



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:25 am BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

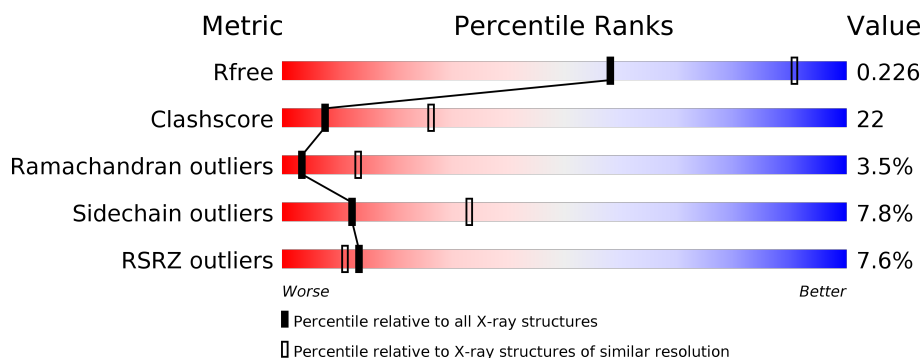
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



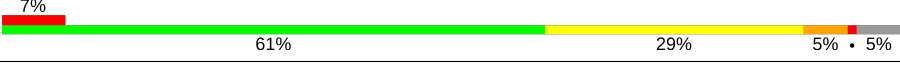
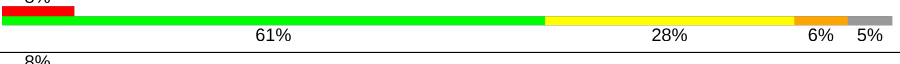


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 ≥ 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>9%</div> <div>62%</div> <div>27%</div> <div>6%</div> <div>5%</div> </div>
1	B	322	<div> <div>6%</div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div>
1	C	322	<div> <div>5%</div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div>
1	D	322	<div> <div>7%</div> <div>62%</div> <div>26%</div> <div>6%</div> <div>5%</div> </div>
1	E	322	<div> <div>6%</div> <div>64%</div> <div>26%</div> <div>5%</div> <div>5%</div> </div>
1	F	322	<div> <div>7%</div> <div>64%</div> <div>27%</div> <div>5%</div> <div>5%</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
4	GOL	A	325	-	-	-	X
4	GOL	A	326	-	-	X	-
4	GOL	B	326	-	-	X	-
4	GOL	B	327	-	-	X	-
4	GOL	C	325	-	-	X	-
4	GOL	F	328	-	-	X	-
4	GOL	G	328	-	-	X	-
4	GOL	H	325	-	-	X	-
4	GOL	I	327	-	-	X	-
4	GOL	I	329	-	-	X	-
4	GOL	J	325	-	-	X	-

2 Entry composition

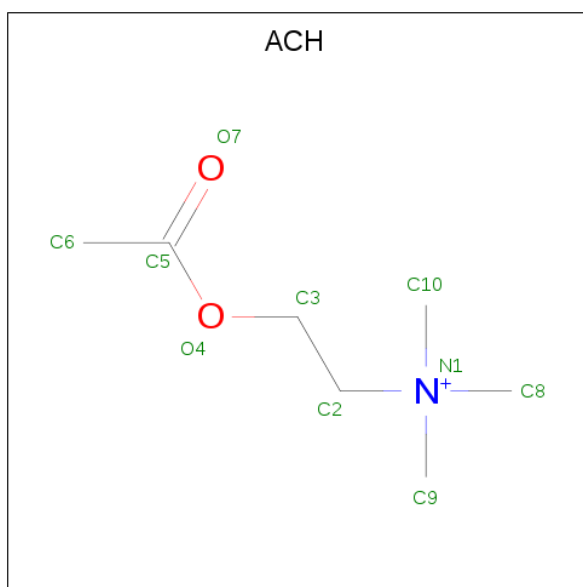
There are 5 unique types of molecules in this entry. The entry contains 25508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₇H₁₆NO₂).



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: C₆H₁₃NO₄S).



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: C₃H₈O₃).



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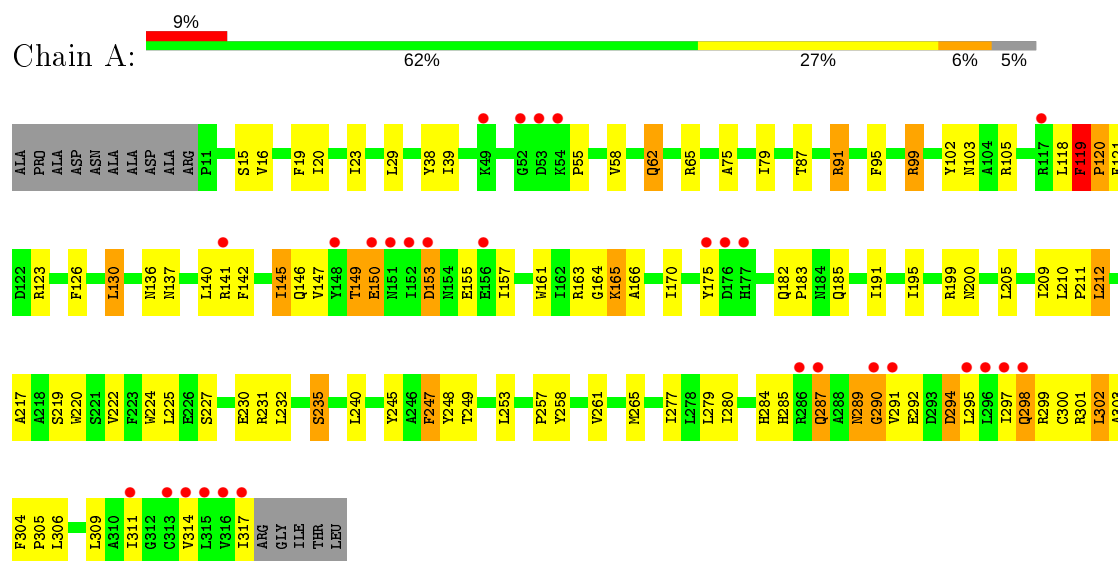
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	12	Total 12	O 12	0	0
5	H	7	Total 7	O 7	0	0
5	I	6	Total 6	O 6	0	0
5	J	7	Total 7	O 7	0	0

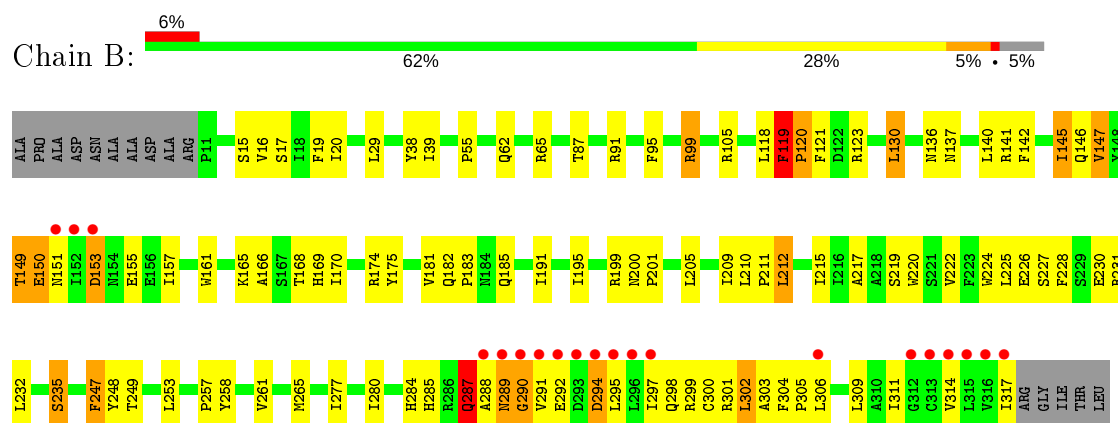
3 Residue-property plots

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.

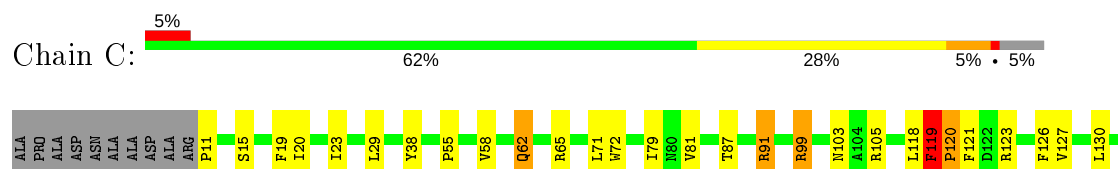
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

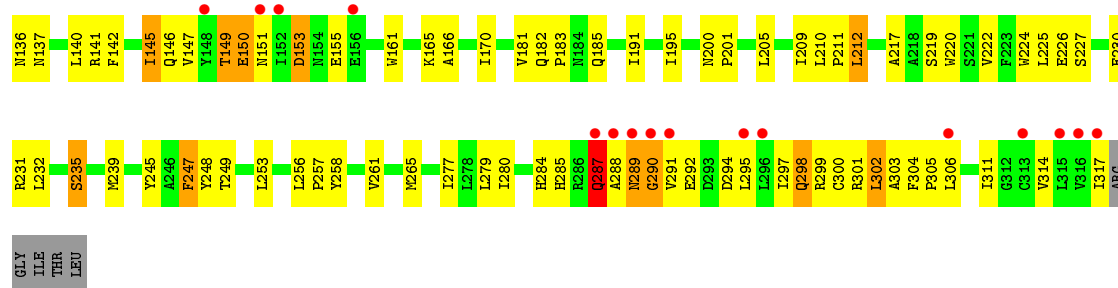


• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

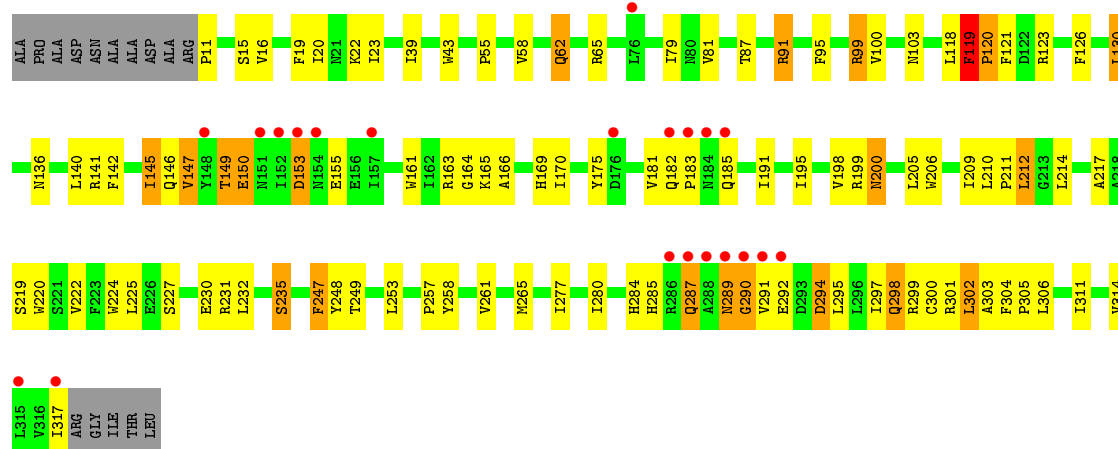


• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

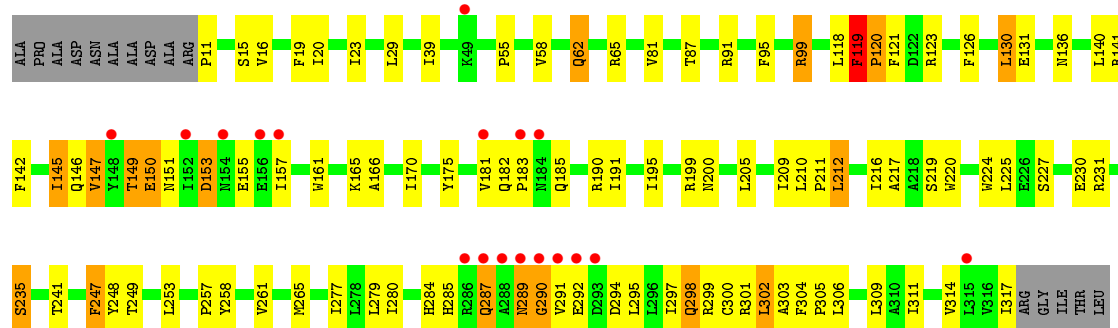




• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

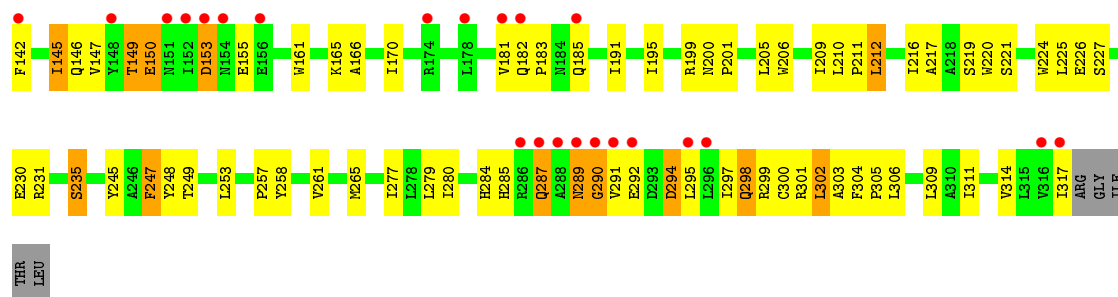


• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

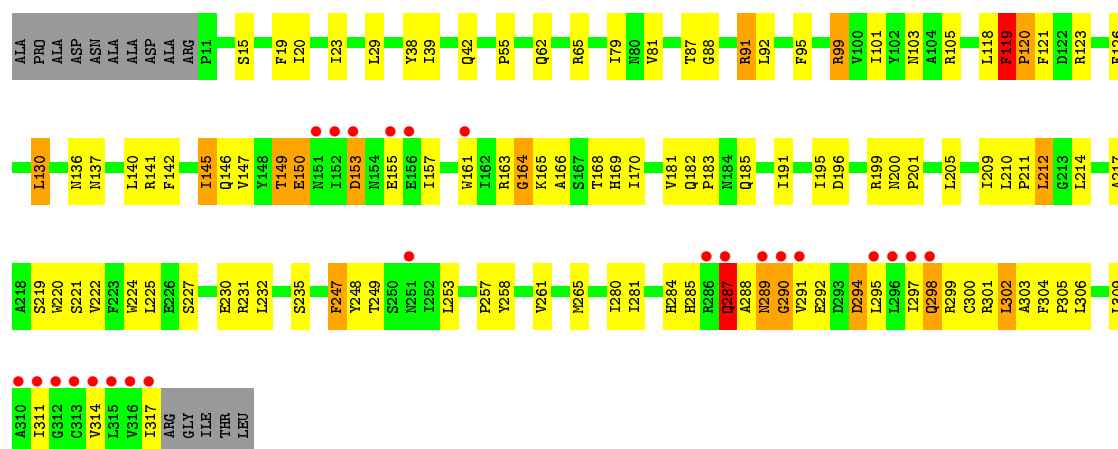


• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

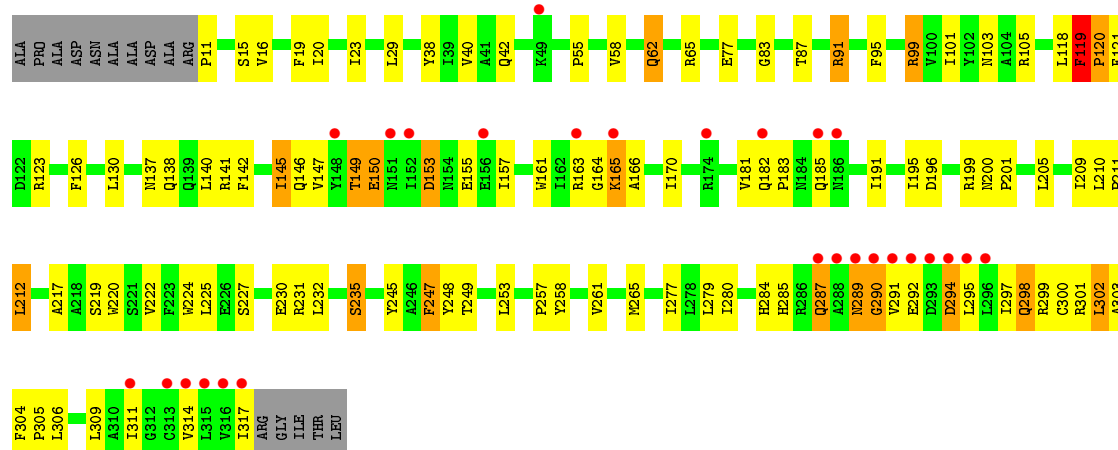




- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

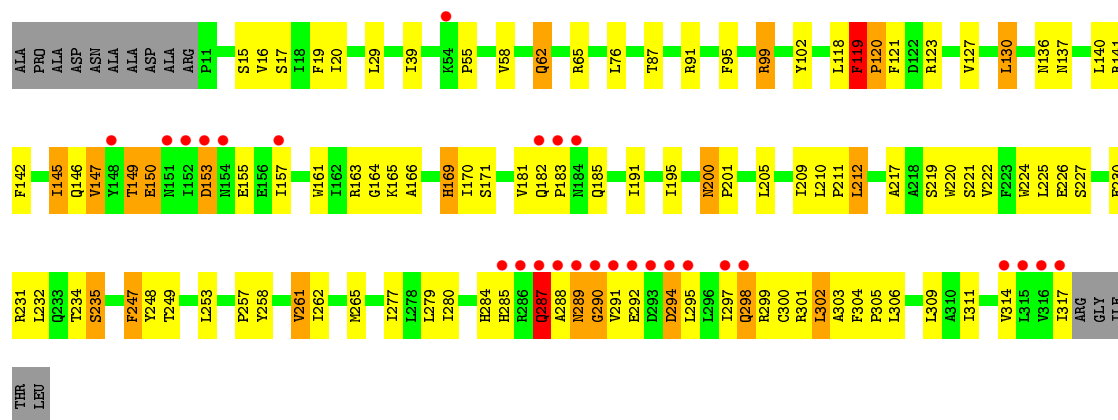


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

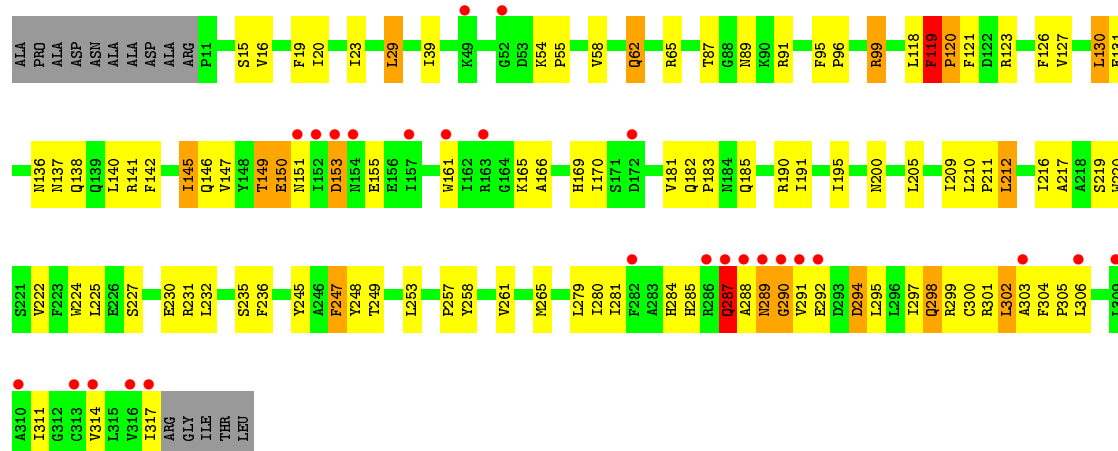


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*





• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.206 , 0.231 0.202 , 0.226	Depositor DCC
R_{free} test set	6262 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25508	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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:A:99:ARG:HG3	1:A:99:ARG:HH11	1.32	0.95
1:J:99:ARG:HG3	1:J:99:ARG:HH11	1.29	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:D:99:ARG:HH11	1:D:99:ARG:HG3	1.33	0.93
1:I:99:ARG:HH11	1:I: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: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:I:137:ASN:HA	4:I:329:GOL:H12	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:A:295:LEU:HA	1:A:298:GLN:HE21	1.44	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: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:147:VAL:HG13	1:E:165:LYS:HE2	1.66	0.78
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.65	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:G:119:PHE:CD2	1:G:120:PRO:HD3	2.21	0.76
1:H:147:VAL:HG13	1:H:165:LYS:HE2	1.67	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:F:119:PHE:CD2	1:F:120:PRO:HD3	2.22	0.74
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.68	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:119:PHE:CD2	1:J:120:PRO:HD3	2.23	0.74
1:J:137:ASN:O	5:J:326:HOH:O	2.05	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:G:145:ILE:CD1	1:G:166:ALA:HB3	2.19	0.73
1:H:137:ASN:HA	4:H:324:GOL:O1	1.89	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:G:105:ARG:HG2	4:H:325:GOL:H11	1.72	0.72
1:I:137:ASN:HA	4:I:329:GOL:O1	1.90	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:A:294:ASP:HB3	1:A:297:ILE:HG22	1.72	0.71
1:C:145:ILE:CD1	1:C:166:ALA:HB3	2.19	0.71
1:C:294:ASP:HB3	1:C:297:ILE:HG22	1.72	0.71
1:G:105:ARG:HG3	4:H:325:GOL:H31	1.72	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:C:231:ARG:HB3	1:C:280:ILE:HD13	1.75	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:E:145:ILE:CD1	1:E:166:ALA:HB3	2.22	0.69
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.74	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:J:145:ILE:HD13	1:J:145:ILE:O	1.94	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:J:294:ASP:HB3	1:J:297:ILE:HG22	1.75	0.68
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.76	0.68
1:H:257:PRO:HG2	1:H:258:TYR:CD2	2.28	0.68
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.75	0.68
1:H:166:ALA:HB2	1:H:195:ILE:HG12	1.74	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:B:119:PHE:CD2	1:B:120:PRO:HD3	2.29	0.67
1:J:138:GLN:HB2	5:J:326:HOH:O	1.94	0.67
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:PRO:HG2	1:I:181:VAL:HG13	1.74	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:G:141:ARG:NH1	5:G:329:HOH:O	2.28	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:D:119:PHE:O	1:D:121:PHE:N	2.24	0.66
1:D:145:ILE:O	1:D:145:ILE:HD13	1.95	0.66
1:G:147:VAL:HG13	1:G:165:LYS:HE2	1.76	0.66
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.10	0.66
1:H:182:GLN:HB3	1:H:183:PRO:HD2	1.76	0.66
1:D:182:GLN:HB3	1:D:183:PRO:HD2	1.77	0.66
1:C:119:PHE:C	1:C:121:PHE:H	1.98	0.66
1:E:147:VAL:CG1	1:E:165:LYS:HE2	2.25	0.66
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.10	0.66
1:I:257:PRO:HG2	1:I:258:TYR:CD2	2.31	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: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:I:231:ARG:HB3	1:I:280:ILE:HD13	1.77	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:C:289:ASN:CG	1:C:290:GLY:H	2.00	0.65
1:G:289:ASN:CG	1:G:290:GLY:H	2.00	0.65
1:I:289:ASN:CG	1:I: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:A:257:PRO:HG2	1:A:258:TYR:CD2	2.30	0.65
1:B:119:PHE:C	1:B:121:PHE:H	2.00	0.65
1:H:137:ASN:HA	4:H:324:GOL:C1	2.27	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:E:289:ASN:CG	1:E:290:GLY:H	2.00	0.65
1:F:289:ASN:CG	1:F:290:GLY:H	1.99	0.65
1:G:147:VAL:CG1	1:G:165:LYS:HE2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:PHE:C	1:J:121:PHE:H	1.99	0.65
1:B:182:GLN:HB3	1:B:183:PRO:HD2	1.77	0.64
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.13	0.64
1:F:206:TRP:CD1	3:F:324:MES:H71	2.33	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:C:145:ILE:O	1:C:145:ILE:HD13	1.98	0.64
1:F:166:ALA:HB2	1:F:195:ILE:HG12	1.79	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:A:182:GLN:HB3	1:A:183:PRO:HD2	1.79	0.64
1:E:145:ILE:HD13	1:E:145:ILE:O	1.97	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:B:224:TRP:NE1	1:B:301:ARG:HB3	2.12	0.63
1:I:147:VAL:CG1	1:I:165:LYS:HE2	2.27	0.63
1:F:257:PRO:HG2	1:F:258:TYR:CD2	2.33	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:B:137:ASN:HA	4:B:327:GOL:H12	1.80	0.63
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.80	0.63
1:J:137:ASN:HA	4:J:325:GOL:C1	2.29	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:B:248:TYR:CD1	1:C:247:PHE:HA	2.35	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:G:248:TYR:CD1	1:H:247:PHE:HA	2.36	0.60
1:I:166:ALA:HB2	1:I:195:ILE:HG12	1.82	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:C:141:ARG:HG3	1:C:142:PHE:CD2	2.35	0.60
1:G:182:GLN:HB3	1:G:183:PRO:HD2	1.81	0.60
1:G:224:TRP:HE1	1:G:301:ARG:HB3	1.66	0.60
1:G:166:ALA:HB2	1:G:195:ILE:HG12	1.83	0.60
1:H:99:ARG:NH1	1:H:99:ARG:HG3	2.13	0.60
1:J:137:ASN:HA	4:J:325:GOL:H2	1.84	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:C:55:PRO:HG2	1:D:181:VAL:HG13	1.83	0.59
1:I:15:SER:HB3	1:I:141:ARG:HD3	1.83	0.59
1:D:99:ARG:NH1	1:D:99:ARG:HG3	2.08	0.59
1:B:302:LEU:O	1:B:306:LEU:HG	2.03	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: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:F:294:ASP:HB3	1:F:297:ILE:CG2	2.31	0.58
1:G:136:ASN:O	4:G:328:GOL:C2	2.47	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:H:20:ILE:HD12	1:H:195:ILE:HD11	1.86	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:F:182:GLN:HB2	1:F:185:GLN:HG2	1.87	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: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:F:227:SER:HB3	1:F:230:GLU:HG3	1.87	0.56
1:J:182:GLN:HB2	1:J:185:GLN:HG2	1.86	0.56
1:A:247:PHE:HA	1:E:248:TYR:CD1	2.41	0.56
1:A:302:LEU:O	1:A:306:LEU:HG	2.05	0.56
1:B:257:PRO:HG2	1:B:258:TYR:HD2	1.71	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:B:145:ILE:HD11	1:B:166:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:HG2	1:B:181:VAL:HG13	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:A:119:PHE:CG	1:A:120:PRO:N	2.75	0.55
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.35	0.55
1:A:118:LEU:O	1:A:119:PHE:O	2.24	0.55
1:A:15:SER:HB3	1:A:141:ARG:HD3	1.88	0.55
1:C:182:GLN:HB2	1:C:185:GLN:HG2	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: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:I:210:LEU:HB3	1:I:211:PRO:CD	2.34	0.55
1:A:75:ALA:HA	4:A:325:GOL:H2	1.88	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: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:A:224:TRP:HE1	1:A:301:ARG:HB3	1.71	0.55
1:B:118:LEU:O	1:B:119:PHE:O	2.24	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: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:A:119:PHE:O	1:A:121:PHE:N	2.33	0.54
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: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:D:314:VAL:HG12	1:D:314:VAL:O	2.08	0.54
1:E:15:SER:HB3	1:E:141:ARG:CD	2.36	0.54
1:E:20:ILE:HD12	1:E:195:ILE:HD11	1.89	0.54
1:J:15:SER:HB3	1:J:141:ARG:HD3	1.89	0.54
1:G:105:ARG:HG2	4:H:325:GOL:C1	2.36	0.54
1:G:314:VAL:O	1:G:314:VAL:HG12	2.08	0.54
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.89	0.54

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:GLU:HG3	1:F:153:ASP:HB2	1.91	0.53
1:H:297:ILE:HG23	1:H:298:GLN:N	2.24	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
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
2:J:323:ACH:H102	2:J:323:ACH:O4	2.08	0.53
1:D:15:SER:HB3	1:D:141:ARG:CG	2.39	0.53
1:F:142:PHE:HA	1:F:170:ILE:HD11	1.90	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:B:119:PHE:O	1:B:121:PHE:N	2.31	0.53
1:E:119:PHE:CG	1:E:120:PRO:N	2.77	0.53
1:J:119:PHE:O	1:J:121:PHE:N	2.32	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:E:15:SER:HB3	1:E:141:ARG:CG	2.39	0.52
1:G:210:LEU:HB3	1:G:211:PRO:CD	2.36	0.52
1:E:150:GLU:HG3	1:E:153:ASP:HB2	1.92	0.52
1:H:212:LEU:HB3	1:H:265:MET:HE1	1.91	0.52
1:D:55:PRO:HG2	1:E:181:VAL:HG13	1.92	0.52
1:F:140:LEU:CD2	5:F:331:HOH:O	2.43	0.52
1:A:314:VAL:O	1:A:314:VAL:HG12	2.09	0.52
1:D:119:PHE:CD2	1:D:120:PRO:CD	2.91	0.52
1:F:119:PHE:CG	1:F:120:PRO:N	2.77	0.52
1:I:142:PHE:HA	1:I:170:ILE:HD11	1.91	0.52
1:J:136:ASN:O	4:J:325:GOL:C2	2.50	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:A:15:SER:HB3	1:A:141:ARG:CG	2.39	0.52
1:B:168:THR:C	1:B:169:HIS:CD2	2.83	0.52
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.40	0.52
1:I:118:LEU:O	1:I:119:PHE:O	2.28	0.52
1:B:19:PHE:CD1	2:B:323:ACH:H61	2.45	0.52
1:H:118:LEU:O	1:H:119:PHE:O	2.28	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:I:102:TYR:HE2	4:I:327:GOL:H2	1.74	0.52
1:D:257:PRO:HG2	1:D:258:TYR:HD2	1.74	0.52
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.40	0.52
1:G:150:GLU:HG3	1:G:153:ASP:HB2	1.92	0.52
1:H:140:LEU:CD2	5:H:331:HOH:O	2.47	0.52
1:G:225:LEU:CD2	1:H:232:LEU:HD23	2.40	0.52
1:I:314:VAL:HG12	1:I:314:VAL:O	2.10	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:I:212:LEU:HB3	1:I:265:MET:HE1	1.91	0.52
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.44	0.51
1:E:118:LEU:O	1:E:119:PHE:O	2.28	0.51
1:E:314:VAL:O	1:E:314:VAL:HG12	2.10	0.51
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.38	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:H:297:ILE:CG2	1:H:298:GLN:N	2.73	0.51
1:D:150:GLU:HG3	1:D:153:ASP:HB2	1.92	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:B:225:LEU:HB2	1:B:231:ARG:HG3	1.92	0.51
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.40	0.51
1:D:210:LEU:CB	1:D:211:PRO:HD3	2.38	0.51
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.93	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: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:J:155:GLU:HB3	1:J:161:TRP:CD1	2.46	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:F:137:ASN:HA	4:F:328:GOL:C1	2.41	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: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:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.51
1:F:301:ARG:HH12	1:G:285:HIS:CE1	2.29	0.51
1:I:182:GLN:HB2	1:I:185:GLN:HG2	1.91	0.51

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PHE:CD2	1:H:120:PRO:CD	2.96	0.49
1:H:212:LEU:HG	1:H:245:TYR:CE2	2.47	0.49
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.76	0.49
1:H:83:GLY:O	4:H:325:GOL:O2	2.31	0.49
1:I:248:TYR:HA	1:J:247:PHE:CE1	2.47	0.49
1:J:297:ILE:CG2	1:J:298:GLN:N	2.75	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: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:A:212:LEU:HB3	1:A:265:MET:HE1	1.93	0.49
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.94	0.49
1:B:205:LEU:HD23	1:B:209:ILE:HD12	1.93	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:F:119:PHE:C	1:F:121:PHE:N	2.65	0.49
1:F:15:SER:HB3	1:F:141:ARG:CD	2.43	0.49
1:H:165:LYS:HD2	1:H:165:LYS:N	2.27	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: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:E:297:ILE:CG2	1:E:298:GLN:N	2.75	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:I:297:ILE:CG2	1:I:298:GLN:N	2.76	0.49
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.67	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:D:248:TYR:CD1	1:E:247:PHE:HA	2.48	0.48
1:E:257:PRO:HG2	1:E:258:TYR:HD2	1.75	0.48
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:H:42:GLN:HG3	1:H:101:ILE:HG12	1.95	0.48
1:J:19:PHE:CD1	2:J:323:ACH:H61	2.48	0.48
1:C:15:SER:HB3	1:C:141:ARG:CD	2.43	0.48
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.76	0.48
1:C:297:ILE:HG23	1:C:298:GLN:N	2.26	0.48
1:E:212:LEU:CD1	1:E:265:MET:HB3	2.43	0.48
1:G:145:ILE:HD11	1:G:166:ALA:HB3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ILE:CG2	1:G:298:GLN:N	2.75	0.48
1:H:205:LEU:HD23	1:H:209:ILE:HD12	1.95	0.48
1:J:15:SER:HB3	1:J:141:ARG:HG2	1.93	0.48
1:C:11:PRO:HD2	5:C:335:HOH:O	2.13	0.48
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.95	0.48
2:D:323:ACH:O4	2:D:323:ACH:H102	2.13	0.48
1:A:232:LEU:HD23	1:E:225:LEU:CD2	2.44	0.48
1:G:119:PHE:C	1:G:121:PHE:N	2.65	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:J:95:PHE:CD2	1:J:99:ARG:HB2	2.49	0.48
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.48	0.48
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.49	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:C:212:LEU:HB3	1:C:265:MET:HE1	1.95	0.48
1:D:297:ILE:C	1:D:299:ARG:N	2.67	0.48
1:E:205:LEU:HD23	1:E:209:ILE:HD12	1.95	0.48
1:I:297:ILE:C	1:I:299:ARG:N	2.67	0.48
1:J:212:LEU:HB3	1:J:265:MET:HE1	1.95	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:A:210:LEU:CB	1:A:211:PRO:HD3	2.39	0.48
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.96	0.48
1:E:217:ALA:HA	1:E:220:TRP:CE3	2.49	0.48
1:H:15:SER:HB3	1:H:141:ARG:CG	2.44	0.48
1:H:210:LEU:CB	1:H:211:PRO:HD3	2.41	0.48
1:J:149:THR:O	1:J:150:GLU:HB3	2.14	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:E:23:ILE:HG21	1:E:126:PHE:CD2	2.49	0.48
1:E:297:ILE:C	1:E:299:ARG:N	2.67	0.48
1:I:145:ILE:CG1	1:I:166:ALA:HB3	2.44	0.48
1:I:145:ILE:HG13	1:I:166:ALA:HB3	1.96	0.48
1:I:235:SER:HB3	1:I:277:ILE:HD11	1.95	0.48
1:I:301:ARG:HH12	1:J:285:HIS:CE1	2.31	0.48
1:F:248:TYR:HD1	1:G:247:PHE:HA	1.78	0.48
1:G:289:ASN:OD1	1:G:292:GLU:HB3	2.14	0.48
1:G:210:LEU:CB	1:G:211:PRO:HD3	2.41	0.47
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:PHE:C	1:I:121:PHE:N	2.67	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: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:E:279:LEU:HD22	1:E:304:PHE:HE2	1.79	0.47
1:E:95:PHE:HB2	1:E:99:ARG:HB2	1.96	0.47
1:F:257:PRO:HG2	1:F:258:TYR:HD2	1.76	0.47
1:G:136:ASN:C	4:G:328:GOL:H2	2.33	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: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
1:I:284:HIS:HD2	1:I:285:HIS:NE2	2.12	0.47
2:I:323:ACH:H102	2:I:323:ACH:O4	2.14	0.47
1:B:145:ILE:HG13	1:B:166:ALA:HB3	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:G:142:PHE:HA	1:G:170:ILE:HD11	1.96	0.47
1:I:305:PRO:O	1:I:309:LEU:HG	2.14	0.47
1:A:149:THR:O	1:A:150:GLU:HB3	2.13	0.47
1:B:137:ASN:CA	4:B:327:GOL:O1	2.62	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:J:19:PHE:CE2	1:J:146:GLN:HG3	2.49	0.47
1:I:55:PRO:HG2	1:J:181:VAL:HG13	1.96	0.47
1:C:145:ILE:HD11	1:C:166:ALA:HB3	1.94	0.47
1:F:29:LEU:HD23	1:F:29:LEU:HA	1.67	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:H:83:GLY:C	4:H:325:GOL:O2	2.52	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:B:145:ILE:CD1	1:B:145:ILE:O	2.59	0.47
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.50	0.47
1:E:289:ASN:OD1	1:E:292:GLU:HB3	2.15	0.47
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.48	0.47
1:G:15:SER:HB3	1:G:141:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:LEU:CD1	5:H:331:HOH:O	2.33	0.47
1:I:119:PHE:CD2	1:I:120:PRO:CD	2.97	0.47
1:A:136:ASN:O	4:A:326:GOL:H11	2.14	0.47
1:E:145:ILE:HD11	1:E:166:ALA:HB3	1.94	0.47
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.95	0.47
1:I:119:PHE:O	1:I:121:PHE:N	2.39	0.47
1:I:76:LEU:H	4:I:327:GOL:C1	2.28	0.47
1:B:168:THR:C	1:B:169:HIS:CG	2.88	0.47
1:G:297:ILE:O	1:G:299:ARG:N	2.48	0.47
2:G:323:ACH:H102	2:G:323:ACH:O4	2.15	0.47
1:J:55:PRO:HB3	1:J:95:PHE:CD1	2.49	0.47
1:D:289:ASN:OD1	1:D:292:GLU:HB3	2.15	0.47
1:F:284:HIS:HD2	1:F:285:HIS:NE2	2.12	0.47
1:F:297:ILE:CG2	1:F:298:GLN:N	2.78	0.47
1:H:149:THR:O	1:H:150:GLU:HB3	2.14	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:B:147:VAL:O	1:B:147:VAL:HG13	2.15	0.46
1:E:15:SER:HB3	1:E:141:ARG:HG2	1.97	0.46
1:B:119:PHE:CD2	1:B:120:PRO:CD	2.98	0.46
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.50	0.46
1:E:149:THR:O	1:E:150:GLU:HB3	2.13	0.46
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.30	0.46
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.97	0.46
1:J:145:ILE:HD11	1:J:166:ALA:HB3	1.97	0.46
1:J:289:ASN:OD1	1:J:292:GLU:HB3	2.15	0.46
1:B:142:PHE:HA	1:B:170:ILE:HD11	1.97	0.46
1:B:95:PHE:HB2	1:B:99:ARG:HB2	1.96	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:D:15:SER:HB3	1:D:141:ARG:CD	2.45	0.46
1:D:297:ILE:O	1:D:299:ARG:N	2.48	0.46
1:G:91:ARG:HD3	1:G:103:ASN:HB3	1.97	0.46
1:I:140:LEU:CD2	5:I:334:HOH:O	2.29	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:J:99:ARG:HH11	1:J:99:ARG:CG	2.12	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:15:SER:HB2	1:D:142:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:ILE:C	1:F:299:ARG:N	2.69	0.46
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.80	0.46
1:J:297:ILE:C	1:J: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:D:297:ILE:CG2	1:D:298:GLN:N	2.78	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
1:H:297:ILE:C	1:H:299:ARG:N	2.68	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:A:227:SER:HB3	1:A:230:GLU:CG	2.45	0.46
1:A:297:ILE:O	1:A:299:ARG:N	2.49	0.46
1:E:297:ILE:O	1:E:299:ARG:N	2.48	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:G:227:SER:HB3	1:G:230:GLU:HG3	1.98	0.46
1:I:248:TYR:HD1	1:J:247:PHE:HA	1.81	0.46
1:A:145:ILE:CG1	1:A:166:ALA:HB3	2.46	0.46
3:A:324:MES:O1S	3:A:324:MES:H51	2.16	0.46
1:B:145:ILE:CG1	1:B:166:ALA:HB3	2.45	0.46
1:B:304:PHE:CB	1:B:305:PRO:HD3	2.46	0.46
1:C:150:GLU:HG3	1:C:153:ASP:CB	2.46	0.46
1:G:145:ILE:HG13	1:G:166:ALA:HB3	1.96	0.46
1:H:77:GLU:O	1:H:130:LEU:HD12	2.15	0.46
1:J:220:TRP:C	1:J:222:VAL:H	2.19	0.46
1:A:289:ASN:OD1	1:A:292:GLU:HB3	2.16	0.45
1:C:227:SER:HB3	1:C:230:GLU:CG	2.45	0.45
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:F:289:ASN:OD1	1:F:292:GLU:HB3	2.16	0.45
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.51	0.45
1:B:220:TRP:C	1:B:222:VAL:H	2.20	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:F:181:VAL:HG13	1:J:55:PRO:HG2	1.97	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:J:205:LEU:HD23	1:J:209:ILE:HD12	1.98	0.45
1:A:95:PHE:CD2	1:A:99:ARG:HB2	2.51	0.45
1:C:289:ASN:CG	1:C:290:GLY:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:SER:HB3	1:D:230:GLU:CG	2.46	0.45
1:F:11:PRO:N	5:F:330:HOH:O	2.49	0.45
1:G:289:ASN:CG	1:G:290:GLY:N	2.69	0.45
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.81	0.45
1:D:15:SER:HB3	1:D:141:ARG:HG2	1.98	0.45
1:D:289:ASN:CG	1:D:290:GLY:N	2.69	0.45
1:D:248:TYR:HD1	1:E:247:PHE:HA	1.81	0.45
1:E:289:ASN:CG	1:E:290:GLY:N	2.69	0.45
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.78	0.45
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.51	0.45
1:C:147:VAL:O	1:C:147:VAL:HG13	2.17	0.45
1:F:289:ASN:HD21	1:F:292:GLU:HB2	1.81	0.45
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.42	0.45
1:G:15:SER:HB3	1:G:141:ARG:CG	2.47	0.45
1:J:227:SER:HB3	1:J:230:GLU:HG3	1.98	0.45
1:J:304:PHE:CB	1:J:305:PRO:HD3	2.46	0.45
1:D:145:ILE:HD12	1:D:166:ALA:HB3	1.97	0.45
1:E:289:ASN:HD21	1:E:292:GLU:HB2	1.81	0.45
1:E:289:ASN:ND2	1:E:292:GLU:HB2	2.32	0.45
1:F:149:THR:O	1:F:150:GLU:HB3	2.16	0.45
1:F:95:PHE:CD2	1:F:99:ARG:HB2	2.52	0.45
1:A:155:GLU:HB3	1:A:161:TRP:CD1	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:E:224:TRP:CE2	1:E:301:ARG:HD3	2.51	0.45
1:F:145:ILE:CG1	1:F:166:ALA:HB3	2.45	0.45
1:J:95:PHE:HB2	1:J:99:ARG:HB2	1.99	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:A:150:GLU:HG3	1:A:153:ASP:CB	2.47	0.45
1:B:289:ASN:CG	1:B:290:GLY:N	2.70	0.45
1:B:95:PHE:CD2	1:B:99:ARG:HB2	2.52	0.45
1:C:212:LEU:HD13	1:C:265:MET:HB3	1.99	0.45
1:D:150:GLU:HG3	1:D:153:ASP:CB	2.47	0.45
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.81	0.45
1:I:279:LEU:HD22	1:I:304:PHE:HE2	1.82	0.45
1:I:297:ILE:O	1:I:299:ARG:N	2.50	0.45
1:A:289:ASN:CG	1:A:290:GLY:N	2.68	0.45
1:A:304:PHE:CB	1:A:305:PRO:HD3	2.47	0.45
1:C:297:ILE:O	1:C:299:ARG:N	2.50	0.45
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.47	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:H:157:ILE:HA	1:H:157:ILE:HD13	1.79	0.45
1:I:150:GLU:HG3	1:I:153:ASP:CB	2.47	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:257:PRO:HG2	1:A:258:TYR:HD2	1.76	0.44
4:C:325:GOL:H32	5:C:326:HOH:O	2.17	0.44
1:G:287:GLN:HB2	1:G:288:ALA:H	1.52	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:I:39:ILE:HD11	1:I:130:LEU:HD11	1.99	0.44
1:J:23:ILE:HG21	1:J:126:PHE:CD2	2.52	0.44
1:B:136:ASN:C	4:B:327:GOL:H32	2.37	0.44
1:C:137:ASN:HA	4:C:325:GOL:O3	2.16	0.44
1:E:150:GLU:HG3	1:E:153:ASP:CB	2.47	0.44
1:G:212:LEU:HD13	1:G:265:MET:HB3	1.98	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: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:J:29:LEU:HA	1:J:29:LEU:HD23	1.69	0.44
1:A:248:TYR:HD1	1:B:247:PHE:HA	1.82	0.44
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.63	0.44
1:B:289:ASN:HD21	1:B:292:GLU:HB2	1.82	0.44
1:C:136:ASN:O	4:C:325:GOL:C2	2.31	0.44
1:C:289:ASN:OD1	1:C:292:GLU:HB3	2.17	0.44
1:D:55:PRO:HB3	1:D:95:PHE:CD1	2.52	0.44
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.51	0.44
1:F:289:ASN:CG	1:F:290:GLY:N	2.68	0.44
1:G:304:PHE:CB	1:G:305:PRO:HD3	2.48	0.44
1:J:150:GLU:HG3	1:J:153:ASP:CB	2.46	0.44
1:D:289:ASN:ND2	1:D:292:GLU:HB2	2.32	0.44
1:E:212:LEU:HA	1:E:212:LEU:HD23	1.81	0.44
2:E:323:ACH:O4	2:E:323:ACH:H102	2.17	0.44
1:G:150:GLU:HG3	1:G:153:ASP:CB	2.47	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:287:GLN:HB2	1:I:288:ALA:H	1.53	0.44
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.57	0.44
1:J:212:LEU:HD13	1:J:265:MET:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CZ	4:A:325:GOL:H12	2.52	0.44
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.53	0.44
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.57	0.44
1:F:289:ASN:ND2	1:F:292:GLU:HB2	2.33	0.44
1:F:102:TYR:OH	4:F:325:GOL:H12	2.17	0.44
1:H:150:GLU:HG3	1:H:153:ASP:CB	2.47	0.44
1:H:58:VAL:CG1	1:H:62:GLN:HB3	2.47	0.44
1:J:287:GLN:HB2	1:J:288:ALA:H	1.54	0.44
1:A:39:ILE:HD11	1:A:130:LEU:HD11	2.00	0.44
1:A:140:LEU:HD13	1:A:191:ILE:CG1	2.40	0.44
1:A:284:HIS:HD2	1:A:285:HIS:NE2	2.15	0.44
1:B:147:VAL:O	1:B:149:THR:N	2.48	0.44
1:B:289:ASN:ND2	1:B:292:GLU:HB2	2.33	0.44
1:D:11:PRO:N	5:D:339:HOH:O	2.50	0.44
1:D:147:VAL:O	1:D:147:VAL:HG13	2.17	0.44
1:E:58:VAL:CG1	1:E:62:GLN:HB3	2.47	0.44
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.87	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:A:205:LEU:HA	1:A:205:LEU:HD23	1.66	0.44
1:A:289:ASN:ND2	1:A:292:GLU:HB2	2.32	0.44
1:B:212:LEU:HD13	1:B:265:MET:HB3	1.99	0.44
1:B:227:SER:HB3	1:B:230:GLU:CG	2.48	0.44
1:B:55:PRO:HG2	1:C:181:VAL:HG13	2.00	0.44
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.82	0.44
1:D:79:ILE:HD13	1:D:79:ILE:HA	1.80	0.44
1:E:291:VAL:O	1:E:291:VAL:HG12	2.17	0.44
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.52	0.44
1:F:225:LEU:HD21	1:G:232:LEU:HD23	1.99	0.44
1:A:212:LEU:HD13	1:A:265:MET:HB3	2.00	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: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: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: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:A:147:VAL:HG13	1:A:147:VAL:O	2.18	0.43
1:B:174:ARG:O	4:B:326:GOL:H31	2.18	0.43
2:B:323:ACH:O4	2:B:323:ACH:H102	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PHE:C	1:H:121:PHE:N	2.63	0.43
1:J:224:TRP:CE2	1:J:301:ARG:HD3	2.53	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:C:19:PHE:CD1	2:C:323:ACH:H61	2.53	0.43
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.83	0.43
1:F:212:LEU:HG	1:F:245:TYR:CE2	2.53	0.43
1:F:304:PHE:CB	1:F:305:PRO:HD3	2.49	0.43
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.53	0.43
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.53	0.43
1:C:311:ILE:O	1:C:311:ILE:HG22	2.18	0.43
1:H:163:ARG:HB2	1:H:196:ASP:HB2	2.00	0.43
1:H:248:TYR:HD1	1:I:247:PHE:HA	1.84	0.43
1:H:289:ASN:ND2	1:H:292:GLU:HB2	2.32	0.43
1:H:311:ILE:O	1:H:311:ILE:HG22	2.18	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:I:163:ARG:HD3	1:I:163:ARG:HA	1.84	0.43
1:I:257:PRO:HG2	1:I:258:TYR:HD2	1.83	0.43
1:I:58:VAL:CG1	1:I:62:GLN:HB3	2.49	0.43
1:F:182:GLN:NE2	1:J:54:LYS:HD2	2.33	0.43
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.31	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.66	0.43
1:I:161:TRP:CZ2	1:I:200:ASN:ND2	2.85	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: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: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:279:LEU:HD22	1:J:304:PHE:HE2	1.84	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:B:155:GLU:HB3	1:B:161:TRP:CD1	2.54	0.43
1:D:284:HIS:HD2	1:D:285:HIS:NE2	2.16	0.43
1:A:240:LEU:HD13	1:E:241:THR:HA	2.01	0.43
1:F:226:GLU:OE2	1:G:284:HIS:NE2	2.45	0.43
1:H:161:TRP:CZ2	1:H:200:ASN:ND2	2.87	0.43
1:H:248:TYR:HA	1:I:247:PHE:CE1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:ASN:CG	1:I:290:GLY:N	2.69	0.43
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.79	0.43
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.53	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:G:305:PRO:O	1:G:309:LEU:HG	2.18	0.43
1:H:304:PHE:CB	1:H:305:PRO:HD3	2.48	0.43
1:I:220:TRP:C	1:I:222:VAL:H	2.21	0.43
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.83	0.43
1:I:99:ARG:CG	1:I:99:ARG:NH1	2.78	0.43
1:D:297:ILE:C	1:D:299:ARG:H	2.21	0.43
1:E:157:ILE:HA	1:E:157:ILE:HD13	1.79	0.43
1:F:140:LEU:CG	5:F:331:HOH:O	2.62	0.43
1:G:145:ILE:CG1	1:G:166:ALA:HB3	2.48	0.43
1:H:305:PRO:O	1:H:309:LEU:HG	2.19	0.43
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.34	0.43
1:A:79:ILE:HA	1:A:79:ILE:HD13	1.83	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:D:224:TRP:CE2	1:D:301:ARG:HD3	2.54	0.43
1:D:95:PHE:HB2	1:D:99:ARG:HB2	1.99	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.78	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:I:155:GLU:HB3	1:I:161:TRP:CD1	2.54	0.43
1:B:38:TYR:CE1	1:B:105:ARG:HD3	2.53	0.42
1:D:304:PHE:CB	1:D:305:PRO:HD3	2.48	0.42
1:E:145:ILE:CG1	1:E:166:ALA:HB3	2.48	0.42
1:H:145:ILE:CG1	1:H:166:ALA:HB3	2.49	0.42
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.84	0.42
1:I:221:SER:HB2	1:J:281:ILE:CD1	2.49	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:E:284:HIS:HD2	1:E:285:HIS:NE2	2.16	0.42
1:H:291:VAL:O	1:H:291:VAL:HG12	2.19	0.42
1:A:95:PHE:HB2	1:A:99:ARG:HB2	2.00	0.42
1:B:119:PHE:HE1	1:B:199:ARG:CZ	2.32	0.42
1:B:39:ILE:HD11	1:B:130:LEU:HD11	2.00	0.42
1:E:210:LEU:CB	1:E:211:PRO:CD	2.95	0.42
1:F:212:LEU:HD13	1:F:265:MET:HB3	1.99	0.42
1:G:23:ILE:HG21	1:G:126:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:ILE:C	1:G:299:ARG:H	2.23	0.42
1:I:140:LEU:CD1	5:I:334:HOH:O	2.53	0.42
1:C:279:LEU:HD22	1:C:304:PHE:HE2	1.83	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: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:H:297:ILE:O	1:H:299:ARG:N	2.52	0.42
1:B:297:ILE:O	1:B:299:ARG:N	2.53	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:F:248:TYR:HA	1:G:247:PHE:CE1	2.55	0.42
1:H:15:SER:HB3	1:H:141:ARG:CD	2.50	0.42
1:I:95:PHE:CD2	1:I:99:ARG:HB2	2.55	0.42
1:C:58:VAL:CG1	1:C:62:GLN:HB3	2.50	0.42
1:F:147:VAL:O	1:F:147:VAL:HG13	2.18	0.42
1:F:311:ILE:O	1:F:311:ILE:HG22	2.20	0.42
1:G:227:SER:HB3	1:G:230:GLU:CG	2.49	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:I:234:THR:HG21	1:J:236:PHE:CE2	2.55	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:J:291:VAL:HG12	1:J:291:VAL:O	2.20	0.42
1:A:311:ILE:HG22	1:A:311:ILE:O	2.20	0.42
1:C:297:ILE:C	1:C:299:ARG:H	2.23	0.42
1:D:220:TRP:C	1:D:222:VAL:H	2.23	0.42
1:E:140:LEU:CG	5:E:336:HOH:O	2.68	0.42
1:E:212:LEU:HD13	1:E:265:MET:HB3	2.01	0.42
1:G:15:SER:HB3	1:G:141:ARG:HG2	2.01	0.42
1:I:297:ILE:C	1:I:299:ARG:H	2.22	0.42
1:J:19:PHE:CG	2:J:323:ACH:H61	2.55	0.42
1:A:291:VAL:O	1:A:291:VAL:HG12	2.19	0.42
1:D:142:PHE:HA	1:D:170:ILE:HD11	2.01	0.42
1:E:95:PHE:CD2	1:E:99:ARG:HB2	2.54	0.42
1:H:38:TYR:CE1	1:H:105:ARG:HD3	2.54	0.42
1:I:137:ASN:CA	4:I:329:GOL:O1	2.64	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

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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:F:55:PRO:HB3	1:F:95:PHE:CD1	2.54	0.42
1:G:39:ILE:HD11	1:G:130:LEU:HD11	2.02	0.42
1:H:138:GLN:N	4:H:324:GOL:H11	2.34	0.42
1:J:136:ASN:C	4:J:325:GOL:H2	2.37	0.42
1:A:297:ILE:C	1:A:299:ARG:H	2.23	0.42
1:C:257:PRO:HG2	1:C:258:TYR:HD2	1.80	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:F:15:SER:HB3	1:F:141:ARG:HG2	2.01	0.42
1:G:200:ASN:HA	1:G:201:PRO:HD3	1.83	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
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.55	0.42
1:J:182:GLN:HB2	1:J:185:GLN:CG	2.49	0.42
1:J:297:ILE:O	1:J:299:ARG:N	2.53	0.42
1:D:43:TRP:CZ2	1:D:100:VAL:HG11	2.55	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
4:G:328:GOL:O3	4:G:328:GOL:O1	2.32	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:F:212:LEU:O	1:F:216:ILE:HG13	2.20	0.41
1:H:119:PHE:HE1	1:H:199:ARG:CZ	2.32	0.41
1:I:147:VAL:O	1:I:149:THR:N	2.49	0.41
1:J:284:HIS:HD2	1:J:285:HIS:CD2	2.37	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:G:284:HIS:HD2	1:G:285:HIS:NE2	2.17	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:B:305:PRO:O	1:B:309:LEU:HG	2.20	0.41
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.86	0.41
1:D:206:TRP:CD2	3:D:325:MES:O2S	2.74	0.41
1:F:291:VAL:HG12	1:F:291:VAL:O	2.20	0.41
1:G:220:TRP:C	1:G:222:VAL:H	2.24	0.41
1:I:311:ILE:O	1:I:311:ILE:HG22	2.21	0.41
1:E:235:SER:HB3	1:E:277:ILE:HD11	2.03	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:J:145:ILE:CG1	1:J:166:ALA:HB3	2.49	0.41
1:B:311:ILE:HG22	1:B:311:ILE:O	2.21	0.41
1:C:71:LEU:HD12	1:C:72:TRP:H	1.84	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:B:200:ASN:HA	1:B:201:PRO:HD3	1.83	0.41
1:C:220:TRP:C	1:C:222:VAL:H	2.24	0.41
1:C:291:VAL:O	1:C:291:VAL:HG12	2.20	0.41
1:D:210:LEU:CB	1:D:211:PRO:CD	2.98	0.41
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.56	0.41
1:F:221:SER:HB2	1:G:281:ILE:CD1	2.50	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:I:261:VAL:HG12	1:I:262:ILE:N	2.35	0.41
1:J:58:VAL:CG1	1:J:62:GLN:HB3	2.50	0.41
1:A:212:LEU:HG	1:A:245:TYR:CE2	2.55	0.41
1:E:131:GLU:HG2	1:E:190:ARG:HB2	2.02	0.41
1:G:205:LEU:HD23	1:G:209:ILE:HD12	2.02	0.41
1:I:212:LEU:HD13	1:I:265:MET:HB3	2.02	0.41
1:J:155:GLU:HB3	1:J:161:TRP:NE1	2.36	0.41
1:A:305:PRO:O	1:A:309:LEU:HG	2.21	0.41
1:A:58:VAL:CG1	1:A:62:GLN:HB3	2.50	0.41
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.83	0.41
1:C:256:LEU:HB3	1:C:257:PRO:HD2	2.02	0.41
1:D:235:SER:HB3	1:D:277:ILE:HD11	2.02	0.41
1:D:311:ILE:HG22	1:D:311:ILE:O	2.20	0.41
1:J:210:LEU:CB	1:J:211:PRO:CD	2.98	0.41
1:A:210:LEU:CB	1:A:211:PRO:CD	2.98	0.41
1:B:215:ILE:HA	1:C:239:MET:HE2	2.03	0.41
1:C:284:HIS:HD2	1:C:285:HIS:CD2	2.39	0.41
1:F:119:PHE:HE1	1:F:199:ARG:CZ	2.34	0.41
1:F:305:PRO:O	1:F:309:LEU:HG	2.21	0.41
1:G:291:VAL:HG12	1:G:291:VAL:O	2.21	0.41
1:H:99:ARG:CG	1:H:99:ARG:NH1	2.82	0.41
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.80	0.41
1:A:38:TYR:CE1	1:A:105:ARG:HD3	2.55	0.40
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.85	0.40
1:C:91:ARG:HD3	1:C:103:ASN:HB3	2.02	0.40
1:C:161:TRP:CZ2	1:C:200:ASN:ND2	2.89	0.40
1:C:226:GLU:OE1	1:C:226:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:O	1:D:145:ILE:CD1	2.68	0.40
1:D:22:LYS:NZ	5:D:331:HOH:O	2.54	0.40
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.98	0.40
1:J:212:LEU:HG	1:J:245:TYR:CE2	2.57	0.40
1:A:225:LEU:HD21	1:B:232:LEU:HD23	2.03	0.40
1:D:119:PHE:HE1	1:D:199:ARG:CZ	2.34	0.40
1:D:58:VAL:CG1	1:D:62:GLN:HB3	2.51	0.40
1:E:295:LEU:HA	1:E:298:GLN:NE2	2.23	0.40
1:F:205:LEU:HA	1:F:205:LEU:HD23	1.65	0.40
1:G:15:SER:HB3	1:G:141:ARG:CD	2.52	0.40
1:H:279:LEU:HD22	1:H:304:PHE:HE2	1.85	0.40
1:D:291:VAL:O	1:D:291:VAL:HG12	2.21	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: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:175:TYR:HH	2:E:323:ACH:H101	1.84	0.40
1:G:137:ASN:HA	4:G:328:GOL:C2	2.52	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%)	4	14
1	B	305/322 (95%)	271 (89%)	24 (8%)	10 (3%)	4	14
1	C	305/322 (95%)	267 (88%)	29 (10%)	9 (3%)	4	16
1	D	305/322 (95%)	269 (88%)	24 (8%)	12 (4%)	3	11
1	E	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	3	13
1	F	305/322 (95%)	268 (88%)	28 (9%)	9 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	3	13
1	H	305/322 (95%)	268 (88%)	27 (9%)	10 (3%)	4	14
1	I	305/322 (95%)	271 (89%)	22 (7%)	12 (4%)	3	11
1	J	305/322 (95%)	267 (88%)	26 (8%)	12 (4%)	3	11
All	All	3050/3220 (95%)	2681 (88%)	263 (9%)	106 (4%)	3	13

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%)	14	37
1	B	275/284 (97%)	253 (92%)	22 (8%)	12	32
1	C	275/284 (97%)	254 (92%)	21 (8%)	13	35
1	D	275/284 (97%)	251 (91%)	24 (9%)	10	29
1	E	275/284 (97%)	253 (92%)	22 (8%)	12	32
1	F	275/284 (97%)	255 (93%)	20 (7%)	14	37
1	G	275/284 (97%)	254 (92%)	21 (8%)	13	35
1	H	275/284 (97%)	256 (93%)	19 (7%)	15	40
1	I	275/284 (97%)	252 (92%)	23 (8%)	11	30
1	J	275/284 (97%)	253 (92%)	22 (8%)	12	32
All	All	2750/2840 (97%)	2536 (92%)	214 (8%)	12	33

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
4	GOL	F	328	-	5,5,5	0.77	0	5,5,5	0.59	0
4	GOL	B	326	-	5,5,5	0.75	0	5,5,5	0.58	0
4	GOL	G	328	-	5,5,5	0.59	0	5,5,5	0.98	0
4	GOL	J	325	-	5,5,5	0.70	0	5,5,5	0.62	0
2	ACH	H	323	-	9,9,9	1.00	1 (11%)	12,12,12	0.89	1 (8%)
4	GOL	F	325	-	5,5,5	0.70	0	5,5,5	0.42	0
4	GOL	G	327	-	3,3,5	0.49	0	2,2,5	0.31	0
2	ACH	G	323	-	9,9,9	1.10	1 (11%)	12,12,12	0.62	0
4	GOL	C	324	-	5,5,5	0.60	0	5,5,5	0.54	0
3	MES	D	325	-	12,12,12	2.24	1 (8%)	14,16,16	2.71	5 (35%)
2	ACH	C	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.78	0
4	GOL	H	324	-	5,5,5	0.45	0	5,5,5	0.77	0
4	GOL	F	327	-	5,5,5	0.83	0	5,5,5	0.29	0
4	GOL	D	327	-	5,5,5	0.69	0	5,5,5	0.55	0
3	MES	A	324	-	12,12,12	2.14	1 (8%)	14,16,16	2.53	7 (50%)
4	GOL	A	326	-	5,5,5	0.77	0	5,5,5	0.30	0
2	ACH	I	323	-	9,9,9	1.01	1 (11%)	12,12,12	0.75	0
3	MES	I	324	-	12,12,12	2.08	1 (8%)	14,16,16	2.44	8 (57%)
3	MES	D	324	-	12,12,12	2.14	1 (8%)	14,16,16	2.44	6 (42%)
2	ACH	J	323	-	9,9,9	1.04	1 (11%)	12,12,12	0.78	0
4	GOL	I	326	-	5,5,5	0.72	0	5,5,5	0.81	0
2	ACH	D	323	-	9,9,9	1.14	1 (11%)	12,12,12	0.86	0
2	ACH	F	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.85	0
4	GOL	I	327	-	5,5,5	0.75	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	F	324	-	12,12,12	2.18	1 (8%)	14,16,16	2.47	7 (50%)
2	ACH	E	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.72	0
3	MES	G	324	-	12,12,12	2.28	1 (8%)	14,16,16	2.49	8 (57%)
4	GOL	G	325	-	5,5,5	0.71	0	5,5,5	0.50	0
4	GOL	E	326	-	5,5,5	0.83	0	5,5,5	0.54	0
4	GOL	D	326	-	5,5,5	0.75	0	5,5,5	0.54	0
2	ACH	A	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.67	0
4	GOL	H	325	-	5,5,5	0.94	0	5,5,5	0.42	0
3	MES	J	324	-	12,12,12	2.25	1 (8%)	14,16,16	2.51	7 (50%)
2	ACH	B	323	-	9,9,9	1.02	1 (11%)	12,12,12	0.74	0
4	GOL	B	327	-	5,5,5	0.81	0	5,5,5	0.67	0
4	GOL	E	325	-	5,5,5	0.78	0	5,5,5	0.31	0
3	MES	E	324	-	12,12,12	2.20	1 (8%)	14,16,16	2.41	7 (50%)
4	GOL	C	325	-	5,5,5	0.73	0	5,5,5	0.70	0
4	GOL	G	326	-	5,5,5	0.64	0	5,5,5	0.42	0
4	GOL	F	326	-	5,5,5	0.65	0	5,5,5	0.55	0
3	MES	B	324	-	12,12,12	2.15	1 (8%)	14,16,16	2.51	7 (50%)
4	GOL	A	325	-	5,5,5	0.73	0	5,5,5	0.59	0
4	GOL	I	325	-	5,5,5	0.76	0	5,5,5	0.40	0
4	GOL	B	325	-	5,5,5	0.68	0	5,5,5	0.64	0
4	GOL	I	328	-	5,5,5	0.69	0	5,5,5	0.46	0
4	GOL	I	329	-	5,5,5	0.83	0	5,5,5	0.57	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
4	GOL	F	328	-	-	4/4/4/4	-
4	GOL	B	326	-	-	2/4/4/4	-
4	GOL	G	328	-	-	1/4/4/4	-
4	GOL	J	325	-	-	0/4/4/4	-
2	ACH	H	323	-	-	0/7/7/7	-
4	GOL	F	325	-	-	2/4/4/4	-
4	GOL	G	327	-	-	1/1/1/4	-
2	ACH	G	323	-	-	1/7/7/7	-
4	GOL	C	324	-	-	4/4/4/4	-
3	MES	D	325	-	-	5/6/14/14	0/1/1/1
2	ACH	C	323	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	324	-	-	2/4/4/4	-
4	GOL	F	327	-	-	0/4/4/4	-
4	GOL	D	327	-	-	2/4/4/4	-
3	MES	A	324	-	-	5/6/14/14	0/1/1/1
4	GOL	A	326	-	-	0/4/4/4	-
2	ACH	I	323	-	-	1/7/7/7	-
3	MES	I	324	-	-	5/6/14/14	0/1/1/1
3	MES	D	324	-	-	4/6/14/14	0/1/1/1
2	ACH	J	323	-	-	0/7/7/7	-
4	GOL	I	326	-	-	1/4/4/4	-
2	ACH	D	323	-	-	0/7/7/7	-
2	ACH	F	323	-	-	0/7/7/7	-
4	GOL	I	327	-	-	0/4/4/4	-
3	MES	F	324	-	-	5/6/14/14	0/1/1/1
2	ACH	E	323	-	-	0/7/7/7	-
3	MES	G	324	-	-	4/6/14/14	0/1/1/1
4	GOL	G	325	-	-	3/4/4/4	-
4	GOL	E	326	-	-	0/4/4/4	-
4	GOL	D	326	-	-	0/4/4/4	-
2	ACH	A	323	-	-	0/7/7/7	-
4	GOL	H	325	-	-	2/4/4/4	-
3	MES	J	324	-	-	1/6/14/14	0/1/1/1
2	ACH	B	323	-	-	1/7/7/7	-
4	GOL	B	327	-	-	3/4/4/4	-
4	GOL	E	325	-	-	0/4/4/4	-
3	MES	E	324	-	-	2/6/14/14	0/1/1/1
4	GOL	C	325	-	-	0/4/4/4	-
4	GOL	G	326	-	-	2/4/4/4	-
4	GOL	F	326	-	-	1/4/4/4	-
3	MES	B	324	-	-	4/6/14/14	0/1/1/1
4	GOL	A	325	-	-	0/4/4/4	-
4	GOL	I	325	-	-	0/4/4/4	-
4	GOL	B	325	-	-	3/4/4/4	-
4	GOL	I	328	-	-	4/4/4/4	-
4	GOL	I	329	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	324	MES	C8-S	-7.55	1.66	1.77
3	J	324	MES	C8-S	-7.49	1.66	1.77
3	D	325	MES	C8-S	-7.44	1.66	1.77
3	E	324	MES	C8-S	-7.28	1.67	1.77
3	F	324	MES	C8-S	-7.14	1.67	1.77
3	B	324	MES	C8-S	-7.12	1.67	1.77
3	D	324	MES	C8-S	-7.07	1.67	1.77
3	A	324	MES	C8-S	-6.98	1.67	1.77
3	I	324	MES	C8-S	-6.84	1.67	1.77
2	E	323	ACH	O4-C5	2.59	1.46	1.33
2	D	323	ACH	O4-C5	2.45	1.45	1.33
2	G	323	ACH	O4-C5	2.44	1.45	1.33
2	B	323	ACH	O4-C5	2.44	1.45	1.33
2	A	323	ACH	O4-C5	2.43	1.45	1.33
2	J	323	ACH	O4-C5	2.43	1.45	1.33
2	I	323	ACH	O4-C5	2.41	1.45	1.33
2	H	323	ACH	O4-C5	2.40	1.45	1.33
2	C	323	ACH	O4-C5	2.32	1.44	1.33
2	F	323	ACH	O4-C5	2.27	1.44	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	325	MES	O3S-S-C8	6.99	117.07	105.77
3	G	324	MES	O1S-S-C8	5.10	113.06	106.92
3	F	324	MES	C5-N4-C3	5.01	120.11	108.83
3	A	324	MES	C5-N4-C3	4.80	119.62	108.83
3	E	324	MES	C5-N4-C3	4.78	119.59	108.83
3	B	324	MES	C5-N4-C3	4.72	119.45	108.83
3	J	324	MES	C5-N4-C3	4.60	119.19	108.83
3	I	324	MES	C5-N4-C3	4.60	119.19	108.83
3	D	324	MES	C5-N4-C3	4.39	118.72	108.83
3	D	324	MES	O3S-S-C8	3.86	112.01	105.77
3	I	324	MES	C7-N4-C5	3.85	121.07	111.23
3	A	324	MES	C7-N4-C5	3.75	120.83	111.23
3	A	324	MES	C6-C5-N4	-3.72	104.46	110.10
3	D	325	MES	C5-N4-C3	3.62	116.98	108.83
3	F	324	MES	C7-N4-C5	3.62	120.50	111.23
3	E	324	MES	C6-C5-N4	-3.59	104.65	110.10
3	J	324	MES	C6-C5-N4	-3.58	104.68	110.10
3	B	324	MES	O1S-S-C8	3.56	111.20	106.92
3	J	324	MES	C2-C3-N4	-3.55	104.71	110.10
3	B	324	MES	C7-N4-C3	3.53	120.27	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	324	MES	C7-N4-C5	3.38	119.88	111.23
3	D	324	MES	O1S-S-C8	3.36	110.96	106.92
3	F	324	MES	O1S-S-C8	3.34	110.94	106.92
3	J	324	MES	O3S-S-C8	3.33	111.15	105.77
3	A	324	MES	O3S-S-C8	3.33	111.15	105.77
3	F	324	MES	C6-C5-N4	-3.29	105.11	110.10
3	I	324	MES	C7-N4-C3	3.29	119.65	111.23
3	D	325	MES	C7-N4-C3	3.29	119.64	111.23
3	A	324	MES	C7-N4-C3	3.23	119.50	111.23
3	G	324	MES	C7-N4-C5	3.21	119.45	111.23
3	E	324	MES	C7-N4-C5	3.21	119.43	111.23
3	G	324	MES	C5-N4-C3	3.20	116.03	108.83
3	E	324	MES	C7-N4-C3	3.18	119.38	111.23
3	J	324	MES	C7-N4-C5	3.18	119.37	111.23
3	F	324	MES	C7-N4-C3	3.16	119.31	111.23
3	G	324	MES	C7-N4-C3	3.11	119.19	111.23
3	J	324	MES	C7-N4-C3	3.06	119.06	111.23
3	B	324	MES	C6-C5-N4	-3.04	105.50	110.10
3	D	324	MES	C7-N4-C5	2.99	118.89	111.23
3	D	324	MES	C7-N4-C3	2.96	118.81	111.23
3	I	324	MES	C6-C5-N4	-2.94	105.64	110.10
3	G	324	MES	C6-C5-N4	-2.84	105.80	110.10
3	D	325	MES	C7-N4-C5	2.82	118.44	111.23
3	D	325	MES	C6-C5-N4	-2.79	105.87	110.10
3	A	324	MES	C2-C3-N4	-2.69	106.02	110.10
3	E	324	MES	C2-C3-N4	-2.61	106.14	110.10
3	I	324	MES	O3S-S-C8	2.54	109.87	105.77
3	E	324	MES	O2S-S-C8	2.49	109.92	106.92
3	B	324	MES	C2-C3-N4	-2.46	106.37	110.10
3	I	324	MES	O2S-S-C8	2.46	109.87	106.92
3	G	324	MES	C6-O1-C2	2.31	117.61	109.89
3	I	324	MES	O1S-S-C8	2.28	109.67	106.92
3	D	324	MES	C2-C3-N4	-2.25	106.69	110.10
3	E	324	MES	O3S-S-C8	2.24	109.39	105.77
3	A	324	MES	O2S-S-C8	2.19	109.55	106.92
3	I	324	MES	C2-C3-N4	-2.18	106.79	110.10
3	G	324	MES	C2-C3-N4	-2.18	106.80	110.10
3	B	324	MES	O3S-S-C8	2.17	109.28	105.77
3	F	324	MES	O2S-S-C8	2.16	109.51	106.92
3	J	324	MES	O1S-S-C8	2.09	109.44	106.92
2	H	323	ACH	O4-C5-C6	2.09	121.51	112.38
3	F	324	MES	C2-C3-N4	-2.03	107.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	324	MES	O1-C2-C3	2.01	116.22	111.80

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	325	MES	C8-C7-N4-C3
3	D	325	MES	N4-C7-C8-S
4	B	325	GOL	C1-C2-C3-O3
4	D	327	GOL	O1-C1-C2-C3
3	A	324	MES	C7-C8-S-O1S
3	A	324	MES	C7-C8-S-O3S
4	G	325	GOL	C1-C2-C3-O3
3	I	324	MES	C8-C7-N4-C3
3	I	324	MES	N4-C7-C8-S
3	I	324	MES	C7-C8-S-O1S
3	I	324	MES	C7-C8-S-O3S
3	F	324	MES	N4-C7-C8-S
3	G	324	MES	N4-C7-C8-S
3	G	324	MES	C7-C8-S-O1S
3	G	324	MES	C7-C8-S-O3S
4	B	327	GOL	O1-C1-C2-C3
3	E	324	MES	N4-C7-C8-S
4	G	326	GOL	C1-C2-C3-O3
3	B	324	MES	N4-C7-C8-S
3	B	324	MES	C7-C8-S-O1S
3	B	324	MES	C7-C8-S-O2S
3	B	324	MES	C7-C8-S-O3S
4	I	328	GOL	C1-C2-C3-O3
4	I	329	GOL	C1-C2-C3-O3
4	C	324	GOL	O2-C2-C3-O3
3	F	324	MES	C7-C8-S-O3S
4	B	326	GOL	C1-C2-C3-O3
4	G	328	GOL	O1-C1-C2-C3
4	F	325	GOL	C1-C2-C3-O3
4	C	324	GOL	O1-C1-C2-C3
4	C	324	GOL	C1-C2-C3-O3
4	B	325	GOL	O1-C1-C2-C3
4	I	326	GOL	O1-C1-C2-C3
4	H	324	GOL	O1-C1-C2-C3
4	H	325	GOL	C1-C2-C3-O3
4	I	328	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	F	325	GOL	O2-C2-C3-O3
4	B	325	GOL	O2-C2-C3-O3
4	D	327	GOL	O1-C1-C2-O2
4	G	325	GOL	O2-C2-C3-O3
4	B	327	GOL	O1-C1-C2-O2
4	I	328	GOL	O2-C2-C3-O3
4	I	329	GOL	O2-C2-C3-O3
3	D	324	MES	C7-C8-S-O3S
3	A	324	MES	N4-C7-C8-S
3	D	325	MES	C8-C7-N4-C5
3	A	324	MES	C8-C7-N4-C3
3	F	324	MES	C8-C7-N4-C3
3	J	324	MES	C8-C7-N4-C5
3	E	324	MES	C8-C7-N4-C3
4	F	328	GOL	O1-C1-C2-O2
4	B	326	GOL	O2-C2-C3-O3
4	H	325	GOL	O2-C2-C3-O3
4	B	327	GOL	O2-C2-C3-O3
4	F	328	GOL	O2-C2-C3-O3
3	A	324	MES	C7-C8-S-O2S
3	I	324	MES	C7-C8-S-O2S
3	D	324	MES	C7-C8-S-O1S
3	D	324	MES	C7-C8-S-O2S
3	F	324	MES	C7-C8-S-O1S
3	F	324	MES	C7-C8-S-O2S
3	G	324	MES	C7-C8-S-O2S
4	H	324	GOL	O1-C1-C2-O2
3	D	324	MES	C8-C7-N4-C3
2	I	323	ACH	N1-C2-C3-O4
4	F	328	GOL	O1-C1-C2-C3
4	F	328	GOL	C1-C2-C3-O3
4	G	326	GOL	O2-C2-C3-O3
4	I	328	GOL	O1-C1-C2-O2
2	G	323	ACH	C2-C3-O4-C5
4	G	327	GOL	O1-C1-C2-O2
2	B	323	ACH	N1-C2-C3-O4
4	C	324	GOL	O1-C1-C2-O2
4	G	325	GOL	O1-C1-C2-O2
4	F	326	GOL	O1-C1-C2-C3
3	D	325	MES	C7-C8-S-O3S
3	D	325	MES	C7-C8-S-O2S

There are no ring outliers.

28 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	328	GOL	4	0
4	B	326	GOL	5	0
4	G	328	GOL	9	0
4	J	325	GOL	7	0
2	H	323	ACH	1	0
4	F	325	GOL	1	0
2	G	323	ACH	1	0
3	D	325	MES	1	0
2	C	323	ACH	3	0
4	H	324	GOL	3	0
4	D	327	GOL	1	0
3	A	324	MES	1	0
4	A	326	GOL	4	0
2	I	323	ACH	3	0
2	J	323	ACH	3	0
2	D	323	ACH	2	0
2	F	323	ACH	2	0
4	I	327	GOL	4	0
3	F	324	MES	2	0
2	E	323	ACH	4	0
4	E	326	GOL	2	0
2	A	323	ACH	2	0
4	H	325	GOL	6	0
2	B	323	ACH	2	0
4	B	327	GOL	7	0
4	C	325	GOL	4	0
4	A	325	GOL	2	0
4	I	329	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, 95th 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 ²)	Q<0.9
1	A	307/322 (95%)	0.18	29 (9%) 8 6	57, 90, 172, 210	0
1	B	307/322 (95%)	0.02	20 (6%) 18 15	52, 87, 172, 213	0
1	C	307/322 (95%)	0.06	16 (5%) 27 24	51, 87, 173, 210	0
1	D	307/322 (95%)	0.02	21 (6%) 17 14	51, 84, 170, 210	0
1	E	307/322 (95%)	0.04	18 (5%) 22 19	54, 88, 170, 208	0
1	F	307/322 (95%)	0.08	24 (7%) 13 10	53, 94, 173, 208	0
1	G	307/322 (95%)	0.10	24 (7%) 13 10	51, 87, 168, 209	0
1	H	307/322 (95%)	0.26	27 (8%) 10 7	55, 89, 174, 208	0
1	I	307/322 (95%)	0.07	27 (8%) 10 7	57, 90, 172, 211	0
1	J	307/322 (95%)	0.05	26 (8%) 10 8	59, 94, 175, 208	0
All	All	3070/3220 (95%)	0.09	232 (7%) 13 11	51, 89, 174, 213	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	23.2
1	A	152	ILE	18.3
1	G	152	ILE	17.0
1	E	291	VAL	12.9
1	H	152	ILE	12.5
1	A	151	ASN	11.6
1	H	290	GLY	11.4
1	B	151	ASN	11.4
1	H	288	ALA	11.4
1	J	291	VAL	10.7
1	H	289	ASN	10.7
1	D	152	ILE	10.4
1	I	152	ILE	10.2

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Mol	Chain	Res	Type	RSRZ
1	G	315	LEU	10.1
1	H	291	VAL	10.0
1	J	152	ILE	9.6
1	C	152	ILE	9.6
1	G	314	VAL	9.1
1	G	151	ASN	9.0
1	I	291	VAL	8.9
1	G	290	GLY	8.5
1	F	152	ILE	8.2
1	F	291	VAL	7.6
1	J	153	ASP	7.6
1	E	290	GLY	7.5
1	B	291	VAL	7.4
1	G	291	VAL	7.3
1	B	313	CYS	7.1
1	H	151	ASN	7.0
1	F	317	ILE	6.9
1	G	317	ILE	6.7
1	F	151	ASN	6.6
1	J	151	ASN	6.5
1	A	291	VAL	6.5
1	F	316	VAL	6.4
1	C	291	VAL	6.2
1	A	317	ILE	6.2
1	I	290	GLY	6.1
1	D	290	GLY	6.1
1	E	152	ILE	6.0
1	F	290	GLY	6.0
1	D	291	VAL	5.9
1	H	292	GLU	5.9
1	H	315	LEU	5.8
1	A	290	GLY	5.8
1	H	314	VAL	5.7
1	D	151	ASN	5.5
1	G	316	VAL	5.5
1	C	317	ILE	5.4
1	A	53	ASP	5.4
1	J	317	ILE	5.4
1	A	316	VAL	5.3
1	C	289	ASN	5.2
1	G	286	ARG	5.1
1	D	153	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	ASN	5.1
1	B	317	ILE	5.1
1	J	306	LEU	5.0
1	I	153	ASP	5.0
1	J	290	GLY	4.9
1	A	296	LEU	4.9
1	B	290	GLY	4.9
1	G	296	LEU	4.9
1	G	313	CYS	4.8
1	F	182	GLN	4.8
1	F	289	ASN	4.8
1	A	153	ASP	4.8
1	A	148	TYR	4.7
1	I	151	ASN	4.7
1	C	316	VAL	4.7
1	B	312	GLY	4.6
1	B	289	ASN	4.6
1	H	317	ILE	4.4
1	F	286	ARG	4.4
1	B	293	ASP	4.4
1	I	293	ASP	4.3
1	B	316	VAL	4.3
1	G	287	GLN	4.2
1	E	289	ASN	4.1
1	E	287	GLN	4.1
1	H	316	VAL	4.1
1	I	317	ILE	4.0
1	J	289	ASN	3.9
1	C	295	LEU	3.9
1	F	181	VAL	3.9
1	A	314	VAL	3.8
1	F	288	ALA	3.8
1	J	154	ASN	3.8
1	I	287	GLN	3.8
1	B	296	LEU	3.8
1	F	148	TYR	3.8
1	I	286	ARG	3.8
1	A	295	LEU	3.7
1	E	288	ALA	3.7
1	J	314	VAL	3.7
1	I	154	ASN	3.7
1	C	288	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	156	GLU	3.7
1	A	313	CYS	3.7
1	I	148	TYR	3.7
1	F	287	GLN	3.7
1	E	49	LYS	3.6
1	E	156	GLU	3.6
1	H	182	GLN	3.6
1	A	117	ARG	3.6
1	F	296	LEU	3.6
1	J	157	ILE	3.6
1	H	185	GLN	3.6
1	B	288	ALA	3.5
1	F	153	ASP	3.5
1	J	310	ALA	3.5
1	A	49	LYS	3.4
1	I	315	LEU	3.4
1	D	154	ASN	3.4
1	G	289	ASN	3.3
1	I	316	VAL	3.3
1	H	313	CYS	3.2
1	C	313	CYS	3.2
1	I	292	GLU	3.1
1	B	314	VAL	3.1
1	I	314	VAL	3.1
1	B	315	LEU	3.1
1	E	148	TYR	3.1
1	E	292	GLU	3.0
1	H	293	ASP	3.0
1	H	295	LEU	3.0
1	A	54	LYS	3.0
1	C	290	GLY	3.0
1	G	311	ILE	3.0
1	I	183	PRO	3.0
1	B	295	LEU	3.0
1	C	296	LEU	2.9
1	F	295	LEU	2.9
1	B	294	ASP	2.9
1	D	289	ASN	2.9
1	A	297	ILE	2.9
1	D	176	ASP	2.9
1	A	176	ASP	2.9
1	D	317	ILE	2.9

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

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Mol	Chain	Res	Type	RSRZ
1	A	286	ARG	2.4
1	C	315	LEU	2.4
1	J	49	LYS	2.4
1	E	184	ASN	2.4
1	D	184	ASN	2.4
1	G	298	GLN	2.4
1	I	294	ASP	2.4
1	I	289	ASN	2.4
1	J	282	PHE	2.4
1	H	287	GLN	2.4
1	H	49	LYS	2.4
1	B	306	LEU	2.3
1	J	161	TRP	2.3
1	I	157	ILE	2.3
1	J	163	ARG	2.3
1	I	182	GLN	2.3
1	F	178	LEU	2.3
1	G	156	GLU	2.3
1	E	154	ASN	2.2
1	G	251	ASN	2.2
1	G	155	GLU	2.2
1	D	185	GLN	2.2
1	H	174	ARG	2.2
1	I	285	HIS	2.2
1	J	286	ARG	2.2
1	I	298	GLN	2.2
1	A	150	GLU	2.2
1	A	156	GLU	2.2
1	H	296	LEU	2.1
1	E	183	PRO	2.1
1	A	177	HIS	2.1
1	B	153	ASP	2.1
1	E	315	LEU	2.1
1	D	157	ILE	2.1
1	D	292	GLU	2.1
1	D	148	TYR	2.1
1	D	288	ALA	2.1
1	J	303	ALA	2.1
1	A	175	TYR	2.1
1	I	297	ILE	2.0
1	D	183	PRO	2.0
1	C	287	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	185	GLN	2.0
1	H	294	ASP	2.0
1	C	156	GLU	2.0
1	A	311	ILE	2.0
1	J	172	ASP	2.0
1	H	186	ASN	2.0
1	F	174	ARG	2.0
1	H	163	ARG	2.0
1	D	315	LEU	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. The B-factors column lists the minimum, median, 95th 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(Å ²)	Q<0.9
4	GOL	B	326	6/6	0.68	0.21	83,110,138,150	0
4	GOL	A	325	6/6	0.73	0.49	69,109,127,135	0
4	GOL	E	325	6/6	0.73	0.22	85,99,110,130	0
4	GOL	I	327	6/6	0.78	0.38	88,92,119,126	0
4	GOL	H	324	6/6	0.79	0.20	56,69,111,111	0
4	GOL	F	325	6/6	0.80	0.38	84,100,114,125	0
4	GOL	C	324	6/6	0.81	0.41	79,89,98,113	0
4	GOL	J	325	6/6	0.82	0.15	64,92,106,114	0
4	GOL	H	325	6/6	0.83	0.57	80,85,104,115	0
4	GOL	B	325	6/6	0.83	0.35	77,88,103,117	0
3	MES	A	324	12/12	0.84	0.14	91,140,168,188	0
4	GOL	F	328	6/6	0.84	0.13	73,86,114,121	0
4	GOL	F	327	6/6	0.84	0.34	77,98,110,119	0
4	GOL	I	329	6/6	0.84	0.19	61,71,110,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	326	6/6	0.85	0.18	79,90,125,127	0
4	GOL	G	325	6/6	0.85	0.28	79,94,101,112	0
3	MES	F	324	12/12	0.86	0.19	106,147,159,185	0
3	MES	D	324	12/12	0.86	0.17	107,132,160,169	0
4	GOL	F	326	6/6	0.86	0.35	83,98,121,143	0
3	MES	D	325	12/12	0.86	0.15	85,140,157,157	0
4	GOL	G	328	6/6	0.87	0.18	50,79,101,104	0
4	GOL	G	326	6/6	0.87	0.29	91,96,115,116	0
3	MES	I	324	12/12	0.87	0.17	109,142,169,177	0
3	MES	J	324	12/12	0.87	0.13	139,157,169,184	0
4	GOL	I	325	6/6	0.88	0.10	88,93,105,121	0
4	GOL	I	328	6/6	0.88	0.77	87,95,119,124	0
4	GOL	B	327	6/6	0.88	0.14	55,62,83,90	0
3	MES	G	324	12/12	0.89	0.14	99,122,143,150	0
3	MES	E	324	12/12	0.90	0.09	123,143,171,178	0
4	GOL	G	327	4/6	0.90	0.34	86,96,104,106	0
4	GOL	I	326	6/6	0.91	0.26	73,91,114,119	0
4	GOL	D	327	6/6	0.91	0.25	51,79,98,109	0
4	GOL	C	325	6/6	0.91	0.13	60,66,78,92	0
4	GOL	D	326	6/6	0.91	0.39	96,100,101,106	0
4	GOL	E	326	6/6	0.92	0.16	67,89,129,133	0
2	ACH	J	323	10/10	0.93	0.20	56,74,82,89	0
3	MES	B	324	12/12	0.94	0.09	120,136,164,175	0
2	ACH	C	323	10/10	0.95	0.23	54,69,74,75	0
2	ACH	E	323	10/10	0.96	0.18	57,76,82,85	0
2	ACH	H	323	10/10	0.97	0.30	57,74,81,83	0
2	ACH	A	323	10/10	0.97	0.23	56,66,76,77	0
2	ACH	G	323	10/10	0.97	0.19	48,68,76,77	0
2	ACH	I	323	10/10	0.97	0.19	54,67,76,80	0
2	ACH	B	323	10/10	0.97	0.18	53,65,78,80	0
2	ACH	D	323	10/10	0.98	0.17	53,62,70,73	0
2	ACH	F	323	10/10	0.99	0.17	48,67,74,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.