



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:44 PM GMT

PDB ID : 3RQW  
Title : Crystal structure of acetylcholine bound to 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 : 2.91 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

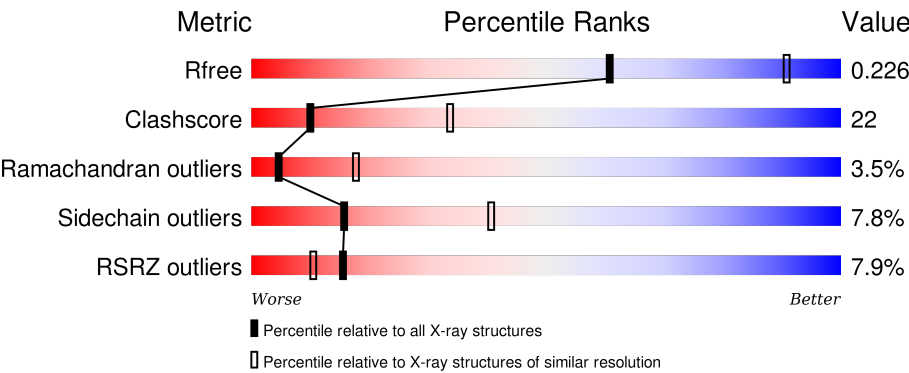
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	322	<div><div>9%</div><div><div></div><div>62%</div><div>27%</div><div>6%</div><div>5%</div></div></div>
1	B	322	<div><div>7%</div><div><div></div><div>62%</div><div>28%</div><div>5%</div><div>• 5%</div></div></div>
1	C	322	<div><div>5%</div><div><div></div><div>62%</div><div>28%</div><div>5%</div><div>• 5%</div></div></div>
1	D	322	<div><div>7%</div><div><div></div><div>62%</div><div>26%</div><div>6%</div><div>5%</div></div></div>
1	E	322	<div><div>6%</div><div><div></div><div>64%</div><div>26%</div><div>5%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	322	
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
4	GOL	A	326	-	-	X	-
4	GOL	B	325	-	-	-	X
4	GOL	B	326	-	-	X	-
4	GOL	B	327	-	-	X	-
4	GOL	C	324	-	-	-	X
4	GOL	C	325	-	-	X	-
4	GOL	F	325	-	-	-	X
4	GOL	F	326	-	-	-	X
4	GOL	F	327	-	-	-	X
4	GOL	F	328	-	-	X	-
4	GOL	G	325	-	-	-	X
4	GOL	G	326	-	-	-	X
4	GOL	G	327	-	-	-	X
4	GOL	G	328	-	-	X	-
4	GOL	H	325	-	-	X	X
4	GOL	I	327	-	-	X	X
4	GOL	I	328	-	-	-	X
4	GOL	I	329	-	-	X	-
4	GOL	J	325	-	-	X	-

## 2 Entry composition

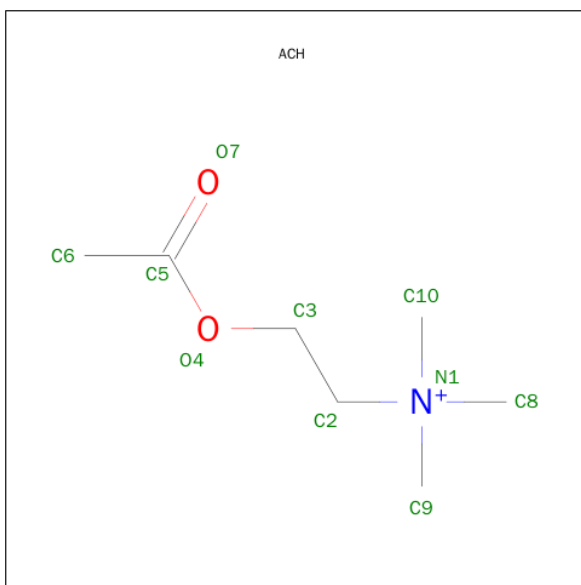
There are 5 unique types of molecules in this entry. The entry contains 25508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINE (three-letter code: ACH) (formula:  $C_7H_{16}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		
2	C	1	Total	C	N	O	0	0
			10	7	1	2		
2	D	1	Total	C	N	O	0	0
			10	7	1	2		
2	E	1	Total	C	N	O	0	0
			10	7	1	2		
2	F	1	Total	C	N	O	0	0
			10	7	1	2		
2	G	1	Total	C	N	O	0	0
			10	7	1	2		
2	H	1	Total	C	N	O	0	0
			10	7	1	2		
2	I	1	Total	C	N	O	0	0
			10	7	1	2		
2	J	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 3 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
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	8	Total O 8 8	0	0
5	C	10	Total O 10 10	0	0
5	D	15	Total O 15 15	0	0
5	E	11	Total O 11 11	0	0
5	F	4	Total O 4 4	0	0

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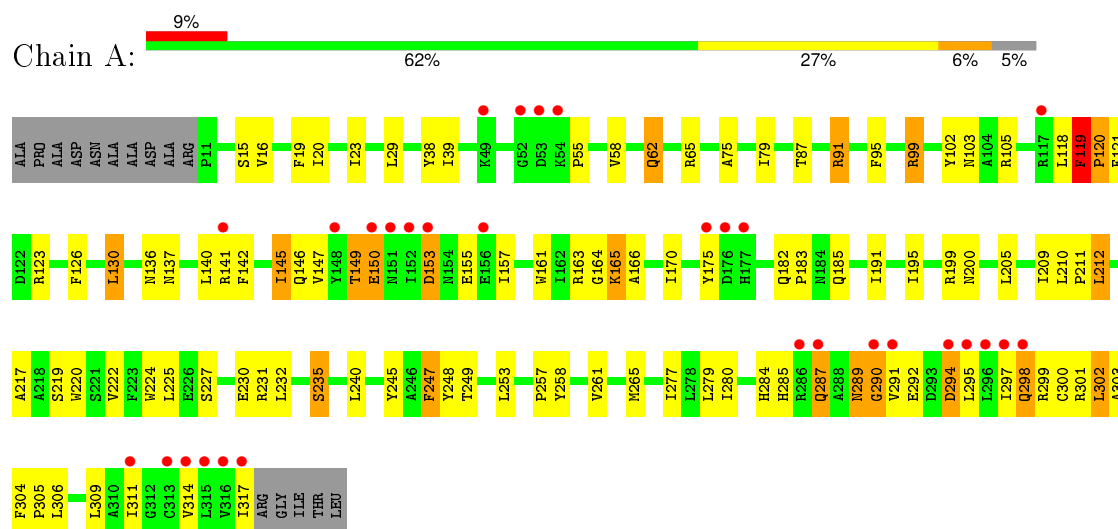
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	12	Total 12	O 12	0	0
5	H	7	Total 7	O 7	0	0
5	I	6	Total 6	O 6	0	0
5	J	7	Total 7	O 7	0	0

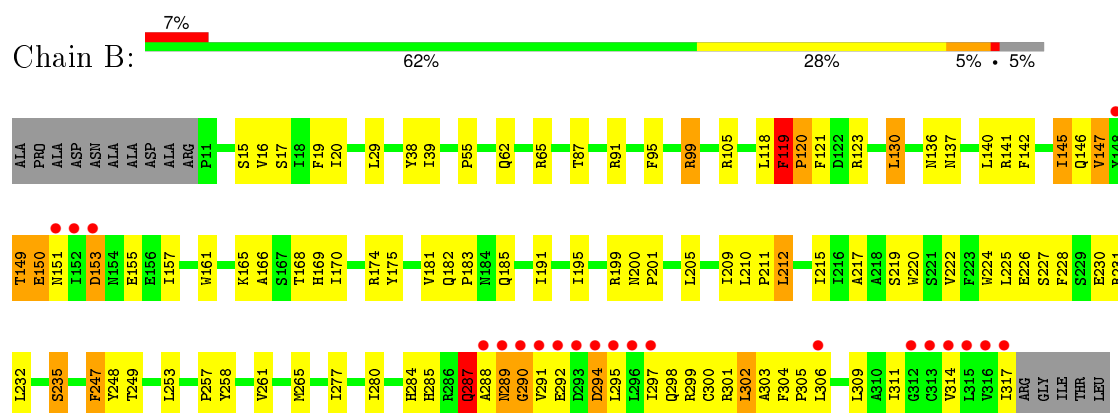
### 3 Residue-property plots [i](#)

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

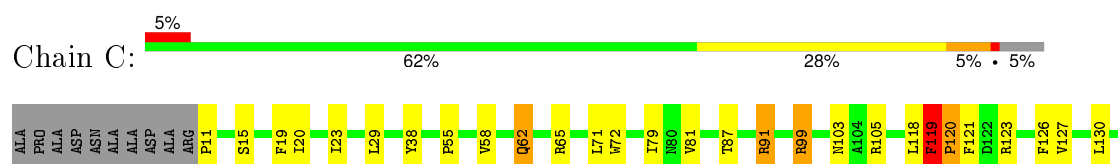
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

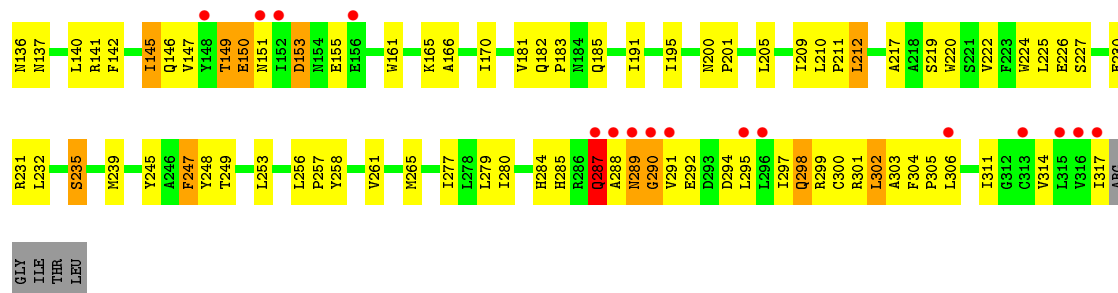


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

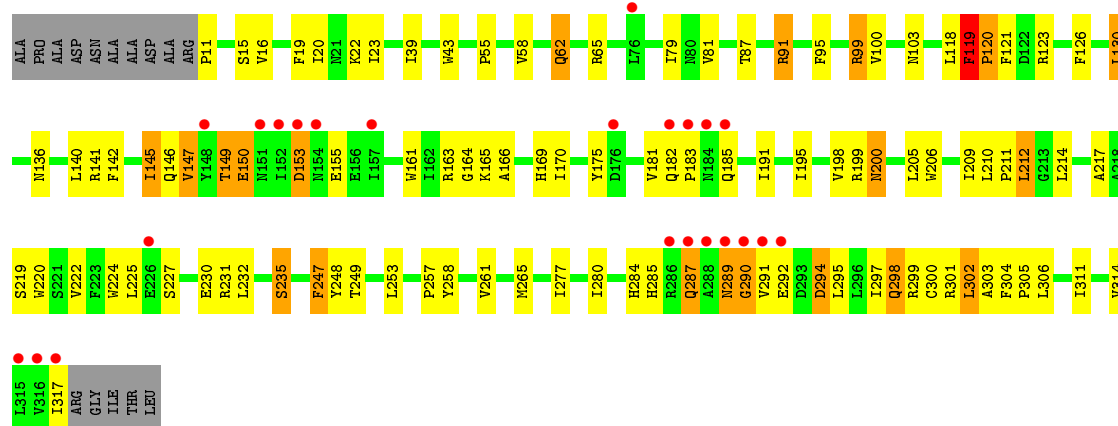


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

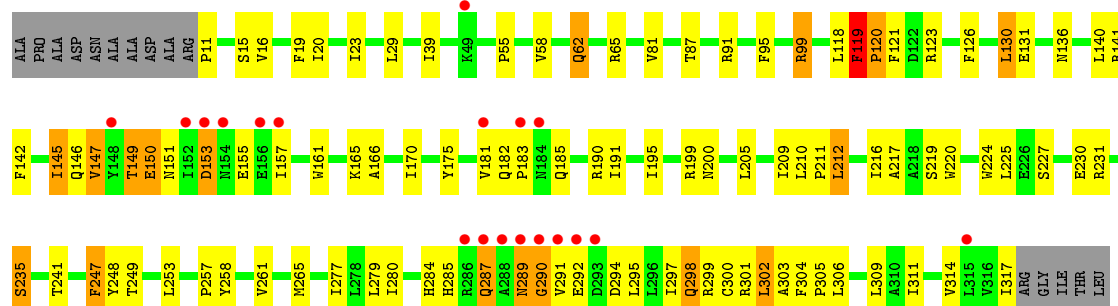




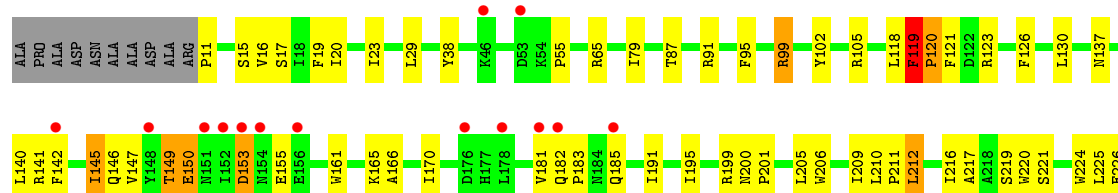
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

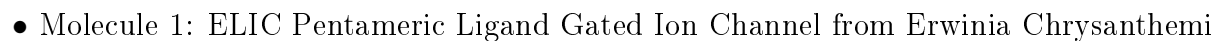


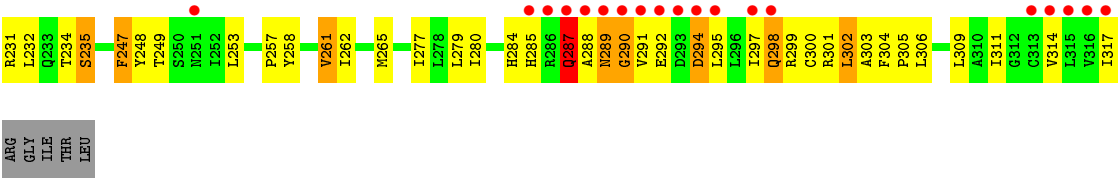
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



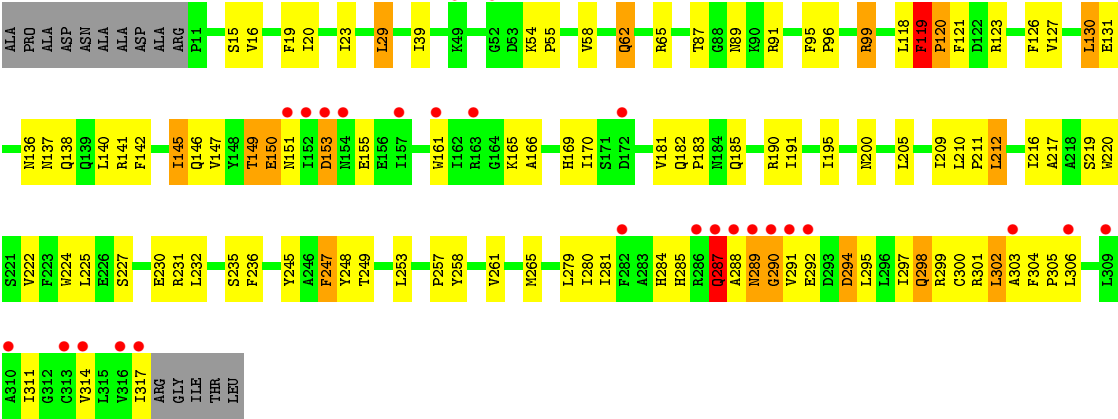
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*







● 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, $\alpha$ , $\beta$ , $\gamma$	105.76Å 266.07Å 111.16Å 90.00° 107.82° 90.00°	Depositor
Resolution (Å)	24.98 – 2.91 29.80 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.98-2.91) 98.0 (29.80-2.91)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.206 , 0.231 0.205 , 0.226	Depositor DCC
$R_{free}$ test set	6260 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.5	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 124569 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: GOL, ACH, 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	0.38	0/2573	0.54	1/3507 (0.0%)
1	B	0.44	0/2573	0.57	1/3507 (0.0%)
1	C	0.43	0/2573	0.57	1/3507 (0.0%)
1	D	0.46	0/2573	0.58	1/3507 (0.0%)
1	E	0.42	0/2573	0.56	1/3507 (0.0%)
1	F	0.41	0/2573	0.55	1/3507 (0.0%)
1	G	0.43	0/2573	0.60	2/3507 (0.1%)
1	H	0.42	0/2573	0.57	1/3507 (0.0%)
1	I	0.43	0/2573	0.58	1/3507 (0.0%)
1	J	0.41	0/2573	0.56	1/3507 (0.0%)
All	All	0.42	0/25730	0.57	11/35070 (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	2
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	2
1	I	0	1
1	J	0	1
All	All	0	12

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	119	PHE	C-N-CD	-7.40	104.31	120.60
1	J	119	PHE	C-N-CD	-7.25	104.66	120.60
1	G	302	LEU	CA-CB-CG	7.10	131.62	115.30
1	E	119	PHE	C-N-CD	-7.04	105.12	120.60
1	G	119	PHE	C-N-CD	-7.01	105.17	120.60
1	B	119	PHE	C-N-CD	-6.93	105.34	120.60
1	A	119	PHE	C-N-CD	-6.67	105.92	120.60
1	D	119	PHE	C-N-CD	-6.39	106.55	120.60
1	H	119	PHE	C-N-CD	-6.33	106.68	120.60
1	F	119	PHE	C-N-CD	-6.07	107.25	120.60
1	C	119	PHE	C-N-CD	-6.04	107.31	120.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PHE	Peptide
1	A	164	GLY	Peptide
1	B	119	PHE	Peptide
1	C	119	PHE	Peptide
1	D	119	PHE	Peptide
1	E	119	PHE	Peptide
1	F	119	PHE	Peptide
1	G	119	PHE	Peptide
1	H	119	PHE	Peptide
1	H	164	GLY	Peptide
1	I	119	PHE	Peptide
1	J	119	PHE	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2478	118	0
1	B	2505	0	2478	121	0
1	C	2505	0	2478	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2505	0	2478	111	0
1	E	2505	0	2478	105	0
1	F	2505	0	2478	115	0
1	G	2505	0	2478	130	0
1	H	2505	0	2478	117	0
1	I	2505	0	2478	121	0
1	J	2505	0	2478	119	0
2	A	10	0	16	2	0
2	B	10	0	16	2	0
2	C	10	0	16	3	0
2	D	10	0	16	2	0
2	E	10	0	16	4	0
2	F	10	0	16	2	0
2	G	10	0	16	1	0
2	H	10	0	16	1	0
2	I	10	0	16	3	0
2	J	10	0	16	3	0
3	A	12	0	12	1	0
3	B	12	0	12	0	0
3	D	24	0	24	1	0
3	E	12	0	12	0	0
3	F	12	0	12	2	0
3	G	12	0	12	0	0
3	I	12	0	12	0	0
3	J	12	0	12	0	0
4	A	12	0	16	6	0
4	B	18	0	24	12	0
4	C	12	0	16	4	0
4	D	12	0	16	1	0
4	E	12	0	16	2	0
4	F	24	0	32	5	0
4	G	22	0	28	9	0
4	H	12	0	16	9	0
4	I	30	0	40	10	0
4	J	6	0	8	7	0
5	A	10	0	0	2	0
5	B	8	0	0	2	0
5	C	10	0	0	4	0
5	D	15	0	0	9	0
5	E	11	0	0	5	0
5	F	4	0	0	5	0
5	G	12	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	7	0	0	5	0
5	I	6	0	0	4	0
5	J	7	0	0	6	0
All	All	25508	0	25260	1114	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 22.

All (1114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASN:O	4:C:325:GOL:H2	1.36	1.20
1:I:140:LEU:HD21	5:I:334:HOH:O	1.48	1.11
1:B:140:LEU:HD11	5:B:332:HOH:O	1.51	1.11
1:D:140:LEU:HD11	5:D:341:HOH:O	1.52	1.09
1:H:140:LEU:HD11	5:H:331:HOH:O	1.52	1.07
1:B:175:TYR:HA	4:B:326:GOL:H12	1.37	1.04
1:G:140:LEU:HD11	5:G:338:HOH:O	1.58	1.02
1:E:140:LEU:HD11	5:E:336:HOH:O	1.61	1.00
1:G:140:LEU:HD21	5:G:338:HOH:O	1.61	0.99
1:D:140:LEU:HD21	5:D:341:HOH:O	1.61	0.98
1:F:140:LEU:HD11	5:F:331:HOH:O	1.62	0.98
1:C:140:LEU:HD21	5:C:333:HOH:O	1.63	0.98
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.46	0.98
1:G:99:ARG:HH11	1:G:99:ARG:HG3	1.28	0.95
1:J:136:ASN:O	4:J:325:GOL:H2	1.65	0.95
1:J:99:ARG:HG3	1:J:99:ARG:HH11	1.29	0.95
1:A:99:ARG:HG3	1:A:99:ARG:HH11	1.32	0.95
1:G:136:ASN:O	4:G:328:GOL:H2	1.66	0.94
1:E:99:ARG:HH11	1:E:99:ARG:HG3	1.31	0.94
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.50	0.94
1:I:99:ARG:HH11	1:I:99:ARG:HG3	1.33	0.93
1:D:99:ARG:HH11	1:D:99:ARG:HG3	1.33	0.93
1:F:99:ARG:HH11	1:F:99:ARG:HG3	1.30	0.93
1:I:136:ASN:O	4:I:329:GOL:H31	1.69	0.93
1:A:140:LEU:HD11	5:A:335:HOH:O	1.69	0.93
1:C:99:ARG:HH11	1:C:99:ARG:HG3	1.33	0.91
1:C:140:LEU:HD11	5:C:333:HOH:O	1.68	0.91
1:F:140:LEU:HD21	5:F:331:HOH:O	1.68	0.90
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.35	0.88
1:H:140:LEU:HD21	5:H:331:HOH:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.57	0.87
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.57	0.86
1:H:99:ARG:HG3	1:H:99:ARG:HH11	1.39	0.85
1:E:295:LEU:HA	1:E:298:GLN:HE21	1.42	0.85
1:G:137:ASN:HA	4:G:328:GOL:O3	1.75	0.85
1:I:295:LEU:HA	1:I:298:GLN:HE21	1.42	0.85
1:I:137:ASN:HA	4:I:329:GOL:C1	2.07	0.84
1:G:295:LEU:HA	1:G:298:GLN:HE21	1.42	0.83
1:B:136:ASN:O	4:B:327:GOL:H32	1.78	0.83
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.60	0.83
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.59	0.83
1:F:11:PRO:HB3	4:F:328:GOL:H12	1.59	0.83
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.58	0.83
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.59	0.82
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.62	0.82
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.60	0.82
1:I:137:ASN:HA	4:I:329:GOL:H12	1.62	0.82
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.61	0.82
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.62	0.82
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.62	0.82
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.60	0.81
1:B:137:ASN:HA	4:B:327:GOL:C1	2.10	0.81
1:C:295:LEU:HA	1:C:298:GLN:HE21	1.46	0.81
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.61	0.81
1:I:145:ILE:CD1	1:I:166:ALA:HB3	2.11	0.81
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.62	0.80
1:A:140:LEU:HD21	5:A:335:HOH:O	1.80	0.80
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.63	0.80
1:I:140:LEU:HD11	5:I:334:HOH:O	1.82	0.80
1:J:140:LEU:HD21	5:J:330:HOH:O	1.80	0.80
1:A:295:LEU:HA	1:A:298:GLN:HE21	1.44	0.80
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.63	0.80
1:D:295:LEU:HA	1:D:298:GLN:HE21	1.45	0.80
1:F:295:LEU:HA	1:F:298:GLN:HE21	1.44	0.80
1:H:300:CYS:HB2	1:H:303:ALA:HB3	1.62	0.80
1:B:145:ILE:CD1	1:B:166:ALA:HB3	2.12	0.79
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.63	0.79
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.63	0.79
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.62	0.79
1:C:147:VAL:HG13	1:C:165:LYS:HE2	1.65	0.79
1:D:145:ILE:CD1	1:D:166:ALA:HB3	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.65	0.78
1:E:147:VAL:HG13	1:E:165:LYS:HE2	1.66	0.78
1:E:140:LEU:HD21	5:E:336:HOH:O	1.84	0.78
1:J:295:LEU:HA	1:J:298:GLN:HE21	1.46	0.77
1:H:295:LEU:HA	1:H:298:GLN:HE21	1.50	0.77
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.66	0.77
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.65	0.77
1:F:294:ASP:HB3	1:F:297:ILE:HG22	1.67	0.76
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.64	0.76
1:C:119:PHE:CD2	1:C:120:PRO:HD3	2.20	0.76
1:H:147:VAL:HG13	1:H:165:LYS:HE2	1.67	0.76
1:G:119:PHE:CD2	1:G:120:PRO:HD3	2.21	0.76
1:B:145:ILE:O	1:B:145:ILE:HD13	1.85	0.76
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.67	0.75
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.69	0.75
1:F:147:VAL:HG13	1:F:165:LYS:HE2	1.68	0.75
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.69	0.75
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.68	0.74
1:F:119:PHE:CD2	1:F:120:PRO:HD3	2.22	0.74
1:B:295:LEU:HA	1:B:298:GLN:HE21	1.52	0.74
1:D:119:PHE:CD2	1:D:120:PRO:HD3	2.22	0.74
1:A:145:ILE:CD1	1:A:166:ALA:HB3	2.17	0.74
1:J:137:ASN:O	5:J:326:HOH:O	2.05	0.74
1:J:119:PHE:CD2	1:J:120:PRO:HD3	2.23	0.74
1:J:140:LEU:HD11	5:J:330:HOH:O	1.87	0.73
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.70	0.73
1:A:119:PHE:CD2	1:A:120:PRO:HD3	2.22	0.73
1:A:147:VAL:HG13	1:A:165:LYS:HE2	1.70	0.73
1:F:145:ILE:CD1	1:F:166:ALA:HB3	2.18	0.73
1:H:137:ASN:HA	4:H:324:GOL:O1	1.89	0.73
1:G:145:ILE:CD1	1:G:166:ALA:HB3	2.19	0.73
1:J:137:ASN:HA	4:J:325:GOL:O1	1.89	0.73
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.69	0.73
1:D:294:ASP:HB3	1:D:297:ILE:HG22	1.71	0.72
1:A:137:ASN:HA	4:A:326:GOL:O1	1.89	0.72
1:I:137:ASN:HA	4:I:329:GOL:O1	1.90	0.72
1:G:105:ARG:HG2	4:H:325:GOL:H11	1.72	0.72
1:B:137:ASN:HA	4:B:327:GOL:O1	1.89	0.72
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.71	0.72
1:D:147:VAL:HG13	1:D:165:LYS:HE2	1.70	0.72
1:G:137:ASN:HA	4:G:328:GOL:C3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASP:HB3	1:C:297:ILE:HG22	1.72	0.71
1:A:294:ASP:HB3	1:A:297:ILE:HG22	1.72	0.71
1:G:105:ARG:HG3	4:H:325:GOL:H31	1.72	0.71
1:C:145:ILE:CD1	1:C:166:ALA:HB3	2.19	0.71
1:J:145:ILE:CD1	1:J:166:ALA:HB3	2.19	0.71
1:G:88:GLY:HA3	4:H:325:GOL:H12	1.72	0.71
1:I:119:PHE:CD2	1:I:120:PRO:HD3	2.25	0.71
1:E:119:PHE:CD2	1:E:120:PRO:HD3	2.26	0.70
1:G:99:ARG:HG3	1:G:99:ARG:NH1	2.05	0.70
1:F:137:ASN:HA	4:F:328:GOL:O1	1.91	0.70
1:G:294:ASP:HB3	1:G:297:ILE:HG22	1.73	0.70
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.72	0.70
1:I:147:VAL:HG13	1:I:165:LYS:HE2	1.72	0.70
1:D:119:PHE:C	1:D:121:PHE:H	1.94	0.69
1:H:119:PHE:CD2	1:H:120:PRO:HD3	2.27	0.69
1:G:145:ILE:O	1:G:145:ILE:HD13	1.93	0.69
1:H:145:ILE:CD1	1:H:166:ALA:HB3	2.22	0.69
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.73	0.69
1:I:294:ASP:HB3	1:I:297:ILE:HG22	1.74	0.69
1:F:145:ILE:HD13	1:F:145:ILE:O	1.92	0.69
1:I:102:TYR:CE2	4:I:327:GOL:H2	2.28	0.69
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.75	0.69
1:E:145:ILE:CD1	1:E:166:ALA:HB3	2.22	0.69
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.08	0.69
1:H:294:ASP:HB3	1:H:297:ILE:HG22	1.73	0.69
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.74	0.69
1:J:145:ILE:HD13	1:J:145:ILE:O	1.94	0.68
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.75	0.68
1:B:294:ASP:HB3	1:B:297:ILE:HG22	1.75	0.68
1:E:166:ALA:HB2	1:E:195:ILE:HG12	1.75	0.68
1:J:147:VAL:HG13	1:J:165:LYS:HE2	1.73	0.68
1:H:257:PRO:HG2	1:H:258:TYR:CD2	2.28	0.68
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.76	0.68
1:H:166:ALA:HB2	1:H:195:ILE:HG12	1.74	0.68
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.75	0.68
1:H:119:PHE:C	1:H:121:PHE:H	1.98	0.68
1:B:141:ARG:HG3	1:B:142:PHE:CD2	2.29	0.68
1:F:99:ARG:HG3	1:F:99:ARG:NH1	2.06	0.67
1:J:138:GLN:HB2	5:J:326:HOH:O	1.94	0.67
1:B:119:PHE:CD2	1:B:120:PRO:HD3	2.29	0.67
1:H:55:PRO:HG2	1:I:181:VAL:HG13	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.29	0.67
1:D:147:VAL:CG1	1:D:165:LYS:HE2	2.24	0.67
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.76	0.67
1:E:257:PRO:HG2	1:E:258:TYR:CD2	2.30	0.67
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.30	0.67
1:J:99:ARG:HG3	1:J:99:ARG:NH1	2.07	0.67
1:I:145:ILE:HD13	1:I:145:ILE:O	1.95	0.67
1:I:182:GLN:HB3	1:I:183:PRO:HD2	1.76	0.67
1:G:141:ARG:NH1	5:G:329:HOH:O	2.28	0.67
1:D:145:ILE:O	1:D:145:ILE:HD13	1.95	0.66
1:D:119:PHE:O	1:D:121:PHE:N	2.24	0.66
1:G:147:VAL:HG13	1:G:165:LYS:HE2	1.76	0.66
1:H:182:GLN:HB3	1:H:183:PRO:HD2	1.76	0.66
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.10	0.66
1:D:182:GLN:HB3	1:D:183:PRO:HD2	1.77	0.66
1:E:147:VAL:CG1	1:E:165:LYS:HE2	2.25	0.66
1:C:119:PHE:C	1:C:121:PHE:H	1.98	0.66
1:I:257:PRO:HG2	1:I:258:TYR:CD2	2.31	0.66
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.10	0.66
1:C:147:VAL:CG1	1:C:165:LYS:HE2	2.26	0.66
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.31	0.66
1:A:289:ASN:CG	1:A:290:GLY:H	1.99	0.66
1:A:145:ILE:HD13	1:A:145:ILE:O	1.95	0.66
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.77	0.66
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.11	0.66
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.78	0.66
1:F:147:VAL:CG1	1:F:165:LYS:HE2	2.25	0.65
1:E:119:PHE:C	1:E:121:PHE:H	1.99	0.65
1:I:289:ASN:CG	1:I:290:GLY:H	2.00	0.65
1:G:289:ASN:CG	1:G:290:GLY:H	2.00	0.65
1:C:289:ASN:CG	1:C:290:GLY:H	2.00	0.65
1:E:141:ARG:HG3	1:E:142:PHE:CD2	2.32	0.65
1:A:147:VAL:CG1	1:A:165:LYS:HE2	2.26	0.65
1:H:137:ASN:HA	4:H:324:GOL:C1	2.27	0.65
1:B:119:PHE:C	1:B:121:PHE:H	2.00	0.65
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.30	0.65
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.30	0.65
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.11	0.65
1:J:119:PHE:C	1:J:121:PHE:H	1.99	0.65
1:G:147:VAL:CG1	1:G:165:LYS:HE2	2.27	0.65
1:E:289:ASN:CG	1:E:290:GLY:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:ASN:CG	1:F:290:GLY:H	1.99	0.65
1:B:182:GLN:HB3	1:B:183:PRO:HD2	1.77	0.64
1:F:206:TRP:CD1	3:F:324:MES:H71	2.33	0.64
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.13	0.64
1:B:289:ASN:CG	1:B:290:GLY:H	2.01	0.64
1:J:182:GLN:HB3	1:J:183:PRO:HD2	1.79	0.64
1:A:166:ALA:HB2	1:A:195:ILE:HG12	1.80	0.64
1:D:289:ASN:CG	1:D:290:GLY:H	2.00	0.64
1:F:166:ALA:HB2	1:F:195:ILE:HG12	1.79	0.64
1:C:145:ILE:O	1:C:145:ILE:HD13	1.98	0.64
1:F:119:PHE:C	1:F:121:PHE:H	2.00	0.64
1:J:166:ALA:HB2	1:J:195:ILE:HG12	1.78	0.64
1:B:136:ASN:O	4:B:327:GOL:C3	2.45	0.64
1:H:289:ASN:CG	1:H:290:GLY:H	2.01	0.64
1:E:145:ILE:HD13	1:E:145:ILE:O	1.97	0.64
1:A:182:GLN:HB3	1:A:183:PRO:HD2	1.79	0.64
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.12	0.64
1:J:289:ASN:CG	1:J:290:GLY:H	2.00	0.64
1:A:119:PHE:C	1:A:121:PHE:H	2.00	0.63
1:I:147:VAL:CG1	1:I:165:LYS:HE2	2.27	0.63
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.12	0.63
1:F:11:PRO:HB3	4:F:328:GOL:C1	2.26	0.63
1:I:119:PHE:C	1:I:121:PHE:H	2.01	0.63
1:F:257:PRO:HG2	1:F:258:TYR:CD2	2.33	0.63
1:B:137:ASN:HA	4:B:327:GOL:H12	1.80	0.63
1:J:137:ASN:HA	4:J:325:GOL:C1	2.29	0.63
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.80	0.63
1:E:182:GLN:HB3	1:E:183:PRO:HD2	1.80	0.63
1:C:182:GLN:HB3	1:C:183:PRO:HD2	1.80	0.62
1:C:118:LEU:O	1:C:119:PHE:O	2.18	0.62
1:I:225:LEU:CD2	1:J:232:LEU:HD23	2.29	0.62
1:B:99:ARG:HG3	1:B:99:ARG:NH1	2.11	0.62
1:H:145:ILE:HD13	1:H:145:ILE:O	1.98	0.62
1:J:147:VAL:CG1	1:J:165:LYS:HE2	2.29	0.62
1:B:175:TYR:HA	4:B:326:GOL:C1	2.22	0.62
1:G:119:PHE:C	1:G:121:PHE:H	2.01	0.62
1:A:141:ARG:HG3	1:A:142:PHE:CD2	2.35	0.62
1:C:119:PHE:O	1:C:121:PHE:N	2.27	0.62
1:F:182:GLN:HB3	1:F:183:PRO:HD2	1.81	0.62
1:I:76:LEU:H	4:I:327:GOL:H12	1.64	0.62
1:J:141:ARG:HG3	1:J:142:PHE:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:ARG:HG3	1:G:142:PHE:CD2	2.34	0.61
1:H:302:LEU:O	1:H:306:LEU:HG	2.00	0.61
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.15	0.61
1:F:141:ARG:HG3	1:F:142:PHE:CD2	2.35	0.61
1:I:99:ARG:HG3	1:I:99:ARG:NH1	2.09	0.61
1:C:99:ARG:HG3	1:C:99:ARG:NH1	2.11	0.61
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.16	0.61
1:H:147:VAL:CG1	1:H:165:LYS:HE2	2.31	0.61
1:F:206:TRP:NE1	3:F:324:MES:H71	2.16	0.61
1:J:89:ASN:ND2	5:J:331:HOH:O	2.33	0.61
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.35	0.61
1:I:166:ALA:HB2	1:I:195:ILE:HG12	1.82	0.60
1:G:248:TYR:CD1	1:H:247:PHE:HA	2.36	0.60
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.16	0.60
1:G:168:THR:C	1:G:169:HIS:ND1	2.54	0.60
1:E:15:SER:HB3	1:E:141:ARG:HD3	1.82	0.60
1:J:257:PRO:HG2	1:J:258:TYR:CD2	2.35	0.60
1:G:224:TRP:HE1	1:G:301:ARG:HB3	1.66	0.60
1:G:182:GLN:HB3	1:G:183:PRO:HD2	1.81	0.60
1:C:141:ARG:HG3	1:C:142:PHE:CD2	2.35	0.60
1:G:166:ALA:HB2	1:G:195:ILE:HG12	1.83	0.60
1:J:137:ASN:HA	4:J:325:GOL:H2	1.84	0.60
1:H:99:ARG:NH1	1:H:99:ARG:HG3	2.13	0.60
1:B:147:VAL:HG13	1:B:165:LYS:HE2	1.83	0.60
1:D:141:ARG:HG3	1:D:142:PHE:CD2	2.37	0.60
1:E:99:ARG:NH1	1:E:99:ARG:HG3	2.08	0.60
1:I:136:ASN:O	4:I:329:GOL:C3	2.48	0.60
1:E:140:LEU:HD13	1:E:191:ILE:CG1	2.29	0.59
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.67	0.59
1:I:15:SER:HB3	1:I:141:ARG:HD3	1.83	0.59
1:C:55:PRO:HG2	1:D:181:VAL:HG13	1.83	0.59
1:D:99:ARG:NH1	1:D:99:ARG:HG3	2.08	0.59
1:E:210:LEU:HB3	1:E:211:PRO:CD	2.33	0.59
1:I:15:SER:HB3	1:I:141:ARG:CG	2.33	0.59
1:B:302:LEU:O	1:B:306:LEU:HG	2.03	0.59
1:F:20:ILE:HD12	1:F:195:ILE:HD11	1.84	0.59
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.32	0.58
1:E:136:ASN:O	4:E:326:GOL:H32	2.03	0.58
1:D:118:LEU:O	1:D:119:PHE:O	2.21	0.58
1:J:302:LEU:O	1:J:306:LEU:HG	2.03	0.58
1:H:165:LYS:H	1:H:165:LYS:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:VAL:HG22	1:I:147:VAL:O	2.03	0.58
1:G:136:ASN:O	4:G:328:GOL:C2	2.47	0.58
1:F:294:ASP:HB3	1:F:297:ILE:CG2	2.31	0.58
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.86	0.58
1:B:147:VAL:CG1	1:B:165:LYS:HE2	2.34	0.58
1:C:302:LEU:O	1:C:306:LEU:HG	2.04	0.58
1:F:247:PHE:HA	1:J:248:TYR:CD1	2.39	0.58
1:D:294:ASP:HB3	1:D:297:ILE:CG2	2.34	0.57
1:F:224:TRP:HE1	1:F:301:ARG:HB3	1.68	0.57
1:F:15:SER:HB3	1:F:141:ARG:HD3	1.87	0.57
1:G:302:LEU:O	1:G:306:LEU:HG	2.04	0.57
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.34	0.57
1:F:225:LEU:CD2	1:G:232:LEU:HD23	2.34	0.57
1:H:294:ASP:HB3	1:H:297:ILE:CG2	2.35	0.57
1:B:140:LEU:HD21	5:B:332:HOH:O	2.04	0.57
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.69	0.57
1:H:147:VAL:O	1:H:147:VAL:HG22	2.04	0.57
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.87	0.57
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.68	0.57
1:F:19:PHE:CD1	2:F:323:ACH:H61	2.40	0.57
1:B:175:TYR:HD1	4:B:326:GOL:H11	1.69	0.56
1:G:294:ASP:HB3	1:G:297:ILE:CG2	2.35	0.56
1:I:145:ILE:HD11	1:I:166:ALA:HB3	1.86	0.56
1:F:182:GLN:HB2	1:F:185:GLN:HG2	1.87	0.56
1:J:15:SER:HB3	1:J:141:ARG:CG	2.35	0.56
1:B:212:LEU:HB3	1:B:265:MET:HE1	1.87	0.56
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.40	0.56
1:F:118:LEU:O	1:F:119:PHE:O	2.23	0.56
1:J:182:GLN:HB2	1:J:185:GLN:HG2	1.86	0.56
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.87	0.56
1:A:247:PHE:HA	1:E:248:TYR:CD1	2.41	0.56
1:B:257:PRO:HG2	1:B:258:TYR:HD2	1.71	0.56
1:A:302:LEU:O	1:A:306:LEU:HG	2.05	0.56
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.36	0.56
1:E:302:LEU:O	1:E:306:LEU:HG	2.05	0.56
1:G:119:PHE:CG	1:G:120:PRO:N	2.73	0.56
1:G:163:ARG:O	1:G:164:GLY:O	2.24	0.56
1:A:20:ILE:HD12	1:A:195:ILE:HD11	1.88	0.56
1:B:248:TYR:HA	1:C:247:PHE:CE1	2.41	0.56
1:H:141:ARG:HG3	1:H:142:PHE:CD2	2.41	0.56
1:A:55:PRO:HG2	1:B:181:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HD11	1:B:166:ALA:HB3	1.87	0.56
1:C:119:PHE:CD2	1:C:120:PRO:CD	2.89	0.56
1:A:294:ASP:HB3	1:A:297:ILE:CG2	2.35	0.55
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.35	0.55
1:A:119:PHE:CG	1:A:120:PRO:N	2.75	0.55
1:A:118:LEU:O	1:A:119:PHE:O	2.24	0.55
1:C:182:GLN:HB2	1:C:185:GLN:HG2	1.88	0.55
1:A:15:SER:HB3	1:A:141:ARG:HD3	1.88	0.55
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.36	0.55
1:G:248:TYR:HA	1:H:247:PHE:CE1	2.42	0.55
1:I:210:LEU:HB3	1:I:211:PRO:CD	2.34	0.55
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.89	0.55
1:H:119:PHE:CG	1:H:120:PRO:N	2.75	0.55
1:I:15:SER:HB3	1:I:141:ARG:CD	2.36	0.55
1:B:119:PHE:CG	1:B:120:PRO:N	2.75	0.55
1:I:141:ARG:HG3	1:I:142:PHE:CD2	2.42	0.55
1:A:75:ALA:HA	4:A:325:GOL:H2	1.88	0.55
1:D:119:PHE:C	1:D:121:PHE:N	2.59	0.55
1:J:119:PHE:CG	1:J:120:PRO:N	2.75	0.55
1:C:147:VAL:HG22	1:C:147:VAL:O	2.07	0.55
1:E:147:VAL:HG22	1:E:147:VAL:O	2.07	0.55
1:B:118:LEU:O	1:B:119:PHE:O	2.24	0.55
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.71	0.55
1:F:248:TYR:CD1	1:G:247:PHE:HA	2.42	0.55
1:E:210:LEU:CB	1:E:211:PRO:HD3	2.34	0.55
1:F:247:PHE:CE1	1:J:248:TYR:HA	2.42	0.55
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.42	0.55
1:C:140:LEU:HD13	1:C:191:ILE:CG1	2.35	0.54
1:C:294:ASP:HB3	1:C:297:ILE:CG2	2.35	0.54
1:D:119:PHE:CG	1:D:120:PRO:N	2.75	0.54
1:A:119:PHE:O	1:A:121:PHE:N	2.33	0.54
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.89	0.54
1:G:182:GLN:HB2	1:G:185:GLN:HG2	1.89	0.54
1:D:147:VAL:O	1:D:147:VAL:HG22	2.07	0.54
1:E:20:ILE:HD12	1:E:195:ILE:HD11	1.89	0.54
1:E:15:SER:HB3	1:E:141:ARG:CD	2.36	0.54
1:J:15:SER:HB3	1:J:141:ARG:HD3	1.89	0.54
1:D:314:VAL:HG12	1:D:314:VAL:O	2.08	0.54
1:G:105:ARG:HG2	4:H:325:GOL:C1	2.36	0.54
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.89	0.54
1:G:314:VAL:O	1:G:314:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:PRO:HG2	1:G:258:TYR:HD2	1.72	0.54
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.71	0.54
1:C:224:TRP:HE1	1:C:301:ARG:HB3	1.73	0.54
1:A:248:TYR:CD1	1:B:247:PHE:HA	2.43	0.54
1:J:210:LEU:HB3	1:J:211:PRO:CD	2.36	0.54
1:B:15:SER:HB3	1:B:141:ARG:HD3	1.89	0.54
1:C:15:SER:HB3	1:C:141:ARG:HD3	1.89	0.54
1:I:302:LEU:O	1:I:306:LEU:HG	2.07	0.54
1:G:147:VAL:HG13	1:G:147:VAL:O	2.07	0.54
1:J:142:PHE:HA	1:J:170:ILE:HD11	1.88	0.54
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.37	0.54
1:D:302:LEU:O	1:D:306:LEU:HG	2.08	0.54
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.37	0.54
1:G:20:ILE:HD12	1:G:195:ILE:HD11	1.90	0.54
1:C:119:PHE:CG	1:C:120:PRO:N	2.76	0.54
1:B:225:LEU:CD2	1:C:232:LEU:HD23	2.38	0.54
1:A:182:GLN:HB2	1:A:185:GLN:HG2	1.89	0.54
1:D:15:SER:HB3	1:D:141:ARG:HD3	1.90	0.54
1:H:142:PHE:HA	1:H:170:ILE:HD11	1.89	0.54
1:F:302:LEU:O	1:F:306:LEU:HG	2.07	0.54
1:F:147:VAL:HG22	1:F:147:VAL:O	2.07	0.54
1:D:182:GLN:HB2	1:D:185:GLN:HG2	1.90	0.54
1:C:20:ILE:HD12	1:C:195:ILE:HD11	1.90	0.53
1:J:96:PRO:HD2	5:J:332:HOH:O	2.08	0.53
1:G:119:PHE:CD2	1:G:120:PRO:CD	2.91	0.53
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.43	0.53
1:I:205:LEU:HD23	1:I:209:ILE:HD12	1.91	0.53
1:I:20:ILE:HD12	1:I:195:ILE:HD11	1.90	0.53
1:A:147:VAL:HG22	1:A:147:VAL:O	2.07	0.53
1:E:182:GLN:HB2	1:E:185:GLN:HG2	1.90	0.53
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.73	0.53
1:H:91:ARG:HD3	1:H:103:ASN:HB3	1.90	0.53
1:F:314:VAL:HG12	1:F:314:VAL:O	2.09	0.53
1:J:294:ASP:HB3	1:J:297:ILE:CG2	2.37	0.53
1:B:182:GLN:HB2	1:B:185:GLN:HG2	1.90	0.53
1:G:168:THR:O	1:G:169:HIS:ND1	2.41	0.53
1:C:142:PHE:HA	1:C:170:ILE:HD11	1.91	0.53
1:F:227:SER:HB3	1:F:230:GLU:CG	2.38	0.53
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.44	0.53
1:H:297:ILE:HG23	1:H:298:GLN:N	2.24	0.53
1:C:15:SER:HB3	1:C:141:ARG:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:VAL:O	1:C:314:VAL:HG12	2.08	0.53
1:F:150:GLU:HG3	1:F:153:ASP:HB2	1.91	0.53
1:F:55:PRO:HG2	1:G:181:VAL:HG13	1.89	0.53
1:I:294:ASP:HB3	1:I:297:ILE:CG2	2.37	0.53
1:A:225:LEU:CD2	1:B:232:LEU:HD23	2.39	0.53
1:B:314:VAL:HG12	1:B:314:VAL:O	2.09	0.53
2:J:323:ACH:H102	2:J:323:ACH:O4	2.08	0.53
1:F:142:PHE:HA	1:F:170:ILE:HD11	1.90	0.53
1:D:15:SER:HB3	1:D:141:ARG:CG	2.39	0.53
1:H:227:SER:HB3	1:H:230:GLU:HG3	1.90	0.53
1:H:140:LEU:HD13	1:H:191:ILE:CG1	2.39	0.53
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.43	0.53
1:J:119:PHE:O	1:J:121:PHE:N	2.32	0.53
1:E:119:PHE:CG	1:E:120:PRO:N	2.77	0.53
1:B:119:PHE:O	1:B:121:PHE:N	2.31	0.53
1:I:225:LEU:HD21	1:J:232:LEU:HD23	1.91	0.53
1:A:210:LEU:HB3	1:A:211:PRO:CD	2.36	0.52
1:G:210:LEU:HB3	1:G:211:PRO:CD	2.36	0.52
1:E:15:SER:HB3	1:E:141:ARG:CG	2.39	0.52
1:H:212:LEU:HB3	1:H:265:MET:HE1	1.91	0.52
1:E:150:GLU:HG3	1:E:153:ASP:HB2	1.92	0.52
1:F:140:LEU:CD2	5:F:331:HOH:O	2.43	0.52
1:D:55:PRO:HG2	1:E:181:VAL:HG13	1.92	0.52
1:J:136:ASN:O	4:J:325:GOL:C2	2.50	0.52
1:F:119:PHE:CG	1:F:120:PRO:N	2.77	0.52
1:D:119:PHE:CD2	1:D:120:PRO:CD	2.91	0.52
1:I:142:PHE:HA	1:I:170:ILE:HD11	1.91	0.52
1:A:314:VAL:O	1:A:314:VAL:HG12	2.09	0.52
1:A:99:ARG:CG	1:A:99:ARG:HH11	2.14	0.52
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.90	0.52
1:D:140:LEU:CD1	5:D:341:HOH:O	2.28	0.52
1:F:119:PHE:CD2	1:F:120:PRO:CD	2.93	0.52
1:J:118:LEU:O	1:J:119:PHE:O	2.28	0.52
1:J:212:LEU:CD1	1:J:265:MET:HB3	2.39	0.52
1:I:118:LEU:O	1:I:119:PHE:O	2.28	0.52
1:A:15:SER:HB3	1:A:141:ARG:CG	2.39	0.52
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.40	0.52
1:B:168:THR:C	1:B:169:HIS:CD2	2.83	0.52
1:H:118:LEU:O	1:H:119:PHE:O	2.28	0.52
1:I:102:TYR:HE2	4:I:327:GOL:H2	1.74	0.52
1:I:15:SER:HB2	1:I:142:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:SER:HB3	1:I:141:ARG:HG2	1.91	0.52
1:B:19:PHE:CD1	2:B:323:ACH:H61	2.45	0.52
1:H:140:LEU:CD2	5:H:331:HOH:O	2.47	0.52
1:D:257:PRO:HG2	1:D:258:TYR:HD2	1.74	0.52
1:G:225:LEU:CD2	1:H:232:LEU:HD23	2.40	0.52
1:G:150:GLU:HG3	1:G:153:ASP:HB2	1.92	0.52
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.40	0.52
1:I:314:VAL:HG12	1:I:314:VAL:O	2.10	0.52
1:I:212:LEU:HB3	1:I:265:MET:HE1	1.91	0.52
1:F:205:LEU:HD23	1:F:209:ILE:HD12	1.91	0.52
1:H:314:VAL:O	1:H:314:VAL:HG12	2.10	0.52
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.38	0.51
1:E:118:LEU:O	1:E:119:PHE:O	2.28	0.51
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.44	0.51
1:E:314:VAL:O	1:E:314:VAL:HG12	2.10	0.51
1:H:297:ILE:CG2	1:H:298:GLN:N	2.73	0.51
1:C:119:PHE:C	1:C:121:PHE:N	2.63	0.51
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.45	0.51
1:D:150:GLU:HG3	1:D:153:ASP:HB2	1.92	0.51
1:D:210:LEU:CB	1:D:211:PRO:HD3	2.38	0.51
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.92	0.51
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.93	0.51
1:A:142:PHE:HA	1:A:170:ILE:HD11	1.92	0.51
1:A:212:LEU:CD1	1:A:265:MET:HB3	2.39	0.51
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.40	0.51
1:D:145:ILE:HG13	1:D:166:ALA:HB3	1.93	0.51
1:G:118:LEU:O	1:G:119:PHE:O	2.29	0.51
1:A:145:ILE:HD11	1:A:166:ALA:HB3	1.92	0.51
1:D:141:ARG:NH1	5:D:329:HOH:O	2.31	0.51
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.46	0.51
1:F:137:ASN:HA	4:F:328:GOL:C1	2.41	0.51
1:A:297:ILE:HG23	1:A:298:GLN:N	2.26	0.51
1:B:15:SER:HB3	1:B:141:ARG:CG	2.40	0.51
1:C:248:TYR:CD1	1:D:247:PHE:HA	2.45	0.51
1:D:95:PHE:CD2	1:D:99:ARG:HB2	2.45	0.51
1:I:150:GLU:HG3	1:I:153:ASP:HB2	1.92	0.51
1:C:15:SER:HB2	1:C:142:PHE:CE1	2.46	0.51
1:D:11:PRO:CD	5:D:339:HOH:O	2.59	0.51
1:I:182:GLN:HB2	1:I:185:GLN:HG2	1.91	0.51
1:F:301:ARG:HH12	1:G:285:HIS:CE1	2.29	0.51
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:ASN:HA	4:J:325:GOL:C2	2.41	0.51
1:G:119:PHE:O	1:G:121:PHE:N	2.33	0.51
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.75	0.51
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.74	0.51
1:H:15:SER:HB3	1:H:141:ARG:HD3	1.93	0.51
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.41	0.51
1:C:210:LEU:HB3	1:C:211:PRO:CD	2.41	0.50
1:F:145:ILE:HD11	1:F:166:ALA:HB3	1.92	0.50
1:I:119:PHE:CG	1:I:120:PRO:N	2.79	0.50
1:F:15:SER:HB3	1:F:141:ARG:CG	2.41	0.50
1:H:227:SER:HB3	1:H:230:GLU:CG	2.40	0.50
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.94	0.50
1:B:119:PHE:C	1:B:121:PHE:N	2.65	0.50
1:H:182:GLN:HB2	1:H:185:GLN:HG2	1.93	0.50
1:D:11:PRO:HD2	5:D:339:HOH:O	2.09	0.50
1:F:38:TYR:CE1	1:F:105:ARG:HD3	2.46	0.50
1:F:235:SER:HB3	1:F:277:ILE:HD11	1.93	0.50
1:A:150:GLU:HG3	1:A:153:ASP:HB2	1.92	0.50
1:G:137:ASN:CA	4:G:328:GOL:O3	2.55	0.50
1:B:150:GLU:HG3	1:B:153:ASP:HB2	1.92	0.50
1:I:19:PHE:CD1	2:I:323:ACH:H61	2.47	0.50
1:J:150:GLU:HG3	1:J:153:ASP:HB2	1.92	0.50
1:E:11:PRO:N	5:E:332:HOH:O	2.43	0.50
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.93	0.50
1:J:119:PHE:C	1:J:121:PHE:N	2.65	0.50
1:B:15:SER:HB3	1:B:141:ARG:HG2	1.93	0.50
1:C:284:HIS:HD2	1:C:285:HIS:NE2	2.09	0.50
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.93	0.50
1:E:297:ILE:HG23	1:E:298:GLN:N	2.26	0.50
1:H:150:GLU:HG3	1:H:153:ASP:HB2	1.92	0.50
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.46	0.50
1:J:314:VAL:HG12	1:J:314:VAL:O	2.10	0.50
1:A:297:ILE:CG2	1:A:298:GLN:N	2.75	0.50
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.92	0.50
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.42	0.50
1:E:227:SER:HB3	1:E:230:GLU:CG	2.41	0.50
2:F:323:ACH:O4	2:F:323:ACH:H102	2.12	0.50
1:D:161:TRP:CZ2	1:D:200:ASN:ND2	2.80	0.50
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.46	0.50
2:D:323:ACH:H101	1:E:175:TYR:CZ	2.46	0.50
1:D:136:ASN:O	4:D:327:GOL:H32	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ILE:HG23	1:G:298:GLN:N	2.27	0.50
1:B:147:VAL:O	1:B:147:VAL:HG22	2.12	0.50
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.47	0.50
1:D:91:ARG:HD3	1:D:103:ASN:HB3	1.94	0.50
1:D:140:LEU:CD2	5:D:341:HOH:O	2.33	0.50
1:B:210:LEU:HB3	1:B:211:PRO:CD	2.37	0.50
1:J:297:ILE:HG23	1:J:298:GLN:N	2.26	0.50
1:A:225:LEU:HB2	1:A:231:ARG:HG3	1.93	0.50
1:B:15:SER:HB2	1:B:142:PHE:CE1	2.47	0.50
1:E:142:PHE:HA	1:E:170:ILE:HD11	1.93	0.50
1:D:212:LEU:HB3	1:D:265:MET:HE1	1.94	0.50
1:G:297:ILE:C	1:G:299:ARG:N	2.66	0.50
1:J:210:LEU:CB	1:J:211:PRO:HD3	2.40	0.50
1:G:119:PHE:HE1	1:G:199:ARG:CZ	2.25	0.50
1:H:119:PHE:O	1:H:121:PHE:N	2.30	0.50
1:H:225:LEU:HB2	1:H:231:ARG:HG3	1.93	0.50
1:J:147:VAL:HG22	1:J:147:VAL:O	2.12	0.50
1:F:212:LEU:HB3	1:F:265:MET:HE1	1.93	0.50
1:H:248:TYR:CD1	1:I:247:PHE:HA	2.46	0.50
1:C:150:GLU:HG3	1:C:153:ASP:HB2	1.92	0.50
1:G:55:PRO:HG2	1:H:181:VAL:HG13	1.93	0.50
1:B:297:ILE:HG23	1:B:298:GLN:N	2.26	0.49
1:J:119:PHE:CD2	1:J:120:PRO:CD	2.94	0.49
1:E:119:PHE:C	1:E:121:PHE:N	2.65	0.49
1:A:247:PHE:CE1	1:E:248:TYR:HA	2.46	0.49
1:G:212:LEU:HB3	1:G:265:MET:HE1	1.94	0.49
1:D:205:LEU:HD23	1:D:209:ILE:HD12	1.93	0.49
1:A:175:TYR:OH	2:E:323:ACH:H101	2.12	0.49
1:B:175:TYR:CD1	4:B:326:GOL:H11	2.45	0.49
1:G:99:ARG:CG	1:G:99:ARG:HH11	2.12	0.49
1:I:297:ILE:HG23	1:I:298:GLN:N	2.27	0.49
1:C:205:LEU:HD23	1:C:209:ILE:HD12	1.95	0.49
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.93	0.49
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.47	0.49
1:A:227:SER:HB3	1:A:230:GLU:HG3	1.94	0.49
1:I:149:THR:O	1:I:150:GLU:HB3	2.12	0.49
1:A:205:LEU:HD23	1:A:209:ILE:HD12	1.93	0.49
1:F:297:ILE:HG23	1:F:298:GLN:N	2.27	0.49
1:F:145:ILE:HG13	1:F:166:ALA:HB3	1.94	0.49
1:H:119:PHE:CD2	1:H:120:PRO:CD	2.96	0.49
1:B:15:SER:HB3	1:B:141:ARG:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SER:HB2	1:A:142:PHE:CE1	2.47	0.49
1:H:212:LEU:HG	1:H:245:TYR:CE2	2.47	0.49
1:J:297:ILE:CG2	1:J:298:GLN:N	2.75	0.49
1:H:83:GLY:O	4:H:325:GOL:O2	2.31	0.49
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.76	0.49
1:I:248:TYR:HA	1:J:247:PHE:CE1	2.47	0.49
1:G:95:PHE:CD2	1:G:99:ARG:HB2	2.47	0.49
1:I:95:PHE:HB2	1:I:99:ARG:HB2	1.94	0.49
1:C:297:ILE:CG2	1:C:298:GLN:N	2.76	0.49
1:D:145:ILE:CG1	1:D:166:ALA:HB3	2.43	0.49
1:G:15:SER:HB2	1:G:142:PHE:CE1	2.48	0.49
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.94	0.49
1:E:15:SER:HB2	1:E:142:PHE:CE1	2.47	0.49
1:G:248:TYR:HD1	1:H:247:PHE:HA	1.77	0.49
1:A:212:LEU:HB3	1:A:265:MET:HE1	1.93	0.49
1:B:205:LEU:HD23	1:B:209:ILE:HD12	1.93	0.49
1:H:165:LYS:HD2	1:H:165:LYS:N	2.27	0.49
1:F:119:PHE:C	1:F:121:PHE:N	2.65	0.49
1:J:15:SER:HB2	1:J:142:PHE:CE1	2.48	0.49
1:J:15:SER:HB3	1:J:141:ARG:CD	2.42	0.49
1:F:15:SER:HB3	1:F:141:ARG:CD	2.43	0.49
1:E:297:ILE:CG2	1:E:298:GLN:N	2.75	0.49
1:I:297:ILE:CG2	1:I:298:GLN:N	2.76	0.49
1:A:119:PHE:CD2	1:A:120:PRO:CD	2.92	0.49
1:E:145:ILE:HG13	1:E:166:ALA:HB3	1.95	0.49
1:A:175:TYR:CZ	2:E:323:ACH:H101	2.47	0.49
1:I:248:TYR:CD1	1:J:247:PHE:HA	2.48	0.49
1:B:297:ILE:CG2	1:B:298:GLN:N	2.75	0.49
1:B:301:ARG:HH12	1:C:285:HIS:CE1	2.31	0.49
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.67	0.49
1:F:119:PHE:O	1:F:121:PHE:N	2.31	0.48
1:H:145:ILE:HD11	1:H:166:ALA:HB3	1.95	0.48
1:E:257:PRO:HG2	1:E:258:TYR:HD2	1.75	0.48
1:J:19:PHE:CD1	2:J:323:ACH:H61	2.48	0.48
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.95	0.48
1:D:248:TYR:CD1	1:E:247:PHE:HA	2.48	0.48
1:G:297:ILE:CG2	1:G:298:GLN:N	2.75	0.48
1:C:297:ILE:HG23	1:C:298:GLN:N	2.26	0.48
1:G:145:ILE:HD11	1:G:166:ALA:HB3	1.93	0.48
1:J:15:SER:HB3	1:J:141:ARG:HG2	1.93	0.48
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:SER:HB3	1:C:141:ARG:CD	2.43	0.48
1:H:205:LEU:HD23	1:H:209:ILE:HD12	1.95	0.48
1:E:212:LEU:CD1	1:E:265:MET:HB3	2.43	0.48
1:G:119:PHE:C	1:G:121:PHE:N	2.65	0.48
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.95	0.48
1:A:232:LEU:HD23	1:E:225:LEU:CD2	2.44	0.48
2:D:323:ACH:O4	2:D:323:ACH:H102	2.13	0.48
1:C:11:PRO:HD2	5:C:335:HOH:O	2.13	0.48
1:J:95:PHE:CD2	1:J:99:ARG:HB2	2.49	0.48
1:D:145:ILE:HD11	1:D:166:ALA:HB3	1.92	0.48
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.48	0.48
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.49	0.48
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.48	0.48
1:F:15:SER:HB2	1:F:142:PHE:CE1	2.48	0.48
1:J:284:HIS:HD2	1:J:285:HIS:NE2	2.12	0.48
1:I:297:ILE:C	1:I:299:ARG:N	2.67	0.48
1:D:297:ILE:C	1:D:299:ARG:N	2.67	0.48
1:J:212:LEU:HB3	1:J:265:MET:HE1	1.95	0.48
1:C:212:LEU:HB3	1:C:265:MET:HE1	1.95	0.48
1:E:205:LEU:HD23	1:E:209:ILE:HD12	1.95	0.48
1:A:210:LEU:CB	1:A:211:PRO:HD3	2.39	0.48
1:H:210:LEU:CB	1:H:211:PRO:HD3	2.41	0.48
1:A:137:ASN:HA	4:A:326:GOL:HO1	1.78	0.48
1:A:15:SER:HB3	1:A:141:ARG:CD	2.43	0.48
1:H:15:SER:HB3	1:H:141:ARG:CG	2.44	0.48
1:J:149:THR:O	1:J:150:GLU:HB3	2.14	0.48
1:E:217:ALA:HA	1:E:220:TRP:CE3	2.49	0.48
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.96	0.48
1:E:297:ILE:C	1:E:299:ARG:N	2.67	0.48
1:I:145:ILE:HG13	1:I:166:ALA:HB3	1.96	0.48
1:I:145:ILE:CG1	1:I:166:ALA:HB3	2.44	0.48
1:I:301:ARG:HH12	1:J:285:HIS:CE1	2.31	0.48
1:A:19:PHE:CD1	2:A:323:ACH:H61	2.49	0.48
1:C:149:THR:O	1:C:150:GLU:HB3	2.12	0.48
1:E:212:LEU:HB3	1:E:265:MET:HE1	1.95	0.48
1:I:235:SER:HB3	1:I:277:ILE:HD11	1.95	0.48
1:E:23:ILE:HG21	1:E:126:PHE:CD2	2.49	0.48
1:G:289:ASN:OD1	1:G:292:GLU:HB3	2.14	0.48
1:F:248:TYR:HD1	1:G:247:PHE:HA	1.78	0.48
1:G:210:LEU:CB	1:G:211:PRO:HD3	2.41	0.47
1:I:119:PHE:C	1:I:121:PHE:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.57	0.47
1:G:136:ASN:C	4:G:328:GOL:H2	2.33	0.47
1:E:95:PHE:HB2	1:E:99:ARG:HB2	1.96	0.47
1:C:297:ILE:C	1:C:299:ARG:N	2.67	0.47
1:E:119:PHE:O	1:E:121:PHE:N	2.38	0.47
1:I:225:LEU:HB2	1:I:231:ARG:HG3	1.96	0.47
1:I:289:ASN:OD1	1:I:292:GLU:HB3	2.14	0.47
1:F:257:PRO:HG2	1:F:258:TYR:HD2	1.76	0.47
1:A:15:SER:HB3	1:A:141:ARG:HG2	1.96	0.47
1:B:149:THR:O	1:B:150:GLU:HB3	2.14	0.47
1:E:279:LEU:HD22	1:E:304:PHE:HE2	1.79	0.47
1:A:297:ILE:C	1:A:299:ARG:N	2.67	0.47
1:D:297:ILE:HG23	1:D:298:GLN:N	2.28	0.47
1:E:119:PHE:CD2	1:E:120:PRO:CD	2.95	0.47
1:H:19:PHE:CD1	2:H:323:ACH:H61	2.49	0.47
2:I:323:ACH:H102	2:I:323:ACH:O4	2.14	0.47
1:I:284:HIS:HD2	1:I:285:HIS:NE2	2.12	0.47
1:B:145:ILE:HG13	1:B:166:ALA:HB3	1.96	0.47
1:G:142:PHE:HA	1:G:170:ILE:HD11	1.96	0.47
1:D:149:THR:O	1:D:150:GLU:HB3	2.14	0.47
1:E:39:ILE:HD11	1:E:130:LEU:HD11	1.96	0.47
1:I:305:PRO:O	1:I:309:LEU:HG	2.14	0.47
1:B:137:ASN:CA	4:B:327:GOL:O1	2.62	0.47
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.49	0.47
1:A:149:THR:O	1:A:150:GLU:HB3	2.13	0.47
1:E:11:PRO:CD	5:E:332:HOH:O	2.63	0.47
1:I:169:HIS:CE1	1:I:171:SER:HB3	2.49	0.47
1:I:55:PRO:HG2	1:J:181:VAL:HG13	1.96	0.47
1:H:95:PHE:CD2	1:H:99:ARG:HB2	2.50	0.47
1:I:210:LEU:CB	1:I:211:PRO:HD3	2.36	0.47
1:H:83:GLY:C	4:H:325:GOL:O2	2.52	0.47
1:C:145:ILE:HD11	1:C:166:ALA:HB3	1.94	0.47
1:G:147:VAL:O	1:G:147:VAL:HG22	2.14	0.47
1:G:149:THR:O	1:G:150:GLU:HB3	2.14	0.47
1:H:11:PRO:N	5:H:328:HOH:O	2.47	0.47
1:F:29:LEU:HD23	1:F:29:LEU:HA	1.67	0.47
1:H:140:LEU:CD1	5:H:331:HOH:O	2.33	0.47
1:B:145:ILE:CD1	1:B:145:ILE:O	2.59	0.47
1:A:136:ASN:O	4:A:326:GOL:H11	2.14	0.47
1:I:119:PHE:CD2	1:I:120:PRO:CD	2.97	0.47
1:I:119:PHE:O	1:I:121:PHE:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:LEU:H	4:I:327:GOL:C1	2.28	0.47
1:E:145:ILE:HD11	1:E:166:ALA:HB3	1.94	0.47
1:G:15:SER:HB3	1:G:141:ARG:HD3	1.96	0.47
1:E:289:ASN:OD1	1:E:292:GLU:HB3	2.15	0.47
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.50	0.47
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.48	0.47
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.95	0.47
1:J:55:PRO:HB3	1:J:95:PHE:CD1	2.49	0.47
1:G:297:ILE:O	1:G:299:ARG:N	2.48	0.47
1:B:168:THR:C	1:B:169:HIS:CG	2.88	0.47
2:G:323:ACH:H102	2:G:323:ACH:O4	2.15	0.47
1:F:297:ILE:CG2	1:F:298:GLN:N	2.78	0.47
1:D:289:ASN:OD1	1:D:292:GLU:HB3	2.15	0.47
1:H:149:THR:O	1:H:150:GLU:HB3	2.14	0.47
1:F:284:HIS:HD2	1:F:285:HIS:NE2	2.12	0.47
1:A:119:PHE:C	1:A:121:PHE:N	2.65	0.47
1:C:15:SER:HB3	1:C:141:ARG:HG2	1.97	0.47
1:E:15:SER:HB3	1:E:141:ARG:HG2	1.97	0.46
1:B:147:VAL:O	1:B:147:VAL:HG13	2.15	0.46
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.50	0.46
1:J:145:ILE:HD11	1:J:166:ALA:HB3	1.97	0.46
1:B:119:PHE:CD2	1:B:120:PRO:CD	2.98	0.46
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.30	0.46
1:J:289:ASN:OD1	1:J:292:GLU:HB3	2.15	0.46
1:E:149:THR:O	1:E:150:GLU:HB3	2.13	0.46
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.97	0.46
1:I:140:LEU:CD2	5:I:334:HOH:O	2.29	0.46
1:B:95:PHE:HB2	1:B:99:ARG:HB2	1.96	0.46
1:D:297:ILE:O	1:D:299:ARG:N	2.48	0.46
1:B:142:PHE:HA	1:B:170:ILE:HD11	1.97	0.46
1:D:15:SER:HB3	1:D:141:ARG:CD	2.45	0.46
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.51	0.46
1:C:38:TYR:CE1	1:C:105:ARG:HD3	2.50	0.46
1:G:91:ARG:HD3	1:G:103:ASN:HB3	1.97	0.46
1:J:99:ARG:HH11	1:J:99:ARG:CG	2.12	0.46
1:A:137:ASN:HA	4:A:326:GOL:C1	2.44	0.46
1:B:289:ASN:OD1	1:B:292:GLU:HB3	2.14	0.46
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.49	0.46
1:F:297:ILE:C	1:F:299:ARG:N	2.69	0.46
1:J:297:ILE:C	1:J:299:ARG:N	2.68	0.46
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:SER:HB2	1:D:142:PHE:CE1	2.51	0.46
1:B:235:SER:HB3	1:B:277:ILE:HD11	1.98	0.46
1:C:287:GLN:HB2	1:C:288:ALA:H	1.54	0.46
1:D:297:ILE:CG2	1:D:298:GLN:N	2.78	0.46
1:H:297:ILE:C	1:H:299:ARG:N	2.68	0.46
1:A:145:ILE:HG13	1:A:166:ALA:HB3	1.96	0.46
1:C:145:ILE:HG13	1:C:166:ALA:HB3	1.98	0.46
1:F:150:GLU:HG3	1:F:153:ASP:CB	2.46	0.46
1:G:161:TRP:CZ2	1:G:200:ASN:ND2	2.83	0.46
2:A:323:ACH:O4	2:A:323:ACH:H102	2.15	0.46
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.51	0.46
1:E:297:ILE:O	1:E:299:ARG:N	2.48	0.46
1:A:297:ILE:O	1:A:299:ARG:N	2.49	0.46
1:H:145:ILE:HG13	1:H:166:ALA:HB3	1.96	0.46
1:J:212:LEU:O	1:J:216:ILE:HG13	2.15	0.46
1:A:227:SER:HB3	1:A:230:GLU:CG	2.45	0.46
1:I:248:TYR:HD1	1:J:247:PHE:HA	1.81	0.46
1:G:227:SER:HB3	1:G:230:GLU:HG3	1.98	0.46
1:B:145:ILE:CG1	1:B:166:ALA:HB3	2.45	0.46
1:A:145:ILE:CG1	1:A:166:ALA:HB3	2.46	0.46
1:G:145:ILE:HG13	1:G:166:ALA:HB3	1.96	0.46
1:C:150:GLU:HG3	1:C:153:ASP:CB	2.46	0.46
1:J:220:TRP:C	1:J:222:VAL:H	2.19	0.46
3:A:324:MES:O1S	3:A:324:MES:H51	2.16	0.46
1:H:77:GLU:O	1:H:130:LEU:HD12	2.15	0.46
1:B:304:PHE:CB	1:B:305:PRO:HD3	2.46	0.46
1:F:210:LEU:CB	1:F:211:PRO:HD3	2.39	0.45
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.51	0.45
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.51	0.45
1:A:289:ASN:OD1	1:A:292:GLU:HB3	2.16	0.45
1:F:289:ASN:OD1	1:F:292:GLU:HB3	2.16	0.45
1:C:227:SER:HB3	1:C:230:GLU:CG	2.45	0.45
1:F:181:VAL:HG13	1:J:55:PRO:HG2	1.97	0.45
2:C:323:ACH:O4	2:C:323:ACH:H102	2.15	0.45
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.61	0.45
1:B:220:TRP:C	1:B:222:VAL:H	2.20	0.45
1:J:205:LEU:HD23	1:J:209:ILE:HD12	1.98	0.45
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.51	0.45
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.99	0.45
1:A:95:PHE:CD2	1:A:99:ARG:HB2	2.51	0.45
1:F:11:PRO:N	5:F:330:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ASN:CG	1:G:290:GLY:N	2.69	0.45
1:C:289:ASN:CG	1:C:290:GLY:N	2.69	0.45
1:D:227:SER:HB3	1:D:230:GLU:CG	2.46	0.45
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.81	0.45
1:E:289:ASN:CG	1:E:290:GLY:N	2.69	0.45
1:D:289:ASN:CG	1:D:290:GLY:N	2.69	0.45
1:D:15:SER:HB3	1:D:141:ARG:HG2	1.98	0.45
1:D:248:TYR:HD1	1:E:247:PHE:HA	1.81	0.45
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.42	0.45
1:C:147:VAL:O	1:C:147:VAL:HG13	2.17	0.45
1:G:15:SER:HB3	1:G:141:ARG:CG	2.47	0.45
1:F:289:ASN:HD21	1:F:292:GLU:HB2	1.81	0.45
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.51	0.45
1:J:304:PHE:CB	1:J:305:PRO:HD3	2.46	0.45
1:J:227:SER:HB3	1:J:230:GLU:HG3	1.98	0.45
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.78	0.45
1:F:95:PHE:CD2	1:F:99:ARG:HB2	2.52	0.45
1:D:145:ILE:HD12	1:D:166:ALA:HB3	1.97	0.45
1:E:289:ASN:ND2	1:E:292:GLU:HB2	2.32	0.45
1:E:289:ASN:HD21	1:E:292:GLU:HB2	1.81	0.45
1:F:149:THR:O	1:F:150:GLU:HB3	2.16	0.45
1:J:95:PHE:HB2	1:J:99:ARG:HB2	1.99	0.45
1:F:145:ILE:CG1	1:F:166:ALA:HB3	2.45	0.45
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.51	0.45
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.98	0.45
1:C:304:PHE:CB	1:C:305:PRO:HD3	2.46	0.45
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.51	0.45
1:G:137:ASN:HA	4:G:328:GOL:H2	1.98	0.45
1:J:145:ILE:HG13	1:J:166:ALA:HB3	1.98	0.45
1:B:95:PHE:CD2	1:B:99:ARG:HB2	2.52	0.45
1:I:297:ILE:O	1:I:299:ARG:N	2.50	0.45
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.81	0.45
1:B:289:ASN:CG	1:B:290:GLY:N	2.70	0.45
1:D:150:GLU:HG3	1:D:153:ASP:CB	2.47	0.45
1:C:212:LEU:HD13	1:C:265:MET:HB3	1.99	0.45
1:A:150:GLU:HG3	1:A:153:ASP:CB	2.47	0.45
1:I:279:LEU:HD22	1:I:304:PHE:HE2	1.82	0.45
1:C:297:ILE:O	1:C:299:ARG:N	2.50	0.45
1:I:150:GLU:HG3	1:I:153:ASP:CB	2.47	0.45
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.47	0.45
1:A:289:ASN:CG	1:A:290:GLY:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ASN:O	4:E:326:GOL:O1	2.32	0.45
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.70	0.45
1:I:304:PHE:CB	1:I:305:PRO:HD3	2.47	0.45
1:J:227:SER:HB3	1:J:230:GLU:CG	2.47	0.45
1:A:304:PHE:CB	1:A:305:PRO:HD3	2.47	0.45
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.79	0.45
4:C:325:GOL:H32	5:C:326:HOH:O	2.17	0.44
1:G:38:TYR:CE1	1:G:105:ARG:HD3	2.52	0.44
1:H:257:PRO:HG2	1:H:258:TYR:HD2	1.78	0.44
1:A:257:PRO:HG2	1:A:258:TYR:HD2	1.76	0.44
1:G:287:GLN:HB2	1:G:288:ALA:H	1.52	0.44
1:J:23:ILE:HG21	1:J:126:PHE:CD2	2.52	0.44
1:I:39:ILE:HD11	1:I:130:LEU:HD11	1.99	0.44
1:C:137:ASN:HA	4:C:325:GOL:O3	2.16	0.44
1:B:136:ASN:C	4:B:327:GOL:H32	2.37	0.44
1:I:289:ASN:HD21	1:I:292:GLU:HB2	1.82	0.44
1:I:289:ASN:ND2	1:I:292:GLU:HB2	2.32	0.44
1:G:212:LEU:HD13	1:G:265:MET:HB3	1.98	0.44
1:E:150:GLU:HG3	1:E:153:ASP:CB	2.47	0.44
1:J:29:LEU:HA	1:J:29:LEU:HD23	1.69	0.44
1:G:311:ILE:O	1:G:311:ILE:HG22	2.18	0.44
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.78	0.44
1:C:136:ASN:O	4:C:325:GOL:C2	2.31	0.44
1:D:55:PRO:HB3	1:D:95:PHE:CD1	2.52	0.44
1:C:289:ASN:OD1	1:C:292:GLU:HB3	2.17	0.44
1:F:289:ASN:CG	1:F:290:GLY:N	2.68	0.44
1:B:289:ASN:HD21	1:B:292:GLU:HB2	1.82	0.44
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.51	0.44
1:A:248:TYR:HD1	1:B:247:PHE:HA	1.82	0.44
1:J:150:GLU:HG3	1:J:153:ASP:CB	2.46	0.44
1:G:304:PHE:CB	1:G:305:PRO:HD3	2.48	0.44
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.63	0.44
1:D:289:ASN:ND2	1:D:292:GLU:HB2	2.32	0.44
1:J:212:LEU:HD13	1:J:265:MET:HB3	1.98	0.44
1:G:150:GLU:HG3	1:G:153:ASP:CB	2.47	0.44
2:E:323:ACH:O4	2:E:323:ACH:H102	2.17	0.44
1:E:212:LEU:HA	1:E:212:LEU:HD23	1.81	0.44
1:I:287:GLN:HB2	1:I:288:ALA:H	1.53	0.44
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.66	0.44
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.53	0.44
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:ASN:ND2	1:F:292:GLU:HB2	2.33	0.44
1:A:102:TYR:CZ	4:A:325:GOL:H12	2.52	0.44
1:H:150:GLU:HG3	1:H:153:ASP:CB	2.47	0.44
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.53	0.44
1:F:102:TYR:OH	4:F:325:GOL:H12	2.17	0.44
1:H:58:VAL:CG1	1:H:62:GLN:HB3	2.47	0.44
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.57	0.44
1:J:287:GLN:HB2	1:J:288:ALA:H	1.54	0.44
1:A:140:LEU:HD13	1:A:191:ILE:CG1	2.40	0.44
1:D:147:VAL:O	1:D:147:VAL:HG13	2.17	0.44
1:B:289:ASN:ND2	1:B:292:GLU:HB2	2.33	0.44
1:B:147:VAL:O	1:B:149:THR:N	2.48	0.44
1:H:40:VAL:HG22	1:H:103:ASN:ND2	2.33	0.44
1:H:220:TRP:C	1:H:222:VAL:H	2.21	0.44
1:D:11:PRO:N	5:D:339:HOH:O	2.50	0.44
1:E:58:VAL:CG1	1:E:62:GLN:HB3	2.47	0.44
1:A:39:ILE:HD11	1:A:130:LEU:HD11	2.00	0.44
1:A:284:HIS:HD2	1:A:285:HIS:NE2	2.15	0.44
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.87	0.44
1:B:55:PRO:HG2	1:C:181:VAL:HG13	2.00	0.44
1:F:225:LEU:HD21	1:G:232:LEU:HD23	1.99	0.44
1:A:289:ASN:ND2	1:A:292:GLU:HB2	2.32	0.44
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.82	0.44
1:B:212:LEU:HD13	1:B:265:MET:HB3	1.99	0.44
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.66	0.44
1:B:227:SER:HB3	1:B:230:GLU:CG	2.48	0.44
1:E:291:VAL:O	1:E:291:VAL:HG12	2.17	0.44
1:D:79:ILE:HD13	1:D:79:ILE:HA	1.80	0.44
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.52	0.44
1:B:297:ILE:C	1:B:299:ARG:N	2.69	0.44
1:C:289:ASN:HD21	1:C:292:GLU:HB2	1.82	0.44
1:A:212:LEU:HD13	1:A:265:MET:HB3	2.00	0.44
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.60	0.44
1:B:226:GLU:OE2	1:C:284:HIS:NE2	2.46	0.44
1:H:15:SER:HB2	1:H:142:PHE:CE1	2.53	0.44
1:I:227:SER:HB3	1:I:230:GLU:CG	2.48	0.44
1:B:287:GLN:HB2	1:B:288:ALA:H	1.55	0.44
1:E:311:ILE:O	1:E:311:ILE:HG22	2.18	0.44
1:B:174:ARG:O	4:B:326:GOL:H31	2.18	0.43
1:A:147:VAL:HG13	1:A:147:VAL:O	2.18	0.43
1:H:119:PHE:C	1:H:121:PHE:N	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:TRP:CE2	1:J:301:ARG:HD3	2.53	0.43
2:B:323:ACH:O4	2:B:323:ACH:H102	2.18	0.43
1:C:19:PHE:CD1	2:C:323:ACH:H61	2.53	0.43
1:F:212:LEU:HG	1:F:245:TYR:CE2	2.53	0.43
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.83	0.43
1:F:304:PHE:CB	1:F:305:PRO:HD3	2.49	0.43
1:B:284:HIS:HD2	1:B:285:HIS:NE2	2.16	0.43
1:B:291:VAL:O	1:B:291:VAL:HG12	2.19	0.43
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.53	0.43
1:H:289:ASN:ND2	1:H:292:GLU:HB2	2.32	0.43
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.53	0.43
1:H:248:TYR:HD1	1:I:247:PHE:HA	1.84	0.43
1:H:163:ARG:HB2	1:H:196:ASP:HB2	2.00	0.43
1:H:311:ILE:O	1:H:311:ILE:HG22	2.18	0.43
1:C:311:ILE:O	1:C:311:ILE:HG22	2.18	0.43
1:I:257:PRO:HG2	1:I:258:TYR:HD2	1.83	0.43
1:C:289:ASN:ND2	1:C:292:GLU:HB2	2.34	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.53	0.43
1:F:182:GLN:NE2	1:J:54:LYS:HD2	2.33	0.43
1:I:163:ARG:HD3	1:I:163:ARG:HA	1.84	0.43
1:I:58:VAL:CG1	1:I:62:GLN:HB3	2.49	0.43
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.31	0.43
1:H:225:LEU:CD2	1:I:232:LEU:HD23	2.48	0.43
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.83	0.43
1:I:161:TRP:CZ2	1:I:200:ASN:ND2	2.85	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.66	0.43
1:C:224:TRP:CE2	1:C:301:ARG:HD3	2.53	0.43
1:E:304:PHE:CB	1:E:305:PRO:HD3	2.49	0.43
1:J:279:LEU:HD22	1:J:304:PHE:HE2	1.84	0.43
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.78	0.43
1:H:284:HIS:HD2	1:H:285:HIS:NE2	2.17	0.43
1:J:311:ILE:O	1:J:311:ILE:HG22	2.19	0.43
1:A:55:PRO:HB3	1:A:95:PHE:CD1	2.53	0.43
1:F:226:GLU:OE2	1:G:284:HIS:NE2	2.45	0.43
1:I:289:ASN:CG	1:I:290:GLY:N	2.69	0.43
1:H:289:ASN:CG	1:H:290:GLY:N	2.70	0.43
1:H:289:ASN:OD1	1:H:292:GLU:HB3	2.19	0.43
1:H:248:TYR:HA	1:I:247:PHE:CE1	2.53	0.43
1:H:161:TRP:CZ2	1:H:200:ASN:ND2	2.87	0.43
1:A:240:LEU:HD13	1:E:241:THR:HA	2.01	0.43
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:HD2	1:D:285:HIS:NE2	2.16	0.43
1:I:99:ARG:CG	1:I:99:ARG:NH1	2.78	0.43
1:B:150:GLU:HG3	1:B:153:ASP:CB	2.48	0.43
1:D:212:LEU:HD13	1:D:265:MET:HB3	2.00	0.43
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.83	0.43
1:I:220:TRP:C	1:I:222:VAL:H	2.21	0.43
1:G:305:PRO:O	1:G:309:LEU:HG	2.18	0.43
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.53	0.43
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.79	0.43
1:H:304:PHE:CB	1:H:305:PRO:HD3	2.48	0.43
1:F:140:LEU:CG	5:F:331:HOH:O	2.62	0.43
1:D:297:ILE:C	1:D:299:ARG:H	2.21	0.43
1:G:145:ILE:CG1	1:G:166:ALA:HB3	2.48	0.43
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.34	0.43
1:H:305:PRO:O	1:H:309:LEU:HG	2.19	0.43
1:E:157:ILE:HA	1:E:157:ILE:HD13	1.79	0.43
1:D:95:PHE:HB2	1:D:99:ARG:HB2	1.99	0.43
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.54	0.43
1:B:168:THR:O	1:B:169:HIS:CG	2.72	0.43
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.61	0.43
1:I:155:GLU:HB3	1:I:161:TRP:CD1	2.54	0.43
1:H:200:ASN:HA	1:H:201:PRO:HD3	1.85	0.43
1:H:235:SER:HB3	1:H:277:ILE:HD11	2.01	0.43
1:A:79:ILE:HA	1:A:79:ILE:HD13	1.83	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.78	0.43
1:H:145:ILE:CG1	1:H:166:ALA:HB3	2.49	0.42
1:E:145:ILE:CG1	1:E:166:ALA:HB3	2.48	0.42
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.84	0.42
1:B:38:TYR:CE1	1:B:105:ARG:HD3	2.53	0.42
1:I:221:SER:HB2	1:J:281:ILE:CD1	2.49	0.42
1:D:304:PHE:CB	1:D:305:PRO:HD3	2.48	0.42
1:B:210:LEU:CB	1:B:211:PRO:HD3	2.40	0.42
1:C:145:ILE:CG1	1:C:166:ALA:HB3	2.49	0.42
1:H:291:VAL:O	1:H:291:VAL:HG12	2.19	0.42
1:E:284:HIS:HD2	1:E:285:HIS:NE2	2.16	0.42
1:I:140:LEU:CD1	5:I:334:HOH:O	2.53	0.42
1:A:95:PHE:HB2	1:A:99:ARG:HB2	2.00	0.42
1:G:297:ILE:C	1:G:299:ARG:H	2.23	0.42
1:E:210:LEU:CB	1:E:211:PRO:CD	2.95	0.42
1:B:119:PHE:HE1	1:B:199:ARG:CZ	2.32	0.42
1:F:212:LEU:HD13	1:F:265:MET:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ILE:HG21	1:G:126:PHE:CD2	2.54	0.42
1:B:39:ILE:HD11	1:B:130:LEU:HD11	2.00	0.42
1:H:297:ILE:O	1:H:299:ARG:N	2.52	0.42
1:G:210:LEU:CB	1:G:211:PRO:CD	2.97	0.42
1:G:284:HIS:HE1	1:G:291:VAL:HG13	1.84	0.42
1:H:212:LEU:HD13	1:H:265:MET:HB3	2.02	0.42
1:E:305:PRO:O	1:E:309:LEU:HG	2.20	0.42
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.54	0.42
1:C:279:LEU:HD22	1:C:304:PHE:HE2	1.83	0.42
1:I:95:PHE:CD2	1:I:99:ARG:HB2	2.55	0.42
1:F:297:ILE:O	1:F:299:ARG:N	2.53	0.42
1:G:119:PHE:CG	1:G:120:PRO:CD	3.02	0.42
1:B:297:ILE:O	1:B:299:ARG:N	2.53	0.42
1:H:15:SER:HB3	1:H:141:ARG:CD	2.50	0.42
1:F:248:TYR:HA	1:G:247:PHE:CE1	2.55	0.42
1:G:95:PHE:HB2	1:G:99:ARG:HB2	2.01	0.42
1:H:55:PRO:HB3	1:H:95:PHE:CD1	2.54	0.42
1:F:147:VAL:O	1:F:147:VAL:HG13	2.18	0.42
1:I:19:PHE:CG	2:I:323:ACH:H61	2.54	0.42
1:J:212:LEU:HA	1:J:212:LEU:HD23	1.88	0.42
1:G:227:SER:HB3	1:G:230:GLU:CG	2.49	0.42
1:I:234:THR:HG21	1:J:236:PHE:CE2	2.55	0.42
1:J:291:VAL:HG12	1:J:291:VAL:O	2.20	0.42
1:F:311:ILE:O	1:F:311:ILE:HG22	2.20	0.42
1:C:58:VAL:CG1	1:C:62:GLN:HB3	2.50	0.42
1:E:140:LEU:CG	5:E:336:HOH:O	2.68	0.42
1:I:297:ILE:C	1:I:299:ARG:H	2.22	0.42
1:C:297:ILE:C	1:C:299:ARG:H	2.23	0.42
1:G:15:SER:HB3	1:G:141:ARG:HG2	2.01	0.42
1:J:19:PHE:CG	2:J:323:ACH:H61	2.55	0.42
1:E:212:LEU:HD13	1:E:265:MET:HB3	2.01	0.42
1:D:220:TRP:C	1:D:222:VAL:H	2.23	0.42
1:A:311:ILE:HG22	1:A:311:ILE:O	2.20	0.42
1:E:95:PHE:CD2	1:E:99:ARG:HB2	2.54	0.42
1:I:137:ASN:CA	4:I:329:GOL:O1	2.64	0.42
1:D:142:PHE:HA	1:D:170:ILE:HD11	2.01	0.42
1:H:38:TYR:CE1	1:H:105:ARG:HD3	2.54	0.42
1:A:291:VAL:O	1:A:291:VAL:HG12	2.19	0.42
1:J:136:ASN:C	4:J:325:GOL:H2	2.37	0.42
1:F:55:PRO:HB3	1:F:95:PHE:CD1	2.54	0.42
1:H:138:GLN:N	4:H:324:GOL:H11	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:PHE:HE1	1:E:199:ARG:CZ	2.33	0.42
1:A:220:TRP:C	1:A:222:VAL:H	2.23	0.42
1:A:279:LEU:HD22	1:A:304:PHE:HE2	1.85	0.42
1:C:235:SER:HB3	1:C:277:ILE:HD11	2.02	0.42
1:G:39:ILE:HD11	1:G:130:LEU:HD11	2.02	0.42
1:A:297:ILE:C	1:A:299:ARG:H	2.23	0.42
1:J:297:ILE:O	1:J:299:ARG:N	2.53	0.42
1:C:257:PRO:HG2	1:C:258:TYR:HD2	1.80	0.42
1:J:182:GLN:HB2	1:J:185:GLN:CG	2.49	0.42
1:F:15:SER:HB3	1:F:141:ARG:HG2	2.01	0.42
2:C:323:ACH:H101	1:D:175:TYR:CZ	2.55	0.42
1:E:212:LEU:O	1:E:216:ILE:HG13	2.19	0.42
1:G:200:ASN:HA	1:G:201:PRO:HD3	1.83	0.42
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.55	0.42
1:G:42:GLN:HG3	1:G:101:ILE:HG12	2.02	0.42
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.80	0.42
4:G:328:GOL:O3	4:G:328:GOL:O1	2.32	0.41
1:E:55:PRO:HB3	1:E:95:PHE:CD1	2.54	0.41
1:G:145:ILE:CD1	1:G:145:ILE:O	2.67	0.41
1:D:43:TRP:CZ2	1:D:100:VAL:HG11	2.55	0.41
1:I:147:VAL:O	1:I:149:THR:N	2.49	0.41
1:H:119:PHE:HE1	1:H:199:ARG:CZ	2.32	0.41
1:J:284:HIS:HD2	1:J:285:HIS:CD2	2.37	0.41
1:F:212:LEU:O	1:F:216:ILE:HG13	2.20	0.41
1:A:235:SER:HB3	1:A:277:ILE:HD11	2.01	0.41
1:C:23:ILE:HG21	1:C:126:PHE:CD2	2.55	0.41
1:C:79:ILE:HA	1:C:79:ILE:HD13	1.84	0.41
1:G:284:HIS:HD2	1:G:285:HIS:NE2	2.17	0.41
1:A:161:TRP:CZ2	1:A:200:ASN:ND2	2.88	0.41
1:D:23:ILE:HG21	1:D:126:PHE:CD2	2.56	0.41
1:J:131:GLU:HG2	1:J:190:ARG:HB2	2.02	0.41
1:A:119:PHE:HE1	1:A:199:ARG:CZ	2.32	0.41
1:C:212:LEU:HG	1:C:245:TYR:CE2	2.56	0.41
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.86	0.41
1:G:220:TRP:C	1:G:222:VAL:H	2.24	0.41
1:B:305:PRO:O	1:B:309:LEU:HG	2.20	0.41
1:D:206:TRP:CD2	3:D:325:MES:O2S	2.74	0.41
1:I:311:ILE:O	1:I:311:ILE:HG22	2.21	0.41
1:F:291:VAL:HG12	1:F:291:VAL:O	2.20	0.41
1:J:145:ILE:CG1	1:J:166:ALA:HB3	2.49	0.41
1:F:161:TRP:CZ2	1:F:200:ASN:ND2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:LEU:HD22	1:F:304:PHE:HE2	1.84	0.41
1:E:235:SER:HB3	1:E:277:ILE:HD11	2.03	0.41
1:G:295:LEU:O	1:G:298:GLN:HG2	2.20	0.41
1:J:166:ALA:CB	1:J:195:ILE:HG12	2.48	0.41
1:C:71:LEU:HD12	1:C:72:TRP:H	1.84	0.41
1:B:311:ILE:HG22	1:B:311:ILE:O	2.21	0.41
1:D:210:LEU:CB	1:D:211:PRO:CD	2.98	0.41
1:G:163:ARG:HB2	1:G:196:ASP:HB2	2.02	0.41
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.97	0.41
1:C:220:TRP:C	1:C:222:VAL:H	2.24	0.41
1:F:221:SER:HB2	1:G:281:ILE:CD1	2.50	0.41
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.56	0.41
1:J:58:VAL:CG1	1:J:62:GLN:HB3	2.50	0.41
1:I:261:VAL:HG12	1:I:262:ILE:N	2.35	0.41
1:C:291:VAL:O	1:C:291:VAL:HG12	2.20	0.41
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.83	0.41
1:J:210:LEU:CB	1:J:211:PRO:CD	2.98	0.41
1:C:256:LEU:HB3	1:C:257:PRO:HD2	2.02	0.41
1:I:212:LEU:HD13	1:I:265:MET:HB3	2.02	0.41
1:A:212:LEU:HG	1:A:245:TYR:CE2	2.55	0.41
1:J:155:GLU:HB3	1:J:161:TRP:NE1	2.36	0.41
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.83	0.41
1:A:305:PRO:O	1:A:309:LEU:HG	2.21	0.41
1:G:205:LEU:HD23	1:G:209:ILE:HD12	2.02	0.41
1:E:131:GLU:HG2	1:E:190:ARG:HB2	2.02	0.41
1:D:235:SER:HB3	1:D:277:ILE:HD11	2.02	0.41
1:A:58:VAL:CG1	1:A:62:GLN:HB3	2.50	0.41
1:D:311:ILE:HG22	1:D:311:ILE:O	2.20	0.41
1:H:99:ARG:CG	1:H:99:ARG:NH1	2.82	0.41
1:A:210:LEU:CB	1:A:211:PRO:CD	2.98	0.41
1:F:119:PHE:HE1	1:F:199:ARG:CZ	2.34	0.41
1:G:291:VAL:HG12	1:G:291:VAL:O	2.21	0.41
1:C:284:HIS:HD2	1:C:285:HIS:CD2	2.39	0.41
1:F:305:PRO:O	1:F:309:LEU:HG	2.21	0.41
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.80	0.41
1:B:215:ILE:HA	1:C:239:MET:HE2	2.03	0.41
1:D:145:ILE:O	1:D:145:ILE:CD1	2.68	0.40
1:J:212:LEU:HG	1:J:245:TYR:CE2	2.57	0.40
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.98	0.40
1:C:161:TRP:CZ2	1:C:200:ASN:ND2	2.89	0.40
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:NZ	5:D:331:HOH:O	2.54	0.40
1:A:38:TYR:CE1	1:A:105:ARG:HD3	2.55	0.40
1:C:226:GLU:OE1	1:C:226:GLU:HA	2.21	0.40
1:C:91:ARG:HD3	1:C:103:ASN:HB3	2.02	0.40
1:E:295:LEU:HA	1:E:298:GLN:NE2	2.23	0.40
1:D:119:PHE:HE1	1:D:199:ARG:CZ	2.34	0.40
1:A:225:LEU:HD21	1:B:232:LEU:HD23	2.03	0.40
1:G:15:SER:HB3	1:G:141:ARG:CD	2.52	0.40
1:F:205:LEU:HA	1:F:205:LEU:HD23	1.65	0.40
1:H:279:LEU:HD22	1:H:304:PHE:HE2	1.85	0.40
1:D:58:VAL:CG1	1:D:62:GLN:HB3	2.51	0.40
1:D:291:VAL:O	1:D:291:VAL:HG12	2.21	0.40
1:D:198:VAL:HG12	1:D:199:ARG:N	2.36	0.40
1:I:221:SER:HB2	1:J:281:ILE:HD11	2.03	0.40
1:A:91:ARG:HD3	1:A:103:ASN:HB3	2.02	0.40
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.71	0.40
1:G:137:ASN:HA	4:G:328:GOL:C2	2.52	0.40
1:A:175:TYR:HH	2:E:323:ACH:H101	1.84	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%)	270 (88%)	25 (8%)	10 (3%)	5	19
1	B	305/322 (95%)	271 (89%)	24 (8%)	10 (3%)	5	19
1	C	305/322 (95%)	267 (88%)	29 (10%)	9 (3%)	5	21
1	D	305/322 (95%)	269 (88%)	24 (8%)	12 (4%)	4	14
1	E	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	4	17
1	F	305/322 (95%)	268 (88%)	28 (9%)	9 (3%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	4	17
1	H	305/322 (95%)	268 (88%)	27 (9%)	10 (3%)	5	19
1	I	305/322 (95%)	271 (89%)	22 (7%)	12 (4%)	4	14
1	J	305/322 (95%)	267 (88%)	26 (8%)	12 (4%)	4	14
All	All	3050/3220 (95%)	2681 (88%)	263 (9%)	106 (4%)	4	18

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	120	PRO
1	A	149	THR
1	A	165	LYS
1	B	119	PHE
1	B	120	PRO
1	C	119	PHE
1	C	120	PRO
1	C	149	THR
1	D	119	PHE
1	D	120	PRO
1	D	149	THR
1	E	119	PHE
1	E	120	PRO
1	E	149	THR
1	F	119	PHE
1	F	120	PRO
1	F	149	THR
1	G	119	PHE
1	G	120	PRO
1	H	119	PHE
1	H	120	PRO
1	H	149	THR
1	H	165	LYS
1	I	119	PHE
1	I	120	PRO
1	I	149	THR
1	J	119	PHE
1	J	120	PRO
1	J	149	THR
1	A	289	ASN
1	B	149	THR

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Mol	Chain	Res	Type
1	B	289	ASN
1	C	289	ASN
1	D	289	ASN
1	E	289	ASN
1	F	289	ASN
1	G	149	THR
1	G	164	GLY
1	G	289	ASN
1	H	289	ASN
1	I	164	GLY
1	I	289	ASN
1	J	169	HIS
1	J	289	ASN
1	A	290	GLY
1	B	290	GLY
1	C	290	GLY
1	D	290	GLY
1	E	290	GLY
1	F	290	GLY
1	G	290	GLY
1	H	153	ASP
1	H	290	GLY
1	I	290	GLY
1	J	290	GLY
1	A	153	ASP
1	A	298	GLN
1	B	153	ASP
1	C	153	ASP
1	D	153	ASP
1	D	298	GLN
1	E	153	ASP
1	E	298	GLN
1	F	153	ASP
1	G	153	ASP
1	H	298	GLN
1	I	153	ASP
1	I	294	ASP
1	J	153	ASP
1	A	287	GLN
1	A	294	ASP
1	B	294	ASP
1	C	298	GLN

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Mol	Chain	Res	Type
1	D	287	GLN
1	D	294	ASP
1	E	151	ASN
1	F	287	GLN
1	F	298	GLN
1	G	221	SER
1	G	294	ASP
1	G	298	GLN
1	H	287	GLN
1	I	287	GLN
1	J	298	GLN
1	B	151	ASN
1	B	287	GLN
1	C	151	ASN
1	C	287	GLN
1	E	200	ASN
1	E	287	GLN
1	F	294	ASP
1	G	287	GLN
1	H	294	ASP
1	I	298	GLN
1	J	151	ASN
1	J	200	ASN
1	J	287	GLN
1	J	294	ASP
1	D	164	GLY
1	D	200	ASN
1	I	147	VAL
1	D	147	VAL
1	I	200	ASN
1	B	147	VAL
1	E	147	VAL

### 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%)	255 (93%)	20 (7%)	17	45
1	B	275/284 (97%)	253 (92%)	22 (8%)	15	39
1	C	275/284 (97%)	254 (92%)	21 (8%)	16	42
1	D	275/284 (97%)	251 (91%)	24 (9%)	13	35
1	E	275/284 (97%)	253 (92%)	22 (8%)	15	39
1	F	275/284 (97%)	255 (93%)	20 (7%)	17	45
1	G	275/284 (97%)	254 (92%)	21 (8%)	16	42
1	H	275/284 (97%)	256 (93%)	19 (7%)	19	48
1	I	275/284 (97%)	252 (92%)	23 (8%)	14	37
1	J	275/284 (97%)	253 (92%)	22 (8%)	15	39
All	All	2750/2840 (97%)	2536 (92%)	214 (8%)	16	41

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	62	GLN
1	A	65	ARG
1	A	87	THR
1	A	91	ARG
1	A	99	ARG
1	A	123	ARG
1	A	130	LEU
1	A	145	ILE
1	A	150	GLU
1	A	212	LEU
1	A	219	SER
1	A	235	SER
1	A	247	PHE
1	A	249	THR
1	A	253	LEU
1	A	261	VAL
1	A	287	GLN
1	A	302	LEU
1	A	317	ILE
1	B	16	VAL
1	B	17	SER
1	B	62	GLN
1	B	65	ARG

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Mol	Chain	Res	Type
1	B	87	THR
1	B	91	ARG
1	B	99	ARG
1	B	123	ARG
1	B	130	LEU
1	B	145	ILE
1	B	150	GLU
1	B	212	LEU
1	B	219	SER
1	B	228	PHE
1	B	235	SER
1	B	247	PHE
1	B	249	THR
1	B	253	LEU
1	B	261	VAL
1	B	287	GLN
1	B	302	LEU
1	B	317	ILE
1	C	62	GLN
1	C	65	ARG
1	C	81	VAL
1	C	87	THR
1	C	91	ARG
1	C	99	ARG
1	C	123	ARG
1	C	127	VAL
1	C	130	LEU
1	C	145	ILE
1	C	150	GLU
1	C	212	LEU
1	C	219	SER
1	C	235	SER
1	C	247	PHE
1	C	249	THR
1	C	253	LEU
1	C	261	VAL
1	C	287	GLN
1	C	302	LEU
1	C	317	ILE
1	D	16	VAL
1	D	62	GLN
1	D	65	ARG

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Mol	Chain	Res	Type
1	D	81	VAL
1	D	87	THR
1	D	91	ARG
1	D	99	ARG
1	D	123	ARG
1	D	130	LEU
1	D	145	ILE
1	D	150	GLU
1	D	163	ARG
1	D	169	HIS
1	D	212	LEU
1	D	214	LEU
1	D	219	SER
1	D	235	SER
1	D	247	PHE
1	D	249	THR
1	D	253	LEU
1	D	261	VAL
1	D	287	GLN
1	D	302	LEU
1	D	317	ILE
1	E	16	VAL
1	E	29	LEU
1	E	62	GLN
1	E	65	ARG
1	E	81	VAL
1	E	87	THR
1	E	91	ARG
1	E	99	ARG
1	E	123	ARG
1	E	130	LEU
1	E	145	ILE
1	E	150	GLU
1	E	212	LEU
1	E	219	SER
1	E	235	SER
1	E	247	PHE
1	E	249	THR
1	E	253	LEU
1	E	261	VAL
1	E	287	GLN
1	E	302	LEU

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Mol	Chain	Res	Type
1	E	317	ILE
1	F	16	VAL
1	F	17	SER
1	F	65	ARG
1	F	87	THR
1	F	91	ARG
1	F	99	ARG
1	F	123	ARG
1	F	130	LEU
1	F	145	ILE
1	F	150	GLU
1	F	212	LEU
1	F	219	SER
1	F	235	SER
1	F	247	PHE
1	F	249	THR
1	F	253	LEU
1	F	261	VAL
1	F	287	GLN
1	F	302	LEU
1	F	317	ILE
1	G	62	GLN
1	G	65	ARG
1	G	81	VAL
1	G	87	THR
1	G	91	ARG
1	G	92	LEU
1	G	99	ARG
1	G	123	ARG
1	G	130	LEU
1	G	145	ILE
1	G	150	GLU
1	G	212	LEU
1	G	214	LEU
1	G	219	SER
1	G	235	SER
1	G	247	PHE
1	G	249	THR
1	G	253	LEU
1	G	261	VAL
1	G	287	GLN
1	G	317	ILE

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Mol	Chain	Res	Type
1	H	16	VAL
1	H	62	GLN
1	H	65	ARG
1	H	87	THR
1	H	91	ARG
1	H	99	ARG
1	H	123	ARG
1	H	145	ILE
1	H	150	GLU
1	H	212	LEU
1	H	219	SER
1	H	235	SER
1	H	247	PHE
1	H	249	THR
1	H	253	LEU
1	H	261	VAL
1	H	287	GLN
1	H	302	LEU
1	H	317	ILE
1	I	16	VAL
1	I	17	SER
1	I	62	GLN
1	I	65	ARG
1	I	87	THR
1	I	91	ARG
1	I	99	ARG
1	I	123	ARG
1	I	127	VAL
1	I	130	LEU
1	I	145	ILE
1	I	150	GLU
1	I	169	HIS
1	I	212	LEU
1	I	219	SER
1	I	235	SER
1	I	247	PHE
1	I	249	THR
1	I	253	LEU
1	I	261	VAL
1	I	287	GLN
1	I	302	LEU
1	I	317	ILE

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Mol	Chain	Res	Type
1	J	16	VAL
1	J	29	LEU
1	J	62	GLN
1	J	65	ARG
1	J	87	THR
1	J	91	ARG
1	J	99	ARG
1	J	123	ARG
1	J	127	VAL
1	J	130	LEU
1	J	145	ILE
1	J	150	GLU
1	J	212	LEU
1	J	219	SER
1	J	235	SER
1	J	247	PHE
1	J	249	THR
1	J	253	LEU
1	J	261	VAL
1	J	287	GLN
1	J	302	LEU
1	J	317	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	200	ASN
1	A	298	GLN
1	B	69	ASN
1	B	151	ASN
1	B	200	ASN
1	B	284	HIS
1	B	285	HIS
1	B	298	GLN
1	C	69	ASN
1	C	151	ASN
1	C	200	ASN
1	C	285	HIS
1	C	298	GLN
1	D	69	ASN
1	D	103	ASN

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Mol	Chain	Res	Type
1	D	200	ASN
1	D	284	HIS
1	D	285	HIS
1	D	298	GLN
1	E	69	ASN
1	E	151	ASN
1	E	200	ASN
1	E	284	HIS
1	E	285	HIS
1	E	298	GLN
1	F	69	ASN
1	F	200	ASN
1	F	284	HIS
1	F	298	GLN
1	G	69	ASN
1	G	200	ASN
1	G	285	HIS
1	G	298	GLN
1	H	69	ASN
1	H	200	ASN
1	H	285	HIS
1	H	298	GLN
1	I	69	ASN
1	I	200	ASN
1	I	284	HIS
1	I	285	HIS
1	I	298	GLN
1	J	69	ASN
1	J	200	ASN
1	J	285	HIS
1	J	298	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

46 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	ACH	A	323	-	9,9,9	1.04	1 (11%)	12,12,12	0.67	0
3	MES	A	324	-	11,12,12	0.77	0	14,16,16	2.46	6 (42%)
4	GOL	A	325	-	5,5,5	0.74	0	5,5,5	0.59	0
4	GOL	A	326	-	5,5,5	0.80	0	5,5,5	0.35	0
2	ACH	B	323	-	9,9,9	0.97	1 (11%)	12,12,12	0.73	0
3	MES	B	324	-	11,12,12	0.66	0	14,16,16	2.70	7 (50%)
4	GOL	B	325	-	5,5,5	0.71	0	5,5,5	0.65	0
4	GOL	B	326	-	5,5,5	0.78	0	5,5,5	0.61	0
4	GOL	B	327	-	5,5,5	0.84	0	5,5,5	0.74	0
2	ACH	C	323	-	9,9,9	1.01	1 (11%)	12,12,12	0.77	0
4	GOL	C	324	-	5,5,5	0.62	0	5,5,5	0.56	0
4	GOL	C	325	-	5,5,5	0.77	0	5,5,5	0.73	0
2	ACH	D	323	-	9,9,9	1.10	1 (11%)	12,12,12	0.84	0
3	MES	D	324	-	11,12,12	0.68	0	14,16,16	2.47	5 (35%)
3	MES	D	325	-	11,12,12	0.72	0	14,16,16	2.16	5 (35%)
4	GOL	D	326	-	5,5,5	0.78	0	5,5,5	0.55	0
4	GOL	D	327	-	5,5,5	0.73	0	5,5,5	0.53	0
2	ACH	E	323	-	9,9,9	1.03	1 (11%)	12,12,12	0.70	0
3	MES	E	324	-	11,12,12	0.66	0	14,16,16	2.51	7 (50%)
4	GOL	E	325	-	5,5,5	0.81	0	5,5,5	0.33	0
4	GOL	E	326	-	5,5,5	0.88	0	5,5,5	0.52	0
2	ACH	F	323	-	9,9,9	1.01	1 (11%)	12,12,12	0.85	0
3	MES	F	324	-	11,12,12	0.73	0	14,16,16	2.71	7 (50%)
4	GOL	F	325	-	5,5,5	0.72	0	5,5,5	0.45	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	F	326	-	5,5,5	0.68	0	5,5,5	0.56	0
4	GOL	F	327	-	5,5,5	0.87	0	5,5,5	0.31	0
4	GOL	F	328	-	5,5,5	0.80	0	5,5,5	0.61	0
2	ACH	G	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.62	0
3	MES	G	324	-	11,12,12	0.70	0	14,16,16	2.90	8 (57%)
4	GOL	G	325	-	5,5,5	0.73	0	5,5,5	0.54	0
4	GOL	G	326	-	5,5,5	0.67	0	5,5,5	0.44	0
4	GOL	G	327	-	3,3,5	0.47	0	2,2,5	0.40	0
4	GOL	G	328	-	5,5,5	0.63	0	5,5,5	1.00	0
2	ACH	H	323	-	9,9,9	0.96	1 (11%)	12,12,12	0.88	1 (8%)
4	GOL	H	324	-	5,5,5	0.49	0	5,5,5	0.79	0
4	GOL	H	325	-	5,5,5	0.96	0	5,5,5	0.45	0
2	ACH	I	323	-	9,9,9	0.97	1 (11%)	12,12,12	0.74	0
3	MES	I	324	-	11,12,12	0.69	0	14,16,16	2.53	7 (50%)
4	GOL	I	325	-	5,5,5	0.80	0	5,5,5	0.42	0
4	GOL	I	326	-	5,5,5	0.74	0	5,5,5	0.85	0
4	GOL	I	327	-	5,5,5	0.78	0	5,5,5	0.40	0
4	GOL	I	328	-	5,5,5	0.72	0	5,5,5	0.48	0
4	GOL	I	329	-	5,5,5	0.86	0	5,5,5	0.62	0
2	ACH	J	323	-	9,9,9	1.00	1 (11%)	12,12,12	0.77	0
3	MES	J	324	-	11,12,12	0.65	0	14,16,16	2.50	6 (42%)
4	GOL	J	325	-	5,5,5	0.74	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	ACH	A	323	-	-	0/7/7/7	0/0/0/0
3	MES	A	324	-	-	0/6/14/14	0/1/1/1
4	GOL	A	325	-	-	0/4/4/4	0/0/0/0
4	GOL	A	326	-	-	0/4/4/4	0/0/0/0
2	ACH	B	323	-	-	0/7/7/7	0/0/0/0
3	MES	B	324	-	-	0/6/14/14	0/1/1/1
4	GOL	B	325	-	-	0/4/4/4	0/0/0/0
4	GOL	B	326	-	-	0/4/4/4	0/0/0/0
4	GOL	B	327	-	-	0/4/4/4	0/0/0/0
2	ACH	C	323	-	-	0/7/7/7	0/0/0/0
4	GOL	C	324	-	-	0/4/4/4	0/0/0/0
4	GOL	C	325	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACH	D	323	-	-	0/7/7/7	0/0/0/0
3	MES	D	324	-	-	0/6/14/14	0/1/1/1
3	MES	D	325	-	-	0/6/14/14	0/1/1/1
4	GOL	D	326	-	-	0/4/4/4	0/0/0/0
4	GOL	D	327	-	-	0/4/4/4	0/0/0/0
2	ACH	E	323	-	-	0/7/7/7	0/0/0/0
3	MES	E	324	-	-	0/6/14/14	0/1/1/1
4	GOL	E	325	-	-	0/4/4/4	0/0/0/0
4	GOL	E	326	-	-	0/4/4/4	0/0/0/0
2	ACH	F	323	-	-	0/7/7/7	0/0/0/0
3	MES	F	324	-	-	0/6/14/14	0/1/1/1
4	GOL	F	325	-	-	0/4/4/4	0/0/0/0
4	GOL	F	326	-	-	0/4/4/4	0/0/0/0
4	GOL	F	327	-	-	0/4/4/4	0/0/0/0
4	GOL	F	328	-	-	0/4/4/4	0/0/0/0
2	ACH	G	323	-	-	0/7/7/7	0/0/0/0
3	MES	G	324	-	-	0/6/14/14	0/1/1/1
4	GOL	G	325	-	-	0/4/4/4	0/0/0/0
4	GOL	G	326	-	-	0/4/4/4	0/0/0/0
4	GOL	G	327	-	-	0/1/1/4	0/0/0/0
4	GOL	G	328	-	-	0/4/4/4	0/0/0/0
2	ACH	H	323	-	-	0/7/7/7	0/0/0/0
4	GOL	H	324	-	-	0/4/4/4	0/0/0/0
4	GOL	H	325	-	-	0/4/4/4	0/0/0/0
2	ACH	I	323	-	-	0/7/7/7	0/0/0/0
3	MES	I	324	-	-	0/6/14/14	0/1/1/1
4	GOL	I	325	-	-	0/4/4/4	0/0/0/0
4	GOL	I	326	-	-	0/4/4/4	0/0/0/0
4	GOL	I	327	-	-	0/4/4/4	0/0/0/0
4	GOL	I	328	-	-	0/4/4/4	0/0/0/0
4	GOL	I	329	-	-	0/4/4/4	0/0/0/0
2	ACH	J	323	-	-	0/7/7/7	0/0/0/0
3	MES	J	324	-	-	0/6/14/14	0/1/1/1
4	GOL	J	325	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	323	ACH	O4-C5	2.13	1.44	1.33
2	C	323	ACH	O4-C5	2.17	1.44	1.33
2	H	323	ACH	O4-C5	2.25	1.45	1.33
2	I	323	ACH	O4-C5	2.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	323	ACH	O4-C5	2.28	1.45	1.33
2	A	323	ACH	O4-C5	2.28	1.45	1.33
2	B	323	ACH	O4-C5	2.29	1.45	1.33
2	G	323	ACH	O4-C5	2.29	1.45	1.33
2	D	323	ACH	O4-C5	2.30	1.45	1.33
2	E	323	ACH	O4-C5	2.43	1.46	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	324	MES	C6-C5-N4	-3.74	104.46	110.12
3	E	324	MES	C6-C5-N4	-3.61	104.65	110.12
3	J	324	MES	C6-C5-N4	-3.60	104.68	110.12
3	J	324	MES	C2-C3-N4	-3.57	104.71	110.12
3	F	324	MES	C6-C5-N4	-3.31	105.11	110.12
3	B	324	MES	C6-C5-N4	-3.05	105.50	110.12
3	D	325	MES	C7-C8-S	-2.98	103.30	112.51
3	I	324	MES	C6-C5-N4	-2.96	105.64	110.12
3	G	324	MES	C6-C5-N4	-2.85	105.80	110.12
3	D	325	MES	C6-C5-N4	-2.81	105.87	110.12
3	A	324	MES	C2-C3-N4	-2.71	106.02	110.12
3	E	324	MES	C2-C3-N4	-2.63	106.14	110.12
3	B	324	MES	C2-C3-N4	-2.48	106.37	110.12
3	D	324	MES	C2-C3-N4	-2.27	106.69	110.12
3	I	324	MES	C2-C3-N4	-2.20	106.79	110.12
3	G	324	MES	C2-C3-N4	-2.19	106.80	110.12
3	F	324	MES	C2-C3-N4	-2.04	107.03	110.12
2	H	323	ACH	O4-C5-C6	2.01	121.51	112.42
3	G	324	MES	O2S-S-C8	2.19	108.77	106.91
3	G	324	MES	C6-O1-C2	2.29	117.61	109.89
3	E	324	MES	O1S-S-C8	2.40	108.95	106.91
3	B	324	MES	O2S-S-C8	2.60	109.12	106.91
3	D	325	MES	C7-N4-C5	2.80	118.44	111.27
3	D	324	MES	C7-N4-C3	2.94	118.81	111.27
3	J	324	MES	O1S-S-C8	2.97	109.44	106.91
3	D	324	MES	C7-N4-C5	2.97	118.89	111.27
3	J	324	MES	C7-N4-C3	3.04	119.06	111.27
3	F	324	MES	O2S-S-C8	3.06	109.51	106.91
3	G	324	MES	C7-N4-C3	3.09	119.19	111.27
3	A	324	MES	O2S-S-C8	3.10	109.55	106.91
3	F	324	MES	C7-N4-C3	3.14	119.31	111.27
3	J	324	MES	C7-N4-C5	3.16	119.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	324	MES	C7-N4-C3	3.16	119.38	111.27
3	E	324	MES	C7-N4-C5	3.19	119.43	111.27
3	G	324	MES	C7-N4-C5	3.19	119.45	111.27
3	A	324	MES	C7-N4-C3	3.21	119.50	111.27
3	I	324	MES	O1S-S-C8	3.24	109.67	106.91
3	D	325	MES	C7-N4-C3	3.26	119.64	111.27
3	I	324	MES	C7-N4-C3	3.27	119.65	111.27
3	G	324	MES	C5-N4-C3	3.29	116.03	108.90
3	B	324	MES	C7-N4-C5	3.36	119.88	111.27
3	I	324	MES	O2S-S-C8	3.48	109.87	106.91
3	B	324	MES	C7-N4-C3	3.51	120.27	111.27
3	E	324	MES	O2S-S-C8	3.53	109.92	106.91
3	F	324	MES	C7-N4-C5	3.60	120.50	111.27
3	A	324	MES	C7-N4-C5	3.73	120.83	111.27
3	D	325	MES	C5-N4-C3	3.73	116.98	108.90
3	I	324	MES	C7-N4-C5	3.82	121.07	111.27
3	D	324	MES	C5-N4-C3	4.53	118.72	108.90
3	F	324	MES	O1S-S-C8	4.73	110.94	106.91
3	I	324	MES	C5-N4-C3	4.75	119.19	108.90
3	J	324	MES	C5-N4-C3	4.75	119.19	108.90
3	D	324	MES	O1S-S-C8	4.75	110.96	106.91
3	B	324	MES	C5-N4-C3	4.87	119.45	108.90
3	E	324	MES	C5-N4-C3	4.94	119.59	108.90
3	A	324	MES	C5-N4-C3	4.95	119.62	108.90
3	B	324	MES	O1S-S-C8	5.03	111.20	106.91
3	F	324	MES	C5-N4-C3	5.18	120.11	108.90
3	G	324	MES	O1S-S-C8	7.21	113.06	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	323	ACH	2	0
3	A	324	MES	1	0
4	A	325	GOL	2	0
4	A	326	GOL	4	0
2	B	323	ACH	2	0
4	B	326	GOL	5	0
4	B	327	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	323	ACH	3	0
4	C	325	GOL	4	0
2	D	323	ACH	2	0
3	D	325	MES	1	0
4	D	327	GOL	1	0
2	E	323	ACH	4	0
4	E	326	GOL	2	0
2	F	323	ACH	2	0
3	F	324	MES	2	0
4	F	325	GOL	1	0
4	F	328	GOL	4	0
2	G	323	ACH	1	0
4	G	328	GOL	9	0
2	H	323	ACH	1	0
4	H	324	GOL	3	0
4	H	325	GOL	6	0
2	I	323	ACH	3	0
4	I	327	GOL	4	0
4	I	329	GOL	6	0
2	J	323	ACH	3	0
4	J	325	GOL	7	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%)	0.19	30 (9%)	10 6	57, 90, 172, 210	0
1	B	307/322 (95%)	0.03	21 (6%)	20 15	52, 87, 172, 213	0
1	C	307/322 (95%)	0.07	16 (5%)	31 25	51, 87, 173, 210	0
1	D	307/322 (95%)	0.02	23 (7%)	17 12	51, 84, 170, 210	0
1	E	307/322 (95%)	0.05	19 (6%)	24 18	54, 88, 170, 208	0
1	F	307/322 (95%)	0.09	25 (8%)	15 10	53, 94, 173, 208	0
1	G	307/322 (95%)	0.11	26 (8%)	13 9	51, 87, 168, 209	0
1	H	307/322 (95%)	0.27	28 (9%)	11 7	55, 89, 174, 208	0
1	I	307/322 (95%)	0.08	30 (9%)	10 6	57, 90, 172, 211	0
1	J	307/322 (95%)	0.06	26 (8%)	13 9	59, 94, 175, 208	0
All	All	3070/3220 (95%)	0.10	244 (7%)	15 10	51, 89, 174, 213	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	23.8
1	A	152	ILE	18.6
1	G	152	ILE	17.3
1	E	291	VAL	13.1
1	H	152	ILE	12.7
1	B	151	ASN	11.8
1	A	151	ASN	11.7
1	H	290	GLY	11.4
1	H	288	ALA	11.3
1	H	289	ASN	11.1
1	J	291	VAL	10.9
1	D	152	ILE	10.6
1	I	152	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
1	G	315	LEU	10.3
1	H	291	VAL	10.1
1	C	152	ILE	9.8
1	J	152	ILE	9.8
1	G	314	VAL	9.2
1	G	151	ASN	9.2
1	I	291	VAL	8.9
1	F	152	ILE	8.4
1	G	290	GLY	8.3
1	F	291	VAL	7.9
1	J	153	ASP	7.8
1	E	290	GLY	7.7
1	B	291	VAL	7.6
1	G	291	VAL	7.4
1	B	313	CYS	7.3
1	H	151	ASN	7.2
1	F	317	ILE	6.9
1	G	317	ILE	6.8
1	J	151	ASN	6.8
1	F	151	ASN	6.7
1	F	316	VAL	6.6
1	A	291	VAL	6.5
1	A	317	ILE	6.4
1	I	290	GLY	6.3
1	C	291	VAL	6.2
1	F	290	GLY	6.1
1	D	290	GLY	6.1
1	E	152	ILE	6.0
1	H	292	GLU	6.0
1	D	291	VAL	5.9
1	H	315	LEU	5.9
1	A	290	GLY	5.7
1	D	151	ASN	5.7
1	H	314	VAL	5.7
1	A	53	ASP	5.6
1	G	316	VAL	5.6
1	C	317	ILE	5.6
1	J	317	ILE	5.5
1	A	316	VAL	5.4
1	C	289	ASN	5.4
1	D	153	ASP	5.3
1	C	151	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	I	153	ASP	5.2
1	B	317	ILE	5.2
1	J	306	LEU	5.1
1	J	290	GLY	5.1
1	B	290	GLY	5.0
1	F	182	GLN	5.0
1	F	289	ASN	5.0
1	G	313	CYS	5.0
1	A	296	LEU	5.0
1	G	296	LEU	5.0
1	A	153	ASP	5.0
1	A	148	TYR	5.0
1	G	286	ARG	4.9
1	I	151	ASN	4.8
1	B	289	ASN	4.8
1	C	316	VAL	4.7
1	B	312	GLY	4.7
1	B	293	ASP	4.5
1	H	317	ILE	4.5
1	I	293	ASP	4.4
1	B	316	VAL	4.3
1	E	289	ASN	4.3
1	G	287	GLN	4.3
1	E	287	GLN	4.2
1	F	286	ARG	4.2
1	I	317	ILE	4.1
1	H	316	VAL	4.1
1	J	289	ASN	4.1
1	J	154	ASN	4.0
1	C	295	LEU	4.0
1	I	287	GLN	3.9
1	F	148	TYR	3.9
1	A	313	CYS	3.9
1	B	296	LEU	3.9
1	I	154	ASN	3.8
1	A	314	VAL	3.8
1	F	181	VAL	3.8
1	F	287	GLN	3.8
1	A	295	LEU	3.8
1	I	148	TYR	3.8
1	F	156	GLU	3.8
1	F	288	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	314	VAL	3.8
1	F	153	ASP	3.7
1	C	288	ALA	3.7
1	E	49	LYS	3.7
1	E	288	ALA	3.7
1	H	182	GLN	3.7
1	F	296	LEU	3.7
1	H	185	GLN	3.7
1	E	156	GLU	3.6
1	I	286	ARG	3.6
1	J	157	ILE	3.6
1	A	49	LYS	3.6
1	I	315	LEU	3.5
1	D	154	ASN	3.5
1	B	288	ALA	3.5
1	J	310	ALA	3.4
1	A	117	ARG	3.4
1	G	289	ASN	3.4
1	H	313	CYS	3.3
1	C	313	CYS	3.3
1	I	316	VAL	3.3
1	H	293	ASP	3.2
1	I	292	GLU	3.2
1	I	314	VAL	3.2
1	H	295	LEU	3.2
1	E	148	TYR	3.1
1	B	315	LEU	3.1
1	B	314	VAL	3.1
1	E	292	GLU	3.1
1	I	183	PRO	3.1
1	A	54	LYS	3.1
1	B	294	ASP	3.1
1	G	311	ILE	3.1
1	C	290	GLY	3.0
1	D	176	ASP	3.0
1	B	295	LEU	3.0
1	D	289	ASN	3.0
1	C	296	LEU	3.0
1	F	295	LEU	3.0
1	A	176	ASP	3.0
1	A	297	ILE	2.9
1	D	317	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	154	ASN	2.9
1	J	309	LEU	2.9
1	B	297	ILE	2.9
1	I	295	LEU	2.9
1	F	292	GLU	2.9
1	G	312	GLY	2.9
1	E	293	ASP	2.9
1	A	315	LEU	2.8
1	E	157	ILE	2.8
1	J	316	VAL	2.8
1	J	292	GLU	2.8
1	G	161	TRP	2.8
1	I	184	ASN	2.8
1	A	298	GLN	2.8
1	E	286	ARG	2.7
1	I	54	LYS	2.7
1	H	148	TYR	2.7
1	G	297	ILE	2.7
1	D	286	ARG	2.7
1	G	153	ASP	2.7
1	D	182	GLN	2.7
1	C	306	LEU	2.7
1	G	295	LEU	2.7
1	D	287	GLN	2.6
1	J	288	ALA	2.6
1	C	148	TYR	2.6
1	J	313	CYS	2.6
1	E	181	VAL	2.6
1	A	141	ARG	2.6
1	F	142	PHE	2.6
1	B	292	GLU	2.6
1	H	156	GLU	2.6
1	H	165	LYS	2.6
1	H	311	ILE	2.6
1	G	310	ALA	2.6
1	D	76	LEU	2.5
1	A	287	GLN	2.5
1	F	46	LYS	2.5
1	G	298	GLN	2.5
1	J	287	GLN	2.5
1	A	52	GLY	2.5
1	I	288	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	52	GLY	2.5
1	D	184	ASN	2.5
1	I	289	ASN	2.5
1	H	287	GLN	2.5
1	J	49	LYS	2.5
1	J	161	TRP	2.5
1	C	315	LEU	2.4
1	E	184	ASN	2.4
1	H	49	LYS	2.4
1	I	294	ASP	2.4
1	J	282	PHE	2.4
1	G	156	GLU	2.4
1	A	286	ARG	2.4
1	G	251	ASN	2.4
1	F	178	LEU	2.3
1	I	157	ILE	2.3
1	B	306	LEU	2.3
1	E	154	ASN	2.3
1	I	182	GLN	2.3
1	G	155	GLU	2.3
1	I	298	GLN	2.3
1	D	185	GLN	2.3
1	A	150	GLU	2.2
1	A	156	GLU	2.2
1	B	153	ASP	2.2
1	J	163	ARG	2.2
1	I	285	HIS	2.2
1	D	292	GLU	2.2
1	H	296	LEU	2.2
1	E	183	PRO	2.2
1	D	148	TYR	2.2
1	E	315	LEU	2.2
1	H	294	ASP	2.2
1	A	177	HIS	2.2
1	F	185	GLN	2.1
1	D	183	PRO	2.1
1	H	174	ARG	2.1
1	J	172	ASP	2.1
1	C	156	GLU	2.1
1	H	46	LYS	2.1
1	J	303	ALA	2.1
1	H	186	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	286	ARG	2.1
1	D	288	ALA	2.1
1	F	53	ASP	2.1
1	D	157	ILE	2.1
1	A	175	TYR	2.1
1	I	297	ILE	2.1
1	C	287	GLN	2.1
1	D	315	LEU	2.1
1	F	176	ASP	2.0
1	G	157	ILE	2.0
1	I	185	GLN	2.0
1	G	292	GLU	2.0
1	B	148	TYR	2.0
1	I	251	ASN	2.0
1	A	294	ASP	2.0
1	E	153	ASP	2.0
1	D	316	VAL	2.0
1	I	313	CYS	2.0
1	A	311	ILE	2.0
1	H	184	ASN	2.0
1	D	226	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
4	GOL	I	328	6/6	0.88	0.77	14.57	87,95,119,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	H	325	6/6	0.83	0.57	11.13	80,85,104,115	0
4	GOL	F	327	6/6	0.84	0.34	10.16	77,98,110,119	0
4	GOL	B	325	6/6	0.83	0.36	8.46	77,88,103,117	0
4	GOL	C	324	6/6	0.81	0.41	5.70	79,89,98,113	0
4	GOL	G	327	4/6	0.90	0.34	5.54	86,96,104,106	0
4	GOL	I	327	6/6	0.78	0.37	3.57	88,92,119,126	0
4	GOL	F	325	6/6	0.81	0.38	2.92	84,100,114,125	0
4	GOL	G	325	6/6	0.85	0.28	2.65	79,94,101,112	0
4	GOL	G	326	6/6	0.87	0.29	2.57	91,96,115,116	0
4	GOL	F	326	6/6	0.86	0.35	2.18	83,98,121,143	0
4	GOL	D	326	6/6	0.91	0.39	1.93	96,100,101,106	0
4	GOL	I	326	6/6	0.91	0.26	1.83	73,91,114,119	0
2	ACH	H	323	10/10	0.97	0.30	1.61	57,74,81,83	0
4	GOL	E	325	6/6	0.73	0.22	1.49	85,99,110,130	0
2	ACH	A	323	10/10	0.97	0.23	0.67	56,66,76,77	0
4	GOL	D	327	6/6	0.91	0.25	0.56	51,79,98,109	0
4	GOL	A	326	6/6	0.85	0.18	0.10	79,90,125,127	0
2	ACH	I	323	10/10	0.97	0.19	0.10	54,67,76,80	0
2	ACH	G	323	10/10	0.97	0.19	0.05	48,68,76,77	0
2	ACH	C	323	10/10	0.95	0.24	0.02	54,69,74,75	0
2	ACH	D	323	10/10	0.98	0.17	-0.13	53,62,70,73	0
2	ACH	B	323	10/10	0.97	0.18	-0.17	53,65,78,80	0
4	GOL	B	326	6/6	0.69	0.21	-0.18	83,110,138,150	0
2	ACH	J	323	10/10	0.93	0.20	-0.25	56,74,82,89	0
2	ACH	F	323	10/10	0.99	0.17	-0.35	48,67,74,76	0
4	GOL	I	329	6/6	0.84	0.19	-0.37	61,71,110,133	0
4	GOL	G	328	6/6	0.86	0.17	-0.56	50,79,101,104	0
4	GOL	E	326	6/6	0.92	0.16	-0.62	67,89,129,133	0
4	GOL	H	324	6/6	0.79	0.20	-0.70	56,69,111,111	0
4	GOL	B	327	6/6	0.88	0.14	-0.77	55,62,83,90	0
4	GOL	C	325	6/6	0.91	0.13	-0.99	60,66,78,92	0
4	GOL	F	328	6/6	0.85	0.13	-1.02	73,86,114,121	0
4	GOL	J	325	6/6	0.82	0.15	-1.05	64,92,106,114	0
2	ACH	E	323	10/10	0.96	0.18	-1.21	57,76,82,85	0
3	MES	B	324	12/12	0.94	0.09	-1.49	120,136,164,175	0
3	MES	I	324	12/12	0.87	0.17	-	109,142,169,177	0
4	GOL	A	325	6/6	0.72	0.49	-	69,109,127,135	0
3	MES	E	324	12/12	0.89	0.09	-	123,143,171,178	0
3	MES	D	324	12/12	0.86	0.17	-	107,132,160,169	0
3	MES	A	324	12/12	0.84	0.14	-	91,140,168,188	0
3	MES	F	324	12/12	0.86	0.19	-	106,147,159,185	0
3	MES	D	325	12/12	0.86	0.15	-	85,140,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	I	325	6/6	0.88	0.10	-	88,93,105,121	0
3	MES	J	324	12/12	0.87	0.13	-	139,157,169,184	0
3	MES	G	324	12/12	0.89	0.14	-	99,122,143,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.