



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:35 AM UTC

PDB ID : 3RQW / pdb_00003rqw
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

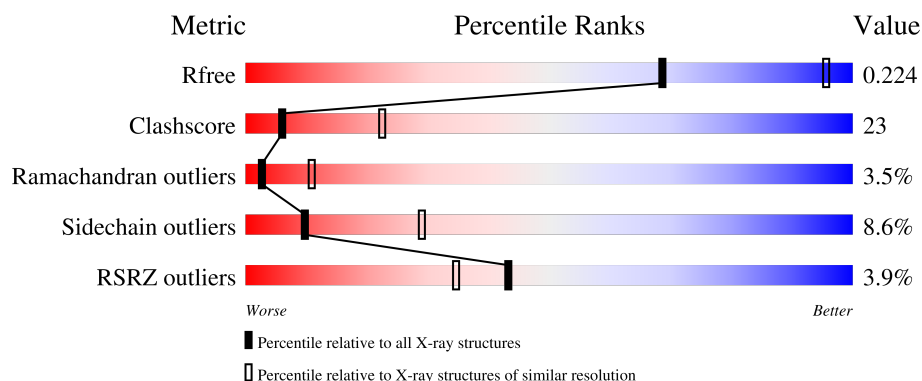
1 Overall quality at a glance

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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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 of 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	7% 60% 29% 6% 5%
1	B	322	4% 61% 30% • • 5%
1	C	322	2% 60% 30% 5% • 5%
1	D	322	2% 60% 29% 7% 5%
1	E	322	4% 61% 29% 5% 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	326	-	-	X	-
4	GOL	B	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

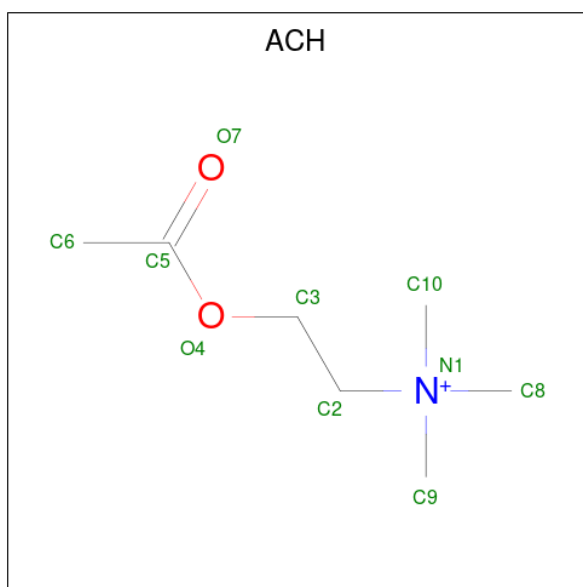
There are 5 unique types of molecules in this entry. The entry contains 25508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ACH) (formula: $C_7H_{16}NO_2$).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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 (CCD ID: 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

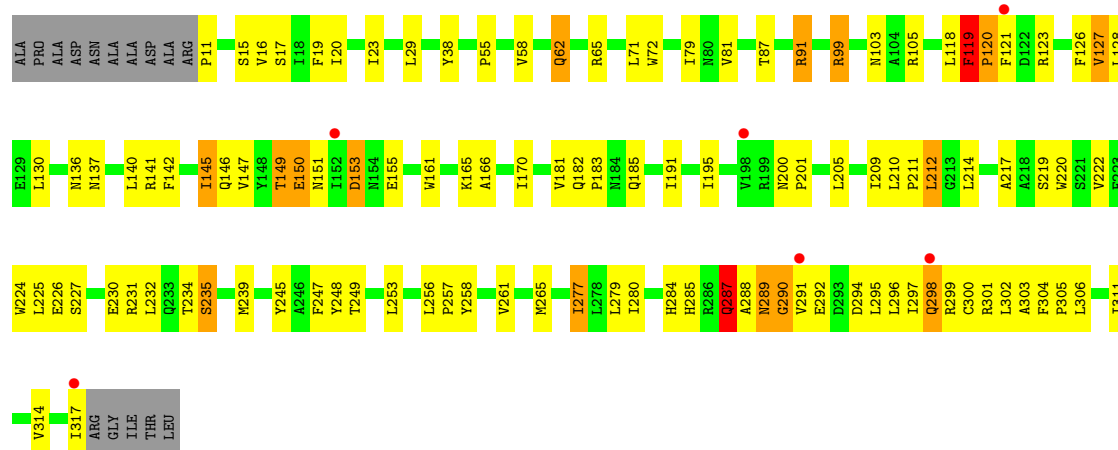
- Molecule 5 is water.

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

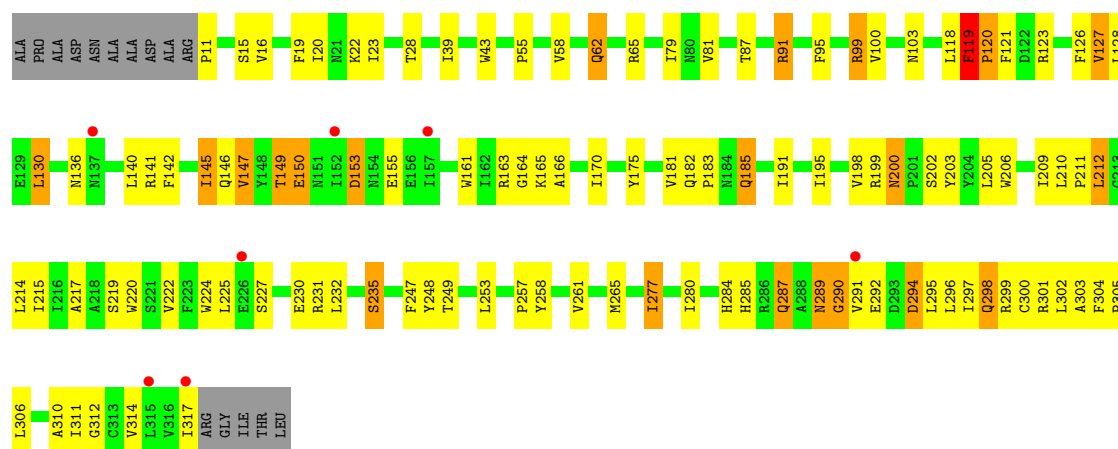
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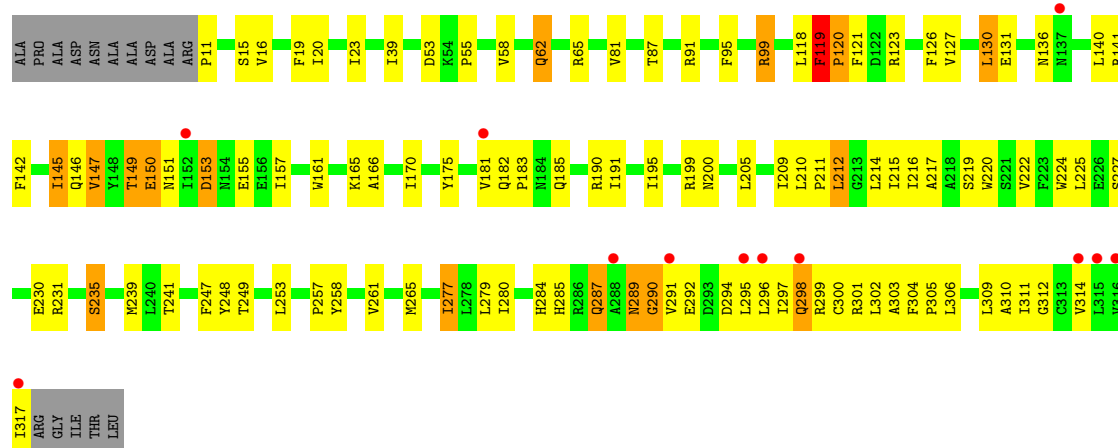
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	12	Total 12	O 12	0	0
5	H	7	Total 7	O 7	0	0
5	I	6	Total 6	O 6	0	0
5	J	7	Total 7	O 7	0	0



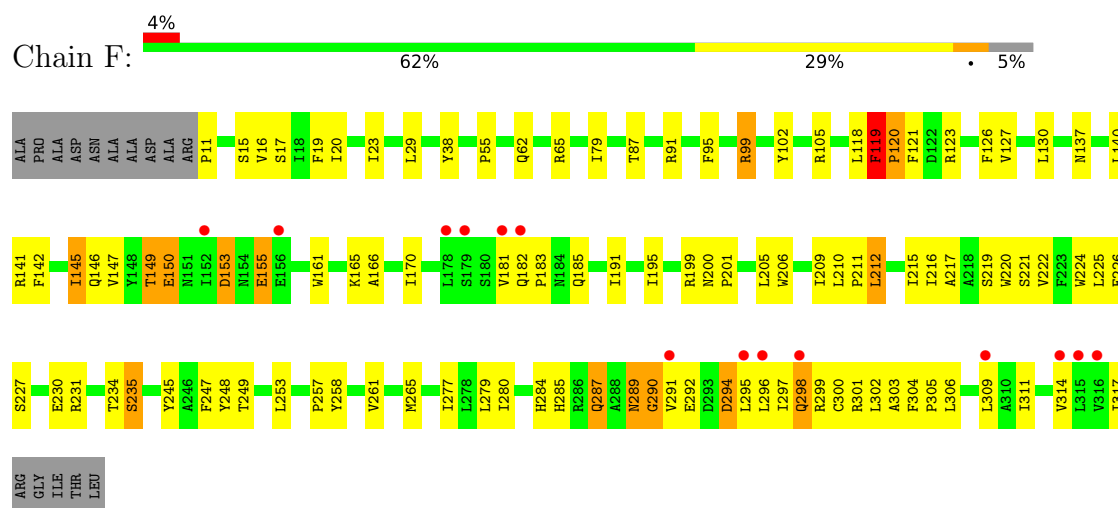
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



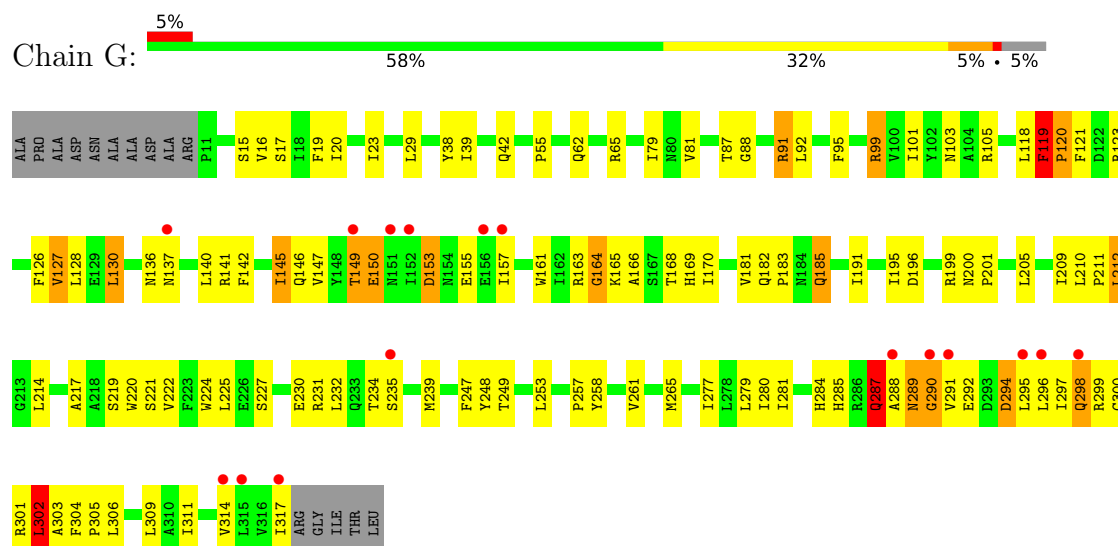
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



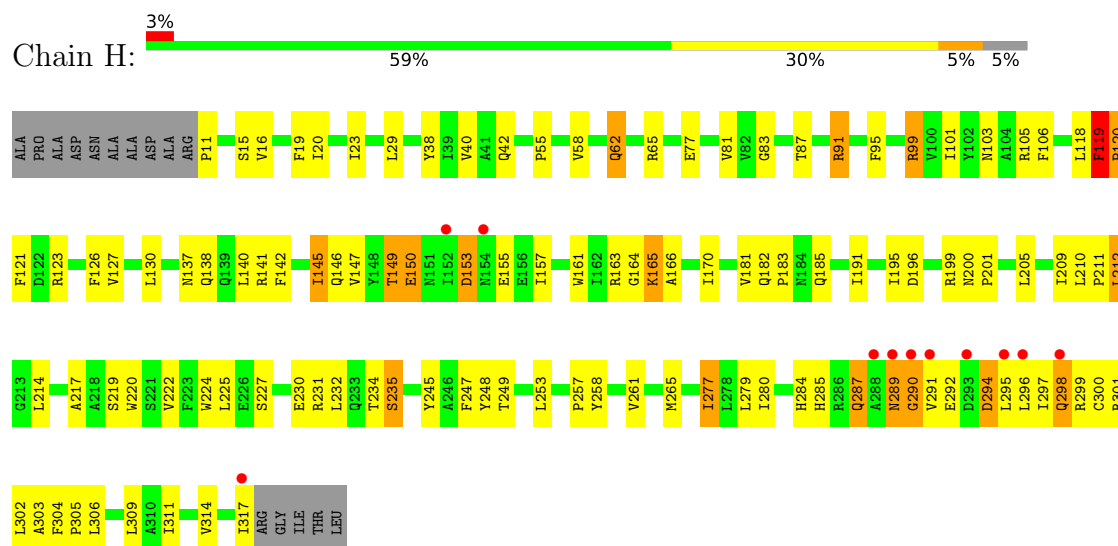
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



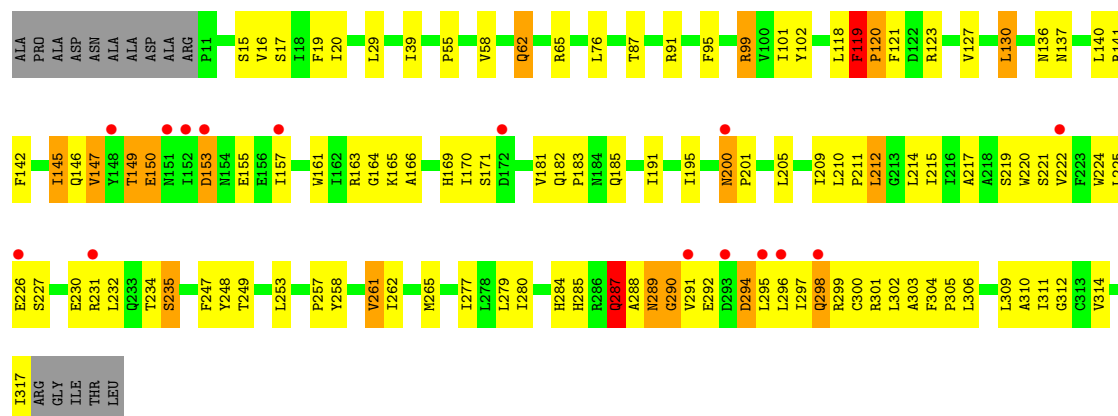
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



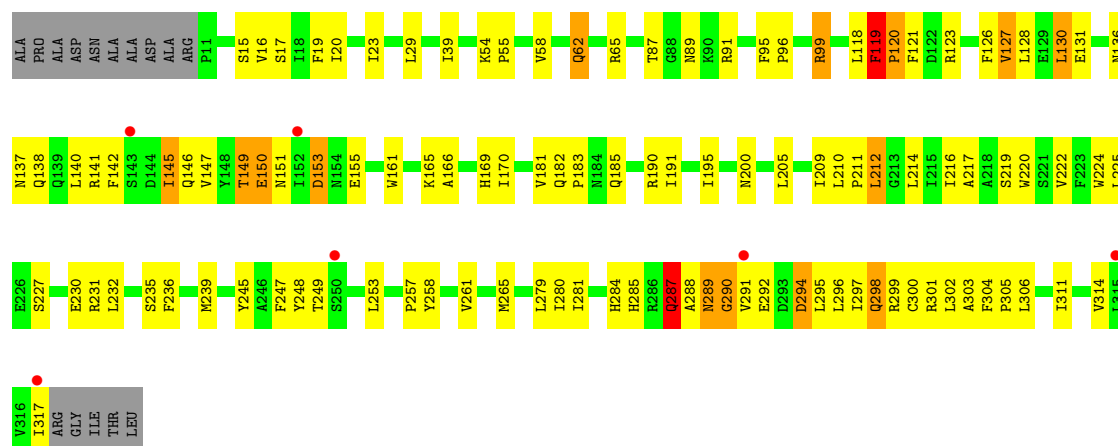
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



Chain I: 5% 60% 30% 5% 5%



Chain J: 2% 61% 30% 5%



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 24.98 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.98-2.91) 97.9 (24.98-2.91)	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 0.203 , 0.224	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)	0.28 , 51.1	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: MES, ACH, GOL

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	0.45	0/2573	0.81	2/3507 (0.1%)
1	B	0.54	0/2573	0.85	2/3507 (0.1%)
1	C	0.51	0/2573	0.84	2/3507 (0.1%)
1	D	0.57	0/2573	0.85	3/3507 (0.1%)
1	E	0.52	0/2573	0.83	3/3507 (0.1%)
1	F	0.48	0/2573	0.84	3/3507 (0.1%)
1	G	0.53	0/2573	0.88	4/3507 (0.1%)
1	H	0.51	0/2573	0.85	2/3507 (0.1%)
1	I	0.51	0/2573	0.87	4/3507 (0.1%)
1	J	0.49	0/2573	0.83	2/3507 (0.1%)
All	All	0.51	0/25730	0.84	27/35070 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	119	PHE	CA-C-N	7.56	129.29	119.84
1	I	119	PHE	C-N-CA	7.56	129.29	119.84
1	F	155	GLU	N-CA-C	-6.85	106.81	114.62
1	E	119	PHE	CA-C-N	6.80	128.34	119.84
1	E	119	PHE	C-N-CA	6.80	128.34	119.84
1	J	119	PHE	CA-C-N	6.50	127.96	119.84
1	J	119	PHE	C-N-CA	6.50	127.96	119.84
1	F	119	PHE	CA-C-N	6.35	127.78	119.84
1	F	119	PHE	C-N-CA	6.35	127.78	119.84
1	G	119	PHE	CA-C-N	6.30	127.71	119.84
1	G	119	PHE	C-N-CA	6.30	127.71	119.84
1	A	119	PHE	CA-C-N	6.08	127.44	119.84
1	A	119	PHE	C-N-CA	6.08	127.44	119.84
1	B	119	PHE	CA-C-N	5.55	126.78	119.84
1	B	119	PHE	C-N-CA	5.55	126.78	119.84
1	H	119	PHE	CA-C-N	5.50	126.71	119.84
1	H	119	PHE	C-N-CA	5.50	126.71	119.84
1	C	119	PHE	CA-C-N	5.39	126.57	119.84
1	C	119	PHE	C-N-CA	5.39	126.57	119.84
1	G	302	LEU	N-CA-C	-5.19	108.21	114.75
1	D	119	PHE	CA-C-N	5.18	126.31	119.84
1	D	119	PHE	C-N-CA	5.18	126.31	119.84
1	G	185	GLN	N-CA-C	5.11	116.99	107.99
1	D	185	GLN	N-CA-C	5.05	116.91	108.23
1	I	119	PHE	C-N-CD	-5.04	104.31	125.00
1	E	53	ASP	N-CA-C	-5.04	104.92	112.54
1	I	101	ILE	N-CA-C	5.02	115.08	107.75

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

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Mol	Chain	Res	Type	Group
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	120	0
1	B	2505	0	2478	126	0
1	C	2505	0	2478	110	0
1	D	2505	0	2478	117	0
1	E	2505	0	2478	112	0
1	F	2505	0	2478	120	0
1	G	2505	0	2478	134	0
1	H	2505	0	2478	120	0
1	I	2505	0	2478	126	0
1	J	2505	0	2478	126	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	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1152) 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:B:140:LEU:HD11	5:B:332:HOH:O	1.51	1.11
1:I:140:LEU:HD21	5:I:334:HOH:O	1.48	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:HG3	1:G:99:ARG:HH11	1.28	0.95
1:J:136:ASN:O	4:J:325:GOL:H2	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HH11	1:A:99:ARG:HG3	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:HG3	1:E:99:ARG:HH11	1.31	0.94
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.50	0.94
1:D:99:ARG:HG3	1:D:99:ARG:HH11	1.33	0.93
1:I:99:ARG:HG3	1:I:99:ARG:HH11	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:HG3	1:C:99:ARG:HH11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:212:LEU:HD13	1:H:265:MET:HE2	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:F:212:LEU:HD13	1:F:265:MET:HE2	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: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:212:LEU:HD13	1:B:265:MET:HE2	1.68	0.76
1:B:145:ILE:HD13	1:B:145:ILE:O	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:C	1:D:121:PHE:H	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:119:PHE:C	1:H:121:PHE:H	1.98	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:A:212:LEU:HD13	1:A:265:MET:HE2	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: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:G:212:LEU:HD13	1:G:265:MET:HE2	1.71	0.71
1:J:145:ILE:CD1	1:J:166:ALA:HB3	2.19	0.71
1:C:119:PHE:C	1:C:121:PHE:H	1.98	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:A:289:ASN:CG	1:A:290:GLY:H	1.99	0.70
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:E:119:PHE:C	1:E:121:PHE:H	1.99	0.70
1:C:289:ASN:CG	1:C:290:GLY:H	2.00	0.70
1:G:289:ASN:CG	1:G:290:GLY:H	2.00	0.70
1:I:289:ASN:CG	1:I:290:GLY:H	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:C	1:B:121:PHE:H	2.00	0.69
1:H:119:PHE:CD2	1:H:120:PRO:HD3	2.27	0.69
1:J:212:LEU:HD13	1:J:265:MET:HE2	1.73	0.69
1:F:289:ASN:CG	1:F:290:GLY:H	1.99	0.69
1:G:145:ILE:HD13	1:G:145:ILE:O	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:E:289:ASN:CG	1:E:290:GLY:H	2.00	0.69
1:I:294:ASP:HB3	1:I:297:ILE:HG22	1.74	0.69
1:J:119:PHE:C	1:J:121:PHE:H	1.99	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:B:289:ASN:CG	1:B:290:GLY:H	2.01	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:A:231:ARG:HB3	1:A:280:ILE:HD13	1.74	0.69
1:D:289:ASN:CG	1:D:290:GLY:H	2.00	0.69
1:F:119:PHE:C	1:F:121:PHE:H	2.00	0.69
1:H:294:ASP:HB3	1:H:297:ILE:HG22	1.73	0.69
1:D:212:LEU:HD13	1:D:265:MET:HE2	1.75	0.68
1:J:145:ILE:O	1:J:145:ILE:HD13	1.94	0.68
1:A:119:PHE:C	1:A:121:PHE:H	2.00	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:289:ASN:CG	1:J:290:GLY:H	2.00	0.68
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.75	0.68
1:I:119:PHE:C	1:I:121:PHE:H	2.01	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: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
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:E:212:LEU:HD13	1:E:265:MET:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:LEU:HD13	1:I:265:MET:HE2	1.75	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:H:289:ASN:CG	1:H:290:GLY:H	2.01	0.67
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.30	0.67
1:G:119:PHE:C	1:G:121:PHE:H	2.01	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:HD13	1:D:145:ILE:O	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: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: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:C:212:LEU:HD13	1:C:265:MET:HE2	1.78	0.65
1:F:147:VAL:CG1	1:F:165:LYS:HE2	2.25	0.65
1:G:168:THR:C	1:G:169:HIS:ND1	2.54	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: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:G:147:VAL:CG1	1:G:165:LYS:HE2	2.27	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: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:C:145:ILE:HD13	1:C:145:ILE:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:ALA:HB2	1:F:195:ILE:HG12	1.79	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: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: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:11:PRO:HB3	4:F:328:GOL:C1	2.26	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: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: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
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:E:15:SER:HB3	1:E:141:ARG:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:H:99:ARG:NH1	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:119:PHE:C	1:D:121:PHE:N	2.59	0.60
1:D:141:ARG:HG3	1:D:142:PHE:CD2	2.37	0.60
1:E:99:ARG:HG3	1:E:99:ARG:NH1	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:HG3	1:D:99:ARG:NH1	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:136:ASN:O	4:E:326:GOL:H32	2.03	0.58
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.32	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:O	1:I:147:VAL:HG22	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:F:247:PHE:HA	1:J:248:TYR:CD1	2.39	0.58
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.69	0.57
1:H:147:VAL:HG22	1:H:147:VAL:O	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:168:THR:C	1:B:169:HIS:CD2	2.83	0.56
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:D:19:PHE:CE2	1:D:146:GLN:HG3	2.40	0.56
1:A:247:PHE:HA	1:E:248:TYR:CD1	2.41	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: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: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: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:15:SER:HB3	1:A:141:ARG:HD3	1.88	0.55
1:A:118:LEU:O	1:A:119:PHE:O	2.24	0.55
1:C:182:GLN:HB2	1:C:185:GLN:HG2	1.88	0.55
1:B:119:PHE:C	1:B:121:PHE:N	2.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:E:147:VAL:HG22	2.07	0.55
1:F:248:TYR:CD1	1:G:247:PHE:HA	2.42	0.55
1:A:119:PHE:C	1:A:121:PHE:N	2.65	0.55
1:E:210:LEU:CB	1:E:211:PRO:HD3	2.34	0.55
1:H:119:PHE:CG	1:H:120:PRO:N	2.75	0.55
1:H:212:LEU:CD1	1:H:265:MET:HE2	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:HG22	1:D:147:VAL:O	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:119:PHE:C	1:G:121:PHE:N	2.65	0.54
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.89	0.54
1:A:248:TYR:CD1	1:B:247:PHE:HA	2.43	0.54
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.71	0.54
1:C:119:PHE:C	1:C:121:PHE:N	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:212:LEU:CD1	1:B:265:MET:HE2	2.37	0.53
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.43	0.53
1:F:212:LEU:CD1	1:F:265:MET:HE2	2.33	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:HG12	1:C:314:VAL:O	2.08	0.53
1:F:150:GLU:HG3	1:F:153:ASP:HB2	1.91	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
1:G:314:VAL:HG12	1:G:314:VAL:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:297:ILE:C	1:I:299:ARG:N	2.67	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:I:215:ILE:HG12	1:J:239:MET:HE3	1.90	0.53
1:I:225:LEU:HD21	1:J:232:LEU:HD23	1.91	0.53
1:J:119:PHE:O	1:J:121:PHE:N	2.32	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:A:297:ILE:C	1:A:299:ARG:N	2.67	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:HG12	1:A:314:VAL:O	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:G:136:ASN:C	4:G:328:GOL:H2	2.33	0.52
1:I:119:PHE:C	1:I:121:PHE:N	2.67	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:HH11	1:A:99:ARG:CG	2.14	0.52
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.90	0.52
1:I:212:LEU:CD1	1:I:265:MET:HE2	2.40	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: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:HB3	1:I:141:ARG:HG2	1.91	0.52
1:I:15:SER:HB2	1:I:142:PHE:CE1	2.45	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:G:225:LEU:CD2	1:H:232:LEU:HD23	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:GLY:C	4:H:325:GOL:O2	2.52	0.52
1:H:140:LEU:CD2	5:H:331:HOH:O	2.47	0.52
1:H:297:ILE:HG23	1:H:298:GLN:N	2.24	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:HG12	1:H:314:VAL:O	2.10	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:H:210:LEU:HB3	1:H:211:PRO:CD	2.38	0.51
1:A:212:LEU:CD1	1:A:265:MET:HE2	2.40	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:B:168:THR:C	1:B:169:HIS:CG	2.88	0.51
1:C:297:ILE:C	1:C:299:ARG:N	2.67	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:E:314:VAL:HG12	1:E:314:VAL:O	2.10	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:E:119:PHE:C	1:E:121:PHE:N	2.65	0.51
1:F:297:ILE:C	1:F:299:ARG:N	2.69	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
1:J:119:PHE:C	1:J:121:PHE:N	2.65	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:297:ILE:C	1:J:299:ARG:N	2.68	0.51
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:137:ASN:HA	4:J:325:GOL:C2	2.41	0.51
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.74	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:D:11:PRO:HD2	5:D:339:HOH:O	2.09	0.50
1:D:297:ILE:C	1:D:299:ARG:N	2.67	0.50
1:F:38:TYR:CE1	1:F:105:ARG:HD3	2.46	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:G:289:ASN:CG	1:G:290:GLY:N	2.69	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:J:220:TRP:C	1:J:222:VAL:H	2.19	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:20:ILE:HD12	1:D:195:ILE:HD11	1.93	0.50
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.93	0.50
1:H:297:ILE:C	1:H:299:ARG:N	2.68	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:B:289:ASN:CG	1:B:290:GLY:N	2.70	0.50
1:D:136:ASN:O	4:D:327:GOL:H32	2.12	0.50
1:D:161:TRP:CZ2	1:D:200:ASN:ND2	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ILE:C	1:E:299:ARG:N	2.67	0.50
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.46	0.50
2:F:323:ACH:H102	2:F:323:ACH:O4	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
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:E:289:ASN:CG	1:E:290:GLY:N	2.69	0.50
1:G:297:ILE:HG23	1:G:298:GLN:N	2.27	0.50
1:G:297:ILE:C	1:G:299:ARG:N	2.66	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:B:220:TRP:C	1:B:222:VAL:H	2.20	0.50
1:D:140:LEU:CD2	5:D:341:HOH:O	2.33	0.50
1:E:142:PHE:HA	1:E:170:ILE:HD11	1.93	0.50
1:F:289:ASN:CG	1:F:290:GLY:N	2.68	0.50
1:B:147:VAL:O	1:B:147:VAL:HG22	2.12	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: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: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:J:119:PHE:CD2	1:J:120:PRO:CD	2.94	0.49
1:J:297:ILE:HG23	1:J:298:GLN:N	2.26	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:215:ILE:CG1	1:J:239:MET:HE3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:CG	1:A:290:GLY:N	2.68	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
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:I:289:ASN:CG	1:I:290:GLY:N	2.69	0.49
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.76	0.49
1:G:212:LEU:CD1	1:G:265:MET:HE2	2.40	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:289:ASN:CG	1:J:290:GLY:N	2.70	0.49
1:J:297:ILE:CG2	1:J:298:GLN:N	2.75	0.49
1:B:136:ASN:C	4:B:327:GOL:H32	2.37	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:D:297:ILE:C	1:D:299:ARG:H	2.21	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: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: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:HB3	1:J:141:ARG:CD	2.42	0.49
1:J:15:SER:HB2	1:J:142:PHE:CE1	2.48	0.49
1:A:119:PHE:CD2	1:A:120:PRO:CD	2.92	0.49
1:A:175:TYR:CZ	2:E:323:ACH:H101	2.47	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:I:248:TYR:CD1	1:J:247:PHE:HA	2.48	0.49
1:B:205:LEU:HD23	1:B:205:LEU:HA	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:H:220:TRP:C	1:H:222:VAL:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PHE:O	1:F:121:PHE:N	2.31	0.48
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.95	0.48
1:H:145:ILE:HD11	1:H:166:ALA:HB3	1.95	0.48
1:I:297:ILE:CG2	1:I:298:GLN:N	2.76	0.48
1:J:19:PHE:CD1	2:J:323:ACH:H61	2.48	0.48
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.76	0.48
1:B:297:ILE:C	1:B:299:ARG:N	2.69	0.48
1:C:15:SER:HB3	1:C:141:ARG:CD	2.43	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
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:A:232:LEU:HD23	1:E:225:LEU:CD2	2.44	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:H102	2:D:323:ACH:O4	2.13	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:H:119:PHE:C	1:H:121:PHE:N	2.63	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:E:205:LEU:HD23	1:E:209:ILE:HD12	1.95	0.48
1:A:15:SER:HB3	1:A:141:ARG:CD	2.43	0.48
1:A:137:ASN:HA	4:A:326:GOL:HO1	1.78	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:23:ILE:HG21	1:E:126:PHE:CD2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:LEU:HA	1:G:29:LEU:HD23	1.57	0.47
1:G:210:LEU:CB	1:G:211:PRO:HD3	2.41	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:95:PHE:HB2	1:E:99:ARG:HB2	1.96	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:F:257:PRO:HG2	1:F:258:TYR:HD2	1.76	0.47
1:I:220:TRP:C	1:I:222:VAL:H	2.21	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: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: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:55:PRO:HG2	1:J:181:VAL:HG13	1.96	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:C:145:ILE:HD11	1:C:166:ALA:HB3	1.94	0.47
1:F:29:LEU:HA	1:F:29:LEU:HD23	1.67	0.47
1:F:119:PHE:C	1:F:121:PHE:N	2.65	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:G:297:ILE:C	1:G:299:ARG:H	2.23	0.47
1:H:11:PRO:N	5:H:328:HOH:O	2.47	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:A:136:ASN:O	4:A:326:GOL:H11	2.14	0.47
1:B:145:ILE:CD1	1:B:145:ILE:O	2.59	0.47
1:D:149:THR:O	1:D:150:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TRP:C	1:D:222:VAL:H	2.23	0.47
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.50	0.47
1:E:145:ILE:HD11	1:E:166:ALA:HB3	1.94	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:F:221:SER:HB2	1:G:281:ILE:HD11	1.95	0.47
1:G:15:SER:HB3	1:G:141:ARG:HD3	1.96	0.47
1:H:140:LEU:CD1	5:H:331:HOH:O	2.33	0.47
1:I:76:LEU:H	4:I:327:GOL:C1	2.28	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:D:289:ASN:CG	1:D:290:GLY:N	2.69	0.47
1:G:297:ILE:O	1:G:299:ARG:N	2.48	0.47
2:G:323:ACH:O4	2:G:323:ACH:H102	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:C:15:SER:HB3	1:C:141:ARG:HG2	1.97	0.47
1:F:215:ILE:HG12	1:G:239:MET:HE3	1.96	0.47
1:J:212:LEU:CD1	1:J:265:MET:HE2	2.42	0.47
1:A:220:TRP:C	1:A:222:VAL:H	2.23	0.46
1:B:147:VAL:HG13	1:B:147:VAL:O	2.15	0.46
1:E:15:SER:HB3	1:E:141:ARG:HG2	1.97	0.46
1:J:136:ASN:C	4:J:325:GOL:H2	2.37	0.46
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.50	0.46
1:B:119:PHE:CD2	1:B:120:PRO:CD	2.98	0.46
1:B:215:ILE:CG1	1:C:239:MET:HE3	2.45	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:95:PHE:HB2	1:B:99:ARG:HB2	1.96	0.46
1:B:142:PHE:HA	1:B:170:ILE:HD11	1.97	0.46
1:C:38:TYR:CE1	1:C:105:ARG:HD3	2.50	0.46
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:149:THR:O	1:H:150:GLU:HB3	2.14	0.46
1:J:99:ARG:HH11	1:J:99:ARG:CG	2.12	0.46
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.49	0.46
1:A:239:MET:HE3	1:E:215:ILE:HG12	1.98	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
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.80	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
2:A:323:ACH:H102	2:A:323:ACH:O4	2.15	0.46
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.51	0.46
1:G:220:TRP:C	1:G:222:VAL:H	2.24	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:C:297:ILE:C	1:C:299:ARG:H	2.23	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:A:297:ILE:C	1:A:299:ARG:H	2.23	0.46
1:E:297:ILE:C	1:E:299:ARG:H	2.24	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:H51	3:A:324:MES:O1S	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:A:289:ASN:OD1	1:A:292:GLU:HB3	2.16	0.45
1:C:220:TRP:C	1:C:222:VAL:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.51	0.45
2:C:323:ACH:H102	2:C:323:ACH:O4	2.15	0.45
1:E:205:LEU:HD23	1:E:205:LEU:HA	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:I:297:ILE:C	1:I:299:ARG:H	2.22	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: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: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:248:TYR:HD1	1:E:247:PHE:HA	1.81	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:F:289:ASN:HD21	1:F:292:GLU:HB2	1.81	0.45
1:G:15:SER:HB3	1:G:141:ARG:CG	2.47	0.45
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.42	0.45
1:H:289:ASN:CG	1:H:290:GLY:N	2.70	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: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:95:PHE:CD2	1:F:99:ARG:HB2	2.52	0.45
1:F:149:THR:O	1:F:150:GLU:HB3	2.16	0.45
4:G:328:GOL:O3	4:G:328:GOL:O1	2.32	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:C:147:VAL:HG13	1:C:147:VAL:O	2.17	0.45
1:D:215:ILE:HG12	1:E:239:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:304:PHE:CB	1:A:305:PRO:HD3	2.47	0.45
1:C:225:LEU:CD2	1:D:232:LEU:HD23	2.47	0.45
1:C:297:ILE:O	1:C:299:ARG:N	2.50	0.45
1:E:136:ASN:O	4:E:326:GOL:O1	2.32	0.45
1:H:157:ILE:HD13	1:H:157:ILE:HA	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:D:212:LEU:CD1	1:D:265:MET:HE2	2.44	0.44
1:G:38:TYR:CE1	1:G:105:ARG:HD3	2.52	0.44
1:G:287:GLN:HB2	1:G:288:ALA:H	1.52	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: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:127:VAL:C	1:G:128:LEU:HD12	2.43	0.44
1:G:212:LEU:HD13	1:G:265:MET:HB3	1.98	0.44
1:G:311:ILE:HG22	1:G:311:ILE:O	2.18	0.44
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.78	0.44
1:I:289:ASN:ND2	1:I:292:GLU:HB2	2.32	0.44
1:I:289:ASN:HD21	1:I:292:GLU:HB2	1.82	0.44
1:J:29:LEU:HA	1:J:29:LEU:HD23	1.69	0.44
1:A:29:LEU:HA	1:A:29:LEU:HD23	1.63	0.44
1:A:248:TYR:HD1	1:B:247:PHE:HA	1.82	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:215:ILE:CG1	1:G:239:MET:HE3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HD23	1:E:212:LEU:HA	1.81	0.44
2:E:323:ACH:H102	2:E:323:ACH:O4	2.17	0.44
1:G:150:GLU:HG3	1:G:153:ASP:CB	2.47	0.44
1:G:205:LEU:HA	1:G:205:LEU:HD23	1.66	0.44
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.53	0.44
1:I:29:LEU:HD23	1:I:29:LEU:HA	1.57	0.44
1:I:287:GLN:HB2	1:I:288:ALA:H	1.53	0.44
1:J:212:LEU:HD13	1:J:265:MET:HB3	1.98	0.44
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:102:TYR:OH	4:F:325:GOL:H12	2.17	0.44
1:F:289:ASN:ND2	1:F:292:GLU:HB2	2.33	0.44
1:H:58:VAL:CG1	1:H:62:GLN:HB3	2.47	0.44
1:H:150:GLU:HG3	1:H:153:ASP:CB	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:HG13	1:D:147:VAL:O	2.17	0.44
1:E:58:VAL:CG1	1:E:62:GLN:HB3	2.47	0.44
1:F:79:ILE:HD13	1:F:79:ILE:HA	1.87	0.44
1:H:40:VAL:HG22	1:H:103:ASN:ND2	2.33	0.44
1:H:297:ILE:C	1:H:299:ARG:H	2.25	0.44
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.66	0.44
1:A:289:ASN:ND2	1:A:292:GLU:HB2	2.32	0.44
1:B:55:PRO:HG2	1:C:181:VAL:HG13	2.00	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:D:79:ILE:HD13	1:D:79:ILE:HA	1.80	0.44
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.82	0.44
1:E:291:VAL:HG12	1:E:291:VAL:O	2.17	0.44
1:F:225:LEU:HD21	1:G:232:LEU:HD23	1.99	0.44
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.52	0.44
1:A:212:LEU:HD13	1:A:265:MET:HB3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLN:HB2	1:B:288:ALA:H	1.55	0.44
1:E:311:ILE:HG22	1:E:311:ILE:O	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
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:HG12	1:B:291:VAL:O	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:HG22	1:C:311:ILE:O	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:HG22	1:H:311:ILE:O	2.18	0.43
1:C:289:ASN:ND2	1:C:292:GLU:HB2	2.34	0.43
1:F:182:GLN:NE2	1:J:54:LYS:HD2	2.33	0.43
1:F:220:TRP:C	1:F:222:VAL:H	2.26	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.53	0.43
1:I:58:VAL:CG1	1:I:62:GLN:HB3	2.49	0.43
1:I:163:ARG:HA	1:I:163:ARG:HD3	1.84	0.43
1:I:257:PRO:HG2	1:I:258:TYR:HD2	1.83	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.66	0.43
1:B:140:LEU:HD13	1:B:191:ILE:CG1	2.31	0.43
1:H:225:LEU:CD2	1:I:232:LEU:HD23	2.48	0.43
1:I:161:TRP:CZ2	1:I:200:ASN:ND2	2.85	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:212:LEU:CD1	1:E:265:MET:HE2	2.45	0.43
1:E:304:PHE:CB	1:E:305:PRO:HD3	2.49	0.43
1:H:163:ARG:HD3	1:H:163:ARG:HA	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:HG22	1:J:311:ILE:O	2.19	0.43
1:A:55:PRO:HB3	1:A:95:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:297:ILE:C	1:B:299:ARG:H	2.27	0.43
1:C:212:LEU:CD1	1:C:265:MET:HE2	2.47	0.43
1:D:127:VAL:C	1:D:128:LEU:HD12	2.43	0.43
1:D:284:HIS:HD2	1:D:285:HIS:NE2	2.16	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:OD1	1:H:292:GLU:HB3	2.19	0.43
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.53	0.43
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.79	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:99:ARG:NH1	1:I:99:ARG:CG	2.78	0.43
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.83	0.43
1:E:157:ILE:HD13	1:E:157:ILE:HA	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:HD13	1:A:79:ILE:HA	1.83	0.43
1:B:168:THR:O	1:B:169:HIS:CG	2.72	0.43
1:D:95:PHE:HB2	1:D:99:ARG:HB2	1.99	0.43
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.61	0.43
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.54	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:F:297:ILE:C	1:F:299:ARG:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:HIS:HD2	1:E:285:HIS:NE2	2.16	0.42
1:H:291:VAL:HG12	1:H:291:VAL:O	2.19	0.42
1:A:95:PHE:HB2	1:A:99:ARG:HB2	2.00	0.42
1:B:39:ILE:HD11	1:B:130:LEU:HD11	2.00	0.42
1:B:119:PHE:HE1	1:B:199:ARG:CZ	2.32	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
1:I:140:LEU:CD1	5:I:334:HOH:O	2.53	0.42
1:B:147:VAL:C	1:B:149:THR:H	2.28	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:J:220:TRP:C	1:J:222:VAL:N	2.78	0.42
1:B:297:ILE:O	1:B:299:ARG:N	2.53	0.42
1:F:248:TYR:HA	1:G:247:PHE:CE1	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: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:HG13	1:F:147:VAL:O	2.18	0.42
1:F:311:ILE:O	1:F:311:ILE:HG22	2.20	0.42
1:G:95:PHE:HB2	1:G:99:ARG:HB2	2.01	0.42
1:G:227:SER:HB3	1:G:230:GLU:CG	2.49	0.42
1:H:55:PRO:HB3	1:H:95:PHE:CD1	2.54	0.42
1:I:19:PHE:CG	2:I:323:ACH:H61	2.54	0.42
1:I:234:THR:HG21	1:J:236:PHE:CE2	2.55	0.42
1:J:212:LEU:HD23	1:J:212:LEU:HA	1.88	0.42
1:J:291:VAL:HG12	1:J:291:VAL:O	2.20	0.42
1:J:297:ILE:C	1:J:299:ARG:H	2.26	0.42
1:A:311:ILE:O	1:A:311:ILE:HG22	2.20	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:J:19:PHE:CG	2:J:323:ACH:H61	2.55	0.42
1:A:291:VAL:HG12	1:A:291:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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: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
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:HD13	1:C:79:ILE:HA	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:B:220:TRP:C	1:B:222:VAL:N	2.78	0.41
1:D:23:ILE:HG21	1:D:126:PHE:CD2	2.56	0.41
1:D:310:ALA:C	1:D:312:GLY:H	2.27	0.41
1:G:284:HIS:HD2	1:G:285:HIS:NE2	2.17	0.41
1:H:106:PHE:CD1	1:H:106:PHE:C	2.98	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:D:202:SER:O	1:D:203:TYR:C	2.63	0.41
1:B:305:PRO:O	1:B:309:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:310:ALA:C	1:E:312:GLY:H	2.28	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:J:145:ILE:CG1	1:J:166:ALA:HB3	2.49	0.41
1:B:310:ALA:C	1:B:312:GLY:H	2.28	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:A:239:MET:HE3	1:E:215:ILE:CG1	2.51	0.41
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.83	0.41
1:C:291:VAL:HG12	1:C:291:VAL:O	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:58:VAL:CG1	1:A:62:GLN:HB3	2.50	0.41
1:A:212:LEU:HG	1:A:245:TYR:CE2	2.55	0.41
1:A:305:PRO:O	1:A:309:LEU:HG	2.21	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:O	1:D:311:ILE:HG22	2.20	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: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:C:284:HIS:HD2	1:C:285:HIS:CD2	2.39	0.41
1:E:220:TRP:C	1:E:222:VAL:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:VAL:O	1:G:291:VAL:HG12	2.21	0.41
1:H:99:ARG:NH1	1:H:99:ARG:CG	2.82	0.41
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.80	0.41
1:J:127:VAL:C	1:J:128:LEU:HD12	2.45	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
1:D:22:LYS:NZ	5:D:331:HOH:O	2.54	0.40
1:D:145:ILE:CD1	1:D:145:ILE:O	2.68	0.40
1:F:212:LEU:HD23	1:F:212:LEU:HA	1.98	0.40
1:I:147:VAL:C	1:I:149:THR:H	2.29	0.40
1:I:310:ALA:C	1:I:312:GLY:H	2.29	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:58:VAL:CG1	1:D:62:GLN:HB3	2.51	0.40
1:D:119:PHE:HE1	1:D:199:ARG:CZ	2.34	0.40
1:D:147:VAL:C	1:D:149:THR:H	2.29	0.40
1:E:295:LEU:HA	1:E:298:GLN:NE2	2.23	0.40
1:F:205:LEU:HD23	1:F:205:LEU:HA	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:HD3	1:A:163:ARG:HA	1.71	0.40
1:C:127:VAL:C	1:C:128:LEU:HD12	2.46	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:G:137:ASN:HA	4:G:328:GOL:C2	2.52	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%)	3	11
1	B	305/322 (95%)	271 (89%)	24 (8%)	10 (3%)	3	11
1	C	305/322 (95%)	267 (88%)	29 (10%)	9 (3%)	3	13
1	D	305/322 (95%)	269 (88%)	24 (8%)	12 (4%)	2	9
1	E	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	2	10
1	F	305/322 (95%)	268 (88%)	28 (9%)	9 (3%)	3	13
1	G	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	2	10
1	H	305/322 (95%)	268 (88%)	27 (9%)	10 (3%)	3	11
1	I	305/322 (95%)	271 (89%)	22 (7%)	12 (4%)	2	9
1	J	305/322 (95%)	267 (88%)	26 (8%)	12 (4%)	2	9
All	All	3050/3220 (95%)	2681 (88%)	263 (9%)	106 (4%)	3	11

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

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Mol	Chain	Res	Type
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
1	B	153	ASP
1	C	153	ASP
1	D	153	ASP
1	D	298	GLN
1	E	153	ASP
1	E	298	GLN

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Mol	Chain	Res	Type
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
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%)	251 (91%)	24 (9%)	9	28
1	B	275/284 (97%)	253 (92%)	22 (8%)	11	32
1	C	275/284 (97%)	250 (91%)	25 (9%)	9	27
1	D	275/284 (97%)	250 (91%)	25 (9%)	9	27
1	E	275/284 (97%)	252 (92%)	23 (8%)	10	30
1	F	275/284 (97%)	253 (92%)	22 (8%)	11	32
1	G	275/284 (97%)	247 (90%)	28 (10%)	7	22
1	H	275/284 (97%)	252 (92%)	23 (8%)	10	30
1	I	275/284 (97%)	253 (92%)	22 (8%)	11	32
1	J	275/284 (97%)	253 (92%)	22 (8%)	11	32
All	All	2750/2840 (97%)	2514 (91%)	236 (9%)	10	29

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	17	SER
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	127	VAL
1	A	130	LEU
1	A	145	ILE
1	A	150	GLU
1	A	212	LEU
1	A	214	LEU
1	A	219	SER
1	A	234	THR

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Mol	Chain	Res	Type
1	A	235	SER
1	A	249	THR
1	A	253	LEU
1	A	261	VAL
1	A	277	ILE
1	A	287	GLN
1	A	296	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	127	VAL
1	B	130	LEU
1	B	145	ILE
1	B	150	GLU
1	B	212	LEU
1	B	214	LEU
1	B	219	SER
1	B	235	SER
1	B	249	THR
1	B	253	LEU
1	B	261	VAL
1	B	287	GLN
1	B	296	LEU
1	B	317	ILE
1	C	16	VAL
1	C	17	SER
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

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Mol	Chain	Res	Type
1	C	150	GLU
1	C	212	LEU
1	C	214	LEU
1	C	219	SER
1	C	234	THR
1	C	235	SER
1	C	249	THR
1	C	253	LEU
1	C	261	VAL
1	C	277	ILE
1	C	287	GLN
1	C	296	LEU
1	C	317	ILE
1	D	16	VAL
1	D	28	THR
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	127	VAL
1	D	130	LEU
1	D	145	ILE
1	D	150	GLU
1	D	163	ARG
1	D	212	LEU
1	D	214	LEU
1	D	219	SER
1	D	235	SER
1	D	249	THR
1	D	253	LEU
1	D	261	VAL
1	D	277	ILE
1	D	287	GLN
1	D	296	LEU
1	D	317	ILE
1	E	16	VAL
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	127	VAL
1	E	130	LEU
1	E	145	ILE
1	E	150	GLU
1	E	212	LEU
1	E	214	LEU
1	E	219	SER
1	E	235	SER
1	E	249	THR
1	E	253	LEU
1	E	261	VAL
1	E	277	ILE
1	E	287	GLN
1	E	296	LEU
1	E	317	ILE
1	F	16	VAL
1	F	17	SER
1	F	62	GLN
1	F	65	ARG
1	F	87	THR
1	F	91	ARG
1	F	99	ARG
1	F	123	ARG
1	F	127	VAL
1	F	130	LEU
1	F	145	ILE
1	F	150	GLU
1	F	212	LEU
1	F	219	SER
1	F	234	THR
1	F	235	SER
1	F	249	THR
1	F	253	LEU
1	F	261	VAL
1	F	287	GLN
1	F	296	LEU
1	F	317	ILE
1	G	16	VAL

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Mol	Chain	Res	Type
1	G	17	SER
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	127	VAL
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	234	THR
1	G	235	SER
1	G	249	THR
1	G	253	LEU
1	G	261	VAL
1	G	277	ILE
1	G	279	LEU
1	G	287	GLN
1	G	296	LEU
1	G	302	LEU
1	G	317	ILE
1	H	16	VAL
1	H	62	GLN
1	H	65	ARG
1	H	81	VAL
1	H	87	THR
1	H	91	ARG
1	H	99	ARG
1	H	123	ARG
1	H	127	VAL
1	H	145	ILE
1	H	150	GLU
1	H	212	LEU
1	H	214	LEU
1	H	219	SER
1	H	234	THR

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Mol	Chain	Res	Type
1	H	235	SER
1	H	249	THR
1	H	253	LEU
1	H	261	VAL
1	H	277	ILE
1	H	287	GLN
1	H	296	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	212	LEU
1	I	214	LEU
1	I	219	SER
1	I	235	SER
1	I	249	THR
1	I	253	LEU
1	I	261	VAL
1	I	287	GLN
1	I	296	LEU
1	I	317	ILE
1	J	16	VAL
1	J	17	SER
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

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Mol	Chain	Res	Type
1	J	212	LEU
1	J	214	LEU
1	J	219	SER
1	J	235	SER
1	J	249	THR
1	J	253	LEU
1	J	261	VAL
1	J	287	GLN
1	J	296	LEU
1	J	317	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	62	GLN
1	A	69	ASN
1	A	200	ASN
1	A	284	HIS
1	A	285	HIS
1	A	298	GLN
1	B	69	ASN
1	B	177	HIS
1	B	200	ASN
1	B	284	HIS
1	B	285	HIS
1	B	298	GLN
1	C	42	GLN
1	C	62	GLN
1	C	69	ASN
1	C	200	ASN
1	C	284	HIS
1	C	285	HIS
1	C	298	GLN
1	D	62	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	62	GLN

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Mol	Chain	Res	Type
1	E	69	ASN
1	E	151	ASN
1	E	169	HIS
1	E	200	ASN
1	E	284	HIS
1	E	285	HIS
1	E	298	GLN
1	F	42	GLN
1	F	69	ASN
1	F	169	HIS
1	F	200	ASN
1	F	284	HIS
1	F	285	HIS
1	F	298	GLN
1	G	69	ASN
1	G	200	ASN
1	G	284	HIS
1	G	285	HIS
1	G	298	GLN
1	H	42	GLN
1	H	62	GLN
1	H	69	ASN
1	H	151	ASN
1	H	169	HIS
1	H	200	ASN
1	H	284	HIS
1	H	285	HIS
1	H	298	GLN
1	I	42	GLN
1	I	62	GLN
1	I	69	ASN
1	I	139	GLN
1	I	200	ASN
1	I	284	HIS
1	I	285	HIS
1	I	298	GLN
1	J	62	GLN
1	J	69	ASN
1	J	151	ASN
1	J	200	ASN
1	J	284	HIS
1	J	285	HIS

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Mol	Chain	Res	Type
1	J	298	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	$\# Z > 2$
4	GOL	F	328	-	5,5,5	0.79	0	5,5,5	0.61	0
4	GOL	E	326	-	5,5,5	0.85	0	5,5,5	0.59	0
4	GOL	F	327	-	5,5,5	0.85	0	5,5,5	0.31	0
4	GOL	I	326	-	5,5,5	0.74	0	5,5,5	0.84	0
2	ACH	C	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.80	0
3	MES	B	324	-	12,12,12	2.20	1 (8%)	15,16,16	2.35	6 (40%)
3	MES	G	324	-	12,12,12	2.33	1 (8%)	15,16,16	2.31	8 (53%)
4	GOL	B	326	-	5,5,5	0.77	0	5,5,5	0.59	0
2	ACH	E	323	-	9,9,9	1.11	1 (11%)	12,12,12	0.73	0
4	GOL	A	325	-	5,5,5	0.74	0	5,5,5	0.61	0
3	MES	D	324	-	12,12,12	2.19	1 (8%)	15,16,16	2.25	6 (40%)
4	GOL	D	326	-	5,5,5	0.76	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACH	B	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.75	0
2	ACH	H	323	-	9,9,9	1.03	1 (11%)	12,12,12	0.91	1 (8%)
4	GOL	E	325	-	5,5,5	0.80	0	5,5,5	0.32	0
2	ACH	D	323	-	9,9,9	1.17	1 (11%)	12,12,12	0.87	1 (8%)
4	GOL	C	324	-	5,5,5	0.61	0	5,5,5	0.56	0
2	ACH	I	323	-	9,9,9	1.03	1 (11%)	12,12,12	0.77	0
3	MES	F	324	-	12,12,12	2.23	1 (8%)	15,16,16	2.33	6 (40%)
4	GOL	G	327	-	3,3,5	0.49	0	2,2,5	0.36	0
3	MES	A	324	-	12,12,12	2.19	1 (8%)	15,16,16	2.38	6 (40%)
2	ACH	J	323	-	9,9,9	1.07	1 (11%)	12,12,12	0.80	0
2	ACH	F	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.87	0
4	GOL	H	325	-	5,5,5	0.96	0	5,5,5	0.43	0
4	GOL	B	325	-	5,5,5	0.69	0	5,5,5	0.67	0
2	ACH	A	323	-	9,9,9	1.11	1 (11%)	12,12,12	0.68	0
4	GOL	F	326	-	5,5,5	0.67	0	5,5,5	0.58	0
4	GOL	G	326	-	5,5,5	0.65	0	5,5,5	0.43	0
3	MES	D	325	-	12,12,12	2.29	1 (8%)	15,16,16	2.39	6 (40%)
4	GOL	I	327	-	5,5,5	0.77	0	5,5,5	0.32	0
4	GOL	C	325	-	5,5,5	0.75	0	5,5,5	0.74	0
4	GOL	I	325	-	5,5,5	0.78	0	5,5,5	0.41	0
4	GOL	I	329	-	5,5,5	0.85	0	5,5,5	0.58	0
4	GOL	G	325	-	5,5,5	0.72	0	5,5,5	0.52	0
3	MES	J	324	-	12,12,12	2.30	1 (8%)	15,16,16	2.39	6 (40%)
2	ACH	G	323	-	9,9,9	1.13	1 (11%)	12,12,12	0.64	0
4	GOL	G	328	-	5,5,5	0.61	0	5,5,5	1.04	1 (20%)
4	GOL	I	328	-	5,5,5	0.70	0	5,5,5	0.48	0
4	GOL	B	327	-	5,5,5	0.83	0	5,5,5	0.69	0
4	GOL	H	324	-	5,5,5	0.46	0	5,5,5	0.80	0
3	MES	I	324	-	12,12,12	2.13	1 (8%)	15,16,16	2.29	6 (40%)
4	GOL	A	326	-	5,5,5	0.79	0	5,5,5	0.30	0
3	MES	E	324	-	12,12,12	2.25	1 (8%)	15,16,16	2.30	6 (40%)
4	GOL	D	327	-	5,5,5	0.71	0	5,5,5	0.59	0
4	GOL	F	325	-	5,5,5	0.71	0	5,5,5	0.42	0
4	GOL	J	325	-	5,5,5	0.72	0	5,5,5	0.64	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	-	-	2/4/4/4	-
4	GOL	E	326	-	-	0/4/4/4	-
4	GOL	F	327	-	-	0/4/4/4	-
4	GOL	I	326	-	-	1/4/4/4	-
2	ACH	C	323	-	-	0/7/7/7	-
3	MES	B	324	-	-	4/6/14/14	0/1/1/1
3	MES	G	324	-	-	4/6/14/14	0/1/1/1
4	GOL	B	326	-	-	2/4/4/4	-
2	ACH	E	323	-	-	0/7/7/7	-
4	GOL	A	325	-	-	0/4/4/4	-
3	MES	D	324	-	-	4/6/14/14	0/1/1/1
4	GOL	D	326	-	-	0/4/4/4	-
2	ACH	B	323	-	-	1/7/7/7	-
2	ACH	H	323	-	-	0/7/7/7	-
4	GOL	E	325	-	-	0/4/4/4	-
2	ACH	D	323	-	-	0/7/7/7	-
4	GOL	C	324	-	-	4/4/4/4	-
2	ACH	I	323	-	-	1/7/7/7	-
3	MES	F	324	-	-	5/6/14/14	0/1/1/1
4	GOL	G	327	-	-	1/1/1/4	-
3	MES	A	324	-	-	5/6/14/14	0/1/1/1
2	ACH	J	323	-	-	0/7/7/7	-
2	ACH	F	323	-	-	0/7/7/7	-
4	GOL	H	325	-	-	2/4/4/4	-
4	GOL	B	325	-	-	3/4/4/4	-
2	ACH	A	323	-	-	0/7/7/7	-
4	GOL	F	326	-	-	0/4/4/4	-
4	GOL	G	326	-	-	2/4/4/4	-
3	MES	D	325	-	-	4/6/14/14	0/1/1/1
4	GOL	I	327	-	-	0/4/4/4	-
4	GOL	C	325	-	-	0/4/4/4	-
4	GOL	I	325	-	-	0/4/4/4	-
4	GOL	I	329	-	-	2/4/4/4	-
4	GOL	G	325	-	-	3/4/4/4	-
3	MES	J	324	-	-	1/6/14/14	0/1/1/1
2	ACH	G	323	-	-	1/7/7/7	-
4	GOL	G	328	-	-	1/4/4/4	-
4	GOL	I	328	-	-	4/4/4/4	-
4	GOL	B	327	-	-	3/4/4/4	-

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	324	MES	C8-S	-7.71	1.66	1.77
3	J	324	MES	C8-S	-7.65	1.66	1.77
3	D	325	MES	C8-S	-7.59	1.66	1.77
3	E	324	MES	C8-S	-7.44	1.67	1.77
3	F	324	MES	C8-S	-7.29	1.67	1.77
3	B	324	MES	C8-S	-7.27	1.67	1.77
3	D	324	MES	C8-S	-7.22	1.67	1.77
3	A	324	MES	C8-S	-7.13	1.67	1.77
3	I	324	MES	C8-S	-6.99	1.67	1.77
2	E	323	ACH	O4-C5	2.66	1.46	1.33
2	D	323	ACH	O4-C5	2.52	1.45	1.33
2	G	323	ACH	O4-C5	2.51	1.45	1.33
2	B	323	ACH	O4-C5	2.50	1.45	1.33
2	A	323	ACH	O4-C5	2.49	1.45	1.33
2	J	323	ACH	O4-C5	2.49	1.45	1.33
2	I	323	ACH	O4-C5	2.47	1.45	1.33
2	H	323	ACH	O4-C5	2.46	1.45	1.33
2	C	323	ACH	O4-C5	2.38	1.44	1.33
2	F	323	ACH	O4-C5	2.33	1.44	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	325	MES	O3S-S-C8	5.66	117.07	106.00
3	F	324	MES	C5-N4-C3	5.23	120.11	108.84
3	A	324	MES	C5-N4-C3	5.01	119.62	108.84
3	E	324	MES	C5-N4-C3	4.99	119.59	108.84
3	B	324	MES	C5-N4-C3	4.92	119.45	108.84
3	J	324	MES	C5-N4-C3	4.81	119.19	108.84
3	I	324	MES	C5-N4-C3	4.80	119.19	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	324	MES	C5-N4-C3	4.58	118.72	108.84
3	G	324	MES	O1S-S-C8	4.19	113.06	106.73
3	D	325	MES	C5-N4-C3	3.78	116.98	108.84
3	A	324	MES	C6-C5-N4	-3.73	104.46	110.12
3	I	324	MES	C7-N4-C5	3.69	121.07	111.24
3	A	324	MES	C7-N4-C5	3.60	120.83	111.24
3	E	324	MES	C6-C5-N4	-3.60	104.65	110.12
3	J	324	MES	C6-C5-N4	-3.58	104.68	110.12
3	J	324	MES	C2-C3-N4	-3.56	104.71	110.12
3	F	324	MES	C7-N4-C5	3.47	120.50	111.24
3	B	324	MES	C7-N4-C3	3.39	120.27	111.24
3	G	324	MES	C5-N4-C3	3.34	116.03	108.84
3	F	324	MES	C6-C5-N4	-3.29	105.11	110.12
3	B	324	MES	C7-N4-C5	3.24	119.88	111.24
3	I	324	MES	C7-N4-C3	3.15	119.65	111.24
3	D	325	MES	C7-N4-C3	3.15	119.64	111.24
3	A	324	MES	C7-N4-C3	3.10	119.50	111.24
3	G	324	MES	C7-N4-C5	3.08	119.45	111.24
3	E	324	MES	C7-N4-C5	3.08	119.43	111.24
3	D	324	MES	O3S-S-C8	3.07	112.01	106.00
3	E	324	MES	C7-N4-C3	3.05	119.38	111.24
3	J	324	MES	C7-N4-C5	3.05	119.37	111.24
3	B	324	MES	C6-C5-N4	-3.04	105.50	110.12
3	F	324	MES	C7-N4-C3	3.03	119.31	111.24
3	G	324	MES	C7-N4-C3	2.99	119.19	111.24
3	B	324	MES	O1S-S-C8	2.96	111.20	106.73
3	I	324	MES	C6-C5-N4	-2.95	105.64	110.12
3	J	324	MES	C7-N4-C3	2.93	119.06	111.24
3	D	324	MES	C7-N4-C5	2.87	118.89	111.24
3	G	324	MES	C6-C5-N4	-2.84	105.80	110.12
3	D	324	MES	C7-N4-C3	2.84	118.81	111.24
3	D	324	MES	O1S-S-C8	2.80	110.96	106.73
3	D	325	MES	C6-C5-N4	-2.80	105.87	110.12
3	F	324	MES	O1S-S-C8	2.79	110.94	106.73
3	D	325	MES	C7-N4-C5	2.70	118.44	111.24
3	A	324	MES	C2-C3-N4	-2.70	106.02	110.12
3	J	324	MES	O3S-S-C8	2.63	111.15	106.00
3	A	324	MES	O3S-S-C8	2.63	111.15	106.00
3	E	324	MES	C2-C3-N4	-2.62	106.14	110.12
3	B	324	MES	C2-C3-N4	-2.47	106.37	110.12
3	G	324	MES	C6-O1-C2	2.39	117.61	109.88
3	D	324	MES	C2-C3-N4	-2.26	106.69	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	324	MES	C2-C3-N4	-2.19	106.79	110.12
3	G	324	MES	C2-C3-N4	-2.18	106.80	110.12
2	H	323	ACH	O4-C5-C6	2.15	121.51	112.38
3	E	324	MES	O2S-S-C8	2.11	109.92	106.73
3	I	324	MES	O2S-S-C8	2.08	109.87	106.73
3	G	324	MES	O1-C2-C3	2.07	116.22	111.77
3	D	325	MES	C6-O1-C2	2.06	116.55	109.88
3	F	324	MES	C2-C3-N4	-2.03	107.03	110.12
2	D	323	ACH	O4-C5-C6	2.01	120.92	112.38
4	G	328	GOL	O2-C2-C3	2.01	117.48	109.18

There are no chirality outliers.

All (73) torsion outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atoms
2	B	323	ACH	N1-C2-C3-O4
2	G	323	ACH	C2-C3-O4-C5
4	C	324	GOL	O1-C1-C2-O2
4	G	327	GOL	O1-C1-C2-O2

There are no ring outliers.

28 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	328	GOL	4	0
4	E	326	GOL	2	0
2	C	323	ACH	3	0
4	B	326	GOL	5	0
2	E	323	ACH	3	0
4	A	325	GOL	2	0
2	B	323	ACH	2	0
2	H	323	ACH	1	0
2	D	323	ACH	2	0
2	I	323	ACH	3	0
3	F	324	MES	2	0
3	A	324	MES	1	0
2	J	323	ACH	3	0
2	F	323	ACH	2	0
4	H	325	GOL	6	0
2	A	323	ACH	2	0
3	D	325	MES	1	0
4	I	327	GOL	4	0
4	C	325	GOL	4	0
4	I	329	GOL	6	0
2	G	323	ACH	1	0
4	G	328	GOL	9	0
4	B	327	GOL	7	0
4	H	324	GOL	3	0
4	A	326	GOL	4	0
4	D	327	GOL	1	0
4	F	325	GOL	1	0
4	J	325	GOL	7	0

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%)	0.15	21 (6%)	23	19	57, 90, 172, 210	0
1	B	307/322 (95%)	-0.03	13 (4%)	40	32	52, 87, 172, 212	0
1	C	307/322 (95%)	-0.06	6 (1%)	65	56	51, 87, 173, 210	0
1	D	307/322 (95%)	-0.08	7 (2%)	61	51	50, 84, 170, 210	0
1	E	307/322 (95%)	-0.07	12 (3%)	43	35	54, 88, 170, 208	0
1	F	307/322 (95%)	-0.07	14 (4%)	37	29	53, 94, 173, 208	0
1	G	307/322 (95%)	-0.03	16 (5%)	33	26	51, 87, 168, 209	0
1	H	307/322 (95%)	-0.13	11 (3%)	46	37	55, 89, 174, 208	0
1	I	307/322 (95%)	0.01	15 (4%)	35	27	57, 90, 172, 211	0
1	J	307/322 (95%)	0.00	6 (1%)	65	56	59, 94, 175, 208	0
All	All	3070/3220 (95%)	-0.03	121 (3%)	43	35	50, 89, 174, 212	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	9.3
1	H	291	VAL	5.7
1	I	152	ILE	5.7
1	D	152	ILE	5.2
1	I	291	VAL	5.1
1	G	152	ILE	4.9
1	A	178	LEU	4.7
1	B	151	ASN	4.3
1	F	181	VAL	4.3
1	E	291	VAL	4.2
1	B	295	LEU	4.2
1	C	291	VAL	4.2
1	E	181	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	291	VAL	4.1
1	B	291	VAL	4.0
1	F	178	LEU	3.9
1	D	157	ILE	3.9
1	G	291	VAL	3.8
1	G	157	ILE	3.8
1	A	291	VAL	3.7
1	I	298	GLN	3.7
1	H	295	LEU	3.6
1	A	288	ALA	3.6
1	A	294	ASP	3.5
1	G	288	ALA	3.5
1	E	314	VAL	3.3
1	A	298	GLN	3.3
1	F	291	VAL	3.3
1	G	315	LEU	3.3
1	F	179	SER	3.3
1	A	292	GLU	3.2
1	G	314	VAL	3.2
1	A	295	LEU	3.1
1	D	291	VAL	3.1
1	E	152	ILE	3.1
1	I	296	LEU	3.1
1	J	143	SER	3.0
1	E	295	LEU	3.0
1	I	157	ILE	3.0
1	C	152	ILE	3.0
1	H	317	ILE	2.9
1	A	152	ILE	2.9
1	H	290	GLY	2.9
1	A	156	GLU	2.9
1	A	317	ILE	2.9
1	G	290	GLY	2.8
1	J	317	ILE	2.8
1	F	314	VAL	2.8
1	C	298	GLN	2.7
1	E	315	LEU	2.7
1	E	317	ILE	2.7
1	E	296	LEU	2.7
1	A	151	ASN	2.7
1	G	235	SER	2.7
1	G	149	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	231	ARG	2.6
1	F	152	ILE	2.6
1	A	175	TYR	2.6
1	J	152	ILE	2.6
1	A	289	ASN	2.6
1	A	181	VAL	2.5
1	H	152	ILE	2.5
1	F	298	GLN	2.5
1	F	309	LEU	2.5
1	G	296	LEU	2.5
1	B	317	ILE	2.5
1	B	148	TYR	2.5
1	G	298	GLN	2.5
1	H	288	ALA	2.5
1	H	154	ASN	2.5
1	A	297	ILE	2.5
1	C	121	PHE	2.5
1	E	298	GLN	2.4
1	I	222	VAL	2.4
1	F	316	VAL	2.4
1	H	296	LEU	2.4
1	I	200	ASN	2.3
1	B	298	GLN	2.3
1	B	164	GLY	2.3
1	E	137	ASN	2.3
1	F	295	LEU	2.3
1	G	151	ASN	2.3
1	D	317	ILE	2.3
1	A	296	LEU	2.3
1	A	315	LEU	2.2
1	B	56	LEU	2.2
1	J	250	SER	2.2
1	B	296	LEU	2.2
1	F	315	LEU	2.2
1	I	226	GLU	2.2
1	C	317	ILE	2.2
1	I	293	ASP	2.2
1	A	183	PRO	2.2
1	B	272	SER	2.2
1	A	286	ARG	2.2
1	E	316	VAL	2.2
1	F	182	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	289	ASN	2.2
1	G	295	LEU	2.2
1	D	226	GLU	2.2
1	F	156	GLU	2.2
1	C	198	VAL	2.1
1	I	153	ASP	2.1
1	F	296	LEU	2.1
1	I	295	LEU	2.1
1	E	288	ALA	2.1
1	I	148	TYR	2.1
1	G	156	GLU	2.1
1	H	298	GLN	2.1
1	G	317	ILE	2.1
1	D	137	ASN	2.1
1	G	137	ASN	2.1
1	I	151	ASN	2.1
1	J	315	LEU	2.1
1	B	149	THR	2.1
1	A	154	ASN	2.0
1	B	315	LEU	2.0
1	D	315	LEU	2.0
1	A	257	PRO	2.0
1	H	293	ASP	2.0
1	I	172	ASP	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	GOL	B	326	6/6	0.61	0.25	83,110,138,150	0
3	MES	A	324	12/12	0.63	0.20	91,140,168,188	0
3	MES	J	324	12/12	0.64	0.21	139,157,169,184	0
4	GOL	D	327	6/6	0.66	0.21	51,79,98,109	0
3	MES	E	324	12/12	0.70	0.17	123,143,171,178	0
3	MES	D	324	12/12	0.71	0.21	107,132,160,169	0
4	GOL	F	325	6/6	0.71	0.18	84,100,114,125	0
4	GOL	J	325	6/6	0.73	0.20	64,92,106,114	0
3	MES	F	324	12/12	0.75	0.14	106,147,159,185	0
4	GOL	A	326	6/6	0.75	0.20	79,90,125,127	0
3	MES	B	324	12/12	0.76	0.17	120,136,164,175	0
4	GOL	I	325	6/6	0.78	0.17	88,93,105,121	0
3	MES	D	325	12/12	0.78	0.15	85,140,157,157	0
4	GOL	B	325	6/6	0.80	0.13	77,88,103,117	0
4	GOL	E	325	6/6	0.80	0.15	85,99,110,130	0
4	GOL	E	326	6/6	0.80	0.17	67,89,129,133	0
3	MES	G	324	12/12	0.81	0.17	99,122,143,150	0
4	GOL	B	327	6/6	0.82	0.17	55,62,83,90	0
4	GOL	H	325	6/6	0.82	0.33	80,85,104,115	0
4	GOL	G	326	6/6	0.83	0.18	91,96,115,116	0
3	MES	I	324	12/12	0.83	0.12	109,142,169,177	0
4	GOL	I	327	6/6	0.84	0.15	88,92,119,126	0
4	GOL	I	329	6/6	0.84	0.20	61,71,110,133	0
4	GOL	F	328	6/6	0.84	0.17	73,86,114,121	0
4	GOL	F	326	6/6	0.85	0.27	83,98,121,143	0
4	GOL	F	327	6/6	0.85	0.16	77,98,110,119	0
4	GOL	A	325	6/6	0.85	0.15	69,109,127,135	0
4	GOL	I	326	6/6	0.86	0.17	73,91,114,119	0
4	GOL	H	324	6/6	0.86	0.14	56,69,111,111	0
4	GOL	C	324	6/6	0.86	0.16	79,89,98,113	0
4	GOL	G	328	6/6	0.86	0.18	50,79,101,104	0
4	GOL	G	325	6/6	0.88	0.10	79,94,101,112	0
4	GOL	C	325	6/6	0.88	0.13	60,66,78,92	0
4	GOL	I	328	6/6	0.90	0.14	87,95,119,124	0
4	GOL	D	326	6/6	0.90	0.15	96,100,101,106	0
4	GOL	G	327	4/6	0.90	0.19	86,96,104,106	0
2	ACH	J	323	10/10	0.92	0.13	56,74,82,89	0
2	ACH	H	323	10/10	0.95	0.10	57,74,81,83	0
2	ACH	C	323	10/10	0.95	0.12	54,69,74,75	0
2	ACH	B	323	10/10	0.96	0.09	53,65,78,80	0
2	ACH	E	323	10/10	0.96	0.11	57,76,82,85	0
2	ACH	G	323	10/10	0.97	0.09	48,68,76,77	0
2	ACH	D	323	10/10	0.97	0.10	53,62,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACH	I	323	10/10	0.97	0.15	54,67,76,80	0
2	ACH	A	323	10/10	0.97	0.08	56,66,76,77	0
2	ACH	F	323	10/10	0.98	0.11	48,67,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.