



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:39 PM GMT

PDB ID : 4TWF
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with bromomemantine
Authors : Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.
Deposited on : 2014-06-30
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

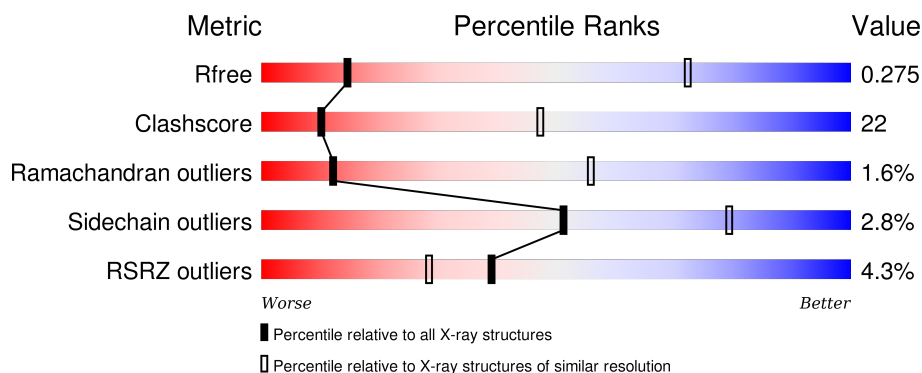
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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. 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	307	<div> <div>3%</div> <div>59%</div> <div>36%</div> <div>• •</div> </div>
1	B	307	<div> <div>4%</div> <div>60%</div> <div>38%</div> <div>•</div> </div>
1	C	307	<div> <div>6%</div> <div>60%</div> <div>37%</div> <div>•</div> </div>
1	D	307	<div> <div>4%</div> <div>68%</div> <div>29%</div> <div>• •</div> </div>
1	E	307	<div> <div>3%</div> <div>59%</div> <div>37%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

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
2	BR7	A	401	-	-	-	X
2	BR7	C	401	-	-	-	X
2	BR7	E	401	-	-	-	X
2	BR7	F	401	-	-	-	X
2	BR7	G	401	-	-	-	X
2	BR7	H	401	-	-	-	X
2	BR7	J	401	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25138 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

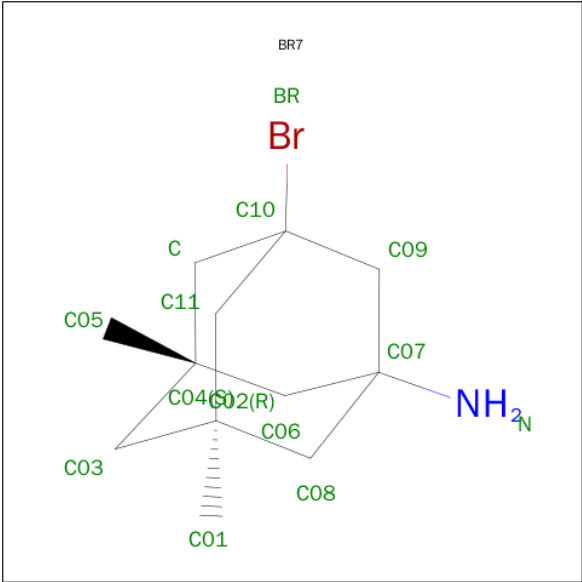
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is Bromomemantine (three-letter code: BR7) (formula: C₁₂H₂₀BrN).

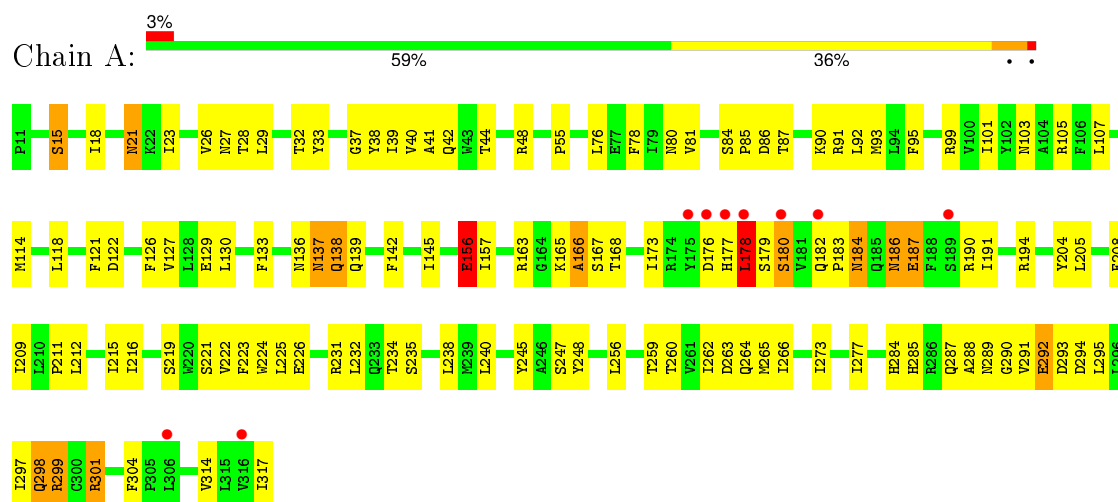


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			14	1	12	1		
2	A	1	Total	Br	C	N	0	0
			14	1	12	1		
2	B	1	Total	Br	C	N	0	0
			14	1	12	1		
2	C	1	Total	Br	C	N	0	0
			14	1	12	1		
2	D	1	Total	Br	C	N	0	0
			14	1	12	1		
2	E	1	Total	Br	C	N	0	0
			14	1	12	1		
2	F	1	Total	Br	C	N	0	0
			14	1	12	1		
2	F	1	Total	Br	C	N	0	0
			14	1	12	1		
2	G	1	Total	Br	C	N	0	0
			14	1	12	1		
2	H	1	Total	Br	C	N	0	0
			14	1	12	1		
2	I	1	Total	Br	C	N	0	0
			14	1	12	1		
2	J	1	Total	Br	C	N	0	0
			14	1	12	1		

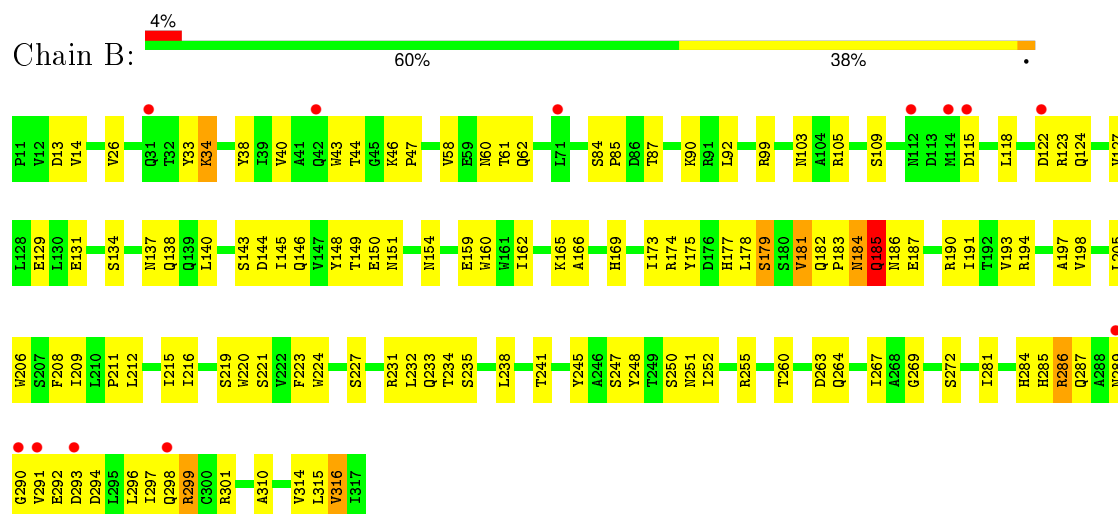
3 Residue-property plots

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: Cys-loop ligand-gated ion channel

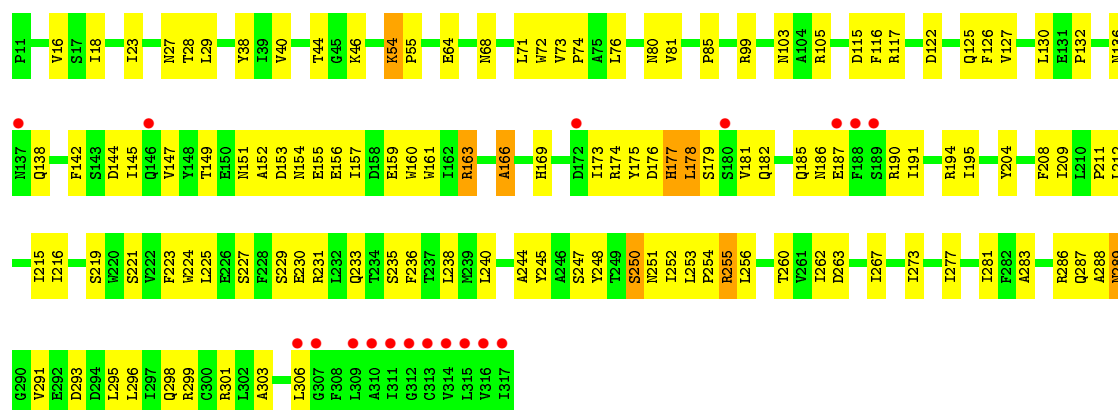


• Molecule 1: Cys-loop ligand-gated ion channel

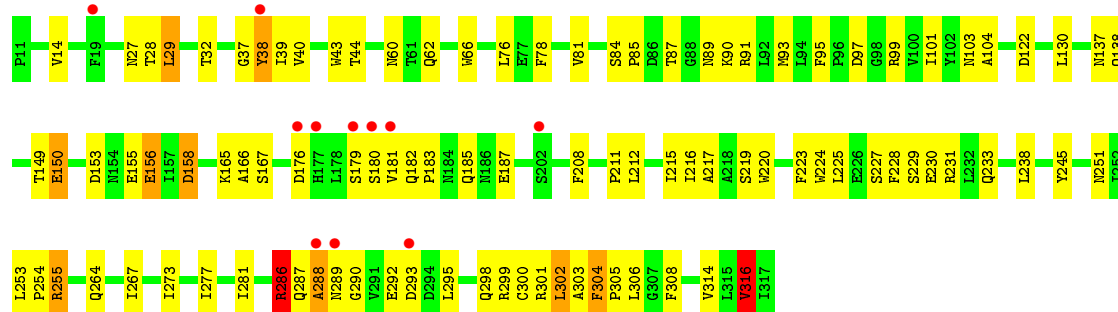


• Molecule 1: Cys-loop ligand-gated ion channel

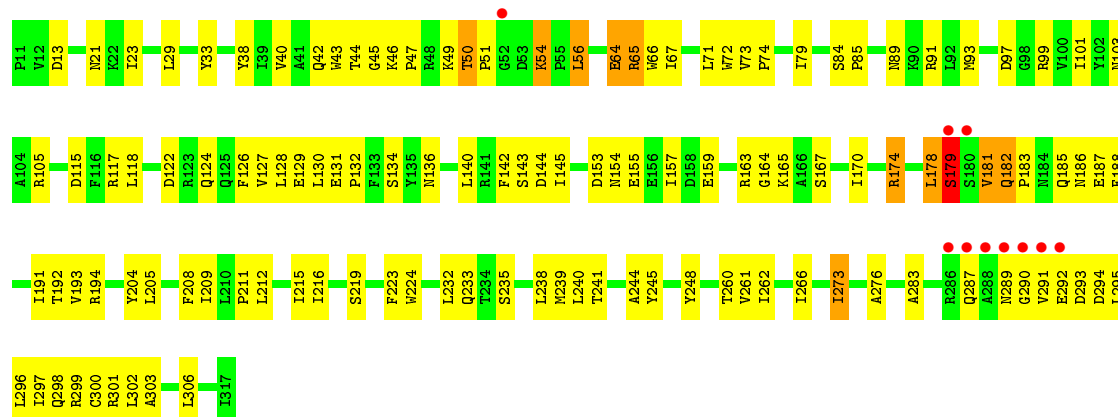




• Molecule 1: Cys-loop ligand-gated ion channel

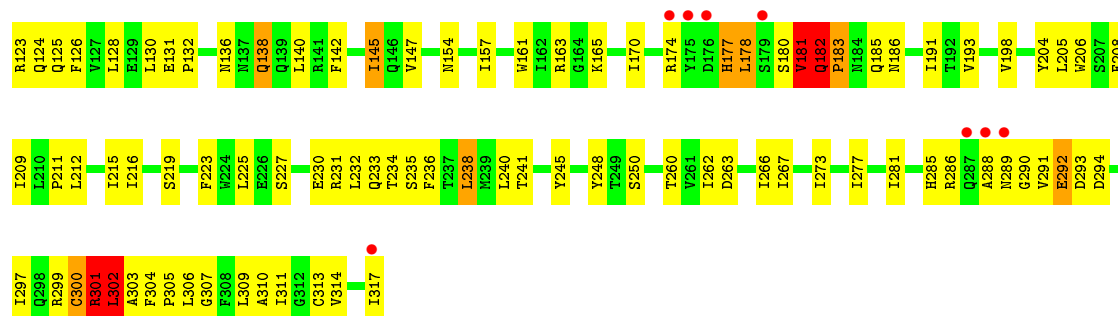


• Molecule 1: Cys-loop ligand-gated ion channel

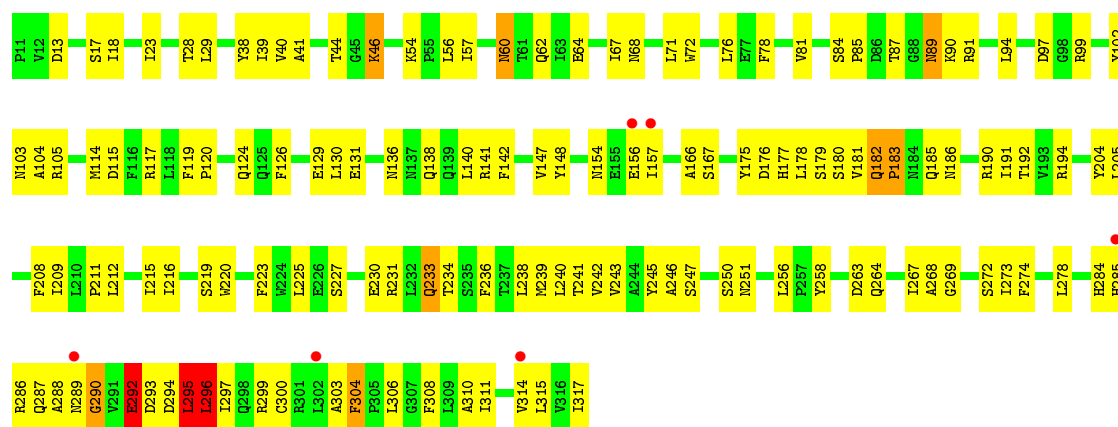


• Molecule 1: Cys-loop ligand-gated ion channel

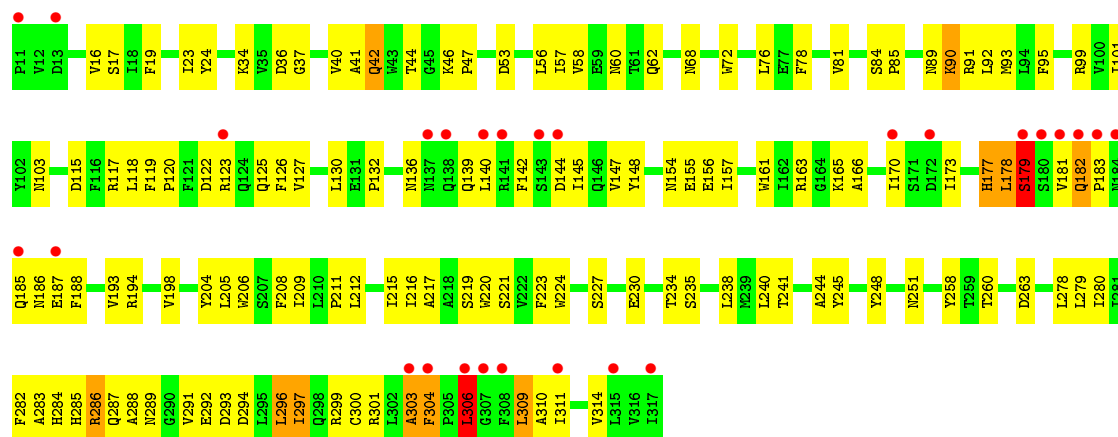




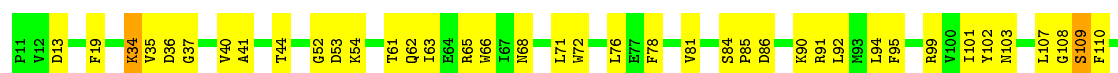
• Molecule 1: Cys-loop ligand-gated ion channel

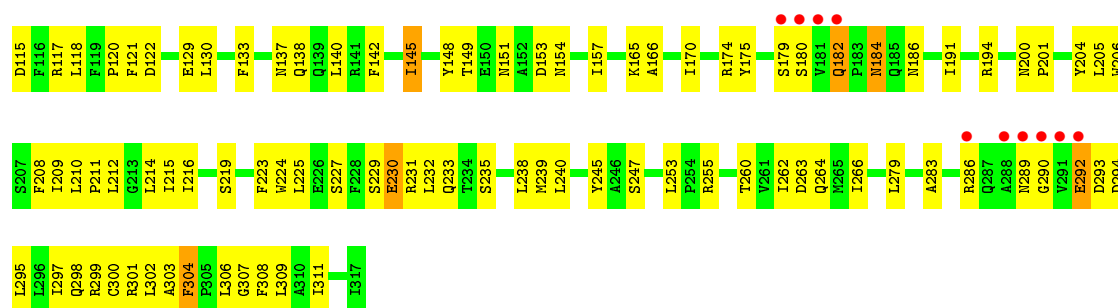


• Molecule 1: Cys-loop ligand-gated ion channel

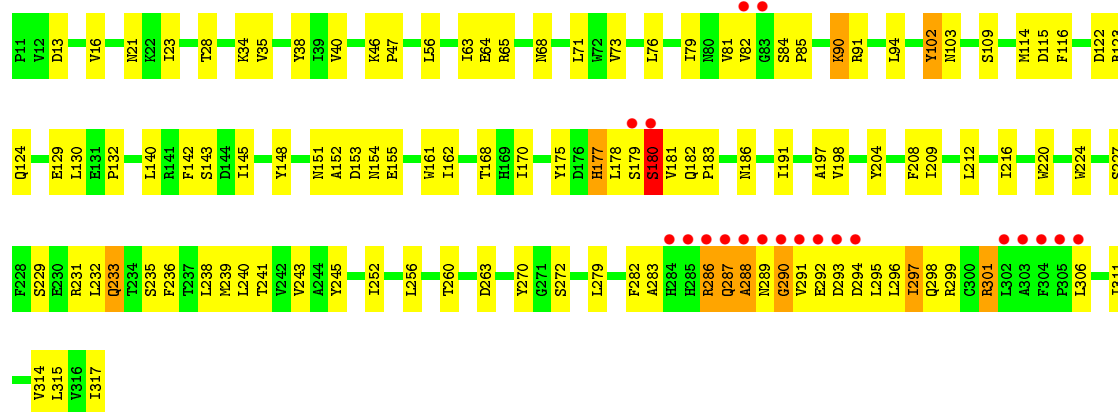


• Molecule 1: Cys-loop ligand-gated ion channel





• Molecule 1: Cys-loop ligand-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.50Å 266.09Å 112.17Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	49.83 – 3.90 49.83 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.83-3.90) 91.1 (49.83-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.250 0.229 , 0.275	Depositor DCC
R_{free} test set	2719 reflections (5.83%)	DCC
Wilson B-factor (Å ²)	109.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 77.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 53593 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	25138	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BR7

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	0.42	0/2564	0.77	3/3495 (0.1%)
1	B	0.43	0/2564	0.75	2/3495 (0.1%)
1	C	0.42	0/2564	0.75	1/3495 (0.0%)
1	D	0.39	0/2564	0.72	0/3495
1	E	0.49	2/2564 (0.1%)	0.82	4/3495 (0.1%)
1	F	0.43	0/2564	0.78	3/3495 (0.1%)
1	G	0.41	0/2564	0.75	4/3495 (0.1%)
1	H	0.45	0/2564	0.80	3/3495 (0.1%)
1	I	0.41	0/2564	0.74	1/3495 (0.0%)
1	J	0.45	0/2564	0.76	3/3495 (0.1%)
All	All	0.43	2/25640 (0.0%)	0.77	24/34950 (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	7
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	5
1	G	0	2
1	H	0	3
1	I	0	2
1	J	0	2
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ILE	CA-CB	-7.06	1.38	1.54
1	E	54	LYS	CE-NZ	5.27	1.62	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	56	LEU	CB-CG-CD1	-13.99	87.22	111.00
1	A	301	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	H	296	LEU	CA-CB-CG	10.74	140.00	115.30
1	H	306	LEU	CA-CB-CG	8.49	134.84	115.30
1	F	178	LEU	CA-CB-CG	7.92	133.51	115.30
1	G	315	LEU	CA-CB-CG	7.64	132.88	115.30
1	G	238	LEU	CA-CB-CG	7.13	131.71	115.30
1	B	34	LYS	CD-CE-NZ	6.49	126.62	111.70
1	C	178	LEU	CA-CB-CG	6.47	130.18	115.30
1	I	182	GLN	CA-CB-CG	6.46	127.60	113.40
1	A	301	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	E	45	GLY	N-CA-C	-6.36	97.20	113.10
1	G	296	LEU	CA-CB-CG	5.79	128.63	115.30
1	J	288	ALA	N-CA-C	5.69	126.37	111.00
1	H	286	ARG	CB-CG-CD	5.64	126.26	111.60
1	F	182	GLN	CA-CB-CG	5.41	125.30	113.40
1	E	56	LEU	CB-CA-C	-5.34	100.06	110.20
1	E	181	VAL	N-CA-C	-5.31	96.67	111.00
1	F	238	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	299	ARG	CA-CB-CG	5.23	124.90	113.40
1	B	181	VAL	N-CA-C	-5.20	96.95	111.00
1	J	178	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	J	178	LEU	CA-CB-CG	5.05	126.93	115.30
1	G	182	GLN	C-N-CD	-5.04	109.51	120.60

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	HIS	Peptide
1	A	178	LEU	Peptide
1	B	177	HIS	Peptide
1	B	178	LEU	Peptide
1	B	179	SER	Peptide
1	B	184	ASN	Peptide
1	B	185	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	286	ARG	Peptide
1	B	316	VAL	Peptide
1	C	177	HIS	Sidechain
1	C	286	ARG	Peptide
1	C	288	ALA	Peptide
1	D	158	ASP	Peptide
1	D	286	ARG	Peptide
1	E	178	LEU	Peptide
1	E	179	SER	Peptide
1	E	46	LYS	Peptide
1	F	177	HIS	Peptide
1	F	180	SER	Peptide
1	F	181	VAL	Peptide
1	F	300	CYS	Peptide
1	F	301	ARG	Peptide
1	G	294	ASP	Peptide
1	G	295	LEU	Peptide
1	H	178	LEU	Peptide
1	H	179	SER	Peptide
1	H	293	ASP	Peptide
1	I	292	GLU	Peptide
1	I	34	LYS	Peptide
1	J	177	HIS	Peptide
1	J	180	SER	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	2497	0	2468	117	0
1	B	2497	0	2468	115	0
1	C	2497	0	2468	118	0
1	D	2497	0	2468	79	0
1	E	2497	0	2468	118	0
1	F	2497	0	2468	126	0
1	G	2497	0	2468	124	0
1	H	2497	0	2468	130	0
1	I	2497	0	2468	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2497	0	2468	116	0
2	A	28	0	40	2	0
2	B	14	0	20	4	0
2	C	14	0	20	5	0
2	D	14	0	20	0	0
2	E	14	0	20	2	0
2	F	28	0	40	1	0
2	G	14	0	20	3	0
2	H	14	0	20	0	0
2	I	14	0	20	1	0
2	J	14	0	20	2	0
All	All	25138	0	24920	1091	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1091) 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:A:221:SER:HA	1:A:301:ARG:HH22	1.15	1.07
1:E:239:MET:HE3	1:E:273:ILE:HG21	1.37	1.06
1:I:63:ILE:HD13	1:I:90:LYS:HE3	1.40	1.04
1:I:299:ARG:HH12	1:I:302:LEU:HD23	1.21	1.01
1:C:298:GLN:O	1:C:301:ARG:NH1	1.98	0.97
1:H:286:ARG:HH12	1:H:297:ILE:HG21	1.29	0.94
1:H:287:GLN:OE1	1:H:292:GLU:N	2.03	0.92
1:F:145:ILE:HD12	1:F:191:ILE:HG21	1.50	0.92
1:J:115:ASP:H	1:J:124:GLN:HE22	0.99	0.91
1:E:223:PHE:HB3	1:E:301:ARG:NH1	1.86	0.90
1:F:301:ARG:HB3	1:F:303:ALA:H	1.32	0.89
1:H:296:LEU:HA	1:H:299:ARG:HB2	1.55	0.88
1:E:235:SER:HA	1:E:238:LEU:HD12	1.56	0.88
1:F:90:LYS:HE2	1:F:104:ALA:HB2	1.53	0.88
1:G:287:GLN:HB2	1:G:292:GLU:HB2	1.53	0.88
1:C:251:ASN:HD21	1:D:251:ASN:HD22	1.18	0.87
1:A:221:SER:HA	1:A:301:ARG:NH2	1.90	0.87
1:F:219:SER:HA	1:F:238:LEU:HD11	1.57	0.87
1:J:220:TRP:HE1	1:J:272:SER:HG	1.18	0.86
1:I:34:LYS:NZ	1:I:35:VAL:O	2.08	0.85
1:C:287:GLN:HG2	1:C:289:ASN:H	1.40	0.85
1:F:182:GLN:HB2	1:F:183:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:OG1	1:E:56:LEU:HD11	1.76	0.85
1:G:156:GLU:OE1	1:H:117:ARG:NH1	2.08	0.85
1:E:182:GLN:H	1:E:183:PRO:HD2	1.42	0.85
1:J:115:ASP:N	1:J:124:GLN:HE22	1.74	0.84
1:J:123:ARG:HD3	1:J:198:VAL:HG22	1.59	0.84
1:E:50:THR:OG1	1:E:54:LYS:NZ	2.09	0.84
1:H:230:GLU:OE2	1:I:229:SER:OG	1.94	0.84
1:C:176:ASP:HB2	1:C:177:HIS:CD2	2.13	0.83
1:H:234:THR:OG1	1:I:233:GLN:NE2	2.11	0.83
1:I:255:ARG:HH11	1:I:255:ARG:HG2	1.43	0.83
1:I:76:LEU:HB3	1:I:130:LEU:HD11	1.60	0.82
1:B:38:TYR:HE1	1:B:105:ARG:HD2	1.44	0.82
1:H:93:MET:HB3	1:H:101:ILE:HB	1.61	0.82
1:I:90:LYS:HD2	1:I:91:ARG:N	1.94	0.82
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.61	0.82
1:H:156:GLU:HG3	1:H:157:ILE:HG13	1.62	0.81
1:F:50:THR:HG21	1:F:54:LYS:O	1.81	0.81
1:I:223:PHE:HE1	1:I:304:PHE:HE2	1.29	0.80
1:J:181:VAL:HG12	1:J:183:PRO:HD2	1.63	0.80
1:J:235:SER:HA	1:J:238:LEU:HD13	1.64	0.80
1:I:34:LYS:CG	1:I:109:SER:HA	2.12	0.80
1:C:153:ASP:OD1	1:C:154:ASN:N	2.15	0.79
1:H:42:GLN:HG2	1:H:101:ILE:HG12	1.63	0.79
1:H:286:ARG:NH1	1:H:297:ILE:HG21	1.98	0.79
2:A:402:BR7:BR	1:C:244:ALA:HA	2.38	0.79
1:C:251:ASN:ND2	1:D:251:ASN:HD22	1.82	0.78
1:D:62:GLN:HE22	1:E:67:ILE:HG22	1.47	0.78
1:I:219:SER:HA	1:I:238:LEU:HD23	1.63	0.78
1:F:174:ARG:NH1	1:F:186:ASN:HB2	1.98	0.78
1:D:97:ASP:OD1	1:D:99:ARG:NH1	2.16	0.77
1:G:287:GLN:HG2	1:G:289:ASN:H	1.49	0.77
1:E:239:MET:CE	1:E:273:ILE:HG21	2.12	0.77
1:D:289:ASN:OD1	1:D:290:GLY:N	2.17	0.77
1:C:229:SER:O	1:C:233:GLN:HG2	1.85	0.77
1:E:145:ILE:HD11	1:E:191:ILE:HG12	1.66	0.77
1:B:34:LYS:HD2	1:B:109:SER:HA	1.64	0.77
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.64	0.77
1:E:298:GLN:O	1:E:301:ARG:NH1	2.18	0.76
1:J:282:PHE:HE2	1:J:297:ILE:HG12	1.50	0.76
1:C:16:VAL:HB	1:C:145:ILE:HD11	1.66	0.76
1:C:301:ARG:HG3	1:C:301:ARG:HH11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:LYS:HG2	1:I:109:SER:HA	1.68	0.75
1:C:40:VAL:HG13	1:C:103:ASN:HD21	1.52	0.74
1:C:298:GLN:C	1:C:301:ARG:HH12	1.90	0.74
1:H:224:TRP:CD1	1:H:301:ARG:HD3	2.23	0.74
1:J:23:ILE:HG12	1:J:35:VAL:HG22	1.68	0.74
1:B:219:SER:HA	1:B:238:LEU:CD2	2.18	0.74
1:G:311:ILE:O	1:G:314:VAL:HG22	1.87	0.74
1:E:239:MET:CE	1:E:273:ILE:HD13	2.18	0.74
1:D:302:LEU:HD23	1:D:305:PRO:HB2	1.70	0.73
1:H:219:SER:HA	1:H:238:LEU:HD22	1.70	0.73
1:G:287:GLN:HB2	1:G:292:GLU:CB	2.19	0.72
1:F:234:THR:OG1	1:G:233:GLN:OE1	2.07	0.72
1:E:219:SER:HA	1:E:238:LEU:HD22	1.72	0.72
1:G:99:ARG:HH11	1:G:99:ARG:HG2	1.54	0.72
1:F:90:LYS:CE	1:F:104:ALA:HB2	2.20	0.72
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.22	0.71
1:D:233:GLN:OE1	1:E:233:GLN:NE2	2.23	0.71
1:E:239:MET:HE3	1:E:273:ILE:CG2	2.17	0.71
1:C:176:ASP:HB2	1:C:177:HIS:HD2	1.55	0.71
1:H:40:VAL:HG13	1:H:103:ASN:HD21	1.55	0.71
1:I:44:THR:HA	1:I:99:ARG:HA	1.71	0.71
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.55	0.71
1:F:181:VAL:HG22	1:F:182:GLN:HA	1.73	0.70
1:A:287:GLN:HG3	1:A:290:GLY:N	2.06	0.70
1:F:289:ASN:OD1	1:F:290:GLY:N	2.24	0.70
1:B:252:ILE:HD11	1:C:250:SER:OG	1.92	0.70
1:B:224:TRP:CE2	1:B:301:ARG:HG2	2.26	0.70
1:H:283:ALA:HA	1:H:286:ARG:CZ	2.21	0.70
1:H:286:ARG:HH21	1:H:294:ASP:H	1.38	0.70
1:I:34:LYS:HE2	1:I:108:GLY:N	2.07	0.70
1:J:90:LYS:NZ	1:J:102:TYR:CD2	2.58	0.70
1:D:229:SER:O	1:D:233:GLN:HG2	1.92	0.70
1:B:223:PHE:HB2	1:B:301:ARG:HD3	1.73	0.70
1:F:116:PHE:CE2	1:F:124:GLN:NE2	2.60	0.70
1:F:178:LEU:HG	1:F:181:VAL:HB	1.73	0.70
1:E:51:PRO:HB2	1:E:54:LYS:HE3	1.73	0.70
1:J:162:ILE:HD13	1:J:197:ALA:HB2	1.74	0.69
1:G:46:LYS:HD3	1:G:46:LYS:N	2.07	0.69
1:B:87:THR:HG21	1:B:90:LYS:NZ	2.06	0.69
1:I:34:LYS:HZ3	1:I:108:GLY:H	1.38	0.69
1:H:145:ILE:HD12	1:H:170:ILE:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:HIS:CD2	1:J:148:TYR:HH	2.10	0.69
1:E:13:ASP:HB3	1:E:143:SER:HB3	1.74	0.69
1:J:286:ARG:NH1	1:J:287:GLN:HA	2.07	0.69
1:E:239:MET:HE1	1:E:273:ILE:HD13	1.75	0.69
1:H:179:SER:HB2	1:H:181:VAL:H	1.57	0.69
1:A:38:TYR:CD2	2:B:401:BR7:H20	2.28	0.69
1:A:42:GLN:HB2	1:A:101:ILE:HG12	1.75	0.69
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.74	0.68
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.75	0.68
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.76	0.68
1:E:153:ASP:OD1	1:E:154:ASN:N	2.24	0.68
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.58	0.68
1:B:38:TYR:CE2	2:C:401:BR7:H20	2.29	0.68
1:J:287:GLN:HE21	1:J:289:ASN:H	1.40	0.67
1:I:165:LYS:HG3	1:I:166:ALA:H	1.60	0.67
1:F:76:LEU:HB3	1:F:130:LEU:HD11	1.76	0.67
1:A:314:VAL:O	1:A:317:ILE:HG22	1.93	0.67
1:I:63:ILE:HD13	1:I:90:LYS:CE	2.22	0.67
1:H:42:GLN:HG2	1:H:101:ILE:HA	1.77	0.67
1:G:178:LEU:HD22	2:G:401:BR7:H2	1.77	0.67
1:I:34:LYS:CE	1:I:108:GLY:H	2.08	0.67
1:A:157:ILE:HD11	1:B:115:ASP:HA	1.76	0.67
2:F:402:BR7:BR	1:H:244:ALA:HA	2.50	0.67
1:F:211:PRO:O	1:F:215:ILE:HG12	1.95	0.67
1:C:208:PHE:O	1:C:245:TYR:OH	2.12	0.66
1:E:145:ILE:HD13	1:E:191:ILE:HG23	1.77	0.66
1:I:34:LYS:HE3	1:I:35:VAL:H	1.60	0.66
1:C:235:SER:HA	1:C:238:LEU:HD13	1.76	0.66
1:A:219:SER:HA	1:A:238:LEU:HD23	1.77	0.66
1:A:224:TRP:CE3	1:B:281:ILE:HG21	2.31	0.66
1:J:220:TRP:NE1	1:J:272:SER:OG	2.20	0.66
1:I:53:ASP:H	1:I:54:LYS:HD2	1.60	0.66
1:F:145:ILE:HD11	1:F:191:ILE:HD13	1.78	0.66
1:A:221:SER:CA	1:A:301:ARG:HH22	2.01	0.66
1:H:241:THR:HA	1:I:240:LEU:HD23	1.78	0.66
1:A:287:GLN:HG2	1:A:289:ASN:H	1.61	0.66
1:E:129:GLU:HG2	1:E:192:THR:HG23	1.77	0.66
1:A:38:TYR:HE1	1:A:105:ARG:HD2	1.60	0.65
1:D:299:ARG:HG2	1:D:299:ARG:HH11	1.62	0.65
1:H:204:TYR:O	1:H:208:PHE:HB2	1.96	0.65
1:C:299:ARG:HA	1:C:301:ARG:NH1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:LYS:HE2	1:I:108:GLY:H	1.58	0.65
1:J:287:GLN:HG2	1:J:288:ALA:N	2.10	0.65
1:B:143:SER:OG	1:B:144:ASP:OD1	2.14	0.65
1:F:303:ALA:O	1:F:307:GLY:N	2.28	0.65
1:F:301:ARG:HB3	1:F:303:ALA:N	2.10	0.64
1:I:34:LYS:NZ	1:I:108:GLY:H	1.95	0.64
1:J:293:ASP:OD1	1:J:293:ASP:N	2.30	0.64
1:A:287:GLN:HA	1:A:292:GLU:OE2	1.97	0.64
1:A:15:SER:HB3	1:A:42:GLN:HG2	1.78	0.64
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.79	0.64
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.30	0.64
1:I:230:GLU:HB3	1:J:233:GLN:HE22	1.61	0.64
1:B:40:VAL:HG13	1:B:103:ASN:HD21	1.61	0.64
1:F:294:ASP:HB2	1:F:297:ILE:HB	1.80	0.64
1:J:297:ILE:HG13	1:J:298:GLN:N	2.11	0.64
1:G:178:LEU:HG	1:G:179:SER:H	1.63	0.64
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.31	0.64
1:I:85:PRO:HA	1:I:108:GLY:HA3	1.80	0.63
1:C:301:ARG:HG3	1:C:301:ARG:NH1	2.12	0.63
1:E:208:PHE:O	1:E:245:TYR:OH	2.16	0.63
1:C:27:ASN:OD1	1:C:255:ARG:NH1	2.31	0.63
1:J:180:SER:O	1:J:180:SER:OG	2.08	0.63
1:H:309:LEU:HG	1:H:310:ALA:N	2.13	0.63
1:F:110:PHE:HE2	1:F:128:LEU:HG	1.64	0.63
1:C:296:LEU:HA	1:C:299:ARG:HB2	1.79	0.63
1:I:230:GLU:OE1	1:J:233:GLN:NE2	2.30	0.63
1:I:227:SER:O	1:I:231:ARG:HG3	1.98	0.63
1:C:149:THR:HG23	1:C:151:ASN:HD22	1.63	0.63
1:I:294:ASP:HB2	1:I:297:ILE:HG12	1.80	0.63
1:D:76:LEU:HB3	1:D:130:LEU:HD11	1.80	0.63
1:I:91:ARG:NH2	1:I:103:ASN:OD1	2.32	0.62
1:J:114:MET:HA	1:J:124:GLN:NE2	2.15	0.62
1:E:298:GLN:O	1:E:301:ARG:CZ	2.47	0.62
1:H:115:ASP:OD2	1:H:117:ARG:NH2	2.29	0.62
1:D:299:ARG:HG2	1:D:299:ARG:NH1	2.14	0.62
1:G:251:ASN:ND2	1:H:251:ASN:ND2	2.47	0.62
1:H:235:SER:HA	1:H:238:LEU:HD12	1.82	0.62
1:E:182:GLN:H	1:E:183:PRO:CD	2.11	0.62
1:I:61:THR:HG21	1:J:64:GLU:HG2	1.80	0.62
1:A:232:LEU:O	1:A:235:SER:OG	2.18	0.62
1:E:93:MET:HB3	1:E:101:ILE:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:ILE:HD13	1:J:90:LYS:HE2	1.81	0.62
1:G:76:LEU:HB3	1:G:130:LEU:HD11	1.82	0.62
2:A:402:BR7:H3	1:E:244:ALA:HA	1.81	0.62
1:I:54:LYS:HD2	1:I:54:LYS:H	1.64	0.62
1:C:256:LEU:HD12	1:C:260:THR:HG22	1.82	0.62
1:H:227:SER:HB3	1:H:230:GLU:HG3	1.81	0.61
1:J:286:ARG:HD2	1:J:287:GLN:N	2.15	0.61
1:F:178:LEU:HD21	1:F:181:VAL:HG21	1.81	0.61
1:J:123:ARG:NH1	1:J:197:ALA:O	2.33	0.61
1:C:175:TYR:CE1	2:C:401:BR7:H4	2.36	0.61
1:G:216:ILE:HD12	1:G:269:GLY:HA2	1.82	0.61
1:C:130:LEU:HB3	1:C:191:ILE:HD12	1.82	0.61
1:G:97:ASP:OD1	1:G:99:ARG:NH1	2.33	0.61
1:B:87:THR:HG21	1:B:90:LYS:HZ2	1.66	0.61
1:J:286:ARG:O	1:J:287:GLN:HB3	2.00	0.61
1:I:63:ILE:HD12	1:I:90:LYS:HG3	1.83	0.61
1:H:81:VAL:HG21	1:H:85:PRO:HG3	1.82	0.61
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.81	0.61
1:J:282:PHE:CE2	1:J:297:ILE:HG12	2.34	0.61
1:I:295:LEU:HA	1:I:298:GLN:HG2	1.83	0.61
1:B:212:LEU:O	1:B:216:ILE:HG12	2.00	0.61
1:J:91:ARG:NH2	1:J:103:ASN:OD1	2.34	0.61
1:H:44:THR:HA	1:H:99:ARG:HA	1.82	0.61
1:B:146:GLN:HB3	1:B:148:TYR:CE1	2.35	0.61
1:G:212:LEU:O	1:G:216:ILE:HG12	2.01	0.60
1:G:208:PHE:O	1:G:245:TYR:OH	2.19	0.60
1:I:299:ARG:HH12	1:I:302:LEU:CD2	2.05	0.60
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.82	0.60
1:G:38:TYR:CE1	1:G:105:ARG:HD2	2.35	0.60
1:F:248:TYR:HB2	1:G:247:SER:HB3	1.82	0.60
1:A:178:LEU:HD13	1:A:180:SER:HA	1.82	0.60
1:G:38:TYR:HE1	1:G:105:ARG:HD2	1.66	0.60
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.83	0.60
1:F:241:THR:HA	1:G:240:LEU:HD23	1.83	0.60
1:J:34:LYS:HZ3	1:J:109:SER:HG	1.50	0.60
1:A:28:THR:HB	1:A:256:LEU:HD21	1.83	0.60
1:F:136:ASN:ND2	1:F:185:GLN:HA	2.16	0.60
1:F:90:LYS:HE3	1:F:102:TYR:OH	2.02	0.60
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.36	0.60
1:G:295:LEU:HD13	1:G:296:LEU:HB3	1.83	0.60
1:F:301:ARG:HG2	1:F:302:LEU:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:CE1	1:G:304:PHE:HE2	2.20	0.60
1:C:219:SER:HA	1:C:238:LEU:HD23	1.83	0.60
1:H:221:SER:HA	1:H:224:TRP:CE3	2.37	0.60
1:B:131:GLU:OE1	1:B:190:ARG:NH2	2.35	0.60
1:B:149:THR:O	1:B:151:ASN:N	2.34	0.60
1:C:54:LYS:HB3	1:C:55:PRO:HD2	1.83	0.60
1:I:255:ARG:CG	1:I:255:ARG:HH11	2.15	0.60
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.84	0.59
1:G:97:ASP:OD2	1:G:99:ARG:NH1	2.35	0.59
1:D:219:SER:HA	1:D:238:LEU:HD11	1.84	0.59
1:B:123:ARG:HD3	1:B:198:VAL:HG22	1.83	0.59
1:F:91:ARG:NH2	1:F:103:ASN:OD1	2.34	0.59
1:B:175:TYR:CE1	2:B:401:BR7:H4	2.37	0.59
1:B:162:ILE:HD13	1:B:197:ALA:HB2	1.84	0.59
1:G:251:ASN:HD21	1:H:251:ASN:ND2	2.00	0.59
1:B:219:SER:HA	1:B:238:LEU:HD22	1.84	0.59
1:A:208:PHE:O	1:A:245:TYR:OH	2.19	0.59
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.85	0.59
1:E:299:ARG:HA	1:E:301:ARG:HG2	1.84	0.59
1:D:211:PRO:O	1:D:215:ILE:HG12	2.02	0.59
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.84	0.59
1:H:283:ALA:HA	1:H:286:ARG:NH2	2.19	0.58
1:G:182:GLN:N	1:G:183:PRO:HD3	2.16	0.58
1:H:287:GLN:HB3	1:H:289:ASN:H	1.66	0.58
1:J:34:LYS:HG2	1:J:109:SER:HA	1.85	0.58
1:I:41:ALA:HB3	1:I:102:TYR:HB3	1.85	0.58
1:E:223:PHE:HB3	1:E:301:ARG:CZ	2.33	0.58
1:G:180:SER:HA	1:G:182:GLN:HE22	1.66	0.58
1:B:138:GLN:HE22	1:B:184:ASN:ND2	2.00	0.58
1:G:289:ASN:OD1	1:G:290:GLY:N	2.33	0.58
1:F:306:LEU:O	1:F:310:ALA:N	2.35	0.58
1:A:212:LEU:O	1:A:216:ILE:HG12	2.02	0.58
1:A:136:ASN:HB2	1:A:187:GLU:HG3	1.85	0.58
1:H:42:GLN:HE21	1:H:101:ILE:HG23	1.68	0.58
1:H:76:LEU:HB3	1:H:130:LEU:HD11	1.85	0.58
1:I:223:PHE:CE1	1:I:304:PHE:HE2	2.17	0.58
1:D:219:SER:HA	1:D:238:LEU:HD21	1.86	0.58
1:F:206:TRP:HZ3	1:G:264:GLN:HE21	1.50	0.58
1:G:54:LYS:HD2	1:G:54:LYS:N	2.18	0.58
1:B:251:ASN:ND2	1:C:251:ASN:OD1	2.36	0.58
1:D:288:ALA:N	1:D:292:GLU:HG3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:ILE:O	1:F:266:ILE:HG12	2.04	0.58
1:F:90:LYS:NZ	1:F:102:TYR:CZ	2.70	0.58
1:G:233:GLN:HA	1:G:236:PHE:HD1	1.68	0.58
1:A:93:MET:HE3	1:A:101:ILE:HB	1.85	0.57
1:I:81:VAL:HG21	1:I:85:PRO:HG3	1.86	0.57
1:I:175:TYR:CD1	2:I:401:BR7:H3	2.39	0.57
1:I:90:LYS:HD2	1:I:91:ARG:H	1.69	0.57
1:H:17:SER:HB2	1:H:40:VAL:HB	1.86	0.57
1:I:219:SER:HA	1:I:238:LEU:CD2	2.33	0.57
1:D:149:THR:HG23	1:D:165:LYS:HE2	1.86	0.57
1:I:148:TYR:OH	1:J:177:HIS:HD2	1.88	0.57
1:E:239:MET:N	1:E:239:MET:HE2	2.19	0.57
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.86	0.57
1:E:145:ILE:CD1	1:E:191:ILE:HG12	2.34	0.57
1:A:87:THR:HG21	1:A:90:LYS:NZ	2.19	0.57
1:A:91:ARG:HH11	1:B:134:SER:HA	1.70	0.57
1:I:289:ASN:HD21	1:I:292:GLU:HG2	1.69	0.57
1:G:28:THR:HB	1:G:256:LEU:HD21	1.87	0.57
1:G:284:HIS:HB3	1:G:285:HIS:HD2	1.70	0.57
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.86	0.57
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.85	0.57
1:A:289:ASN:OD1	1:A:290:GLY:N	2.27	0.57
1:E:289:ASN:OD1	1:E:290:GLY:N	2.35	0.57
1:B:260:THR:O	1:B:264:GLN:HG3	2.05	0.57
1:J:295:LEU:HA	1:J:298:GLN:HG2	1.86	0.57
1:H:208:PHE:O	1:H:245:TYR:OH	2.21	0.57
1:I:137:ASN:HA	1:I:140:LEU:O	2.04	0.57
1:H:300:CYS:HG	1:H:304:PHE:HE2	1.52	0.57
1:I:115:ASP:OD2	1:I:117:ARG:NH2	2.38	0.56
1:D:208:PHE:O	1:D:245:TYR:OH	2.21	0.56
1:E:211:PRO:O	1:E:215:ILE:HG12	2.04	0.56
1:A:44:THR:HA	1:A:99:ARG:HA	1.87	0.56
1:B:208:PHE:O	1:B:245:TYR:OH	2.22	0.56
1:G:90:LYS:HD3	1:G:102:TYR:OH	2.05	0.56
1:H:221:SER:HA	1:H:224:TRP:HE3	1.70	0.56
1:G:136:ASN:HD21	1:G:138:GLN:HB2	1.70	0.56
1:E:179:SER:HB2	1:E:181:VAL:H	1.69	0.56
1:G:263:ASP:O	1:G:267:ILE:HG13	2.05	0.56
1:F:16:VAL:HA	1:F:40:VAL:O	2.05	0.56
1:H:248:TYR:HB2	1:I:247:SER:HB3	1.86	0.56
1:E:40:VAL:HG13	1:E:103:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:ARG:HH11	1:J:287:GLN:HA	1.71	0.56
1:F:145:ILE:CD1	1:F:191:ILE:HD13	2.34	0.56
1:B:159:GLU:OE2	1:C:29:LEU:HD21	2.05	0.56
1:D:212:LEU:O	1:D:216:ILE:HG12	2.04	0.56
1:F:227:SER:HB3	1:F:230:GLU:OE2	2.04	0.56
1:H:211:PRO:O	1:H:215:ILE:HG12	2.06	0.56
1:I:211:PRO:O	1:I:215:ILE:HG12	2.06	0.56
1:C:224:TRP:CD1	1:C:301:ARG:HD3	2.40	0.56
1:J:282:PHE:CE2	1:J:297:ILE:HG21	2.40	0.56
1:I:165:LYS:HG3	1:I:166:ALA:N	2.20	0.56
1:A:184:ASN:O	1:A:187:GLU:HG2	2.05	0.56
1:A:263:ASP:OD1	1:A:264:GLN:N	2.38	0.56
1:I:34:LYS:CE	1:I:35:VAL:H	2.19	0.56
1:A:295:LEU:HA	1:A:298:GLN:HE22	1.71	0.56
1:D:38:TYR:CD2	2:E:401:BR7:H20	2.41	0.56
1:E:49:LYS:HD2	1:E:50:THR:H	1.71	0.55
1:C:177:HIS:N	1:C:177:HIS:CD2	2.74	0.55
1:D:149:THR:HG21	1:D:165:LYS:O	2.05	0.55
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.40	0.55
1:A:211:PRO:O	1:A:215:ILE:HG12	2.06	0.55
1:E:91:ARG:NH2	1:E:103:ASN:OD1	2.40	0.55
1:G:176:ASP:OD1	1:G:177:HIS:N	2.37	0.55
1:J:123:ARG:CD	1:J:198:VAL:HG22	2.33	0.55
1:J:102:TYR:HD2	1:J:103:ASN:N	2.05	0.55
1:B:232:LEU:O	1:B:235:SER:OG	2.23	0.55
1:E:115:ASP:O	1:E:124:GLN:NE2	2.39	0.55
1:J:142:PHE:CD2	1:J:191:ILE:HG13	2.42	0.55
1:F:289:ASN:OD1	1:F:291:VAL:N	2.38	0.55
1:F:110:PHE:CE2	1:F:128:LEU:HG	2.41	0.55
1:F:281:ILE:HG21	1:J:224:TRP:CZ3	2.41	0.55
1:C:212:LEU:O	1:C:216:ILE:HG12	2.05	0.55
1:H:118:LEU:HD11	1:H:122:ASP:HA	1.87	0.55
1:E:67:ILE:HG23	1:E:71:LEU:O	2.06	0.55
1:B:224:TRP:CD1	1:B:301:ARG:NE	2.74	0.55
1:E:44:THR:HA	1:E:99:ARG:HA	1.89	0.55
1:J:123:ARG:HD2	1:J:197:ALA:O	2.06	0.55
1:D:38:TYR:CE2	2:E:401:BR7:H20	2.41	0.55
1:H:284:HIS:CD2	1:H:291:VAL:HG13	2.41	0.55
1:A:186:ASN:N	1:A:186:ASN:OD1	2.39	0.55
1:D:137:ASN:ND2	1:D:187:GLU:OE1	2.37	0.55
1:C:251:ASN:HD21	1:D:251:ASN:ND2	1.96	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:O	1:A:292:GLU:HG2	2.06	0.55
1:G:284:HIS:HB3	1:G:285:HIS:CD2	2.42	0.55
1:E:165:LYS:N	1:E:165:LYS:HD2	2.22	0.55
1:G:99:ARG:HG2	1:G:99:ARG:NH1	2.21	0.55
1:I:54:LYS:HD2	1:I:54:LYS:N	2.20	0.55
1:F:181:VAL:O	1:F:182:GLN:NE2	2.40	0.54
1:I:304:PHE:HA	1:I:307:GLY:H	1.71	0.54
1:G:44:THR:HA	1:G:99:ARG:HA	1.89	0.54
1:B:44:THR:HA	1:B:99:ARG:HA	1.89	0.54
1:E:299:ARG:C	1:E:301:ARG:H	2.10	0.54
1:F:90:LYS:HE3	1:F:102:TYR:CZ	2.42	0.54
1:D:91:ARG:HH11	1:E:134:SER:HA	1.72	0.54
1:B:173:ILE:O	1:B:187:GLU:HA	2.07	0.54
1:G:154:ASN:O	1:G:157:ILE:HG22	2.08	0.54
1:B:223:PHE:HB2	1:B:301:ARG:CD	2.36	0.54
1:E:174:ARG:HB2	1:E:187:GLU:HG2	1.87	0.54
1:A:165:LYS:O	1:A:165:LYS:HG2	2.06	0.54
1:F:132:PRO:HD3	1:F:142:PHE:CE2	2.42	0.54
1:I:101:ILE:HD13	1:J:179:SER:HB2	1.88	0.54
1:C:211:PRO:HG2	1:C:245:TYR:OH	2.08	0.54
1:E:287:GLN:HA	1:E:292:GLU:HB3	1.90	0.54
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.89	0.54
1:A:224:TRP:N	1:A:301:ARG:HH11	2.04	0.54
1:H:279:LEU:O	1:H:283:ALA:N	2.28	0.54
1:F:212:LEU:O	1:F:216:ILE:HG12	2.07	0.54
1:A:81:VAL:O	1:E:105:ARG:NH2	2.41	0.54
1:F:223:PHE:HE2	1:F:300:CYS:HG	1.54	0.54
1:I:299:ARG:C	1:I:301:ARG:H	2.11	0.54
1:A:260:THR:N	1:A:263:ASP:OD2	2.33	0.54
1:G:129:GLU:HG2	1:G:192:THR:HG23	1.89	0.54
1:J:155:GLU:O	1:J:161:TRP:NE1	2.40	0.54
1:G:91:ARG:NH2	1:G:103:ASN:OD1	2.41	0.54
1:C:299:ARG:HA	1:C:301:ARG:HH11	1.73	0.54
1:A:15:SER:O	1:A:41:ALA:HA	2.07	0.54
1:G:216:ILE:O	1:G:219:SER:HB3	2.08	0.54
1:J:34:LYS:NZ	1:J:109:SER:OG	2.34	0.54
1:F:136:ASN:ND2	1:F:138:GLN:HG3	2.22	0.54
1:B:314:VAL:C	1:B:316:VAL:H	2.11	0.54
1:D:300:CYS:HG	1:D:304:PHE:HE2	1.55	0.54
1:A:235:SER:HA	1:A:238:LEU:HD13	1.89	0.54
1:C:132:PRO:HD3	1:C:142:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HD2	2:B:401:BR7:H20	1.72	0.54
1:C:99:ARG:NH2	1:D:180:SER:OG	2.40	0.54
1:J:301:ARG:HD2	1:J:301:ARG:O	2.08	0.54
1:H:144:ASP:O	1:H:145:ILE:HG13	2.08	0.53
1:I:95:PHE:HE2	1:J:181:VAL:CG2	2.20	0.53
1:F:23:ILE:HG12	1:F:35:VAL:HG22	1.90	0.53
1:J:286:ARG:HG3	1:J:294:ASP:OD2	2.09	0.53
1:E:154:ASN:HB3	1:E:157:ILE:HD13	1.88	0.53
1:D:37:GLY:C	1:D:38:TYR:HD1	2.11	0.53
1:I:174:ARG:HA	1:I:186:ASN:O	2.08	0.53
1:G:296:LEU:HA	1:G:299:ARG:HB3	1.90	0.53
1:B:263:ASP:O	1:B:267:ILE:HG13	2.08	0.53
1:F:182:GLN:HB2	1:F:183:PRO:CD	2.35	0.53
1:J:283:ALA:HB2	1:J:297:ILE:HD11	1.91	0.53
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.24	0.53
1:B:224:TRP:CD2	1:B:301:ARG:HG2	2.42	0.53
1:B:289:ASN:OD1	1:B:290:GLY:N	2.35	0.53
1:C:251:ASN:HB3	1:C:252:ILE:HD13	1.91	0.53
1:E:50:THR:HG1	1:E:56:LEU:HD11	1.70	0.53
1:F:236:PHE:CE2	1:J:238:LEU:HD11	2.43	0.53
1:G:97:ASP:CG	1:G:99:ARG:NH1	2.62	0.53
1:G:223:PHE:HE1	1:G:304:PHE:HE2	1.55	0.53
1:I:232:LEU:O	1:I:235:SER:OG	2.21	0.53
1:F:46:LYS:HD2	1:F:47:PRO:N	2.23	0.53
1:A:294:ASP:OD2	1:A:297:ILE:HB	2.08	0.53
1:F:154:ASN:O	1:F:157:ILE:HG22	2.09	0.53
1:I:34:LYS:HE3	1:I:107:LEU:HD12	1.90	0.53
1:J:279:LEU:O	1:J:282:PHE:HB3	2.08	0.53
1:C:221:SER:HA	1:C:224:TRP:HE3	1.73	0.53
1:H:286:ARG:NH2	1:H:294:ASP:HB3	2.24	0.53
1:E:295:LEU:HA	1:E:298:GLN:HG2	1.91	0.53
1:H:16:VAL:HB	1:H:145:ILE:HG12	1.91	0.53
1:H:303:ALA:O	1:H:306:LEU:HG	2.09	0.53
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.90	0.53
1:J:227:SER:O	1:J:231:ARG:NH1	2.42	0.53
1:E:299:ARG:HG3	1:E:299:ARG:HH11	1.74	0.53
1:F:174:ARG:CZ	1:F:186:ASN:HB2	2.39	0.53
1:I:54:LYS:CD	1:I:54:LYS:H	2.22	0.53
1:A:180:SER:O	1:A:180:SER:OG	2.20	0.53
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.44	0.53
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ASP:N	1:D:176:ASP:OD1	2.39	0.53
1:C:46:LYS:HD3	1:C:46:LYS:N	2.24	0.53
1:D:122:ASP:N	1:D:122:ASP:OD1	2.42	0.53
1:J:132:PRO:HG3	1:J:140:LEU:HD22	1.90	0.52
1:H:294:ASP:HB3	1:H:297:ILE:HB	1.90	0.52
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.91	0.52
1:A:226:GLU:OE2	1:B:285:HIS:CE1	2.62	0.52
1:C:219:SER:HA	1:C:238:LEU:CD2	2.39	0.52
1:G:233:GLN:O	1:G:236:PHE:HB2	2.09	0.52
1:G:181:VAL:C	1:G:183:PRO:HD3	2.30	0.52
1:B:26:VAL:HG21	1:B:160:TRP:CZ2	2.44	0.52
1:I:212:LEU:O	1:I:216:ILE:HG12	2.10	0.52
1:E:33:TYR:OH	1:E:127:VAL:N	2.37	0.52
1:A:224:TRP:CG	1:A:301:ARG:HD3	2.45	0.52
1:G:157:ILE:HD12	1:H:258:TYR:CE2	2.45	0.52
1:B:238:LEU:HD21	1:C:236:PHE:CE2	2.44	0.52
1:C:295:LEU:O	1:C:299:ARG:HG3	2.09	0.52
1:B:40:VAL:HG13	1:B:103:ASN:ND2	2.23	0.52
1:A:91:ARG:HB3	1:A:103:ASN:HB2	1.91	0.52
1:F:260:THR:HG23	1:F:263:ASP:OD2	2.10	0.52
1:D:93:MET:HB3	1:D:101:ILE:HB	1.92	0.52
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.92	0.52
1:C:159:GLU:HG2	1:C:160:TRP:CD1	2.45	0.52
1:F:90:LYS:HE2	1:F:104:ALA:CB	2.32	0.52
1:F:112:ASN:ND2	1:F:125:GLN:O	2.43	0.52
1:B:14:VAL:HG22	1:B:43:TRP:HB3	1.91	0.52
1:B:118:LEU:CD1	1:B:122:ASP:HA	2.40	0.52
1:A:221:SER:C	1:A:301:ARG:HH12	2.13	0.52
1:B:38:TYR:HE2	2:C:401:BR7:H6	1.74	0.52
1:I:92:LEU:HD13	1:I:94:LEU:HD21	1.92	0.52
1:G:105:ARG:NH2	1:H:81:VAL:O	2.43	0.52
1:H:224:TRP:CE2	1:H:301:ARG:HB3	2.45	0.51
1:A:136:ASN:N	1:A:139:GLN:OE1	2.43	0.51
1:J:151:ASN:OD1	1:J:152:ALA:N	2.43	0.51
1:D:97:ASP:CG	1:D:99:ARG:NH1	2.64	0.51
1:I:65:ARG:NH2	1:J:68:ASN:HD22	2.07	0.51
1:D:40:VAL:HG13	1:D:103:ASN:ND2	2.25	0.51
1:F:157:ILE:HD13	1:G:115:ASP:HA	1.91	0.51
1:B:87:THR:CG2	1:B:90:LYS:HZ2	2.22	0.51
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.58	0.51
1:F:240:LEU:HD23	1:J:241:THR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:PHE:O	1:J:245:TYR:OH	2.29	0.51
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.92	0.51
1:C:223:PHE:HB3	1:C:301:ARG:HG2	1.92	0.51
1:B:216:ILE:O	1:B:219:SER:HB3	2.10	0.51
1:B:224:TRP:CD1	1:C:281:ILE:HG21	2.46	0.51
1:F:227:SER:HB3	1:F:230:GLU:HG3	1.93	0.51
1:B:38:TYR:CE1	1:B:105:ARG:HD2	2.35	0.51
1:B:33:TYR:C	1:B:34:LYS:HD3	2.30	0.51
1:C:44:THR:HA	1:C:99:ARG:HA	1.93	0.51
1:F:157:ILE:HD11	1:G:114:MET:O	2.10	0.51
1:A:27:ASN:HB3	1:A:32:THR:HB	1.93	0.51
1:J:28:THR:HB	1:J:256:LEU:HD21	1.92	0.51
1:G:242:VAL:HG21	1:G:273:ILE:HD11	1.93	0.51
1:C:156:GLU:CD	1:C:156:GLU:H	2.14	0.51
1:G:211:PRO:O	1:G:215:ILE:HG12	2.11	0.51
1:G:274:PHE:O	1:G:278:LEU:HG	2.10	0.51
1:C:176:ASP:CB	1:C:177:HIS:HD2	2.22	0.51
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.10	0.51
1:I:34:LYS:CE	1:I:107:LEU:HD12	2.40	0.51
1:D:220:TRP:CE3	1:D:305:PRO:HB3	2.45	0.51
1:D:303:ALA:O	1:D:306:LEU:HG	2.11	0.51
1:E:72:TRP:CH2	1:E:140:LEU:HD12	2.46	0.51
1:H:283:ALA:HA	1:H:286:ARG:NH1	2.26	0.50
1:A:38:TYR:CE1	1:A:105:ARG:HD2	2.43	0.50
1:H:306:LEU:O	1:H:309:LEU:HB3	2.10	0.50
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.46	0.50
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.46	0.50
1:D:298:GLN:HG3	1:D:298:GLN:O	2.11	0.50
1:H:289:ASN:CG	1:H:292:GLU:HB3	2.31	0.50
1:F:136:ASN:HD21	1:F:138:GLN:HG3	1.76	0.50
1:G:90:LYS:HE3	1:G:104:ALA:HB1	1.92	0.50
1:C:295:LEU:HA	1:C:298:GLN:HG2	1.94	0.50
1:I:52:GLY:HA3	1:I:54:LYS:HD3	1.94	0.50
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.92	0.50
1:G:131:GLU:OE1	1:G:190:ARG:NH2	2.38	0.50
1:A:87:THR:HG21	1:A:90:LYS:HZ2	1.76	0.50
1:D:29:LEU:CD1	1:D:255:ARG:NH1	2.74	0.50
1:H:125:GLN:HE22	1:H:194:ARG:HH11	1.58	0.50
1:A:224:TRP:H	1:A:301:ARG:HH11	1.59	0.50
1:J:115:ASP:H	1:J:124:GLN:NE2	1.84	0.50
1:C:211:PRO:O	1:C:215:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLN:CG	1:A:289:ASN:H	2.24	0.50
1:J:71:LEU:HD22	1:J:73:VAL:CG2	2.42	0.50
1:J:153:ASP:CG	1:J:154:ASN:H	2.15	0.50
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.94	0.50
1:C:221:SER:HA	1:C:224:TRP:CE3	2.46	0.50
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.94	0.50
1:I:90:LYS:NZ	1:I:102:TYR:CD1	2.80	0.50
1:I:95:PHE:HB2	1:I:99:ARG:O	2.12	0.50
1:G:178:LEU:CD2	2:G:401:BR7:H2	2.41	0.50
1:C:29:LEU:HB2	1:C:255:ARG:HD2	1.94	0.50
1:G:91:ARG:HB3	1:G:103:ASN:HB2	1.93	0.50
1:A:55:PRO:HG3	1:A:95:PHE:CE2	2.47	0.50
1:E:91:ARG:HB3	1:E:103:ASN:HB2	1.94	0.50
1:F:223:PHE:HE2	1:F:300:CYS:SG	2.35	0.50
1:I:138:GLN:NE2	1:I:184:ASN:HB3	2.27	0.50
1:J:186:ASN:OD1	1:J:186:ASN:N	2.45	0.50
1:D:27:ASN:HB3	1:D:32:THR:HB	1.93	0.50
1:G:239:MET:HA	1:G:273:ILE:HD13	1.93	0.49
1:F:185:GLN:HG3	1:F:185:GLN:O	2.11	0.49
1:G:64:GLU:HA	1:G:67:ILE:HD12	1.94	0.49
1:E:299:ARG:NH1	1:E:299:ARG:HG3	2.27	0.49
1:C:81:VAL:HG21	1:C:85:PRO:HG3	1.93	0.49
1:C:16:VAL:HB	1:C:145:ILE:CD1	2.39	0.49
1:D:91:ARG:HB3	1:D:103:ASN:HB2	1.94	0.49
1:F:36:ASP:HB2	1:F:107:LEU:HD13	1.93	0.49
1:G:293:ASP:N	1:G:293:ASP:OD1	2.44	0.49
1:H:282:PHE:CD2	1:H:286:ARG:HD3	2.47	0.49
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.47	0.49
1:F:116:PHE:CD2	1:F:124:GLN:NE2	2.80	0.49
1:I:142:PHE:CD2	1:I:191:ILE:HG13	2.47	0.49
1:I:279:LEU:O	1:I:283:ALA:N	2.36	0.49
1:B:87:THR:HG21	1:B:90:LYS:HZ1	1.77	0.49
1:C:132:PRO:HD3	1:C:142:PHE:HE2	1.77	0.49
1:A:122:ASP:N	1:A:122:ASP:OD1	2.44	0.49
1:F:142:PHE:HB3	1:F:170:ILE:HD13	1.94	0.49
1:I:306:LEU:HA	1:I:309:LEU:HB2	1.95	0.49
1:H:36:ASP:OD2	1:H:37:GLY:N	2.45	0.49
1:E:296:LEU:HA	1:E:299:ARG:HB3	1.95	0.49
1:A:93:MET:HB3	1:A:101:ILE:HB	1.94	0.49
1:J:229:SER:O	1:J:233:GLN:HG3	2.11	0.49
1:I:260:THR:N	1:I:263:ASP:OD2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:SER:HB3	1:J:252:ILE:HD11	1.95	0.49
1:C:38:TYR:CE2	1:C:105:ARG:HD2	2.48	0.49
1:H:16:VAL:HA	1:H:40:VAL:O	2.13	0.49
1:I:95:PHE:HE2	1:J:181:VAL:HG21	1.77	0.49
1:G:233:GLN:HA	1:G:236:PHE:CD1	2.48	0.49
1:A:219:SER:HA	1:A:238:LEU:CD2	2.40	0.49
1:G:114:MET:HB3	1:G:124:GLN:NE2	2.27	0.49
1:I:204:TYR:O	1:I:208:PHE:HB2	2.13	0.49
1:C:18:ILE:HB	1:C:147:VAL:HG22	1.93	0.49
1:E:295:LEU:HA	1:E:298:GLN:OE1	2.12	0.49
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.47	0.49
1:I:295:LEU:O	1:I:299:ARG:HB2	2.13	0.48
1:E:295:LEU:HA	1:E:298:GLN:CD	2.34	0.48
1:G:223:PHE:HE1	1:G:304:PHE:CE2	2.31	0.48
1:C:125:GLN:OE1	1:C:194:ARG:HD3	2.13	0.48
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.48	0.48
1:I:40:VAL:HG22	1:I:103:ASN:ND2	2.28	0.48
1:F:181:VAL:HG22	1:F:182:GLN:CA	2.43	0.48
1:B:211:PRO:O	1:B:215:ILE:HG12	2.12	0.48
1:I:63:ILE:CD1	1:I:90:LYS:HG3	2.43	0.48
1:E:72:TRP:HH2	1:E:140:LEU:HD12	1.78	0.48
1:J:314:VAL:O	1:J:317:ILE:HG13	2.13	0.48
1:A:29:LEU:HD21	1:E:159:GLU:OE2	2.13	0.48
1:C:231:ARG:NH2	1:C:293:ASP:OD1	2.46	0.48
1:I:255:ARG:CG	1:I:255:ARG:NH1	2.75	0.48
1:C:76:LEU:HB3	1:C:130:LEU:HD21	1.93	0.48
1:H:224:TRP:CZ2	1:H:301:ARG:HB3	2.49	0.48
1:A:176:ASP:OD1	1:A:176:ASP:N	2.46	0.48
1:F:178:LEU:HD11	1:F:181:VAL:HG23	1.95	0.48
1:B:129:GLU:OE1	1:B:190:ARG:HD3	2.12	0.48
1:G:90:LYS:HZ2	1:G:104:ALA:HB1	1.77	0.48
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.42	0.48
1:I:34:LYS:HG3	1:I:109:SER:HA	1.94	0.48
1:F:123:ARG:HD2	1:F:198:VAL:HG22	1.96	0.48
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.14	0.48
1:A:78:PHE:O	1:A:81:VAL:HG12	2.14	0.48
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.95	0.48
1:H:182:GLN:H	1:H:183:PRO:CD	2.27	0.48
1:D:39:ILE:HD11	1:D:78:PHE:CE1	2.49	0.48
1:B:299:ARG:O	1:B:299:ARG:HG3	2.13	0.48
1:I:115:ASP:OD2	1:I:117:ARG:NE	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ILE:HD12	1:I:191:ILE:HG21	1.96	0.48
1:C:136:ASN:OD1	1:C:138:GLN:HB2	2.14	0.48
1:I:293:ASP:OD1	1:I:293:ASP:N	2.45	0.48
1:A:133:PHE:CE1	1:E:89:ASN:HB2	2.48	0.48
1:J:287:GLN:HG3	1:J:292:GLU:H	1.78	0.48
1:E:212:LEU:O	1:E:216:ILE:HG12	2.14	0.48
1:H:78:PHE:O	1:H:81:VAL:HG12	2.14	0.48
1:E:40:VAL:HG22	1:E:103:ASN:ND2	2.29	0.48
1:A:284:HIS:HB3	1:A:285:HIS:CD2	2.49	0.48
1:G:56:LEU:HD12	1:G:57:ILE:H	1.79	0.48
1:I:34:LYS:CD	1:I:35:VAL:H	2.27	0.48
1:H:42:GLN:HG2	1:H:101:ILE:CG1	2.40	0.48
1:B:221:SER:HA	1:B:301:ARG:NH2	2.28	0.48
1:B:287:GLN:HA	1:B:292:GLU:HB3	1.96	0.48
1:A:18:ILE:HD13	1:A:39:ILE:HG23	1.96	0.48
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.43	0.48
1:D:84:SER:HA	1:D:85:PRO:HD3	1.57	0.48
1:G:178:LEU:HG	1:G:179:SER:N	2.29	0.48
1:A:215:ILE:O	1:A:219:SER:N	2.46	0.48
1:A:26:VAL:HG13	1:A:114:MET:HE1	1.96	0.48
1:A:156:GLU:HG3	1:A:156:GLU:H	1.34	0.48
1:D:264:GLN:HA	1:D:267:ILE:HD12	1.95	0.48
1:A:223:PHE:HB2	1:A:301:ARG:HD2	1.96	0.47
1:C:144:ASP:O	1:C:145:ILE:HG13	2.14	0.47
1:H:215:ILE:O	1:H:219:SER:N	2.45	0.47
1:I:289:ASN:OD1	1:I:290:GLY:N	2.46	0.47
1:A:259:THR:HA	1:A:263:ASP:OD2	2.14	0.47
1:B:58:VAL:HB	1:B:92:LEU:HB2	1.95	0.47
1:G:17:SER:HB2	1:G:40:VAL:HB	1.96	0.47
1:E:235:SER:O	1:E:239:MET:HE2	2.15	0.47
1:I:223:PHE:CZ	1:I:279:LEU:HD21	2.49	0.47
1:E:142:PHE:CD2	1:E:191:ILE:HG13	2.49	0.47
1:F:204:TYR:O	1:F:209:ILE:HG12	2.14	0.47
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.96	0.47
1:A:21:ASN:HD22	1:A:37:GLY:HA2	1.79	0.47
1:D:253:LEU:HG	1:D:254:PRO:HD2	1.95	0.47
1:F:122:ASP:OD1	1:F:122:ASP:N	2.42	0.47
1:G:287:GLN:CB	1:G:292:GLU:HB2	2.36	0.47
1:I:86:ASP:N	1:I:107:LEU:O	2.36	0.47
1:E:51:PRO:HD2	1:E:54:LYS:NZ	2.29	0.47
1:C:40:VAL:HA	1:C:103:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:ARG:HG2	1:I:231:ARG:HH11	1.78	0.47
1:A:226:GLU:OE2	1:B:285:HIS:NE2	2.47	0.47
1:D:87:THR:HG21	1:D:90:LYS:HE3	1.96	0.47
1:D:62:GLN:O	1:D:66:TRP:HD1	1.98	0.47
1:G:46:LYS:H	1:G:46:LYS:HD3	1.78	0.47
1:C:263:ASP:O	1:C:267:ILE:HG13	2.14	0.47
1:D:153:ASP:HA	1:D:155:GLU:OE2	2.15	0.47
1:D:150:GLU:HG2	1:D:150:GLU:H	1.47	0.47
1:H:154:ASN:HA	1:H:156:GLU:HG2	1.95	0.47
1:E:118:LEU:CD1	1:E:122:ASP:HA	2.45	0.47
1:H:291:VAL:O	1:H:291:VAL:HG12	2.15	0.47
1:E:174:ARG:HA	1:E:186:ASN:O	2.14	0.47
1:F:263:ASP:O	1:F:267:ILE:HG13	2.15	0.47
1:H:224:TRP:NE1	1:H:301:ARG:HD3	2.30	0.47
1:J:63:ILE:HD13	1:J:90:LYS:CE	2.45	0.47
1:F:123:ARG:CZ	1:F:198:VAL:HG13	2.45	0.47
1:C:185:GLN:OE1	1:C:185:GLN:N	2.47	0.47
1:B:169:HIS:CE1	1:B:194:ARG:HH11	2.33	0.47
1:E:64:GLU:OE1	1:E:65:ARG:N	2.48	0.47
1:F:92:LEU:HA	1:F:92:LEU:HD23	1.73	0.47
1:A:224:TRP:H	1:A:301:ARG:NH1	2.12	0.47
1:B:255:ARG:HH11	1:B:255:ARG:CG	2.28	0.47
1:C:178:LEU:CG	1:C:179:SER:H	2.28	0.47
1:D:185:GLN:N	1:D:185:GLN:OE1	2.48	0.47
1:A:287:GLN:HG2	1:A:288:ALA:N	2.29	0.47
1:C:29:LEU:CB	1:C:255:ARG:HD2	2.45	0.47
1:E:122:ASP:HB2	1:E:124:GLN:HE21	1.79	0.47
1:B:294:ASP:HB3	1:B:297:ILE:HB	1.96	0.47
1:G:241:THR:HA	1:H:240:LEU:HD23	1.95	0.47
1:H:178:LEU:HD21	1:H:186:ASN:HA	1.97	0.47
1:J:286:ARG:HD2	1:J:286:ARG:C	2.34	0.47
1:J:295:LEU:HD23	1:J:295:LEU:O	2.15	0.46
1:B:234:THR:O	1:B:238:LEU:HD12	2.15	0.46
1:G:87:THR:HG23	1:G:90:LYS:NZ	2.30	0.46
1:E:122:ASP:N	1:E:122:ASP:OD1	2.48	0.46
1:J:212:LEU:O	1:J:216:ILE:HG12	2.15	0.46
1:D:273:ILE:O	1:D:277:ILE:HG12	2.15	0.46
1:A:299:ARG:C	1:A:301:ARG:H	2.18	0.46
1:I:216:ILE:O	1:I:219:SER:HB3	2.15	0.46
1:I:121:PHE:HZ	1:I:205:LEU:HD21	1.79	0.46
1:J:84:SER:HA	1:J:85:PRO:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASP:CG	1:B:143:SER:HB3	2.36	0.46
1:B:169:HIS:CE1	1:B:194:ARG:NH1	2.83	0.46
1:C:178:LEU:HD21	1:C:181:VAL:HG13	1.96	0.46
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.50	0.46
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.60	0.46
1:F:16:VAL:HB	1:F:145:ILE:HD11	1.97	0.46
1:F:236:PHE:CD2	1:J:238:LEU:HD11	2.50	0.46
1:C:155:GLU:O	1:C:161:TRP:NE1	2.48	0.46
1:E:40:VAL:HG13	1:E:103:ASN:ND2	2.29	0.46
1:H:136:ASN:HA	1:H:188:PHE:CD1	2.50	0.46
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.98	0.46
1:H:41:ALA:C	1:H:42:GLN:HG3	2.35	0.46
1:J:71:LEU:HD22	1:J:73:VAL:HG22	1.97	0.46
1:F:288:ALA:HB3	1:F:292:GLU:OE2	2.16	0.46
1:C:251:ASN:ND2	1:D:251:ASN:ND2	2.58	0.46
1:D:89:ASN:O	1:D:104:ALA:HA	2.16	0.46
1:D:228:PHE:HA	1:D:231:ARG:CZ	2.46	0.46
1:A:240:LEU:HD23	1:E:241:THR:HA	1.97	0.46
1:I:255:ARG:HG2	1:I:255:ARG:NH1	2.20	0.46
1:H:90:LYS:HA	1:H:103:ASN:O	2.16	0.46
1:A:38:TYR:HE1	1:A:105:ARG:CD	2.26	0.46
1:G:90:LYS:HZ2	1:G:104:ALA:CA	2.29	0.46
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.98	0.46
1:F:301:ARG:HD2	1:F:303:ALA:HB2	1.97	0.46
1:I:307:GLY:O	1:I:311:ILE:HG13	2.15	0.46
1:H:118:LEU:CD1	1:H:122:ASP:HA	2.45	0.46
1:B:61:THR:HG21	1:C:64:GLU:HG3	1.97	0.46
1:H:19:PHE:CE1	1:H:148:TYR:HD2	2.34	0.46
1:C:248:TYR:O	1:C:252:ILE:HG12	2.16	0.46
1:J:233:GLN:HA	1:J:236:PHE:HD1	1.81	0.46
1:A:208:PHE:HE2	1:A:248:TYR:CZ	2.34	0.46
1:A:95:PHE:CZ	1:B:181:VAL:HB	2.51	0.46
1:C:71:LEU:HD22	1:C:73:VAL:HG22	1.98	0.46
1:A:80:ASN:ND2	1:A:127:VAL:O	2.45	0.46
1:B:284:HIS:HA	1:B:293:ASP:OD1	2.16	0.46
1:A:223:PHE:H	1:A:301:ARG:NH1	2.13	0.46
1:I:90:LYS:HD2	1:I:90:LYS:C	2.36	0.46
1:I:224:TRP:CD1	1:I:301:ARG:HD3	2.50	0.46
1:C:216:ILE:O	1:C:219:SER:HB3	2.16	0.46
1:I:78:PHE:O	1:I:81:VAL:HG12	2.15	0.46
1:F:128:LEU:HB2	1:F:193:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:315:LEU:HD12	1:J:315:LEU:HA	1.55	0.46
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.98	0.46
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.99	0.46
1:G:216:ILE:HD12	1:G:269:GLY:CA	2.46	0.46
1:B:174:ARG:NH2	1:I:13:ASP:OD1	2.48	0.46
1:J:123:ARG:NH1	1:J:197:ALA:H	2.14	0.45
1:A:42:GLN:CB	1:A:101:ILE:HG12	2.46	0.45
1:J:311:ILE:HA	1:J:314:VAL:HG23	1.97	0.45
1:A:234:THR:OG1	1:B:233:GLN:NE2	2.49	0.45
1:C:204:TYR:O	1:C:209:ILE:HG12	2.16	0.45
1:I:149:THR:O	1:I:151:ASN:N	2.45	0.45
1:J:175:TYR:CE1	2:J:401:BR7:H4	2.51	0.45
1:B:146:GLN:N	1:B:146:GLN:OE1	2.49	0.45
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.51	0.45
1:I:36:ASP:OD1	1:I:37:GLY:N	2.49	0.45
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.59	0.45
1:E:182:GLN:N	1:E:183:PRO:HD2	2.21	0.45
1:C:176:ASP:C	1:C:177:HIS:HD2	2.19	0.45
1:H:42:GLN:CG	1:H:101:ILE:HG12	2.42	0.45
1:D:227:SER:HB3	1:D:230:GLU:CG	2.46	0.45
1:H:119:PHE:CD1	1:H:120:PRO:HA	2.51	0.45
1:D:44:THR:HA	1:D:99:ARG:HA	1.98	0.45
1:E:118:LEU:HD11	1:E:122:ASP:HA	1.98	0.45
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.99	0.45
1:H:72:TRP:HH2	1:H:140:LEU:HD12	1.82	0.45
1:E:84:SER:HA	1:E:85:PRO:HD3	1.85	0.45
1:H:286:ARG:HH21	1:H:294:ASP:N	2.10	0.45
1:H:72:TRP:CH2	1:H:140:LEU:HD12	2.52	0.45
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.99	0.45
1:J:16:VAL:HA	1:J:40:VAL:O	2.17	0.45
1:G:239:MET:O	1:G:243:VAL:HG23	2.17	0.45
1:D:180:SER:OG	1:D:180:SER:O	2.27	0.45
1:D:181:VAL:HG11	1:D:185:GLN:HB2	1.98	0.45
1:E:178:LEU:HD21	1:E:185:GLN:O	2.17	0.45
1:G:287:GLN:HG2	1:G:288:ALA:N	2.31	0.45
1:B:38:TYR:CD2	2:C:401:BR7:H20	2.51	0.45
1:B:62:GLN:HE22	1:C:68:ASN:CG	2.18	0.45
1:J:46:LYS:HA	1:J:47:PRO:HD3	1.80	0.45
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.51	0.45
1:B:186:ASN:N	1:B:186:ASN:OD1	2.47	0.45
1:I:62:GLN:O	1:I:66:TRP:HD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:N	1:A:301:ARG:NH1	2.65	0.45
1:H:278:LEU:O	1:H:282:PHE:N	2.30	0.45
1:H:286:ARG:HH12	1:H:297:ILE:CG2	2.15	0.45
1:G:183:PRO:HG2	1:G:185:GLN:H	1.81	0.45
1:C:169:HIS:CD2	1:C:169:HIS:C	2.91	0.45
1:A:222:VAL:HG13	1:A:223:PHE:CD2	2.51	0.44
1:I:95:PHE:CE2	1:J:181:VAL:HG23	2.52	0.44
1:C:16:VAL:HA	1:C:40:VAL:O	2.17	0.44
1:B:299:ARG:C	1:B:301:ARG:H	2.18	0.44
1:D:216:ILE:O	1:D:219:SER:HB2	2.17	0.44
1:B:137:ASN:ND2	1:B:187:GLU:OE2	2.47	0.44
1:A:33:TYR:OH	1:A:127:VAL:N	2.41	0.44
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.99	0.44
1:I:153:ASP:OD1	1:I:154:ASN:N	2.50	0.44
1:F:208:PHE:O	1:F:245:TYR:OH	2.33	0.44
1:H:56:LEU:HD12	1:H:57:ILE:N	2.32	0.44
1:F:90:LYS:CE	1:F:102:TYR:CZ	3.01	0.44
1:F:216:ILE:O	1:F:219:SER:HB3	2.17	0.44
1:G:181:VAL:HG22	1:G:183:PRO:HD3	1.99	0.44
1:J:182:GLN:N	1:J:183:PRO:CD	2.80	0.44
1:B:122:ASP:N	1:B:122:ASP:OD1	2.49	0.44
1:G:186:ASN:N	1:G:186:ASN:OD1	2.51	0.44
1:H:286:ARG:O	1:H:287:GLN:NE2	2.51	0.44
1:F:178:LEU:CG	1:F:181:VAL:HB	2.45	0.44
1:B:137:ASN:HA	1:B:140:LEU:O	2.18	0.44
1:A:194:ARG:HH11	1:A:194:ARG:HG3	1.83	0.44
1:B:206:TRP:CD1	1:B:206:TRP:N	2.84	0.44
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.82	0.44
1:H:285:HIS:O	1:H:285:HIS:CG	2.70	0.44
1:H:286:ARG:O	1:H:286:ARG:CG	2.65	0.44
1:I:294:ASP:HB2	1:I:297:ILE:CG1	2.48	0.44
1:E:132:PRO:HD3	1:E:142:PHE:CE2	2.52	0.44
1:B:175:TYR:CD1	2:B:401:BR7:H4	2.52	0.44
1:G:175:TYR:CE1	2:G:401:BR7:H4	2.53	0.44
1:B:40:VAL:HG22	1:B:103:ASN:ND2	2.33	0.44
1:A:248:TYR:HE1	1:B:250:SER:OG	2.01	0.44
1:G:136:ASN:ND2	1:G:138:GLN:H	2.15	0.44
1:F:39:ILE:HD11	1:F:78:PHE:CE1	2.52	0.44
1:E:232:LEU:O	1:E:235:SER:OG	2.32	0.44
1:I:34:LYS:HD3	1:I:108:GLY:O	2.17	0.44
1:A:216:ILE:O	1:A:219:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:SER:HA	1:H:85:PRO:HD3	1.72	0.44
1:F:132:PRO:HG3	1:F:140:LEU:HD22	2.00	0.44
1:I:186:ASN:OD1	1:I:186:ASN:N	2.50	0.44
1:C:283:ALA:O	1:C:293:ASP:HA	2.17	0.44
1:F:313:CYS:O	1:F:317:ILE:HG12	2.18	0.44
1:B:174:ARG:HA	1:B:186:ASN:O	2.17	0.44
1:H:223:PHE:CE1	1:H:304:PHE:HZ	2.36	0.44
1:J:175:TYR:CD1	2:J:401:BR7:H3	2.52	0.44
1:E:240:LEU:HA	1:E:240:LEU:HD22	1.64	0.44
1:F:40:VAL:HG22	1:F:103:ASN:ND2	2.33	0.44
1:I:61:THR:HG21	1:J:64:GLU:CG	2.47	0.44
1:H:287:GLN:OE1	1:H:292:GLU:HG2	2.18	0.44
1:F:40:VAL:HG13	1:F:103:ASN:HD21	1.83	0.44
1:E:42:GLN:HG3	1:E:101:ILE:HA	1.99	0.44
1:I:308:PHE:HA	1:I:311:ILE:HD12	1.99	0.44
1:I:52:GLY:HA3	1:I:54:LYS:NZ	2.33	0.44
1:G:90:LYS:NZ	1:G:104:ALA:HB1	2.32	0.44
1:I:145:ILE:HG22	1:I:170:ILE:HD11	2.00	0.44
1:B:127:VAL:HA	1:B:193:VAL:O	2.18	0.44
1:H:136:ASN:ND2	1:H:139:GLN:HG3	2.33	0.44
1:B:286:ARG:HD3	1:B:286:ARG:HA	1.28	0.44
1:E:130:LEU:HB3	1:E:191:ILE:HB	2.00	0.43
1:E:212:LEU:HD23	1:E:245:TYR:CE2	2.53	0.43
1:G:269:GLY:O	1:G:273:ILE:HG13	2.17	0.43
1:J:132:PRO:CG	1:J:140:LEU:HD22	2.48	0.43
1:J:153:ASP:OD1	1:J:154:ASN:N	2.42	0.43
1:E:224:TRP:CD1	1:E:224:TRP:N	2.85	0.43
1:C:289:ASN:CG	1:C:291:VAL:H	2.21	0.43
1:C:154:ASN:HB3	1:C:157:ILE:HG12	1.98	0.43
1:F:123:ARG:C	1:F:124:GLN:HG2	2.39	0.43
1:F:260:THR:H	1:F:263:ASP:HB2	1.83	0.43
1:G:230:GLU:O	1:G:234:THR:OG1	2.18	0.43
1:G:18:ILE:HB	1:G:147:VAL:HG22	2.01	0.43
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.99	0.43
1:E:145:ILE:HD13	1:E:191:ILE:CG2	2.45	0.43
1:C:103:ASN:HA	1:C:103:ASN:HD22	1.60	0.43
1:F:177:HIS:CE1	1:J:148:TYR:HH	2.31	0.43
1:J:301:ARG:HD2	1:J:301:ARG:C	2.39	0.43
1:I:118:LEU:HD11	1:I:122:ASP:HA	1.99	0.43
1:E:47:PRO:HG3	1:E:97:ASP:O	2.18	0.43
1:B:165:LYS:O	1:B:165:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:SER:HA	1:E:238:LEU:CD2	2.46	0.43
1:G:314:VAL:O	1:G:317:ILE:HG12	2.19	0.43
1:D:165:LYS:HD2	1:D:165:LYS:HA	1.83	0.43
1:F:62:GLN:OE1	1:F:65:ARG:HD3	2.18	0.43
1:F:65:ARG:HD2	1:G:68:ASN:ND2	2.33	0.43
1:C:303:ALA:HA	1:C:306:LEU:HD23	2.01	0.43
1:H:173:ILE:O	1:H:187:GLU:HA	2.18	0.43
1:A:291:VAL:O	1:A:293:ASP:N	2.51	0.43
1:I:299:ARG:HG2	1:I:301:ARG:CZ	2.49	0.43
1:D:220:TRP:CZ2	1:D:308:PHE:HD2	2.35	0.43
1:E:155:GLU:OE1	1:E:163:ARG:NH1	2.49	0.43
1:A:142:PHE:CD2	1:A:191:ILE:HG13	2.53	0.43
1:E:273:ILE:O	1:E:276:ALA:N	2.51	0.43
1:F:181:VAL:HG22	1:F:182:GLN:N	2.34	0.43
1:H:91:ARG:HB3	1:H:103:ASN:HB2	2.01	0.43
1:D:289:ASN:OD1	1:D:292:GLU:HG2	2.17	0.43
1:E:145:ILE:HD12	1:E:170:ILE:HG12	2.00	0.43
1:C:255:ARG:O	1:C:255:ARG:HG2	2.11	0.43
1:G:204:TYR:O	1:G:208:PHE:HB2	2.19	0.43
1:A:137:ASN:N	1:A:187:GLU:OE1	2.51	0.43
1:E:300:CYS:HA	1:E:303:ALA:HB3	2.00	0.43
1:H:286:ARG:NH1	1:H:297:ILE:HD13	2.34	0.43
1:I:34:LYS:HZ2	1:I:110:PHE:HE1	1.66	0.43
1:C:145:ILE:HD12	1:C:191:ILE:HG12	2.00	0.43
1:G:136:ASN:CG	1:G:185:GLN:HG3	2.39	0.43
1:D:28:THR:HG21	1:D:254:PRO:HB2	2.00	0.43
1:A:166:ALA:HA	1:A:194:ARG:O	2.18	0.43
1:B:84:SER:HA	1:B:85:PRO:HD3	1.79	0.43
1:J:204:TYR:O	1:J:209:ILE:HG12	2.19	0.43
1:F:44:THR:HA	1:F:99:ARG:HA	2.00	0.43
1:F:165:LYS:HA	1:F:165:LYS:HD2	1.57	0.43
1:J:296:LEU:HD12	1:J:296:LEU:H	1.83	0.43
1:J:295:LEU:HA	1:J:298:GLN:CG	2.49	0.43
1:J:40:VAL:HG22	1:J:103:ASN:ND2	2.33	0.43
1:A:121:PHE:HZ	1:A:205:LEU:HD21	1.82	0.43
1:H:125:GLN:HE22	1:H:194:ARG:HD3	1.84	0.43
1:B:165:LYS:HA	1:B:165:LYS:HD2	1.89	0.43
1:H:89:ASN:HB2	1:I:133:PHE:CE1	2.54	0.43
1:J:13:ASP:HB3	1:J:143:SER:HB3	2.01	0.43
1:G:117:ARG:HG2	1:G:258:TYR:CD1	2.53	0.43
1:I:302:LEU:HD12	1:I:303:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:TYR:O	1:C:186:ASN:HB2	2.19	0.43
1:F:42:GLN:OE1	1:G:179:SER:OG	2.36	0.43
1:H:300:CYS:SG	1:H:304:PHE:HE2	2.42	0.43
1:D:286:ARG:HD3	1:D:286:ARG:HA	1.59	0.43
1:I:40:VAL:HG13	1:I:103:ASN:ND2	2.34	0.43
1:F:301:ARG:HH11	1:F:303:ALA:HB2	1.84	0.43
1:E:56:LEU:O	1:E:93:MET:HA	2.19	0.43
1:D:227:SER:HB3	1:D:230:GLU:HG3	2.01	0.43
1:B:220:TRP:NE1	1:B:272:SER:OG	2.42	0.43
1:C:174:ARG:HB3	1:C:187:GLU:HG2	1.99	0.42
1:G:90:LYS:CE	1:G:104:ALA:HB1	2.48	0.42
1:D:286:ARG:NH1	1:D:287:GLN:NE2	2.67	0.42
1:F:174:ARG:HH12	1:F:186:ASN:HD22	1.65	0.42
1:A:129:GLU:OE2	1:A:190:ARG:NH1	2.52	0.42
1:G:78:PHE:O	1:G:81:VAL:HG12	2.20	0.42
1:B:26:VAL:HG21	1:B:160:TRP:HZ2	1.83	0.42
1:B:118:LEU:HD12	1:B:122:ASP:HA	2.00	0.42
1:J:65:ARG:HA	1:J:68:ASN:OD1	2.19	0.42
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.78	0.42
1:B:227:SER:O	1:B:231:ARG:NH1	2.52	0.42
1:H:206:TRP:CD1	1:H:206:TRP:N	2.87	0.42
1:H:165:LYS:HG3	1:H:165:LYS:O	2.19	0.42
1:E:262:ILE:O	1:E:266:ILE:HG12	2.19	0.42
1:D:95:PHE:HB2	1:D:99:ARG:O	2.18	0.42
1:F:123:ARG:CD	1:F:198:VAL:HG22	2.48	0.42
1:C:155:GLU:HB3	1:C:161:TRP:CG	2.54	0.42
1:A:204:TYR:O	1:A:208:PHE:HB2	2.19	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.79	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.85	0.42
1:A:76:LEU:HB3	1:A:130:LEU:HD11	2.00	0.42
1:H:260:THR:H	1:H:263:ASP:HB2	1.84	0.42
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.79	0.42
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.00	0.42
1:H:119:PHE:CG	1:H:120:PRO:HA	2.54	0.42
1:G:227:SER:HB3	1:G:230:GLU:CD	2.39	0.42
1:C:115:ASP:OD2	1:C:117:ARG:NE	2.50	0.42
1:I:225:LEU:HD21	1:J:232:LEU:HD22	2.02	0.42
1:J:21:ASN:ND2	1:J:38:TYR:HE1	2.17	0.42
1:J:260:THR:H	1:J:263:ASP:HB2	1.84	0.42
1:H:279:LEU:HD23	1:H:279:LEU:HA	1.90	0.42
1:H:288:ALA:C	1:H:289:ASN:HD22	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:LEU:HA	1:E:298:GLN:CG	2.48	0.42
1:H:91:ARG:NH2	1:H:103:ASN:OD1	2.52	0.42
1:C:16:VAL:HB	1:C:145:ILE:CG1	2.50	0.42
1:D:224:TRP:CD1	1:D:301:ARG:HD3	2.55	0.42
1:A:137:ASN:OD1	1:A:138:GLN:HG2	2.18	0.42
1:F:240:LEU:HD21	1:J:240:LEU:HD13	2.01	0.42
1:H:182:GLN:H	1:H:183:PRO:HD2	1.84	0.42
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.49	0.42
1:E:136:ASN:HA	1:E:188:PHE:CD2	2.54	0.42
1:E:283:ALA:O	1:E:293:ASP:HA	2.20	0.42
1:J:282:PHE:HD2	1:J:297:ILE:HD13	1.83	0.42
1:J:287:GLN:NE2	1:J:290:GLY:N	2.68	0.42
1:F:248:TYR:HE1	1:G:250:SER:HG	1.63	0.42
1:G:136:ASN:ND2	1:G:185:GLN:HG3	2.35	0.42
1:G:268:ALA:HB1	1:G:308:PHE:HE1	1.84	0.42
1:H:123:ARG:CD	1:H:198:VAL:HG22	2.50	0.42
1:F:311:ILE:HA	1:F:314:VAL:HB	2.01	0.42
1:A:84:SER:HA	1:A:85:PRO:HD3	1.86	0.42
1:J:233:GLN:HA	1:J:236:PHE:CD1	2.54	0.42
1:F:248:TYR:CE1	1:G:246:ALA:HB1	2.54	0.42
1:C:178:LEU:HG	1:C:179:SER:H	1.84	0.42
1:F:24:TYR:CE2	1:F:34:LYS:HD2	2.55	0.42
1:B:291:VAL:O	1:B:291:VAL:HG22	2.20	0.42
1:A:157:ILE:HD11	1:B:115:ASP:CA	2.47	0.42
1:I:208:PHE:O	1:I:245:TYR:OH	2.38	0.42
1:D:155:GLU:CD	1:D:155:GLU:H	2.23	0.42
1:I:118:LEU:CD1	1:I:122:ASP:HA	2.49	0.42
1:A:262:ILE:O	1:A:266:ILE:HG12	2.20	0.42
1:C:227:SER:HB3	1:C:230:GLU:HG3	2.01	0.42
1:I:286:ARG:HD3	1:I:286:ARG:HA	1.80	0.42
1:I:95:PHE:CE2	1:J:181:VAL:CG2	3.02	0.42
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.82	0.42
1:J:82:VAL:HB	1:J:109:SER:CB	2.50	0.42
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.48	0.42
1:F:273:ILE:O	1:F:277:ILE:HG12	2.20	0.42
1:E:117:ARG:O	1:E:260:THR:HA	2.20	0.42
1:E:293:ASP:O	1:E:295:LEU:N	2.53	0.41
1:I:283:ALA:HA	1:I:297:ILE:HD11	2.01	0.41
1:D:223:PHE:HB3	1:D:301:ARG:HG2	2.02	0.41
1:A:40:VAL:HG22	1:A:103:ASN:HD22	1.85	0.41
1:F:227:SER:HB3	1:F:230:GLU:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ILE:HD13	1:J:224:TRP:CZ3	2.55	0.41
1:C:72:TRP:CZ2	1:C:74:PRO:HB3	2.55	0.41
1:B:145:ILE:HD12	1:B:191:ILE:HG21	2.02	0.41
1:A:182:GLN:N	1:A:183:PRO:CD	2.83	0.41
1:H:95:PHE:HE1	1:H:101:ILE:HD12	1.85	0.41
1:I:223:PHE:HE1	1:I:304:PHE:CE2	2.20	0.41
1:B:221:SER:HA	1:B:301:ARG:CZ	2.50	0.41
1:A:40:VAL:HG22	1:A:103:ASN:ND2	2.34	0.41
1:D:137:ASN:OD1	1:D:138:GLN:N	2.53	0.41
1:B:314:VAL:O	1:B:316:VAL:N	2.51	0.41
1:C:166:ALA:HA	1:C:194:ARG:O	2.20	0.41
1:G:306:LEU:O	1:G:310:ALA:N	2.50	0.41
1:J:56:LEU:HD23	1:J:94:LEU:HD12	2.03	0.41
1:F:18:ILE:HB	1:F:147:VAL:HG22	2.01	0.41
1:E:302:LEU:O	1:E:306:LEU:HG	2.19	0.41
1:B:182:GLN:N	1:B:183:PRO:CD	2.83	0.41
1:G:148:TYR:OH	1:H:177:HIS:CE1	2.74	0.41
1:B:184:ASN:O	1:B:186:ASN:N	2.54	0.41
1:H:19:PHE:N	1:H:19:PHE:CD1	2.88	0.41
1:I:19:PHE:O	1:I:37:GLY:HA3	2.20	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
1:J:76:LEU:HB3	1:J:130:LEU:HD11	2.02	0.41
1:F:232:LEU:O	1:F:235:SER:OG	2.38	0.41
1:A:273:ILE:O	1:A:277:ILE:HG12	2.21	0.41
1:F:56:LEU:HD12	1:F:57:ILE:N	2.35	0.41
1:B:46:LYS:HA	1:B:47:PRO:HD3	1.95	0.41
1:C:273:ILE:O	1:C:277:ILE:HG12	2.20	0.41
1:F:123:ARG:NH1	1:F:198:VAL:HG13	2.35	0.41
1:D:91:ARG:NH2	1:D:103:ASN:OD1	2.53	0.41
1:C:303:ALA:O	1:C:306:LEU:HG	2.20	0.41
1:A:145:ILE:HG23	1:A:168:THR:HG21	2.03	0.41
1:I:71:LEU:HD12	1:I:72:TRP:N	2.36	0.41
1:H:132:PRO:HD3	1:H:142:PHE:CE2	2.56	0.41
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.50	0.41
1:F:302:LEU:N	1:F:305:PRO:HD2	2.35	0.41
1:H:230:GLU:OE2	1:I:229:SER:CB	2.67	0.41
1:C:175:TYR:HE1	2:C:401:BR7:H15	1.85	0.41
1:I:120:PRO:HG2	1:I:121:PHE:CE2	2.55	0.41
1:B:123:ARG:C	1:B:124:GLN:HG2	2.40	0.41
1:F:285:HIS:O	1:F:285:HIS:CG	2.74	0.41
1:H:286:ARG:O	1:H:286:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:GLN:N	1:E:183:PRO:CD	2.78	0.41
1:J:289:ASN:OD1	1:J:290:GLY:N	2.44	0.41
1:I:262:ILE:O	1:I:266:ILE:HG12	2.21	0.41
1:I:206:TRP:CD1	1:I:210:LEU:HD12	2.54	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.02	0.41
1:J:79:ILE:HB	1:J:129:GLU:HB2	2.02	0.41
1:G:220:TRP:NE1	1:G:272:SER:OG	2.49	0.41
1:C:28:THR:HG22	1:C:116:PHE:CE1	2.55	0.41
1:F:84:SER:HA	1:F:85:PRO:HD3	1.86	0.41
1:E:291:VAL:HG12	1:E:291:VAL:O	2.20	0.41
1:F:304:PHE:HB3	1:F:305:PRO:HD3	2.03	0.41
1:B:216:ILE:HD12	1:B:269:GLY:HA2	2.01	0.41
1:G:54:LYS:HD2	1:G:54:LYS:H	1.86	0.41
1:C:166:ALA:HB2	1:C:195:ILE:HG12	2.02	0.41
1:H:92:LEU:HD23	1:H:92:LEU:HA	1.85	0.41
1:F:161:TRP:HE3	1:F:163:ARG:HH21	1.66	0.41
1:I:214:LEU:HD12	1:J:270:TYR:HB3	2.02	0.41
1:F:91:ARG:HB3	1:F:103:ASN:HB2	2.03	0.41
1:I:121:PHE:CZ	1:I:205:LEU:HD21	2.55	0.41
1:J:90:LYS:HE3	1:J:91:ARG:N	2.36	0.41
1:G:242:VAL:CG2	1:G:273:ILE:HD11	2.50	0.41
1:H:46:LYS:HA	1:H:47:PRO:HD3	1.95	0.41
1:A:247:SER:HB3	1:E:248:TYR:HB2	2.03	0.41
1:F:130:LEU:HD12	1:F:131:GLU:H	1.86	0.41
1:E:164:GLY:C	1:E:165:LYS:HD2	2.41	0.41
1:A:133:PHE:CD1	1:E:89:ASN:HB2	2.55	0.41
1:F:205:LEU:HD23	1:F:209:ILE:HG13	2.02	0.41
1:H:311:ILE:O	1:H:314:VAL:HB	2.20	0.41
1:C:122:ASP:N	1:C:122:ASP:OD1	2.49	0.41
1:H:212:LEU:O	1:H:216:ILE:HG12	2.21	0.41
1:C:163:ARG:HB3	1:C:163:ARG:HE	1.63	0.41
1:H:185:GLN:OE1	1:H:185:GLN:N	2.54	0.41
1:A:225:LEU:HB2	1:A:231:ARG:HG3	2.03	0.41
1:H:280:ILE:O	1:H:283:ALA:HB3	2.21	0.41
1:E:296:LEU:HA	1:E:296:LEU:HD12	1.91	0.41
1:F:181:VAL:CG2	1:F:182:GLN:N	2.84	0.41
1:D:302:LEU:HA	1:D:305:PRO:HG2	2.03	0.41
1:H:208:PHE:HE2	1:H:248:TYR:CZ	2.39	0.41
1:F:306:LEU:HA	1:F:309:LEU:HB2	2.03	0.41
1:B:289:ASN:OD1	1:B:292:GLU:N	2.54	0.41
1:C:125:GLN:HE22	1:C:194:ARG:HE	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:VAL:HG21	1:H:193:VAL:HG11	2.03	0.41
1:C:208:PHE:HE2	1:C:248:TYR:CZ	2.40	0.40
1:G:157:ILE:HD13	1:H:115:ASP:HA	2.03	0.40
1:B:310:ALA:O	1:B:314:VAL:HG23	2.21	0.40
1:H:145:ILE:HD12	1:H:170:ILE:CD1	2.47	0.40
1:A:287:GLN:HG2	1:A:289:ASN:N	2.32	0.40
1:A:212:LEU:HD11	1:A:265:MET:HB3	2.03	0.40
1:A:178:LEU:HB2	1:A:179:SER:O	2.21	0.40
1:H:163:ARG:HG3	1:H:198:VAL:HG23	2.02	0.40
1:J:145:ILE:HG22	1:J:170:ILE:HD11	2.02	0.40
1:B:241:THR:HA	1:C:240:LEU:HD23	2.02	0.40
1:H:24:TYR:CE2	1:H:34:LYS:HD2	2.56	0.40
1:G:142:PHE:CD2	1:G:191:ILE:HG13	2.56	0.40
1:J:239:MET:O	1:J:243:VAL:HG23	2.21	0.40
1:G:72:TRP:HH2	1:G:140:LEU:HD12	1.87	0.40
1:A:222:VAL:O	1:A:225:LEU:HB2	2.22	0.40
1:F:299:ARG:C	1:F:301:ARG:N	2.74	0.40
1:I:84:SER:HA	1:I:85:PRO:HD3	1.71	0.40
1:C:174:ARG:HA	1:C:186:ASN:O	2.21	0.40
1:J:40:VAL:HG13	1:J:103:ASN:HD21	1.86	0.40
1:F:286:ARG:NE	1:F:294:ASP:OD2	2.55	0.40
1:B:181:VAL:O	1:B:185:GLN:HB2	2.21	0.40
1:J:116:PHE:HD2	1:J:122:ASP:OD2	2.05	0.40
1:D:314:VAL:C	1:D:316:VAL:N	2.75	0.40
1:F:181:VAL:HG13	1:F:182:GLN:NE2	2.35	0.40
1:H:40:VAL:HG12	1:H:42:GLN:NE2	2.37	0.40
1:B:208:PHE:HE1	1:B:248:TYR:CZ	2.40	0.40
1:G:41:ALA:HB3	1:G:102:TYR:HB3	2.04	0.40
1:B:118:LEU:HG	1:B:118:LEU:H	1.76	0.40
1:B:127:VAL:HG22	1:B:194:ARG:HG2	2.03	0.40
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.97	0.40
1:D:293:ASP:O	1:D:295:LEU:HD23	2.22	0.40
1:G:119:PHE:CD1	1:G:120:PRO:HA	2.56	0.40
1:G:60:ASN:OD1	1:G:89:ASN:HB3	2.21	0.40
1:J:123:ARG:NH1	1:J:124:GLN:O	2.54	0.40
1:E:144:ASP:C	1:E:145:ILE:HG13	2.42	0.40
1:B:34:LYS:HE2	1:B:109:SER:OG	2.21	0.40
1:E:204:TYR:HA	1:E:208:PHE:HD1	1.85	0.40
1:C:253:LEU:HG	1:C:254:PRO:HD2	2.03	0.40
1:J:153:ASP:CG	1:J:154:ASN:N	2.74	0.40
1:G:39:ILE:HG21	1:G:39:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASN:ND2	1:C:127:VAL:O	2.40	0.40
1:E:43:TRP:HH2	1:E:73:VAL:HG13	1.86	0.40
1:A:86:ASP:HB3	1:A:107:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	305/307 (99%)	278 (91%)	23 (8%)	4 (1%)	15 59
1	B	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	9 52
1	C	305/307 (99%)	281 (92%)	20 (7%)	4 (1%)	15 59
1	D	305/307 (99%)	273 (90%)	23 (8%)	9 (3%)	5 44
1	E	305/307 (99%)	277 (91%)	26 (8%)	2 (1%)	26 70
1	F	305/307 (99%)	280 (92%)	20 (7%)	5 (2%)	12 56
1	G	305/307 (99%)	280 (92%)	18 (6%)	7 (2%)	8 50
1	H	305/307 (99%)	280 (92%)	19 (6%)	6 (2%)	9 52
1	I	305/307 (99%)	276 (90%)	25 (8%)	4 (1%)	15 59
1	J	305/307 (99%)	279 (92%)	24 (8%)	2 (1%)	26 70
All	All	3050/3070 (99%)	2784 (91%)	217 (7%)	49 (2%)	12 56

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	GLU
1	B	154	ASN
1	B	179	SER
1	B	185	GLN

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Mol	Chain	Res	Type
1	C	152	ALA
1	D	156	GLU
1	D	179	SER
1	D	288	ALA
1	E	179	SER
1	F	181	VAL
1	F	182	GLN
1	F	302	LEU
1	G	295	LEU
1	H	179	SER
1	H	303	ALA
1	I	179	SER
1	A	156	GLU
1	A	180	SER
1	E	182	GLN
1	F	301	ARG
1	G	183	PRO
1	H	304	PHE
1	I	184	ASN
1	J	287	GLN
1	A	166	ALA
1	C	289	ASN
1	D	60	ASN
1	H	166	ALA
1	B	166	ALA
1	C	166	ALA
1	C	182	GLN
1	D	166	ALA
1	F	183	PRO
1	G	292	GLU
1	I	109	SER
1	J	290	GLY
1	B	60	ASN
1	D	182	GLN
1	G	166	ALA
1	H	60	ASN
1	G	60	ASN
1	H	182	GLN
1	I	304	PHE
1	A	304	PHE
1	G	304	PHE
1	G	290	GLY

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Mol	Chain	Res	Type
1	D	183	PRO
1	D	304	PHE
1	D	316	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	274/274 (100%)	260 (95%)	14 (5%)	29	68
1	B	274/274 (100%)	271 (99%)	3 (1%)	80	90
1	C	274/274 (100%)	270 (98%)	4 (2%)	72	89
1	D	274/274 (100%)	264 (96%)	10 (4%)	42	76
1	E	274/274 (100%)	268 (98%)	6 (2%)	60	84
1	F	274/274 (100%)	267 (97%)	7 (3%)	54	81
1	G	274/274 (100%)	266 (97%)	8 (3%)	50	79
1	H	274/274 (100%)	267 (97%)	7 (3%)	54	81
1	I	274/274 (100%)	265 (97%)	9 (3%)	45	77
1	J	274/274 (100%)	264 (96%)	10 (4%)	42	76
All	All	2740/2740 (100%)	2662 (97%)	78 (3%)	51	79

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	21	ASN
1	A	48	ARG
1	A	118	LEU
1	A	137	ASN
1	A	138	GLN
1	A	156	GLU
1	A	167	SER
1	A	178	LEU
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	186	ASN
1	A	187	GLU
1	A	292	GLU
1	A	298	GLN
1	B	296	LEU
1	B	298	GLN
1	B	299	ARG
1	C	54	LYS
1	C	163	ARG
1	C	250	SER
1	C	255	ARG
1	D	29	LEU
1	D	38	TYR
1	D	150	GLU
1	D	156	GLU
1	D	158	ASP
1	D	167	SER
1	D	255	ARG
1	D	286	ARG
1	D	302	LEU
1	D	316	VAL
1	E	29	LEU
1	E	50	THR
1	E	64	GLU
1	E	65	ARG
1	E	174	ARG
1	E	179	SER
1	F	50	THR
1	F	138	GLN
1	F	145	ILE
1	F	233	GLN
1	F	292	GLU
1	F	293	ASP
1	F	302	LEU
1	G	46	LYS
1	G	89	ASN
1	G	233	GLN
1	G	286	ARG
1	G	292	GLU
1	G	295	LEU
1	G	296	LEU
1	G	297	ILE

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Mol	Chain	Res	Type
1	H	42	GLN
1	H	53	ASP
1	H	90	LYS
1	H	177	HIS
1	H	297	ILE
1	H	306	LEU
1	H	309	LEU
1	I	129	GLU
1	I	145	ILE
1	I	157	ILE
1	I	180	SER
1	I	182	GLN
1	I	194	ARG
1	I	230	GLU
1	I	239	MET
1	I	264	GLN
1	J	90	LYS
1	J	102	TYR
1	J	180	SER
1	J	233	GLN
1	J	286	ARG
1	J	291	VAL
1	J	297	ILE
1	J	299	ARG
1	J	301	ARG
1	J	306	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	285	HIS
1	B	62	GLN
1	B	103	ASN
1	B	169	HIS
1	B	184	ASN
1	B	185	GLN
1	B	233	GLN
1	C	103	ASN
1	C	151	ASN
1	C	169	HIS
1	C	177	HIS

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Mol	Chain	Res	Type
1	C	285	HIS
1	C	287	GLN
1	D	62	GLN
1	D	182	GLN
1	D	251	ASN
1	D	287	GLN
1	E	139	GLN
1	E	186	ASN
1	F	151	ASN
1	F	182	GLN
1	F	185	GLN
1	F	186	ASN
1	G	124	GLN
1	G	136	ASN
1	G	182	GLN
1	G	251	ASN
1	G	285	HIS
1	H	42	GLN
1	H	125	GLN
1	H	251	ASN
1	H	289	ASN
1	I	184	ASN
1	I	233	GLN
1	I	264	GLN
1	J	124	GLN
1	J	177	HIS
1	J	185	GLN
1	J	233	GLN
1	J	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	BR7	A	401	-	13,16,16	3.98	9 (69%)	19,30,30	2.38	9 (47%)
2	BR7	A	402	-	13,16,16	4.38	11 (84%)	19,30,30	3.02	7 (36%)
2	BR7	B	401	-	13,16,16	4.22	11 (84%)	19,30,30	2.69	6 (31%)
2	BR7	C	401	-	13,16,16	4.28	11 (84%)	19,30,30	2.41	6 (31%)
2	BR7	D	401	-	13,16,16	4.19	8 (61%)	19,30,30	1.92	5 (26%)
2	BR7	E	401	-	13,16,16	4.06	11 (84%)	19,30,30	2.42	6 (31%)
2	BR7	F	401	-	13,16,16	4.02	8 (61%)	19,30,30	2.05	7 (36%)
2	BR7	F	402	-	13,16,16	4.25	10 (76%)	19,30,30	2.50	8 (42%)
2	BR7	G	401	-	13,16,16	4.18	9 (69%)	19,30,30	2.35	8 (42%)
2	BR7	H	401	-	13,16,16	4.08	9 (69%)	19,30,30	2.04	8 (42%)
2	BR7	I	401	-	13,16,16	4.18	9 (69%)	19,30,30	2.06	6 (31%)
2	BR7	J	401	-	13,16,16	3.98	8 (61%)	19,30,30	2.44	7 (36%)

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	BR7	A	401	-	-	0/0/36/36	0/0/3/3
2	BR7	A	402	-	-	0/0/36/36	0/0/3/3
2	BR7	B	401	-	-	0/0/36/36	0/0/3/3
2	BR7	C	401	-	-	0/0/36/36	0/0/3/3
2	BR7	D	401	-	-	0/0/36/36	0/0/3/3
2	BR7	E	401	-	-	0/0/36/36	0/0/3/3
2	BR7	F	401	-	-	0/0/36/36	0/0/3/3
2	BR7	F	402	-	-	0/0/36/36	0/0/3/3
2	BR7	G	401	-	-	0/0/36/36	0/0/3/3
2	BR7	H	401	-	-	0/0/36/36	0/0/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BR7	I	401	-	-	0/0/36/36	0/0/3/3
2	BR7	J	401	-	-	0/0/36/36	0/0/3/3

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BR7	C09-C10	-12.28	1.37	1.53
2	C	401	BR7	C09-C10	-12.13	1.38	1.53
2	F	402	BR7	C09-C10	-12.10	1.38	1.53
2	I	401	BR7	C09-C10	-12.06	1.38	1.53
2	D	401	BR7	C09-C10	-12.05	1.38	1.53
2	H	401	BR7	C09-C10	-12.00	1.38	1.53
2	G	401	BR7	C09-C10	-11.89	1.38	1.53
2	B	401	BR7	C09-C10	-11.78	1.38	1.53
2	F	401	BR7	C09-C10	-11.70	1.38	1.53
2	A	401	BR7	C09-C10	-11.41	1.38	1.53
2	J	401	BR7	C09-C10	-11.39	1.38	1.53
2	E	401	BR7	C09-C10	-11.24	1.39	1.53
2	J	401	BR7	C11-C02	-4.54	1.47	1.53
2	E	401	BR7	C11-C02	-4.50	1.47	1.53
2	B	401	BR7	C11-C02	-4.48	1.47	1.53
2	D	401	BR7	C03-C02	-4.44	1.47	1.53
2	B	401	BR7	C03-C02	-4.30	1.47	1.53
2	I	401	BR7	C11-C02	-4.27	1.47	1.53
2	G	401	BR7	C11-C02	-4.23	1.48	1.53
2	I	401	BR7	C03-C02	-4.20	1.48	1.53
2	H	401	BR7	C03-C02	-4.13	1.48	1.53
2	C	401	BR7	C03-C02	-4.07	1.48	1.53
2	G	401	BR7	C03-C02	-4.06	1.48	1.53
2	A	401	BR7	C11-C02	-4.05	1.48	1.53
2	C	401	BR7	C11-C02	-4.04	1.48	1.53
2	D	401	BR7	C11-C02	-4.03	1.48	1.53
2	F	401	BR7	C11-C02	-4.02	1.48	1.53
2	A	402	BR7	C11-C02	-3.95	1.48	1.53
2	A	401	BR7	C03-C02	-3.86	1.48	1.53
2	F	402	BR7	C11-C02	-3.85	1.48	1.53
2	E	401	BR7	C03-C02	-3.82	1.48	1.53
2	J	401	BR7	C03-C02	-3.81	1.48	1.53
2	F	402	BR7	C03-C02	-3.79	1.48	1.53
2	F	401	BR7	C03-C02	-3.79	1.48	1.53
2	H	401	BR7	C11-C02	-3.76	1.48	1.53
2	A	402	BR7	C03-C02	-3.55	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BR7	C08-C02	-3.48	1.49	1.53
2	C	401	BR7	C08-C02	-3.41	1.49	1.53
2	A	402	BR7	C-C04	-3.32	1.49	1.53
2	A	402	BR7	C-C10	-3.19	1.49	1.53
2	F	402	BR7	C08-C02	-3.13	1.49	1.53
2	J	401	BR7	C08-C02	-3.06	1.49	1.53
2	F	401	BR7	C08-C02	-3.05	1.49	1.53
2	G	401	BR7	C08-C02	-3.01	1.49	1.53
2	B	401	BR7	C03-C04	-2.98	1.49	1.53
2	F	402	BR7	C-C04	-2.98	1.49	1.53
2	F	402	BR7	C05-C04	-2.96	1.47	1.54
2	C	401	BR7	C03-C04	-2.95	1.49	1.53
2	A	402	BR7	C06-C04	-2.88	1.49	1.53
2	I	401	BR7	C08-C02	-2.87	1.49	1.53
2	D	401	BR7	C08-C02	-2.87	1.49	1.53
2	E	401	BR7	C-C04	-2.86	1.49	1.53
2	A	402	BR7	C05-C04	-2.86	1.48	1.54
2	A	401	BR7	C08-C02	-2.85	1.49	1.53
2	H	401	BR7	C08-C02	-2.80	1.49	1.53
2	D	401	BR7	C03-C04	-2.80	1.49	1.53
2	G	401	BR7	C-C04	-2.76	1.49	1.53
2	G	401	BR7	C03-C04	-2.74	1.50	1.53
2	B	401	BR7	C-C04	-2.73	1.50	1.53
2	E	401	BR7	C08-C02	-2.71	1.50	1.53
2	B	401	BR7	C-C10	-2.71	1.49	1.53
2	C	401	BR7	C06-C04	-2.69	1.50	1.53
2	J	401	BR7	C06-C04	-2.65	1.50	1.53
2	E	401	BR7	C05-C04	-2.63	1.48	1.54
2	B	401	BR7	C08-C02	-2.61	1.50	1.53
2	A	401	BR7	C-C04	-2.57	1.50	1.53
2	F	402	BR7	C06-C04	-2.57	1.50	1.53
2	F	402	BR7	C03-C04	-2.56	1.50	1.53
2	E	401	BR7	C03-C04	-2.52	1.50	1.53
2	F	402	BR7	C-C10	-2.52	1.50	1.53
2	F	401	BR7	C03-C04	-2.52	1.50	1.53
2	I	401	BR7	C06-C04	-2.51	1.50	1.53
2	A	401	BR7	C-C10	-2.51	1.50	1.53
2	I	401	BR7	C05-C04	-2.51	1.48	1.54
2	C	401	BR7	C-C10	-2.50	1.50	1.53
2	D	401	BR7	C01-C02	-2.48	1.48	1.54
2	F	402	BR7	C01-C02	-2.46	1.49	1.54
2	D	401	BR7	C05-C04	-2.45	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	BR7	C05-C04	-2.44	1.49	1.54
2	G	401	BR7	C01-C02	-2.43	1.49	1.54
2	C	401	BR7	C05-C04	-2.43	1.49	1.54
2	I	401	BR7	C01-C02	-2.40	1.49	1.54
2	B	401	BR7	C01-C02	-2.40	1.49	1.54
2	G	401	BR7	C-C10	-2.39	1.50	1.53
2	E	401	BR7	C06-C04	-2.39	1.50	1.53
2	A	401	BR7	C06-C04	-2.38	1.50	1.53
2	H	401	BR7	C05-C04	-2.38	1.49	1.54
2	A	402	BR7	C01-C02	-2.37	1.49	1.54
2	F	401	BR7	C-C04	-2.37	1.50	1.53
2	E	401	BR7	C-C10	-2.34	1.50	1.53
2	A	401	BR7	C05-C04	-2.32	1.49	1.54
2	G	401	BR7	C05-C04	-2.29	1.49	1.54
2	B	401	BR7	C11-C10	-2.29	1.50	1.53
2	A	402	BR7	C03-C04	-2.29	1.50	1.53
2	H	401	BR7	C-C04	-2.27	1.50	1.53
2	I	401	BR7	C-C04	-2.27	1.50	1.53
2	E	401	BR7	C11-C10	-2.23	1.50	1.53
2	B	401	BR7	C05-C04	-2.23	1.49	1.54
2	C	401	BR7	C01-C02	-2.21	1.49	1.54
2	F	401	BR7	C01-C02	-2.20	1.49	1.54
2	H	401	BR7	C03-C04	-2.19	1.50	1.53
2	H	401	BR7	C06-C04	-2.18	1.50	1.53
2	F	401	BR7	C05-C04	-2.16	1.49	1.54
2	C	401	BR7	C11-C10	-2.16	1.50	1.53
2	I	401	BR7	C03-C04	-2.16	1.50	1.53
2	H	401	BR7	C01-C02	-2.15	1.49	1.54
2	B	401	BR7	C06-C04	-2.15	1.50	1.53
2	E	401	BR7	C01-C02	-2.15	1.49	1.54
2	A	402	BR7	C11-C10	-2.12	1.50	1.53
2	C	401	BR7	C-C04	-2.11	1.50	1.53
2	A	401	BR7	C01-C02	-2.09	1.49	1.54
2	D	401	BR7	C-C04	-2.08	1.50	1.53
2	J	401	BR7	C01-C02	-2.07	1.49	1.54
2	J	401	BR7	C-C04	-2.05	1.50	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	BR7	BR-C10-C	-7.82	101.75	108.42
2	B	401	BR7	C-C04-C03	-6.50	100.99	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	BR7	C-C04-C03	-5.63	102.07	109.06
2	E	401	BR7	C-C04-C03	-5.58	102.13	109.06
2	F	402	BR7	BR-C10-C	-4.36	104.70	108.42
2	A	402	BR7	C-C04-C03	-4.10	103.97	109.06
2	J	401	BR7	C-C04-C03	-3.78	104.37	109.06
2	I	401	BR7	C-C04-C03	-3.73	104.42	109.06
2	F	401	BR7	C-C04-C03	-3.67	104.50	109.06
2	A	401	BR7	C-C04-C03	-3.65	104.52	109.06
2	G	401	BR7	C-C04-C03	-3.60	104.58	109.06
2	A	401	BR7	BR-C10-C	-3.56	105.39	108.42
2	F	402	BR7	C-C04-C03	-3.50	104.71	109.06
2	H	401	BR7	C-C04-C03	-3.50	104.72	109.06
2	D	401	BR7	C-C04-C03	-3.42	104.81	109.06
2	H	401	BR7	C06-C04-C	-3.27	104.99	109.06
2	J	401	BR7	C03-C02-C11	-3.18	105.11	109.06
2	I	401	BR7	C06-C04-C	-2.93	105.42	109.06
2	F	401	BR7	C06-C04-C	-2.90	105.46	109.06
2	G	401	BR7	C06-C04-C	-2.89	105.47	109.06
2	D	401	BR7	C06-C04-C	-2.83	105.55	109.06
2	J	401	BR7	C06-C04-C	-2.79	105.59	109.06
2	F	402	BR7	C06-C04-C	-2.74	105.65	109.06
2	A	401	BR7	C03-C02-C11	-2.66	105.76	109.06
2	I	401	BR7	C08-C02-C11	-2.60	105.83	109.06
2	G	401	BR7	C08-C02-C11	-2.59	105.84	109.06
2	A	401	BR7	C06-C04-C	-2.51	105.94	109.06
2	G	401	BR7	C03-C02-C11	-2.43	106.04	109.06
2	B	401	BR7	C06-C04-C	-2.39	106.09	109.06
2	F	402	BR7	C08-C02-C11	-2.36	106.13	109.06
2	C	401	BR7	C06-C04-C	-2.35	106.14	109.06
2	A	402	BR7	C08-C02-C11	-2.32	106.18	109.06
2	F	401	BR7	C03-C02-C11	-2.18	106.35	109.06
2	H	401	BR7	C03-C02-C11	-2.18	106.35	109.06
2	E	401	BR7	C01-C02-C11	-2.17	107.30	110.69
2	H	401	BR7	C08-C02-C11	-2.15	106.39	109.06
2	F	401	BR7	C08-C02-C11	-2.14	106.40	109.06
2	J	401	BR7	C08-C02-C11	-2.14	106.40	109.06
2	E	401	BR7	C08-C02-C11	-2.13	106.42	109.06
2	A	401	BR7	C08-C02-C11	-2.09	106.46	109.06
2	C	401	BR7	C03-C02-C11	-2.08	106.48	109.06
2	B	401	BR7	BR-C10-C	-2.04	106.68	108.42
2	A	402	BR7	C03-C02-C08	2.12	111.69	109.06
2	G	401	BR7	C05-C04-C06	2.26	114.22	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	BR7	BR-C10-C09	2.42	110.49	108.42
2	A	401	BR7	BR-C10-C11	2.46	110.52	108.42
2	A	401	BR7	C03-C02-C08	2.55	112.22	109.06
2	A	402	BR7	BR-C10-C11	2.60	110.64	108.42
2	B	401	BR7	C03-C02-C08	2.65	112.35	109.06
2	E	401	BR7	C03-C02-C08	2.67	112.38	109.06
2	J	401	BR7	C03-C02-C08	2.69	112.39	109.06
2	F	401	BR7	C06-C04-C03	2.74	112.47	109.06
2	D	401	BR7	BR-C10-C09	2.75	110.77	108.42
2	I	401	BR7	C03-C02-C08	2.81	112.55	109.06
2	G	401	BR7	C06-C04-C03	2.88	112.63	109.06
2	H	401	BR7	C03-C02-C08	2.94	112.70	109.06
2	C	401	BR7	C03-C02-C08	3.05	112.85	109.06
2	F	401	BR7	C03-C02-C08	3.37	113.25	109.06
2	A	401	BR7	C06-C04-C03	3.41	113.29	109.06
2	F	402	BR7	C03-C02-C08	3.42	113.31	109.06
2	D	401	BR7	C03-C02-C08	3.53	113.44	109.06
2	A	402	BR7	C06-C04-C03	3.58	113.50	109.06
2	H	401	BR7	C06-C04-C03	3.70	113.65	109.06
2	D	401	BR7	C06-C04-C03	3.71	113.66	109.06
2	F	402	BR7	BR-C10-C11	3.80	111.66	108.42
2	F	402	BR7	C06-C04-C03	3.80	113.78	109.06
2	H	401	BR7	BR-C10-C11	3.82	111.68	108.42
2	I	401	BR7	C06-C04-C03	3.95	113.97	109.06
2	E	401	BR7	C06-C04-C03	3.97	113.99	109.06
2	J	401	BR7	C06-C04-C03	4.10	114.15	109.06
2	G	401	BR7	C03-C02-C08	4.11	114.16	109.06
2	I	401	BR7	BR-C10-C09	4.20	112.01	108.42
2	C	401	BR7	C06-C04-C03	4.46	114.59	109.06
2	F	401	BR7	BR-C10-C09	4.46	112.23	108.42
2	B	401	BR7	C06-C04-C03	4.99	115.25	109.06
2	F	402	BR7	BR-C10-C09	5.16	112.83	108.42
2	C	401	BR7	BR-C10-C09	5.33	112.97	108.42
2	G	401	BR7	BR-C10-C09	5.83	113.40	108.42
2	A	401	BR7	BR-C10-C09	5.99	113.54	108.42
2	B	401	BR7	BR-C10-C09	6.06	113.59	108.42
2	J	401	BR7	BR-C10-C09	6.25	113.76	108.42
2	E	401	BR7	BR-C10-C09	6.33	113.83	108.42
2	A	402	BR7	BR-C10-C09	7.30	114.65	108.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	BR7	2	0
2	B	401	BR7	4	0
2	C	401	BR7	5	0
2	E	401	BR7	2	0
2	F	402	BR7	1	0
2	G	401	BR7	3	0
2	I	401	BR7	1	0
2	J	401	BR7	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/307 (100%)	-0.17	9 (2%) 55 42	89, 136, 232, 324	0
1	B	307/307 (100%)	-0.10	12 (3%) 43 32	78, 123, 237, 352	0
1	C	307/307 (100%)	-0.24	18 (5%) 26 17	71, 119, 234, 291	0
1	D	307/307 (100%)	-0.10	11 (3%) 46 35	73, 121, 228, 325	0
1	E	307/307 (100%)	-0.23	10 (3%) 50 38	83, 129, 235, 381	0
1	F	307/307 (100%)	-0.18	8 (2%) 59 47	84, 138, 250, 372	0
1	G	307/307 (100%)	-0.15	6 (1%) 68 57	78, 122, 221, 324	0
1	H	307/307 (100%)	-0.08	27 (8%) 12 8	79, 133, 250, 378	0
1	I	307/307 (100%)	-0.23	10 (3%) 50 38	76, 131, 234, 327	0
1	J	307/307 (100%)	-0.19	20 (6%) 22 14	91, 139, 272, 347	0
All	All	3070/3070 (100%)	-0.17	131 (4%) 39 28	71, 129, 243, 381	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ASP	10.2
1	E	290	GLY	10.1
1	I	179	SER	8.8
1	I	180	SER	8.6
1	A	177	HIS	7.8
1	J	290	GLY	6.8
1	C	313	CYS	6.3
1	C	180	SER	5.8
1	H	180	SER	5.6
1	J	306	LEU	5.3
1	J	305	PRO	5.3
1	J	291	VAL	4.8
1	D	177	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	289	ASN	4.7
1	F	287	GLN	4.7
1	E	291	VAL	4.4
1	J	286	ARG	4.3
1	E	287	GLN	4.2
1	F	288	ALA	4.2
1	E	288	ALA	4.1
1	F	176	ASP	4.1
1	E	289	ASN	4.0
1	F	317	ILE	4.0
1	H	306	LEU	3.9
1	J	180	SER	3.9
1	F	179	SER	3.9
1	H	137	ASN	3.9
1	A	178	LEU	3.8
1	C	314	VAL	3.8
1	I	291	VAL	3.8
1	I	289	ASN	3.8
1	J	304	PHE	3.7
1	J	287	GLN	3.7
1	F	174	ARG	3.7
1	G	156	GLU	3.7
1	C	317	ILE	3.6
1	G	285	HIS	3.6
1	D	179	SER	3.5
1	E	180	SER	3.5
1	I	181	VAL	3.5
1	C	146	GLN	3.5
1	A	182	GLN	3.4
1	C	187	GLU	3.4
1	C	306	LEU	3.4
1	A	175	TYR	3.4
1	D	180	SER	3.4
1	I	288	ALA	3.4
1	F	175	TYR	3.4
1	J	303	ALA	3.3
1	B	291	VAL	3.3
1	H	123	ARG	3.2
1	B	31	GLN	3.2
1	C	172	ASP	3.2
1	B	293	ASP	3.1
1	J	285	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	308	PHE	3.1
1	H	181	VAL	3.1
1	C	315	LEU	3.0
1	H	179	SER	3.0
1	H	303	ALA	3.0
1	J	284	HIS	3.0
1	C	316	VAL	3.0
1	H	184	ASN	3.0
1	D	202	SER	3.0
1	C	311	ILE	2.9
1	B	122	ASP	2.9
1	B	289	ASN	2.9
1	B	290	GLY	2.8
1	D	176	ASP	2.8
1	B	112	ASN	2.8
1	J	179	SER	2.8
1	H	11	PRO	2.8
1	I	290	GLY	2.8
1	H	182	GLN	2.8
1	J	302	LEU	2.6
1	B	298	GLN	2.6
1	H	140	LEU	2.6
1	H	317	ILE	2.6
1	D	288	ALA	2.6
1	C	312	GLY	2.6
1	J	288	ALA	2.6
1	B	114	MET	2.6
1	B	115	ASP	2.5
1	E	52	GLY	2.5
1	G	314	VAL	2.5
1	I	286	ARG	2.5
1	A	306	LEU	2.5
1	H	185	GLN	2.5
1	H	307	GLY	2.5
1	H	187	GLU	2.5
1	H	141	ARG	2.5
1	C	309	LEU	2.4
1	J	294	ASP	2.4
1	J	82	VAL	2.4
1	A	189	SER	2.4
1	B	71	LEU	2.4
1	J	83	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	302	LEU	2.3
1	E	292	GLU	2.3
1	C	310	ALA	2.3
1	J	293	ASP	2.3
1	D	293	ASP	2.3
1	H	183	PRO	2.3
1	G	289	ASN	2.3
1	H	172	ASP	2.3
1	D	19	PHE	2.3
1	E	179	SER	2.2
1	G	157	ILE	2.2
1	H	138	GLN	2.2
1	C	307	GLY	2.2
1	J	292	GLU	2.2
1	H	143	SER	2.2
1	H	304	PHE	2.2
1	C	188	PHE	2.2
1	A	316	VAL	2.2
1	D	38	TYR	2.2
1	H	13	ASP	2.2
1	I	292	GLU	2.1
1	D	289	ASN	2.1
1	H	144	ASP	2.1
1	I	182	GLN	2.1
1	H	170	ILE	2.1
1	H	315	LEU	2.1
1	C	189	SER	2.1
1	A	180	SER	2.1
1	F	289	ASN	2.1
1	B	42	GLN	2.1
1	D	181	VAL	2.1
1	H	311	ILE	2.0
1	C	137	ASN	2.0
1	E	286	ARG	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	BR7	G	401	14/14	0.98	0.41	1.89	77,115,131,268	0
2	BR7	E	401	14/14	0.96	0.61	1.50	84,110,120,309	0
2	BR7	H	401	14/14	0.96	0.41	1.45	129,141,153,250	0
2	BR7	J	401	14/14	0.96	0.48	1.34	98,112,125,194	0
2	BR7	C	401	14/14	0.95	0.46	1.26	111,127,145,217	0
2	BR7	D	401	14/14	0.98	0.38	1.02	98,111,119,277	0
2	BR7	F	401	14/14	0.94	0.42	0.98	99,129,135,272	0
2	BR7	A	401	14/14	0.94	0.43	0.68	112,142,147,354	0
2	BR7	A	402	14/14	0.97	0.27	0.62	98,109,129,224	0
2	BR7	F	402	14/14	0.94	0.24	-0.13	110,131,138,389	0
2	BR7	B	401	14/14	0.96	0.17	-0.26	104,108,119,265	0
2	BR7	I	401	14/14	0.97	0.15	-0.78	86,100,119,321	0

6.5 Other polymers [i](#)

There are no such residues in this entry.