



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:26 pm BST

PDB ID : 3RQU  
Title : Crystal structure of a prokaryotic pentameric ligand-gated ion channel, ELIC  
Authors : Pan, J.J.; Chen, Q.; Yoshida, K.; Cohen, A.; Kong, X.P.; Xu, Y.; Tang, P.  
Deposited on : 2011-04-28  
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

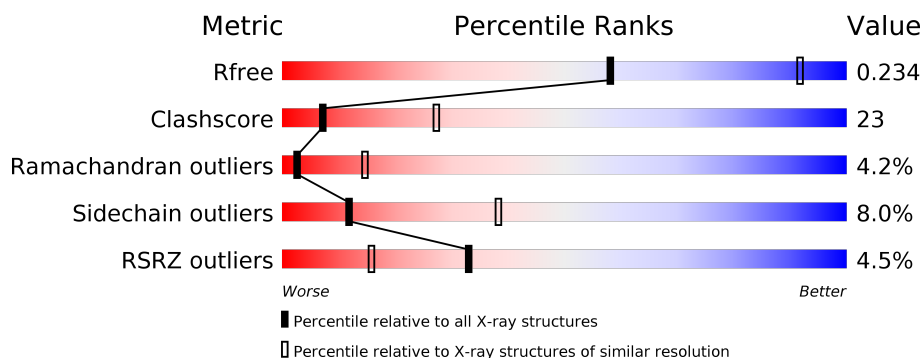
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 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.






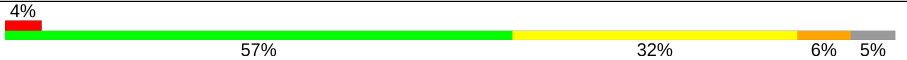
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	322	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>6% • 5%</div> </div> </div>
1	B	322	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>33%</div> <div>6% 5%</div> </div> </div>
1	C	322	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>6% 5%</div> </div> </div>
1	D	322	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>6% 5%</div> </div> </div>
1	E	322	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>31%</div> <div>6% • 5%</div> </div> </div>
1	F	322	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>6% 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	322	
1	H	322	
1	I	322	
1	J	322	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	326	-	-	X	-
3	GOL	E	324	-	-	X	-
3	GOL	F	323	-	-	X	-
3	GOL	G	325	-	-	X	-
3	GOL	H	323	-	-	X	-
3	GOL	I	326	-	-	X	-
3	GOL	J	325	-	-	X	-

## 2 Entry composition

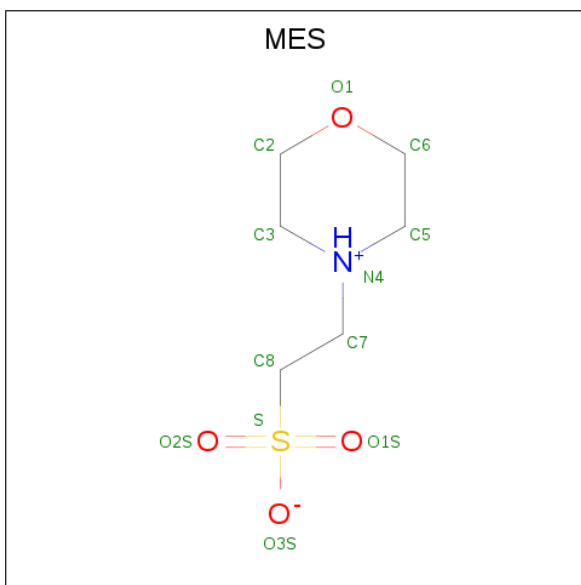
There are 4 unique types of molecules in this entry. The entry contains 25308 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			5	3	2		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

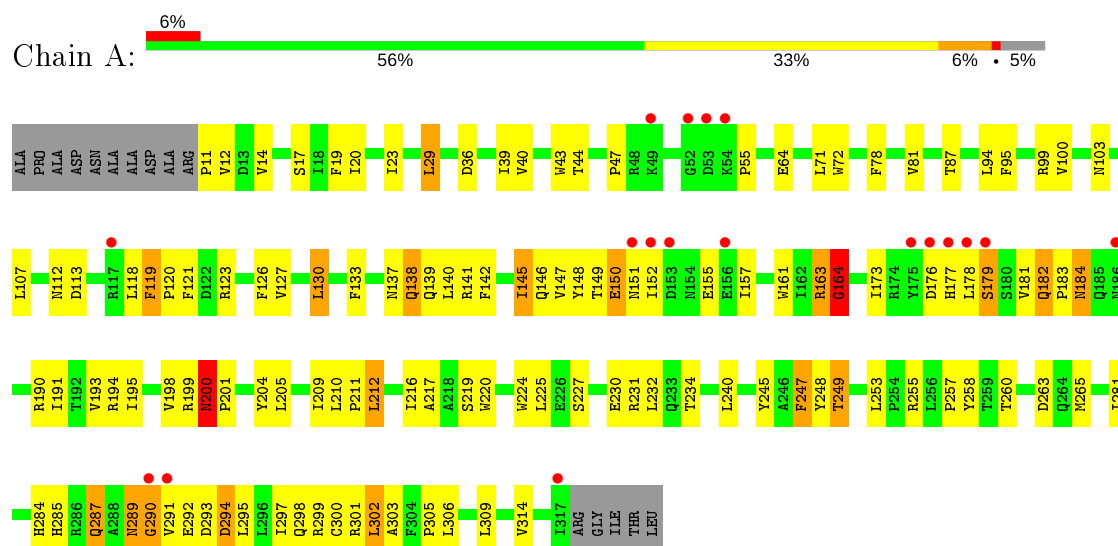
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	6	Total	O	0	0
			6	6		
4	C	4	Total	O	0	0
			4	4		
4	D	6	Total	O	0	0
			6	6		
4	E	5	Total	O	0	0
			5	5		
4	F	2	Total	O	0	0
			2	2		
4	G	7	Total	O	0	0
			7	7		
4	H	5	Total	O	0	0
			5	5		
4	I	4	Total	O	0	0
			4	4		
4	J	5	Total	O	0	0
			5	5		

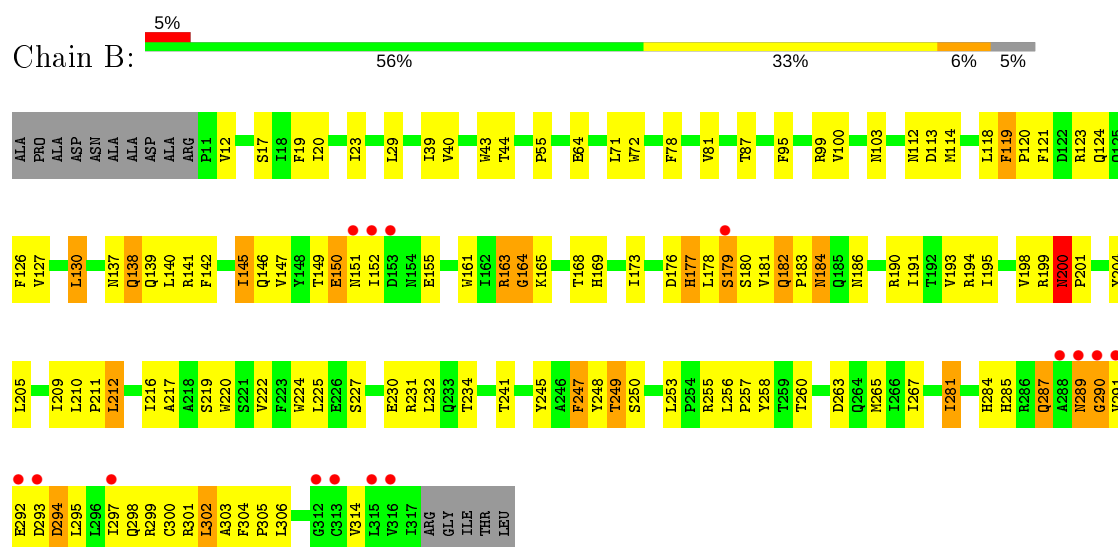
### 3 Residue-property plots [i](#)

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: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



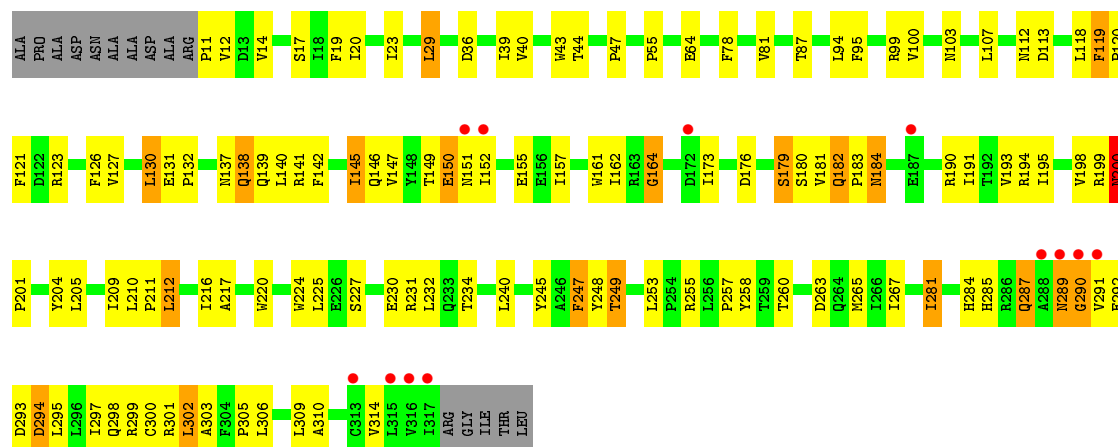
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



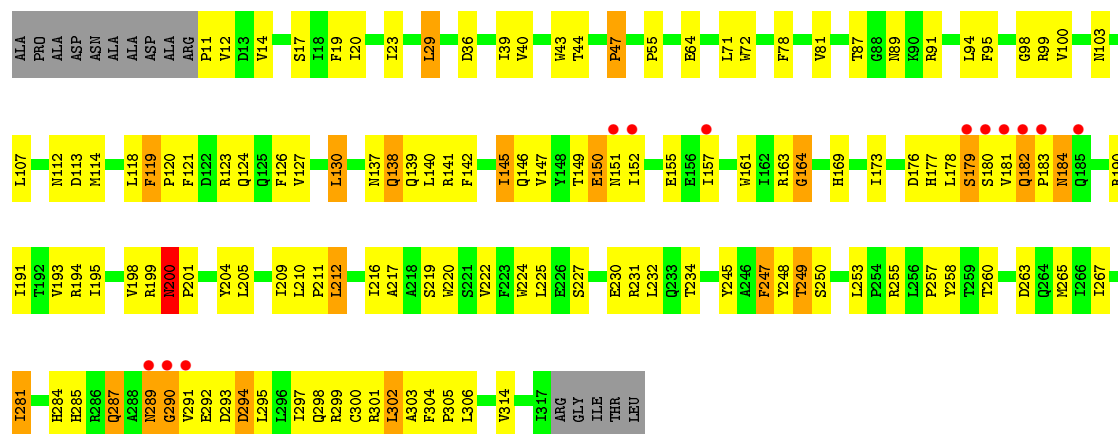
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



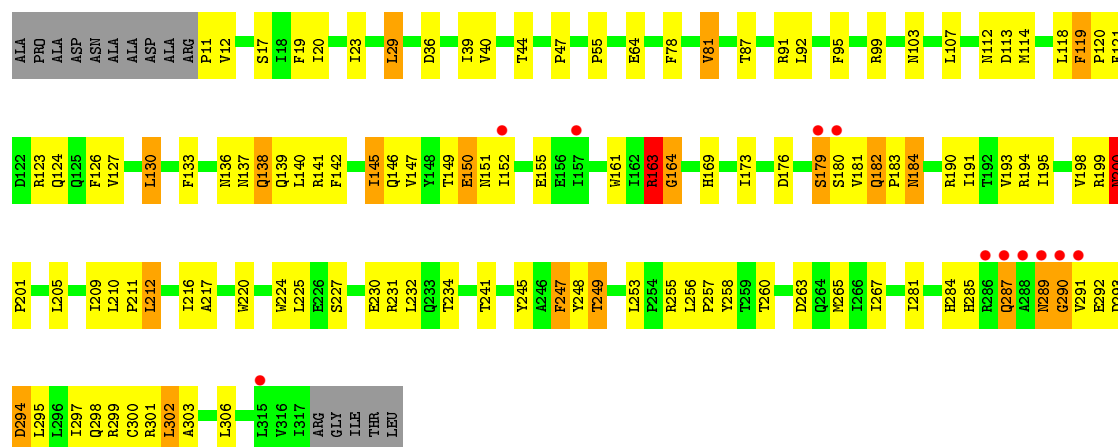




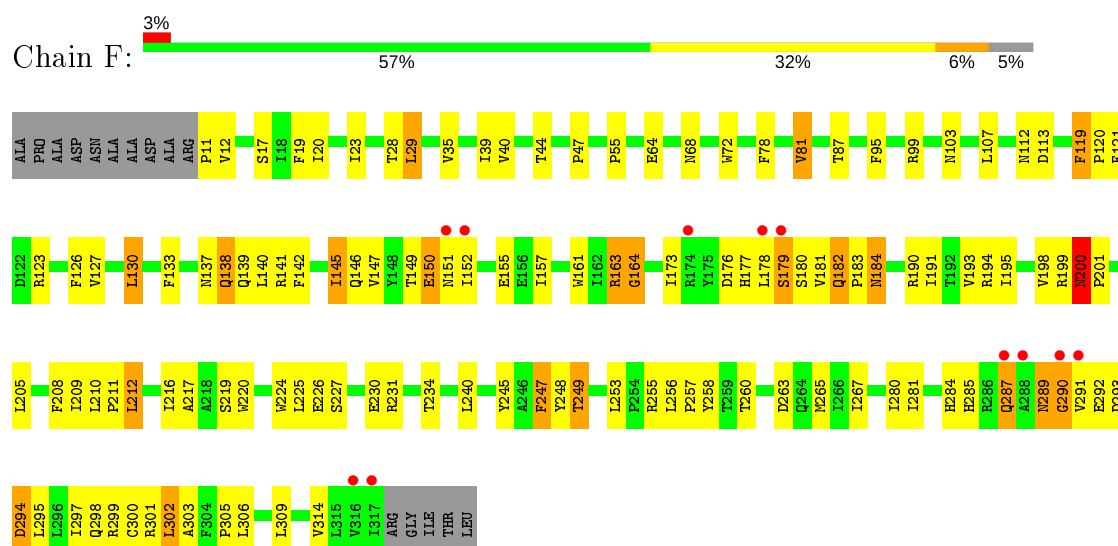
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



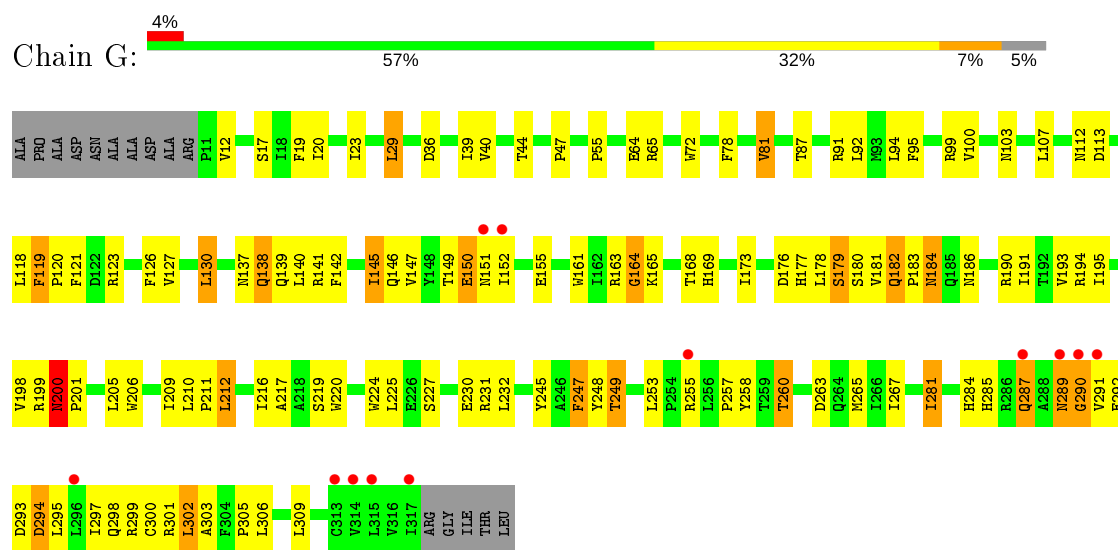
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



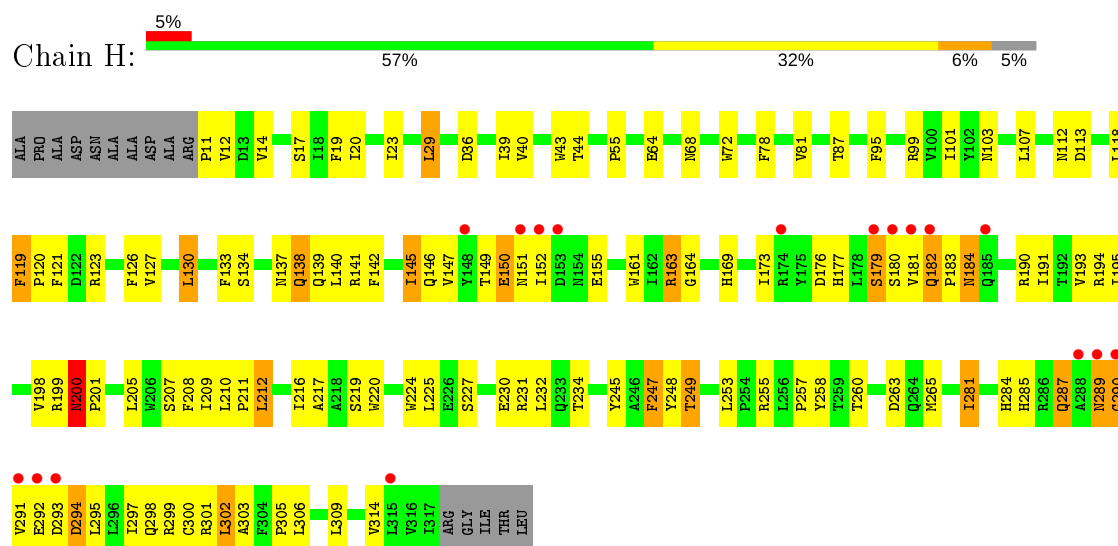
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



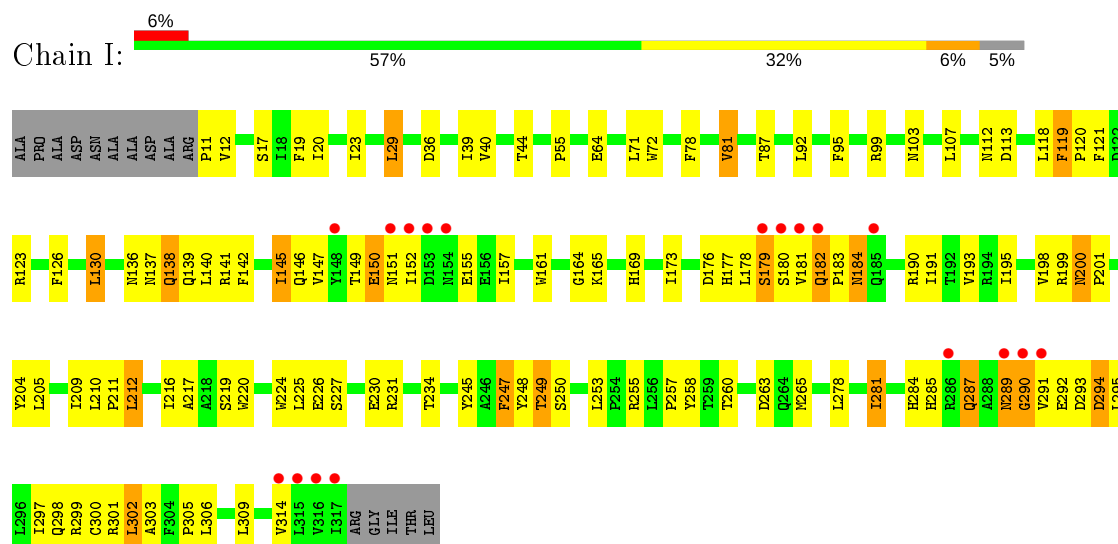
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



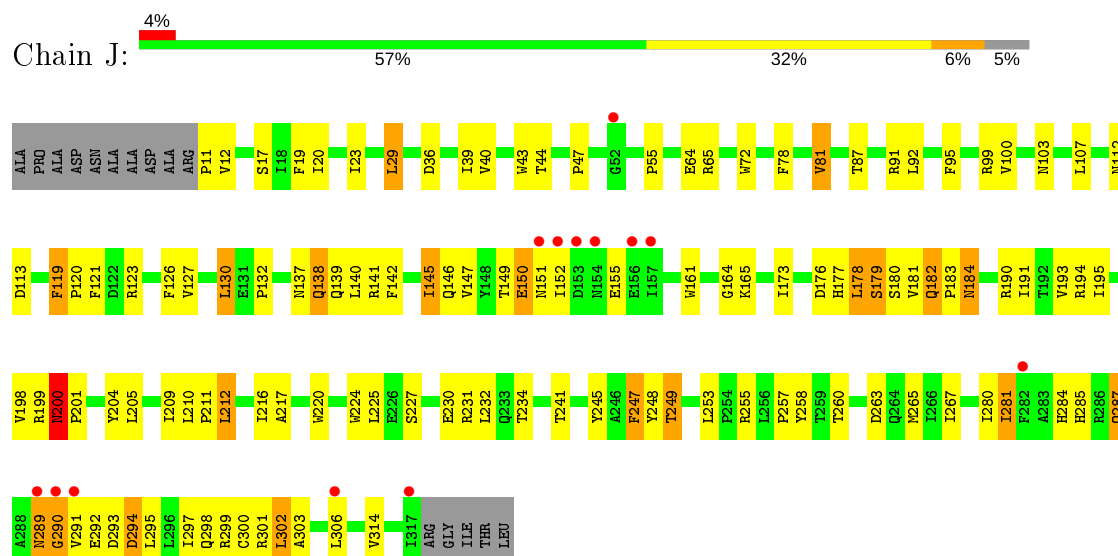
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.29 Å   266.97 Å   111.07 Å 90.00°   107.53°   90.00°	Depositor
Resolution (Å)	24.99 – 3.09 29.78 – 3.09	Depositor EDS
% Data completeness (in resolution range)	91.5 (24.99-3.09) 97.5 (29.78-3.09)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.11 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.209   ,   0.240 0.207   ,   0.234	Depositor DCC
$R_{free}$ test set	5174 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.3	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 69.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

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

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	0.32	0/2573	0.49	0/3507
1	B	0.35	0/2573	0.53	0/3507
1	C	0.34	0/2573	0.51	0/3507
1	D	0.36	0/2573	0.52	0/3507
1	E	0.34	0/2573	0.50	0/3507
1	F	0.34	0/2573	0.50	0/3507
1	G	0.35	0/2573	0.52	0/3507
1	H	0.34	0/2573	0.51	0/3507
1	I	0.36	0/2573	0.52	1/3507 (0.0%)
1	J	0.34	0/2573	0.50	0/3507
All	All	0.35	0/25730	0.51	1/35070 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
1	I	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	LYS	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLY	Peptide
1	H	164	GLY	Peptide
1	I	164	GLY	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	2505	0	2478	122	0
1	B	2505	0	2478	129	0
1	C	2505	0	2478	117	0
1	D	2505	0	2478	133	0
1	E	2505	0	2478	120	0
1	F	2505	0	2478	121	0
1	G	2505	0	2478	128	0
1	H	2505	0	2478	115	0
1	I	2505	0	2478	122	0
1	J	2505	0	2478	123	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	1	0
2	G	24	0	24	1	0
2	I	12	0	12	0	0
3	A	6	0	8	3	0
3	B	30	0	40	3	0
3	C	6	0	8	3	0
3	D	17	0	21	11	0
3	E	12	0	16	9	0
3	F	6	0	8	5	0
3	G	6	0	8	6	0
3	H	6	0	8	4	0
3	I	18	0	24	9	0
3	J	18	0	24	7	0
4	A	5	0	0	2	0
4	B	6	0	0	2	0
4	C	4	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	0	4	0
4	E	5	0	0	3	0
4	F	2	0	0	2	0
4	G	7	0	0	2	0
4	H	5	0	0	3	0
4	I	4	0	0	2	0
4	J	5	0	0	3	0
All	All	25308	0	25029	1134	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 (1134) 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:B:123:ARG:HG2	1:B:198:VAL:HG12	1.30	1.12
1:J:123:ARG:HG2	1:J:198:VAL:HG12	1.32	1.11
1:J:11:PRO:HB3	3:J:325:GOL:H12	1.33	1.10
1:I:123:ARG:HG2	1:I:198:VAL:HG12	1.34	1.09
1:C:123:ARG:HG2	1:C:198:VAL:HG12	1.34	1.08
1:F:123:ARG:HG2	1:F:198:VAL:HG12	1.33	1.07
1:E:123:ARG:HG2	1:E:198:VAL:HG12	1.31	1.06
1:G:123:ARG:HG2	1:G:198:VAL:HG12	1.37	1.06
1:I:140:LEU:HD21	4:I:329:HOH:O	1.56	1.05
1:A:123:ARG:HG2	1:A:198:VAL:HG12	1.33	1.05
1:D:123:ARG:HG2	1:D:198:VAL:HG12	1.36	1.05
1:H:123:ARG:HG2	1:H:198:VAL:HG12	1.39	1.05
1:D:140:LEU:HD11	4:D:331:HOH:O	1.62	0.98
1:H:137:ASN:HA	3:H:323:GOL:H2	1.47	0.96
1:H:140:LEU:HD21	4:H:327:HOH:O	1.65	0.96
1:A:137:ASN:HA	3:A:324:GOL:H31	1.47	0.96
1:G:140:LEU:HD21	4:G:331:HOH:O	1.66	0.94
1:A:140:LEU:HD11	4:A:328:HOH:O	1.69	0.93
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.51	0.92
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.36	0.89
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.54	0.89
1:E:295:LEU:HA	1:E:298:GLN:HE21	1.38	0.89
1:F:140:LEU:HD11	4:F:325:HOH:O	1.71	0.89
1:G:224:TRP:HE1	1:G:301:ARG:HB3	1.37	0.89
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.55	0.88
1:J:140:LEU:HD11	4:J:329:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.56	0.88
1:E:137:ASN:HA	3:E:324:GOL:H2	1.56	0.87
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.39	0.87
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.56	0.87
1:D:137:ASN:HA	3:D:326:GOL:H2	1.53	0.87
1:E:140:LEU:HD11	4:E:327:HOH:O	1.74	0.87
1:J:11:PRO:HB3	3:J:325:GOL:C1	2.04	0.87
1:B:140:LEU:HD21	4:B:333:HOH:O	1.75	0.86
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.58	0.86
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.38	0.86
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.39	0.86
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.41	0.86
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.39	0.86
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.41	0.85
1:D:140:LEU:HD21	4:D:331:HOH:O	1.76	0.85
1:G:295:LEU:HA	1:G:298:GLN:HE21	1.42	0.85
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.59	0.85
1:C:224:TRP:HE1	1:C:301:ARG:HB3	1.41	0.85
1:G:140:LEU:HD11	4:G:331:HOH:O	1.77	0.85
1:H:137:ASN:HA	3:H:323:GOL:C2	2.07	0.84
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.59	0.84
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.59	0.84
1:I:295:LEU:HA	1:I:298:GLN:HE21	1.40	0.84
1:B:163:ARG:O	1:B:164:GLY:O	1.95	0.84
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.59	0.84
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.60	0.83
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.58	0.83
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.61	0.83
1:A:163:ARG:O	1:A:164:GLY:O	1.96	0.83
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.61	0.83
1:F:224:TRP:HE1	1:F:301:ARG:HB3	1.43	0.83
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.60	0.83
1:E:11:PRO:HB3	3:E:324:GOL:H32	1.59	0.83
1:H:300:CYS:HB2	1:H:303:ALA:HB3	1.61	0.82
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.61	0.82
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.60	0.82
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.62	0.82
1:D:137:ASN:HA	3:D:326:GOL:C1	2.10	0.81
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.61	0.81
1:D:295:LEU:HA	1:D:298:GLN:HE21	1.46	0.81
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:ASN:HA	3:J:325:GOL:C1	2.11	0.81
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.62	0.80
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.62	0.80
1:C:205:LEU:HD23	1:C:209:ILE:HG13	1.64	0.80
1:A:295:LEU:HA	1:A:298:GLN:HE21	1.45	0.80
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.63	0.80
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.64	0.79
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.63	0.79
1:D:137:ASN:HA	3:D:326:GOL:C2	2.12	0.79
1:J:295:LEU:HA	1:J:298:GLN:HE21	1.46	0.79
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.65	0.79
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.65	0.79
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.65	0.79
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.63	0.79
1:C:140:LEU:HD21	4:C:327:HOH:O	1.81	0.79
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.64	0.79
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.65	0.79
1:F:295:LEU:HA	1:F:298:GLN:HE21	1.46	0.78
1:F:163:ARG:O	1:F:164:GLY:O	2.01	0.78
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.64	0.78
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.63	0.78
1:H:295:LEU:HA	1:H:298:GLN:HE21	1.49	0.77
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.66	0.77
1:C:295:LEU:HA	1:C:298:GLN:HE21	1.49	0.77
1:F:140:LEU:HD21	4:F:325:HOH:O	1.84	0.77
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.65	0.77
1:C:140:LEU:HD11	4:C:327:HOH:O	1.85	0.76
1:E:11:PRO:HB3	3:E:324:GOL:C3	2.16	0.76
1:B:140:LEU:HD11	4:B:333:HOH:O	1.85	0.75
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.66	0.75
1:I:39:ILE:HD11	1:I:130:LEU:HD11	1.67	0.74
1:G:119:PHE:HB3	1:G:120:PRO:HD3	1.70	0.73
1:B:295:LEU:HA	1:B:298:GLN:HE21	1.53	0.73
1:H:137:ASN:CA	3:H:323:GOL:H2	2.18	0.73
1:J:137:ASN:HA	3:J:325:GOL:H11	1.69	0.73
1:E:295:LEU:HA	1:E:298:GLN:NE2	2.04	0.72
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.72	0.72
1:B:182:GLN:H	1:B:183:PRO:CD	2.04	0.71
1:D:145:ILE:HG21	1:D:193:VAL:HG11	1.72	0.71
1:E:39:ILE:HD11	1:E:130:LEU:HD11	1.73	0.71
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:LEU:CD2	1:J:232:LEU:HD23	2.21	0.70
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.73	0.70
1:E:182:GLN:H	1:E:183:PRO:CD	2.05	0.70
1:G:137:ASN:HA	3:G:325:GOL:C2	2.21	0.70
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.72	0.70
1:A:39:ILE:HD11	1:A:130:LEU:HD11	1.74	0.70
1:D:119:PHE:HB3	1:D:120:PRO:HD3	1.71	0.70
1:E:137:ASN:HA	3:E:324:GOL:C2	2.20	0.70
1:A:294:ASP:HB2	1:A:297:ILE:HG22	1.74	0.70
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.73	0.70
1:H:182:GLN:H	1:H:183:PRO:CD	2.05	0.70
1:B:145:ILE:HG21	1:B:193:VAL:HG11	1.74	0.70
1:I:119:PHE:HB3	1:I:120:PRO:HD3	1.74	0.70
1:A:182:GLN:H	1:A:183:PRO:CD	2.05	0.69
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.73	0.69
1:B:294:ASP:HB2	1:B:297:ILE:HG22	1.74	0.69
1:D:182:GLN:H	1:D:183:PRO:CD	2.05	0.69
1:H:119:PHE:HB3	1:H:120:PRO:HD3	1.73	0.69
1:J:182:GLN:H	1:J:183:PRO:CD	2.06	0.69
1:E:137:ASN:HA	3:E:324:GOL:C3	2.22	0.69
1:F:182:GLN:H	1:F:183:PRO:CD	2.05	0.69
1:J:294:ASP:HB2	1:J:297:ILE:HG22	1.74	0.69
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.74	0.69
1:B:137:ASN:HA	3:B:328:GOL:C1	2.23	0.69
1:C:182:GLN:H	1:C:183:PRO:CD	2.06	0.69
1:H:145:ILE:HG21	1:H:193:VAL:HG11	1.76	0.68
1:A:145:ILE:HG21	1:A:193:VAL:HG11	1.74	0.68
1:I:295:LEU:HA	1:I:298:GLN:NE2	2.07	0.68
1:G:295:LEU:HA	1:G:298:GLN:NE2	2.08	0.68
1:I:137:ASN:HA	3:I:326:GOL:C3	2.24	0.68
1:H:39:ILE:HD11	1:H:130:LEU:HD11	1.74	0.68
1:B:119:PHE:HB3	1:B:120:PRO:HD3	1.75	0.68
1:I:182:GLN:H	1:I:183:PRO:CD	2.07	0.68
1:C:119:PHE:HB3	1:C:120:PRO:HD3	1.76	0.68
1:B:212:LEU:HB3	1:B:265:MET:HE1	1.77	0.67
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.10	0.67
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.74	0.67
1:I:199:ARG:O	1:I:201:PRO:HD3	1.94	0.67
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.60	0.67
1:G:182:GLN:H	1:G:183:PRO:CD	2.07	0.67
1:I:294:ASP:HB2	1:I:297:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASN:HA	3:C:324:GOL:O1	1.95	0.67
1:H:140:LEU:HD11	4:H:327:HOH:O	1.94	0.67
1:J:119:PHE:HB3	1:J:120:PRO:HD3	1.76	0.67
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.08	0.67
1:J:145:ILE:HG21	1:J:193:VAL:HG11	1.76	0.67
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.10	0.67
1:E:294:ASP:HB2	1:E:297:ILE:HG22	1.76	0.67
1:H:212:LEU:HB3	1:H:265:MET:HE1	1.77	0.67
1:A:119:PHE:HB3	1:A:120:PRO:HD3	1.75	0.66
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.31	0.66
1:D:137:ASN:CA	3:D:326:GOL:H2	2.24	0.66
1:C:39:ILE:HD11	1:C:130:LEU:HD11	1.78	0.66
1:D:137:ASN:HA	3:D:326:GOL:O1	1.94	0.66
1:E:119:PHE:HB3	1:E:120:PRO:HD3	1.78	0.66
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.31	0.66
1:F:145:ILE:HG21	1:F:193:VAL:HG11	1.77	0.66
1:J:295:LEU:HA	1:J:298:GLN:NE2	2.11	0.66
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.31	0.65
1:E:210:LEU:HB3	1:E:211:PRO:CD	2.26	0.65
1:A:295:LEU:HA	1:A:298:GLN:NE2	2.11	0.65
1:C:145:ILE:HG21	1:C:193:VAL:HG11	1.76	0.65
1:E:137:ASN:HA	3:E:324:GOL:O3	1.97	0.65
1:F:137:ASN:HA	3:F:323:GOL:H31	1.78	0.65
1:G:137:ASN:HA	3:G:325:GOL:O1	1.95	0.65
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.09	0.65
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.12	0.65
1:D:295:LEU:HA	1:D:298:GLN:NE2	2.11	0.65
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.11	0.65
1:B:248:TYR:HA	1:C:247:PHE:CE1	2.31	0.65
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.09	0.65
1:I:212:LEU:HB3	1:I:265:MET:HE1	1.79	0.65
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.10	0.65
1:G:145:ILE:HG21	1:G:193:VAL:HG11	1.79	0.64
1:I:40:VAL:HG22	1:I:103:ASN:HD22	1.62	0.64
1:I:145:ILE:HG21	1:I:193:VAL:HG11	1.77	0.64
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.33	0.64
1:E:199:ARG:O	1:E:201:PRO:HD3	1.97	0.64
1:D:11:PRO:HB3	3:D:326:GOL:H11	1.79	0.64
1:D:199:ARG:O	1:D:201:PRO:HD3	1.97	0.64
1:F:247:PHE:CE1	1:J:248:TYR:HA	2.32	0.64
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ILE:HD11	1:G:130:LEU:HD11	1.79	0.64
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.11	0.64
1:A:212:LEU:HB3	1:A:265:MET:HE1	1.80	0.64
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.63	0.64
1:F:295:LEU:HA	1:F:298:GLN:NE2	2.12	0.64
1:F:119:PHE:HB3	1:F:120:PRO:HD3	1.79	0.63
1:H:248:TYR:HA	1:I:247:PHE:CE1	2.33	0.63
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.33	0.63
1:H:182:GLN:H	1:H:183:PRO:HD2	1.63	0.63
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.33	0.63
1:E:182:GLN:H	1:E:183:PRO:HD2	1.63	0.63
1:I:11:PRO:HB3	3:I:326:GOL:C3	2.29	0.63
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.79	0.63
1:A:140:LEU:HD21	4:A:328:HOH:O	1.98	0.63
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.34	0.63
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.34	0.63
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.80	0.62
1:C:295:LEU:HA	1:C:298:GLN:NE2	2.14	0.62
1:E:224:TRP:NE1	1:E:301:ARG:HD3	2.13	0.62
1:H:295:LEU:HA	1:H:298:GLN:NE2	2.13	0.62
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.17	0.62
1:F:145:ILE:H	1:F:145:ILE:HD12	1.64	0.62
1:F:20:ILE:HD12	1:F:195:ILE:HD11	1.81	0.62
1:G:179:SER:HB2	1:G:181:VAL:HG12	1.81	0.62
1:G:212:LEU:HB3	1:G:265:MET:HE1	1.80	0.62
1:A:182:GLN:H	1:A:183:PRO:HD2	1.64	0.62
1:G:248:TYR:HA	1:H:247:PHE:CE1	2.34	0.62
1:D:182:GLN:H	1:D:183:PRO:HD2	1.64	0.62
1:G:20:ILE:HD12	1:G:195:ILE:HD11	1.81	0.62
1:J:145:ILE:HD12	1:J:145:ILE:H	1.64	0.62
1:J:182:GLN:H	1:J:183:PRO:HD2	1.65	0.62
1:B:182:GLN:H	1:B:183:PRO:HD2	1.64	0.62
1:C:212:LEU:HB3	1:C:265:MET:HE1	1.82	0.62
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.35	0.62
1:D:163:ARG:O	1:D:164:GLY:O	2.17	0.62
1:C:20:ILE:HD12	1:C:195:ILE:HD11	1.81	0.62
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.81	0.62
1:F:248:TYR:HD1	1:G:247:PHE:HA	1.64	0.62
1:D:212:LEU:HB3	1:D:265:MET:HE1	1.82	0.61
1:F:39:ILE:HD11	1:F:130:LEU:HD11	1.81	0.61
1:F:284:HIS:HD2	1:F:285:HIS:CE1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.82	0.61
1:A:248:TYR:HD1	1:B:247:PHE:HA	1.65	0.61
1:C:182:GLN:H	1:C:183:PRO:HD2	1.64	0.61
1:F:182:GLN:H	1:F:183:PRO:HD2	1.64	0.61
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.30	0.61
1:I:182:GLN:H	1:I:183:PRO:HD2	1.66	0.61
1:H:179:SER:HB2	1:H:181:VAL:HG12	1.82	0.61
1:E:212:LEU:HB3	1:E:265:MET:HE1	1.81	0.61
1:H:145:ILE:H	1:H:145:ILE:HD12	1.65	0.61
1:H:248:TYR:HD1	1:I:247:PHE:HA	1.66	0.61
1:I:210:LEU:HB3	1:I:211:PRO:CD	2.29	0.61
1:I:11:PRO:HB3	3:I:326:GOL:H32	1.83	0.61
1:E:145:ILE:HD12	1:E:145:ILE:H	1.66	0.61
1:E:145:ILE:HG21	1:E:193:VAL:HG11	1.81	0.61
1:E:224:TRP:CD1	1:E:301:ARG:HD3	2.36	0.61
1:F:248:TYR:HA	1:G:247:PHE:CE1	2.36	0.61
1:B:145:ILE:HD12	1:B:145:ILE:H	1.65	0.61
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.35	0.61
1:G:141:ARG:HG2	1:G:142:PHE:CD2	2.36	0.61
1:J:132:PRO:HD3	4:J:329:HOH:O	2.00	0.61
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.83	0.60
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.20	0.60
1:J:179:SER:HB2	1:J:181:VAL:HG12	1.81	0.60
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.83	0.60
1:G:248:TYR:HD1	1:H:247:PHE:HA	1.65	0.60
1:A:179:SER:HB2	1:A:181:VAL:HG12	1.83	0.60
1:D:23:ILE:HG21	1:D:126:PHE:CD1	2.37	0.60
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.36	0.60
1:F:179:SER:HB2	1:F:181:VAL:HG12	1.84	0.60
1:G:145:ILE:H	1:G:145:ILE:HD12	1.65	0.60
1:G:182:GLN:H	1:G:183:PRO:HD2	1.65	0.60
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.36	0.60
1:C:145:ILE:HD12	1:C:145:ILE:H	1.66	0.60
1:E:140:LEU:HD21	4:E:327:HOH:O	2.02	0.60
1:F:224:TRP:CE3	1:G:281:ILE:HG23	2.37	0.59
1:A:20:ILE:HD12	1:A:195:ILE:HD11	1.82	0.59
1:A:247:PHE:CE1	1:E:248:TYR:HA	2.37	0.59
1:B:199:ARG:O	1:B:201:PRO:HD3	2.02	0.59
1:B:224:TRP:NE1	1:B:301:ARG:HD3	2.17	0.59
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.37	0.59
1:E:20:ILE:HD12	1:E:195:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:ILE:HG21	1:J:126:PHE:CD1	2.37	0.59
1:A:145:ILE:H	1:A:145:ILE:HD12	1.66	0.59
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.85	0.59
1:C:179:SER:HB2	1:C:181:VAL:HG12	1.84	0.59
1:C:199:ARG:O	1:C:201:PRO:HD3	2.03	0.59
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.36	0.59
1:D:179:SER:HB2	1:D:181:VAL:HG12	1.83	0.59
1:H:295:LEU:H	1:H:295:LEU:HD12	1.67	0.59
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.84	0.59
1:E:295:LEU:HD12	1:E:295:LEU:H	1.67	0.59
1:I:179:SER:HB2	1:I:181:VAL:HG12	1.85	0.59
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.32	0.59
1:C:295:LEU:H	1:C:295:LEU:HD12	1.68	0.59
1:F:295:LEU:H	1:F:295:LEU:HD12	1.68	0.59
1:A:199:ARG:O	1:A:201:PRO:HD3	2.03	0.59
1:A:294:ASP:HB2	1:A:297:ILE:CG2	2.33	0.59
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.38	0.58
1:I:212:LEU:O	1:I:216:ILE:HG13	2.03	0.58
1:J:212:LEU:HB3	1:J:265:MET:HE1	1.84	0.58
1:B:141:ARG:HG2	1:B:142:PHE:CD2	2.38	0.58
1:E:179:SER:HB2	1:E:181:VAL:HG12	1.85	0.58
1:I:152:ILE:HG23	1:I:155:GLU:OE1	2.03	0.58
1:A:232:LEU:HD23	1:E:225:LEU:CD2	2.34	0.58
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.33	0.58
1:J:141:ARG:HG2	1:J:142:PHE:CD2	2.38	0.58
1:A:295:LEU:HD12	1:A:295:LEU:H	1.68	0.58
1:B:137:ASN:HA	3:B:328:GOL:O1	2.03	0.58
1:F:212:LEU:O	1:F:216:ILE:HG13	2.04	0.58
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.34	0.58
1:F:294:ASP:HB2	1:F:297:ILE:CG2	2.32	0.58
1:J:295:LEU:H	1:J:295:LEU:HD12	1.68	0.58
1:G:225:LEU:CD2	1:H:232:LEU:HD23	2.34	0.58
1:H:224:TRP:CD1	1:H:301:ARG:HD3	2.38	0.58
1:I:295:LEU:H	1:I:295:LEU:HD12	1.67	0.58
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.38	0.58
1:F:212:LEU:HB3	1:F:265:MET:HE1	1.84	0.58
1:I:225:LEU:HD21	1:J:232:LEU:HD23	1.85	0.58
1:B:179:SER:HB2	1:B:181:VAL:HG12	1.86	0.58
1:C:212:LEU:O	1:C:216:ILE:HG13	2.03	0.58
1:E:163:ARG:O	1:E:164:GLY:O	2.21	0.58
1:E:257:PRO:HG2	1:E:258:TYR:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:VAL:HG22	1:I:103:ASN:ND2	2.17	0.58
1:J:294:ASP:HB2	1:J:297:ILE:CG2	2.33	0.58
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.39	0.57
1:H:224:TRP:NE1	1:H:301:ARG:HD3	2.18	0.57
1:D:152:ILE:HG23	1:D:155:GLU:OE1	2.04	0.57
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.86	0.57
1:B:224:TRP:CD1	1:B:301:ARG:HD3	2.40	0.57
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.84	0.57
1:G:294:ASP:HB2	1:G:297:ILE:CG2	2.33	0.57
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.85	0.57
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.86	0.57
1:E:294:ASP:HB2	1:E:297:ILE:CG2	2.34	0.57
1:I:294:ASP:HB2	1:I:297:ILE:CG2	2.34	0.57
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.70	0.57
1:G:224:TRP:NE1	1:G:301:ARG:HD3	2.19	0.57
1:D:295:LEU:HD12	1:D:295:LEU:H	1.69	0.57
1:E:40:VAL:HG22	1:E:103:ASN:HD22	1.69	0.57
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.34	0.57
1:B:212:LEU:O	1:B:216:ILE:HG13	2.05	0.57
1:D:294:ASP:HB2	1:D:297:ILE:CG2	2.33	0.57
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.87	0.57
1:E:260:THR:HG23	1:E:263:ASP:OD2	2.05	0.57
1:G:137:ASN:HA	3:G:325:GOL:H2	1.87	0.57
1:H:257:PRO:HG2	1:H:258:TYR:CD2	2.39	0.57
1:F:225:LEU:CD2	1:G:232:LEU:HD23	2.35	0.57
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.35	0.57
1:G:295:LEU:H	1:G:295:LEU:HD12	1.67	0.57
1:B:295:LEU:HD12	1:B:295:LEU:H	1.70	0.57
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.86	0.57
1:G:137:ASN:HA	3:G:325:GOL:C1	2.35	0.57
1:J:199:ARG:O	1:J:201:PRO:HD3	2.05	0.57
1:A:210:LEU:HB3	1:A:211:PRO:CD	2.33	0.56
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.39	0.56
1:I:248:TYR:HA	1:J:247:PHE:CE1	2.40	0.56
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.40	0.56
1:I:257:PRO:HG2	1:I:258:TYR:CD2	2.41	0.56
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.41	0.56
1:B:145:ILE:HG21	1:B:193:VAL:CG1	2.36	0.56
1:E:141:ARG:HG2	1:E:142:PHE:CD2	2.41	0.56
1:F:289:ASN:CG	1:F:290:GLY:H	2.08	0.56
1:G:224:TRP:CD1	1:G:301:ARG:HD3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.88	0.56
1:C:210:LEU:HB3	1:C:211:PRO:CD	2.35	0.56
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.41	0.56
1:G:78:PHE:O	1:G:81:VAL:HG22	2.06	0.56
1:G:210:LEU:HB3	1:G:211:PRO:CD	2.35	0.56
1:J:224:TRP:NE1	1:J:301:ARG:HD3	2.21	0.56
1:G:141:ARG:HG2	1:G:142:PHE:HD2	1.70	0.56
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.88	0.56
1:G:289:ASN:CG	1:G:290:GLY:H	2.08	0.56
1:J:302:LEU:O	1:J:306:LEU:HG	2.06	0.56
1:A:225:LEU:HB2	1:A:231:ARG:HG3	1.88	0.55
1:C:141:ARG:HG2	1:C:142:PHE:CD2	2.41	0.55
1:F:257:PRO:HG2	1:F:258:TYR:CD2	2.40	0.55
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.42	0.55
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.41	0.55
1:A:212:LEU:O	1:A:216:ILE:HG13	2.07	0.55
1:D:145:ILE:HG21	1:D:193:VAL:CG1	2.36	0.55
1:F:99:ARG:NH1	1:G:180:SER:HB3	2.21	0.55
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.88	0.55
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.42	0.55
1:I:284:HIS:HD2	1:I:285:HIS:CE1	2.24	0.55
1:B:168:THR:O	1:B:169:HIS:CG	2.59	0.55
1:D:260:THR:HG23	1:D:263:ASP:OD2	2.06	0.55
1:E:137:ASN:CA	3:E:324:GOL:H2	2.34	0.55
1:A:224:TRP:NE1	1:A:301:ARG:HD3	2.20	0.55
1:B:137:ASN:HA	3:B:328:GOL:H12	1.87	0.55
1:C:302:LEU:O	1:C:306:LEU:HG	2.07	0.55
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.42	0.55
1:G:284:HIS:HD2	1:G:285:HIS:CE1	2.25	0.55
1:A:141:ARG:HG2	1:A:142:PHE:CD2	2.41	0.55
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.87	0.55
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.41	0.55
1:H:289:ASN:CG	1:H:290:GLY:H	2.10	0.55
1:I:44:THR:HA	1:I:99:ARG:HA	1.89	0.55
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.34	0.55
1:D:99:ARG:NH1	1:E:180:SER:HB3	2.22	0.55
1:J:289:ASN:CG	1:J:290:GLY:H	2.09	0.55
1:B:295:LEU:HA	1:B:298:GLN:NE2	2.19	0.55
1:C:140:LEU:HD13	1:C:191:ILE:CG1	2.35	0.55
1:C:284:HIS:HD2	1:C:285:HIS:CE1	2.24	0.55
1:C:289:ASN:CG	1:C:290:GLY:H	2.11	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ARG:O	1:F:201:PRO:HD3	2.06	0.54
1:F:227:SER:HB3	1:F:230:GLU:CG	2.37	0.54
1:G:44:THR:HA	1:G:99:ARG:HA	1.89	0.54
1:H:225:LEU:HB2	1:H:231:ARG:HG3	1.88	0.54
1:I:225:LEU:HB2	1:I:231:ARG:HG3	1.89	0.54
1:J:149:THR:HG22	1:J:150:GLU:H	1.73	0.54
1:B:12:VAL:H	1:B:138:GLN:HA	1.73	0.54
1:D:212:LEU:O	1:D:216:ILE:HG13	2.08	0.54
1:D:224:TRP:NE1	1:D:301:ARG:HD3	2.22	0.54
1:E:284:HIS:HD2	1:E:285:HIS:CE1	2.26	0.54
1:F:141:ARG:HG2	1:F:142:PHE:CD2	2.42	0.54
1:H:227:SER:HB3	1:H:230:GLU:CG	2.37	0.54
1:A:284:HIS:HD2	1:A:285:HIS:CE1	2.25	0.54
1:A:224:TRP:CD1	1:A:301:ARG:HD3	2.42	0.54
1:C:11:PRO:N	4:C:326:HOH:O	2.40	0.54
1:E:40:VAL:HG22	1:E:103:ASN:ND2	2.22	0.54
1:J:141:ARG:HG2	1:J:142:PHE:HD2	1.73	0.54
1:J:210:LEU:HB3	1:J:211:PRO:CD	2.35	0.54
1:B:225:LEU:CD2	1:C:232:LEU:HD23	2.37	0.54
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.73	0.54
1:G:206:TRP:CD2	2:G:324:MES:O3S	2.61	0.54
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.43	0.54
1:G:302:LEU:O	1:G:306:LEU:HG	2.08	0.54
1:H:212:LEU:O	1:H:216:ILE:HG13	2.08	0.54
1:A:145:ILE:HG21	1:A:193:VAL:CG1	2.38	0.54
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.42	0.54
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.26	0.54
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.43	0.54
1:D:248:TYR:HD1	1:E:247:PHE:HA	1.73	0.54
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.88	0.54
1:J:284:HIS:HD2	1:J:285:HIS:CE1	2.26	0.54
1:B:289:ASN:CG	1:B:290:GLY:H	2.10	0.54
1:D:12:VAL:H	1:D:138:GLN:HA	1.73	0.54
1:A:44:THR:HA	1:A:99:ARG:HA	1.90	0.54
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.43	0.54
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.43	0.54
1:I:152:ILE:HA	1:I:155:GLU:CD	2.28	0.54
1:B:141:ARG:HG2	1:B:142:PHE:HD2	1.73	0.53
1:J:224:TRP:CD1	1:J:301:ARG:HD3	2.42	0.53
1:J:44:THR:HA	1:J:99:ARG:HA	1.90	0.53
1:A:289:ASN:CG	1:A:290:GLY:H	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:H	1:D:145:ILE:HD12	1.72	0.53
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.89	0.53
1:D:11:PRO:HB3	3:D:326:GOL:C1	2.38	0.53
1:E:289:ASN:CG	1:E:290:GLY:H	2.11	0.53
1:H:302:LEU:O	1:H:306:LEU:HG	2.08	0.53
1:I:289:ASN:CG	1:I:290:GLY:H	2.11	0.53
1:B:284:HIS:HD2	1:B:285:HIS:CE1	2.26	0.53
1:B:302:LEU:O	1:B:306:LEU:HG	2.08	0.53
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.90	0.53
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.90	0.53
1:D:44:THR:HA	1:D:99:ARG:HA	1.89	0.53
1:E:217:ALA:HA	1:E:220:TRP:CE3	2.44	0.53
1:G:173:ILE:HD13	1:G:190:ARG:HB3	1.89	0.53
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.35	0.53
1:C:44:THR:HA	1:C:99:ARG:HA	1.90	0.53
1:D:302:LEU:O	1:D:306:LEU:HG	2.08	0.53
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.91	0.53
1:I:224:TRP:CE3	1:J:281:ILE:HG23	2.43	0.53
1:J:212:LEU:O	1:J:216:ILE:HG13	2.07	0.53
1:H:199:ARG:O	1:H:201:PRO:HD3	2.08	0.53
1:H:99:ARG:NH1	1:I:180:SER:HB3	2.24	0.53
1:A:127:VAL:HG22	1:A:194:ARG:HG2	1.91	0.53
1:A:302:LEU:O	1:A:306:LEU:HG	2.09	0.53
1:C:224:TRP:NE1	1:C:301:ARG:HD3	2.23	0.53
1:F:127:VAL:HG22	1:F:194:ARG:HG2	1.91	0.53
1:G:147:VAL:HG13	1:G:147:VAL:O	2.08	0.53
1:H:40:VAL:HG22	1:H:103:ASN:HD22	1.73	0.53
1:D:289:ASN:CG	1:D:290:GLY:H	2.11	0.53
1:E:141:ARG:HG2	1:E:142:PHE:HD2	1.74	0.53
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.27	0.53
1:H:149:THR:HG22	1:H:150:GLU:H	1.74	0.53
1:H:183:PRO:O	1:H:184:ASN:HB2	2.09	0.53
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.39	0.53
1:I:145:ILE:HG21	1:I:193:VAL:CG1	2.39	0.53
1:C:145:ILE:HG21	1:C:193:VAL:CG1	2.38	0.52
1:C:227:SER:HB3	1:C:230:GLU:CG	2.39	0.52
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.90	0.52
1:G:152:ILE:HG23	1:G:155:GLU:OE1	2.09	0.52
1:H:141:ARG:HG2	1:H:142:PHE:CD2	2.43	0.52
1:D:141:ARG:HG2	1:D:142:PHE:CD2	2.44	0.52
1:I:20:ILE:HD12	1:I:195:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:HG22	1:C:150:GLU:H	1.74	0.52
1:F:12:VAL:H	1:F:138:GLN:HA	1.73	0.52
1:I:141:ARG:HG2	1:I:142:PHE:CD2	2.44	0.52
1:C:147:VAL:HG13	1:C:147:VAL:O	2.10	0.52
1:B:224:TRP:CE3	1:C:281:ILE:HG23	2.45	0.52
1:D:227:SER:HB3	1:D:230:GLU:CG	2.40	0.52
1:G:199:ARG:O	1:G:201:PRO:HD3	2.09	0.52
1:I:183:PRO:O	1:I:184:ASN:HB2	2.08	0.52
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.44	0.52
1:D:284:HIS:HD2	1:D:285:HIS:CE1	2.28	0.52
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.44	0.52
1:J:140:LEU:HD13	1:J:191:ILE:CG1	2.35	0.52
1:J:145:ILE:HG21	1:J:193:VAL:CG1	2.39	0.52
1:D:137:ASN:HB3	3:D:326:GOL:O1	2.10	0.52
1:E:44:THR:HA	1:E:99:ARG:HA	1.92	0.52
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.45	0.52
1:B:40:VAL:HG22	1:B:103:ASN:HD22	1.74	0.52
1:D:224:TRP:CD1	1:D:301:ARG:HD3	2.44	0.52
1:E:145:ILE:HG21	1:E:193:VAL:CG1	2.39	0.52
1:I:225:LEU:HD23	1:J:232:LEU:HD23	1.92	0.52
1:A:152:ILE:HG23	1:A:155:GLU:OE1	2.10	0.52
1:B:210:LEU:HB3	1:B:211:PRO:CD	2.36	0.52
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.45	0.51
1:E:149:THR:HG22	1:E:150:GLU:H	1.74	0.51
1:I:224:TRP:NE1	1:I:301:ARG:HD3	2.25	0.51
1:I:302:LEU:O	1:I:306:LEU:HG	2.10	0.51
1:A:141:ARG:HG2	1:A:142:PHE:HD2	1.75	0.51
1:C:141:ARG:HG2	1:C:142:PHE:HD2	1.75	0.51
1:E:78:PHE:O	1:E:81:VAL:HG22	2.10	0.51
1:F:149:THR:HG22	1:F:150:GLU:H	1.75	0.51
1:A:40:VAL:HG22	1:A:103:ASN:HD22	1.74	0.51
1:J:227:SER:O	1:J:231:ARG:HD3	2.11	0.51
1:H:145:ILE:HG21	1:H:193:VAL:CG1	2.39	0.51
1:A:225:LEU:CD2	1:B:232:LEU:HD23	2.41	0.51
1:B:227:SER:HB3	1:B:230:GLU:CG	2.40	0.51
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.46	0.51
1:H:284:HIS:HD2	1:H:285:HIS:CE1	2.28	0.51
1:I:248:TYR:HD1	1:J:247:PHE:HA	1.74	0.51
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.91	0.51
1:B:287:GLN:HE21	1:B:287:GLN:C	2.14	0.51
1:A:227:SER:HB3	1:A:230:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PRO:O	1:B:184:ASN:HB2	2.11	0.51
1:C:99:ARG:NH1	1:D:180:SER:HB3	2.25	0.51
1:F:141:ARG:HG2	1:F:142:PHE:HD2	1.76	0.51
1:F:40:VAL:HG22	1:F:103:ASN:HD22	1.76	0.51
1:G:127:VAL:HG22	1:G:194:ARG:HG2	1.92	0.51
1:H:287:GLN:C	1:H:287:GLN:HE21	2.14	0.51
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.91	0.51
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.92	0.51
1:B:147:VAL:O	1:B:147:VAL:HG13	2.11	0.51
1:D:147:VAL:O	1:D:147:VAL:HG13	2.11	0.51
1:E:302:LEU:O	1:E:306:LEU:HG	2.10	0.51
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.93	0.51
1:I:78:PHE:O	1:I:81:VAL:HG22	2.10	0.51
1:A:12:VAL:H	1:A:138:GLN:HA	1.76	0.51
1:A:183:PRO:O	1:A:184:ASN:HB2	2.10	0.51
1:C:224:TRP:CD1	1:C:301:ARG:HD3	2.45	0.51
1:A:137:ASN:HB3	3:A:324:GOL:H12	1.93	0.51
1:A:78:PHE:O	1:A:81:VAL:HG22	2.11	0.51
1:B:55:PRO:HB3	1:B:95:PHE:CD2	2.45	0.51
1:F:183:PRO:O	1:F:184:ASN:HB2	2.10	0.51
1:F:44:THR:HA	1:F:99:ARG:HA	1.93	0.51
1:H:44:THR:HA	1:H:99:ARG:HA	1.92	0.51
1:A:149:THR:HG22	1:A:150:GLU:H	1.75	0.50
1:B:152:ILE:HG23	1:B:155:GLU:OE1	2.11	0.50
1:F:40:VAL:HG22	1:F:103:ASN:ND2	2.26	0.50
1:G:149:THR:HG22	1:G:150:GLU:H	1.77	0.50
1:B:40:VAL:HG22	1:B:103:ASN:ND2	2.26	0.50
1:C:183:PRO:O	1:C:184:ASN:HB2	2.11	0.50
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.93	0.50
1:E:183:PRO:O	1:E:184:ASN:HB2	2.10	0.50
1:E:12:VAL:H	1:E:138:GLN:HA	1.76	0.50
1:E:210:LEU:CB	1:E:211:PRO:HD3	2.33	0.50
1:F:302:LEU:O	1:F:306:LEU:HG	2.12	0.50
1:F:78:PHE:O	1:F:81:VAL:HG22	2.12	0.50
1:D:183:PRO:O	1:D:184:ASN:HB2	2.11	0.50
1:D:40:VAL:HG22	1:D:103:ASN:HD22	1.77	0.50
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.47	0.50
1:F:152:ILE:HG23	1:F:155:GLU:OE1	2.12	0.50
1:A:40:VAL:HG22	1:A:103:ASN:ND2	2.27	0.50
1:B:78:PHE:O	1:B:81:VAL:HG22	2.12	0.50
1:D:137:ASN:CB	3:D:326:GOL:O1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.47	0.50
1:G:112:ASN:OD1	1:G:113:ASP:N	2.44	0.50
1:I:182:GLN:N	1:I:183:PRO:CD	2.75	0.50
1:B:44:THR:HA	1:B:99:ARG:HA	1.92	0.50
1:H:152:ILE:HG23	1:H:155:GLU:OE1	2.12	0.50
1:H:260:THR:HG23	1:H:263:ASP:OD2	2.11	0.50
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.76	0.50
1:E:152:ILE:HG23	1:E:155:GLU:OE1	2.11	0.50
1:F:260:THR:HG23	1:F:263:ASP:OD2	2.12	0.50
1:I:145:ILE:HD12	1:I:145:ILE:H	1.75	0.50
1:J:183:PRO:O	1:J:184:ASN:HB2	2.11	0.50
1:A:260:THR:HG23	1:A:263:ASP:OD2	2.11	0.49
1:E:227:SER:HB3	1:E:230:GLU:CG	2.41	0.49
1:I:247:PHE:CD2	1:J:247:PHE:CE2	2.99	0.49
1:B:127:VAL:HG22	1:B:194:ARG:HG2	1.94	0.49
1:C:152:ILE:HG23	1:C:155:GLU:OE1	2.11	0.49
1:D:11:PRO:HD2	4:D:330:HOH:O	2.12	0.49
1:G:227:SER:HB3	1:G:230:GLU:CG	2.42	0.49
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.45	0.49
1:D:141:ARG:HG2	1:D:142:PHE:HD2	1.78	0.49
1:G:99:ARG:NH1	1:H:180:SER:HB3	2.27	0.49
1:I:149:THR:HG22	1:I:150:GLU:H	1.77	0.49
1:I:227:SER:HB3	1:I:230:GLU:CG	2.41	0.49
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.48	0.49
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.12	0.49
1:F:224:TRP:CD1	1:F:301:ARG:HD3	2.47	0.49
1:J:12:VAL:H	1:J:138:GLN:HA	1.77	0.49
1:C:112:ASN:OD1	1:C:113:ASP:N	2.45	0.49
1:C:11:PRO:CD	4:C:326:HOH:O	2.61	0.49
1:F:210:LEU:CB	1:F:211:PRO:HD3	2.36	0.49
1:H:141:ARG:HG2	1:H:142:PHE:HD2	1.76	0.49
1:I:55:PRO:HB3	1:I:95:PHE:CD2	2.47	0.49
1:D:152:ILE:HA	1:D:155:GLU:CD	2.32	0.49
1:E:147:VAL:HG13	1:E:147:VAL:O	2.12	0.49
1:F:224:TRP:NE1	1:F:301:ARG:HD3	2.27	0.49
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.42	0.49
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.30	0.49
1:H:40:VAL:HG22	1:H:103:ASN:ND2	2.27	0.49
1:E:245:TYR:O	1:E:249:THR:HB	2.13	0.49
1:F:68:ASN:ND2	1:J:65:ARG:HD2	2.28	0.49
1:C:212:LEU:HG	1:C:245:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:N	1:D:138:GLN:HA	2.28	0.49
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.47	0.49
1:F:182:GLN:N	1:F:183:PRO:CD	2.74	0.49
1:G:168:THR:C	1:G:169:HIS:ND1	2.66	0.49
1:G:183:PRO:O	1:G:184:ASN:HB2	2.11	0.49
1:E:12:VAL:N	1:E:138:GLN:HA	2.28	0.49
1:I:224:TRP:CD1	1:I:301:ARG:HD3	2.47	0.49
1:C:40:VAL:HG22	1:C:103:ASN:ND2	2.28	0.48
1:D:43:TRP:CZ2	1:D:100:VAL:HG11	2.47	0.48
1:I:136:ASN:O	3:I:326:GOL:H12	2.12	0.48
1:J:29:LEU:HD23	1:J:29:LEU:HA	1.69	0.48
1:E:140:LEU:HD13	1:E:191:ILE:CG1	2.41	0.48
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.32	0.48
1:I:11:PRO:HB3	3:I:326:GOL:H31	1.95	0.48
1:I:12:VAL:H	1:I:138:GLN:HA	1.78	0.48
1:D:78:PHE:O	1:D:81:VAL:HG22	2.13	0.48
1:F:137:ASN:HA	3:F:323:GOL:C3	2.44	0.48
1:F:29:LEU:HD23	1:F:29:LEU:HA	1.73	0.48
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.48	0.48
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.43	0.48
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.48	0.48
1:G:12:VAL:H	1:G:138:GLN:HA	1.76	0.48
1:G:145:ILE:HG21	1:G:193:VAL:CG1	2.43	0.48
1:G:289:ASN:OD1	1:G:292:GLU:HB3	2.13	0.48
1:H:112:ASN:OD1	1:H:113:ASP:N	2.46	0.48
1:B:112:ASN:OD1	1:B:113:ASP:N	2.47	0.48
1:D:71:LEU:HD12	1:D:72:TRP:N	2.28	0.48
1:F:145:ILE:HG21	1:F:193:VAL:CG1	2.40	0.48
1:H:137:ASN:HA	3:H:323:GOL:C1	2.43	0.48
1:J:227:SER:HB3	1:J:230:GLU:CG	2.43	0.48
1:C:40:VAL:HG22	1:C:103:ASN:HD22	1.78	0.48
1:G:212:LEU:O	1:G:216:ILE:HG13	2.12	0.48
1:H:212:LEU:HG	1:H:245:TYR:CE2	2.48	0.48
1:J:152:ILE:HG23	1:J:155:GLU:OE1	2.13	0.48
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.62	0.48
1:H:78:PHE:O	1:H:81:VAL:HG22	2.13	0.48
1:A:247:PHE:CD1	1:E:248:TYR:HA	2.48	0.48
1:A:287:GLN:HE21	1:A:287:GLN:C	2.17	0.48
1:A:99:ARG:NH1	1:B:180:SER:HB3	2.29	0.48
1:E:55:PRO:HB3	1:E:95:PHE:CD2	2.49	0.48
1:G:163:ARG:O	1:G:164:GLY:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:ASN:C	1:G:200:ASN:HD22	2.16	0.48
1:G:225:LEU:HD21	1:H:232:LEU:HD23	1.95	0.48
1:A:11:PRO:HB3	3:A:324:GOL:O1	2.14	0.48
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.43	0.48
1:D:40:VAL:HG22	1:D:103:ASN:ND2	2.29	0.48
1:E:212:LEU:O	1:E:216:ILE:HG13	2.13	0.48
1:H:147:VAL:O	1:H:147:VAL:HG22	2.14	0.48
1:I:287:GLN:HE21	1:I:287:GLN:C	2.17	0.48
1:E:152:ILE:HA	1:E:155:GLU:CD	2.34	0.47
1:E:182:GLN:N	1:E:183:PRO:CD	2.74	0.47
1:E:297:ILE:CG2	1:E:298:GLN:N	2.77	0.47
1:F:12:VAL:N	1:F:138:GLN:HA	2.29	0.47
1:A:210:LEU:CB	1:A:211:PRO:HD3	2.39	0.47
1:A:112:ASN:OD1	1:A:113:ASP:N	2.47	0.47
1:B:12:VAL:N	1:B:138:GLN:HA	2.29	0.47
1:H:182:GLN:N	1:H:183:PRO:CD	2.74	0.47
1:I:137:ASN:HA	3:I:326:GOL:O3	2.14	0.47
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.13	0.47
1:A:152:ILE:HA	1:A:155:GLU:CD	2.35	0.47
1:A:182:GLN:N	1:A:183:PRO:CD	2.74	0.47
1:B:182:GLN:N	1:B:183:PRO:CD	2.73	0.47
1:G:152:ILE:HA	1:G:155:GLU:CD	2.34	0.47
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.15	0.47
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.64	0.47
1:J:257:PRO:HG2	1:J:258:TYR:CD2	2.48	0.47
1:B:200:ASN:C	1:B:200:ASN:HD22	2.18	0.47
1:C:227:SER:O	1:C:231:ARG:HD3	2.14	0.47
1:D:140:LEU:HD22	1:D:191:ILE:HD11	1.96	0.47
1:F:147:VAL:HG22	1:F:147:VAL:O	2.13	0.47
1:G:55:PRO:HB3	1:G:95:PHE:CD2	2.50	0.47
1:A:232:LEU:HD23	1:E:225:LEU:HD21	1.96	0.47
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.96	0.47
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.95	0.47
1:G:40:VAL:HG22	1:G:103:ASN:HD22	1.79	0.47
1:B:149:THR:HG22	1:B:150:GLU:H	1.78	0.47
1:D:147:VAL:O	1:D:147:VAL:HG22	2.15	0.47
1:D:137:ASN:N	3:D:326:GOL:H2	2.30	0.47
1:G:168:THR:O	1:G:169:HIS:CG	2.67	0.47
1:H:224:TRP:CE3	1:I:281:ILE:HG23	2.49	0.47
1:A:240:LEU:CD1	1:E:241:THR:HA	2.44	0.47
1:D:212:LEU:HA	1:D:212:LEU:HD23	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:TYR:O	1:H:249:THR:HB	2.14	0.47
1:B:204:TYR:O	1:B:209:ILE:HG12	2.15	0.47
1:B:260:THR:HG23	1:B:263:ASP:OD2	2.14	0.47
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.45	0.47
1:E:212:LEU:HG	1:E:245:TYR:CE2	2.49	0.47
1:F:247:PHE:CD1	1:J:248:TYR:HA	2.49	0.47
1:H:227:SER:HB3	1:H:230:GLU:HG3	1.96	0.47
1:I:136:ASN:O	3:I:326:GOL:C1	2.63	0.47
1:J:260:THR:HG23	1:J:263:ASP:OD2	2.15	0.47
1:G:224:TRP:CE3	1:H:281:ILE:HG23	2.50	0.47
1:J:182:GLN:N	1:J:183:PRO:CD	2.74	0.47
1:J:40:VAL:HG22	1:J:103:ASN:HD22	1.80	0.47
1:A:212:LEU:HG	1:A:245:TYR:CE2	2.50	0.47
1:J:152:ILE:HA	1:J:155:GLU:CD	2.35	0.47
1:A:227:SER:HB3	1:A:230:GLU:HG3	1.97	0.46
1:C:137:ASN:HA	3:C:324:GOL:HO1	1.80	0.46
1:F:212:LEU:HG	1:F:245:TYR:CE2	2.50	0.46
1:G:147:VAL:O	1:G:147:VAL:HG22	2.14	0.46
1:H:14:VAL:HG22	1:H:43:TRP:HB3	1.96	0.46
1:I:212:LEU:HG	1:I:245:TYR:CE2	2.50	0.46
1:J:137:ASN:HA	3:J:325:GOL:C2	2.45	0.46
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.97	0.46
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.50	0.46
1:C:78:PHE:O	1:C:81:VAL:HG22	2.14	0.46
1:G:287:GLN:HE21	1:G:287:GLN:C	2.18	0.46
1:I:140:LEU:HD11	4:I:329:HOH:O	2.14	0.46
1:I:147:VAL:HG22	1:I:147:VAL:O	2.15	0.46
1:A:147:VAL:HG13	1:A:147:VAL:O	2.15	0.46
1:E:29:LEU:HA	1:E:29:LEU:HD23	1.69	0.46
1:F:200:ASN:HD22	1:F:200:ASN:C	2.19	0.46
1:F:287:GLN:HE21	1:F:287:GLN:C	2.19	0.46
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.81	0.46
1:A:200:ASN:HD22	1:A:200:ASN:C	2.19	0.46
1:D:149:THR:HG22	1:D:150:GLU:H	1.78	0.46
1:D:182:GLN:N	1:D:183:PRO:CD	2.74	0.46
1:E:136:ASN:O	3:E:324:GOL:O1	2.25	0.46
1:J:287:GLN:C	1:J:287:GLN:HE21	2.19	0.46
1:A:224:TRP:CE3	1:B:281:ILE:HG23	2.50	0.46
1:A:55:PRO:HB3	1:A:95:PHE:CD2	2.50	0.46
1:B:225:LEU:HD23	1:C:232:LEU:HD23	1.97	0.46
1:B:248:TYR:HA	1:C:247:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.97	0.46
1:F:140:LEU:HD13	1:F:191:ILE:CG1	2.36	0.46
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.46	0.46
1:E:289:ASN:OD1	1:E:292:GLU:HB3	2.16	0.46
1:G:182:GLN:N	1:G:183:PRO:CD	2.75	0.46
1:H:152:ILE:HA	1:H:155:GLU:CD	2.36	0.46
1:G:248:TYR:HA	1:H:247:PHE:CD1	2.50	0.46
1:H:297:ILE:C	1:H:299:ARG:N	2.69	0.46
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.45	0.46
1:I:297:ILE:CG2	1:I:298:GLN:N	2.78	0.46
1:A:12:VAL:N	1:A:138:GLN:HA	2.30	0.46
1:B:168:THR:O	1:B:169:HIS:CD2	2.69	0.46
1:E:136:ASN:O	3:E:324:GOL:H2	2.16	0.46
1:F:297:ILE:CG2	1:F:298:GLN:N	2.78	0.46
1:H:248:TYR:HE1	1:I:250:SER:HG	1.64	0.46
1:J:12:VAL:N	1:J:138:GLN:HA	2.31	0.46
1:C:12:VAL:H	1:C:138:GLN:HA	1.79	0.46
1:C:12:VAL:N	1:C:138:GLN:HA	2.30	0.46
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.97	0.46
1:C:287:GLN:C	1:C:287:GLN:HE21	2.19	0.46
1:E:297:ILE:HG23	1:E:298:GLN:N	2.31	0.46
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.51	0.46
1:D:140:LEU:HD13	1:D:191:ILE:CG1	2.38	0.46
1:F:137:ASN:HA	3:F:323:GOL:C2	2.46	0.46
1:H:227:SER:O	1:H:231:ARG:HD3	2.16	0.46
1:J:212:LEU:CD1	1:J:265:MET:HB3	2.46	0.46
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.81	0.46
1:A:212:LEU:CD1	1:A:265:MET:HB3	2.45	0.46
1:B:227:SER:O	1:B:231:ARG:HD3	2.16	0.46
1:C:297:ILE:C	1:C:299:ARG:N	2.69	0.46
1:C:297:ILE:CG2	1:C:298:GLN:N	2.79	0.46
1:D:227:SER:O	1:D:231:ARG:HD3	2.16	0.46
1:F:112:ASN:OD1	1:F:113:ASP:N	2.48	0.46
1:H:297:ILE:CG2	1:H:298:GLN:N	2.78	0.46
1:I:141:ARG:HG2	1:I:142:PHE:HD2	1.80	0.46
1:D:284:HIS:HE1	1:D:291:VAL:HG13	1.81	0.45
1:D:287:GLN:C	1:D:287:GLN:HE21	2.19	0.45
1:J:289:ASN:OD1	1:J:292:GLU:HB3	2.16	0.45
1:A:147:VAL:O	1:A:147:VAL:HG22	2.15	0.45
1:B:241:THR:HA	1:C:240:LEU:CD1	2.46	0.45
1:G:12:VAL:N	1:G:138:GLN:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:CD1	1:J:241:THR:HA	2.46	0.45
1:A:289:ASN:OD1	1:A:292:GLU:HB3	2.16	0.45
1:D:11:PRO:CD	4:D:330:HOH:O	2.64	0.45
1:D:289:ASN:OD1	1:D:292:GLU:HB3	2.16	0.45
1:E:112:ASN:OD1	1:E:113:ASP:N	2.49	0.45
1:F:137:ASN:HA	3:F:323:GOL:O1	2.17	0.45
1:I:72:TRP:HH2	1:I:138:GLN:HG3	1.81	0.45
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.84	0.45
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.85	0.45
1:B:289:ASN:OD1	1:B:292:GLU:HB3	2.16	0.45
1:H:72:TRP:HH2	1:H:138:GLN:HG3	1.81	0.45
1:I:137:ASN:HB3	3:I:326:GOL:O3	2.16	0.45
1:A:245:TYR:O	1:A:249:THR:HB	2.17	0.45
1:A:297:ILE:CG2	1:A:298:GLN:N	2.79	0.45
1:C:94:LEU:HD23	1:C:100:VAL:HG22	1.98	0.45
1:F:72:TRP:HH2	1:F:138:GLN:HG3	1.81	0.45
1:F:55:PRO:HB3	1:F:95:PHE:CD2	2.52	0.45
1:I:210:LEU:CB	1:I:211:PRO:HD3	2.37	0.45
1:J:200:ASN:HD22	1:J:200:ASN:C	2.19	0.45
1:B:297:ILE:CG2	1:B:298:GLN:N	2.79	0.45
1:E:212:LEU:CD1	1:E:265:MET:HB3	2.47	0.45
1:E:287:GLN:C	1:E:287:GLN:HE21	2.20	0.45
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.98	0.45
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.80	0.45
1:C:289:ASN:OD1	1:C:292:GLU:HB3	2.16	0.45
1:D:249:THR:HG22	1:D:250:SER:N	2.32	0.45
1:G:147:VAL:CG1	1:G:165:LYS:HE2	2.47	0.45
1:J:212:LEU:HA	1:J:212:LEU:HD23	1.74	0.45
1:A:227:SER:O	1:A:231:ARG:HD3	2.16	0.45
1:A:36:ASP:HB2	1:A:107:LEU:HD13	1.99	0.45
1:B:245:TYR:O	1:B:249:THR:HB	2.16	0.45
1:C:152:ILE:HA	1:C:155:GLU:CD	2.37	0.45
1:D:91:ARG:HB2	1:E:133:PHE:CE2	2.52	0.45
1:F:227:SER:O	1:F:231:ARG:HD3	2.17	0.45
1:F:263:ASP:O	1:F:267:ILE:HG13	2.16	0.45
1:I:289:ASN:OD1	1:I:292:GLU:HB3	2.15	0.45
1:B:152:ILE:HA	1:B:155:GLU:CD	2.36	0.45
1:C:297:ILE:C	1:C:299:ARG:H	2.20	0.45
1:D:112:ASN:OD1	1:D:113:ASP:N	2.49	0.45
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.82	0.45
1:D:300:CYS:C	1:D:302:LEU:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:VAL:O	1:F:147:VAL:HG13	2.16	0.45
1:F:152:ILE:HA	1:F:155:GLU:CD	2.36	0.45
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.51	0.45
1:H:297:ILE:HG23	1:H:298:GLN:N	2.32	0.45
1:J:137:ASN:HB3	3:J:325:GOL:O1	2.17	0.45
1:J:212:LEU:HG	1:J:245:TYR:CE2	2.52	0.45
1:B:147:VAL:O	1:B:147:VAL:HG22	2.17	0.45
1:B:168:THR:C	1:B:169:HIS:CD2	2.90	0.45
1:C:137:ASN:O	1:C:138:GLN:HB3	2.17	0.45
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.35	0.45
1:E:182:GLN:O	1:E:183:PRO:C	2.55	0.45
1:F:245:TYR:O	1:F:249:THR:HB	2.17	0.45
1:G:297:ILE:CG2	1:G:298:GLN:N	2.79	0.45
1:J:147:VAL:HG22	1:J:147:VAL:O	2.17	0.45
1:B:163:ARG:HD2	1:B:163:ARG:HA	1.63	0.44
1:B:168:THR:C	1:B:169:HIS:CG	2.91	0.44
1:B:71:LEU:HD12	1:B:72:TRP:N	2.33	0.44
1:C:200:ASN:HD22	1:C:200:ASN:C	2.19	0.44
1:G:305:PRO:O	1:G:309:LEU:HD13	2.17	0.44
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.35	0.44
1:I:12:VAL:N	1:I:138:GLN:HA	2.33	0.44
1:C:182:GLN:N	1:C:183:PRO:CD	2.74	0.44
1:G:297:ILE:C	1:G:299:ARG:N	2.70	0.44
1:G:72:TRP:HH2	1:G:138:GLN:HG3	1.80	0.44
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.82	0.44
1:J:291:VAL:HG12	1:J:291:VAL:O	2.18	0.44
1:B:249:THR:HG22	1:B:250:SER:N	2.33	0.44
1:E:293:ASP:O	1:E:295:LEU:N	2.51	0.44
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.72	0.44
1:F:289:ASN:OD1	1:F:292:GLU:HB3	2.18	0.44
1:F:293:ASP:O	1:F:295:LEU:N	2.50	0.44
1:J:137:ASN:CA	3:J:325:GOL:H11	2.45	0.44
1:H:182:GLN:O	1:H:183:PRO:C	2.55	0.44
1:I:305:PRO:O	1:I:309:LEU:HD13	2.17	0.44
1:J:205:LEU:HD23	1:J:205:LEU:HA	1.86	0.44
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.84	0.44
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.36	0.44
1:B:173:ILE:HD13	1:B:190:ARG:CB	2.47	0.44
1:D:297:ILE:CG2	1:D:298:GLN:N	2.81	0.44
1:G:173:ILE:HD13	1:G:190:ARG:CB	2.47	0.44
1:I:112:ASN:OD1	1:I:113:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:297:ILE:C	1:J:299:ARG:N	2.71	0.44
1:C:263:ASP:O	1:C:267:ILE:HG13	2.17	0.44
1:D:178:LEU:HA	1:D:178:LEU:HD23	1.85	0.44
1:D:200:ASN:C	1:D:200:ASN:HD22	2.20	0.44
1:F:180:SER:HB3	1:J:99:ARG:NH1	2.32	0.44
1:H:200:ASN:HD22	1:H:200:ASN:C	2.20	0.44
1:B:297:ILE:C	1:B:299:ARG:N	2.71	0.44
1:G:119:PHE:CB	1:G:120:PRO:HD3	2.44	0.44
1:G:212:LEU:HG	1:G:245:TYR:CE2	2.53	0.44
1:G:293:ASP:O	1:G:295:LEU:N	2.50	0.44
1:G:40:VAL:HG22	1:G:103:ASN:ND2	2.32	0.44
2:D:323:MES:H82	2:D:323:MES:H31	1.80	0.44
1:E:11:PRO:CD	4:E:328:HOH:O	2.65	0.44
1:A:140:LEU:HD13	1:A:191:ILE:CG1	2.41	0.44
1:A:148:TYR:OH	1:B:177:HIS:HE1	2.01	0.44
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.71	0.44
1:A:297:ILE:C	1:A:299:ARG:N	2.71	0.44
1:D:157:ILE:HA	1:D:157:ILE:HD13	1.84	0.44
1:D:297:ILE:C	1:D:299:ARG:H	2.21	0.44
1:F:284:HIS:HD2	1:F:285:HIS:HE1	1.61	0.44
1:G:291:VAL:HG12	1:G:291:VAL:O	2.18	0.44
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.33	0.44
1:J:40:VAL:HG22	1:J:103:ASN:ND2	2.33	0.44
1:C:289:ASN:HD21	1:C:292:GLU:HB2	1.83	0.43
1:D:199:ARG:O	1:D:201:PRO:CD	2.66	0.43
1:E:227:SER:O	1:E:231:ARG:HD3	2.18	0.43
1:A:247:PHE:CE2	1:E:247:PHE:CD2	3.04	0.43
1:F:163:ARG:HA	1:F:163:ARG:HD2	1.58	0.43
1:J:182:GLN:O	1:J:183:PRO:C	2.57	0.43
1:A:182:GLN:O	1:A:183:PRO:C	2.57	0.43
1:F:300:CYS:C	1:F:302:LEU:H	2.21	0.43
1:I:155:GLU:HB3	1:I:161:TRP:CD1	2.52	0.43
1:J:227:SER:HB3	1:J:230:GLU:HG3	2.00	0.43
1:D:118:LEU:O	1:D:119:PHE:C	2.57	0.43
1:D:293:ASP:O	1:D:295:LEU:N	2.51	0.43
1:E:140:LEU:HD22	1:E:191:ILE:HD11	2.00	0.43
1:E:147:VAL:HG22	1:E:147:VAL:O	2.18	0.43
1:F:208:PHE:CE2	1:F:248:TYR:CE2	3.06	0.43
1:G:94:LEU:HD23	1:G:100:VAL:HG22	1.99	0.43
1:F:225:LEU:HD23	1:G:232:LEU:HD23	1.99	0.43
1:J:297:ILE:CG2	1:J:298:GLN:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:PRO:HB3	1:J:95:PHE:CD2	2.53	0.43
1:B:43:TRP:CZ2	1:B:100:VAL:HG11	2.54	0.43
1:C:284:HIS:HE1	1:C:291:VAL:HG13	1.84	0.43
1:D:210:LEU:CB	1:D:211:PRO:HD3	2.39	0.43
1:E:200:ASN:C	1:E:200:ASN:HD22	2.21	0.43
1:E:289:ASN:HD21	1:E:292:GLU:HB2	1.82	0.43
1:F:297:ILE:HG23	1:F:298:GLN:N	2.33	0.43
1:I:199:ARG:O	1:I:201:PRO:CD	2.65	0.43
1:G:118:LEU:O	1:G:119:PHE:C	2.56	0.43
1:G:263:ASP:O	1:G:267:ILE:HG13	2.19	0.43
1:I:212:LEU:HD23	1:I:212:LEU:HA	1.72	0.43
1:I:248:TYR:HA	1:J:247:PHE:CD1	2.53	0.43
1:J:112:ASN:OD1	1:J:113:ASP:N	2.52	0.43
1:A:72:TRP:HH2	1:A:138:GLN:HG3	1.83	0.43
1:D:249:THR:CG2	1:D:250:SER:N	2.82	0.43
1:E:173:ILE:N	1:E:173:ILE:HD12	2.34	0.43
1:E:297:ILE:C	1:E:299:ARG:N	2.71	0.43
1:F:157:ILE:HA	1:F:157:ILE:HD13	1.79	0.43
1:F:289:ASN:HD21	1:F:292:GLU:HB2	1.84	0.43
1:F:291:VAL:HG12	1:F:291:VAL:O	2.18	0.43
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.86	0.43
1:A:293:ASP:O	1:A:295:LEU:N	2.52	0.43
1:A:248:TYR:CD1	1:B:247:PHE:HA	2.50	0.43
1:B:72:TRP:HH2	1:B:138:GLN:HG3	1.83	0.43
1:C:305:PRO:O	1:C:309:LEU:HD13	2.19	0.43
1:D:297:ILE:C	1:D:299:ARG:N	2.72	0.43
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.49	0.43
1:H:291:VAL:O	1:H:291:VAL:HG12	2.18	0.43
1:A:297:ILE:HG23	1:A:298:GLN:N	2.33	0.43
1:I:137:ASN:HA	3:I:326:GOL:H32	1.97	0.43
1:I:71:LEU:HD12	1:I:72:TRP:N	2.33	0.43
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.66	0.43
1:B:173:ILE:CD1	1:B:190:ARG:HB3	2.49	0.43
1:C:137:ASN:HA	3:C:324:GOL:C1	2.48	0.43
1:E:118:LEU:O	1:E:119:PHE:C	2.56	0.43
1:F:226:GLU:OE2	1:G:284:HIS:NE2	2.51	0.43
1:H:163:ARG:HA	1:H:163:ARG:HD2	1.55	0.43
1:I:227:SER:O	1:I:231:ARG:HD3	2.18	0.43
1:I:293:ASP:O	1:I:295:LEU:N	2.52	0.43
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.83	0.43
1:B:147:VAL:CG1	1:B:165:LYS:HE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HG23	1:B:298:GLN:N	2.34	0.43
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.84	0.43
1:J:297:ILE:C	1:J:299:ARG:H	2.22	0.43
1:J:78:PHE:O	1:J:81:VAL:HG22	2.19	0.43
1:A:209:ILE:HG12	1:A:209:ILE:H	1.69	0.42
1:C:118:LEU:O	1:C:119:PHE:C	2.57	0.42
1:D:114:MET:HE2	1:D:124:GLN:HG2	2.01	0.42
1:G:289:ASN:CG	1:G:290:GLY:N	2.72	0.42
1:H:11:PRO:N	4:H:325:HOH:O	2.52	0.42
1:H:12:VAL:N	1:H:138:GLN:HA	2.34	0.42
1:H:297:ILE:C	1:H:299:ARG:H	2.22	0.42
1:I:147:VAL:HG13	1:I:147:VAL:O	2.18	0.42
1:I:297:ILE:HG23	1:I:298:GLN:N	2.33	0.42
1:J:147:VAL:CG1	1:J:165:LYS:HE2	2.49	0.42
1:A:297:ILE:C	1:A:299:ARG:H	2.22	0.42
1:F:297:ILE:C	1:F:299:ARG:N	2.72	0.42
1:H:287:GLN:CA	1:H:287:GLN:HE21	2.32	0.42
1:G:65:ARG:HD2	1:H:68:ASN:ND2	2.34	0.42
1:I:204:TYR:O	1:I:209:ILE:HG12	2.19	0.42
1:I:284:HIS:HD2	1:I:285:HIS:HE1	1.67	0.42
1:B:249:THR:CG2	1:B:250:SER:N	2.82	0.42
1:E:256:LEU:HB3	1:E:257:PRO:HD2	2.00	0.42
1:G:224:TRP:CD1	1:G:224:TRP:N	2.87	0.42
1:G:297:ILE:HG23	1:G:298:GLN:N	2.34	0.42
1:I:182:GLN:O	1:I:183:PRO:C	2.57	0.42
1:B:212:LEU:HG	1:B:245:TYR:CE2	2.54	0.42
1:C:291:VAL:O	1:C:291:VAL:HG12	2.19	0.42
1:D:314:VAL:HG12	1:D:314:VAL:O	2.19	0.42
1:E:297:ILE:C	1:E:299:ARG:H	2.23	0.42
1:G:209:ILE:H	1:G:209:ILE:HG12	1.72	0.42
1:G:91:ARG:HD2	1:H:134:SER:HB3	2.01	0.42
1:B:182:GLN:O	1:B:183:PRO:C	2.58	0.42
1:B:291:VAL:O	1:B:291:VAL:HG12	2.20	0.42
1:B:314:VAL:HG12	1:B:314:VAL:O	2.19	0.42
1:C:182:GLN:O	1:C:183:PRO:C	2.56	0.42
1:C:314:VAL:O	1:C:314:VAL:HG12	2.20	0.42
1:F:145:ILE:H	1:F:145:ILE:CD1	2.28	0.42
1:F:247:PHE:HA	1:J:248:TYR:CD1	2.49	0.42
1:F:248:TYR:HA	1:G:247:PHE:CD1	2.54	0.42
1:F:35:VAL:O	1:F:107:LEU:HD12	2.20	0.42
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:291:VAL:O	1:I:291:VAL:HG12	2.19	0.42
1:J:293:ASP:O	1:J:295:LEU:N	2.52	0.42
1:C:11:PRO:HD2	4:C:326:HOH:O	2.18	0.42
1:C:14:VAL:HG22	1:C:43:TRP:HB3	2.02	0.42
1:C:297:ILE:HG23	1:C:298:GLN:N	2.33	0.42
1:D:204:TYR:O	1:D:209:ILE:HG12	2.19	0.42
1:F:305:PRO:O	1:F:309:LEU:HD13	2.20	0.42
1:G:178:LEU:HD12	1:G:186:ASN:HA	2.02	0.42
1:I:297:ILE:C	1:I:299:ARG:N	2.72	0.42
1:J:245:TYR:O	1:J:249:THR:HB	2.19	0.42
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.31	0.42
1:C:162:ILE:HG22	1:C:164:GLY:H	1.85	0.42
1:G:297:ILE:C	1:G:299:ARG:H	2.21	0.42
1:G:36:ASP:HB2	1:G:107:LEU:HD13	2.01	0.42
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.52	0.42
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.84	0.42
1:F:182:GLN:O	1:F:183:PRO:C	2.58	0.42
1:J:284:HIS:HE1	1:J:291:VAL:HG13	1.85	0.42
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.84	0.42
1:B:220:TRP:C	1:B:222:VAL:H	2.24	0.42
1:B:256:LEU:HB3	1:B:257:PRO:HD2	2.01	0.42
1:A:232:LEU:HD23	1:E:225:LEU:HD23	2.01	0.42
1:G:137:ASN:CA	3:G:325:GOL:H2	2.49	0.42
1:H:12:VAL:H	1:H:138:GLN:HA	1.83	0.42
1:E:291:VAL:HG12	1:E:291:VAL:O	2.19	0.42
1:G:227:SER:HB3	1:G:230:GLU:HG3	2.00	0.42
1:G:227:SER:O	1:G:231:ARG:HD3	2.19	0.42
1:G:245:TYR:O	1:G:249:THR:HB	2.19	0.42
1:H:289:ASN:OD1	1:H:292:GLU:HB3	2.19	0.42
1:I:119:PHE:CB	1:I:120:PRO:HD3	2.47	0.42
1:I:289:ASN:HD21	1:I:292:GLU:HB2	1.84	0.42
1:J:140:LEU:HD22	1:J:191:ILE:HD11	2.02	0.42
1:B:145:ILE:CD1	1:B:145:ILE:H	2.29	0.41
1:B:150:GLU:O	1:B:150:GLU:OE1	2.38	0.41
1:A:148:TYR:OH	1:B:177:HIS:CE1	2.73	0.41
1:F:224:TRP:CZ3	1:G:281:ILE:HG23	2.55	0.41
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.64	0.41
1:I:209:ILE:H	1:I:209:ILE:HG12	1.69	0.41
1:J:210:LEU:CB	1:J:211:PRO:HD3	2.41	0.41
1:A:289:ASN:CG	1:A:290:GLY:N	2.73	0.41
1:A:71:LEU:HD12	1:A:72:TRP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.78	0.41
1:D:225:LEU:CD2	1:E:232:LEU:HD23	2.49	0.41
1:D:297:ILE:HG23	1:D:298:GLN:N	2.34	0.41
1:D:137:ASN:CA	3:D:326:GOL:O1	2.66	0.41
1:I:130:LEU:HA	1:I:130:LEU:HD23	1.88	0.41
1:J:231:ARG:HB3	1:J:280:ILE:HD13	2.02	0.41
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.85	0.41
1:C:36:ASP:HB2	1:C:107:LEU:HD13	2.03	0.41
1:C:173:ILE:HD12	1:C:173:ILE:N	2.35	0.41
1:C:245:TYR:O	1:C:249:THR:HB	2.21	0.41
1:E:212:LEU:HA	1:E:212:LEU:HD23	1.66	0.41
1:F:314:VAL:O	1:F:314:VAL:HG12	2.21	0.41
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.66	0.41
1:H:118:LEU:O	1:H:119:PHE:C	2.57	0.41
1:H:205:LEU:HD23	1:H:205:LEU:HA	1.86	0.41
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.69	0.41
1:H:208:PHE:CE2	1:H:248:TYR:CE2	3.08	0.41
1:H:36:ASP:HB2	1:H:107:LEU:HD13	2.01	0.41
1:I:118:LEU:O	1:I:119:PHE:C	2.58	0.41
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.69	0.41
1:F:11:PRO:HB3	3:F:323:GOL:H32	2.02	0.41
1:G:137:ASN:CB	3:G:325:GOL:O1	2.69	0.41
1:J:263:ASP:O	1:J:267:ILE:HG13	2.20	0.41
1:A:118:LEU:O	1:A:119:PHE:C	2.58	0.41
1:B:99:ARG:NH1	1:C:180:SER:HB3	2.36	0.41
1:D:14:VAL:HG22	1:D:43:TRP:HB3	2.03	0.41
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.76	0.41
1:E:114:MET:HE2	1:E:124:GLN:HG2	2.03	0.41
1:F:297:ILE:C	1:F:299:ARG:H	2.23	0.41
1:G:248:TYR:CD1	1:H:247:PHE:HA	2.52	0.41
1:C:310:ALA:O	1:C:314:VAL:HG23	2.21	0.41
1:D:94:LEU:HD23	1:D:100:VAL:HG22	2.02	0.41
1:D:47:PRO:HA	1:D:98:GLY:HA2	2.02	0.41
1:F:209:ILE:H	1:F:209:ILE:HG12	1.68	0.41
1:F:256:LEU:HB3	1:F:257:PRO:HD2	2.03	0.41
1:G:287:GLN:HE21	1:G:287:GLN:CA	2.33	0.41
1:I:245:TYR:O	1:I:249:THR:HB	2.21	0.41
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.86	0.41
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.82	0.41
1:A:225:LEU:HD23	1:B:232:LEU:HD23	2.02	0.41
1:A:300:CYS:C	1:A:302:LEU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ASP:O	1:C:295:LEU:N	2.54	0.41
1:G:182:GLN:O	1:G:183:PRO:C	2.57	0.41
1:F:248:TYR:CD1	1:G:247:PHE:HA	2.51	0.41
1:J:43:TRP:CZ2	1:J:100:VAL:HG11	2.56	0.41
1:A:291:VAL:O	1:A:291:VAL:HG12	2.20	0.41
1:C:147:VAL:HG22	1:C:147:VAL:O	2.21	0.41
1:D:182:GLN:O	1:D:183:PRO:C	2.57	0.41
1:D:209:ILE:H	1:D:209:ILE:HG12	1.65	0.41
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.63	0.41
1:D:36:ASP:HB2	1:D:107:LEU:HD13	2.02	0.41
1:I:278:LEU:HD23	1:I:278:LEU:HA	1.86	0.41
1:I:99:ARG:NH1	1:J:180:SER:HB3	2.36	0.41
1:B:263:ASP:O	1:B:267:ILE:HG13	2.21	0.41
1:C:131:GLU:HA	1:C:132:PRO:HD3	1.96	0.41
1:D:89:ASN:HB2	1:E:133:PHE:CE1	2.55	0.41
1:G:212:LEU:HD23	1:G:212:LEU:HA	1.70	0.41
1:H:182:GLN:N	1:H:183:PRO:HD2	2.34	0.41
1:H:55:PRO:HB3	1:H:95:PHE:CD2	2.55	0.41
1:J:147:VAL:HG13	1:J:147:VAL:O	2.20	0.41
1:J:297:ILE:HG23	1:J:298:GLN:N	2.35	0.41
1:A:173:ILE:HD13	1:A:190:ARG:CB	2.49	0.41
1:A:305:PRO:O	1:A:309:LEU:HD13	2.21	0.41
1:A:314:VAL:O	1:A:314:VAL:HG12	2.21	0.41
1:C:224:TRP:CE3	1:D:281:ILE:HG23	2.55	0.41
1:D:145:ILE:H	1:D:145:ILE:CD1	2.32	0.41
1:F:178:LEU:HD23	1:F:178:LEU:HA	1.83	0.41
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.86	0.41
1:J:178:LEU:HA	1:J:178:LEU:HD23	1.81	0.41
1:J:224:TRP:CD1	1:J:224:TRP:N	2.88	0.41
1:J:92:LEU:HD23	1:J:92:LEU:HA	1.90	0.41
1:A:284:HIS:HE1	1:A:291:VAL:HG13	1.86	0.41
1:C:204:TYR:O	1:C:209:ILE:HG12	2.21	0.41
1:C:212:LEU:HA	1:C:212:LEU:HD23	1.72	0.41
1:D:220:TRP:C	1:D:222:VAL:H	2.24	0.41
1:D:291:VAL:O	1:D:291:VAL:HG12	2.21	0.41
1:D:289:ASN:ND2	1:D:292:GLU:HB2	2.36	0.41
1:D:71:LEU:HD12	1:D:72:TRP:H	1.86	0.41
1:H:248:TYR:HA	1:I:247:PHE:CD1	2.55	0.41
1:H:305:PRO:O	1:H:309:LEU:HD13	2.21	0.41
1:I:178:LEU:HA	1:I:178:LEU:HD23	1.85	0.41
1:I:314:VAL:HG12	1:I:314:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ILE:CD1	1:J:145:ILE:H	2.29	0.41
1:J:204:TYR:O	1:J:209:ILE:HG12	2.20	0.41
1:A:14:VAL:HG22	1:A:43:TRP:HB3	2.03	0.40
1:B:293:ASP:O	1:B:295:LEU:N	2.54	0.40
1:B:300:CYS:C	1:B:302:LEU:H	2.24	0.40
1:D:263:ASP:O	1:D:267:ILE:HG13	2.21	0.40
1:F:231:ARG:HB3	1:F:280:ILE:HD13	2.03	0.40
1:H:293:ASP:O	1:H:295:LEU:N	2.54	0.40
1:H:314:VAL:O	1:H:314:VAL:HG12	2.20	0.40
1:A:248:TYR:HA	1:B:247:PHE:CD1	2.56	0.40
1:B:297:ILE:C	1:B:299:ARG:H	2.24	0.40
1:B:304:PHE:CB	1:B:305:PRO:HD3	2.52	0.40
1:C:224:TRP:CD1	1:C:224:TRP:N	2.89	0.40
1:D:245:TYR:O	1:D:249:THR:HB	2.21	0.40
1:E:263:ASP:O	1:E:267:ILE:HG13	2.20	0.40
1:I:36:ASP:HB2	1:I:107:LEU:HD13	2.03	0.40
1:J:173:ILE:HD13	1:J:190:ARG:CB	2.49	0.40
1:J:72:TRP:HH2	1:J:138:GLN:HG3	1.86	0.40
1:A:204:TYR:O	1:A:209:ILE:HG12	2.22	0.40
1:A:94:LEU:HD23	1:A:100:VAL:HG22	2.04	0.40
1:B:114:MET:CE	1:B:124:GLN:HG2	2.50	0.40
1:D:304:PHE:HB2	1:D:305:PRO:HD3	2.03	0.40
1:E:173:ILE:HD13	1:E:190:ARG:CB	2.50	0.40
1:F:284:HIS:CD2	1:F:285:HIS:CE1	3.06	0.40
1:H:101:ILE:CD1	1:I:179:SER:HB3	2.51	0.40
1:I:224:TRP:CD1	1:I:224:TRP:N	2.89	0.40
1:J:314:VAL:HG12	1:J:314:VAL:O	2.21	0.40
1:C:173:ILE:HD13	1:C:190:ARG:CB	2.51	0.40
1:D:287:GLN:CA	1:D:287:GLN:HE21	2.34	0.40
1:E:173:ILE:CD1	1:E:190:ARG:HB3	2.50	0.40
1:H:147:VAL:HG13	1:H:147:VAL:O	2.21	0.40
1:G:225:LEU:HD23	1:H:232:LEU:HD23	2.03	0.40
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.85	0.40
1:I:92:LEU:HA	1:I:92:LEU:HD23	1.88	0.40
1:J:140:LEU:CD1	4:J:329:HOH:O	2.50	0.40
1:A:145:ILE:H	1:A:145:ILE:CD1	2.30	0.40
1:B:178:LEU:HD12	1:B:186:ASN:HA	2.02	0.40
1:C:210:LEU:CB	1:C:211:PRO:HD3	2.43	0.40
1:C:55:PRO:HB3	1:C:95:PHE:CD2	2.56	0.40
1:E:199:ARG:O	1:E:201:PRO:CD	2.67	0.40
1:D:248:TYR:HA	1:E:247:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:ILE:HD13	1:I:190:ARG:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/322 (95%)	256 (84%)	36 (12%)	13 (4%)	2	14
1	B	305/322 (95%)	254 (83%)	39 (13%)	12 (4%)	3	16
1	C	305/322 (95%)	257 (84%)	35 (12%)	13 (4%)	2	14
1	D	305/322 (95%)	255 (84%)	37 (12%)	13 (4%)	2	14
1	E	305/322 (95%)	252 (83%)	38 (12%)	15 (5%)	2	12
1	F	305/322 (95%)	254 (83%)	38 (12%)	13 (4%)	2	14
1	G	305/322 (95%)	258 (85%)	34 (11%)	13 (4%)	2	14
1	H	305/322 (95%)	257 (84%)	36 (12%)	12 (4%)	3	16
1	I	305/322 (95%)	257 (84%)	37 (12%)	11 (4%)	3	18
1	J	305/322 (95%)	256 (84%)	36 (12%)	13 (4%)	2	14
All	All	3050/3220 (95%)	2556 (84%)	366 (12%)	128 (4%)	3	15

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	151	ASN
1	A	164	GLY
1	A	182	GLN
1	A	184	ASN
1	B	119	PHE

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Mol	Chain	Res	Type
1	B	138	GLN
1	B	151	ASN
1	B	164	GLY
1	B	182	GLN
1	B	184	ASN
1	C	119	PHE
1	C	151	ASN
1	C	182	GLN
1	C	184	ASN
1	D	119	PHE
1	D	138	GLN
1	D	151	ASN
1	D	164	GLY
1	D	182	GLN
1	D	184	ASN
1	E	119	PHE
1	E	151	ASN
1	E	182	GLN
1	E	184	ASN
1	F	119	PHE
1	F	151	ASN
1	F	164	GLY
1	F	182	GLN
1	F	184	ASN
1	G	119	PHE
1	G	151	ASN
1	G	182	GLN
1	G	184	ASN
1	H	119	PHE
1	H	151	ASN
1	H	182	GLN
1	H	184	ASN
1	I	119	PHE
1	I	151	ASN
1	I	182	GLN
1	I	184	ASN
1	J	119	PHE
1	J	151	ASN
1	J	182	GLN
1	J	184	ASN
1	A	138	GLN
1	A	179	SER

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Mol	Chain	Res	Type
1	A	289	ASN
1	A	294	ASP
1	B	179	SER
1	B	289	ASN
1	B	294	ASP
1	C	138	GLN
1	C	179	SER
1	C	289	ASN
1	C	294	ASP
1	D	179	SER
1	D	200	ASN
1	D	289	ASN
1	D	294	ASP
1	E	138	GLN
1	E	164	GLY
1	E	179	SER
1	E	200	ASN
1	E	289	ASN
1	E	294	ASP
1	F	138	GLN
1	F	179	SER
1	F	289	ASN
1	F	294	ASP
1	G	138	GLN
1	G	164	GLY
1	G	179	SER
1	G	289	ASN
1	G	294	ASP
1	H	138	GLN
1	H	179	SER
1	H	289	ASN
1	H	294	ASP
1	I	138	GLN
1	I	179	SER
1	I	289	ASN
1	I	294	ASP
1	J	138	GLN
1	J	164	GLY
1	J	179	SER
1	J	289	ASN
1	J	294	ASP
1	I	200	ASN

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Mol	Chain	Res	Type
1	A	200	ASN
1	B	176	ASP
1	E	163	ARG
1	E	169	HIS
1	E	176	ASP
1	F	176	ASP
1	H	176	ASP
1	I	176	ASP
1	J	176	ASP
1	J	200	ASN
1	A	176	ASP
1	A	290	GLY
1	B	200	ASN
1	C	200	ASN
1	D	176	ASP
1	E	290	GLY
1	F	200	ASN
1	F	290	GLY
1	G	176	ASP
1	G	200	ASN
1	H	200	ASN
1	H	290	GLY
1	B	290	GLY
1	C	176	ASP
1	C	290	GLY
1	D	47	PRO
1	D	290	GLY
1	G	290	GLY
1	H	169	HIS
1	I	290	GLY
1	J	290	GLY
1	E	47	PRO
1	F	47	PRO
1	G	47	PRO
1	J	47	PRO
1	A	47	PRO
1	C	47	PRO
1	C	164	GLY

### 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	275/284 (97%)	253 (92%)	22 (8%)	12	38
1	B	275/284 (97%)	252 (92%)	23 (8%)	11	36
1	C	275/284 (97%)	256 (93%)	19 (7%)	15	44
1	D	275/284 (97%)	253 (92%)	22 (8%)	12	38
1	E	275/284 (97%)	254 (92%)	21 (8%)	13	40
1	F	275/284 (97%)	251 (91%)	24 (9%)	10	35
1	G	275/284 (97%)	253 (92%)	22 (8%)	12	38
1	H	275/284 (97%)	252 (92%)	23 (8%)	11	36
1	I	275/284 (97%)	252 (92%)	23 (8%)	11	36
1	J	275/284 (97%)	253 (92%)	22 (8%)	12	38
All	All	2750/2840 (97%)	2529 (92%)	221 (8%)	12	38

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	29	LEU
1	A	64	GLU
1	A	87	THR
1	A	121	PHE
1	A	130	LEU
1	A	139	GLN
1	A	145	ILE
1	A	150	GLU
1	A	163	ARG
1	A	177	HIS
1	A	200	ASN
1	A	212	LEU
1	A	219	SER
1	A	234	THR
1	A	247	PHE

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Mol	Chain	Res	Type
1	A	249	THR
1	A	253	LEU
1	A	255	ARG
1	A	281	ILE
1	A	287	GLN
1	A	302	LEU
1	B	17	SER
1	B	29	LEU
1	B	64	GLU
1	B	87	THR
1	B	118	LEU
1	B	121	PHE
1	B	130	LEU
1	B	139	GLN
1	B	145	ILE
1	B	150	GLU
1	B	163	ARG
1	B	177	HIS
1	B	200	ASN
1	B	212	LEU
1	B	219	SER
1	B	234	THR
1	B	247	PHE
1	B	249	THR
1	B	253	LEU
1	B	255	ARG
1	B	281	ILE
1	B	287	GLN
1	B	302	LEU
1	C	17	SER
1	C	29	LEU
1	C	64	GLU
1	C	87	THR
1	C	121	PHE
1	C	130	LEU
1	C	139	GLN
1	C	145	ILE
1	C	150	GLU
1	C	200	ASN
1	C	212	LEU
1	C	234	THR
1	C	247	PHE

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Mol	Chain	Res	Type
1	C	249	THR
1	C	253	LEU
1	C	255	ARG
1	C	281	ILE
1	C	287	GLN
1	C	302	LEU
1	D	17	SER
1	D	29	LEU
1	D	64	GLU
1	D	87	THR
1	D	121	PHE
1	D	130	LEU
1	D	139	GLN
1	D	145	ILE
1	D	150	GLU
1	D	169	HIS
1	D	177	HIS
1	D	200	ASN
1	D	212	LEU
1	D	219	SER
1	D	234	THR
1	D	247	PHE
1	D	249	THR
1	D	253	LEU
1	D	255	ARG
1	D	281	ILE
1	D	287	GLN
1	D	302	LEU
1	E	17	SER
1	E	29	LEU
1	E	64	GLU
1	E	81	VAL
1	E	87	THR
1	E	121	PHE
1	E	130	LEU
1	E	139	GLN
1	E	145	ILE
1	E	150	GLU
1	E	163	ARG
1	E	200	ASN
1	E	212	LEU
1	E	234	THR

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Mol	Chain	Res	Type
1	E	247	PHE
1	E	249	THR
1	E	253	LEU
1	E	255	ARG
1	E	281	ILE
1	E	287	GLN
1	E	302	LEU
1	F	17	SER
1	F	28	THR
1	F	29	LEU
1	F	64	GLU
1	F	81	VAL
1	F	87	THR
1	F	121	PHE
1	F	130	LEU
1	F	139	GLN
1	F	145	ILE
1	F	150	GLU
1	F	163	ARG
1	F	177	HIS
1	F	200	ASN
1	F	212	LEU
1	F	219	SER
1	F	234	THR
1	F	247	PHE
1	F	249	THR
1	F	253	LEU
1	F	255	ARG
1	F	281	ILE
1	F	287	GLN
1	F	302	LEU
1	G	17	SER
1	G	29	LEU
1	G	64	GLU
1	G	81	VAL
1	G	87	THR
1	G	121	PHE
1	G	130	LEU
1	G	139	GLN
1	G	145	ILE
1	G	150	GLU
1	G	177	HIS

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Mol	Chain	Res	Type
1	G	200	ASN
1	G	212	LEU
1	G	219	SER
1	G	247	PHE
1	G	249	THR
1	G	253	LEU
1	G	255	ARG
1	G	260	THR
1	G	281	ILE
1	G	287	GLN
1	G	302	LEU
1	H	17	SER
1	H	29	LEU
1	H	64	GLU
1	H	87	THR
1	H	121	PHE
1	H	130	LEU
1	H	139	GLN
1	H	145	ILE
1	H	150	GLU
1	H	163	ARG
1	H	177	HIS
1	H	200	ASN
1	H	207	SER
1	H	212	LEU
1	H	219	SER
1	H	234	THR
1	H	247	PHE
1	H	249	THR
1	H	253	LEU
1	H	255	ARG
1	H	281	ILE
1	H	287	GLN
1	H	302	LEU
1	I	17	SER
1	I	29	LEU
1	I	64	GLU
1	I	81	VAL
1	I	87	THR
1	I	121	PHE
1	I	130	LEU
1	I	139	GLN

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Mol	Chain	Res	Type
1	I	145	ILE
1	I	150	GLU
1	I	169	HIS
1	I	177	HIS
1	I	200	ASN
1	I	212	LEU
1	I	219	SER
1	I	234	THR
1	I	247	PHE
1	I	249	THR
1	I	253	LEU
1	I	255	ARG
1	I	281	ILE
1	I	287	GLN
1	I	302	LEU
1	J	17	SER
1	J	29	LEU
1	J	64	GLU
1	J	81	VAL
1	J	87	THR
1	J	121	PHE
1	J	130	LEU
1	J	139	GLN
1	J	145	ILE
1	J	150	GLU
1	J	177	HIS
1	J	178	LEU
1	J	200	ASN
1	J	212	LEU
1	J	234	THR
1	J	247	PHE
1	J	249	THR
1	J	253	LEU
1	J	255	ARG
1	J	281	ILE
1	J	287	GLN
1	J	302	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	62	GLN
1	A	103	ASN
1	A	124	GLN
1	A	200	ASN
1	A	251	ASN
1	A	284	HIS
1	A	285	HIS
1	A	287	GLN
1	A	298	GLN
1	B	62	GLN
1	B	103	ASN
1	B	124	GLN
1	B	138	GLN
1	B	177	HIS
1	B	200	ASN
1	B	251	ASN
1	B	284	HIS
1	B	285	HIS
1	B	287	GLN
1	B	298	GLN
1	C	62	GLN
1	C	103	ASN
1	C	124	GLN
1	C	177	HIS
1	C	200	ASN
1	C	251	ASN
1	C	284	HIS
1	C	285	HIS
1	C	287	GLN
1	C	298	GLN
1	D	62	GLN
1	D	103	ASN
1	D	177	HIS
1	D	200	ASN
1	D	251	ASN
1	D	284	HIS
1	D	285	HIS
1	D	287	GLN
1	D	298	GLN
1	E	62	GLN
1	E	103	ASN
1	E	200	ASN

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Mol	Chain	Res	Type
1	E	251	ASN
1	E	284	HIS
1	E	285	HIS
1	E	287	GLN
1	E	298	GLN
1	F	62	GLN
1	F	103	ASN
1	F	124	GLN
1	F	151	ASN
1	F	200	ASN
1	F	251	ASN
1	F	284	HIS
1	F	285	HIS
1	F	287	GLN
1	F	298	GLN
1	G	42	GLN
1	G	62	GLN
1	G	103	ASN
1	G	124	GLN
1	G	177	HIS
1	G	200	ASN
1	G	251	ASN
1	G	285	HIS
1	G	287	GLN
1	G	298	GLN
1	H	42	GLN
1	H	62	GLN
1	H	103	ASN
1	H	177	HIS
1	H	200	ASN
1	H	251	ASN
1	H	285	HIS
1	H	287	GLN
1	H	298	GLN
1	I	42	GLN
1	I	62	GLN
1	I	103	ASN
1	I	138	GLN
1	I	200	ASN
1	I	251	ASN
1	I	284	HIS
1	I	285	HIS

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Mol	Chain	Res	Type
1	I	287	GLN
1	I	298	GLN
1	J	62	GLN
1	J	103	ASN
1	J	124	GLN
1	J	177	HIS
1	J	200	ASN
1	J	251	ASN
1	J	285	HIS
1	J	287	GLN
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](#)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MES	G	323	-	12,12,12	2.22	1 (8%)	14,16,16	2.31	6 (42%)
3	GOL	D	326	-	5,5,5	0.66	0	5,5,5	0.71	0
3	GOL	J	324	-	5,5,5	0.82	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MES	C	323	-	12,12,12	2.19	1 (8%)	14,16,16	2.60	6 (42%)
3	GOL	B	328	-	5,5,5	0.81	0	5,5,5	0.37	0
3	GOL	B	324	-	5,5,5	0.65	0	5,5,5	0.78	0
3	GOL	I	325	-	5,5,5	0.75	0	5,5,5	0.45	0
2	MES	I	323	-	12,12,12	2.16	1 (8%)	14,16,16	2.20	6 (42%)
2	MES	A	323	-	12,12,12	2.22	1 (8%)	14,16,16	2.32	8 (57%)
2	MES	B	323	-	12,12,12	2.14	1 (8%)	14,16,16	2.64	7 (50%)
3	GOL	B	326	-	5,5,5	0.83	0	5,5,5	0.27	0
2	MES	D	323	-	12,12,12	2.24	1 (8%)	14,16,16	2.56	6 (42%)
3	GOL	D	325	-	3,4,5	0.62	0	1,4,5	0.46	0
3	GOL	A	324	-	5,5,5	0.89	0	5,5,5	0.28	0
3	GOL	I	326	-	5,5,5	0.92	0	5,5,5	0.30	0
3	GOL	B	325	-	5,5,5	0.87	0	5,5,5	0.50	0
3	GOL	I	324	-	5,5,5	0.79	0	5,5,5	0.35	0
3	GOL	E	324	-	5,5,5	0.96	0	5,5,5	0.39	0
3	GOL	B	327	-	5,5,5	0.84	0	5,5,5	0.28	0
2	MES	G	324	-	12,12,12	2.13	1 (8%)	14,16,16	2.65	7 (50%)
3	GOL	J	325	-	5,5,5	0.90	0	5,5,5	0.54	0
3	GOL	E	323	-	5,5,5	0.85	0	5,5,5	0.34	0
3	GOL	C	324	-	5,5,5	0.73	0	5,5,5	0.66	0
3	GOL	H	323	-	5,5,5	0.92	0	5,5,5	0.39	0
3	GOL	J	323	-	5,5,5	0.90	0	5,5,5	0.23	0
3	GOL	D	324	-	5,5,5	0.78	0	5,5,5	0.34	0
3	GOL	F	323	-	5,5,5	0.92	0	5,5,5	0.23	0
3	GOL	G	325	-	5,5,5	0.64	0	5,5,5	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	G	323	-	-	2/6/14/14	0/1/1/1
3	GOL	D	326	-	-	2/4/4/4	-
3	GOL	J	324	-	-	0/4/4/4	-
2	MES	C	323	-	-	5/6/14/14	0/1/1/1
3	GOL	B	328	-	-	4/4/4/4	-
3	GOL	B	324	-	-	2/4/4/4	-
3	GOL	I	325	-	-	2/4/4/4	-
2	MES	I	323	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	A	323	-	-	0/6/14/14	0/1/1/1
2	MES	B	323	-	-	5/6/14/14	0/1/1/1
3	GOL	B	326	-	-	0/4/4/4	-
2	MES	D	323	-	-	2/6/14/14	0/1/1/1
3	GOL	D	325	-	-	1/2/2/4	-
3	GOL	A	324	-	-	2/4/4/4	-
3	GOL	I	326	-	-	2/4/4/4	-
3	GOL	B	325	-	-	0/4/4/4	-
3	GOL	I	324	-	-	0/4/4/4	-
3	GOL	E	324	-	-	0/4/4/4	-
3	GOL	B	327	-	-	2/4/4/4	-
2	MES	G	324	-	-	2/6/14/14	0/1/1/1
3	GOL	J	325	-	-	2/4/4/4	-
3	GOL	E	323	-	-	0/4/4/4	-
3	GOL	C	324	-	-	3/4/4/4	-
3	GOL	H	323	-	-	0/4/4/4	-
3	GOL	J	323	-	-	0/4/4/4	-
3	GOL	D	324	-	-	0/4/4/4	-
3	GOL	F	323	-	-	2/4/4/4	-
3	GOL	G	325	-	-	3/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	323	MES	C8-S	-7.44	1.66	1.77
2	G	323	MES	C8-S	-7.41	1.67	1.77
2	A	323	MES	C8-S	-7.37	1.67	1.77
2	C	323	MES	C8-S	-7.22	1.67	1.77
2	I	323	MES	C8-S	-7.13	1.67	1.77
2	B	323	MES	C8-S	-7.10	1.67	1.77
2	G	324	MES	C8-S	-7.04	1.67	1.77

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	323	MES	O2S-S-C8	5.77	113.87	106.92
2	G	323	MES	C5-N4-C3	4.84	119.72	108.83
2	C	323	MES	C5-N4-C3	4.77	119.56	108.83
2	G	324	MES	C5-N4-C3	4.71	119.42	108.83
2	B	323	MES	C5-N4-C3	4.68	119.37	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	324	MES	O1S-S-C8	4.55	112.39	106.92
2	D	323	MES	C5-N4-C3	4.45	118.84	108.83
2	I	323	MES	C5-N4-C3	4.40	118.74	108.83
2	A	323	MES	C5-N4-C3	4.38	118.69	108.83
2	C	323	MES	O1S-S-C8	4.30	112.09	106.92
2	B	323	MES	O2S-S-C8	3.87	111.57	106.92
2	G	324	MES	C7-N4-C5	3.77	120.88	111.23
2	C	323	MES	C7-N4-C5	3.74	120.80	111.23
2	C	323	MES	C6-C5-N4	-3.67	104.53	110.10
2	G	324	MES	C6-C5-N4	-3.66	104.55	110.10
2	B	323	MES	C7-N4-C5	3.56	120.34	111.23
2	A	323	MES	C6-C5-N4	-3.54	104.74	110.10
2	B	323	MES	C7-N4-C3	3.52	120.23	111.23
2	B	323	MES	C6-C5-N4	-3.41	104.94	110.10
2	G	324	MES	C7-N4-C3	3.31	119.69	111.23
2	C	323	MES	C7-N4-C3	3.14	119.27	111.23
2	G	323	MES	C7-N4-C3	3.09	119.13	111.23
2	D	323	MES	C7-N4-C5	3.01	118.93	111.23
2	D	323	MES	C7-N4-C3	3.00	118.92	111.23
2	G	323	MES	C7-N4-C5	2.99	118.89	111.23
2	B	323	MES	C2-C3-N4	-2.90	105.71	110.10
2	I	323	MES	O3S-S-C8	2.87	110.41	105.77
2	I	323	MES	C7-N4-C5	2.84	118.50	111.23
2	D	323	MES	C2-C3-N4	-2.83	105.81	110.10
2	A	323	MES	C2-C3-N4	-2.79	105.87	110.10
2	I	323	MES	C7-N4-C3	2.78	118.35	111.23
2	G	323	MES	O1S-S-C8	2.78	110.26	106.92
2	B	323	MES	O3S-S-C8	2.70	110.14	105.77
2	I	323	MES	C2-C3-N4	-2.70	106.02	110.10
2	G	323	MES	C2-C3-N4	-2.65	106.08	110.10
2	A	323	MES	O3S-S-C8	2.63	110.03	105.77
2	A	323	MES	C7-N4-C5	2.61	117.91	111.23
2	C	323	MES	C2-C3-N4	-2.59	106.17	110.10
2	A	323	MES	C7-N4-C3	2.54	117.72	111.23
2	G	323	MES	O3S-S-C8	2.45	109.73	105.77
2	A	323	MES	O2S-S-C8	2.37	109.77	106.92
2	G	324	MES	C2-C3-N4	-2.37	106.51	110.10
2	D	323	MES	C6-C5-N4	-2.18	106.80	110.10
2	A	323	MES	O1S-S-C8	2.12	109.47	106.92
2	I	323	MES	O2S-S-C8	2.09	109.44	106.92
2	G	324	MES	O3S-S-C8	2.01	109.01	105.77

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	323	MES	N4-C7-C8-S
2	C	323	MES	N4-C7-C8-S
3	B	324	GOL	O1-C1-C2-C3
2	I	323	MES	N4-C7-C8-S
2	B	323	MES	N4-C7-C8-S
2	B	323	MES	C7-C8-S-O2S
3	A	324	GOL	O1-C1-C2-C3
3	I	326	GOL	C1-C2-C3-O3
2	G	324	MES	N4-C7-C8-S
3	C	324	GOL	O1-C1-C2-C3
3	G	325	GOL	C1-C2-C3-O3
3	G	325	GOL	O2-C2-C3-O3
3	A	324	GOL	O1-C1-C2-O2
2	C	323	MES	C7-C8-S-O3S
2	B	323	MES	C7-C8-S-O3S
3	D	326	GOL	O1-C1-C2-C3
3	F	323	GOL	O1-C1-C2-C3
3	D	326	GOL	O1-C1-C2-O2
3	F	323	GOL	O1-C1-C2-O2
3	I	326	GOL	O2-C2-C3-O3
3	C	324	GOL	O1-C1-C2-O2
2	D	323	MES	N4-C7-C8-S
2	G	323	MES	C8-C7-N4-C3
2	C	323	MES	C8-C7-N4-C3
2	B	323	MES	C8-C7-N4-C3
2	D	323	MES	C8-C7-N4-C5
2	G	324	MES	C8-C7-N4-C3
3	B	328	GOL	O1-C1-C2-O2
3	B	328	GOL	O2-C2-C3-O3
3	B	324	GOL	O1-C1-C2-O2
3	D	325	GOL	C1-C2-C3-O3
3	J	325	GOL	O1-C1-C2-O2
3	C	324	GOL	O2-C2-C3-O3
3	G	325	GOL	O1-C1-C2-O2
3	B	328	GOL	C1-C2-C3-O3
3	I	325	GOL	C1-C2-C3-O3
2	C	323	MES	C7-C8-S-O1S
2	C	323	MES	C7-C8-S-O2S
2	B	323	MES	C7-C8-S-O1S
3	I	325	GOL	O2-C2-C3-O3
3	J	325	GOL	O1-C1-C2-C3
3	B	328	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	327	GOL	C1-C2-C3-O3
3	B	327	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	326	GOL	11	0
3	B	328	GOL	3	0
2	D	323	MES	1	0
3	A	324	GOL	3	0
3	I	326	GOL	9	0
3	E	324	GOL	9	0
2	G	324	MES	1	0
3	J	325	GOL	7	0
3	C	324	GOL	3	0
3	H	323	GOL	4	0
3	F	323	GOL	5	0
3	G	325	GOL	6	0

## 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	307/322 (95%)	-0.14	18 (5%)	22	10	66, 102, 183, 215	0
1	B	307/322 (95%)	-0.29	15 (4%)	29	13	64, 98, 186, 214	0
1	C	307/322 (95%)	-0.26	12 (3%)	39	19	59, 101, 186, 212	0
1	D	307/322 (95%)	-0.23	12 (3%)	39	19	57, 97, 182, 217	0
1	E	307/322 (95%)	-0.25	11 (3%)	42	21	67, 102, 185, 212	0
1	F	307/322 (95%)	-0.23	11 (3%)	42	21	63, 106, 184, 210	0
1	G	307/322 (95%)	-0.22	12 (3%)	39	19	62, 98, 188, 215	0
1	H	307/322 (95%)	-0.08	17 (5%)	25	11	65, 101, 185, 217	0
1	I	307/322 (95%)	-0.16	18 (5%)	22	10	63, 100, 187, 215	0
1	J	307/322 (95%)	-0.21	13 (4%)	36	18	70, 106, 188, 213	0
All	All	3070/3220 (95%)	-0.20	139 (4%)	33	16	57, 101, 187, 217	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	291	VAL	10.5
1	F	317	ILE	9.4
1	G	315	LEU	9.2
1	E	291	VAL	9.0
1	H	180	SER	8.6
1	B	291	VAL	8.4
1	B	290	GLY	8.4
1	H	290	GLY	7.8
1	B	152	ILE	7.6
1	A	151	ASN	7.6
1	A	152	ILE	7.5
1	J	152	ILE	7.0
1	H	152	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	H	288	ALA	6.7
1	G	314	VAL	5.8
1	H	289	ASN	5.6
1	G	290	GLY	5.5
1	E	290	GLY	5.5
1	H	151	ASN	5.4
1	J	151	ASN	5.4
1	G	151	ASN	5.2
1	J	153	ASP	5.1
1	I	291	VAL	5.1
1	D	181	VAL	5.0
1	I	179	SER	4.9
1	C	290	GLY	4.8
1	F	152	ILE	4.8
1	I	153	ASP	4.8
1	J	290	GLY	4.7
1	A	179	SER	4.7
1	B	151	ASN	4.7
1	I	290	GLY	4.7
1	G	287	GLN	4.7
1	G	152	ILE	4.7
1	F	151	ASN	4.6
1	B	315	LEU	4.6
1	J	291	VAL	4.5
1	H	185	GLN	4.5
1	F	179	SER	4.5
1	I	180	SER	4.5
1	D	151	ASN	4.4
1	F	291	VAL	4.3
1	I	152	ILE	4.3
1	D	180	SER	4.3
1	H	292	GLU	4.2
1	I	181	VAL	4.1
1	A	54	LYS	4.1
1	B	289	ASN	4.1
1	C	151	ASN	4.0
1	I	151	ASN	4.0
1	I	315	LEU	4.0
1	J	306	LEU	3.9
1	D	290	GLY	3.9
1	D	179	SER	3.9
1	H	181	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLY	3.8
1	C	317	ILE	3.7
1	C	288	ALA	3.6
1	C	316	VAL	3.6
1	G	317	ILE	3.6
1	H	182	GLN	3.5
1	A	186	ASN	3.4
1	B	313	CYS	3.4
1	C	172	ASP	3.4
1	B	153	ASP	3.4
1	E	287	GLN	3.3
1	F	316	VAL	3.3
1	A	317	ILE	3.3
1	C	291	VAL	3.3
1	D	183	PRO	3.2
1	I	148	TYR	3.2
1	A	153	ASP	3.2
1	J	317	ILE	3.1
1	I	185	GLN	3.1
1	E	288	ALA	3.1
1	F	178	LEU	3.1
1	A	49	LYS	3.0
1	E	180	SER	3.0
1	D	291	VAL	3.0
1	C	152	ILE	3.0
1	H	315	LEU	3.0
1	G	313	CYS	3.0
1	C	289	ASN	3.0
1	J	157	ILE	3.0
1	D	152	ILE	2.9
1	A	178	LEU	2.9
1	J	156	GLU	2.9
1	H	179	SER	2.9
1	A	291	VAL	2.9
1	E	179	SER	2.8
1	A	175	TYR	2.8
1	F	290	GLY	2.8
1	H	148	TYR	2.7
1	A	53	ASP	2.7
1	C	315	LEU	2.7
1	D	182	GLN	2.7
1	I	182	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	289	ASN	2.7
1	I	154	ASN	2.7
1	F	287	GLN	2.6
1	F	174	ARG	2.5
1	F	288	ALA	2.5
1	E	286	ARG	2.5
1	B	288	ALA	2.5
1	A	52	GLY	2.5
1	J	52	GLY	2.5
1	G	296	LEU	2.5
1	B	312	GLY	2.5
1	H	153	ASP	2.5
1	I	317	ILE	2.4
1	D	185	GLN	2.4
1	A	177	HIS	2.4
1	H	174	ARG	2.4
1	G	291	VAL	2.3
1	B	316	VAL	2.3
1	C	313	CYS	2.3
1	J	154	ASN	2.3
1	A	176	ASP	2.3
1	H	293	ASP	2.3
1	E	289	ASN	2.3
1	E	157	ILE	2.3
1	B	292	GLU	2.3
1	I	289	ASN	2.2
1	D	289	ASN	2.2
1	B	293	ASP	2.2
1	A	156	GLU	2.2
1	B	179	SER	2.2
1	A	117	ARG	2.1
1	I	316	VAL	2.1
1	G	255	ARG	2.1
1	E	152	ILE	2.1
1	C	187	GLU	2.1
1	B	297	ILE	2.1
1	E	315	LEU	2.1
1	G	289	ASN	2.1
1	J	282	PHE	2.0
1	D	157	ILE	2.0
1	I	286	ARG	2.0
1	I	314	VAL	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 ⓘ

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	I	325	6/6	0.65	0.40	83,106,125,132	0
3	GOL	B	326	6/6	0.80	0.36	85,106,135,150	0
2	MES	A	323	12/12	0.81	0.15	110,139,173,180	0
2	MES	C	323	12/12	0.81	0.15	107,156,192,200	0
3	GOL	I	324	6/6	0.84	0.13	82,97,100,127	0
3	GOL	J	324	6/6	0.85	0.26	103,116,132,140	0
2	MES	G	324	12/12	0.85	0.13	110,141,172,181	0
3	GOL	B	324	6/6	0.87	0.43	82,87,123,125	0
3	GOL	B	325	6/6	0.87	0.29	84,105,116,130	0
2	MES	D	323	12/12	0.88	0.12	112,149,168,177	0
3	GOL	J	323	6/6	0.88	0.14	118,131,137,145	0
3	GOL	J	325	6/6	0.90	0.12	67,76,88,104	0
3	GOL	A	324	6/6	0.90	0.17	97,106,124,125	0
3	GOL	D	324	6/6	0.90	0.28	88,89,113,120	0
3	GOL	B	327	6/6	0.91	0.21	87,105,117,126	0
2	MES	I	323	12/12	0.91	0.13	118,142,164,175	0
2	MES	G	323	12/12	0.91	0.12	113,142,161,180	0
3	GOL	E	323	6/6	0.91	0.12	98,115,130,131	0
3	GOL	C	324	6/6	0.91	0.12	75,87,118,122	0
3	GOL	D	325	5/6	0.91	0.67	81,92,115,128	0
3	GOL	E	324	6/6	0.91	0.14	73,82,112,133	0
3	GOL	B	328	6/6	0.92	0.10	63,80,104,110	0
2	MES	B	323	12/12	0.93	0.10	118,141,154,175	0
3	GOL	G	325	6/6	0.93	0.13	70,89,109,128	0
3	GOL	D	326	6/6	0.94	0.14	46,75,116,116	0
3	GOL	H	323	6/6	0.95	0.13	53,91,104,104	0
3	GOL	I	326	6/6	0.95	0.10	52,88,106,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	F	323	6/6	0.96	0.10	68,92,107,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.