



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:29 PM GMT

PDB ID : 3RQW
Title : Crystal structure of acetylcholine bound to a prokaryotic pentameric ligand-gated ion channel, ELIC
Authors : Pan, J.J.; Chen, Q.; Yoshida, K.; Cohen, A.; Kong, X.P.; Xu, Y.; Tang, P.
Deposited on : 2011-04-28
Resolution : 2.91 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

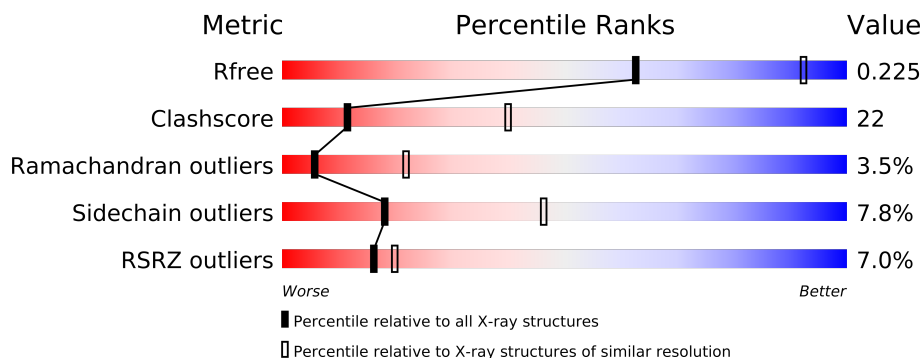
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACH	I	323	-	X
4	GOL	A	325	-	X
4	GOL	B	325	-	X
4	GOL	C	324	-	X
4	GOL	D	326	-	X
4	GOL	F	325	-	X
4	GOL	F	326	-	X
4	GOL	F	327	-	X
4	GOL	G	325	-	X
4	GOL	G	326	-	X
4	GOL	G	327	-	X
4	GOL	H	325	-	X
4	GOL	I	326	-	X
4	GOL	I	327	-	X
4	GOL	I	328	-	X

2 Entry composition

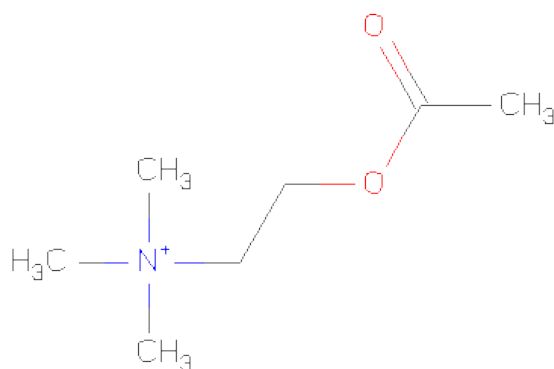
There are 5 unique types of molecules in this entry. The entry contains 25508 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*.

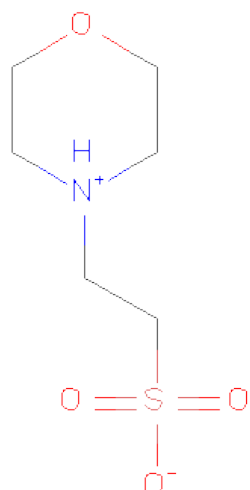
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505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

- Molecule 2 is ACETYLCHOLINE (three-letter code: ACH) (formula: $C_7H_{16}NO_2$).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (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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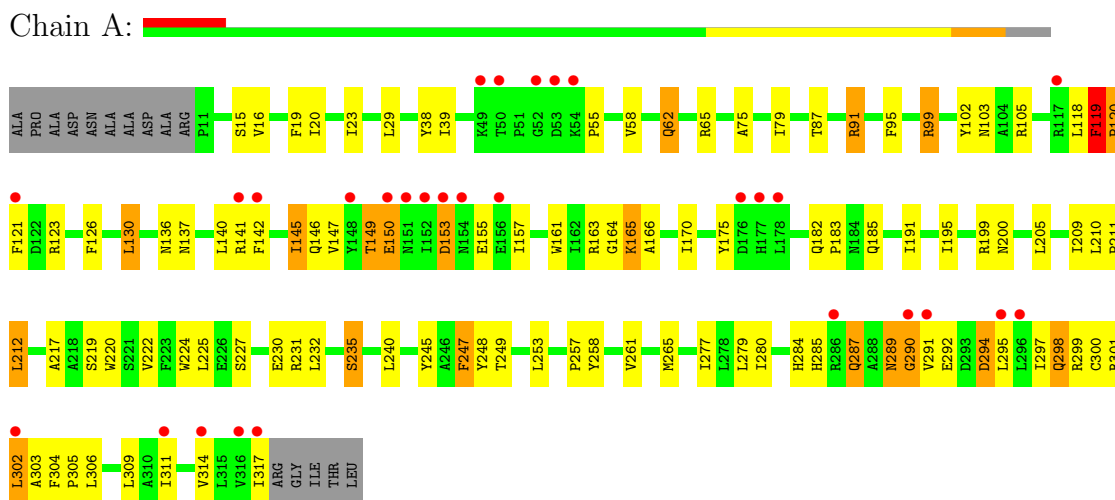
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	12	Total 12	O 12	0	0
5	H	7	Total 7	O 7	0	0
5	I	6	Total 6	O 6	0	0
5	J	7	Total 7	O 7	0	0

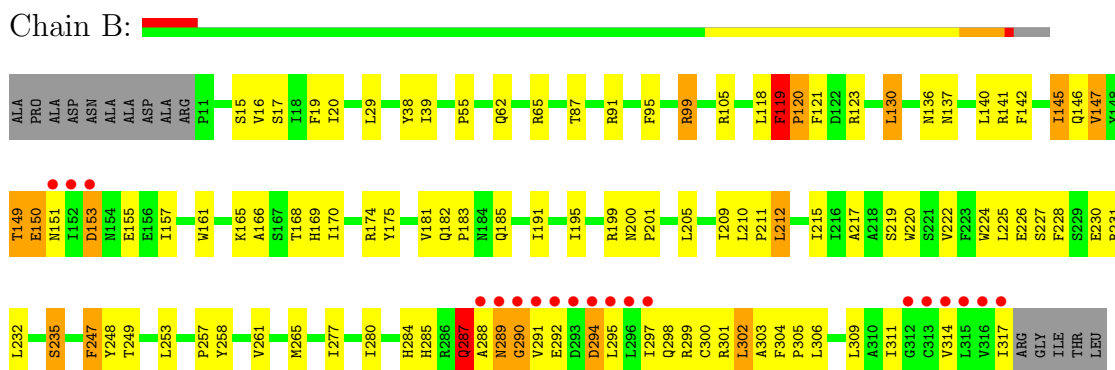
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

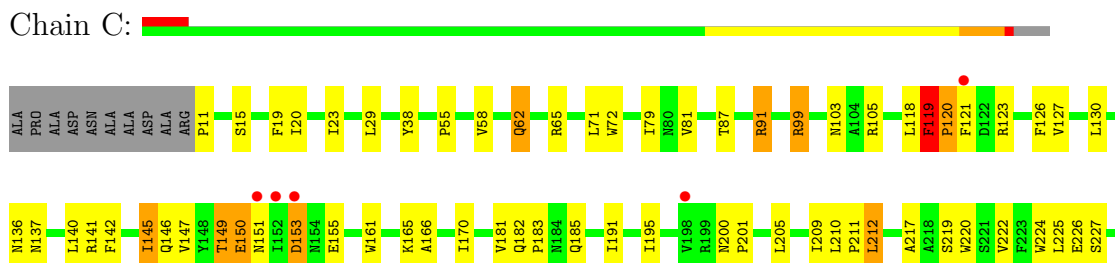
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

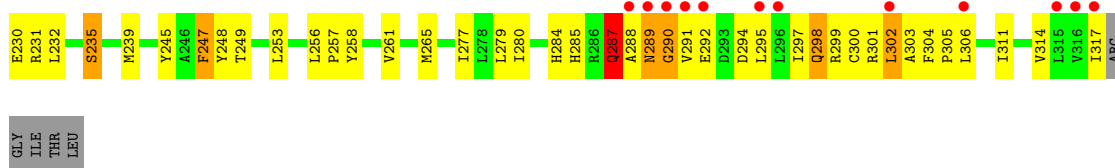


• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



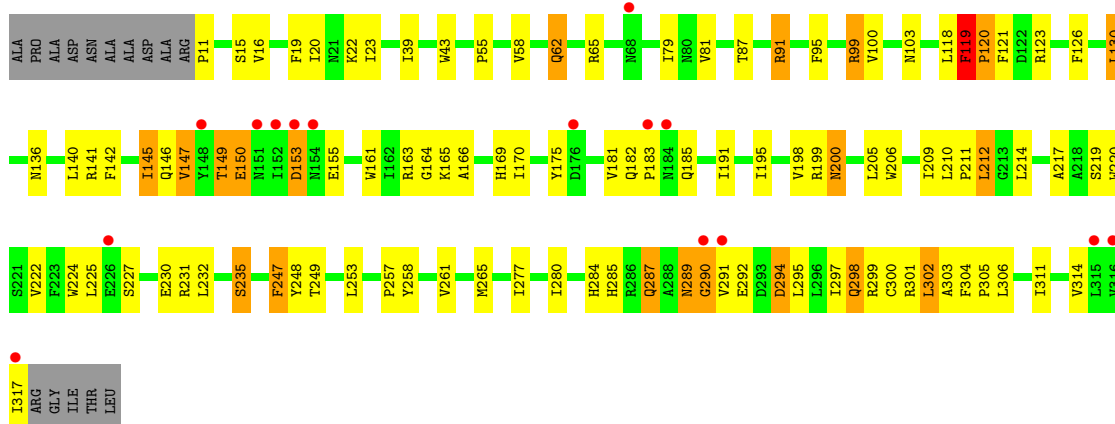
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*





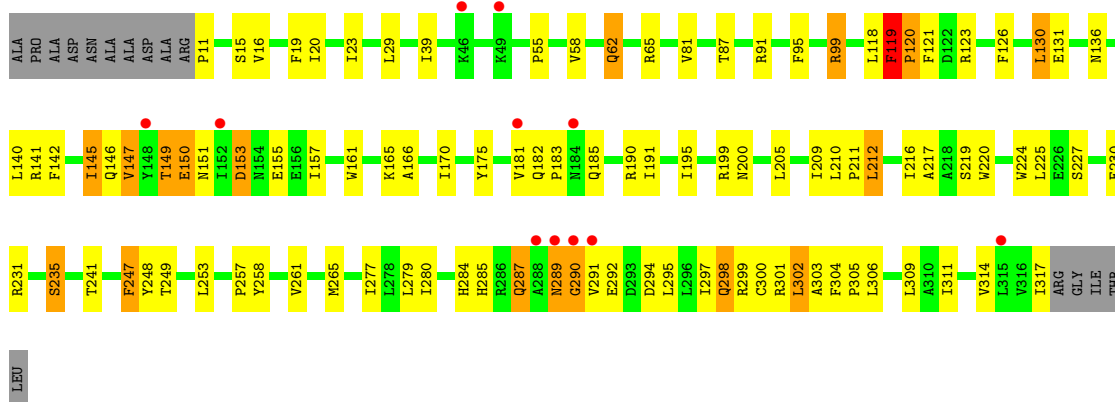
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

Chain D:



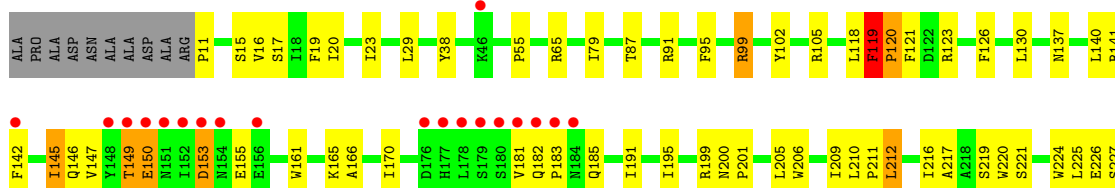
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

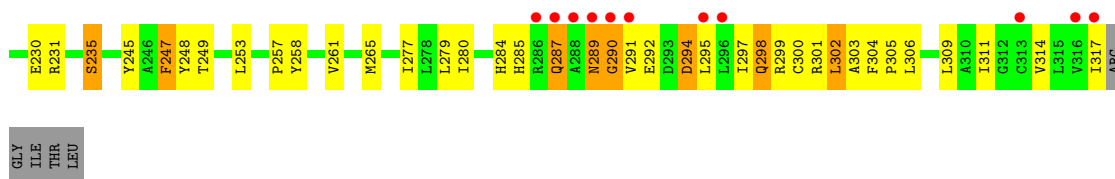
Chain E:



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

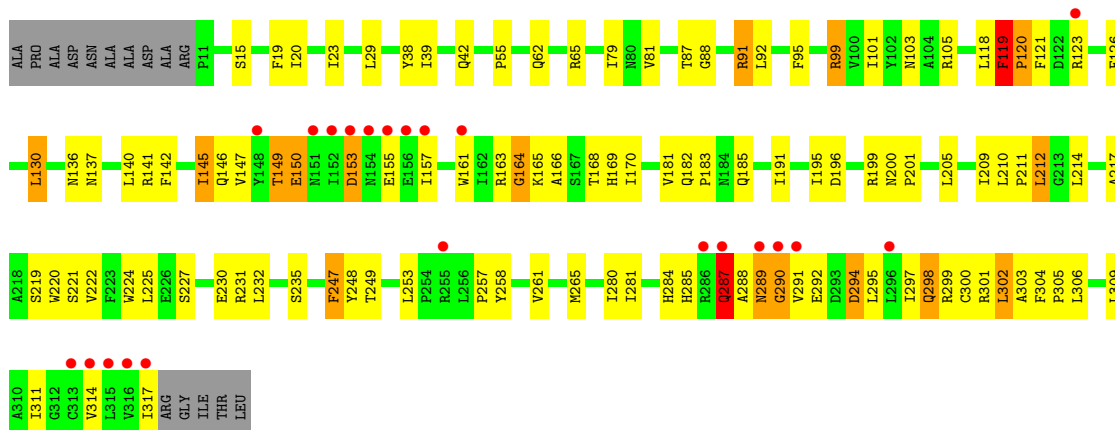
Chain F:





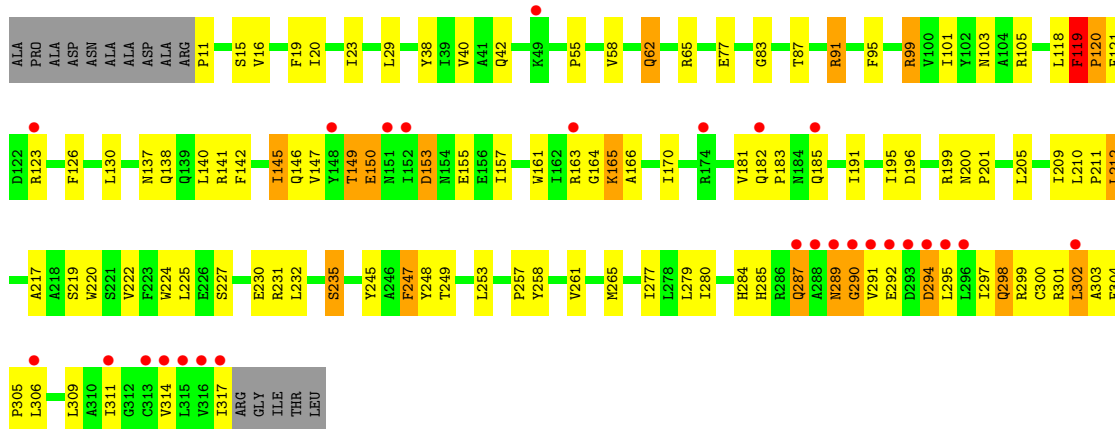
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

Chain G:



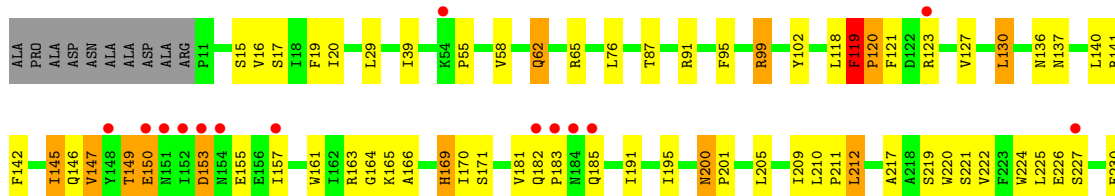
- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

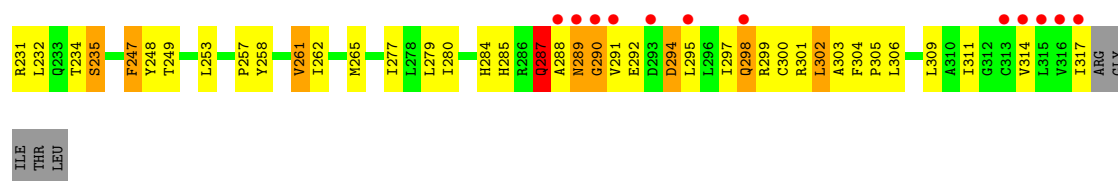
Chain H:



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

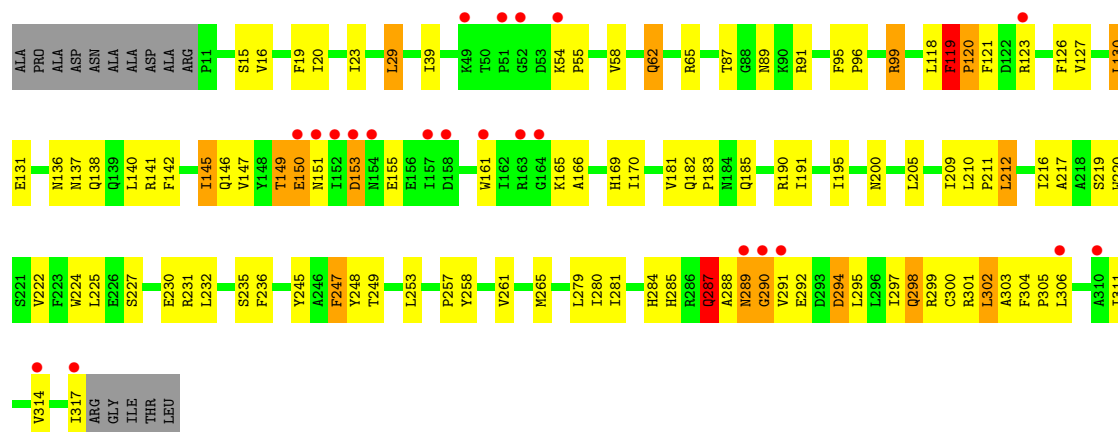
Chain I:





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

Chain J:



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 , 0.225	Depositor DCC
R_{free} test set	6264 reflections (5.03%)	DCC
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 , 62.9	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 124569 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25508	wwPDB-VP
Average B, all atoms (Å 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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	4	0	0	5	0
5	G	12	0	0	3	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (1114) close contacts within the same asymmetric unit are listed below.

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.57	0.87
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.57	0.86
1:H:99:ARG:HG3	1:H:99:ARG:HH11	1.39	0.85
1:E:295:LEU:HA	1:E:298:GLN:HE21	1.42	0.85
1:G:137:ASN:HA	4:G:328:GOL:O3	1.75	0.85
1:I:295:LEU:HA	1:I:298:GLN:HE21	1.42	0.85
1:I:137:ASN:HA	4:I:329:GOL:C1	2.07	0.84
1:G:295:LEU:HA	1:G:298:GLN:HE21	1.42	0.83
1:B:136:ASN:O	4:B:327:GOL:H32	1.78	0.83
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.60	0.83
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.59	0.83
1:F:11:PRO:HB3	4:F:328:GOL:H12	1.59	0.83
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.58	0.83
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.59	0.82
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.62	0.82
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.60	0.82
1:I:137:ASN:HA	4:I:329:GOL:H12	1.62	0.82
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.61	0.82
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.62	0.82
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.62	0.82
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.60	0.81
1:B:137:ASN:HA	4:B:327:GOL:C1	2.10	0.81
1:C:295:LEU:HA	1:C:298:GLN:HE21	1.46	0.81
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.61	0.81
1:I:145:ILE:CD1	1:I:166:ALA:HB3	2.11	0.81
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.62	0.80
1:A:140:LEU:HD21	5:A:335:HOH:O	1.80	0.80
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.63	0.80
1:I:140:LEU:HD11	5:I:334:HOH:O	1.82	0.80
1:J:140:LEU:HD21	5:J:330:HOH:O	1.80	0.80
1:A:295:LEU:HA	1:A:298:GLN:HE21	1.44	0.80
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.63	0.80
1:D:295:LEU:HA	1:D:298:GLN:HE21	1.45	0.80
1:F:295:LEU:HA	1:F:298:GLN:HE21	1.44	0.80
1:H:300:CYS:HB2	1:H:303:ALA:HB3	1.62	0.80
1:B:145:ILE:CD1	1:B:166:ALA:HB3	2.12	0.79
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.63	0.79
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.63	0.79
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.62	0.79
1:C:147:VAL:HG13	1:C:165:LYS:HE2	1.65	0.79
1:D:145:ILE:CD1	1:D:166:ALA:HB3	2.13	0.79
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:147:VAL:HG13	1:E:165:LYS:HE2	1.66	0.78
1:E:140:LEU:HD21	5:E:336:HOH:O	1.84	0.78
1:J:295:LEU:HA	1:J:298:GLN:HE21	1.46	0.77
1:H:295:LEU:HA	1:H:298:GLN:HE21	1.50	0.77
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.66	0.77
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.65	0.77
1:F:294:ASP:HB3	1:F:297:ILE:HG22	1.67	0.76
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.64	0.76
1:C:119:PHE:CD2	1:C:120:PRO:HD3	2.20	0.76
1:H:147:VAL:HG13	1:H:165:LYS:HE2	1.67	0.76
1:G:119:PHE:CD2	1:G:120:PRO:HD3	2.21	0.76
1:B:145:ILE:O	1:B:145:ILE:HD13	1.85	0.76
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.67	0.75
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.69	0.75
1:F:147:VAL:HG13	1:F:165:LYS:HE2	1.68	0.75
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.69	0.75
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.68	0.74
1:F:119:PHE:CD2	1:F:120:PRO:HD3	2.22	0.74
1:B:295:LEU:HA	1:B:298:GLN:HE21	1.52	0.74
1:D:119:PHE:CD2	1:D:120:PRO:HD3	2.22	0.74
1:A:145:ILE:CD1	1:A:166:ALA:HB3	2.17	0.74
1:J:137:ASN:O	5:J:326:HOH:O	2.05	0.74
1:J:119:PHE:CD2	1:J:120:PRO:HD3	2.23	0.74
1:J:140:LEU:HD11	5:J:330:HOH:O	1.87	0.73
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.70	0.73
1:A:119:PHE:CD2	1:A:120:PRO:HD3	2.22	0.73
1:A:147:VAL:HG13	1:A:165:LYS:HE2	1.70	0.73
1:F:145:ILE:CD1	1:F:166:ALA:HB3	2.18	0.73
1:H:137:ASN:HA	4:H:324:GOL:O1	1.89	0.73
1:G:145:ILE:CD1	1:G:166:ALA:HB3	2.19	0.73
1:J:137:ASN:HA	4:J:325:GOL:O1	1.89	0.73
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.69	0.73
1:D:294:ASP:HB3	1:D:297:ILE:HG22	1.71	0.72
1:A:137:ASN:HA	4:A:326:GOL:O1	1.89	0.72
1:I:137:ASN:HA	4:I:329:GOL:O1	1.90	0.72
1:G:105:ARG:HG2	4:H:325:GOL:H11	1.72	0.72
1:B:137:ASN:HA	4:B:327:GOL:O1	1.89	0.72
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.71	0.72
1:D:147:VAL:HG13	1:D:165:LYS:HE2	1.70	0.72
1:G:137:ASN:HA	4:G:328:GOL:C3	2.20	0.72
1:C:294:ASP:HB3	1:C:297:ILE:HG22	1.72	0.71
1:A:294:ASP:HB3	1:A:297:ILE:HG22	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:105:ARG:HG3	4:H:325:GOL:H31	1.72	0.71
1:C:145:ILE:CD1	1:C:166:ALA:HB3	2.19	0.71
1:J:145:ILE:CD1	1:J:166:ALA:HB3	2.19	0.71
1:G:88:GLY:HA3	4:H:325:GOL:H12	1.72	0.71
1:I:119:PHE:CD2	1:I:120:PRO:HD3	2.25	0.71
1:E:119:PHE:CD2	1:E:120:PRO:HD3	2.26	0.70
1:G:99:ARG:HG3	1:G:99:ARG:NH1	2.05	0.70
1:F:137:ASN:HA	4:F:328:GOL:O1	1.91	0.70
1:G:294:ASP:HB3	1:G:297:ILE:HG22	1.73	0.70
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.72	0.70
1:I:147:VAL:HG13	1:I:165:LYS:HE2	1.72	0.70
1:D:119:PHE:C	1:D:121:PHE:H	1.94	0.69
1:H:119:PHE:CD2	1:H:120:PRO:HD3	2.27	0.69
1:G:145:ILE:O	1:G:145:ILE:HD13	1.93	0.69
1:H:145:ILE:CD1	1:H:166:ALA:HB3	2.22	0.69
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.73	0.69
1:I:294:ASP:HB3	1:I:297:ILE:HG22	1.74	0.69
1:F:145:ILE:HD13	1:F:145:ILE:O	1.92	0.69
1:I:102:TYR:CE2	4:I:327:GOL:H2	2.28	0.69
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.75	0.69
1:E:145:ILE:CD1	1:E:166:ALA:HB3	2.22	0.69
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.08	0.69
1:H:294:ASP:HB3	1:H:297:ILE:HG22	1.73	0.69
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.74	0.69
1:J:145:ILE:HD13	1:J:145:ILE:O	1.94	0.68
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.75	0.68
1:B:294:ASP:HB3	1:B:297:ILE:HG22	1.75	0.68
1:E:166:ALA:HB2	1:E:195:ILE:HG12	1.75	0.68
1:J:147:VAL:HG13	1:J:165:LYS:HE2	1.73	0.68
1:H:257:PRO:HG2	1:H:258:TYR:CD2	2.28	0.68
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.76	0.68
1:H:166:ALA:HB2	1:H:195:ILE:HG12	1.74	0.68
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.75	0.68
1:H:119:PHE:C	1:H:121:PHE:H	1.98	0.68
1:B:141:ARG:HG3	1:B:142:PHE:CD2	2.29	0.68
1:F:99:ARG:HG3	1:F:99:ARG:NH1	2.06	0.67
1:J:138:GLN:HB2	5:J:326:HOH:O	1.94	0.67
1:B:119:PHE:CD2	1:B:120:PRO:HD3	2.29	0.67
1:H:55:PRO:HG2	1:I:181:VAL:HG13	1.74	0.67
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.29	0.67
1:D:147:VAL:CG1	1:D:165:LYS:HE2	2.24	0.67
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:257:PRO:HG2	1:E:258:TYR:CD2	2.30	0.67
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.30	0.67
1:J:99:ARG:HG3	1:J:99:ARG:NH1	2.07	0.67
1:I:145:ILE:HD13	1:I:145:ILE:O	1.95	0.67
1:I:182:GLN:HB3	1:I:183:PRO:HD2	1.76	0.67
1:G:141:ARG:NH1	5:G:329:HOH:O	2.28	0.67
1:D:145:ILE:O	1:D:145:ILE:HD13	1.95	0.66
1:D:119:PHE:O	1:D:121:PHE:N	2.24	0.66
1:G:147:VAL:HG13	1:G:165:LYS:HE2	1.76	0.66
1:H:182:GLN:HB3	1:H:183:PRO:HD2	1.76	0.66
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.10	0.66
1:D:182:GLN:HB3	1:D:183:PRO:HD2	1.77	0.66
1:E:147:VAL:CG1	1:E:165:LYS:HE2	2.25	0.66
1:C:119:PHE:C	1:C:121:PHE:H	1.98	0.66
1:I:257:PRO:HG2	1:I:258:TYR:CD2	2.31	0.66
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.10	0.66
1:C:147:VAL:CG1	1:C:165:LYS:HE2	2.26	0.66
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.31	0.66
1:A:289:ASN:CG	1:A:290:GLY:H	1.99	0.66
1:A:145:ILE:HD13	1:A:145:ILE:O	1.95	0.66
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.77	0.66
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.11	0.66
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.78	0.66
1:F:147:VAL:CG1	1:F:165:LYS:HE2	2.25	0.65
1:E:119:PHE:C	1:E:121:PHE:H	1.99	0.65
1:I:289:ASN:CG	1:I:290:GLY:H	2.00	0.65
1:G:289:ASN:CG	1:G:290:GLY:H	2.00	0.65
1:C:289:ASN:CG	1:C:290:GLY:H	2.00	0.65
1:E:141:ARG:HG3	1:E:142:PHE:CD2	2.32	0.65
1:A:147:VAL:CG1	1:A:165:LYS:HE2	2.26	0.65
1:H:137:ASN:HA	4:H:324:GOL:C1	2.27	0.65
1:B:119:PHE:C	1:B:121:PHE:H	2.00	0.65
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.30	0.65
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.30	0.65
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.11	0.65
1:J:119:PHE:C	1:J:121:PHE:H	1.99	0.65
1:G:147:VAL:CG1	1:G:165:LYS:HE2	2.27	0.65
1:E:289:ASN:CG	1:E:290:GLY:H	2.00	0.65
1:F:289:ASN:CG	1:F:290:GLY:H	1.99	0.65
1:B:182:GLN:HB3	1:B:183:PRO:HD2	1.77	0.64
1:F:206:TRP:CD1	3:F:324:MES:H71	2.33	0.64
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.13	0.64

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:99:ARG:HG3	1:C:99:ARG:NH1	2.11	0.61
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.16	0.61
1:H:147:VAL:CG1	1:H:165:LYS:HE2	2.31	0.61
1:F:206:TRP:NE1	3:F:324:MES:H71	2.16	0.61
1:J:89:ASN:ND2	5:J:331:HOH:O	2.33	0.61
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.35	0.61
1:I:166:ALA:HB2	1:I:195:ILE:HG12	1.82	0.60
1:G:248:TYR:CD1	1:H:247:PHE:HA	2.36	0.60
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.16	0.60
1:G:168:THR:C	1:G:169:HIS:ND1	2.54	0.60
1:E:15:SER:HB3	1:E:141:ARG:HD3	1.82	0.60
1:J:257:PRO:HG2	1:J:258:TYR:CD2	2.35	0.60
1:G:224:TRP:HE1	1:G:301:ARG:HB3	1.66	0.60
1:G:182:GLN:HB3	1:G:183:PRO:HD2	1.81	0.60
1:C:141:ARG:HG3	1:C:142:PHE:CD2	2.35	0.60
1:G:166:ALA:HB2	1:G:195:ILE:HG12	1.83	0.60
1:J:137:ASN:HA	4:J:325:GOL:H2	1.84	0.60
1:H:99:ARG:NH1	1:H:99:ARG:HG3	2.13	0.60
1:B:147:VAL:HG13	1:B:165:LYS:HE2	1.83	0.60
1:D:141:ARG:HG3	1:D:142:PHE:CD2	2.37	0.60
1:E:99:ARG:NH1	1:E:99:ARG:HG3	2.08	0.60
1:I:136:ASN:O	4:I:329:GOL:C3	2.48	0.60
1:E:140:LEU:HD13	1:E:191:ILE:CG1	2.29	0.59
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.67	0.59
1:I:15:SER:HB3	1:I:141:ARG:HD3	1.83	0.59
1:C:55:PRO:HG2	1:D:181:VAL:HG13	1.83	0.59
1:D:99:ARG:NH1	1:D:99:ARG:HG3	2.08	0.59
1:E:210:LEU:HB3	1:E:211:PRO:CD	2.33	0.59
1:I:15:SER:HB3	1:I:141:ARG:CG	2.33	0.59
1:B:302:LEU:O	1:B:306:LEU:HG	2.03	0.59
1:F:20:ILE:HD12	1:F:195:ILE:HD11	1.84	0.59
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.32	0.58
1:E:136:ASN:O	4:E:326:GOL:H32	2.03	0.58
1:D:118:LEU:O	1:D:119:PHE:O	2.21	0.58
1:J:302:LEU:O	1:J:306:LEU:HG	2.03	0.58
1:H:165:LYS:H	1:H:165:LYS:HD2	1.67	0.58
1:I:147:VAL:HG22	1:I:147:VAL:O	2.03	0.58
1:G:136:ASN:O	4:G:328:GOL:C2	2.47	0.58
1:F:294:ASP:HB3	1:F:297:ILE:CG2	2.31	0.58
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.86	0.58
1:B:147:VAL:CG1	1:B:165:LYS:HE2	2.34	0.58
1:C:302:LEU:O	1:C:306:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:247:PHE:HA	1:J:248:TYR:CD1	2.39	0.58
1:D:294:ASP:HB3	1:D:297:ILE:CG2	2.34	0.57
1:F:224:TRP:HE1	1:F:301:ARG:HB3	1.68	0.57
1:F:15:SER:HB3	1:F:141:ARG:HD3	1.87	0.57
1:G:302:LEU:O	1:G:306:LEU:HG	2.04	0.57
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.34	0.57
1:F:225:LEU:CD2	1:G:232:LEU:HD23	2.34	0.57
1:H:294:ASP:HB3	1:H:297:ILE:CG2	2.35	0.57
1:B:140:LEU:HD21	5:B:332:HOH:O	2.04	0.57
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.69	0.57
1:H:147:VAL:O	1:H:147:VAL:HG22	2.04	0.57
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.87	0.57
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.68	0.57
1:F:19:PHE:CD1	2:F:323:ACH:H61	2.40	0.57
1:B:175:TYR:HD1	4:B:326:GOL:H11	1.69	0.56
1:G:294:ASP:HB3	1:G:297:ILE:CG2	2.35	0.56
1:I:145:ILE:HD11	1:I:166:ALA:HB3	1.86	0.56
1:F:182:GLN:HB2	1:F:185:GLN:HG2	1.87	0.56
1:J:15:SER:HB3	1:J:141:ARG:CG	2.35	0.56
1:B:212:LEU:HB3	1:B:265:MET:HE1	1.87	0.56
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.40	0.56
1:F:118:LEU:O	1:F:119:PHE:O	2.23	0.56
1:J:182:GLN:HB2	1:J:185:GLN:HG2	1.86	0.56
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.87	0.56
1:A:247:PHE:HA	1:E:248:TYR:CD1	2.41	0.56
1:B:257:PRO:HG2	1:B:258:TYR:HD2	1.71	0.56
1:A:302:LEU:O	1:A:306:LEU:HG	2.05	0.56
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.36	0.56
1:E:302:LEU:O	1:E:306:LEU:HG	2.05	0.56
1:G:119:PHE:CG	1:G:120:PRO:N	2.73	0.56
1:G:163:ARG:O	1:G:164:GLY:O	2.24	0.56
1:A:20:ILE:HD12	1:A:195:ILE:HD11	1.88	0.56
1:B:248:TYR:HA	1:C:247:PHE:CE1	2.41	0.56
1:H:141:ARG:HG3	1:H:142:PHE:CD2	2.41	0.56
1:A:55:PRO:HG2	1:B:181:VAL:HG13	1.87	0.56
1:B:145:ILE:HD11	1:B:166:ALA:HB3	1.87	0.56
1:C:119:PHE:CD2	1:C:120:PRO:CD	2.89	0.56
1:A:294:ASP:HB3	1:A:297:ILE:CG2	2.35	0.55
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.35	0.55
1:A:119:PHE:CG	1:A:120:PRO:N	2.75	0.55
1:A:118:LEU:O	1:A:119:PHE:O	2.24	0.55
1:C:182:GLN:HB2	1:C:185:GLN:HG2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:SER:HB3	1:A:141:ARG:HD3	1.88	0.55
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.36	0.55
1:G:248:TYR:HA	1:H:247:PHE:CE1	2.42	0.55
1:I:210:LEU:HB3	1:I:211:PRO:CD	2.34	0.55
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.89	0.55
1:H:119:PHE:CG	1:H:120:PRO:N	2.75	0.55
1:I:15:SER:HB3	1:I:141:ARG:CD	2.36	0.55
1:B:119:PHE:CG	1:B:120:PRO:N	2.75	0.55
1:I:141:ARG:HG3	1:I:142:PHE:CD2	2.42	0.55
1:A:75:ALA:HA	4:A:325:GOL:H2	1.88	0.55
1:D:119:PHE:C	1:D:121:PHE:N	2.59	0.55
1:J:119:PHE:CG	1:J:120:PRO:N	2.75	0.55
1:C:147:VAL:HG22	1:C:147:VAL:O	2.07	0.55
1:E:147:VAL:HG22	1:E:147:VAL:O	2.07	0.55
1:B:118:LEU:O	1:B:119:PHE:O	2.24	0.55
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.71	0.55
1:F:248:TYR:CD1	1:G:247:PHE:HA	2.42	0.55
1:E:210:LEU:CB	1:E:211:PRO:HD3	2.34	0.55
1:F:247:PHE:CE1	1:J:248:TYR:HA	2.42	0.55
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.42	0.55
1:C:140:LEU:HD13	1:C:191:ILE:CG1	2.35	0.54
1:C:294:ASP:HB3	1:C:297:ILE:CG2	2.35	0.54
1:D:119:PHE:CG	1:D:120:PRO:N	2.75	0.54
1:A:119:PHE:O	1:A:121:PHE:N	2.33	0.54
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.89	0.54
1:G:182:GLN:HB2	1:G:185:GLN:HG2	1.89	0.54
1:D:147:VAL:O	1:D:147:VAL:HG22	2.07	0.54
1:E:20:ILE:HD12	1:E:195:ILE:HD11	1.89	0.54
1:E:15:SER:HB3	1:E:141:ARG:CD	2.36	0.54
1:J:15:SER:HB3	1:J:141:ARG:HD3	1.89	0.54
1:D:314:VAL:HG12	1:D:314:VAL:O	2.08	0.54
1:G:105:ARG:HG2	4:H:325:GOL:C1	2.36	0.54
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.89	0.54
1:G:314:VAL:O	1:G:314:VAL:HG12	2.08	0.54
1:G:257:PRO:HG2	1:G:258:TYR:HD2	1.72	0.54
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.71	0.54
1:C:224:TRP:HE1	1:C:301:ARG:HB3	1.73	0.54
1:A:248:TYR:CD1	1:B:247:PHE:HA	2.43	0.54
1:J:210:LEU:HB3	1:J:211:PRO:CD	2.36	0.54
1:B:15:SER:HB3	1:B:141:ARG:HD3	1.89	0.54
1:C:15:SER:HB3	1:C:141:ARG:HD3	1.89	0.54
1:I:302:LEU:O	1:I:306:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:147:VAL:HG13	1:G:147:VAL:O	2.07	0.54
1:J:142:PHE:HA	1:J:170:ILE:HD11	1.88	0.54
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.37	0.54
1:D:302:LEU:O	1:D:306:LEU:HG	2.08	0.54
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.37	0.54
1:G:20:ILE:HD12	1:G:195:ILE:HD11	1.90	0.54
1:C:119:PHE:CG	1:C:120:PRO:N	2.76	0.54
1:B:225:LEU:CD2	1:C:232:LEU:HD23	2.38	0.54
1:A:182:GLN:HB2	1:A:185:GLN:HG2	1.89	0.54
1:D:15:SER:HB3	1:D:141:ARG:HD3	1.90	0.54
1:H:142:PHE:HA	1:H:170:ILE:HD11	1.89	0.54
1:F:302:LEU:O	1:F:306:LEU:HG	2.07	0.54
1:F:147:VAL:HG22	1:F:147:VAL:O	2.07	0.54
1:D:182:GLN:HB2	1:D:185:GLN:HG2	1.90	0.54
1:C:20:ILE:HD12	1:C:195:ILE:HD11	1.90	0.53
1:J:96:PRO:HD2	5:J:332:HOH:O	2.08	0.53
1:G:119:PHE:CD2	1:G:120:PRO:CD	2.91	0.53
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.43	0.53
1:I:205:LEU:HD23	1:I:209:ILE:HD12	1.91	0.53
1:I:20:ILE:HD12	1:I:195:ILE:HD11	1.90	0.53
1:A:147:VAL:HG22	1:A:147:VAL:O	2.07	0.53
1:E:182:GLN:HB2	1:E:185:GLN:HG2	1.90	0.53
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.73	0.53
1:H:91:ARG:HD3	1:H:103:ASN:HB3	1.90	0.53
1:F:314:VAL:HG12	1:F:314:VAL:O	2.09	0.53
1:J:294:ASP:HB3	1:J:297:ILE:CG2	2.37	0.53
1:B:182:GLN:HB2	1:B:185:GLN:HG2	1.90	0.53
1:G:168:THR:O	1:G:169:HIS:ND1	2.41	0.53
1:C:142:PHE:HA	1:C:170:ILE:HD11	1.91	0.53
1:F:227:SER:HB3	1:F:230:GLU:CG	2.38	0.53
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.44	0.53
1:H:297:ILE:HG23	1:H:298:GLN:N	2.24	0.53
1:C:15:SER:HB3	1:C:141:ARG:CG	2.39	0.53
1:C:314:VAL:O	1:C:314:VAL:HG12	2.08	0.53
1:F:150:GLU:HG3	1:F:153:ASP:HB2	1.91	0.53
1:F:55:PRO:HG2	1:G:181:VAL:HG13	1.89	0.53
1:I:294:ASP:HB3	1:I:297:ILE:CG2	2.37	0.53
1:A:225:LEU:CD2	1:B:232:LEU:HD23	2.39	0.53
1:B:314:VAL:HG12	1:B:314:VAL:O	2.09	0.53
2:J:323:ACH:H102	2:J:323:ACH:O4	2.08	0.53
1:F:142:PHE:HA	1:F:170:ILE:HD11	1.90	0.53
1:D:15:SER:HB3	1:D:141:ARG:CG	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:227:SER:HB3	1:H:230:GLU:HG3	1.90	0.53
1:H:140:LEU:HD13	1:H:191:ILE:CG1	2.39	0.53
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.43	0.53
1:J:119:PHE:O	1:J:121:PHE:N	2.32	0.53
1:E:119:PHE:CG	1:E:120:PRO:N	2.77	0.53
1:B:119:PHE:O	1:B:121:PHE:N	2.31	0.53
1:I:225:LEU:HD21	1:J:232:LEU:HD23	1.91	0.53
1:A:210:LEU:HB3	1:A:211:PRO:CD	2.36	0.52
1:G:210:LEU:HB3	1:G:211:PRO:CD	2.36	0.52
1:E:15:SER:HB3	1:E:141:ARG:CG	2.39	0.52
1:H:212:LEU:HB3	1:H:265:MET:HE1	1.91	0.52
1:E:150:GLU:HG3	1:E:153:ASP:HB2	1.92	0.52
1:F:140:LEU:CD2	5:F:331:HOH:O	2.43	0.52
1:D:55:PRO:HG2	1:E:181:VAL:HG13	1.92	0.52
1:J:136:ASN:O	4:J:325:GOL:C2	2.50	0.52
1:F:119:PHE:CG	1:F:120:PRO:N	2.77	0.52
1:D:119:PHE:CD2	1:D:120:PRO:CD	2.91	0.52
1:I:142:PHE:HA	1:I:170:ILE:HD11	1.91	0.52
1:A:314:VAL:O	1:A:314:VAL:HG12	2.09	0.52
1:A:99:ARG:CG	1:A:99:ARG:HH11	2.14	0.52
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.90	0.52
1:D:140:LEU:CD1	5:D:341:HOH:O	2.28	0.52
1:F:119:PHE:CD2	1:F:120:PRO:CD	2.93	0.52
1:J:118:LEU:O	1:J:119:PHE:O	2.28	0.52
1:J:212:LEU:CD1	1:J:265:MET:HB3	2.39	0.52
1:I:118:LEU:O	1:I:119:PHE:O	2.28	0.52
1:A:15:SER:HB3	1:A:141:ARG:CG	2.39	0.52
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.40	0.52
1:B:168:THR:C	1:B:169:HIS:CD2	2.83	0.52
1:H:118:LEU:O	1:H:119:PHE:O	2.28	0.52
1:I:102:TYR:HE2	4:I:327:GOL:H2	1.74	0.52
1:I:15:SER:HB2	1:I:142:PHE:CE1	2.45	0.52
1:I:15:SER:HB3	1:I:141:ARG:HG2	1.91	0.52
1:B:19:PHE:CD1	2:B:323:ACH:H61	2.45	0.52
1:H:140:LEU:CD2	5:H:331:HOH:O	2.47	0.52
1:D:257:PRO:HG2	1:D:258:TYR:HD2	1.74	0.52
1:G:225:LEU:CD2	1:H:232:LEU:HD23	2.40	0.52
1:G:150:GLU:HG3	1:G:153:ASP:HB2	1.92	0.52
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.40	0.52
1:I:314:VAL:HG12	1:I:314:VAL:O	2.10	0.52
1:I:212:LEU:HB3	1:I:265:MET:HE1	1.91	0.52
1:F:205:LEU:HD23	1:F:209:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:314:VAL:O	1:H:314:VAL:HG12	2.10	0.52
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.38	0.51
1:E:118:LEU:O	1:E:119:PHE:O	2.28	0.51
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.44	0.51
1:E:314:VAL:O	1:E:314:VAL:HG12	2.10	0.51
1:H:297:ILE:CG2	1:H:298:GLN:N	2.73	0.51
1:C:119:PHE:C	1:C:121:PHE:N	2.63	0.51
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.45	0.51
1:D:150:GLU:HG3	1:D:153:ASP:HB2	1.92	0.51
1:D:210:LEU:CB	1:D:211:PRO:HD3	2.38	0.51
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.92	0.51
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.93	0.51
1:A:142:PHE:HA	1:A:170:ILE:HD11	1.92	0.51
1:A:212:LEU:CD1	1:A:265:MET:HB3	2.39	0.51
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.40	0.51
1:D:145:ILE:HG13	1:D:166:ALA:HB3	1.93	0.51
1:G:118:LEU:O	1:G:119:PHE:O	2.29	0.51
1:A:145:ILE:HD11	1:A:166:ALA:HB3	1.92	0.51
1:D:141:ARG:NH1	5:D:329:HOH:O	2.31	0.51
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.46	0.51
1:F:137:ASN:HA	4:F:328:GOL:C1	2.41	0.51
1:A:297:ILE:HG23	1:A:298:GLN:N	2.26	0.51
1:B:15:SER:HB3	1:B:141:ARG:CG	2.40	0.51
1:C:248:TYR:CD1	1:D:247:PHE:HA	2.45	0.51
1:D:95:PHE:CD2	1:D:99:ARG:HB2	2.45	0.51
1:I:150:GLU:HG3	1:I:153:ASP:HB2	1.92	0.51
1:C:15:SER:HB2	1:C:142:PHE:CE1	2.46	0.51
1:D:11:PRO:CD	5:D:339:HOH:O	2.59	0.51
1:I:182:GLN:HB2	1:I:185:GLN:HG2	1.91	0.51
1:F:301:ARG:HH12	1:G:285:HIS:CE1	2.29	0.51
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.51
1:J:137:ASN:HA	4:J:325:GOL:C2	2.41	0.51
1:G:119:PHE:O	1:G:121:PHE:N	2.33	0.51
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.75	0.51
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.74	0.51
1:H:15:SER:HB3	1:H:141:ARG:HD3	1.93	0.51
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.41	0.51
1:C:210:LEU:HB3	1:C:211:PRO:CD	2.41	0.50
1:F:145:ILE:HD11	1:F:166:ALA:HB3	1.92	0.50
1:I:119:PHE:CG	1:I:120:PRO:N	2.79	0.50
1:F:15:SER:HB3	1:F:141:ARG:CG	2.41	0.50
1:H:227:SER:HB3	1:H:230:GLU:CG	2.40	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.94	0.50
1:B:119:PHE:C	1:B:121:PHE:N	2.65	0.50
1:H:182:GLN:HB2	1:H:185:GLN:HG2	1.93	0.50
1:D:11:PRO:HD2	5:D:339:HOH:O	2.09	0.50
1:F:38:TYR:CE1	1:F:105:ARG:HD3	2.46	0.50
1:F:235:SER:HB3	1:F:277:ILE:HD11	1.93	0.50
1:A:150:GLU:HG3	1:A:153:ASP:HB2	1.92	0.50
1:G:137:ASN:CA	4:G:328:GOL:O3	2.55	0.50
1:B:150:GLU:HG3	1:B:153:ASP:HB2	1.92	0.50
1:I:19:PHE:CD1	2:I:323:ACH:H61	2.47	0.50
1:J:150:GLU:HG3	1:J:153:ASP:HB2	1.92	0.50
1:E:11:PRO:N	5:E:332:HOH:O	2.43	0.50
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.93	0.50
1:J:119:PHE:C	1:J:121:PHE:N	2.65	0.50
1:B:15:SER:HB3	1:B:141:ARG:HG2	1.93	0.50
1:C:284:HIS:HD2	1:C:285:HIS:NE2	2.09	0.50
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.93	0.50
1:E:297:ILE:HG23	1:E:298:GLN:N	2.26	0.50
1:H:150:GLU:HG3	1:H:153:ASP:HB2	1.92	0.50
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.46	0.50
1:J:314:VAL:HG12	1:J:314:VAL:O	2.10	0.50
1:A:297:ILE:CG2	1:A:298:GLN:N	2.75	0.50
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.92	0.50
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.42	0.50
1:E:227:SER:HB3	1:E:230:GLU:CG	2.41	0.50
2:F:323:ACH:O4	2:F:323:ACH:H102	2.12	0.50
1:D:161:TRP:CZ2	1:D:200:ASN:ND2	2.80	0.50
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.46	0.50
2:D:323:ACH:H101	1:E:175:TYR:CZ	2.46	0.50
1:D:136:ASN:O	4:D:327:GOL:H32	2.12	0.50
1:G:297:ILE:HG23	1:G:298:GLN:N	2.27	0.50
1:B:147:VAL:O	1:B:147:VAL:HG22	2.12	0.50
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.47	0.50
1:D:91:ARG:HD3	1:D:103:ASN:HB3	1.94	0.50
1:D:140:LEU:CD2	5:D:341:HOH:O	2.33	0.50
1:B:210:LEU:HB3	1:B:211:PRO:CD	2.37	0.50
1:J:297:ILE:HG23	1:J:298:GLN:N	2.26	0.50
1:A:225:LEU:HB2	1:A:231:ARG:HG3	1.93	0.50
1:B:15:SER:HB2	1:B:142:PHE:CE1	2.47	0.50
1:E:142:PHE:HA	1:E:170:ILE:HD11	1.93	0.50
1:D:212:LEU:HB3	1:D:265:MET:HE1	1.94	0.50
1:G:297:ILE:C	1:G:299:ARG:N	2.66	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:210:LEU:CB	1:J:211:PRO:HD3	2.40	0.50
1:G:119:PHE:HE1	1:G:199:ARG:CZ	2.25	0.50
1:H:119:PHE:O	1:H:121:PHE:N	2.30	0.50
1:H:225:LEU:HB2	1:H:231:ARG:HG3	1.93	0.50
1:J:147:VAL:HG22	1:J:147:VAL:O	2.12	0.50
1:F:212:LEU:HB3	1:F:265:MET:HE1	1.93	0.50
1:H:248:TYR:CD1	1:I:247:PHE:HA	2.46	0.50
1:C:150:GLU:HG3	1:C:153:ASP:HB2	1.92	0.50
1:G:55:PRO:HG2	1:H:181:VAL:HG13	1.93	0.50
1:B:297:ILE:HG23	1:B:298:GLN:N	2.26	0.49
1:J:119:PHE:CD2	1:J:120:PRO:CD	2.94	0.49
1:E:119:PHE:C	1:E:121:PHE:N	2.65	0.49
1:A:247:PHE:CE1	1:E:248:TYR:HA	2.46	0.49
1:G:212:LEU:HB3	1:G:265:MET:HE1	1.94	0.49
1:D:205:LEU:HD23	1:D:209:ILE:HD12	1.93	0.49
1:A:175:TYR:OH	2:E:323:ACH:H101	2.12	0.49
1:B:175:TYR:CD1	4:B:326:GOL:H11	2.45	0.49
1:G:99:ARG:CG	1:G:99:ARG:HH11	2.12	0.49
1:I:297:ILE:HG23	1:I:298:GLN:N	2.27	0.49
1:C:205:LEU:HD23	1:C:209:ILE:HD12	1.95	0.49
1:C:227:SER:HB3	1:C:230:GLU:HG3	1.93	0.49
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.47	0.49
1:A:227:SER:HB3	1:A:230:GLU:HG3	1.94	0.49
1:I:149:THR:O	1:I:150:GLU:HB3	2.12	0.49
1:A:205:LEU:HD23	1:A:209:ILE:HD12	1.93	0.49
1:F:297:ILE:HG23	1:F:298:GLN:N	2.27	0.49
1:F:145:ILE:HG13	1:F:166:ALA:HB3	1.94	0.49
1:H:119:PHE:CD2	1:H:120:PRO:CD	2.96	0.49
1:B:15:SER:HB3	1:B:141:ARG:CD	2.42	0.49
1:A:15:SER:HB2	1:A:142:PHE:CE1	2.47	0.49
1:H:212:LEU:HG	1:H:245:TYR:CE2	2.47	0.49
1:J:297:ILE:CG2	1:J:298:GLN:N	2.75	0.49
1:H:83:GLY:O	4:H:325:GOL:O2	2.31	0.49
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.76	0.49
1:I:248:TYR:HA	1:J:247:PHE:CE1	2.47	0.49
1:G:95:PHE:CD2	1:G:99:ARG:HB2	2.47	0.49
1:I:95:PHE:HB2	1:I:99:ARG:HB2	1.94	0.49
1:C:297:ILE:CG2	1:C:298:GLN:N	2.76	0.49
1:D:145:ILE:CG1	1:D:166:ALA:HB3	2.43	0.49
1:G:15:SER:HB2	1:G:142:PHE:CE1	2.48	0.49
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.94	0.49
1:E:15:SER:HB2	1:E:142:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:248:TYR:HD1	1:H:247:PHE:HA	1.77	0.49
1:A:212:LEU:HB3	1:A:265:MET:HE1	1.93	0.49
1:B:205:LEU:HD23	1:B:209:ILE:HD12	1.93	0.49
1:H:165:LYS:HD2	1:H:165:LYS:N	2.27	0.49
1:F:119:PHE:C	1:F:121:PHE:N	2.65	0.49
1:J:15:SER:HB2	1:J:142:PHE:CE1	2.48	0.49
1:J:15:SER:HB3	1:J:141:ARG:CD	2.42	0.49
1:F:15:SER:HB3	1:F:141:ARG:CD	2.43	0.49
1:E:297:ILE:CG2	1:E:298:GLN:N	2.75	0.49
1:I:297:ILE:CG2	1:I:298:GLN:N	2.76	0.49
1:A:119:PHE:CD2	1:A:120:PRO:CD	2.92	0.49
1:E:145:ILE:HG13	1:E:166:ALA:HB3	1.95	0.49
1:A:175:TYR:CZ	2:E:323:ACH:H101	2.47	0.49
1:I:248:TYR:CD1	1:J:247:PHE:HA	2.48	0.49
1:B:297:ILE:CG2	1:B:298:GLN:N	2.75	0.49
1:B:301:ARG:HH12	1:C:285:HIS:CE1	2.31	0.49
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.67	0.49
1:F:119:PHE:O	1:F:121:PHE:N	2.31	0.48
1:H:145:ILE:HD11	1:H:166:ALA:HB3	1.95	0.48
1:E:257:PRO:HG2	1:E:258:TYR:HD2	1.75	0.48
1:J:19:PHE:CD1	2:J:323:ACH:H61	2.48	0.48
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.95	0.48
1:D:248:TYR:CD1	1:E:247:PHE:HA	2.48	0.48
1:G:297:ILE:CG2	1:G:298:GLN:N	2.75	0.48
1:C:297:ILE:HG23	1:C:298:GLN:N	2.26	0.48
1:G:145:ILE:HD11	1:G:166:ALA:HB3	1.93	0.48
1:J:15:SER:HB3	1:J:141:ARG:HG2	1.93	0.48
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.76	0.48
1:C:15:SER:HB3	1:C:141:ARG:CD	2.43	0.48
1:H:205:LEU:HD23	1:H:209:ILE:HD12	1.95	0.48
1:E:212:LEU:CD1	1:E:265:MET:HB3	2.43	0.48
1:G:119:PHE:C	1:G:121:PHE:N	2.65	0.48
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.95	0.48
1:A:232:LEU:HD23	1:E:225:LEU:CD2	2.44	0.48
2:D:323:ACH:O4	2:D:323:ACH:H102	2.13	0.48
1:C:11:PRO:HD2	5:C:335:HOH:O	2.13	0.48
1:J:95:PHE:CD2	1:J:99:ARG:HB2	2.49	0.48
1:D:145:ILE:HD11	1:D:166:ALA:HB3	1.92	0.48
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.48	0.48
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.49	0.48
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.48	0.48
1:F:15:SER:HB2	1:F:142:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:284:HIS:HD2	1:J:285:HIS:NE2	2.12	0.48
1:I:297:ILE:C	1:I:299:ARG:N	2.67	0.48
1:D:297:ILE:C	1:D:299:ARG:N	2.67	0.48
1:J:212:LEU:HB3	1:J:265:MET:HE1	1.95	0.48
1:C:212:LEU:HB3	1:C:265:MET:HE1	1.95	0.48
1:E:205:LEU:HD23	1:E:209:ILE:HD12	1.95	0.48
1:A:210:LEU:CB	1:A:211:PRO:HD3	2.39	0.48
1:H:210:LEU:CB	1:H:211:PRO:HD3	2.41	0.48
1:A:137:ASN:HA	4:A:326:GOL:HO1	1.78	0.48
1:A:15:SER:HB3	1:A:141:ARG:CD	2.43	0.48
1:H:15:SER:HB3	1:H:141:ARG:CG	2.44	0.48
1:J:149:THR:O	1:J:150:GLU:HB3	2.14	0.48
1:E:217:ALA:HA	1:E:220:TRP:CE3	2.49	0.48
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.96	0.48
1:E:297:ILE:C	1:E:299:ARG:N	2.67	0.48
1:I:145:ILE:HG13	1:I:166:ALA:HB3	1.96	0.48
1:I:145:ILE:CG1	1:I:166:ALA:HB3	2.44	0.48
1:I:301:ARG:HH12	1:J:285:HIS:CE1	2.31	0.48
1:A:19:PHE:CD1	2:A:323:ACH:H61	2.49	0.48
1:C:149:THR:O	1:C:150:GLU:HB3	2.12	0.48
1:E:212:LEU:HB3	1:E:265:MET:HE1	1.95	0.48
1:I:235:SER:HB3	1:I:277:ILE:HD11	1.95	0.48
1:E:23:ILE:HG21	1:E:126:PHE:CD2	2.49	0.48
1:G:289:ASN:OD1	1:G:292:GLU:HB3	2.14	0.48
1:F:248:TYR:HD1	1:G:247:PHE:HA	1.78	0.48
1:G:210:LEU:CB	1:G:211:PRO:HD3	2.41	0.47
1:I:119:PHE:C	1:I:121:PHE:N	2.67	0.47
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.57	0.47
1:G:136:ASN:C	4:G:328:GOL:H2	2.33	0.47
1:E:95:PHE:HB2	1:E:99:ARG:HB2	1.96	0.47
1:C:297:ILE:C	1:C:299:ARG:N	2.67	0.47
1:E:119:PHE:O	1:E:121:PHE:N	2.38	0.47
1:I:225:LEU:HB2	1:I:231:ARG:HG3	1.96	0.47
1:I:289:ASN:OD1	1:I:292:GLU:HB3	2.14	0.47
1:F:257:PRO:HG2	1:F:258:TYR:HD2	1.76	0.47
1:A:15:SER:HB3	1:A:141:ARG:HG2	1.96	0.47
1:B:149:THR:O	1:B:150:GLU:HB3	2.14	0.47
1:E:279:LEU:HD22	1:E:304:PHE:HE2	1.79	0.47
1:A:297:ILE:C	1:A:299:ARG:N	2.67	0.47
1:D:297:ILE:HG23	1:D:298:GLN:N	2.28	0.47
1:E:119:PHE:CD2	1:E:120:PRO:CD	2.95	0.47
1:H:19:PHE:CD1	2:H:323:ACH:H61	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:323:ACH:H102	2:I:323:ACH:O4	2.14	0.47
1:I:284:HIS:HD2	1:I:285:HIS:NE2	2.12	0.47
1:B:145:ILE:HG13	1:B:166:ALA:HB3	1.96	0.47
1:G:142:PHE:HA	1:G:170:ILE:HD11	1.96	0.47
1:D:149:THR:O	1:D:150:GLU:HB3	2.14	0.47
1:E:39:ILE:HD11	1:E:130:LEU:HD11	1.96	0.47
1:I:305:PRO:O	1:I:309:LEU:HG	2.14	0.47
1:B:137:ASN:CA	4:B:327:GOL:O1	2.62	0.47
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.49	0.47
1:A:149:THR:O	1:A:150:GLU:HB3	2.13	0.47
1:E:11:PRO:CD	5:E:332:HOH:O	2.63	0.47
1:I:169:HIS:CE1	1:I:171:SER:HB3	2.49	0.47
1:I:55:PRO:HG2	1:J:181:VAL:HG13	1.96	0.47
1:H:95:PHE:CD2	1:H:99:ARG:HB2	2.50	0.47
1:I:210:LEU:CB	1:I:211:PRO:HD3	2.36	0.47
1:H:83:GLY:C	4:H:325:GOL:O2	2.52	0.47
1:C:145:ILE:HD11	1:C:166:ALA:HB3	1.94	0.47
1:G:147:VAL:O	1:G:147:VAL:HG22	2.14	0.47
1:G:149:THR:O	1:G:150:GLU:HB3	2.14	0.47
1:H:11:PRO:N	5:H:328:HOH:O	2.47	0.47
1:F:29:LEU:HD23	1:F:29:LEU:HA	1.67	0.47
1:H:140:LEU:CD1	5:H:331:HOH:O	2.33	0.47
1:B:145:ILE:CD1	1:B:145:ILE:O	2.59	0.47
1:A:136:ASN:O	4:A:326:GOL:H11	2.14	0.47
1:I:119:PHE:CD2	1:I:120:PRO:CD	2.97	0.47
1:I:119:PHE:O	1:I:121:PHE:N	2.39	0.47
1:I:76:LEU:H	4:I:327:GOL:C1	2.28	0.47
1:E:145:ILE:HD11	1:E:166:ALA:HB3	1.94	0.47
1:G:15:SER:HB3	1:G:141:ARG:HD3	1.96	0.47
1:E:289:ASN:OD1	1:E:292:GLU:HB3	2.15	0.47
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.50	0.47
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.48	0.47
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.95	0.47
1:J:55:PRO:HB3	1:J:95:PHE:CD1	2.49	0.47
1:G:297:ILE:O	1:G:299:ARG:N	2.48	0.47
1:B:168:THR:C	1:B:169:HIS:CG	2.88	0.47
2:G:323:ACH:H102	2:G:323:ACH:O4	2.15	0.47
1:F:297:ILE:CG2	1:F:298:GLN:N	2.78	0.47
1:D:289:ASN:OD1	1:D:292:GLU:HB3	2.15	0.47
1:H:149:THR:O	1:H:150:GLU:HB3	2.14	0.47
1:F:284:HIS:HD2	1:F:285:HIS:NE2	2.12	0.47
1:A:119:PHE:C	1:A:121:PHE:N	2.65	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:SER:HB3	1:C:141:ARG:HG2	1.97	0.47
1:E:15:SER:HB3	1:E:141:ARG:HG2	1.97	0.46
1:B:147:VAL:O	1:B:147:VAL:HG13	2.15	0.46
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.50	0.46
1:J:145:ILE:HD11	1:J:166:ALA:HB3	1.97	0.46
1:B:119:PHE:CD2	1:B:120:PRO:CD	2.98	0.46
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.30	0.46
1:J:289:ASN:OD1	1:J:292:GLU:HB3	2.15	0.46
1:E:149:THR:O	1:E:150:GLU:HB3	2.13	0.46
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.97	0.46
1:I:140:LEU:CD2	5:I:334:HOH:O	2.29	0.46
1:B:95:PHE:HB2	1:B:99:ARG:HB2	1.96	0.46
1:D:297:ILE:O	1:D:299:ARG:N	2.48	0.46
1:B:142:PHE:HA	1:B:170:ILE:HD11	1.97	0.46
1:D:15:SER:HB3	1:D:141:ARG:CD	2.45	0.46
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.51	0.46
1:C:38:TYR:CE1	1:C:105:ARG:HD3	2.50	0.46
1:G:91:ARG:HD3	1:G:103:ASN:HB3	1.97	0.46
1:J:99:ARG:HH11	1:J:99:ARG:CG	2.12	0.46
1:A:137:ASN:HA	4:A:326:GOL:C1	2.44	0.46
1:B:289:ASN:OD1	1:B:292:GLU:HB3	2.14	0.46
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.49	0.46
1:F:297:ILE:C	1:F:299:ARG:N	2.69	0.46
1:J:297:ILE:C	1:J:299:ARG:N	2.68	0.46
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.80	0.46
1:D:15:SER:HB2	1:D:142:PHE:CE1	2.51	0.46
1:B:235:SER:HB3	1:B:277:ILE:HD11	1.98	0.46
1:C:287:GLN:HB2	1:C:288:ALA:H	1.54	0.46
1:D:297:ILE:CG2	1:D:298:GLN:N	2.78	0.46
1:H:297:ILE:C	1:H:299:ARG:N	2.68	0.46
1:A:145:ILE:HG13	1:A:166:ALA:HB3	1.96	0.46
1:C:145:ILE:HG13	1:C:166:ALA:HB3	1.98	0.46
1:F:150:GLU:HG3	1:F:153:ASP:CB	2.46	0.46
1:G:161:TRP:CZ2	1:G:200:ASN:ND2	2.83	0.46
2:A:323:ACH:O4	2:A:323:ACH:H102	2.15	0.46
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.51	0.46
1:E:297:ILE:O	1:E:299:ARG:N	2.48	0.46
1:A:297:ILE:O	1:A:299:ARG:N	2.49	0.46
1:H:145:ILE:HG13	1:H:166:ALA:HB3	1.96	0.46
1:J:212:LEU:O	1:J:216:ILE:HG13	2.15	0.46
1:A:227:SER:HB3	1:A:230:GLU:CG	2.45	0.46
1:I:248:TYR:HD1	1:J:247:PHE:HA	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:227:SER:HB3	1:G:230:GLU:HG3	1.98	0.46
1:B:145:ILE:CG1	1:B:166:ALA:HB3	2.45	0.46
1:A:145:ILE:CG1	1:A:166:ALA:HB3	2.46	0.46
1:G:145:ILE:HG13	1:G:166:ALA:HB3	1.96	0.46
1:C:150:GLU:HG3	1:C:153:ASP:CB	2.46	0.46
1:J:220:TRP:C	1:J:222:VAL:H	2.19	0.46
3:A:324:MES:O1S	3:A:324:MES:H51	2.16	0.46
1:H:77:GLU:O	1:H:130:LEU:HD12	2.15	0.46
1:B:304:PHE:CB	1:B:305:PRO:HD3	2.46	0.46
1:F:210:LEU:CB	1:F:211:PRO:HD3	2.39	0.45
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.51	0.45
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.51	0.45
1:A:289:ASN:OD1	1:A:292:GLU:HB3	2.16	0.45
1:F:289:ASN:OD1	1:F:292:GLU:HB3	2.16	0.45
1:C:227:SER:HB3	1:C:230:GLU:CG	2.45	0.45
1:F:181:VAL:HG13	1:J:55:PRO:HG2	1.97	0.45
2:C:323:ACH:O4	2:C:323:ACH:H102	2.15	0.45
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.61	0.45
1:B:220:TRP:C	1:B:222:VAL:H	2.20	0.45
1:J:205:LEU:HD23	1:J:209:ILE:HD12	1.98	0.45
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.51	0.45
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.99	0.45
1:A:95:PHE:CD2	1:A:99:ARG:HB2	2.51	0.45
1:F:11:PRO:N	5:F:330:HOH:O	2.49	0.45
1:G:289:ASN:CG	1:G:290:GLY:N	2.69	0.45
1:C:289:ASN:CG	1:C:290:GLY:N	2.69	0.45
1:D:227:SER:HB3	1:D:230:GLU:CG	2.46	0.45
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.81	0.45
1:E:289:ASN:CG	1:E:290:GLY:N	2.69	0.45
1:D:289:ASN:CG	1:D:290:GLY:N	2.69	0.45
1:D:15:SER:HB3	1:D:141:ARG:HG2	1.98	0.45
1:D:248:TYR:HD1	1:E:247:PHE:HA	1.81	0.45
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.42	0.45
1:C:147:VAL:O	1:C:147:VAL:HG13	2.17	0.45
1:G:15:SER:HB3	1:G:141:ARG:CG	2.47	0.45
1:F:289:ASN:HD21	1:F:292:GLU:HB2	1.81	0.45
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.51	0.45
1:J:304:PHE:CB	1:J:305:PRO:HD3	2.46	0.45
1:J:227:SER:HB3	1:J:230:GLU:HG3	1.98	0.45
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.78	0.45
1:F:95:PHE:CD2	1:F:99:ARG:HB2	2.52	0.45
1:D:145:ILE:HD12	1:D:166:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:289:ASN:ND2	1:E:292:GLU:HB2	2.32	0.45
1:E:289:ASN:HD21	1:E:292:GLU:HB2	1.81	0.45
1:F:149:THR:O	1:F:150:GLU:HB3	2.16	0.45
1:J:95:PHE:HB2	1:J:99:ARG:HB2	1.99	0.45
1:F:145:ILE:CG1	1:F:166:ALA:HB3	2.45	0.45
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.51	0.45
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.98	0.45
1:C:304:PHE:CB	1:C:305:PRO:HD3	2.46	0.45
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.51	0.45
1:G:137:ASN:HA	4:G:328:GOL:H2	1.98	0.45
1:J:145:ILE:HG13	1:J:166:ALA:HB3	1.98	0.45
1:B:95:PHE:CD2	1:B:99:ARG:HB2	2.52	0.45
1:I:297:ILE:O	1:I:299:ARG:N	2.50	0.45
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.81	0.45
1:B:289:ASN:CG	1:B:290:GLY:N	2.70	0.45
1:D:150:GLU:HG3	1:D:153:ASP:CB	2.47	0.45
1:C:212:LEU:HD13	1:C:265:MET:HB3	1.99	0.45
1:A:150:GLU:HG3	1:A:153:ASP:CB	2.47	0.45
1:I:279:LEU:HD22	1:I:304:PHE:HE2	1.82	0.45
1:C:297:ILE:O	1:C:299:ARG:N	2.50	0.45
1:I:150:GLU:HG3	1:I:153:ASP:CB	2.47	0.45
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.47	0.45
1:A:289:ASN:CG	1:A:290:GLY:N	2.68	0.45
1:E:136:ASN:O	4:E:326:GOL:O1	2.32	0.45
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.70	0.45
1:I:304:PHE:CB	1:I:305:PRO:HD3	2.47	0.45
1:J:227:SER:HB3	1:J:230:GLU:CG	2.47	0.45
1:A:304:PHE:CB	1:A:305:PRO:HD3	2.47	0.45
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.79	0.45
4:C:325:GOL:H32	5:C:326:HOH:O	2.17	0.44
1:G:38:TYR:CE1	1:G:105:ARG:HD3	2.52	0.44
1:H:257:PRO:HG2	1:H:258:TYR:HD2	1.78	0.44
1:A:257:PRO:HG2	1:A:258:TYR:HD2	1.76	0.44
1:G:287:GLN:HB2	1:G:288:ALA:H	1.52	0.44
1:J:23:ILE:HG21	1:J:126:PHE:CD2	2.52	0.44
1:I:39:ILE:HD11	1:I:130:LEU:HD11	1.99	0.44
1:C:137:ASN:HA	4:C:325:GOL:O3	2.16	0.44
1:B:136:ASN:C	4:B:327:GOL:H32	2.37	0.44
1:I:289:ASN:HD21	1:I:292:GLU:HB2	1.82	0.44
1:I:289:ASN:ND2	1:I:292:GLU:HB2	2.32	0.44
1:G:212:LEU:HD13	1:G:265:MET:HB3	1.98	0.44
1:E:150:GLU:HG3	1:E:153:ASP:CB	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:29:LEU:HA	1:J:29:LEU:HD23	1.69	0.44
1:G:311:ILE:O	1:G:311:ILE:HG22	2.18	0.44
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.78	0.44
1:C:136:ASN:O	4:C:325:GOL:C2	2.31	0.44
1:D:55:PRO:HB3	1:D:95:PHE:CD1	2.52	0.44
1:C:289:ASN:OD1	1:C:292:GLU:HB3	2.17	0.44
1:F:289:ASN:CG	1:F:290:GLY:N	2.68	0.44
1:B:289:ASN:HD21	1:B:292:GLU:HB2	1.82	0.44
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.51	0.44
1:A:248:TYR:HD1	1:B:247:PHE:HA	1.82	0.44
1:J:150:GLU:HG3	1:J:153:ASP:CB	2.46	0.44
1:G:304:PHE:CB	1:G:305:PRO:HD3	2.48	0.44
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.63	0.44
1:D:289:ASN:ND2	1:D:292:GLU:HB2	2.32	0.44
1:J:212:LEU:HD13	1:J:265:MET:HB3	1.98	0.44
1:G:150:GLU:HG3	1:G:153:ASP:CB	2.47	0.44
2:E:323:ACH:O4	2:E:323:ACH:H102	2.17	0.44
1:E:212:LEU:HA	1:E:212:LEU:HD23	1.81	0.44
1:I:287:GLN:HB2	1:I:288:ALA:H	1.53	0.44
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.66	0.44
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.53	0.44
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.57	0.44
1:F:289:ASN:ND2	1:F:292:GLU:HB2	2.33	0.44
1:A:102:TYR:CZ	4:A:325:GOL:H12	2.52	0.44
1:H:150:GLU:HG3	1:H:153:ASP:CB	2.47	0.44
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.53	0.44
1:F:102:TYR:OH	4:F:325:GOL:H12	2.17	0.44
1:H:58:VAL:CG1	1:H:62:GLN:HB3	2.47	0.44
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.57	0.44
1:J:287:GLN:HB2	1:J:288:ALA:H	1.54	0.44
1:A:140:LEU:HD13	1:A:191:ILE:CG1	2.40	0.44
1:D:147:VAL:O	1:D:147:VAL:HG13	2.17	0.44
1:B:289:ASN:ND2	1:B:292:GLU:HB2	2.33	0.44
1:B:147:VAL:O	1:B:149:THR:N	2.48	0.44
1:H:40:VAL:HG22	1:H:103:ASN:ND2	2.33	0.44
1:H:220:TRP:C	1:H:222:VAL:H	2.21	0.44
1:D:11:PRO:N	5:D:339:HOH:O	2.50	0.44
1:E:58:VAL:CG1	1:E:62:GLN:HB3	2.47	0.44
1:A:39:ILE:HD11	1:A:130:LEU:HD11	2.00	0.44
1:A:284:HIS:HD2	1:A:285:HIS:NE2	2.15	0.44
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.87	0.44
1:B:55:PRO:HG2	1:C:181:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:225:LEU:HD21	1:G:232:LEU:HD23	1.99	0.44
1:A:289:ASN:ND2	1:A:292:GLU:HB2	2.32	0.44
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.82	0.44
1:B:212:LEU:HD13	1:B:265:MET:HB3	1.99	0.44
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.66	0.44
1:B:227:SER:HB3	1:B:230:GLU:CG	2.48	0.44
1:E:291:VAL:O	1:E:291:VAL:HG12	2.17	0.44
1:D:79:ILE:HD13	1:D:79:ILE:HA	1.80	0.44
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.52	0.44
1:B:297:ILE:C	1:B:299:ARG:N	2.69	0.44
1:C:289:ASN:HD21	1:C:292:GLU:HB2	1.82	0.44
1:A:212:LEU:HD13	1:A:265:MET:HB3	2.00	0.44
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.60	0.44
1:B:226:GLU:OE2	1:C:284:HIS:NE2	2.46	0.44
1:H:15:SER:HB2	1:H:142:PHE:CE1	2.53	0.44
1:I:227:SER:HB3	1:I:230:GLU:CG	2.48	0.44
1:B:287:GLN:HB2	1:B:288:ALA:H	1.55	0.44
1:E:311:ILE:O	1:E:311:ILE:HG22	2.18	0.44
1:B:174:ARG:O	4:B:326:GOL:H31	2.18	0.43
1:A:147:VAL:HG13	1:A:147:VAL:O	2.18	0.43
1:H:119:PHE:C	1:H:121:PHE:N	2.63	0.43
1:J:224:TRP:CE2	1:J:301:ARG:HD3	2.53	0.43
2:B:323:ACH:O4	2:B:323:ACH:H102	2.18	0.43
1:C:19:PHE:CD1	2:C:323:ACH:H61	2.53	0.43
1:F:212:LEU:HG	1:F:245:TYR:CE2	2.53	0.43
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.83	0.43
1:F:304:PHE:CB	1:F:305:PRO:HD3	2.49	0.43
1:B:284:HIS:HD2	1:B:285:HIS:NE2	2.16	0.43
1:B:291:VAL:O	1:B:291:VAL:HG12	2.19	0.43
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.53	0.43
1:H:289:ASN:ND2	1:H:292:GLU:HB2	2.32	0.43
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.53	0.43
1:H:248:TYR:HD1	1:I:247:PHE:HA	1.84	0.43
1:H:163:ARG:HB2	1:H:196:ASP:HB2	2.00	0.43
1:H:311:ILE:O	1:H:311:ILE:HG22	2.18	0.43
1:C:311:ILE:O	1:C:311:ILE:HG22	2.18	0.43
1:I:257:PRO:HG2	1:I:258:TYR:HD2	1.83	0.43
1:C:289:ASN:ND2	1:C:292:GLU:HB2	2.34	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.53	0.43
1:F:182:GLN:NE2	1:J:54:LYS:HD2	2.33	0.43
1:I:163:ARG:HD3	1:I:163:ARG:HA	1.84	0.43
1:I:58:VAL:CG1	1:I:62:GLN:HB3	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.31	0.43
1:H:225:LEU:CD2	1:I:232:LEU:HD23	2.48	0.43
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.83	0.43
1:I:161:TRP:CZ2	1:I:200:ASN:ND2	2.85	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.66	0.43
1:C:224:TRP:CE2	1:C:301:ARG:HD3	2.53	0.43
1:E:304:PHE:CB	1:E:305:PRO:HD3	2.49	0.43
1:J:279:LEU:HD22	1:J:304:PHE:HE2	1.84	0.43
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.78	0.43
1:H:284:HIS:HD2	1:H:285:HIS:NE2	2.17	0.43
1:J:311:ILE:O	1:J:311:ILE:HG22	2.19	0.43
1:A:55:PRO:HB3	1:A:95:PHE:CD1	2.53	0.43
1:F:226:GLU:OE2	1:G:284:HIS:NE2	2.45	0.43
1:I:289:ASN:CG	1:I:290:GLY:N	2.69	0.43
1:H:289:ASN:CG	1:H:290:GLY:N	2.70	0.43
1:H:289:ASN:OD1	1:H:292:GLU:HB3	2.19	0.43
1:H:248:TYR:HA	1:I:247:PHE:CE1	2.53	0.43
1:H:161:TRP:CZ2	1:H:200:ASN:ND2	2.87	0.43
1:A:240:LEU:HD13	1:E:241:THR:HA	2.01	0.43
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.54	0.43
1:D:284:HIS:HD2	1:D:285:HIS:NE2	2.16	0.43
1:I:99:ARG:CG	1:I:99:ARG:NH1	2.78	0.43
1:B:150:GLU:HG3	1:B:153:ASP:CB	2.48	0.43
1:D:212:LEU:HD13	1:D:265:MET:HB3	2.00	0.43
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.83	0.43
1:I:220:TRP:C	1:I:222:VAL:H	2.21	0.43
1:G:305:PRO:O	1:G:309:LEU:HG	2.18	0.43
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.53	0.43
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.79	0.43
1:H:304:PHE:CB	1:H:305:PRO:HD3	2.48	0.43
1:F:140:LEU:CG	5:F:331:HOH:O	2.62	0.43
1:D:297:ILE:C	1:D:299:ARG:H	2.21	0.43
1:G:145:ILE:CG1	1:G:166:ALA:HB3	2.48	0.43
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.34	0.43
1:H:305:PRO:O	1:H:309:LEU:HG	2.19	0.43
1:E:157:ILE:HA	1:E:157:ILE:HD13	1.79	0.43
1:D:95:PHE:HB2	1:D:99:ARG:HB2	1.99	0.43
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.54	0.43
1:B:168:THR:O	1:B:169:HIS:CG	2.72	0.43
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.61	0.43
1:I:155:GLU:HB3	1:I:161:TRP:CD1	2.54	0.43
1:H:200:ASN:HA	1:H:201:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:235:SER:HB3	1:H:277:ILE:HD11	2.01	0.43
1:A:79:ILE:HA	1:A:79:ILE:HD13	1.83	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.78	0.43
1:H:145:ILE:CG1	1:H:166:ALA:HB3	2.49	0.42
1:E:145:ILE:CG1	1:E:166:ALA:HB3	2.48	0.42
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.84	0.42
1:B:38:TYR:CE1	1:B:105:ARG:HD3	2.53	0.42
1:I:221:SER:HB2	1:J:281:ILE:CD1	2.49	0.42
1:D:304:PHE:CB	1:D:305:PRO:HD3	2.48	0.42
1:B:210:LEU:CB	1:B:211:PRO:HD3	2.40	0.42
1:C:145:ILE:CG1	1:C:166:ALA:HB3	2.49	0.42
1:H:291:VAL:O	1:H:291:VAL:HG12	2.19	0.42
1:E:284:HIS:HD2	1:E:285:HIS:NE2	2.16	0.42
1:I:140:LEU:CD1	5:I:334:HOH:O	2.53	0.42
1:A:95:PHE:HB2	1:A:99:ARG:HB2	2.00	0.42
1:G:297:ILE:C	1:G:299:ARG:H	2.23	0.42
1:E:210:LEU:CB	1:E:211:PRO:CD	2.95	0.42
1:B:119:PHE:HE1	1:B:199:ARG:CZ	2.32	0.42
1:F:212:LEU:HD13	1:F:265:MET:HB3	1.99	0.42
1:G:23:ILE:HG21	1:G:126:PHE:CD2	2.54	0.42
1:B:39:ILE:HD11	1:B:130:LEU:HD11	2.00	0.42
1:H:297:ILE:O	1:H:299:ARG:N	2.52	0.42
1:G:210:LEU:CB	1:G:211:PRO:CD	2.97	0.42
1:G:284:HIS:HE1	1:G:291:VAL:HG13	1.84	0.42
1:H:212:LEU:HD13	1:H:265:MET:HB3	2.02	0.42
1:E:305:PRO:O	1:E:309:LEU:HG	2.20	0.42
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.54	0.42
1:C:279:LEU:HD22	1:C:304:PHE:HE2	1.83	0.42
1:I:95:PHE:CD2	1:I:99:ARG:HB2	2.55	0.42
1:F:297:ILE:O	1:F:299:ARG:N	2.53	0.42
1:G:119:PHE:CG	1:G:120:PRO:CD	3.02	0.42
1:B:297:ILE:O	1:B:299:ARG:N	2.53	0.42
1:H:15:SER:HB3	1:H:141:ARG:CD	2.50	0.42
1:F:248:TYR:HA	1:G:247:PHE:CE1	2.55	0.42
1:G:95:PHE:HB2	1:G:99:ARG:HB2	2.01	0.42
1:H:55:PRO:HB3	1:H:95:PHE:CD1	2.54	0.42
1:F:147:VAL:O	1:F:147:VAL:HG13	2.18	0.42
1:I:19:PHE:CG	2:I:323:ACH:H61	2.54	0.42
1:J:212:LEU:HA	1:J:212:LEU:HD23	1.88	0.42
1:G:227:SER:HB3	1:G:230:GLU:CG	2.49	0.42
1:I:234:THR:HG21	1:J:236:PHE:CE2	2.55	0.42
1:J:291:VAL:HG12	1:J:291:VAL:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:311:ILE:O	1:F:311:ILE:HG22	2.20	0.42
1:C:58:VAL:CG1	1:C:62:GLN:HB3	2.50	0.42
1:E:140:LEU:CG	5:E:336:HOH:O	2.68	0.42
1:I:297:ILE:C	1:I:299:ARG:H	2.22	0.42
1:C:297:ILE:C	1:C:299:ARG:H	2.23	0.42
1:G:15:SER:HB3	1:G:141:ARG:HG2	2.01	0.42
1:J:19:PHE:CG	2:J:323:ACH:H61	2.55	0.42
1:E:212:LEU:HD13	1:E:265:MET:HB3	2.01	0.42
1:D:220:TRP:C	1:D:222:VAL:H	2.23	0.42
1:A:311:ILE:HG22	1:A:311:ILE:O	2.20	0.42
1:E:95:PHE:CD2	1:E:99:ARG:HB2	2.54	0.42
1:I:137:ASN:CA	4:I:329:GOL:O1	2.64	0.42
1:D:142:PHE:HA	1:D:170:ILE:HD11	2.01	0.42
1:H:38:TYR:CE1	1:H:105:ARG:HD3	2.54	0.42
1:A:291:VAL:O	1:A:291:VAL:HG12	2.19	0.42
1:J:136:ASN:C	4:J:325:GOL:H2	2.37	0.42
1:F:55:PRO:HB3	1:F:95:PHE:CD1	2.54	0.42
1:H:138:GLN:N	4:H:324:GOL:H11	2.34	0.42
1:E:119:PHE:HE1	1:E:199:ARG:CZ	2.33	0.42
1:A:220:TRP:C	1:A:222:VAL:H	2.23	0.42
1:A:279:LEU:HD22	1:A:304:PHE:HE2	1.85	0.42
1:C:235:SER:HB3	1:C:277:ILE:HD11	2.02	0.42
1:G:39:ILE:HD11	1:G:130:LEU:HD11	2.02	0.42
1:A:297:ILE:C	1:A:299:ARG:H	2.23	0.42
1:J:297:ILE:O	1:J:299:ARG:N	2.53	0.42
1:C:257:PRO:HG2	1:C:258:TYR:HD2	1.80	0.42
1:J:182:GLN:HB2	1:J:185:GLN:CG	2.49	0.42
1:F:15:SER:HB3	1:F:141:ARG:HG2	2.01	0.42
2:C:323:ACH:H101	1:D:175:TYR:CZ	2.55	0.42
1:E:212:LEU:O	1:E:216:ILE:HG13	2.19	0.42
1:G:200:ASN:HA	1:G:201:PRO:HD3	1.83	0.42
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.55	0.42
1:G:42:GLN:HG3	1:G:101:ILE:HG12	2.02	0.42
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.80	0.42
4:G:328:GOL:O3	4:G:328:GOL:O1	2.32	0.41
1:E:55:PRO:HB3	1:E:95:PHE:CD1	2.54	0.41
1:G:145:ILE:CD1	1:G:145:ILE:O	2.67	0.41
1:D:43:TRP:CZ2	1:D:100:VAL:HG11	2.55	0.41
1:I:147:VAL:O	1:I:149:THR:N	2.49	0.41
1:H:119:PHE:HE1	1:H:199:ARG:CZ	2.32	0.41
1:J:284:HIS:HD2	1:J:285:HIS:CD2	2.37	0.41
1:F:212:LEU:O	1:F:216:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:SER:HB3	1:A:277:ILE:HD11	2.01	0.41
1:C:23:ILE:HG21	1:C:126:PHE:CD2	2.55	0.41
1:C:79:ILE:HA	1:C:79:ILE:HD13	1.84	0.41
1:G:284:HIS:HD2	1:G:285:HIS:NE2	2.17	0.41
1:A:161:TRP:CZ2	1:A:200:ASN:ND2	2.88	0.41
1:D:23:ILE:HG21	1:D:126:PHE:CD2	2.56	0.41
1:J:131:GLU:HG2	1:J:190:ARG:HB2	2.02	0.41
1:A:119:PHE:HE1	1:A:199:ARG:CZ	2.32	0.41
1:C:212:LEU:HG	1:C:245:TYR:CE2	2.56	0.41
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.86	0.41
1:G:220:TRP:C	1:G:222:VAL:H	2.24	0.41
1:B:305:PRO:O	1:B:309:LEU:HG	2.20	0.41
1:D:206:TRP:CD2	3:D:325:MES:O2S	2.74	0.41
1:I:311:ILE:O	1:I:311:ILE:HG22	2.21	0.41
1:F:291:VAL:HG12	1:F:291:VAL:O	2.20	0.41
1:J:145:ILE:CG1	1:J:166:ALA:HB3	2.49	0.41
1:F:161:TRP:CZ2	1:F:200:ASN:ND2	2.89	0.41
1:F:279:LEU:HD22	1:F:304:PHE:HE2	1.84	0.41
1:E:235:SER:HB3	1:E:277:ILE:HD11	2.03	0.41
1:G:295:LEU:O	1:G:298:GLN:HG2	2.20	0.41
1:J:166:ALA:CB	1:J:195:ILE:HG12	2.48	0.41
1:C:71:LEU:HD12	1:C:72:TRP:H	1.84	0.41
1:B:311:ILE:HG22	1:B:311:ILE:O	2.21	0.41
1:D:210:LEU:CB	1:D:211:PRO:CD	2.98	0.41
1:G:163:ARG:HB2	1:G:196:ASP:HB2	2.02	0.41
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.97	0.41
1:C:220:TRP:C	1:C:222:VAL:H	2.24	0.41
1:F:221:SER:HB2	1:G:281:ILE:CD1	2.50	0.41
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.56	0.41
1:J:58:VAL:CG1	1:J:62:GLN:HB3	2.50	0.41
1:I:261:VAL:HG12	1:I:262:ILE:N	2.35	0.41
1:C:291:VAL:O	1:C:291:VAL:HG12	2.20	0.41
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.83	0.41
1:J:210:LEU:CB	1:J:211:PRO:CD	2.98	0.41
1:C:256:LEU:HB3	1:C:257:PRO:HD2	2.02	0.41
1:I:212:LEU:HD13	1:I:265:MET:HB3	2.02	0.41
1:A:212:LEU:HG	1:A:245:TYR:CE2	2.55	0.41
1:J:155:GLU:HB3	1:J:161:TRP:NE1	2.36	0.41
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.83	0.41
1:A:305:PRO:O	1:A:309:LEU:HG	2.21	0.41
1:G:205:LEU:HD23	1:G:209:ILE:HD12	2.02	0.41
1:E:131:GLU:HG2	1:E:190:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:235:SER:HB3	1:D:277:ILE:HD11	2.02	0.41
1:A:58:VAL:CG1	1:A:62:GLN:HB3	2.50	0.41
1:D:311:ILE:HG22	1:D:311:ILE:O	2.20	0.41
1:H:99:ARG:CG	1:H:99:ARG:NH1	2.82	0.41
1:A:210:LEU:CB	1:A:211:PRO:CD	2.98	0.41
1:F:119:PHE:HE1	1:F:199:ARG:CZ	2.34	0.41
1:G:291:VAL:HG12	1:G:291:VAL:O	2.21	0.41
1:C:284:HIS:HD2	1:C:285:HIS:CD2	2.39	0.41
1:F:305:PRO:O	1:F:309:LEU:HG	2.21	0.41
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.80	0.41
1:B:215:ILE:HA	1:C:239:MET:HE2	2.03	0.41
1:D:145:ILE:O	1:D:145:ILE:CD1	2.68	0.40
1:J:212:LEU:HG	1:J:245:TYR:CE2	2.57	0.40
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.98	0.40
1:C:161:TRP:CZ2	1:C:200:ASN:ND2	2.89	0.40
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.85	0.40
1:D:22:LYS:NZ	5:D:331:HOH:O	2.54	0.40
1:A:38:TYR:CE1	1:A:105:ARG:HD3	2.55	0.40
1:C:226:GLU:OE1	1:C:226:GLU:HA	2.21	0.40
1:C:91:ARG:HD3	1:C:103:ASN:HB3	2.02	0.40
1:E:295:LEU:HA	1:E:298:GLN:NE2	2.23	0.40
1:D:119:PHE:HE1	1:D:199:ARG:CZ	2.34	0.40
1:A:225:LEU:HD21	1:B:232:LEU:HD23	2.03	0.40
1:G:15:SER:HB3	1:G:141:ARG:CD	2.52	0.40
1:F:205:LEU:HA	1:F:205:LEU:HD23	1.65	0.40
1:H:279:LEU:HD22	1:H:304:PHE:HE2	1.85	0.40
1:D:58:VAL:CG1	1:D:62:GLN:HB3	2.51	0.40
1:D:291:VAL:O	1:D:291:VAL:HG12	2.21	0.40
1:D:198:VAL:HG12	1:D:199:ARG:N	2.36	0.40
1:I:221:SER:HB2	1:J:281:ILE:HD11	2.03	0.40
1:A:91:ARG:HD3	1:A:103:ASN:HB3	2.02	0.40
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.71	0.40
1:G:137:ASN:HA	4:G:328:GOL:C2	2.52	0.40
1:A:175:TYR:HH	2:E:323:ACH:H101	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/322 (95%)	270 (88%)	25 (8%)	10 (3%)	6	23
1	B	305/322 (95%)	271 (89%)	24 (8%)	10 (3%)	6	23
1	C	305/322 (95%)	267 (88%)	29 (10%)	9 (3%)	7	26
1	D	305/322 (95%)	269 (88%)	24 (8%)	12 (4%)	5	17
1	E	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	5	21
1	F	305/322 (95%)	268 (88%)	28 (9%)	9 (3%)	7	26
1	G	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	5	21
1	H	305/322 (95%)	268 (88%)	27 (9%)	10 (3%)	6	23
1	I	305/322 (95%)	271 (89%)	22 (7%)	12 (4%)	5	17
1	J	305/322 (95%)	267 (88%)	26 (8%)	12 (4%)	5	17
All	All	3050/3220 (95%)	2681 (88%)	263 (9%)	106 (4%)	6	22

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	20	50
1	B	275/284 (97%)	253 (92%)	22 (8%)	17	45
1	C	275/284 (97%)	254 (92%)	21 (8%)	19	48
1	D	275/284 (97%)	251 (91%)	24 (9%)	15	41
1	E	275/284 (97%)	253 (92%)	22 (8%)	17	45
1	F	275/284 (97%)	255 (93%)	20 (7%)	20	50
1	G	275/284 (97%)	254 (92%)	21 (8%)	19	48
1	H	275/284 (97%)	256 (93%)	19 (7%)	22	53
1	I	275/284 (97%)	252 (92%)	23 (8%)	16	42
1	J	275/284 (97%)	253 (92%)	22 (8%)	17	45
All	All	2750/2840 (97%)	2536 (92%)	214 (8%)	18	46

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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

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Mol	Chain	Res	Type
1	J	69	ASN
1	J	200	ASN
1	J	285	HIS
1	J	298	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACH	A	323	-	9,9,9	1.02	1 (11%)	12,12,12	0.64	0
3	MES	A	324	-	12,12,12	2.10	1 (8%)	16,16,16	2.38	5 (31%)
4	GOL	A	325	-	5,5,5	0.72	0	5,5,5	0.67	0
4	GOL	A	326	-	5,5,5	0.78	0	5,5,5	0.41	0
2	ACH	B	323	-	9,9,9	0.96	1 (11%)	12,12,12	0.71	0
3	MES	B	324	-	12,12,12	2.06	1 (8%)	16,16,16	2.29	5 (31%)
4	GOL	B	325	-	5,5,5	0.70	0	5,5,5	0.70	0
4	GOL	B	326	-	5,5,5	0.76	0	5,5,5	0.69	0
4	GOL	B	327	-	5,5,5	0.82	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACH	C	323	-	9,9,9	1.00	1 (11%)	12,12,12	0.74	0
4	GOL	C	324	-	5,5,5	0.61	0	5,5,5	0.64	0
4	GOL	C	325	-	5,5,5	0.75	0	5,5,5	0.80	0
2	ACH	D	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.82	0
3	MES	D	324	-	12,12,12	2.09	1 (8%)	16,16,16	2.40	9 (56%)
3	MES	D	325	-	12,12,12	2.16	1 (8%)	16,16,16	2.44	7 (43%)
4	GOL	D	326	-	5,5,5	0.76	0	5,5,5	0.62	0
4	GOL	D	327	-	5,5,5	0.71	0	5,5,5	0.57	0
2	ACH	E	323	-	9,9,9	1.02	1 (11%)	12,12,12	0.68	0
3	MES	E	324	-	12,12,12	2.09	1 (8%)	16,16,16	2.36	6 (37%)
4	GOL	E	325	-	5,5,5	0.79	0	5,5,5	0.41	0
4	GOL	E	326	-	5,5,5	0.85	0	5,5,5	0.53	0
2	ACH	F	323	-	9,9,9	1.00	1 (11%)	12,12,12	0.82	0
3	MES	F	324	-	12,12,12	2.10	1 (8%)	16,16,16	2.26	5 (31%)
4	GOL	F	325	-	5,5,5	0.70	0	5,5,5	0.52	0
4	GOL	F	326	-	5,5,5	0.67	0	5,5,5	0.62	0
4	GOL	F	327	-	5,5,5	0.85	0	5,5,5	0.37	0
4	GOL	F	328	-	5,5,5	0.78	0	5,5,5	0.68	0
2	ACH	G	323	-	9,9,9	1.04	1 (11%)	12,12,12	0.59	0
3	MES	G	324	-	12,12,12	2.18	1 (8%)	16,16,16	2.54	12 (75%)
4	GOL	G	325	-	5,5,5	0.72	0	5,5,5	0.62	0
4	GOL	G	326	-	5,5,5	0.66	0	5,5,5	0.52	0
4	GOL	G	327	-	2,3,5	8.66	1 (50%)	0,2,5	0.00	-
4	GOL	G	328	-	5,5,5	0.62	0	5,5,5	1.06	1 (20%)
2	ACH	H	323	-	9,9,9	0.94	1 (11%)	12,12,12	0.86	0
4	GOL	H	324	-	5,5,5	0.48	0	5,5,5	0.87	0
4	GOL	H	325	-	5,5,5	0.93	0	5,5,5	0.43	0
2	ACH	I	323	-	9,9,9	0.95	1 (11%)	12,12,12	0.72	0
3	MES	I	324	-	12,12,12	2.02	1 (8%)	16,16,16	2.26	6 (37%)
4	GOL	I	325	-	5,5,5	0.78	0	5,5,5	0.50	0
4	GOL	I	326	-	5,5,5	0.73	0	5,5,5	0.92	0
4	GOL	I	327	-	5,5,5	0.76	0	5,5,5	0.44	0
4	GOL	I	328	-	5,5,5	0.70	0	5,5,5	0.54	0
4	GOL	I	329	-	5,5,5	0.84	0	5,5,5	0.63	0
2	ACH	J	323	-	9,9,9	0.98	1 (11%)	12,12,12	0.74	0
3	MES	J	324	-	12,12,12	2.15	1 (8%)	16,16,16	2.52	6 (37%)
4	GOL	J	325	-	5,5,5	0.72	0	5,5,5	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	327	GOL	O2-C2	12.22	1.38	1.25
3	G	324	MES	C8-S	-6.46	1.66	1.78
3	J	324	MES	C8-S	-6.42	1.66	1.78
3	D	325	MES	C8-S	-6.37	1.66	1.78
3	E	324	MES	C8-S	-6.25	1.67	1.78
3	F	324	MES	C8-S	-6.14	1.67	1.78
3	B	324	MES	C8-S	-6.12	1.67	1.78
3	D	324	MES	C8-S	-6.08	1.67	1.78
3	A	324	MES	C8-S	-6.01	1.67	1.78
3	I	324	MES	C8-S	-5.90	1.67	1.78
2	E	323	ACH	O4-C5	2.36	1.46	1.33
2	D	323	ACH	O4-C5	2.23	1.45	1.33
2	G	323	ACH	O4-C5	2.22	1.45	1.33
2	B	323	ACH	O4-C5	2.22	1.45	1.33
2	A	323	ACH	O4-C5	2.21	1.45	1.33
2	J	323	ACH	O4-C5	2.21	1.45	1.33
2	I	323	ACH	O4-C5	2.19	1.45	1.33
2	H	323	ACH	O4-C5	2.19	1.45	1.33
2	C	323	ACH	O4-C5	2.11	1.44	1.33
2	F	323	ACH	O4-C5	2.07	1.44	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	324	MES	C5-N4-C3	5.22	120.11	109.75
3	A	324	MES	C5-N4-C3	4.98	119.62	109.75
3	E	324	MES	C5-N4-C3	4.96	119.59	109.75
3	B	324	MES	C5-N4-C3	4.89	119.45	109.75
3	J	324	MES	C5-N4-C3	4.76	119.19	109.75
3	I	324	MES	C5-N4-C3	4.76	119.19	109.75
3	D	324	MES	C5-N4-C3	4.52	118.72	109.75
3	D	325	MES	O3S-S-C8	4.29	117.07	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	324	MES	C6-C5-N4	-4.29	104.46	109.96
3	E	324	MES	C6-C5-N4	-4.14	104.65	109.96
3	J	324	MES	C6-C5-N4	-4.12	104.68	109.96
3	G	324	MES	O1-C2-C3	4.10	116.22	111.34
3	J	324	MES	C2-C3-N4	-4.09	104.71	109.96
3	F	324	MES	C6-C5-N4	-3.78	105.11	109.96
3	D	325	MES	C5-N4-C3	3.65	116.98	109.75
3	I	324	MES	C7-N4-C5	3.60	121.07	111.66
3	A	324	MES	C7-N4-C5	3.51	120.83	111.66
3	B	324	MES	C6-C5-N4	-3.48	105.50	109.96
3	G	324	MES	C8-C7-N4	-3.42	106.58	112.44
3	J	324	MES	C8-C7-N4	-3.39	106.64	112.44
3	F	324	MES	C7-N4-C5	3.38	120.50	111.66
3	D	325	MES	C7-C8-S	-3.38	103.30	112.49
3	I	324	MES	C6-C5-N4	-3.37	105.64	109.96
3	D	324	MES	O1-C6-C5	3.34	115.32	111.34
3	B	324	MES	C7-N4-C3	3.29	120.27	111.66
3	G	324	MES	C6-C5-N4	-3.24	105.80	109.96
3	D	325	MES	C6-C5-N4	-3.19	105.87	109.96
3	G	324	MES	C5-N4-C3	3.17	116.03	109.75
3	B	324	MES	C7-N4-C5	3.14	119.88	111.66
3	E	324	MES	C8-C7-N4	-3.10	107.12	112.44
3	A	324	MES	C2-C3-N4	-3.07	106.02	109.96
3	I	324	MES	C7-N4-C3	3.06	119.65	111.66
3	G	324	MES	O1-C6-C5	3.06	114.98	111.34
3	D	325	MES	C7-N4-C3	3.05	119.64	111.66
3	D	325	MES	O1-C2-C3	3.01	114.93	111.34
3	A	324	MES	C7-N4-C3	3.00	119.50	111.66
3	G	324	MES	C7-N4-C5	2.98	119.45	111.66
3	E	324	MES	C2-C3-N4	-2.98	106.14	109.96
3	E	324	MES	C7-N4-C5	2.97	119.43	111.66
3	E	324	MES	C7-N4-C3	2.95	119.38	111.66
3	J	324	MES	C7-N4-C5	2.95	119.37	111.66
3	F	324	MES	C7-N4-C3	2.93	119.31	111.66
3	D	324	MES	O1-C2-C3	2.92	114.82	111.34
3	G	324	MES	C7-N4-C3	2.88	119.19	111.66
3	J	324	MES	C7-N4-C3	2.83	119.06	111.66
3	B	324	MES	C2-C3-N4	-2.80	106.37	109.96
3	D	324	MES	C7-N4-C5	2.76	118.89	111.66
3	D	324	MES	C7-N4-C3	2.74	118.81	111.66
3	D	325	MES	C7-N4-C5	2.59	118.44	111.66
3	D	324	MES	C2-C3-N4	-2.55	106.69	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	324	MES	C2-C3-N4	-2.47	106.79	109.96
3	G	324	MES	C2-C3-N4	-2.46	106.80	109.96
3	D	324	MES	O3S-S-C8	2.33	112.01	105.99
3	F	324	MES	C2-C3-N4	-2.28	107.03	109.96
3	G	324	MES	C6-O1-C2	2.26	117.61	109.90
3	D	324	MES	C8-C7-N4	-2.19	108.68	112.44
3	G	324	MES	O1S-S-C8	2.17	113.06	106.36
3	G	324	MES	O2S-S-O1S	-2.16	108.26	112.44
3	D	324	MES	C7-C8-S	-2.15	106.62	112.49
3	I	324	MES	C8-C7-N4	-2.12	108.80	112.44
3	G	324	MES	C7-C8-S	-2.12	106.72	112.49
4	G	328	GOL	O2-C2-C3	2.03	117.48	108.22

There are no chirality outliers.

There are no torsion outliers.

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	324	MES	C2-C3-C5-C6-N4-O1
3	E	324	MES	C2-C3-C5-C6-N4-O1
3	A	324	MES	C2-C3-C5-C6-N4-O1
3	F	324	MES	C2-C3-C5-C6-N4-O1
3	I	324	MES	C2-C3-C5-C6-N4-O1
3	B	324	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.16	29 (9%) 9 11	57, 90, 172, 210	0
1	B	307/322 (95%)	-0.05	19 (6%) 20 24	52, 87, 172, 213	0
1	C	307/322 (95%)	-0.06	17 (5%) 24 29	51, 87, 173, 210	0
1	D	307/322 (95%)	-0.07	15 (4%) 28 34	51, 84, 170, 210	0
1	E	307/322 (95%)	-0.13	11 (3%) 41 48	54, 88, 170, 208	0
1	F	307/322 (95%)	0.10	30 (9%) 8 10	53, 94, 173, 208	0
1	G	307/322 (95%)	0.00	22 (7%) 15 18	51, 87, 168, 209	0
1	H	307/322 (95%)	0.18	27 (8%) 10 12	55, 89, 174, 208	0
1	I	307/322 (95%)	0.09	26 (8%) 11 13	57, 90, 172, 211	0
1	J	307/322 (95%)	-0.08	22 (7%) 15 18	59, 94, 175, 208	0
All	All	3070/3220 (95%)	0.01	218 (7%) 16 19	51, 89, 174, 213	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	ILE	21.8
1	B	152	ILE	20.4
1	G	152	ILE	15.9
1	H	288	ALA	12.2
1	F	317	ILE	12.0
1	H	290	GLY	11.6
1	H	291	VAL	11.6
1	H	289	ASN	10.5
1	J	291	VAL	10.3
1	F	152	ILE	9.9
1	F	316	VAL	9.8
1	G	317	ILE	9.8
1	E	291	VAL	9.5

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Mol	Chain	Res	Type	RSRZ
1	G	314	VAL	9.0
1	A	151	ASN	8.8
1	H	152	ILE	8.7
1	I	152	ILE	8.7
1	D	152	ILE	8.6
1	B	291	VAL	8.3
1	A	153	ASP	8.1
1	G	315	LEU	8.1
1	H	292	GLU	8.1
1	I	153	ASP	7.9
1	G	291	VAL	7.3
1	F	151	ASN	7.1
1	G	290	GLY	7.1
1	C	289	ASN	7.0
1	C	291	VAL	7.0
1	B	151	ASN	6.9
1	H	315	LEU	6.8
1	F	296	LEU	6.8
1	C	152	ILE	6.7
1	I	317	ILE	6.7
1	G	151	ASN	6.6
1	J	152	ILE	6.6
1	A	290	GLY	6.6
1	J	153	ASP	6.6
1	B	290	GLY	6.5
1	J	151	ASN	6.5
1	B	289	ASN	6.4
1	F	148	TYR	6.4
1	I	291	VAL	6.4
1	J	290	GLY	6.3
1	I	154	ASN	6.3
1	H	314	VAL	6.2
1	F	182	GLN	6.1
1	E	290	GLY	6.1
1	I	148	TYR	6.0
1	G	316	VAL	6.0
1	A	53	ASP	5.9
1	F	181	VAL	5.8
1	A	291	VAL	5.8
1	B	313	CYS	5.7
1	F	291	VAL	5.6
1	B	317	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	153	ASP	5.6
1	D	291	VAL	5.4
1	I	316	VAL	5.3
1	H	317	ILE	5.2
1	F	290	GLY	5.2
1	I	290	GLY	5.2
1	C	288	ALA	5.1
1	A	296	LEU	5.1
1	C	295	LEU	5.0
1	I	315	LEU	5.0
1	H	293	ASP	5.0
1	F	289	ASN	4.9
1	B	288	ALA	4.9
1	J	317	ILE	4.9
1	I	314	VAL	4.9
1	J	163	ARG	4.8
1	G	296	LEU	4.8
1	D	153	ASP	4.8
1	C	317	ILE	4.8
1	J	154	ASN	4.8
1	F	288	ALA	4.7
1	A	317	ILE	4.7
1	A	54	LYS	4.7
1	J	157	ILE	4.6
1	A	177	HIS	4.5
1	H	295	LEU	4.4
1	H	151	ASN	4.4
1	F	154	ASN	4.3
1	I	151	ASN	4.3
1	D	151	ASN	4.2
1	B	153	ASP	4.2
1	A	148	TYR	4.2
1	F	295	LEU	4.2
1	D	317	ILE	4.1
1	C	316	VAL	4.1
1	B	296	LEU	3.9
1	H	316	VAL	3.9
1	A	49	LYS	3.9
1	F	156	GLU	3.9
1	I	184	ASN	3.8
1	G	313	CYS	3.8
1	F	179	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	306	LEU	3.7
1	F	149	THR	3.7
1	F	150	GLU	3.7
1	D	148	TYR	3.7
1	E	148	TYR	3.7
1	H	296	LEU	3.6
1	J	161	TRP	3.6
1	D	176	ASP	3.6
1	H	182	GLN	3.6
1	D	184	ASN	3.6
1	A	154	ASN	3.6
1	D	290	GLY	3.5
1	H	185	GLN	3.5
1	I	185	GLN	3.5
1	B	316	VAL	3.5
1	F	178	LEU	3.5
1	I	288	ALA	3.5
1	H	163	ARG	3.5
1	A	117	ARG	3.4
1	A	52	GLY	3.4
1	A	176	ASP	3.4
1	B	312	GLY	3.3
1	C	290	GLY	3.2
1	D	226	GLU	3.2
1	B	314	VAL	3.2
1	D	154	ASN	3.1
1	I	289	ASN	3.1
1	A	302	LEU	3.1
1	G	153	ASP	3.1
1	F	286	ARG	3.1
1	H	294	ASP	3.0
1	I	295	LEU	3.0
1	J	289	ASN	3.0
1	J	52	GLY	3.0
1	B	293	ASP	3.0
1	H	311	ILE	3.0
1	D	316	VAL	2.9
1	G	156	GLU	2.9
1	D	183	PRO	2.9
1	A	314	VAL	2.9
1	I	293	ASP	2.9
1	A	150	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	289	ASN	2.9
1	G	286	ARG	2.8
1	I	183	PRO	2.8
1	F	313	CYS	2.8
1	H	313	CYS	2.8
1	E	181	VAL	2.8
1	A	286	ARG	2.8
1	A	121	PHE	2.8
1	G	154	ASN	2.8
1	A	316	VAL	2.8
1	G	157	ILE	2.8
1	J	158	ASP	2.8
1	C	296	LEU	2.8
1	H	302	LEU	2.8
1	F	142	PHE	2.7
1	D	68	ASN	2.7
1	E	152	ILE	2.7
1	J	123	ARG	2.7
1	A	156	GLU	2.7
1	C	292	GLU	2.7
1	E	288	ALA	2.6
1	A	295	LEU	2.6
1	G	155	GLU	2.6
1	B	297	ILE	2.6
1	F	287	GLN	2.6
1	F	183	PRO	2.6
1	D	315	LEU	2.6
1	E	184	ASN	2.6
1	I	298	GLN	2.6
1	I	150	GLU	2.6
1	I	313	CYS	2.5
1	J	310	ALA	2.5
1	B	295	LEU	2.5
1	I	54	LYS	2.5
1	F	180	SER	2.5
1	I	157	ILE	2.5
1	G	287	GLN	2.5
1	G	123	ARG	2.5
1	H	123	ARG	2.5
1	C	151	ASN	2.5
1	H	148	TYR	2.5
1	F	176	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	161	TRP	2.4
1	A	311	ILE	2.4
1	H	49	LYS	2.4
1	E	49	LYS	2.4
1	B	315	LEU	2.4
1	G	148	TYR	2.4
1	C	302	LEU	2.3
1	J	314	VAL	2.3
1	G	255	ARG	2.3
1	F	184	ASN	2.3
1	A	50	THR	2.3
1	A	142	PHE	2.3
1	I	182	GLN	2.3
1	B	294	ASP	2.2
1	J	164	GLY	2.2
1	G	289	ASN	2.2
1	F	46	LYS	2.2
1	A	178	LEU	2.2
1	C	153	ASP	2.2
1	J	54	LYS	2.2
1	C	121	PHE	2.2
1	B	292	GLU	2.2
1	I	123	ARG	2.1
1	C	306	LEU	2.1
1	E	315	LEU	2.1
1	H	306	LEU	2.1
1	A	141	ARG	2.1
1	E	46	LYS	2.1
1	J	49	LYS	2.1
1	H	174	ARG	2.1
1	C	315	LEU	2.1
1	J	51	PRO	2.0
1	C	198	VAL	2.0
1	H	287	GLN	2.0
1	I	227	SER	2.0
1	J	150	GLU	2.0
1	F	177	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	325	6/6	0.41	12.48	69,109,127,135	0
4	GOL	H	325	6/6	0.45	12.17	80,85,104,115	0
4	GOL	I	328	6/6	0.56	10.63	87,95,119,124	0
4	GOL	B	325	6/6	0.33	8.44	77,88,103,117	0
4	GOL	F	327	6/6	0.26	6.54	77,98,110,119	0
4	GOL	G	327	4/6	0.30	5.63	86,96,104,106	0
4	GOL	G	325	6/6	0.27	5.09	79,94,101,112	0
4	GOL	I	327	6/6	0.42	4.41	88,92,119,126	0
4	GOL	C	324	6/6	0.33	3.93	79,89,98,113	0
4	GOL	G	326	6/6	0.30	3.60	91,96,115,116	0
4	GOL	F	325	6/6	0.36	3.49	84,100,114,125	0
4	GOL	D	326	6/6	0.38	2.56	96,100,101,106	0
4	GOL	I	326	6/6	0.28	2.07	73,91,114,119	0
2	ACH	I	323	10/10	0.23	2.05	54,67,76,80	0
4	GOL	F	326	6/6	0.29	2.01	83,98,121,143	0
4	GOL	E	325	6/6	0.19	1.38	85,99,110,130	0
2	ACH	H	323	10/10	0.23	1.07	57,74,81,83	0
4	GOL	A	326	6/6	0.19	1.05	79,90,125,127	0
2	ACH	A	323	10/10	0.21	0.90	56,66,76,77	0
4	GOL	D	327	6/6	0.24	0.60	51,79,98,109	0
2	ACH	D	323	10/10	0.16	0.29	53,62,70,73	0
4	GOL	B	327	6/6	0.16	0.25	55,62,83,90	0
2	ACH	C	323	10/10	0.23	0.21	54,69,74,75	0
2	ACH	J	323	10/10	0.22	0.14	56,74,82,89	0
2	ACH	B	323	10/10	0.17	0.13	53,65,78,80	0
4	GOL	B	326	6/6	0.21	-0.09	83,110,138,150	0
2	ACH	G	323	10/10	0.16	-0.14	48,68,76,77	0
3	MES	F	324	12/12	0.15	-0.14	106,147,159,185	0
3	MES	D	325	12/12	0.16	-0.15	85,140,157,157	0
3	MES	I	324	12/12	0.18	-0.21	109,142,169,177	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MES	G	324	12/12	0.17	-0.21	99,122,143,150	0
3	MES	D	324	12/12	0.18	-0.29	107,132,160,169	0
3	MES	A	324	12/12	0.14	-0.33	91,140,168,188	0
2	ACH	F	323	10/10	0.15	-0.42	48,67,74,76	0
4	GOL	E	326	6/6	0.14	-0.55	67,89,129,133	0
4	GOL	F	328	6/6	0.13	-0.56	73,86,114,121	0
4	GOL	I	329	6/6	0.19	-0.57	61,71,110,133	0
4	GOL	H	324	6/6	0.19	-0.62	56,69,111,111	0
2	ACH	E	323	10/10	0.20	-0.70	57,76,82,85	0
4	GOL	C	325	6/6	0.13	-0.82	60,66,78,92	0
4	GOL	J	325	6/6	0.12	-1.05	64,92,106,114	0
4	GOL	G	328	6/6	0.13	-1.11	50,79,101,104	0
3	MES	B	324	12/12	0.09	-1.32	120,136,164,175	0
3	MES	J	324	12/12	0.12	-1.39	139,157,169,184	0
3	MES	E	324	12/12	0.09	-1.53	123,143,171,178	0
4	GOL	I	325	6/6	0.11	-1.68	88,93,105,121	0

6.5 Other polymers ⓘ

There are no such residues in this entry.