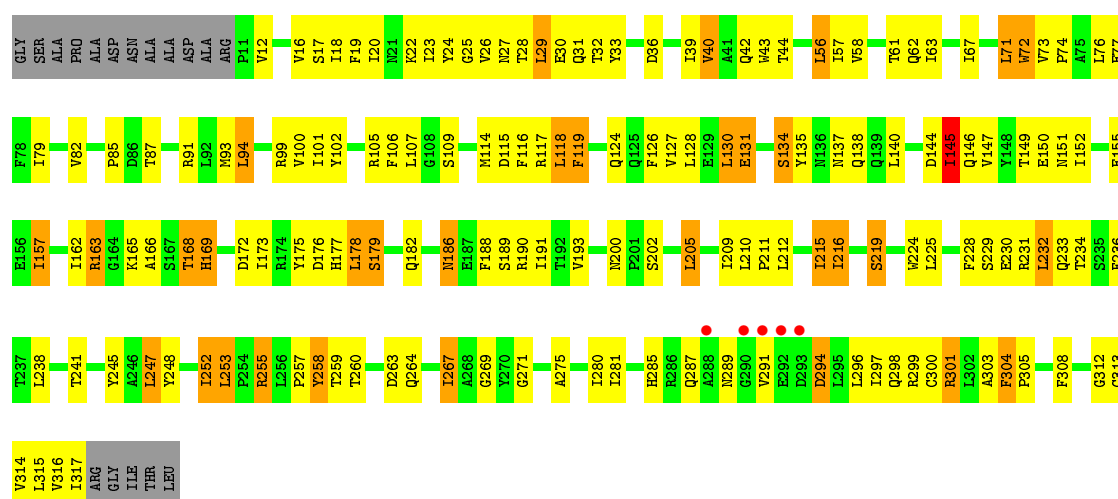




• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



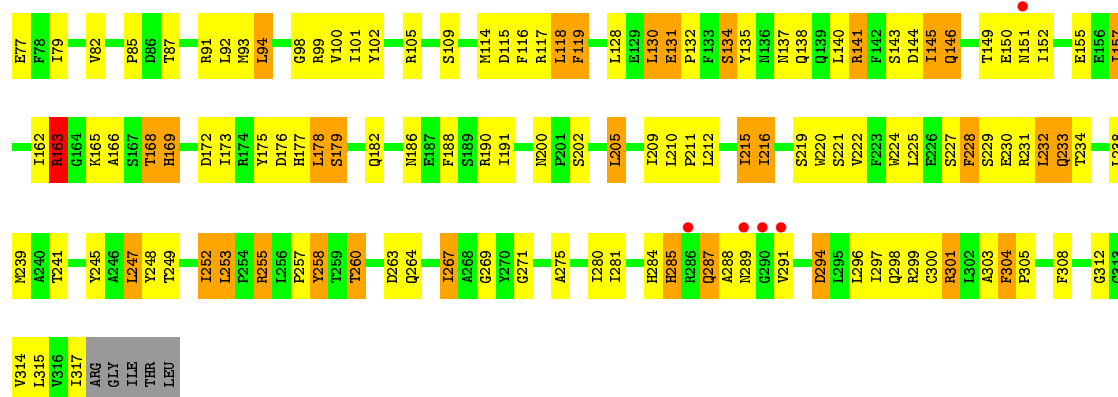
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



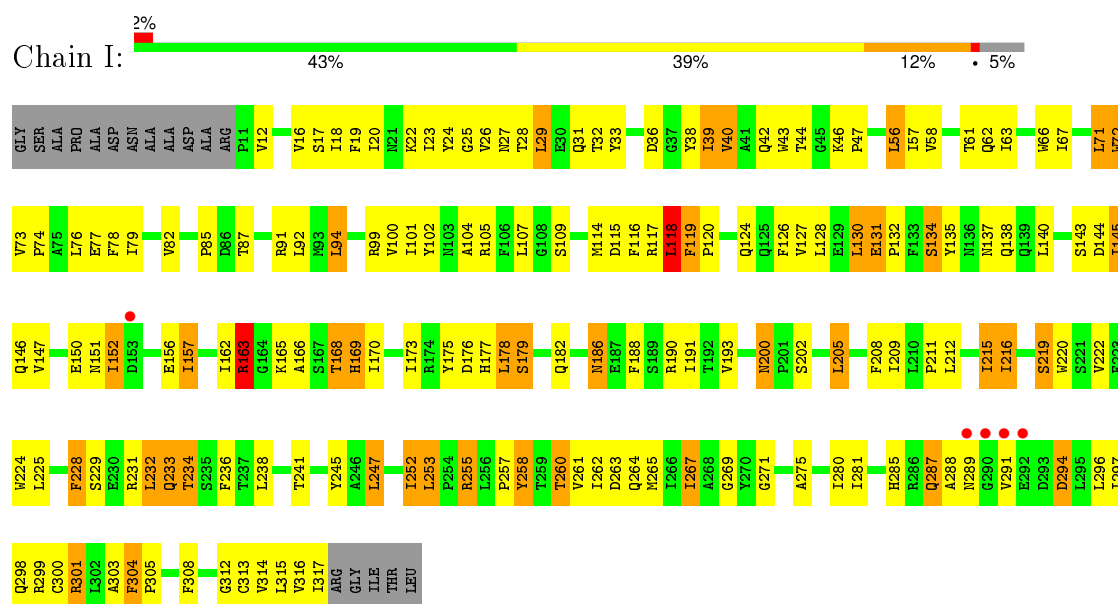
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



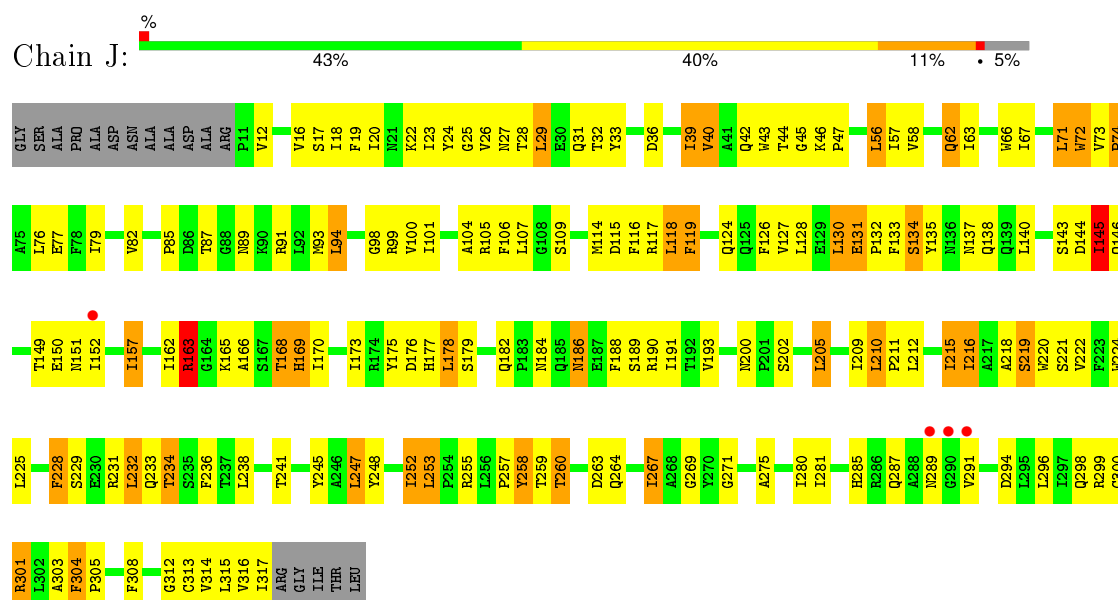




• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.57Å 267.43Å 111.16Å 90.00° 108.64° 90.00°	Depositor
Resolution (Å)	19.99 – 4.20 19.99 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.99-4.20) 99.9 (19.99-4.20)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 4.21Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_897)	Depositor
R, $R_{free}$	0.220 , 0.249 0.193 , 0.228	Depositor DCC
$R_{free}$ test set	2101 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	117.0	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 80.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42056 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.56	0/2566	0.77	3/3498 (0.1%)
1	B	0.59	0/2566	0.79	2/3498 (0.1%)
1	C	0.57	0/2566	0.78	3/3498 (0.1%)
1	D	0.61	0/2566	0.79	2/3498 (0.1%)
1	E	0.58	0/2566	0.77	3/3498 (0.1%)
1	F	0.57	0/2566	0.78	3/3498 (0.1%)
1	G	0.58	0/2566	0.79	3/3498 (0.1%)
1	H	0.60	0/2566	0.78	3/3498 (0.1%)
1	I	0.61	0/2566	0.80	3/3498 (0.1%)
1	J	0.60	0/2566	0.79	3/3498 (0.1%)
All	All	0.59	0/25660	0.78	28/34980 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	12	VAL	CB-CA-C	-6.49	99.07	111.40
1	I	205	LEU	CA-CB-CG	-6.39	100.60	115.30
1	J	205	LEU	CA-CB-CG	-6.17	101.11	115.30
1	B	12	VAL	CB-CA-C	-5.95	100.09	111.40
1	F	205	LEU	CA-CB-CG	-5.92	101.69	115.30
1	H	205	LEU	CA-CB-CG	-5.89	101.75	115.30
1	G	12	VAL	CB-CA-C	-5.86	100.27	111.40
1	D	12	VAL	CB-CA-C	-5.82	100.34	111.40
1	C	12	VAL	CB-CA-C	-5.78	100.42	111.40
1	A	205	LEU	CA-CB-CG	-5.75	102.06	115.30
1	D	205	LEU	CA-CB-CG	-5.73	102.12	115.30
1	G	205	LEU	CA-CB-CG	-5.67	102.25	115.30
1	B	205	LEU	CA-CB-CG	-5.60	102.42	115.30
1	C	29	LEU	CA-CB-CG	5.59	128.17	115.30
1	J	12	VAL	CB-CA-C	-5.57	100.81	111.40
1	A	12	VAL	CB-CA-C	-5.53	100.90	111.40
1	C	205	LEU	CA-CB-CG	-5.51	102.62	115.30
1	H	12	VAL	CB-CA-C	-5.51	100.93	111.40
1	F	12	VAL	CB-CA-C	-5.50	100.95	111.40
1	H	29	LEU	CA-CB-CG	5.40	127.72	115.30
1	F	29	LEU	CA-CB-CG	5.37	127.65	115.30
1	E	205	LEU	CA-CB-CG	-5.32	103.08	115.30
1	E	12	VAL	CB-CA-C	-5.22	101.48	111.40
1	A	29	LEU	CA-CB-CG	5.15	127.15	115.30
1	E	29	LEU	CB-CG-CD2	5.12	119.71	111.00
1	I	29	LEU	CA-CB-CG	5.12	127.07	115.30
1	G	29	LEU	CB-CG-CD2	5.07	119.62	111.00
1	J	29	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Peptide
1	B	137	ASN	Peptide
1	C	137	ASN	Peptide
1	D	137	ASN	Peptide
1	E	137	ASN	Peptide
1	F	137	ASN	Peptide
1	G	137	ASN	Peptide
1	H	137	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	I	137	ASN	Peptide
1	J	137	ASN	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	2499	0	2474	104	0
1	B	2499	0	2474	118	0
1	C	2499	0	2474	110	0
1	D	2499	0	2474	113	0
1	E	2499	0	2474	102	0
1	F	2499	0	2474	103	0
1	G	2499	0	2473	109	0
1	H	2499	0	2473	108	0
1	I	2499	0	2473	121	0
1	J	2499	0	2474	111	0
2	F	1	0	0	0	0
All	All	24991	0	24737	994	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 20.

All (994) 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:J:62:GLN:HA	1:J:62:GLN:HE21	1.10	1.10
1:D:140:LEU:HD22	1:D:191:ILE:HD11	1.52	0.91
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.38	0.89
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.38	0.89
1:C:224:TRP:HE1	1:C:301:ARG:HB3	1.38	0.87
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.54	0.87
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.56	0.86
1:G:140:LEU:HD22	1:G:191:ILE:HD11	1.57	0.86
1:J:62:GLN:HA	1:J:62:GLN:NE2	1.91	0.86
1:B:140:LEU:HD22	1:B:191:ILE:HD11	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:TRP:HE1	1:F:301:ARG:HB3	1.40	0.85
1:G:224:TRP:HE1	1:G:301:ARG:HB3	1.42	0.85
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.40	0.85
1:A:140:LEU:HD22	1:A:191:ILE:HD11	1.59	0.85
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.38	0.85
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.40	0.85
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.58	0.84
1:D:216:ILE:HD11	1:D:269:GLY:HA2	1.60	0.84
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.43	0.83
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.58	0.83
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.58	0.83
1:I:140:LEU:HD22	1:I:191:ILE:HD11	1.61	0.83
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.43	0.82
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.61	0.82
1:G:260:THR:H	1:G:263:ASP:HB2	1.46	0.81
1:B:216:ILE:HD11	1:B:269:GLY:HA2	1.63	0.80
1:E:260:THR:H	1:E:263:ASP:HB2	1.47	0.80
1:E:216:ILE:HD11	1:E:269:GLY:HA2	1.63	0.79
1:C:157:ILE:HD11	1:D:115:ASP:HA	1.66	0.78
1:H:157:ILE:HD11	1:I:115:ASP:HA	1.66	0.78
1:I:260:THR:H	1:I:263:ASP:HB2	1.49	0.78
1:A:216:ILE:HD11	1:A:269:GLY:HA2	1.66	0.78
1:F:260:THR:H	1:F:263:ASP:HB2	1.48	0.78
1:C:216:ILE:HD11	1:C:269:GLY:HA2	1.66	0.78
1:H:44:THR:HG23	1:H:99:ARG:HB3	1.66	0.78
1:G:216:ILE:HD11	1:G:269:GLY:HA2	1.65	0.77
1:H:140:LEU:HD22	1:H:191:ILE:HD11	1.64	0.77
1:F:216:ILE:HD11	1:F:269:GLY:HA2	1.64	0.77
1:H:224:TRP:NE1	1:H:301:ARG:HB3	1.99	0.77
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.67	0.77
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.65	0.77
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.00	0.77
1:D:260:THR:H	1:D:263:ASP:HB2	1.50	0.77
1:B:169:HIS:ND1	1:I:168:THR:HB	1.99	0.76
1:A:157:ILE:HD11	1:B:115:ASP:HA	1.67	0.76
1:C:224:TRP:HE3	1:D:281:ILE:HG13	1.50	0.76
1:J:44:THR:HG23	1:J:99:ARG:HB3	1.67	0.76
1:J:260:THR:H	1:J:263:ASP:HB2	1.49	0.76
1:I:216:ILE:HD11	1:I:269:GLY:HA2	1.68	0.76
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.00	0.76
1:J:216:ILE:HD11	1:J:269:GLY:HA2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:PHE:O	1:G:312:GLY:N	2.19	0.76
1:G:44:THR:HG23	1:G:99:ARG:HB3	1.67	0.76
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.02	0.75
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.01	0.75
1:F:44:THR:HG23	1:F:99:ARG:HB3	1.68	0.75
1:D:44:THR:HG23	1:D:99:ARG:HB3	1.68	0.74
1:D:308:PHE:O	1:D:312:GLY:N	2.21	0.74
1:E:308:PHE:O	1:E:312:GLY:N	2.21	0.74
1:A:308:PHE:O	1:A:312:GLY:N	2.21	0.74
1:J:140:LEU:HD22	1:J:191:ILE:HD11	1.68	0.73
1:C:140:LEU:HD22	1:C:191:ILE:HD11	1.70	0.73
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.03	0.73
1:H:308:PHE:O	1:H:312:GLY:N	2.20	0.73
1:A:44:THR:HG23	1:A:99:ARG:HB3	1.71	0.73
1:G:224:TRP:HE3	1:H:281:ILE:HG13	1.52	0.73
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.69	0.73
1:H:216:ILE:HD11	1:H:269:GLY:HA2	1.69	0.73
1:F:308:PHE:O	1:F:312:GLY:N	2.19	0.73
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.03	0.73
1:G:157:ILE:HD11	1:H:115:ASP:HA	1.71	0.73
1:B:260:THR:H	1:B:263:ASP:HB2	1.53	0.73
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.71	0.73
1:B:308:PHE:O	1:B:312:GLY:N	2.21	0.73
1:C:308:PHE:O	1:C:312:GLY:N	2.21	0.72
1:B:157:ILE:HD11	1:C:115:ASP:HA	1.70	0.72
1:I:44:THR:HG23	1:I:99:ARG:HB3	1.71	0.72
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.02	0.72
1:F:157:ILE:HD11	1:G:115:ASP:HA	1.71	0.72
1:I:308:PHE:O	1:I:312:GLY:N	2.21	0.72
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.04	0.72
1:C:260:THR:H	1:C:263:ASP:HB2	1.52	0.72
1:J:308:PHE:O	1:J:312:GLY:N	2.20	0.72
1:E:31:GLN:HG2	1:E:114:MET:HB2	1.70	0.72
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.03	0.71
1:H:260:THR:H	1:H:263:ASP:HB2	1.53	0.71
1:E:44:THR:HG23	1:E:99:ARG:HB3	1.72	0.71
1:E:140:LEU:HD22	1:E:191:ILE:HD11	1.73	0.71
1:F:140:LEU:HD22	1:F:191:ILE:HD11	1.72	0.71
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.73	0.70
1:G:247:LEU:HD12	1:H:247:LEU:HD11	1.72	0.70
1:C:44:THR:HG23	1:C:99:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:H	1:A:263:ASP:HB2	1.55	0.70
1:B:44:THR:HG23	1:B:99:ARG:HB3	1.72	0.70
1:B:31:GLN:HG2	1:B:114:MET:HB2	1.73	0.70
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.74	0.70
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.75	0.69
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.74	0.68
1:H:224:TRP:HE3	1:I:281:ILE:HG13	1.57	0.68
1:A:314:VAL:HG13	1:A:317:ILE:HD12	1.75	0.68
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.76	0.68
1:D:314:VAL:HG13	1:D:317:ILE:HD12	1.76	0.68
1:F:115:ASP:HA	1:J:157:ILE:HD11	1.75	0.68
1:J:314:VAL:HG13	1:J:317:ILE:HD12	1.75	0.67
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.76	0.67
1:I:31:GLN:HG2	1:I:114:MET:HB2	1.77	0.67
1:A:179:SER:O	1:A:182:GLN:NE2	2.28	0.67
1:H:31:GLN:HG2	1:H:114:MET:HB2	1.76	0.67
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.77	0.66
1:E:22:LYS:HE3	1:E:24:TYR:HD1	1.61	0.66
1:F:281:ILE:HG13	1:J:224:TRP:HE3	1.60	0.66
1:H:314:VAL:HG13	1:H:317:ILE:HD12	1.77	0.66
1:C:79:ILE:HD11	1:C:131:GLU:HB3	1.77	0.66
1:F:56:LEU:HD22	1:F:57:ILE:H	1.60	0.66
1:G:56:LEU:HD22	1:G:57:ILE:H	1.59	0.66
1:D:157:ILE:HD11	1:E:115:ASP:HA	1.76	0.66
1:C:314:VAL:HG13	1:C:317:ILE:HD12	1.78	0.66
1:B:314:VAL:HG13	1:B:317:ILE:HD12	1.77	0.66
1:J:31:GLN:HG2	1:J:114:MET:HB2	1.79	0.66
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.78	0.65
1:J:42:GLN:HB2	1:J:101:ILE:HG12	1.78	0.65
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.78	0.65
1:G:314:VAL:HG13	1:G:317:ILE:HD12	1.78	0.65
1:A:247:LEU:HD11	1:E:247:LEU:HD12	1.79	0.65
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.77	0.65
1:E:44:THR:HA	1:E:99:ARG:HA	1.79	0.65
1:I:314:VAL:HG13	1:I:317:ILE:HD12	1.78	0.65
1:J:16:VAL:HG11	1:J:191:ILE:HD13	1.79	0.65
1:C:247:LEU:HD12	1:D:247:LEU:HD11	1.79	0.65
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.79	0.65
1:G:173:ILE:HD13	1:G:190:ARG:HB3	1.78	0.65
1:F:314:VAL:HG13	1:F:317:ILE:HD12	1.78	0.64
1:A:27:ASN:HB3	1:A:32:THR:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ASN:HB3	1:G:32:THR:HB	1.80	0.64
1:E:314:VAL:HG13	1:E:317:ILE:HD12	1.78	0.64
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.78	0.64
1:I:219:SER:HA	1:I:238:LEU:HD21	1.78	0.64
1:I:157:ILE:HD11	1:J:115:ASP:HA	1.79	0.64
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.80	0.64
1:C:179:SER:O	1:C:182:GLN:NE2	2.31	0.64
1:I:79:ILE:HD11	1:I:131:GLU:HB3	1.80	0.63
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.81	0.63
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.79	0.63
1:C:212:LEU:HD23	1:C:245:TYR:CE2	2.34	0.63
1:D:175:TYR:CE1	1:D:188:PHE:HD1	2.17	0.63
1:B:224:TRP:HE3	1:C:281:ILE:HG13	1.63	0.63
1:F:179:SER:O	1:F:182:GLN:NE2	2.32	0.63
1:J:179:SER:O	1:J:182:GLN:NE2	2.31	0.63
1:E:19:PHE:CE1	1:E:146:GLN:HG3	2.34	0.63
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.81	0.63
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.79	0.63
1:C:17:SER:HB2	1:C:40:VAL:HG23	1.81	0.63
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.81	0.62
1:E:219:SER:HA	1:E:238:LEU:HD21	1.81	0.62
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.80	0.62
1:F:224:TRP:HE3	1:G:281:ILE:HG13	1.64	0.62
1:B:116:PHE:HB2	1:B:258:TYR:HE1	1.64	0.62
1:I:56:LEU:HD22	1:I:57:ILE:H	1.63	0.62
1:J:56:LEU:HD22	1:J:57:ILE:H	1.65	0.62
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.80	0.62
1:H:91:ARG:HD2	1:I:134:SER:HB3	1.80	0.62
1:F:175:TYR:CE1	1:F:188:PHE:HD1	2.17	0.62
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.81	0.62
1:E:22:LYS:HE3	1:E:24:TYR:CD1	2.35	0.62
1:G:22:LYS:HE3	1:G:24:TYR:HD1	1.64	0.62
1:C:31:GLN:HG2	1:C:114:MET:HB2	1.82	0.62
1:C:56:LEU:HD22	1:C:57:ILE:H	1.65	0.62
1:C:16:VAL:HG11	1:C:191:ILE:HD13	1.81	0.62
1:G:179:SER:O	1:G:182:GLN:NE2	2.32	0.61
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.82	0.61
1:B:27:ASN:HB3	1:B:32:THR:HB	1.82	0.61
1:C:219:SER:HA	1:C:238:LEU:HD21	1.81	0.61
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.83	0.61
1:J:219:SER:HA	1:J:238:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:THR:HA	1:I:99:ARG:HA	1.83	0.61
1:C:252:ILE:HD13	1:D:255:ARG:HG3	1.81	0.61
1:B:19:PHE:CE1	1:B:146:GLN:HG3	2.36	0.61
1:A:31:GLN:HG2	1:A:114:MET:HB2	1.82	0.61
1:J:22:LYS:HE3	1:J:24:TYR:HD1	1.64	0.61
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.83	0.61
1:G:116:PHE:HB2	1:G:258:TYR:HE1	1.66	0.61
1:E:16:VAL:HG11	1:E:191:ILE:HD13	1.83	0.61
1:D:31:GLN:HG2	1:D:114:MET:HB2	1.81	0.61
1:A:115:ASP:HA	1:E:157:ILE:HD11	1.83	0.61
1:D:264:GLN:HA	1:D:267:ILE:HG13	1.82	0.61
1:F:31:GLN:HG2	1:F:114:MET:HB2	1.82	0.60
1:E:76:LEU:HB3	1:E:130:LEU:HD21	1.83	0.60
1:A:219:SER:HA	1:A:238:LEU:HD21	1.84	0.60
1:B:42:GLN:HB2	1:B:101:ILE:HG12	1.82	0.60
1:F:16:VAL:HG11	1:F:191:ILE:HD13	1.83	0.60
1:A:56:LEU:HD22	1:A:57:ILE:H	1.66	0.60
1:A:116:PHE:HB2	1:A:258:TYR:HE1	1.66	0.60
1:C:42:GLN:HB2	1:C:101:ILE:HG12	1.84	0.60
1:A:247:LEU:HD12	1:B:247:LEU:HD11	1.84	0.60
1:C:175:TYR:CE1	1:C:188:PHE:HD1	2.19	0.60
1:A:72:TRP:CZ2	1:A:74:PRO:HG3	2.37	0.60
1:D:247:LEU:HD12	1:E:247:LEU:HD11	1.83	0.60
1:G:79:ILE:HD11	1:G:131:GLU:HB3	1.83	0.60
1:H:42:GLN:HB2	1:H:101:ILE:HG12	1.84	0.60
1:I:264:GLN:HA	1:I:267:ILE:HG13	1.83	0.60
1:D:17:SER:HB2	1:D:40:VAL:HG23	1.84	0.60
1:H:17:SER:HB2	1:H:40:VAL:HG23	1.82	0.60
1:I:42:GLN:HB2	1:I:101:ILE:HG12	1.84	0.60
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.83	0.60
1:D:219:SER:HA	1:D:238:LEU:HD21	1.83	0.60
1:J:116:PHE:HB2	1:J:258:TYR:HE1	1.66	0.60
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.84	0.60
1:B:179:SER:O	1:B:182:GLN:NE2	2.34	0.59
1:F:42:GLN:HB2	1:F:101:ILE:HG12	1.83	0.59
1:I:179:SER:O	1:I:182:GLN:NE2	2.35	0.59
1:D:27:ASN:HB3	1:D:32:THR:HB	1.83	0.59
1:E:179:SER:O	1:E:182:GLN:NE2	2.35	0.59
1:F:27:ASN:HB3	1:F:32:THR:HB	1.85	0.59
1:A:16:VAL:HG11	1:A:191:ILE:HD13	1.85	0.59
1:I:116:PHE:HB2	1:I:258:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:THR:HA	1:C:99:ARG:HA	1.83	0.59
1:D:56:LEU:HD22	1:D:57:ILE:H	1.68	0.59
1:H:19:PHE:CE1	1:H:146:GLN:HG3	2.38	0.59
1:A:76:LEU:HB3	1:A:130:LEU:HD21	1.85	0.59
1:G:42:GLN:HB2	1:G:101:ILE:HG12	1.84	0.59
1:H:175:TYR:CE1	1:H:188:PHE:HD1	2.21	0.59
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.83	0.59
1:B:22:LYS:HE3	1:B:24:TYR:HD1	1.67	0.59
1:A:175:TYR:CE1	1:A:188:PHE:HD1	2.20	0.59
1:D:131:GLU:OE2	1:D:175:TYR:OH	2.20	0.59
1:D:179:SER:O	1:D:182:GLN:NE2	2.35	0.59
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.83	0.59
1:E:27:ASN:HB3	1:E:32:THR:HB	1.84	0.59
1:D:116:PHE:HB2	1:D:258:TYR:HE1	1.67	0.58
1:H:72:TRP:CZ2	1:H:74:PRO:HG3	2.38	0.58
1:E:212:LEU:HD23	1:E:245:TYR:CE2	2.37	0.58
1:I:22:LYS:HE3	1:I:24:TYR:HD1	1.67	0.58
1:A:264:GLN:HA	1:A:267:ILE:HG13	1.84	0.58
1:G:31:GLN:HG2	1:G:114:MET:HB2	1.86	0.58
1:A:281:ILE:HG13	1:E:224:TRP:HE3	1.68	0.58
1:B:175:TYR:CE1	1:B:188:PHE:HD1	2.21	0.58
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.86	0.58
1:H:79:ILE:HD11	1:H:131:GLU:HB3	1.84	0.58
1:H:44:THR:HA	1:H:99:ARG:HA	1.85	0.58
1:F:17:SER:HB2	1:F:40:VAL:HG23	1.85	0.58
1:A:226:GLU:OE2	1:B:284:HIS:NE2	2.36	0.58
1:G:264:GLN:HA	1:G:267:ILE:HG13	1.86	0.58
1:I:72:TRP:CZ2	1:I:74:PRO:HG3	2.38	0.58
1:H:94:LEU:HB3	1:H:100:VAL:HG22	1.84	0.58
1:H:16:VAL:HG11	1:H:191:ILE:HD13	1.86	0.57
1:F:19:PHE:CE1	1:F:146:GLN:HG3	2.39	0.57
1:C:205:LEU:HD23	1:C:209:ILE:HG13	1.86	0.57
1:G:168:THR:O	1:G:169:HIS:HB2	2.04	0.57
1:C:116:PHE:HB2	1:C:258:TYR:HE1	1.69	0.57
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.86	0.57
1:H:116:PHE:HB2	1:H:258:TYR:HE1	1.69	0.57
1:C:264:GLN:HA	1:C:267:ILE:HG13	1.87	0.57
1:B:22:LYS:HE3	1:B:24:TYR:CD1	2.40	0.57
1:I:71:LEU:HD22	1:I:72:TRP:O	2.04	0.57
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.86	0.57
1:E:175:TYR:CE1	1:E:188:PHE:HD1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:HD11	1:D:131:GLU:HB3	1.85	0.57
1:G:22:LYS:HE3	1:G:24:TYR:CD1	2.40	0.57
1:F:116:PHE:HB2	1:F:258:TYR:HE1	1.68	0.57
1:I:17:SER:HB2	1:I:40:VAL:HG23	1.86	0.57
1:J:264:GLN:HA	1:J:267:ILE:HG13	1.87	0.57
1:H:264:GLN:HA	1:H:267:ILE:HG13	1.86	0.57
1:D:72:TRP:CZ2	1:D:74:PRO:HG3	2.40	0.57
1:J:62:GLN:CA	1:J:62:GLN:HE21	1.98	0.56
1:J:175:TYR:CE1	1:J:188:PHE:HD1	2.23	0.56
1:J:22:LYS:HE3	1:J:24:TYR:CD1	2.39	0.56
1:J:44:THR:HA	1:J:99:ARG:HA	1.87	0.56
1:F:76:LEU:HB3	1:F:130:LEU:HD21	1.87	0.56
1:B:219:SER:HA	1:B:238:LEU:HD21	1.86	0.56
1:F:219:SER:HA	1:F:238:LEU:HD21	1.86	0.56
1:A:44:THR:HA	1:A:99:ARG:HA	1.87	0.56
1:F:28:THR:HA	1:F:116:PHE:HE1	1.70	0.56
1:F:22:LYS:HE3	1:F:24:TYR:HD1	1.68	0.56
1:C:94:LEU:HB3	1:C:100:VAL:HG22	1.86	0.56
1:H:27:ASN:HB3	1:H:32:THR:HB	1.86	0.56
1:D:42:GLN:HB2	1:D:101:ILE:HG12	1.86	0.56
1:I:94:LEU:HB3	1:I:100:VAL:HG22	1.86	0.56
1:G:224:TRP:CE3	1:H:281:ILE:HG13	2.36	0.56
1:H:219:SER:HA	1:H:238:LEU:HD21	1.86	0.56
1:H:179:SER:O	1:H:182:GLN:NE2	2.38	0.56
1:D:212:LEU:HD23	1:D:245:TYR:CE2	2.40	0.56
1:B:252:ILE:HD13	1:C:255:ARG:HG3	1.88	0.56
1:I:175:TYR:CE1	1:I:188:PHE:HD1	2.24	0.56
1:A:212:LEU:HD23	1:A:245:TYR:CE2	2.41	0.56
1:I:27:ASN:HB3	1:I:32:THR:HB	1.88	0.56
1:E:264:GLN:HA	1:E:267:ILE:HG13	1.88	0.56
1:B:94:LEU:HB3	1:B:100:VAL:HG22	1.88	0.56
1:E:116:PHE:HB2	1:E:258:TYR:HE1	1.71	0.56
1:I:16:VAL:HG11	1:I:191:ILE:HD13	1.87	0.56
1:F:44:THR:HA	1:F:99:ARG:HA	1.88	0.56
1:G:175:TYR:CE1	1:G:188:PHE:HD1	2.24	0.56
1:A:19:PHE:CE1	1:A:146:GLN:HG3	2.41	0.55
1:D:298:GLN:HG3	1:D:299:ARG:HG3	1.88	0.55
1:H:22:LYS:HE3	1:H:24:TYR:HD1	1.71	0.55
1:F:72:TRP:CZ2	1:F:74:PRO:HG3	2.40	0.55
1:F:67:ILE:HG22	1:J:62:GLN:OE1	2.06	0.55
1:E:178:LEU:HD11	1:E:182:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HE3	1:A:24:TYR:HD1	1.72	0.55
1:D:19:PHE:CE1	1:D:146:GLN:HG3	2.41	0.55
1:I:22:LYS:HE3	1:I:24:TYR:CD1	2.40	0.55
1:H:115:ASP:OD2	1:H:117:ARG:NE	2.38	0.55
1:B:264:GLN:HA	1:B:267:ILE:HG13	1.88	0.55
1:E:42:GLN:HB2	1:E:101:ILE:HG12	1.88	0.55
1:C:22:LYS:HE3	1:C:24:TYR:HD1	1.70	0.55
1:B:16:VAL:HG11	1:B:191:ILE:HD13	1.87	0.55
1:I:212:LEU:HD23	1:I:245:TYR:CE2	2.42	0.55
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.88	0.55
1:G:72:TRP:CZ2	1:G:74:PRO:HG3	2.41	0.55
1:I:72:TRP:HZ3	1:I:135:TYR:CZ	2.25	0.55
1:H:252:ILE:HD13	1:I:255:ARG:HG3	1.89	0.55
1:C:19:PHE:CE1	1:C:146:GLN:HG3	2.41	0.55
1:J:27:ASN:HB3	1:J:32:THR:HB	1.87	0.55
1:H:212:LEU:HD23	1:H:245:TYR:CE2	2.42	0.55
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.25	0.54
1:B:17:SER:HB2	1:B:40:VAL:HG23	1.88	0.54
1:C:27:ASN:HB3	1:C:32:THR:HB	1.87	0.54
1:J:298:GLN:HG3	1:J:299:ARG:HG3	1.89	0.54
1:I:115:ASP:OD2	1:I:117:ARG:NE	2.38	0.54
1:J:19:PHE:CE1	1:J:146:GLN:HG3	2.42	0.54
1:B:76:LEU:HB3	1:B:130:LEU:HD21	1.89	0.54
1:D:94:LEU:HB3	1:D:100:VAL:HG22	1.89	0.54
1:I:19:PHE:CE1	1:I:146:GLN:HG3	2.42	0.54
1:C:224:TRP:CE3	1:D:281:ILE:HG13	2.35	0.54
1:B:72:TRP:CZ2	1:B:74:PRO:HG3	2.42	0.54
1:C:115:ASP:OD2	1:C:117:ARG:NE	2.38	0.54
1:A:247:LEU:HD23	1:E:248:TYR:HB2	1.89	0.54
1:E:28:THR:HA	1:E:116:PHE:HE1	1.73	0.54
1:G:16:VAL:HG11	1:G:191:ILE:HD13	1.90	0.54
1:F:247:LEU:HD11	1:J:247:LEU:HD12	1.89	0.54
1:G:44:THR:HA	1:G:99:ARG:HA	1.89	0.54
1:B:247:LEU:HD12	1:C:247:LEU:HD11	1.89	0.54
1:B:178:LEU:HD11	1:B:182:GLN:HG2	1.89	0.54
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.89	0.54
1:B:298:GLN:HG3	1:B:299:ARG:HG3	1.89	0.54
1:B:168:THR:O	1:B:169:HIS:HB2	2.06	0.54
1:A:178:LEU:HD11	1:A:182:GLN:HG2	1.90	0.54
1:C:22:LYS:HE3	1:C:24:TYR:CD1	2.43	0.54
1:E:56:LEU:HD22	1:E:57:ILE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.42	0.54
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.90	0.54
1:B:131:GLU:OE2	1:B:175:TYR:OH	2.23	0.54
1:C:304:PHE:HD1	1:C:305:PRO:HD3	1.72	0.54
1:D:76:LEU:HB3	1:D:130:LEU:HD21	1.90	0.54
1:I:298:GLN:HG3	1:I:299:ARG:HG3	1.89	0.53
1:D:44:THR:HA	1:D:99:ARG:HA	1.90	0.53
1:D:226:GLU:OE2	1:E:284:HIS:NE2	2.41	0.53
1:E:215:ILE:HG21	1:E:241:THR:HG21	1.90	0.53
1:A:17:SER:HB2	1:A:40:VAL:HG23	1.90	0.53
1:I:131:GLU:OE2	1:I:175:TYR:OH	2.26	0.53
1:D:28:THR:HA	1:D:116:PHE:HE1	1.74	0.53
1:H:178:LEU:HD11	1:H:182:GLN:HG2	1.90	0.53
1:H:22:LYS:HE3	1:H:24:TYR:CD1	2.43	0.53
1:B:304:PHE:HD1	1:B:305:PRO:HD3	1.74	0.53
1:G:252:ILE:HD13	1:H:255:ARG:HG3	1.90	0.53
1:I:165:LYS:HD3	1:I:166:ALA:H	1.73	0.53
1:C:28:THR:HA	1:C:116:PHE:HE1	1.74	0.53
1:G:17:SER:HB2	1:G:40:VAL:HG23	1.90	0.53
1:G:298:GLN:HG3	1:G:299:ARG:HG3	1.91	0.53
1:F:22:LYS:HE3	1:F:24:TYR:CD1	2.44	0.53
1:J:28:THR:HA	1:J:116:PHE:HE1	1.72	0.53
1:G:219:SER:HA	1:G:238:LEU:HD21	1.90	0.53
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.91	0.53
1:E:17:SER:HB2	1:E:40:VAL:HG23	1.91	0.53
1:A:304:PHE:HD1	1:A:305:PRO:HD3	1.74	0.53
1:D:16:VAL:HG11	1:D:191:ILE:HD13	1.90	0.53
1:F:61:THR:HG22	1:F:62:GLN:HE21	1.74	0.53
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.89	0.53
1:J:17:SER:HB2	1:J:40:VAL:HG23	1.91	0.53
1:J:119:PHE:HB2	1:J:260:THR:HB	1.91	0.53
1:B:71:LEU:HD22	1:B:72:TRP:O	2.09	0.53
1:E:298:GLN:HG3	1:E:299:ARG:HG3	1.91	0.53
1:I:28:THR:HA	1:I:116:PHE:HE1	1.73	0.53
1:J:178:LEU:HD11	1:J:182:GLN:HG2	1.92	0.52
1:F:281:ILE:HG13	1:J:224:TRP:CE3	2.44	0.52
1:F:252:ILE:HD13	1:G:255:ARG:HG3	1.90	0.52
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.91	0.52
1:F:212:LEU:HD23	1:F:245:TYR:CE2	2.45	0.52
1:H:28:THR:HA	1:H:116:PHE:HE1	1.74	0.52
1:G:165:LYS:HD3	1:G:166:ALA:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:304:PHE:HD1	1:I:305:PRO:HD3	1.75	0.52
1:A:42:GLN:HB2	1:A:101:ILE:HG12	1.91	0.52
1:H:56:LEU:HD22	1:H:57:ILE:H	1.74	0.52
1:C:178:LEU:HD11	1:C:182:GLN:HG2	1.91	0.52
1:G:178:LEU:HD11	1:G:182:GLN:HG2	1.91	0.52
1:F:94:LEU:HB3	1:F:100:VAL:HG22	1.92	0.52
1:F:264:GLN:HA	1:F:267:ILE:HG13	1.92	0.52
1:B:212:LEU:HD23	1:B:245:TYR:CE2	2.44	0.52
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.91	0.52
1:H:76:LEU:HB3	1:H:130:LEU:HD21	1.91	0.52
1:A:22:LYS:HE3	1:A:24:TYR:CD1	2.45	0.52
1:G:212:LEU:HD23	1:G:245:TYR:CE2	2.44	0.52
1:E:115:ASP:OD2	1:E:117:ARG:NE	2.39	0.52
1:I:211:PRO:O	1:I:215:ILE:HG13	2.10	0.52
1:H:298:GLN:HG3	1:H:299:ARG:HG3	1.92	0.52
1:A:79:ILE:HD11	1:A:131:GLU:HB3	1.92	0.52
1:F:105:ARG:HD3	1:G:77:GLU:OE2	2.10	0.52
1:G:28:THR:HA	1:G:116:PHE:HE1	1.75	0.51
1:J:260:THR:N	1:J:263:ASP:HB2	2.23	0.51
1:I:178:LEU:HD11	1:I:182:GLN:HG2	1.91	0.51
1:G:19:PHE:CE1	1:G:146:GLN:HG3	2.45	0.51
1:G:76:LEU:HB3	1:G:130:LEU:HD21	1.92	0.51
1:F:298:GLN:HG3	1:F:299:ARG:HG3	1.92	0.51
1:D:117:ARG:O	1:D:119:PHE:N	2.43	0.51
1:F:178:LEU:HD11	1:F:182:GLN:HG2	1.92	0.51
1:D:178:LEU:HD11	1:D:182:GLN:HG2	1.92	0.51
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.28	0.51
1:C:232:LEU:HD21	1:C:281:ILE:HD13	1.91	0.51
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.33	0.51
1:B:165:LYS:HD3	1:B:166:ALA:H	1.74	0.51
1:H:63:ILE:O	1:H:67:ILE:HD12	2.09	0.51
1:H:224:TRP:CE3	1:I:281:ILE:HG13	2.42	0.51
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.76	0.51
1:D:140:LEU:HD12	1:D:189:SER:O	2.10	0.51
1:B:152:ILE:HD11	1:I:152:ILE:HD12	1.92	0.51
1:I:157:ILE:HD13	1:J:258:TYR:CE2	2.46	0.51
1:J:36:ASP:HB2	1:J:107:LEU:HD12	1.93	0.51
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.11	0.51
1:C:298:GLN:HG3	1:C:299:ARG:HG3	1.91	0.51
1:H:247:LEU:HD12	1:I:247:LEU:HD11	1.91	0.51
1:B:44:THR:HA	1:B:99:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:PRO:O	1:E:215:ILE:HG13	2.11	0.51
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.92	0.51
1:G:71:LEU:HD22	1:G:72:TRP:O	2.11	0.51
1:F:247:LEU:HD12	1:G:247:LEU:HD11	1.92	0.51
1:I:260:THR:N	1:I:263:ASP:HB2	2.23	0.50
1:J:116:PHE:HB2	1:J:258:TYR:CE1	2.46	0.50
1:J:211:PRO:O	1:J:215:ILE:HG13	2.11	0.50
1:F:211:PRO:O	1:F:215:ILE:HG13	2.11	0.50
1:B:56:LEU:HD22	1:B:57:ILE:H	1.76	0.50
1:A:298:GLN:HG3	1:A:299:ARG:HG3	1.93	0.50
1:G:248:TYR:HB2	1:H:247:LEU:HD23	1.93	0.50
1:A:36:ASP:HB2	1:A:107:LEU:HD12	1.93	0.50
1:J:76:LEU:HB3	1:J:130:LEU:HD21	1.92	0.50
1:G:230:GLU:HB3	1:H:233:GLN:NE2	2.25	0.50
1:D:232:LEU:HD13	1:D:236:PHE:HE1	1.77	0.50
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.37	0.50
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.29	0.50
1:C:72:TRP:CZ2	1:C:74:PRO:HG3	2.47	0.50
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.94	0.50
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.93	0.50
1:J:131:GLU:OE2	1:J:175:TYR:OH	2.28	0.50
1:A:71:LEU:HD22	1:A:72:TRP:O	2.11	0.50
1:G:211:PRO:O	1:G:215:ILE:HG13	2.12	0.50
1:J:304:PHE:HD1	1:J:305:PRO:HD3	1.77	0.50
1:E:168:THR:O	1:E:169:HIS:HB2	2.12	0.50
1:F:258:TYR:CE2	1:J:157:ILE:HD13	2.47	0.49
1:A:94:LEU:HB3	1:A:100:VAL:HG22	1.94	0.49
1:I:76:LEU:HB3	1:I:130:LEU:HD21	1.94	0.49
1:F:168:THR:O	1:F:169:HIS:HB2	2.11	0.49
1:J:23:ILE:HG21	1:J:126:PHE:CD1	2.47	0.49
1:F:304:PHE:HD1	1:F:305:PRO:HD3	1.77	0.49
1:G:260:THR:H	1:G:263:ASP:CB	2.22	0.49
1:B:119:PHE:HB2	1:B:260:THR:HB	1.93	0.49
1:I:247:LEU:HD12	1:J:247:LEU:HD11	1.94	0.49
1:G:56:LEU:HD22	1:G:57:ILE:N	2.24	0.49
1:J:71:LEU:HD22	1:J:72:TRP:O	2.12	0.49
1:A:115:ASP:OD2	1:A:117:ARG:NE	2.38	0.49
1:B:28:THR:HA	1:B:116:PHE:HE1	1.77	0.49
1:D:66:TRP:O	1:D:71:LEU:HB2	2.12	0.49
1:G:232:LEU:HD13	1:G:236:PHE:HE1	1.76	0.49
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LEU:HD22	1:E:72:TRP:O	2.13	0.49
1:F:56:LEU:HD22	1:F:57:ILE:N	2.25	0.49
1:H:131:GLU:OE2	1:H:175:TYR:OH	2.28	0.49
1:A:165:LYS:HD3	1:A:166:ALA:H	1.77	0.49
1:C:76:LEU:HB3	1:C:130:LEU:HD21	1.93	0.49
1:E:304:PHE:HD1	1:E:305:PRO:HD3	1.76	0.49
1:D:165:LYS:HD3	1:D:166:ALA:H	1.76	0.49
1:H:304:PHE:HD1	1:H:305:PRO:HD3	1.76	0.49
1:B:248:TYR:HB2	1:C:247:LEU:HD23	1.94	0.49
1:F:72:TRP:HZ3	1:F:135:TYR:CZ	2.30	0.49
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.47	0.49
1:A:64:GLU:HG3	1:E:61:THR:HG21	1.95	0.49
1:I:56:LEU:HD22	1:I:57:ILE:N	2.27	0.49
1:J:212:LEU:HD23	1:J:245:TYR:CE2	2.47	0.49
1:C:228:PHE:HE1	1:C:281:ILE:HD12	1.78	0.49
1:F:247:LEU:HA	1:F:247:LEU:HD22	1.56	0.49
1:A:258:TYR:CE2	1:E:157:ILE:HD13	2.48	0.49
1:D:115:ASP:OD2	1:D:117:ARG:NE	2.40	0.48
1:D:211:PRO:O	1:D:215:ILE:HG13	2.12	0.48
1:G:94:LEU:HB3	1:G:100:VAL:HG22	1.95	0.48
1:A:224:TRP:HE3	1:B:281:ILE:HG13	1.78	0.48
1:B:116:PHE:HB2	1:B:258:TYR:CE1	2.46	0.48
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.60	0.48
1:F:299:ARG:HA	1:F:301:ARG:HG3	1.96	0.48
1:J:299:ARG:HA	1:J:301:ARG:HG3	1.96	0.48
1:I:228:PHE:HE1	1:I:281:ILE:HD12	1.78	0.48
1:F:71:LEU:HD22	1:F:72:TRP:O	2.13	0.48
1:G:72:TRP:HZ3	1:G:135:TYR:CZ	2.31	0.48
1:D:247:LEU:HD22	1:D:247:LEU:HA	1.57	0.48
1:D:232:LEU:HD21	1:D:281:ILE:HD13	1.96	0.48
1:I:224:TRP:HE3	1:J:281:ILE:HG13	1.77	0.48
1:G:117:ARG:O	1:G:119:PHE:N	2.46	0.48
1:D:260:THR:N	1:D:263:ASP:HB2	2.24	0.48
1:J:94:LEU:HB3	1:J:100:VAL:HG22	1.95	0.48
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.56	0.48
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.32	0.48
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.95	0.48
1:F:248:TYR:HB2	1:G:247:LEU:HD23	1.96	0.48
1:C:56:LEU:HD22	1:C:57:ILE:N	2.28	0.48
1:F:89:ASN:H	1:F:105:ARG:HB3	1.79	0.48
1:A:252:ILE:HD13	1:B:255:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:LEU:HD22	1:I:247:LEU:HA	1.61	0.48
1:C:230:GLU:HB3	1:D:233:GLN:NE2	2.29	0.48
1:G:225:LEU:HA	1:G:225:LEU:HD23	1.75	0.48
1:H:249:THR:HG23	1:H:253:LEU:HD22	1.96	0.47
1:G:215:ILE:HG21	1:G:241:THR:HG21	1.96	0.47
1:F:165:LYS:HD3	1:F:166:ALA:H	1.79	0.47
1:B:105:ARG:HG3	1:B:106:PHE:N	2.29	0.47
1:H:225:LEU:HA	1:H:225:LEU:HD23	1.77	0.47
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.96	0.47
1:H:252:ILE:HG22	1:H:253:LEU:HD13	1.97	0.47
1:E:72:TRP:CZ2	1:E:74:PRO:HG3	2.50	0.47
1:B:211:PRO:O	1:B:215:ILE:HG13	2.13	0.47
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.96	0.47
1:B:226:GLU:OE2	1:C:284:HIS:NE2	2.47	0.47
1:A:232:LEU:HD13	1:A:236:PHE:HE1	1.79	0.47
1:F:232:LEU:HD21	1:F:281:ILE:HD13	1.96	0.47
1:E:260:THR:N	1:E:263:ASP:HB2	2.23	0.47
1:G:215:ILE:HG23	1:H:239:MET:HG2	1.96	0.47
1:D:252:ILE:HD13	1:E:255:ARG:HG3	1.97	0.47
1:I:58:VAL:HG12	1:I:63:ILE:CD1	2.45	0.47
1:G:115:ASP:OD2	1:G:117:ARG:NE	2.39	0.47
1:I:143:SER:HB2	1:I:170:ILE:HD11	1.96	0.47
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.33	0.47
1:H:116:PHE:HB2	1:H:258:TYR:CE1	2.50	0.47
1:E:143:SER:HB3	1:E:168:THR:HG21	1.96	0.47
1:H:105:ARG:HD3	1:I:77:GLU:OE2	2.14	0.47
1:C:168:THR:O	1:C:169:HIS:HB2	2.14	0.47
1:A:255:ARG:HG3	1:E:252:ILE:HD13	1.96	0.47
1:G:260:THR:N	1:G:263:ASP:HB2	2.23	0.47
1:H:66:TRP:O	1:H:71:LEU:HB2	2.14	0.47
1:F:215:ILE:HG21	1:F:241:THR:HG21	1.96	0.47
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.95	0.47
1:E:165:LYS:HD3	1:E:166:ALA:H	1.80	0.47
1:I:232:LEU:HD13	1:I:236:PHE:HE1	1.79	0.47
1:F:228:PHE:HE1	1:F:281:ILE:HD12	1.79	0.47
1:I:140:LEU:HD13	1:I:191:ILE:CG1	2.39	0.47
1:E:119:PHE:HB2	1:E:260:THR:HB	1.96	0.47
1:A:119:PHE:HB2	1:A:260:THR:HB	1.96	0.47
1:D:116:PHE:HB2	1:D:258:TYR:CE1	2.49	0.47
1:J:215:ILE:HG21	1:J:241:THR:HG21	1.96	0.47
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.59	0.47
1:J:271:GLY:O	1:J:275:ALA:N	2.48	0.47
1:J:33:TYR:OH	1:J:127:VAL:N	2.43	0.47
1:C:210:LEU:HD23	1:C:211:PRO:N	2.29	0.47
1:B:230:GLU:OE1	1:C:229:SER:OG	2.33	0.47
1:H:140:LEU:HD13	1:H:191:ILE:CG1	2.36	0.47
1:J:56:LEU:HD22	1:J:57:ILE:N	2.29	0.47
1:B:61:THR:HG21	1:C:64:GLU:HG3	1.97	0.47
1:G:304:PHE:HD1	1:G:305:PRO:HD3	1.79	0.47
1:D:304:PHE:HD1	1:D:305:PRO:HD3	1.79	0.47
1:J:168:THR:O	1:J:169:HIS:HB2	2.14	0.47
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.60	0.47
1:B:232:LEU:HD21	1:B:281:ILE:HD13	1.96	0.47
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.15	0.47
1:F:117:ARG:O	1:F:119:PHE:N	2.48	0.47
1:I:238:LEU:HD12	1:I:238:LEU:HA	1.84	0.47
1:D:22:LYS:HE3	1:D:24:TYR:CD1	2.50	0.47
1:H:168:THR:O	1:H:169:HIS:HB2	2.14	0.47
1:C:232:LEU:HD13	1:C:236:PHE:HE1	1.80	0.46
1:A:27:ASN:ND2	1:A:30:GLU:HB2	2.30	0.46
1:F:36:ASP:HB2	1:F:107:LEU:HD12	1.98	0.46
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.50	0.46
1:D:63:ILE:O	1:D:67:ILE:HD12	2.15	0.46
1:D:124:GLN:OE1	1:D:124:GLN:HA	2.14	0.46
1:D:225:LEU:HA	1:D:225:LEU:HD23	1.74	0.46
1:H:71:LEU:HD22	1:H:72:TRP:O	2.16	0.46
1:D:72:TRP:CZ3	1:D:135:TYR:CZ	3.04	0.46
1:H:143:SER:HB3	1:H:168:THR:HG21	1.96	0.46
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.51	0.46
1:B:294:ASP:HB3	1:B:297:ILE:HB	1.97	0.46
1:E:140:LEU:HD12	1:E:189:SER:O	2.15	0.46
1:I:72:TRP:CZ3	1:I:135:TYR:CZ	3.04	0.46
1:I:63:ILE:O	1:I:67:ILE:HD12	2.15	0.46
1:H:119:PHE:HB2	1:H:260:THR:HB	1.96	0.46
1:H:248:TYR:HB2	1:I:247:LEU:HD23	1.96	0.46
1:D:131:GLU:OE1	1:D:190:ARG:NE	2.45	0.46
1:D:264:GLN:O	1:D:267:ILE:N	2.48	0.46
1:I:215:ILE:HG21	1:I:241:THR:HG21	1.97	0.46
1:D:210:LEU:HD23	1:D:211:PRO:N	2.30	0.46
1:C:211:PRO:O	1:C:215:ILE:HG13	2.15	0.46
1:C:165:LYS:HD3	1:C:166:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.67	0.46
1:A:299:ARG:HA	1:A:301:ARG:HG3	1.97	0.46
1:F:205:LEU:HA	1:F:205:LEU:HD23	1.60	0.46
1:D:36:ASP:HB2	1:D:107:LEU:HD12	1.96	0.46
1:J:225:LEU:HA	1:J:225:LEU:HD23	1.69	0.46
1:A:105:ARG:HD3	1:B:77:GLU:OE2	2.16	0.46
1:B:140:LEU:HD12	1:B:189:SER:O	2.15	0.46
1:C:247:LEU:HA	1:C:247:LEU:HD22	1.53	0.46
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.97	0.46
1:D:140:LEU:HD13	1:D:191:ILE:CG1	2.38	0.46
1:F:140:LEU:HD12	1:F:189:SER:O	2.14	0.46
1:B:117:ARG:O	1:B:119:PHE:N	2.49	0.46
1:G:247:LEU:CD1	1:H:247:LEU:HD11	2.43	0.46
1:F:116:PHE:HB2	1:F:258:TYR:CE1	2.50	0.46
1:J:205:LEU:HD23	1:J:205:LEU:HA	1.57	0.46
1:D:228:PHE:HE1	1:D:281:ILE:HD12	1.81	0.46
1:A:28:THR:HA	1:A:116:PHE:HE1	1.79	0.46
1:A:211:PRO:O	1:A:215:ILE:HG13	2.15	0.46
1:J:124:GLN:OE1	1:J:124:GLN:HA	2.15	0.46
1:J:163:ARG:HD3	1:J:163:ARG:HA	1.85	0.46
1:G:264:GLN:O	1:G:267:ILE:N	2.49	0.45
1:I:116:PHE:HB2	1:I:258:TYR:CE1	2.49	0.45
1:E:215:ILE:HG21	1:E:241:THR:CG2	2.45	0.45
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.68	0.45
1:F:210:LEU:HD23	1:F:211:PRO:N	2.31	0.45
1:D:61:THR:HG22	1:D:62:GLN:HE21	1.81	0.45
1:I:232:LEU:HD21	1:I:281:ILE:HD13	1.97	0.45
1:I:178:LEU:HD23	1:I:186:ASN:HB3	1.97	0.45
1:J:66:TRP:O	1:J:71:LEU:HB2	2.17	0.45
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.98	0.45
1:H:232:LEU:HD21	1:H:281:ILE:HD13	1.98	0.45
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.98	0.45
1:J:232:LEU:HD13	1:J:236:PHE:HE1	1.80	0.45
1:F:260:THR:N	1:F:263:ASP:HB2	2.25	0.45
1:F:63:ILE:O	1:F:67:ILE:HD12	2.17	0.45
1:G:228:PHE:HE1	1:G:281:ILE:HD12	1.82	0.45
1:J:131:GLU:HA	1:J:132:PRO:HD2	1.71	0.45
1:F:45:GLY:O	1:F:98:GLY:HA3	2.17	0.45
1:A:116:PHE:HB2	1:A:258:TYR:CE1	2.48	0.45
1:A:168:THR:O	1:A:169:HIS:HB2	2.17	0.45
1:E:228:PHE:HE1	1:E:281:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:LEU:HD21	1:E:281:ILE:HD13	1.97	0.45
1:F:119:PHE:HB2	1:F:260:THR:HB	1.99	0.45
1:F:27:ASN:ND2	1:F:30:GLU:HB2	2.31	0.45
1:B:118:LEU:HG	1:B:118:LEU:H	1.37	0.45
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.81	0.45
1:G:33:TYR:OH	1:G:127:VAL:N	2.43	0.45
1:J:165:LYS:HD3	1:J:166:ALA:H	1.81	0.45
1:I:36:ASP:HB2	1:I:107:LEU:HD12	1.99	0.45
1:B:232:LEU:HD13	1:B:236:PHE:HE1	1.81	0.45
1:C:119:PHE:HB2	1:C:260:THR:HB	1.97	0.45
1:F:178:LEU:HD23	1:F:186:ASN:HB3	1.97	0.45
1:E:178:LEU:HD23	1:E:186:ASN:HB3	1.99	0.45
1:H:57:ILE:CG1	1:H:93:MET:HG3	2.47	0.45
1:B:57:ILE:HG12	1:B:93:MET:HG3	1.98	0.45
1:E:94:LEU:HB3	1:E:100:VAL:HG22	1.99	0.45
1:J:45:GLY:O	1:J:98:GLY:HA3	2.16	0.45
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.61	0.45
1:D:33:TYR:OH	1:D:127:VAL:N	2.46	0.45
1:G:140:LEU:HD12	1:G:189:SER:O	2.17	0.45
1:H:228:PHE:HE1	1:H:281:ILE:HD12	1.82	0.45
1:J:228:PHE:HE1	1:J:281:ILE:HD12	1.82	0.45
1:D:224:TRP:HE3	1:E:281:ILE:HG13	1.82	0.45
1:D:119:PHE:HB2	1:D:260:THR:HB	1.98	0.45
1:D:247:LEU:CD1	1:E:247:LEU:HD11	2.47	0.45
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.67	0.45
1:D:45:GLY:O	1:D:98:GLY:HA3	2.17	0.45
1:H:215:ILE:HG21	1:H:241:THR:HG21	1.98	0.45
1:E:224:TRP:HA	1:E:301:ARG:NH1	2.32	0.45
1:J:260:THR:HG23	1:J:263:ASP:OD2	2.17	0.45
1:C:143:SER:HB3	1:C:168:THR:HG21	1.99	0.45
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.99	0.45
1:E:222:VAL:HG23	1:E:234:THR:HG22	1.97	0.45
1:G:58:VAL:HG12	1:G:63:ILE:CD1	2.47	0.45
1:J:232:LEU:HD21	1:J:281:ILE:HD13	1.99	0.44
1:J:247:LEU:HD22	1:J:247:LEU:HA	1.60	0.44
1:A:56:LEU:HD22	1:A:57:ILE:N	2.32	0.44
1:H:72:TRP:HZ3	1:H:135:TYR:CZ	2.35	0.44
1:G:72:TRP:CE2	1:G:74:PRO:HG3	2.53	0.44
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.51	0.44
1:I:252:ILE:HG22	1:I:253:LEU:HD13	1.99	0.44
1:C:46:LYS:HA	1:C:47:PRO:HD3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:THR:H	1:E:263:ASP:CB	2.24	0.44
1:A:72:TRP:CE2	1:A:74:PRO:HG3	2.53	0.44
1:F:300:CYS:HB2	1:F:303:ALA:HB3	2.00	0.44
1:J:252:ILE:HG22	1:J:253:LEU:HD13	1.99	0.44
1:B:299:ARG:HA	1:B:301:ARG:HG3	1.99	0.44
1:A:281:ILE:HG13	1:E:224:TRP:CE3	2.50	0.44
1:C:215:ILE:HG21	1:C:241:THR:HG21	1.98	0.44
1:J:39:ILE:HG22	1:J:104:ALA:HB3	1.99	0.44
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.71	0.44
1:G:232:LEU:HD21	1:G:281:ILE:HD13	1.99	0.44
1:J:232:LEU:O	1:J:234:THR:N	2.51	0.44
1:G:116:PHE:HB2	1:G:258:TYR:CE1	2.48	0.44
1:C:72:TRP:CZ3	1:C:135:TYR:CZ	3.06	0.44
1:H:165:LYS:HD3	1:H:166:ALA:H	1.82	0.44
1:A:287:GLN:HB2	1:A:288:ALA:H	1.66	0.44
1:G:61:THR:HG22	1:G:62:GLN:HE21	1.82	0.44
1:I:232:LEU:O	1:I:234:THR:N	2.50	0.44
1:F:157:ILE:HD13	1:G:258:TYR:CE2	2.52	0.44
1:E:172:ASP:C	1:E:173:ILE:HD12	2.38	0.44
1:A:131:GLU:HA	1:A:132:PRO:HD2	1.78	0.44
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.58	0.44
1:D:22:LYS:HE3	1:D:24:TYR:HD1	1.83	0.44
1:G:300:CYS:HB2	1:G:303:ALA:HB3	2.00	0.44
1:G:163:ARG:HA	1:G:163:ARG:HD3	1.83	0.44
1:J:117:ARG:O	1:J:119:PHE:N	2.50	0.44
1:G:178:LEU:HD23	1:G:186:ASN:HB3	1.99	0.44
1:B:234:THR:OG1	1:C:233:GLN:HG2	2.18	0.44
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.53	0.44
1:G:105:ARG:HG3	1:G:106:PHE:N	2.32	0.44
1:A:140:LEU:HD13	1:A:191:ILE:CG1	2.43	0.44
1:H:260:THR:HG23	1:H:263:ASP:OD2	2.18	0.44
1:E:131:GLU:OE1	1:E:190:ARG:NE	2.45	0.44
1:H:172:ASP:C	1:H:173:ILE:HD12	2.38	0.44
1:G:105:ARG:HD3	1:H:77:GLU:OE2	2.17	0.44
1:I:119:PHE:HB2	1:I:260:THR:HB	1.99	0.44
1:F:239:MET:HG2	1:J:215:ILE:HG23	2.00	0.44
1:G:215:ILE:HG21	1:G:241:THR:CG2	2.48	0.44
1:B:210:LEU:HD23	1:B:211:PRO:N	2.32	0.44
1:C:299:ARG:HA	1:C:301:ARG:HG3	1.99	0.43
1:C:178:LEU:HD23	1:C:186:ASN:HB3	2.00	0.43
1:J:143:SER:HB3	1:J:168:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:TYR:OH	1:D:107:LEU:HD11	2.18	0.43
1:D:118:LEU:HG	1:D:118:LEU:H	1.39	0.43
1:H:260:THR:N	1:H:263:ASP:HB2	2.28	0.43
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.59	0.43
1:F:24:TYR:OH	1:F:107:LEU:HD11	2.17	0.43
1:H:211:PRO:O	1:H:215:ILE:HG13	2.18	0.43
1:I:61:THR:HG22	1:I:62:GLN:HE21	1.82	0.43
1:A:63:ILE:O	1:A:67:ILE:HD12	2.18	0.43
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.67	0.43
1:D:253:LEU:HD12	1:D:253:LEU:HA	1.78	0.43
1:D:71:LEU:HD22	1:D:72:TRP:O	2.18	0.43
1:A:58:VAL:HG12	1:A:63:ILE:CD1	2.49	0.43
1:A:118:LEU:HG	1:A:118:LEU:H	1.36	0.43
1:B:224:TRP:CE3	1:C:281:ILE:HG13	2.48	0.43
1:F:271:GLY:O	1:F:275:ALA:N	2.52	0.43
1:B:39:ILE:HG22	1:B:104:ALA:HB3	2.00	0.43
1:E:204:TYR:O	1:E:208:PHE:HB3	2.18	0.43
1:C:118:LEU:HG	1:C:118:LEU:H	1.38	0.43
1:B:238:LEU:HD13	1:C:236:PHE:HD2	1.83	0.43
1:J:115:ASP:OD2	1:J:117:ARG:NE	2.46	0.43
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.17	0.43
1:C:116:PHE:HB2	1:C:258:TYR:CE1	2.50	0.43
1:B:215:ILE:HG21	1:B:241:THR:HG21	1.99	0.43
1:C:313:CYS:O	1:C:316:VAL:HG22	2.18	0.43
1:G:36:ASP:HB2	1:G:107:LEU:HD12	2.00	0.43
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.59	0.43
1:C:294:ASP:HB3	1:C:297:ILE:HB	2.01	0.43
1:H:300:CYS:HB2	1:H:303:ALA:HB3	2.00	0.43
1:J:216:ILE:O	1:J:219:SER:HB3	2.18	0.43
1:C:248:TYR:HB2	1:D:247:LEU:HD23	2.00	0.43
1:D:56:LEU:HD22	1:D:57:ILE:N	2.32	0.43
1:I:313:CYS:O	1:I:316:VAL:HG22	2.18	0.43
1:I:156:GLU:HA	1:I:200:ASN:HD21	1.82	0.43
1:A:207:SER:HB2	1:B:259:THR:HG22	2.00	0.43
1:F:260:THR:O	1:F:264:GLN:HG3	2.18	0.43
1:A:66:TRP:O	1:A:71:LEU:HB2	2.19	0.43
1:E:178:LEU:HD13	1:E:182:GLN:HE21	1.83	0.43
1:I:72:TRP:CE2	1:I:74:PRO:HG3	2.54	0.43
1:H:253:LEU:HA	1:H:253:LEU:HD12	1.77	0.43
1:G:210:LEU:HD23	1:G:211:PRO:N	2.34	0.43
1:H:45:GLY:O	1:H:98:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:LEU:HA	1:I:225:LEU:HD23	1.74	0.43
1:G:313:CYS:O	1:G:316:VAL:HG22	2.19	0.43
1:B:228:PHE:HA	1:B:231:ARG:HH11	1.84	0.43
1:G:131:GLU:OE2	1:G:175:TYR:OH	2.31	0.43
1:H:131:GLU:HA	1:H:132:PRO:HD2	1.72	0.43
1:A:215:ILE:HG21	1:A:241:THR:HG21	2.00	0.43
1:F:220:TRP:C	1:F:222:VAL:H	2.22	0.43
1:F:225:LEU:HA	1:F:225:LEU:HD23	1.73	0.43
1:C:222:VAL:HG23	1:C:234:THR:HG22	1.99	0.43
1:A:228:PHE:HA	1:A:231:ARG:HH11	1.84	0.43
1:A:178:LEU:HD23	1:A:186:ASN:HB3	1.99	0.43
1:D:178:LEU:HD23	1:D:186:ASN:HB3	2.01	0.43
1:H:227:SER:HB3	1:H:230:GLU:HG3	2.01	0.43
1:I:287:GLN:HB2	1:I:288:ALA:H	1.67	0.43
1:B:264:GLN:O	1:B:267:ILE:N	2.52	0.43
1:G:314:VAL:HA	1:G:317:ILE:HG13	2.00	0.43
1:H:58:VAL:HG12	1:H:63:ILE:CD1	2.48	0.43
1:H:230:GLU:HB3	1:I:233:GLN:NE2	2.34	0.43
1:H:220:TRP:C	1:H:222:VAL:H	2.22	0.43
1:B:271:GLY:O	1:B:275:ALA:N	2.50	0.43
1:C:224:TRP:HA	1:C:301:ARG:NH1	2.34	0.42
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.78	0.42
1:A:314:VAL:HA	1:A:317:ILE:HG13	2.00	0.42
1:J:314:VAL:HA	1:J:317:ILE:HG13	2.01	0.42
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.62	0.42
1:G:58:VAL:HG12	1:G:63:ILE:HD12	2.01	0.42
1:D:156:GLU:HA	1:D:200:ASN:HD21	1.84	0.42
1:C:253:LEU:HD12	1:C:253:LEU:HA	1.84	0.42
1:A:232:LEU:HD21	1:A:281:ILE:HD13	2.01	0.42
1:C:140:LEU:HD13	1:C:191:ILE:CG1	2.38	0.42
1:H:117:ARG:O	1:H:119:PHE:N	2.52	0.42
1:G:27:ASN:ND2	1:G:30:GLU:HB2	2.34	0.42
1:B:27:ASN:OD1	1:B:28:THR:N	2.51	0.42
1:B:178:LEU:HD23	1:B:186:ASN:HB3	2.01	0.42
1:G:72:TRP:CZ3	1:G:135:TYR:CZ	3.07	0.42
1:J:72:TRP:CZ2	1:J:74:PRO:HG3	2.53	0.42
1:H:210:LEU:HD23	1:H:211:PRO:N	2.35	0.42
1:C:300:CYS:HB2	1:C:303:ALA:HB3	2.00	0.42
1:C:163:ARG:HD3	1:C:163:ARG:HA	1.79	0.42
1:A:313:CYS:O	1:A:316:VAL:HG22	2.19	0.42
1:C:117:ARG:O	1:C:119:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:THR:O	1:C:264:GLN:HG3	2.19	0.42
1:A:247:LEU:HA	1:A:247:LEU:HD22	1.50	0.42
1:H:205:LEU:HD23	1:H:205:LEU:HA	1.63	0.42
1:D:215:ILE:HG21	1:D:241:THR:HG21	2.01	0.42
1:H:61:THR:HG22	1:H:62:GLN:HE21	1.83	0.42
1:H:299:ARG:HA	1:H:301:ARG:HG3	2.00	0.42
1:I:66:TRP:O	1:I:71:LEU:HB2	2.19	0.42
1:A:24:TYR:OH	1:A:107:LEU:HD11	2.19	0.42
1:C:105:ARG:HG3	1:C:106:PHE:N	2.34	0.42
1:E:61:THR:HG22	1:E:62:GLN:HE21	1.84	0.42
1:D:284:HIS:HD2	1:D:285:HIS:CE1	2.37	0.42
1:I:300:CYS:HB2	1:I:303:ALA:HB3	2.00	0.42
1:J:220:TRP:C	1:J:222:VAL:H	2.23	0.42
1:A:117:ARG:O	1:A:119:PHE:N	2.52	0.42
1:A:247:LEU:HD11	1:E:247:LEU:CD1	2.48	0.42
1:E:294:ASP:HB3	1:E:297:ILE:HB	2.01	0.42
1:B:46:LYS:HA	1:B:47:PRO:HD3	1.90	0.42
1:D:143:SER:HB3	1:D:168:THR:HG21	2.02	0.42
1:A:228:PHE:HE1	1:A:281:ILE:HD12	1.85	0.42
1:G:119:PHE:HB2	1:G:260:THR:HB	2.02	0.42
1:G:172:ASP:C	1:G:173:ILE:HD12	2.40	0.42
1:A:143:SER:HB3	1:A:168:THR:HG21	2.01	0.42
1:I:124:GLN:HA	1:I:124:GLN:OE1	2.18	0.42
1:I:163:ARG:HD3	1:I:163:ARG:HA	1.80	0.42
1:B:224:TRP:CD1	1:B:301:ARG:HB3	2.54	0.42
1:I:117:ARG:O	1:I:119:PHE:N	2.52	0.42
1:B:172:ASP:C	1:B:173:ILE:HD12	2.40	0.42
1:I:314:VAL:HA	1:I:317:ILE:HG13	2.02	0.42
1:E:252:ILE:HG22	1:E:253:LEU:HD13	2.00	0.42
1:E:271:GLY:O	1:E:275:ALA:N	2.52	0.42
1:G:260:THR:O	1:G:264:GLN:HG3	2.20	0.42
1:H:157:ILE:HD13	1:I:258:TYR:CE2	2.54	0.42
1:I:168:THR:O	1:I:169:HIS:HB2	2.19	0.42
1:B:131:GLU:HA	1:B:132:PRO:HD2	1.77	0.42
1:E:116:PHE:HB2	1:E:258:TYR:CE1	2.52	0.42
1:E:36:ASP:HB2	1:E:107:LEU:HD12	2.00	0.42
1:B:36:ASP:HB2	1:B:107:LEU:HD12	2.00	0.42
1:D:313:CYS:O	1:D:316:VAL:HG22	2.20	0.42
1:I:39:ILE:HG22	1:I:104:ALA:HB3	2.01	0.42
1:C:232:LEU:O	1:C:234:THR:N	2.53	0.42
1:H:224:TRP:CD1	1:H:301:ARG:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:TRP:HA	1:F:301:ARG:NH1	2.35	0.42
1:I:143:SER:HB3	1:I:168:THR:HG21	2.00	0.42
1:H:178:LEU:HD13	1:H:182:GLN:HE21	1.85	0.42
1:C:32:THR:HA	1:C:110:PHE:O	2.19	0.42
1:G:63:ILE:O	1:G:67:ILE:HD12	2.20	0.42
1:B:313:CYS:O	1:B:316:VAL:HG22	2.20	0.42
1:C:45:GLY:O	1:C:98:GLY:HA3	2.19	0.42
1:G:294:ASP:HB3	1:G:297:ILE:HB	2.00	0.42
1:F:213:GLY:O	1:F:217:ALA:N	2.48	0.42
1:E:45:GLY:O	1:E:98:GLY:HA3	2.19	0.42
1:F:145:ILE:HG21	1:F:193:VAL:HG11	2.01	0.42
1:E:216:ILE:HD13	1:E:216:ILE:HA	1.94	0.42
1:B:260:THR:O	1:B:264:GLN:HG3	2.20	0.42
1:H:216:ILE:O	1:H:219:SER:HB3	2.20	0.42
1:E:131:GLU:OE2	1:E:175:TYR:OH	2.30	0.42
1:I:264:GLN:O	1:I:267:ILE:N	2.53	0.42
1:F:66:TRP:O	1:F:71:LEU:HB2	2.20	0.42
1:I:62:GLN:NE2	1:I:62:GLN:HA	2.35	0.42
1:D:284:HIS:HD2	1:D:285:HIS:ND1	2.17	0.42
1:D:294:ASP:HB3	1:D:297:ILE:HB	2.02	0.42
1:F:232:LEU:O	1:F:234:THR:N	2.54	0.41
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.84	0.41
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.88	0.41
1:I:147:VAL:HB	1:I:165:LYS:NZ	2.35	0.41
1:B:57:ILE:CG1	1:B:93:MET:HG3	2.50	0.41
1:B:105:ARG:HD3	1:C:77:GLU:OE2	2.20	0.41
1:B:61:THR:HG21	1:C:64:GLU:CG	2.50	0.41
1:J:63:ILE:O	1:J:67:ILE:HD12	2.20	0.41
1:J:89:ASN:H	1:J:105:ARG:HB3	1.85	0.41
1:A:294:ASP:HB3	1:A:297:ILE:HB	2.01	0.41
1:F:216:ILE:O	1:F:219:SER:HB3	2.20	0.41
1:B:115:ASP:OD2	1:B:117:ARG:NE	2.48	0.41
1:G:147:VAL:HB	1:G:165:LYS:NZ	2.35	0.41
1:C:215:ILE:HG23	1:D:239:MET:HG2	2.03	0.41
1:I:120:PRO:HD3	1:I:261:VAL:HB	2.01	0.41
1:D:105:ARG:HG3	1:D:106:PHE:N	2.34	0.41
1:A:271:GLY:O	1:A:275:ALA:N	2.53	0.41
1:A:213:GLY:O	1:A:217:ALA:N	2.49	0.41
1:H:287:GLN:HB2	1:H:288:ALA:H	1.67	0.41
1:B:124:GLN:HA	1:B:124:GLN:OE1	2.19	0.41
1:J:46:LYS:HA	1:J:47:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:GLU:HA	1:I:132:PRO:HD2	1.75	0.41
1:C:38:TYR:HD2	1:C:105:ARG:HA	1.86	0.41
1:B:230:GLU:HB3	1:C:233:GLN:NE2	2.35	0.41
1:I:145:ILE:HG21	1:I:193:VAL:HG11	2.02	0.41
1:E:63:ILE:O	1:E:67:ILE:HD12	2.20	0.41
1:B:33:TYR:OH	1:B:127:VAL:N	2.46	0.41
1:D:72:TRP:CZ3	1:D:135:TYR:CE1	3.08	0.41
1:E:210:LEU:HD23	1:E:211:PRO:N	2.35	0.41
1:D:58:VAL:O	1:D:63:ILE:HD11	2.20	0.41
1:B:287:GLN:HB2	1:B:288:ALA:H	1.61	0.41
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.81	0.41
1:J:145:ILE:HG21	1:J:193:VAL:HG11	2.02	0.41
1:B:72:TRP:CZ3	1:B:135:TYR:CZ	3.09	0.41
1:B:72:TRP:CE2	1:B:74:PRO:HG3	2.56	0.41
1:J:58:VAL:HG12	1:J:63:ILE:HD12	2.02	0.41
1:C:207:SER:HB2	1:D:259:THR:HG22	2.02	0.41
1:B:45:GLY:O	1:B:98:GLY:HA3	2.20	0.41
1:I:38:TYR:HD2	1:I:105:ARG:HA	1.86	0.41
1:D:120:PRO:HD3	1:D:261:VAL:HB	2.02	0.41
1:I:46:LYS:HA	1:I:47:PRO:HD3	1.80	0.41
1:H:294:ASP:HB3	1:H:297:ILE:HB	2.01	0.41
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.76	0.41
1:G:247:LEU:HA	1:G:247:LEU:HD22	1.60	0.41
1:A:260:THR:O	1:A:264:GLN:HG3	2.20	0.41
1:F:72:TRP:CE2	1:F:74:PRO:HG3	2.56	0.41
1:A:230:GLU:OE1	1:B:229:SER:OG	2.38	0.41
1:D:271:GLY:O	1:D:275:ALA:N	2.54	0.41
1:D:314:VAL:HA	1:D:317:ILE:HG13	2.02	0.41
1:J:57:ILE:CG1	1:J:93:MET:HG3	2.50	0.41
1:H:40:VAL:HA	1:H:102:TYR:O	2.20	0.41
1:D:238:LEU:HD13	1:E:236:PHE:CD2	2.55	0.41
1:D:72:TRP:CE2	1:D:74:PRO:HG3	2.56	0.41
1:I:220:TRP:C	1:I:222:VAL:H	2.24	0.41
1:H:271:GLY:O	1:H:275:ALA:N	2.52	0.41
1:I:118:LEU:H	1:I:118:LEU:HG	1.42	0.41
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.67	0.41
1:I:228:PHE:HA	1:I:231:ARG:HH11	1.86	0.41
1:D:216:ILE:HD13	1:D:216:ILE:HA	1.93	0.41
1:E:260:THR:HG23	1:E:263:ASP:OD2	2.21	0.41
1:F:247:LEU:HD23	1:J:248:TYR:HB2	2.03	0.41
1:A:264:GLN:O	1:A:267:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:VAL:HA	1:C:317:ILE:HG13	2.02	0.41
1:B:284:HIS:HD2	1:B:285:HIS:ND1	2.19	0.41
1:I:40:VAL:HA	1:I:102:TYR:O	2.20	0.41
1:C:19:PHE:CD1	1:C:19:PHE:N	2.89	0.41
1:E:313:CYS:O	1:E:316:VAL:HG22	2.21	0.41
1:H:228:PHE:HA	1:H:231:ARG:HH11	1.86	0.41
1:B:260:THR:HG23	1:B:263:ASP:OD2	2.21	0.41
1:E:312:GLY:HA2	1:E:315:LEU:HB2	2.03	0.41
1:C:119:PHE:O	1:C:121:PHE:N	2.54	0.41
1:H:314:VAL:HA	1:H:317:ILE:HG13	2.03	0.41
1:G:57:ILE:CG1	1:G:93:MET:HG3	2.51	0.41
1:J:182:GLN:O	1:J:184:ASN:N	2.54	0.41
1:A:73:VAL:HA	1:A:74:PRO:HD3	1.95	0.41
1:A:131:GLU:OE2	1:A:175:TYR:OH	2.32	0.41
1:F:36:ASP:OD1	1:F:105:ARG:NH2	2.53	0.41
1:J:210:LEU:HD23	1:J:211:PRO:N	2.35	0.41
1:F:147:VAL:HB	1:F:165:LYS:NZ	2.36	0.41
1:F:255:ARG:HG3	1:J:252:ILE:HD13	2.03	0.41
1:J:105:ARG:HG3	1:J:106:PHE:N	2.35	0.41
1:A:13:ASP:HB3	1:A:141:ARG:HE	1.85	0.41
1:F:26:VAL:HG21	1:F:160:TRP:HZ2	1.85	0.41
1:E:300:CYS:HB2	1:E:303:ALA:HB3	2.03	0.41
1:H:284:HIS:HD2	1:H:285:HIS:CE1	2.39	0.41
1:J:313:CYS:O	1:J:316:VAL:HG22	2.21	0.41
1:G:253:LEU:HD12	1:G:253:LEU:HA	1.84	0.41
1:C:228:PHE:HA	1:C:231:ARG:HH11	1.86	0.41
1:D:228:PHE:HA	1:D:231:ARG:HH11	1.86	0.41
1:H:247:LEU:HA	1:H:247:LEU:HD22	1.67	0.41
1:A:260:THR:HG23	1:A:263:ASP:OD2	2.21	0.41
1:J:178:LEU:HD23	1:J:186:ASN:HB3	2.02	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.88	0.41
1:F:131:GLU:HA	1:F:132:PRO:HD2	1.79	0.41
1:B:38:TYR:HD2	1:B:105:ARG:HA	1.86	0.41
1:I:105:ARG:HD3	1:J:77:GLU:OE2	2.21	0.41
1:E:105:ARG:HG3	1:E:106:PHE:N	2.36	0.41
1:I:216:ILE:O	1:I:219:SER:HB3	2.21	0.40
1:C:224:TRP:CD1	1:C:301:ARG:HB3	2.55	0.40
1:J:228:PHE:HA	1:J:231:ARG:HH11	1.84	0.40
1:F:140:LEU:HD13	1:F:191:ILE:CG1	2.46	0.40
1:B:119:PHE:C	1:B:121:PHE:H	2.24	0.40
1:I:212:LEU:HD11	1:I:265:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:OD1	1:C:105:ARG:NH2	2.54	0.40
1:J:143:SER:HB2	1:J:170:ILE:HD11	2.03	0.40
1:I:253:LEU:HD12	1:I:253:LEU:HA	1.80	0.40
1:J:58:VAL:HG12	1:J:63:ILE:CD1	2.50	0.40
1:G:145:ILE:HG21	1:G:193:VAL:HG11	2.02	0.40
1:F:13:ASP:HB3	1:F:141:ARG:HE	1.86	0.40
1:D:260:THR:HG23	1:D:263:ASP:OD2	2.20	0.40
1:G:216:ILE:HA	1:G:216:ILE:HD13	1.95	0.40
1:G:61:THR:HG21	1:H:64:GLU:HG3	2.03	0.40
1:E:287:GLN:HB2	1:E:288:ALA:H	1.66	0.40
1:D:220:TRP:C	1:D:222:VAL:H	2.24	0.40
1:I:271:GLY:O	1:I:275:ALA:N	2.53	0.40
1:A:163:ARG:HD3	1:A:163:ARG:HA	1.82	0.40
1:I:294:ASP:HB3	1:I:297:ILE:HB	2.03	0.40
1:B:224:TRP:HA	1:B:301:ARG:NH1	2.36	0.40
1:I:236:PHE:C	1:I:238:LEU:H	2.25	0.40
1:B:228:PHE:HE1	1:B:281:ILE:HD12	1.86	0.40
1:D:143:SER:HB2	1:D:170:ILE:HD11	2.02	0.40
1:C:61:THR:HG22	1:C:62:GLN:HE21	1.87	0.40
1:E:184:ASN:O	1:E:185:GLN:HG3	2.22	0.40
1:G:271:GLY:O	1:G:275:ALA:N	2.54	0.40
1:I:33:TYR:OH	1:I:127:VAL:N	2.50	0.40
1:G:116:PHE:HE2	1:G:124:GLN:HE21	1.69	0.40
1:B:260:THR:N	1:B:263:ASP:HB2	2.28	0.40
1:J:140:LEU:HD12	1:J:189:SER:O	2.22	0.40
1:C:119:PHE:C	1:C:121:PHE:H	2.24	0.40
1:C:182:GLN:O	1:C:184:ASN:N	2.54	0.40
1:E:56:LEU:HD22	1:E:57:ILE:N	2.36	0.40
1:D:39:ILE:HG22	1:D:104:ALA:HB3	2.03	0.40
1:A:68:ASN:ND2	1:E:65:ARG:HD2	2.36	0.40
1:H:13:ASP:HB3	1:H:141:ARG:HE	1.85	0.40
1:E:117:ARG:O	1:E:119:PHE:N	2.55	0.40
1:F:260:THR:HG23	1:F:263:ASP:OD2	2.21	0.40
1:B:143:SER:HB3	1:B:168:THR:HG21	2.04	0.40
1:B:32:THR:HA	1:B:110:PHE:O	2.21	0.40
1:I:178:LEU:HD13	1:I:182:GLN:HE21	1.87	0.40
1:F:72:TRP:CZ3	1:F:135:TYR:CE1	3.09	0.40
1:G:40:VAL:HA	1:G:102:TYR:O	2.22	0.40
1:J:215:ILE:HG21	1:J:241:THR:CG2	2.52	0.40
1:B:56:LEU:HD22	1:B:57:ILE:N	2.37	0.40
1:I:77:GLU:HG2	1:I:78:PHE:N	2.37	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	305/324 (94%)	235 (77%)	53 (17%)	17 (6%)	2	29
1	B	305/324 (94%)	230 (75%)	56 (18%)	19 (6%)	2	27
1	C	305/324 (94%)	233 (76%)	56 (18%)	16 (5%)	2	31
1	D	305/324 (94%)	233 (76%)	55 (18%)	17 (6%)	2	29
1	E	305/324 (94%)	235 (77%)	50 (16%)	20 (7%)	1	25
1	F	305/324 (94%)	235 (77%)	51 (17%)	19 (6%)	2	27
1	G	305/324 (94%)	232 (76%)	57 (19%)	16 (5%)	2	31
1	H	305/324 (94%)	234 (77%)	52 (17%)	19 (6%)	2	27
1	I	305/324 (94%)	235 (77%)	55 (18%)	15 (5%)	3	32
1	J	305/324 (94%)	232 (76%)	55 (18%)	18 (6%)	2	28
All	All	3050/3240 (94%)	2334 (76%)	540 (18%)	176 (6%)	2	28

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	169	HIS
1	A	202	SER
1	B	119	PHE
1	B	151	ASN
1	B	169	HIS
1	B	202	SER
1	C	151	ASN
1	C	169	HIS
1	C	202	SER
1	D	118	LEU
1	D	151	ASN

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Mol	Chain	Res	Type
1	D	169	HIS
1	D	200	ASN
1	D	202	SER
1	E	151	ASN
1	E	169	HIS
1	E	202	SER
1	F	118	LEU
1	F	151	ASN
1	F	169	HIS
1	F	202	SER
1	G	151	ASN
1	G	169	HIS
1	G	202	SER
1	H	151	ASN
1	H	169	HIS
1	H	202	SER
1	I	118	LEU
1	I	151	ASN
1	I	169	HIS
1	I	202	SER
1	J	151	ASN
1	J	169	HIS
1	J	202	SER
1	A	25	GLY
1	A	118	LEU
1	A	176	ASP
1	A	289	ASN
1	B	25	GLY
1	B	118	LEU
1	B	176	ASP
1	B	289	ASN
1	C	25	GLY
1	C	118	LEU
1	C	119	PHE
1	C	176	ASP
1	C	289	ASN
1	D	25	GLY
1	D	119	PHE
1	D	176	ASP
1	D	289	ASN
1	E	25	GLY
1	E	118	LEU

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Mol	Chain	Res	Type
1	E	176	ASP
1	E	289	ASN
1	F	25	GLY
1	F	119	PHE
1	F	176	ASP
1	F	233	GLN
1	F	289	ASN
1	G	25	GLY
1	G	118	LEU
1	G	119	PHE
1	G	176	ASP
1	G	289	ASN
1	H	25	GLY
1	H	118	LEU
1	H	176	ASP
1	H	289	ASN
1	I	25	GLY
1	I	176	ASP
1	I	200	ASN
1	I	289	ASN
1	J	25	GLY
1	J	118	LEU
1	J	119	PHE
1	J	176	ASP
1	J	289	ASN
1	A	85	PRO
1	A	119	PHE
1	A	233	GLN
1	B	85	PRO
1	B	233	GLN
1	C	233	GLN
1	D	233	GLN
1	E	85	PRO
1	E	119	PHE
1	E	200	ASN
1	E	233	GLN
1	G	233	GLN
1	H	119	PHE
1	H	233	GLN
1	I	85	PRO
1	I	233	GLN
1	J	85	PRO

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Mol	Chain	Res	Type
1	J	233	GLN
1	A	163	ARG
1	A	301	ARG
1	C	85	PRO
1	C	141	ARG
1	C	163	ARG
1	D	85	PRO
1	D	301	ARG
1	E	141	ARG
1	E	163	ARG
1	F	85	PRO
1	F	163	ARG
1	F	200	ASN
1	F	301	ARG
1	G	85	PRO
1	H	85	PRO
1	H	141	ARG
1	H	163	ARG
1	H	301	ARG
1	I	119	PHE
1	I	301	ARG
1	J	163	ARG
1	J	200	ASN
1	J	301	ARG
1	A	155	GLU
1	A	200	ASN
1	A	257	PRO
1	B	141	ARG
1	B	155	GLU
1	B	200	ASN
1	B	257	PRO
1	C	257	PRO
1	D	163	ARG
1	D	257	PRO
1	E	232	LEU
1	F	141	ARG
1	F	155	GLU
1	G	155	GLU
1	G	200	ASN
1	G	257	PRO
1	G	301	ARG
1	H	200	ASN

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Mol	Chain	Res	Type
1	I	163	ARG
1	J	218	ALA
1	J	221	SER
1	J	257	PRO
1	A	152	ILE
1	B	152	ILE
1	B	163	ARG
1	B	221	SER
1	C	200	ASN
1	D	47	PRO
1	E	47	PRO
1	E	152	ILE
1	E	257	PRO
1	E	301	ARG
1	F	257	PRO
1	G	145	ILE
1	H	152	ILE
1	H	155	GLU
1	H	221	SER
1	H	257	PRO
1	I	152	ILE
1	C	152	ILE
1	D	152	ILE
1	G	152	ILE
1	J	152	ILE
1	B	145	ILE
1	C	145	ILE
1	F	152	ILE
1	A	145	ILE
1	D	145	ILE
1	E	145	ILE
1	H	145	ILE
1	B	47	PRO
1	E	181	VAL
1	F	47	PRO
1	F	145	ILE
1	I	257	PRO
1	J	145	ILE

### 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	274/284 (96%)	218 (80%)	56 (20%)	1	12
1	B	274/284 (96%)	219 (80%)	55 (20%)	1	13
1	C	274/284 (96%)	217 (79%)	57 (21%)	1	11
1	D	274/284 (96%)	217 (79%)	57 (21%)	1	11
1	E	274/284 (96%)	220 (80%)	54 (20%)	1	13
1	F	274/284 (96%)	218 (80%)	56 (20%)	1	12
1	G	274/284 (96%)	221 (81%)	53 (19%)	2	14
1	H	274/284 (96%)	219 (80%)	55 (20%)	1	13
1	I	274/284 (96%)	219 (80%)	55 (20%)	1	13
1	J	274/284 (96%)	217 (79%)	57 (21%)	1	11
All	All	2740/2840 (96%)	2185 (80%)	555 (20%)	1	12

All (555) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	ILE
1	A	26	VAL
1	A	29	LEU
1	A	39	ILE
1	A	40	VAL
1	A	43	TRP
1	A	56	LEU
1	A	71	LEU
1	A	72	TRP
1	A	73	VAL
1	A	82	VAL
1	A	87	THR
1	A	94	LEU
1	A	107	LEU
1	A	109	SER

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Mol	Chain	Res	Type
1	A	118	LEU
1	A	128	LEU
1	A	130	LEU
1	A	131	GLU
1	A	134	SER
1	A	138	GLN
1	A	144	ASP
1	A	145	ILE
1	A	149	THR
1	A	150	GLU
1	A	157	ILE
1	A	162	ILE
1	A	163	ARG
1	A	168	THR
1	A	177	HIS
1	A	178	LEU
1	A	179	SER
1	A	186	ASN
1	A	210	LEU
1	A	215	ILE
1	A	216	ILE
1	A	219	SER
1	A	228	PHE
1	A	229	SER
1	A	232	LEU
1	A	234	THR
1	A	247	LEU
1	A	252	ILE
1	A	253	LEU
1	A	255	ARG
1	A	258	TYR
1	A	260	THR
1	A	267	ILE
1	A	285	HIS
1	A	287	GLN
1	A	291	VAL
1	A	294	ASP
1	A	296	LEU
1	A	304	PHE
1	A	315	LEU
1	B	18	ILE
1	B	20	ILE

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Mol	Chain	Res	Type
1	B	26	VAL
1	B	29	LEU
1	B	39	ILE
1	B	40	VAL
1	B	43	TRP
1	B	56	LEU
1	B	71	LEU
1	B	72	TRP
1	B	73	VAL
1	B	82	VAL
1	B	87	THR
1	B	94	LEU
1	B	109	SER
1	B	118	LEU
1	B	128	LEU
1	B	130	LEU
1	B	131	GLU
1	B	134	SER
1	B	138	GLN
1	B	144	ASP
1	B	145	ILE
1	B	149	THR
1	B	150	GLU
1	B	157	ILE
1	B	162	ILE
1	B	163	ARG
1	B	168	THR
1	B	177	HIS
1	B	178	LEU
1	B	179	SER
1	B	186	ASN
1	B	215	ILE
1	B	216	ILE
1	B	219	SER
1	B	228	PHE
1	B	229	SER
1	B	232	LEU
1	B	234	THR
1	B	247	LEU
1	B	252	ILE
1	B	253	LEU
1	B	255	ARG

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Mol	Chain	Res	Type
1	B	258	TYR
1	B	260	THR
1	B	262	ILE
1	B	267	ILE
1	B	285	HIS
1	B	287	GLN
1	B	291	VAL
1	B	294	ASP
1	B	296	LEU
1	B	304	PHE
1	B	315	LEU
1	C	18	ILE
1	C	20	ILE
1	C	26	VAL
1	C	29	LEU
1	C	39	ILE
1	C	40	VAL
1	C	43	TRP
1	C	56	LEU
1	C	71	LEU
1	C	72	TRP
1	C	73	VAL
1	C	82	VAL
1	C	87	THR
1	C	94	LEU
1	C	107	LEU
1	C	109	SER
1	C	118	LEU
1	C	128	LEU
1	C	130	LEU
1	C	131	GLU
1	C	134	SER
1	C	138	GLN
1	C	144	ASP
1	C	145	ILE
1	C	149	THR
1	C	150	GLU
1	C	157	ILE
1	C	162	ILE
1	C	163	ARG
1	C	168	THR
1	C	177	HIS

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Mol	Chain	Res	Type
1	C	178	LEU
1	C	179	SER
1	C	186	ASN
1	C	210	LEU
1	C	215	ILE
1	C	216	ILE
1	C	219	SER
1	C	228	PHE
1	C	229	SER
1	C	232	LEU
1	C	234	THR
1	C	247	LEU
1	C	252	ILE
1	C	253	LEU
1	C	255	ARG
1	C	258	TYR
1	C	259	THR
1	C	260	THR
1	C	267	ILE
1	C	285	HIS
1	C	287	GLN
1	C	291	VAL
1	C	294	ASP
1	C	296	LEU
1	C	304	PHE
1	C	315	LEU
1	D	18	ILE
1	D	20	ILE
1	D	26	VAL
1	D	29	LEU
1	D	39	ILE
1	D	40	VAL
1	D	43	TRP
1	D	56	LEU
1	D	71	LEU
1	D	72	TRP
1	D	73	VAL
1	D	82	VAL
1	D	87	THR
1	D	94	LEU
1	D	109	SER
1	D	118	LEU

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Mol	Chain	Res	Type
1	D	128	LEU
1	D	130	LEU
1	D	131	GLU
1	D	134	SER
1	D	138	GLN
1	D	144	ASP
1	D	145	ILE
1	D	149	THR
1	D	150	GLU
1	D	157	ILE
1	D	162	ILE
1	D	163	ARG
1	D	168	THR
1	D	177	HIS
1	D	178	LEU
1	D	179	SER
1	D	186	ASN
1	D	208	PHE
1	D	215	ILE
1	D	216	ILE
1	D	219	SER
1	D	228	PHE
1	D	229	SER
1	D	232	LEU
1	D	234	THR
1	D	247	LEU
1	D	252	ILE
1	D	253	LEU
1	D	255	ARG
1	D	258	TYR
1	D	259	THR
1	D	260	THR
1	D	262	ILE
1	D	267	ILE
1	D	285	HIS
1	D	287	GLN
1	D	291	VAL
1	D	294	ASP
1	D	296	LEU
1	D	304	PHE
1	D	315	LEU
1	E	18	ILE

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Mol	Chain	Res	Type
1	E	20	ILE
1	E	26	VAL
1	E	29	LEU
1	E	39	ILE
1	E	40	VAL
1	E	43	TRP
1	E	56	LEU
1	E	71	LEU
1	E	72	TRP
1	E	73	VAL
1	E	82	VAL
1	E	87	THR
1	E	94	LEU
1	E	109	SER
1	E	118	LEU
1	E	128	LEU
1	E	130	LEU
1	E	131	GLU
1	E	134	SER
1	E	138	GLN
1	E	144	ASP
1	E	145	ILE
1	E	149	THR
1	E	150	GLU
1	E	157	ILE
1	E	162	ILE
1	E	163	ARG
1	E	168	THR
1	E	177	HIS
1	E	178	LEU
1	E	179	SER
1	E	186	ASN
1	E	215	ILE
1	E	216	ILE
1	E	219	SER
1	E	228	PHE
1	E	229	SER
1	E	232	LEU
1	E	234	THR
1	E	247	LEU
1	E	252	ILE
1	E	253	LEU

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Mol	Chain	Res	Type
1	E	255	ARG
1	E	258	TYR
1	E	259	THR
1	E	267	ILE
1	E	285	HIS
1	E	287	GLN
1	E	291	VAL
1	E	294	ASP
1	E	296	LEU
1	E	304	PHE
1	E	315	LEU
1	F	16	VAL
1	F	18	ILE
1	F	20	ILE
1	F	26	VAL
1	F	29	LEU
1	F	39	ILE
1	F	40	VAL
1	F	43	TRP
1	F	56	LEU
1	F	71	LEU
1	F	72	TRP
1	F	73	VAL
1	F	82	VAL
1	F	87	THR
1	F	94	LEU
1	F	107	LEU
1	F	109	SER
1	F	118	LEU
1	F	128	LEU
1	F	130	LEU
1	F	131	GLU
1	F	134	SER
1	F	138	GLN
1	F	144	ASP
1	F	145	ILE
1	F	149	THR
1	F	150	GLU
1	F	157	ILE
1	F	162	ILE
1	F	163	ARG
1	F	168	THR

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Mol	Chain	Res	Type
1	F	177	HIS
1	F	178	LEU
1	F	179	SER
1	F	186	ASN
1	F	215	ILE
1	F	216	ILE
1	F	219	SER
1	F	228	PHE
1	F	229	SER
1	F	232	LEU
1	F	234	THR
1	F	247	LEU
1	F	252	ILE
1	F	253	LEU
1	F	255	ARG
1	F	258	TYR
1	F	259	THR
1	F	267	ILE
1	F	285	HIS
1	F	287	GLN
1	F	291	VAL
1	F	294	ASP
1	F	296	LEU
1	F	304	PHE
1	F	315	LEU
1	G	18	ILE
1	G	20	ILE
1	G	26	VAL
1	G	29	LEU
1	G	39	ILE
1	G	40	VAL
1	G	43	TRP
1	G	56	LEU
1	G	71	LEU
1	G	72	TRP
1	G	73	VAL
1	G	82	VAL
1	G	87	THR
1	G	94	LEU
1	G	109	SER
1	G	118	LEU
1	G	128	LEU

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Mol	Chain	Res	Type
1	G	130	LEU
1	G	131	GLU
1	G	134	SER
1	G	138	GLN
1	G	144	ASP
1	G	145	ILE
1	G	149	THR
1	G	150	GLU
1	G	157	ILE
1	G	162	ILE
1	G	163	ARG
1	G	168	THR
1	G	177	HIS
1	G	178	LEU
1	G	179	SER
1	G	186	ASN
1	G	215	ILE
1	G	216	ILE
1	G	219	SER
1	G	229	SER
1	G	232	LEU
1	G	234	THR
1	G	247	LEU
1	G	252	ILE
1	G	253	LEU
1	G	255	ARG
1	G	258	TYR
1	G	259	THR
1	G	267	ILE
1	G	285	HIS
1	G	287	GLN
1	G	291	VAL
1	G	294	ASP
1	G	296	LEU
1	G	304	PHE
1	G	315	LEU
1	H	18	ILE
1	H	20	ILE
1	H	26	VAL
1	H	29	LEU
1	H	39	ILE
1	H	40	VAL

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Mol	Chain	Res	Type
1	H	43	TRP
1	H	56	LEU
1	H	71	LEU
1	H	72	TRP
1	H	73	VAL
1	H	74	PRO
1	H	82	VAL
1	H	87	THR
1	H	94	LEU
1	H	109	SER
1	H	118	LEU
1	H	128	LEU
1	H	130	LEU
1	H	131	GLU
1	H	134	SER
1	H	138	GLN
1	H	144	ASP
1	H	145	ILE
1	H	146	GLN
1	H	149	THR
1	H	150	GLU
1	H	157	ILE
1	H	162	ILE
1	H	163	ARG
1	H	168	THR
1	H	177	HIS
1	H	178	LEU
1	H	179	SER
1	H	186	ASN
1	H	215	ILE
1	H	216	ILE
1	H	228	PHE
1	H	229	SER
1	H	232	LEU
1	H	234	THR
1	H	247	LEU
1	H	252	ILE
1	H	253	LEU
1	H	255	ARG
1	H	258	TYR
1	H	260	THR
1	H	267	ILE

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Mol	Chain	Res	Type
1	H	285	HIS
1	H	287	GLN
1	H	291	VAL
1	H	294	ASP
1	H	296	LEU
1	H	304	PHE
1	H	315	LEU
1	I	18	ILE
1	I	20	ILE
1	I	26	VAL
1	I	29	LEU
1	I	39	ILE
1	I	40	VAL
1	I	43	TRP
1	I	56	LEU
1	I	71	LEU
1	I	72	TRP
1	I	73	VAL
1	I	82	VAL
1	I	87	THR
1	I	94	LEU
1	I	109	SER
1	I	118	LEU
1	I	128	LEU
1	I	130	LEU
1	I	131	GLU
1	I	134	SER
1	I	138	GLN
1	I	144	ASP
1	I	145	ILE
1	I	150	GLU
1	I	157	ILE
1	I	162	ILE
1	I	163	ARG
1	I	168	THR
1	I	177	HIS
1	I	178	LEU
1	I	179	SER
1	I	186	ASN
1	I	208	PHE
1	I	215	ILE
1	I	216	ILE

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Mol	Chain	Res	Type
1	I	219	SER
1	I	228	PHE
1	I	229	SER
1	I	232	LEU
1	I	234	THR
1	I	247	LEU
1	I	252	ILE
1	I	253	LEU
1	I	255	ARG
1	I	258	TYR
1	I	260	THR
1	I	262	ILE
1	I	267	ILE
1	I	285	HIS
1	I	287	GLN
1	I	291	VAL
1	I	294	ASP
1	I	296	LEU
1	I	304	PHE
1	I	315	LEU
1	J	18	ILE
1	J	20	ILE
1	J	26	VAL
1	J	29	LEU
1	J	39	ILE
1	J	40	VAL
1	J	43	TRP
1	J	56	LEU
1	J	62	GLN
1	J	71	LEU
1	J	72	TRP
1	J	73	VAL
1	J	74	PRO
1	J	82	VAL
1	J	87	THR
1	J	94	LEU
1	J	109	SER
1	J	118	LEU
1	J	128	LEU
1	J	130	LEU
1	J	131	GLU
1	J	134	SER

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Mol	Chain	Res	Type
1	J	138	GLN
1	J	144	ASP
1	J	145	ILE
1	J	149	THR
1	J	150	GLU
1	J	157	ILE
1	J	162	ILE
1	J	163	ARG
1	J	168	THR
1	J	177	HIS
1	J	178	LEU
1	J	186	ASN
1	J	210	LEU
1	J	215	ILE
1	J	216	ILE
1	J	219	SER
1	J	228	PHE
1	J	229	SER
1	J	232	LEU
1	J	234	THR
1	J	247	LEU
1	J	252	ILE
1	J	253	LEU
1	J	255	ARG
1	J	258	TYR
1	J	259	THR
1	J	260	THR
1	J	267	ILE
1	J	285	HIS
1	J	287	GLN
1	J	291	VAL
1	J	294	ASP
1	J	296	LEU
1	J	304	PHE
1	J	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	284	HIS
1	C	62	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	251	ASN
1	C	284	HIS
1	D	62	GLN
1	D	284	HIS
1	E	251	ASN
1	F	251	ASN
1	F	284	HIS
1	G	284	HIS
1	H	284	HIS
1	I	62	GLN
1	I	284	HIS
1	J	62	GLN
1	J	251	ASN
1	J	284	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](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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 ⓘ

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	307/324 (94%)	-0.55	2 (0%) 89 84	83, 137, 287, 353	0
1	B	307/324 (94%)	-0.56	1 (0%) 94 92	80, 134, 284, 357	0
1	C	307/324 (94%)	-0.44	9 (2%) 55 43	80, 135, 285, 355	0
1	D	307/324 (94%)	-0.54	4 (1%) 79 71	79, 135, 285, 354	0
1	E	307/324 (94%)	-0.52	5 (1%) 74 65	79, 138, 287, 356	0
1	F	307/324 (94%)	-0.57	2 (0%) 89 84	81, 137, 284, 360	0
1	G	307/324 (94%)	-0.56	5 (1%) 74 65	81, 135, 281, 354	0
1	H	307/324 (94%)	-0.53	5 (1%) 74 65	82, 136, 286, 357	0
1	I	307/324 (94%)	-0.49	5 (1%) 74 65	80, 135, 286, 351	0
1	J	307/324 (94%)	-0.55	4 (1%) 79 71	81, 136, 282, 356	0
All	All	3070/3240 (94%)	-0.53	42 (1%) 78 69	79, 136, 287, 360	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	290	GLY	7.0
1	C	291	VAL	5.9
1	I	291	VAL	5.8
1	C	290	GLY	4.8
1	C	289	ASN	4.6
1	H	291	VAL	4.5
1	C	151	ASN	4.3
1	J	152	ILE	3.8
1	J	291	VAL	3.5
1	C	288	ALA	3.4
1	H	151	ASN	3.2
1	E	152	ILE	3.2
1	G	293	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	290	GLY	3.1
1	A	151	ASN	3.0
1	C	292	GLU	3.0
1	G	291	VAL	2.9
1	J	290	GLY	2.8
1	C	152	ILE	2.8
1	H	286	ARG	2.8
1	I	289	ASN	2.7
1	D	180	SER	2.6
1	E	153	ASP	2.6
1	A	152	ILE	2.6
1	D	295	LEU	2.6
1	G	292	GLU	2.5
1	F	152	ILE	2.5
1	B	290	GLY	2.5
1	G	290	GLY	2.5
1	H	289	ASN	2.4
1	I	292	GLU	2.3
1	F	151	ASN	2.3
1	E	151	ASN	2.3
1	D	291	VAL	2.2
1	G	288	ALA	2.2
1	E	306	LEU	2.2
1	D	154	ASN	2.1
1	I	153	ASP	2.1
1	J	289	ASN	2.1
1	C	293	ASP	2.1
1	E	290	GLY	2.1
1	C	303	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	F	323	1/1	0.93	0.33	-	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.