



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:52 am BST

PDB ID : 3UQ4
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) mutant F247L (F16L)
Authors : Gonzalez-Gutierrez, G.; Lukk, T.; Agarwal, V.; Papke, D.; Nair, S.K.; Grosman, C.
Deposited on : 2011-11-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

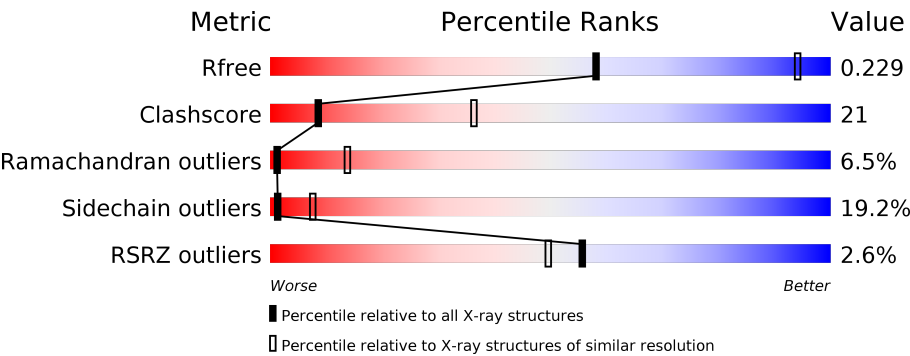
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	324	<div><div>2%</div><div><div></div><div>45%</div><div>37%</div><div>11%</div><div>• 5%</div></div></div>
1	B	324	<div><div>2%</div><div><div></div><div>44%</div><div>37%</div><div>12%</div><div>• 5%</div></div></div>
1	C	324	<div><div>2%</div><div><div></div><div>47%</div><div>36%</div><div>10%</div><div>• 5%</div></div></div>
1	D	324	<div><div>2%</div><div><div></div><div>46%</div><div>36%</div><div>11%</div><div>• 5%</div></div></div>
1	E	324	<div><div>3%</div><div><div></div><div>44%</div><div>39%</div><div>10%</div><div>• 5%</div></div></div>
1	F	324	<div><div>2%</div><div><div></div><div>45%</div><div>36%</div><div>13%</div><div>• 5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	324	
1	H	324	
1	I	324	
1	J	324	

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	NA	A	323	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25022 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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
A	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
A	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
B	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
B	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
B	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
C	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
C	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
C	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
D	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
D	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
E	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
E	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
E	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
F	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
F	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
F	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
G	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
G	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
G	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
H	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
H	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
H	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
I	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
I	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
I	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4
J	-1	GLY	-	EXPRESSION TAG	UNP E0SJQ4
J	0	SER	-	EXPRESSION TAG	UNP E0SJQ4
J	247	LEU	PHE	ENGINEERED MUTATION	UNP E0SJQ4

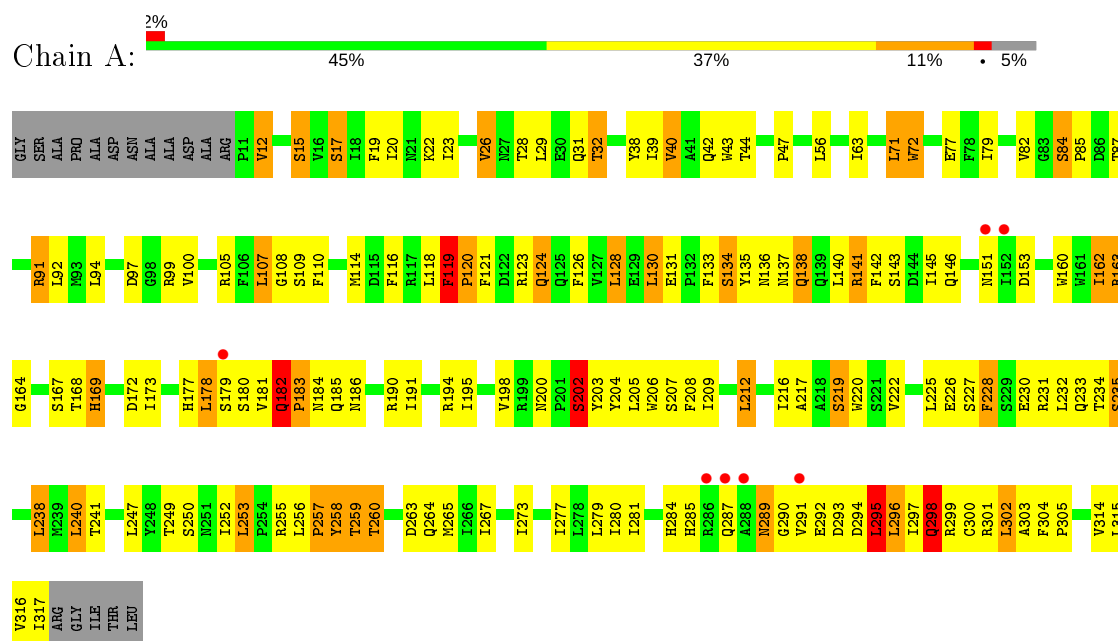
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

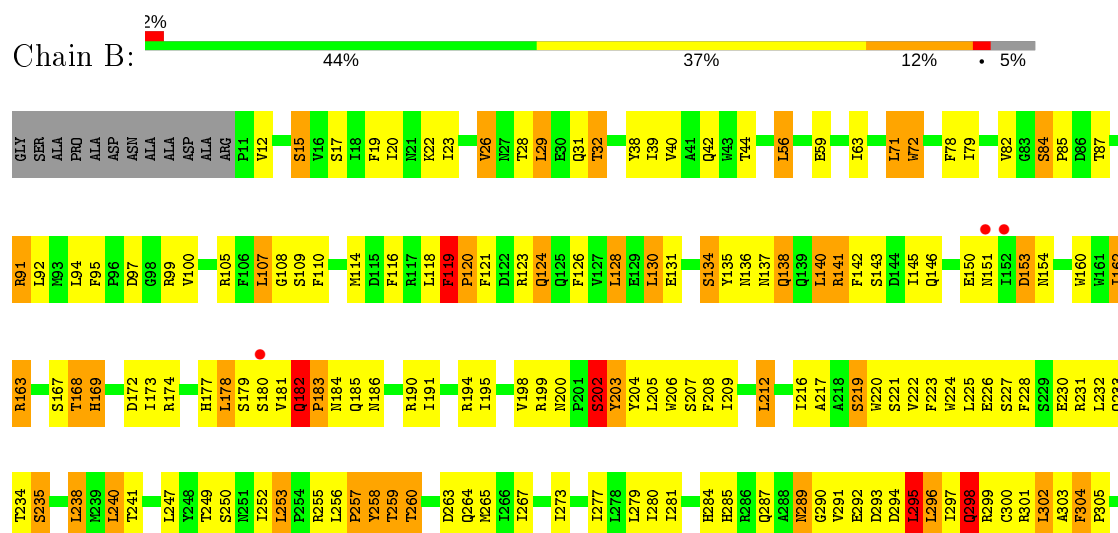
3 Residue-property plots

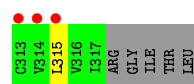
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

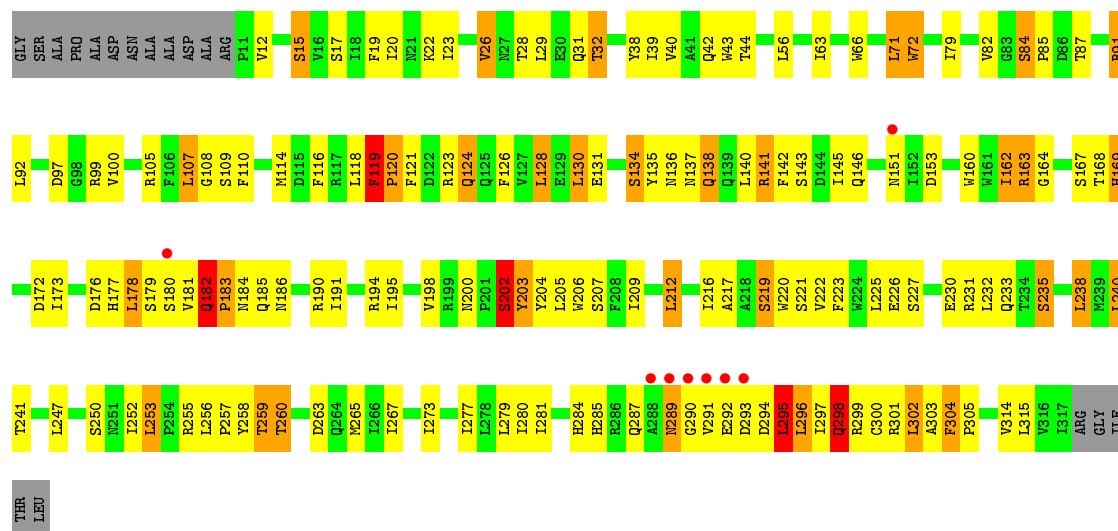


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

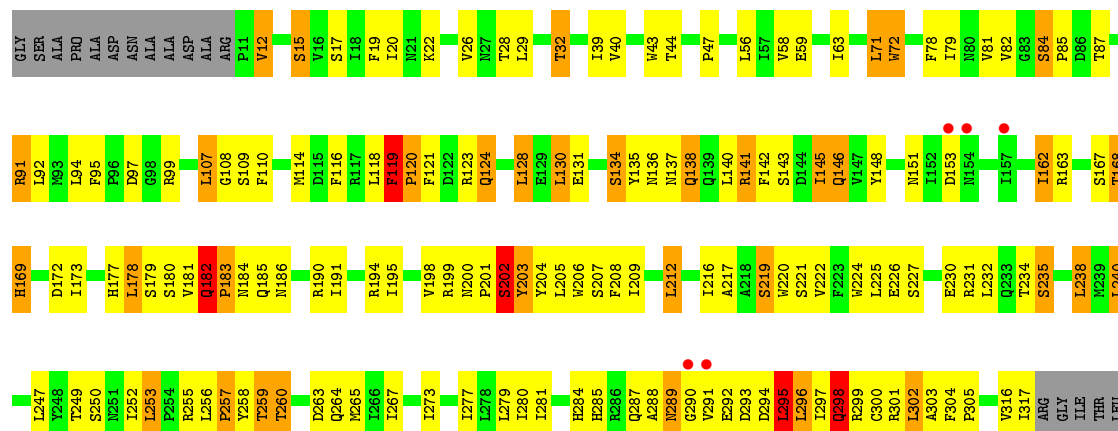




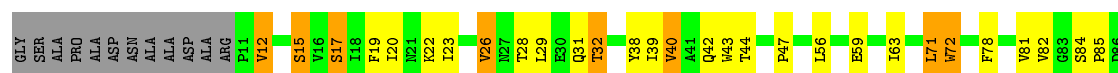
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

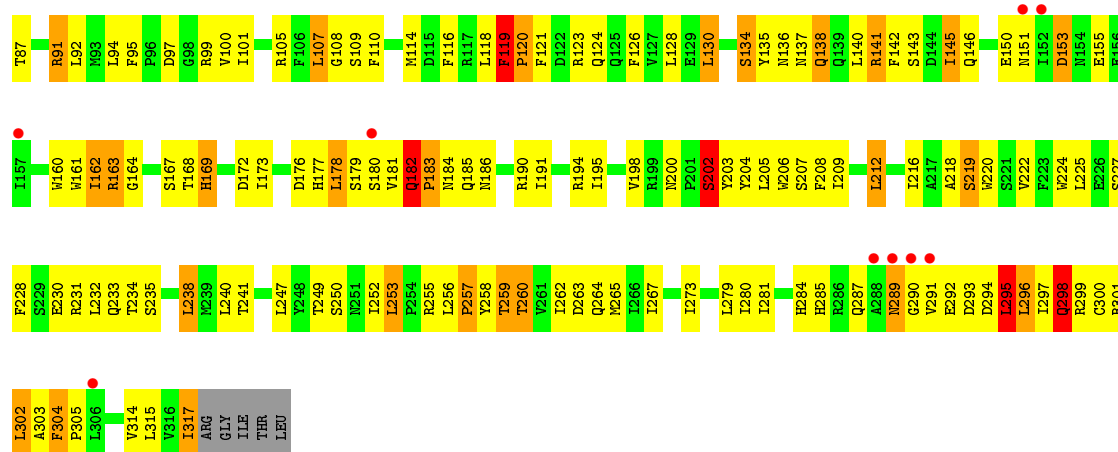


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

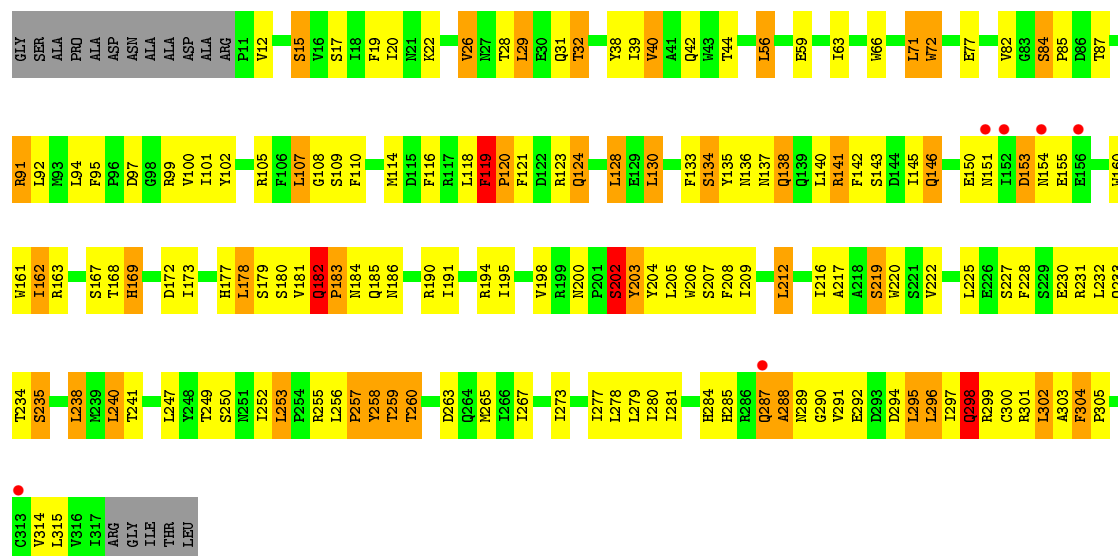
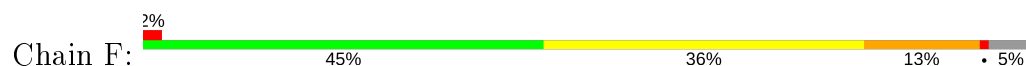


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

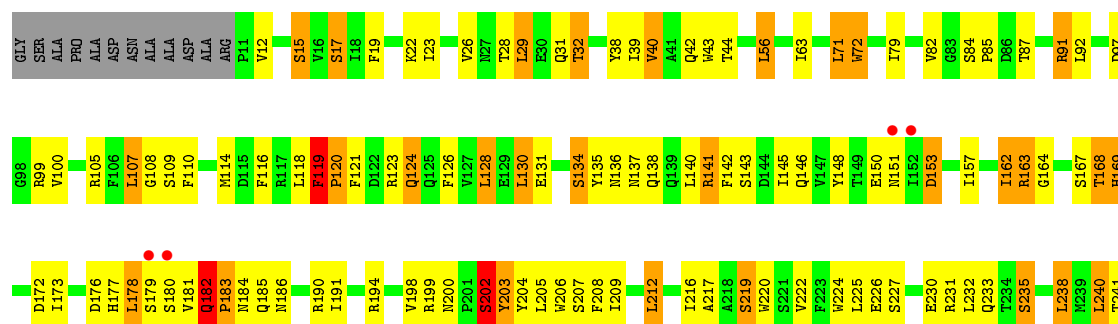


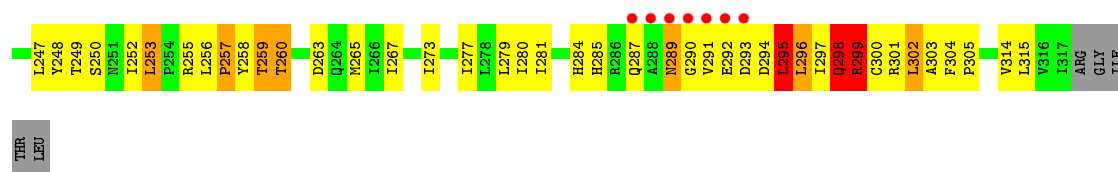


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

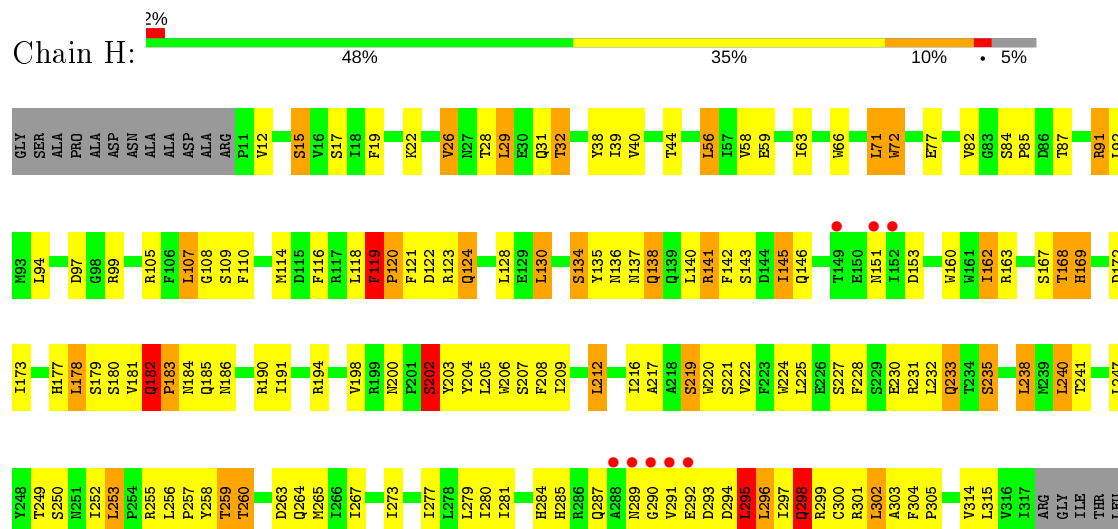


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

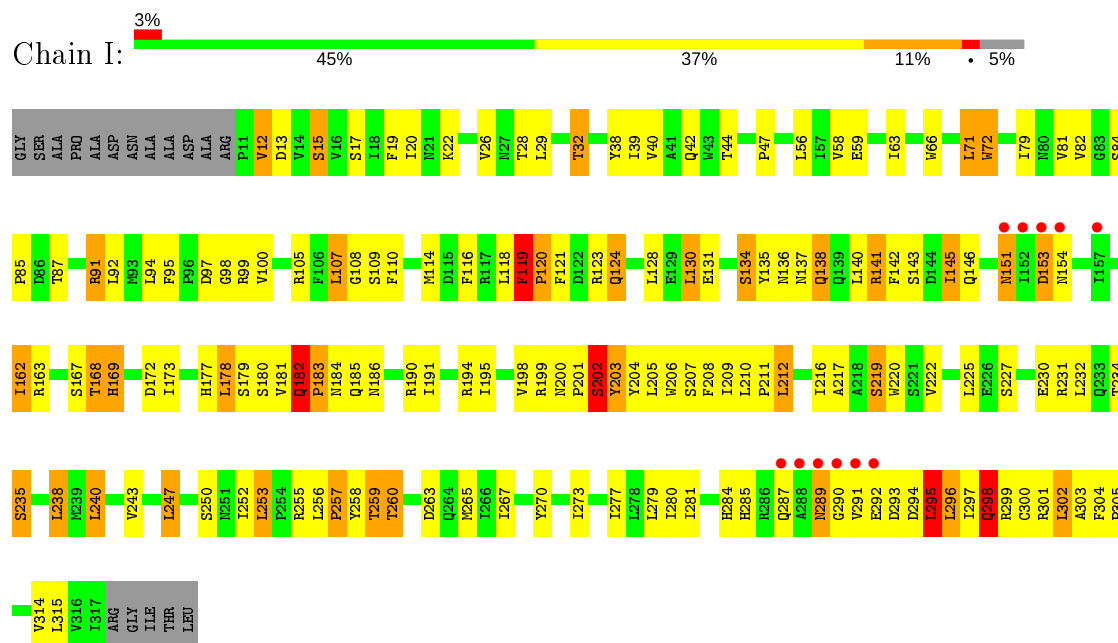




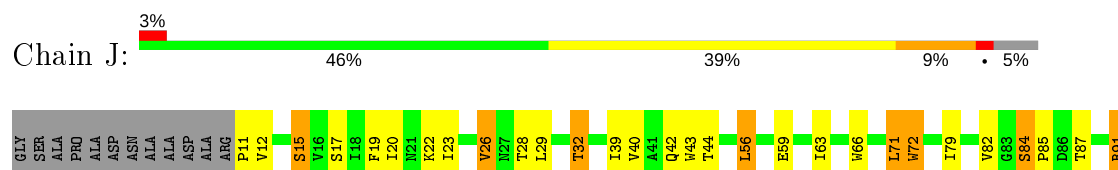
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 266.94Å 110.84Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	19.93 – 3.50 19.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-3.50) 99.8 (19.93-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.52Å)	Xtriage
Refinement program	PHENIX dev_897, REFMAC	Depositor
R, R_{free}	0.215 , 0.239 0.204 , 0.229	Depositor DCC
R_{free} test set	3594 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25022	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: NA

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	0.69	0/2569	0.85	2/3502 (0.1%)
1	B	0.70	0/2569	0.87	2/3502 (0.1%)
1	C	0.70	0/2569	0.84	1/3502 (0.0%)
1	D	0.73	0/2569	0.88	2/3502 (0.1%)
1	E	0.73	0/2569	0.85	2/3502 (0.1%)
1	F	0.69	0/2569	0.85	1/3502 (0.0%)
1	G	0.73	0/2569	1.02	4/3502 (0.1%)
1	H	0.71	1/2569 (0.0%)	0.85	2/3502 (0.1%)
1	I	0.71	0/2569	0.87	2/3502 (0.1%)
1	J	0.70	0/2569	0.85	1/3502 (0.0%)
All	All	0.71	1/25690 (0.0%)	0.87	19/35020 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
All	All	0	30

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	233	GLN	CG-CD	5.49	1.63	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	299	ARG	NE-CZ-NH1	-22.37	109.12	120.30
1	G	299	ARG	NE-CZ-NH2	21.64	131.12	120.30
1	G	299	ARG	CD-NE-CZ	10.27	137.97	123.60
1	J	119	PHE	C-N-CD	-9.47	99.76	120.60
1	D	119	PHE	C-N-CD	-9.39	99.95	120.60
1	E	119	PHE	C-N-CD	-9.30	100.15	120.60
1	B	119	PHE	C-N-CD	-9.27	100.20	120.60
1	H	119	PHE	C-N-CD	-9.16	100.44	120.60
1	F	119	PHE	C-N-CD	-9.13	100.50	120.60
1	I	119	PHE	C-N-CD	-8.83	101.17	120.60
1	C	119	PHE	C-N-CD	-8.73	101.38	120.60
1	A	119	PHE	C-N-CD	-8.58	101.72	120.60
1	G	119	PHE	C-N-CD	-8.30	102.35	120.60
1	E	12	VAL	CB-CA-C	-6.08	99.85	111.40
1	D	12	VAL	CB-CA-C	-5.71	100.55	111.40
1	B	140	LEU	CB-CG-CD2	5.27	119.96	111.00
1	H	145	ILE	CB-CA-C	-5.16	101.28	111.60
1	A	12	VAL	CB-CA-C	-5.12	101.67	111.40
1	I	12	VAL	CB-CA-C	-5.07	101.77	111.40

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PHE	Peptide
1	A	137	ASN	Peptide
1	A	298	GLN	Peptide
1	B	119	PHE	Peptide
1	B	137	ASN	Peptide
1	B	298	GLN	Peptide
1	C	119	PHE	Peptide
1	C	137	ASN	Peptide
1	C	298	GLN	Peptide
1	D	119	PHE	Peptide
1	D	137	ASN	Peptide
1	D	298	GLN	Peptide
1	E	119	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	137	ASN	Peptide
1	E	298	GLN	Peptide
1	F	119	PHE	Peptide
1	F	137	ASN	Peptide
1	F	298	GLN	Peptide
1	G	119	PHE	Peptide
1	G	137	ASN	Peptide
1	G	298	GLN	Peptide
1	H	119	PHE	Peptide
1	H	137	ASN	Peptide
1	H	298	GLN	Peptide
1	I	119	PHE	Peptide
1	I	137	ASN	Peptide
1	I	298	GLN	Peptide
1	J	119	PHE	Peptide
1	J	137	ASN	Peptide
1	J	298	GLN	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	2502	0	2480	108	0
1	B	2502	0	2480	120	0
1	C	2502	0	2480	104	0
1	D	2502	0	2480	110	0
1	E	2502	0	2480	112	0
1	F	2502	0	2480	115	0
1	G	2502	0	2480	112	0
1	H	2502	0	2480	111	0
1	I	2502	0	2480	113	0
1	J	2502	0	2480	104	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0
All	All	25022	0	24800	1031	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 21.

All (1031) 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:I:300:CYS:HA	1:I:303:ALA:HB3	1.53	0.91
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.54	0.89
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.54	0.89
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.55	0.88
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.56	0.87
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.57	0.86
1:B:300:CYS:HA	1:B:303:ALA:HB3	1.58	0.86
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.56	0.85
1:B:174:ARG:NH1	1:I:13:ASP:OD1	2.09	0.85
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.58	0.85
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.56	0.85
1:C:205:LEU:HD23	1:C:209:ILE:HG13	1.58	0.85
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.58	0.85
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.58	0.84
1:G:300:CYS:HA	1:G:303:ALA:HB3	1.56	0.84
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.59	0.83
1:F:300:CYS:HA	1:F:303:ALA:HB3	1.59	0.83
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.61	0.83
1:H:91:ARG:HD3	1:I:134:SER:HB3	1.59	0.83
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.61	0.83
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.60	0.82
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.60	0.82
1:C:91:ARG:HD3	1:D:134:SER:HB3	1.61	0.82
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.62	0.81
1:I:91:ARG:HD3	1:J:134:SER:HB3	1.61	0.81
1:G:247:LEU:HB3	1:H:247:LEU:HD11	1.65	0.79
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.63	0.78
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.65	0.78
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.66	0.77
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.67	0.76
1:D:294:ASP:O	1:D:296:LEU:N	2.18	0.75
1:B:174:ARG:NH2	1:I:13:ASP:OD2	2.15	0.75
1:A:134:SER:HB3	1:E:91:ARG:HD3	1.67	0.75
1:A:247:LEU:HD11	1:E:247:LEU:HB3	1.68	0.74
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.69	0.74
1:A:178:LEU:HD11	1:A:186:ASN:HB3	1.70	0.74
1:F:91:ARG:HD3	1:G:134:SER:HB3	1.70	0.73
1:F:247:LEU:HD11	1:J:247:LEU:HB3	1.69	0.73
1:E:168:THR:HG22	1:E:169:HIS:H	1.53	0.73
1:B:294:ASP:O	1:B:296:LEU:N	2.18	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ASP:O	1:E:296:LEU:N	2.18	0.72
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.71	0.72
1:C:212:LEU:HD12	1:C:265:MET:HB3	1.72	0.72
1:I:212:LEU:HD12	1:I:265:MET:HB3	1.71	0.72
1:A:91:ARG:HD3	1:B:134:SER:HB3	1.72	0.72
1:F:178:LEU:HD11	1:F:186:ASN:HB3	1.72	0.72
1:G:202:SER:OG	1:G:203:TYR:N	2.20	0.72
1:B:91:ARG:HD3	1:C:134:SER:HB3	1.71	0.71
1:C:294:ASP:O	1:C:296:LEU:N	2.20	0.71
1:D:212:LEU:HD12	1:D:265:MET:HB3	1.70	0.71
1:I:294:ASP:O	1:I:296:LEU:N	2.19	0.71
1:D:178:LEU:HD11	1:D:186:ASN:HB3	1.73	0.71
1:F:168:THR:HG22	1:F:169:HIS:H	1.54	0.71
1:G:178:LEU:HD11	1:G:186:ASN:HB3	1.71	0.71
1:H:294:ASP:O	1:H:296:LEU:N	2.17	0.71
1:B:163:ARG:HG3	1:I:151:ASN:HD22	1.56	0.71
1:J:178:LEU:HD11	1:J:186:ASN:HB3	1.73	0.71
1:J:294:ASP:O	1:J:296:LEU:N	2.19	0.71
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.71	0.70
1:E:123:ARG:HG2	1:E:198:VAL:HG22	1.72	0.70
1:E:178:LEU:HD11	1:E:186:ASN:HB3	1.73	0.70
1:H:182:GLN:H	1:H:183:PRO:HD2	1.56	0.70
1:F:294:ASP:O	1:F:296:LEU:N	2.19	0.70
1:C:178:LEU:HD11	1:C:186:ASN:HB3	1.73	0.70
1:H:212:LEU:HD12	1:H:265:MET:HB3	1.74	0.70
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.73	0.70
1:B:169:HIS:ND1	1:I:168:THR:HB	2.06	0.70
1:B:178:LEU:HD11	1:B:186:ASN:HB3	1.73	0.70
1:J:182:GLN:H	1:J:183:PRO:HD2	1.57	0.70
1:E:182:GLN:H	1:E:183:PRO:HD2	1.56	0.70
1:H:178:LEU:HD11	1:H:186:ASN:HB3	1.73	0.70
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.74	0.69
1:C:182:GLN:H	1:C:183:PRO:HD2	1.56	0.69
1:G:212:LEU:HD12	1:G:265:MET:HB3	1.73	0.69
1:F:134:SER:HB3	1:J:91:ARG:HD3	1.73	0.69
1:A:182:GLN:H	1:A:183:PRO:HD2	1.57	0.69
1:I:178:LEU:HD11	1:I:186:ASN:HB3	1.74	0.69
1:E:212:LEU:HD12	1:E:265:MET:HB3	1.74	0.69
1:B:182:GLN:H	1:B:183:PRO:HD2	1.57	0.69
1:F:182:GLN:H	1:F:183:PRO:HD2	1.58	0.69
1:G:91:ARG:HD3	1:H:134:SER:HB3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:LEU:HD12	1:J:265:MET:HB3	1.74	0.69
1:D:259:THR:HG22	1:D:263:ASP:HB3	1.74	0.69
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.74	0.69
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.73	0.69
1:D:316:VAL:HG23	1:D:317:ILE:HG12	1.74	0.69
1:D:182:GLN:H	1:D:183:PRO:HD2	1.57	0.68
1:E:302:LEU:HD12	1:E:305:PRO:HG2	1.75	0.68
1:J:182:GLN:O	1:J:184:ASN:N	2.25	0.68
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.75	0.68
1:G:182:GLN:H	1:G:183:PRO:HD2	1.57	0.68
1:A:123:ARG:HG2	1:A:198:VAL:HG22	1.75	0.68
1:I:182:GLN:H	1:I:183:PRO:HD2	1.59	0.68
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.77	0.67
1:I:259:THR:HG22	1:I:263:ASP:HB3	1.76	0.67
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.75	0.67
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.76	0.67
1:F:212:LEU:HD12	1:F:265:MET:HB3	1.75	0.67
1:H:39:ILE:HD11	1:H:130:LEU:HD11	1.75	0.67
1:B:202:SER:OG	1:B:203:TYR:N	2.25	0.67
1:G:168:THR:HG22	1:G:169:HIS:H	1.58	0.67
1:D:119:PHE:C	1:D:121:PHE:H	1.98	0.67
1:F:63:ILE:HD11	1:F:91:ARG:HA	1.77	0.66
1:A:294:ASP:O	1:A:296:LEU:N	2.19	0.66
1:A:202:SER:OG	1:A:203:TYR:N	2.29	0.66
1:I:99:ARG:HH21	1:J:180:SER:HB3	1.59	0.66
1:C:168:THR:HG22	1:C:169:HIS:H	1.59	0.66
1:H:168:THR:HG22	1:H:169:HIS:H	1.60	0.66
1:A:212:LEU:HD12	1:A:265:MET:HB3	1.78	0.66
1:F:202:SER:OG	1:F:203:TYR:N	2.28	0.65
1:C:39:ILE:HD11	1:C:130:LEU:HD11	1.78	0.65
1:E:212:LEU:O	1:E:216:ILE:HG12	1.95	0.65
1:A:180:SER:HB3	1:E:99:ARG:HH21	1.61	0.65
1:J:168:THR:HG22	1:J:169:HIS:H	1.60	0.65
1:F:182:GLN:O	1:F:184:ASN:N	2.28	0.65
1:A:168:THR:HG22	1:A:169:HIS:H	1.62	0.65
1:A:28:THR:HB	1:A:256:LEU:HD21	1.79	0.65
1:B:247:LEU:HB3	1:C:247:LEU:HD11	1.79	0.65
1:F:247:LEU:HB3	1:G:247:LEU:HD11	1.78	0.65
1:H:123:ARG:HG2	1:H:198:VAL:HG22	1.77	0.65
1:I:39:ILE:HD11	1:I:130:LEU:HD11	1.78	0.65
1:D:202:SER:OG	1:D:203:TYR:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ILE:HD11	1:F:130:LEU:HD11	1.79	0.65
1:G:168:THR:O	1:G:169:HIS:HB2	1.97	0.65
1:C:182:GLN:O	1:C:184:ASN:N	2.28	0.64
1:A:298:GLN:N	1:A:298:GLN:OE1	2.30	0.64
1:E:289:ASN:HD21	1:E:292:GLU:HB2	1.62	0.64
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.79	0.64
1:G:123:ARG:HG2	1:G:198:VAL:HG22	1.79	0.64
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.80	0.64
1:I:119:PHE:C	1:I:121:PHE:H	2.00	0.64
1:I:162:ILE:H	1:I:162:ILE:HD13	1.61	0.64
1:J:259:THR:HG22	1:J:263:ASP:HB3	1.79	0.64
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.79	0.64
1:D:302:LEU:HD12	1:D:305:PRO:HG2	1.79	0.64
1:C:202:SER:OG	1:C:203:TYR:N	2.29	0.64
1:B:168:THR:O	1:B:169:HIS:HB2	1.98	0.63
1:G:39:ILE:HD11	1:G:130:LEU:HD11	1.80	0.63
1:G:182:GLN:O	1:G:184:ASN:N	2.31	0.63
1:H:28:THR:HB	1:H:256:LEU:HD21	1.78	0.63
1:D:226:GLU:OE2	1:E:284:HIS:NE2	2.31	0.63
1:G:173:ILE:HD13	1:G:190:ARG:HB3	1.79	0.63
1:J:302:LEU:HD12	1:J:305:PRO:HG2	1.80	0.63
1:B:168:THR:HG22	1:B:169:HIS:H	1.62	0.63
1:D:182:GLN:O	1:D:184:ASN:N	2.30	0.63
1:E:202:SER:OG	1:E:203:TYR:N	2.29	0.63
1:E:39:ILE:HD11	1:E:130:LEU:HD11	1.79	0.63
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.81	0.63
1:I:182:GLN:O	1:I:184:ASN:N	2.31	0.63
1:D:289:ASN:HD21	1:D:292:GLU:HB2	1.63	0.63
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.81	0.63
1:A:182:GLN:O	1:A:184:ASN:N	2.28	0.62
1:B:298:GLN:N	1:B:298:GLN:OE1	2.32	0.62
1:C:119:PHE:C	1:C:121:PHE:H	2.02	0.62
1:C:289:ASN:HD21	1:C:292:GLU:HB2	1.64	0.62
1:D:91:ARG:HD3	1:E:134:SER:HB3	1.79	0.62
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.80	0.62
1:H:202:SER:OG	1:H:203:TYR:N	2.26	0.62
1:D:298:GLN:OE1	1:D:298:GLN:N	2.32	0.62
1:F:28:THR:HB	1:F:256:LEU:HD21	1.80	0.62
1:H:298:GLN:N	1:H:298:GLN:OE1	2.32	0.62
1:A:212:LEU:O	1:A:216:ILE:HG12	2.00	0.62
1:C:63:ILE:HD11	1:C:91:ARG:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:THR:HA	1:I:99:ARG:HA	1.81	0.62
1:B:259:THR:HG22	1:B:263:ASP:HB3	1.81	0.62
1:C:136:ASN:N	1:C:136:ASN:OD1	2.31	0.62
1:C:44:THR:HA	1:C:99:ARG:HA	1.81	0.62
1:F:123:ARG:HG2	1:F:198:VAL:HG22	1.82	0.62
1:F:289:ASN:HD21	1:F:292:GLU:HB2	1.65	0.62
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.82	0.62
1:C:162:ILE:H	1:C:162:ILE:HD13	1.65	0.62
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.82	0.62
1:H:252:ILE:HG22	1:H:253:LEU:HD13	1.82	0.62
1:A:39:ILE:HD11	1:A:130:LEU:HD11	1.82	0.61
1:H:259:THR:HG22	1:H:263:ASP:HB3	1.80	0.61
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.81	0.61
1:H:182:GLN:O	1:H:184:ASN:N	2.27	0.61
1:G:294:ASP:O	1:G:296:LEU:N	2.24	0.61
1:B:289:ASN:HD21	1:B:292:GLU:HB2	1.66	0.61
1:D:168:THR:HG22	1:D:169:HIS:H	1.65	0.61
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.80	0.61
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.64	0.61
1:D:123:ARG:HG2	1:D:198:VAL:HG22	1.83	0.61
1:J:298:GLN:N	1:J:298:GLN:OE1	2.34	0.61
1:G:162:ILE:HD13	1:G:162:ILE:H	1.65	0.61
1:J:162:ILE:H	1:J:162:ILE:HD13	1.66	0.61
1:A:63:ILE:HD11	1:A:91:ARG:HA	1.83	0.61
1:E:259:THR:HG22	1:E:263:ASP:HB3	1.81	0.61
1:H:119:PHE:C	1:H:121:PHE:H	2.04	0.61
1:H:44:THR:HA	1:H:99:ARG:HA	1.83	0.61
1:I:63:ILE:HD11	1:I:91:ARG:HA	1.82	0.61
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.83	0.61
1:D:162:ILE:HD13	1:D:162:ILE:H	1.65	0.61
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.82	0.61
1:H:212:LEU:O	1:H:216:ILE:HG12	2.00	0.61
1:B:212:LEU:O	1:B:216:ILE:HG12	2.00	0.61
1:D:227:SER:HB3	1:D:230:GLU:HB2	1.83	0.61
1:G:259:THR:HG22	1:G:263:ASP:HB3	1.83	0.61
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.83	0.60
1:F:252:ILE:HG22	1:F:253:LEU:HD13	1.83	0.60
1:A:302:LEU:HD12	1:A:305:PRO:HG2	1.82	0.60
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.83	0.60
1:G:302:LEU:HD12	1:G:305:PRO:HG2	1.84	0.60
1:A:162:ILE:H	1:A:162:ILE:HD13	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:THR:HA	1:E:99:ARG:HA	1.83	0.60
1:G:119:PHE:C	1:G:121:PHE:H	2.04	0.60
1:E:28:THR:HB	1:E:256:LEU:HD21	1.82	0.60
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.83	0.60
1:F:259:THR:HG22	1:F:263:ASP:HB3	1.82	0.60
1:G:298:GLN:N	1:G:298:GLN:OE1	2.35	0.60
1:D:28:THR:HB	1:D:256:LEU:HD21	1.83	0.60
1:E:119:PHE:C	1:E:121:PHE:H	2.05	0.60
1:B:119:PHE:C	1:B:121:PHE:H	2.06	0.60
1:E:298:GLN:OE1	1:E:298:GLN:N	2.34	0.60
1:F:302:LEU:HD12	1:F:305:PRO:HG2	1.83	0.60
1:F:180:SER:HB3	1:J:99:ARG:HH21	1.67	0.60
1:F:162:ILE:HD13	1:F:162:ILE:H	1.67	0.59
1:H:107:LEU:HD12	1:H:108:GLY:N	2.17	0.59
1:B:28:THR:HB	1:B:256:LEU:HD21	1.84	0.59
1:B:44:THR:HA	1:B:99:ARG:HA	1.84	0.59
1:D:136:ASN:OD1	1:D:136:ASN:N	2.35	0.59
1:I:79:ILE:HD11	1:I:131:GLU:HB3	1.84	0.59
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.83	0.59
1:E:182:GLN:O	1:E:184:ASN:N	2.30	0.59
1:B:169:HIS:CG	1:I:168:THR:HB	2.37	0.59
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.84	0.59
1:I:107:LEU:HD12	1:I:108:GLY:N	2.17	0.59
1:C:259:THR:HG22	1:C:263:ASP:HB3	1.83	0.59
1:A:119:PHE:C	1:A:121:PHE:H	2.05	0.59
1:C:302:LEU:HD12	1:C:305:PRO:HG2	1.84	0.59
1:E:181:VAL:HG21	1:E:185:GLN:HB2	1.85	0.59
1:H:63:ILE:HD11	1:H:91:ARG:HA	1.84	0.59
1:I:289:ASN:HD21	1:I:292:GLU:HB2	1.68	0.59
1:I:302:LEU:HD12	1:I:305:PRO:HG2	1.85	0.59
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.20	0.59
1:B:162:ILE:HD13	1:B:162:ILE:H	1.66	0.59
1:A:259:THR:HG22	1:A:263:ASP:HB3	1.83	0.58
1:J:260:THR:HG23	1:J:263:ASP:OD2	2.03	0.58
1:I:28:THR:HB	1:I:256:LEU:HD21	1.84	0.58
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.38	0.58
1:B:226:GLU:OE2	1:C:284:HIS:NE2	2.36	0.58
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.85	0.58
1:B:302:LEU:HD12	1:B:305:PRO:HG2	1.86	0.58
1:I:225:LEU:HB2	1:I:231:ARG:HG3	1.85	0.58
1:A:44:THR:HA	1:A:99:ARG:HA	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:O	1:B:184:ASN:N	2.33	0.58
1:C:298:GLN:N	1:C:298:GLN:OE1	2.36	0.58
1:F:298:GLN:OE1	1:F:298:GLN:N	2.36	0.58
1:G:141:ARG:HG2	1:G:142:PHE:CD2	2.38	0.58
1:J:212:LEU:O	1:J:216:ILE:HG12	2.02	0.58
1:J:289:ASN:HD21	1:J:292:GLU:HB2	1.69	0.58
1:A:227:SER:HB3	1:A:230:GLU:HB2	1.85	0.58
1:A:226:GLU:OE2	1:B:284:HIS:NE2	2.33	0.58
1:C:141:ARG:HG2	1:C:142:PHE:CD2	2.39	0.58
1:I:298:GLN:N	1:I:298:GLN:OE1	2.36	0.58
1:F:44:THR:HA	1:F:99:ARG:HA	1.84	0.58
1:C:79:ILE:HD11	1:C:131:GLU:HB3	1.85	0.58
1:J:63:ILE:HD11	1:J:91:ARG:HA	1.86	0.58
1:B:263:ASP:O	1:B:267:ILE:HG13	2.04	0.57
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.68	0.57
1:G:226:GLU:OE2	1:H:284:HIS:NE2	2.37	0.57
1:E:162:ILE:HD13	1:E:162:ILE:H	1.69	0.57
1:I:123:ARG:HG2	1:I:198:VAL:HG22	1.85	0.57
1:G:212:LEU:O	1:G:216:ILE:HG12	2.05	0.57
1:H:260:THR:HG23	1:H:263:ASP:OD2	2.04	0.57
1:J:44:THR:HA	1:J:99:ARG:HA	1.85	0.57
1:D:44:THR:HA	1:D:99:ARG:HA	1.86	0.57
1:H:136:ASN:OD1	1:H:136:ASN:N	2.38	0.57
1:G:44:THR:HA	1:G:99:ARG:HA	1.85	0.57
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.40	0.57
1:J:298:GLN:O	1:J:301:ARG:HG3	2.05	0.57
1:A:141:ARG:HG2	1:A:142:PHE:CD2	2.40	0.57
1:H:289:ASN:HD21	1:H:292:GLU:HB2	1.69	0.57
1:F:240:LEU:HD23	1:J:241:THR:HA	1.87	0.57
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.84	0.56
1:H:143:SER:HB3	1:H:168:THR:HG21	1.87	0.56
1:A:225:LEU:HB2	1:A:231:ARG:HG3	1.87	0.56
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.35	0.56
1:B:63:ILE:HD11	1:B:91:ARG:HA	1.87	0.56
1:D:247:LEU:HB3	1:E:247:LEU:HD11	1.88	0.56
1:F:99:ARG:HH21	1:G:180:SER:HB3	1.71	0.56
1:A:181:VAL:HG21	1:A:185:GLN:HB2	1.87	0.56
1:D:63:ILE:HD11	1:D:91:ARG:HA	1.87	0.56
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.87	0.56
1:F:141:ARG:HG2	1:F:142:PHE:CD2	2.41	0.56
1:G:181:VAL:HG21	1:G:185:GLN:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:THR:HB	1:G:256:LEU:HD21	1.87	0.56
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.88	0.56
1:H:247:LEU:HB3	1:I:247:LEU:HD11	1.87	0.56
1:B:123:ARG:HG2	1:B:198:VAL:HG22	1.87	0.56
1:B:141:ARG:HG2	1:B:142:PHE:CD2	2.40	0.56
1:B:28:THR:HA	1:B:116:PHE:CE1	2.41	0.56
1:H:181:VAL:HG21	1:H:185:GLN:HB2	1.88	0.56
1:J:141:ARG:HG2	1:J:142:PHE:CD2	2.40	0.56
1:A:107:LEU:HD12	1:A:108:GLY:N	2.21	0.56
1:B:143:SER:HB3	1:B:168:THR:HG21	1.87	0.56
1:C:107:LEU:HD12	1:C:108:GLY:N	2.21	0.56
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.24	0.56
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.88	0.56
1:C:238:LEU:HB3	1:C:273:ILE:HD13	1.86	0.55
1:D:212:LEU:O	1:D:216:ILE:HG12	2.06	0.55
1:B:204:TYR:O	1:B:209:ILE:HG12	2.07	0.55
1:I:72:TRP:HZ3	1:I:135:TYR:CZ	2.24	0.55
1:I:212:LEU:O	1:I:216:ILE:HG12	2.05	0.55
1:J:181:VAL:HG21	1:J:185:GLN:HB2	1.88	0.55
1:G:63:ILE:HD11	1:G:91:ARG:HA	1.89	0.55
1:E:141:ARG:HG2	1:E:142:PHE:CD2	2.41	0.55
1:C:28:THR:HB	1:C:256:LEU:HD21	1.89	0.55
1:F:28:THR:HA	1:F:116:PHE:CE1	2.42	0.55
1:I:202:SER:OG	1:I:203:TYR:N	2.39	0.55
1:A:252:ILE:HG22	1:A:253:LEU:HD13	1.89	0.55
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.41	0.55
1:I:252:ILE:HG22	1:I:253:LEU:HD13	1.89	0.55
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.42	0.55
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.23	0.55
1:A:263:ASP:O	1:A:267:ILE:HG13	2.06	0.55
1:C:247:LEU:HB3	1:D:247:LEU:HD11	1.88	0.55
1:H:227:SER:HB3	1:H:230:GLU:HB2	1.88	0.55
1:I:181:VAL:HG21	1:I:185:GLN:HB2	1.89	0.55
1:G:63:ILE:HG12	1:G:92:LEU:HG	1.88	0.54
1:H:302:LEU:HD12	1:H:305:PRO:HG2	1.89	0.54
1:C:38:TYR:CE2	1:C:105:ARG:HD3	2.43	0.54
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.90	0.54
1:F:72:TRP:HZ3	1:F:135:TYR:CZ	2.26	0.54
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.89	0.54
1:E:107:LEU:HD12	1:E:108:GLY:N	2.23	0.54
1:E:136:ASN:N	1:E:136:ASN:OD1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASP:O	1:D:267:ILE:HG13	2.08	0.54
1:J:119:PHE:C	1:J:121:PHE:H	2.10	0.54
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.90	0.54
1:J:28:THR:HB	1:J:256:LEU:HD21	1.88	0.54
1:J:63:ILE:HG12	1:J:92:LEU:HG	1.90	0.54
1:C:297:ILE:O	1:C:300:CYS:N	2.41	0.54
1:H:162:ILE:H	1:H:162:ILE:HD13	1.73	0.54
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.42	0.54
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.88	0.54
1:D:141:ARG:HG2	1:D:142:PHE:CD2	2.43	0.54
1:D:216:ILE:O	1:D:219:SER:HB3	2.08	0.54
1:D:260:THR:HG23	1:D:263:ASP:OD2	2.08	0.54
1:E:143:SER:HB3	1:E:168:THR:HG21	1.90	0.54
1:F:181:VAL:HG21	1:F:185:GLN:HB2	1.89	0.54
1:G:204:TYR:O	1:G:209:ILE:HG12	2.07	0.54
1:B:63:ILE:HG12	1:B:92:LEU:HG	1.90	0.54
1:E:238:LEU:HB3	1:E:273:ILE:HD13	1.90	0.54
1:G:241:THR:HA	1:H:240:LEU:HD23	1.89	0.54
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.26	0.53
1:D:247:LEU:HD13	1:E:247:LEU:HD11	1.89	0.53
1:H:225:LEU:HB2	1:H:231:ARG:HG3	1.89	0.53
1:J:136:ASN:OD1	1:J:136:ASN:N	2.41	0.53
1:B:181:VAL:HG21	1:B:185:GLN:HB2	1.90	0.53
1:G:136:ASN:N	1:G:136:ASN:OD1	2.41	0.53
1:B:136:ASN:OD1	1:B:136:ASN:N	2.40	0.53
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.38	0.53
1:I:141:ARG:HG2	1:I:142:PHE:CD2	2.43	0.53
1:D:234:THR:HG21	1:E:233:GLN:HG2	1.90	0.53
1:F:212:LEU:O	1:F:216:ILE:HG12	2.09	0.53
1:D:107:LEU:HD12	1:D:108:GLY:N	2.22	0.53
1:A:247:LEU:HB3	1:B:247:LEU:HD11	1.89	0.53
1:D:28:THR:HA	1:D:116:PHE:CE1	2.44	0.53
1:G:235:SER:HB2	1:G:277:ILE:HD11	1.91	0.53
1:H:255:ARG:O	1:H:256:LEU:HD23	2.09	0.53
1:I:168:THR:HG22	1:I:169:HIS:H	1.73	0.53
1:D:79:ILE:HD11	1:D:131:GLU:HB3	1.91	0.52
1:I:143:SER:HB3	1:I:168:THR:HG21	1.91	0.52
1:J:28:THR:HA	1:J:116:PHE:CE1	2.43	0.52
1:C:212:LEU:O	1:C:216:ILE:HG12	2.08	0.52
1:C:297:ILE:O	1:C:299:ARG:N	2.42	0.52
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:202:SER:OG	1:J:203:TYR:N	2.40	0.52
1:C:114:MET:HE2	1:C:124:GLN:HG2	1.91	0.52
1:C:72:TRP:O	1:C:72:TRP:CD1	2.63	0.52
1:H:216:ILE:O	1:H:219:SER:HB3	2.10	0.52
1:H:97:ASP:OD1	1:H:99:ARG:NH1	2.42	0.52
1:I:247:LEU:HB3	1:J:247:LEU:HD11	1.91	0.52
1:F:119:PHE:C	1:F:121:PHE:H	2.12	0.52
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.44	0.52
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.27	0.52
1:E:297:ILE:O	1:E:300:CYS:N	2.42	0.52
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.45	0.52
1:G:227:SER:HB3	1:G:230:GLU:HB2	1.92	0.52
1:H:141:ARG:HG2	1:H:142:PHE:CD2	2.44	0.52
1:I:81:VAL:HG21	1:I:85:PRO:HG3	1.92	0.52
1:F:168:THR:O	1:F:169:HIS:HB2	2.10	0.52
1:G:72:TRP:HZ3	1:G:135:TYR:CZ	2.27	0.52
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.90	0.52
1:I:298:GLN:O	1:I:301:ARG:HG3	2.09	0.52
1:G:32:THR:HA	1:G:110:PHE:O	2.10	0.52
1:I:234:THR:HG21	1:J:233:GLN:HG2	1.92	0.52
1:E:263:ASP:O	1:E:267:ILE:HG13	2.10	0.52
1:I:97:ASP:OD1	1:I:99:ARG:NH1	2.43	0.52
1:C:241:THR:OG1	1:D:240:LEU:HD23	2.10	0.51
1:I:227:SER:HB3	1:I:230:GLU:HB2	1.92	0.51
1:J:107:LEU:HD12	1:J:108:GLY:N	2.25	0.51
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.45	0.51
1:D:298:GLN:O	1:D:301:ARG:HG3	2.10	0.51
1:F:238:LEU:HB3	1:F:273:ILE:HD13	1.92	0.51
1:H:204:TYR:O	1:H:209:ILE:HG12	2.10	0.51
1:A:143:SER:HB3	1:A:168:THR:HG21	1.92	0.51
1:A:162:ILE:CD1	1:A:162:ILE:H	2.23	0.51
1:B:163:ARG:HG3	1:I:151:ASN:ND2	2.25	0.51
1:C:162:ILE:H	1:C:162:ILE:CD1	2.23	0.51
1:D:140:LEU:HD22	1:D:191:ILE:HD11	1.92	0.51
1:G:263:ASP:O	1:G:267:ILE:HG13	2.10	0.51
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.10	0.51
1:A:136:ASN:OD1	1:A:136:ASN:N	2.41	0.51
1:G:238:LEU:HB3	1:G:273:ILE:HD13	1.92	0.51
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.28	0.51
1:A:20:ILE:HD12	1:A:195:ILE:HD11	1.93	0.51
1:A:260:THR:HG23	1:A:263:ASP:OD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ILE:H	1:G:162:ILE:CD1	2.24	0.51
1:H:28:THR:HA	1:H:116:PHE:CE1	2.46	0.51
1:F:216:ILE:O	1:F:219:SER:HB3	2.11	0.51
1:B:227:SER:HB3	1:B:230:GLU:HB2	1.92	0.51
1:A:114:MET:HE2	1:A:124:GLN:HG2	1.93	0.51
1:G:72:TRP:CD1	1:G:72:TRP:O	2.64	0.51
1:C:168:THR:O	1:C:169:HIS:HB2	2.10	0.51
1:D:162:ILE:CD1	1:D:162:ILE:H	2.24	0.51
1:D:238:LEU:HB3	1:D:273:ILE:HD13	1.92	0.51
1:E:297:ILE:O	1:E:299:ARG:N	2.44	0.51
1:I:238:LEU:HB3	1:I:273:ILE:HD13	1.93	0.51
1:C:252:ILE:HG22	1:C:253:LEU:HD13	1.92	0.50
1:C:260:THR:HG23	1:C:263:ASP:OD2	2.11	0.50
1:F:143:SER:HB3	1:F:168:THR:HG21	1.93	0.50
1:H:284:HIS:HD2	1:H:285:HIS:CE1	2.28	0.50
1:E:28:THR:HA	1:E:116:PHE:CE1	2.46	0.50
1:A:235:SER:HB2	1:A:277:ILE:HD11	1.93	0.50
1:A:284:HIS:HD2	1:A:285:HIS:CE1	2.28	0.50
1:A:297:ILE:O	1:A:299:ARG:N	2.44	0.50
1:B:32:THR:HA	1:B:110:PHE:O	2.11	0.50
1:B:298:GLN:O	1:B:301:ARG:HG3	2.12	0.50
1:H:72:TRP:HZ3	1:H:135:TYR:CZ	2.29	0.50
1:I:294:ASP:C	1:I:296:LEU:H	2.12	0.50
1:J:97:ASP:OD1	1:J:99:ARG:NH1	2.44	0.50
1:D:78:PHE:O	1:D:81:VAL:HG12	2.12	0.50
1:E:204:TYR:O	1:E:209:ILE:HG12	2.12	0.50
1:I:71:LEU:HD22	1:I:72:TRP:O	2.11	0.50
1:C:28:THR:HA	1:C:116:PHE:CE1	2.47	0.50
1:F:263:ASP:O	1:F:267:ILE:HG13	2.12	0.50
1:I:204:TYR:O	1:I:209:ILE:HG12	2.12	0.50
1:I:28:THR:HA	1:I:116:PHE:CE1	2.46	0.50
1:I:72:TRP:CD1	1:I:72:TRP:C	2.85	0.50
1:D:181:VAL:HG21	1:D:185:GLN:HB2	1.93	0.50
1:G:114:MET:HE2	1:G:124:GLN:HG2	1.94	0.50
1:I:297:ILE:O	1:I:299:ARG:N	2.45	0.50
1:F:255:ARG:O	1:F:256:LEU:HD23	2.11	0.50
1:D:204:TYR:O	1:D:209:ILE:HG12	2.12	0.50
1:A:42:GLN:HA	1:A:100:VAL:O	2.12	0.49
1:D:99:ARG:HH21	1:E:180:SER:HB3	1.77	0.49
1:E:63:ILE:HD11	1:E:91:ARG:HA	1.94	0.49
1:F:297:ILE:O	1:F:300:CYS:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:293:ASP:HB3	1:J:295:LEU:HD13	1.94	0.49
1:D:143:SER:HB3	1:D:168:THR:HG21	1.93	0.49
1:E:71:LEU:HD22	1:E:72:TRP:O	2.12	0.49
1:G:230:GLU:HG2	1:H:233:GLN:OE1	2.12	0.49
1:H:235:SER:HB2	1:H:277:ILE:HD11	1.94	0.49
1:H:72:TRP:CD1	1:H:72:TRP:O	2.65	0.49
1:J:168:THR:O	1:J:169:HIS:HB2	2.13	0.49
1:C:227:SER:HB3	1:C:230:GLU:HB2	1.94	0.49
1:E:31:GLN:HG2	1:E:114:MET:HB2	1.93	0.49
1:H:297:ILE:O	1:H:299:ARG:N	2.45	0.49
1:J:252:ILE:HG22	1:J:253:LEU:HD13	1.94	0.49
1:C:181:VAL:HG21	1:C:185:GLN:HB2	1.94	0.49
1:D:235:SER:HB2	1:D:277:ILE:HD11	1.93	0.49
1:G:297:ILE:O	1:G:300:CYS:N	2.46	0.49
1:I:255:ARG:O	1:I:256:LEU:HD23	2.13	0.49
1:J:227:SER:HB3	1:J:230:GLU:HB2	1.94	0.49
1:J:72:TRP:CD1	1:J:72:TRP:O	2.64	0.49
1:D:284:HIS:HD2	1:D:285:HIS:CE1	2.30	0.49
1:D:297:ILE:O	1:D:300:CYS:N	2.45	0.49
1:E:227:SER:HB3	1:E:230:GLU:HB2	1.95	0.49
1:F:298:GLN:O	1:F:301:ARG:HG3	2.13	0.49
1:H:212:LEU:HB3	1:H:265:MET:HE1	1.95	0.49
1:J:204:TYR:O	1:J:209:ILE:HG12	2.11	0.49
1:J:235:SER:HB2	1:J:277:ILE:HD11	1.93	0.49
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.94	0.49
1:D:63:ILE:HG12	1:D:92:LEU:HG	1.95	0.49
1:F:136:ASN:N	1:F:136:ASN:OD1	2.44	0.49
1:I:72:TRP:CD1	1:I:72:TRP:O	2.66	0.49
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.48	0.49
1:D:293:ASP:HB3	1:D:295:LEU:HD13	1.94	0.49
1:F:217:ALA:HA	1:F:220:TRP:CE3	2.47	0.49
1:G:293:ASP:HB3	1:G:295:LEU:HD13	1.95	0.49
1:I:136:ASN:N	1:I:136:ASN:OD1	2.46	0.49
1:B:72:TRP:CZ3	1:B:135:TYR:CZ	3.00	0.49
1:E:26:VAL:HG21	1:E:160:TRP:HE1	1.78	0.49
1:F:162:ILE:CD1	1:F:162:ILE:H	2.25	0.49
1:F:227:SER:HB3	1:F:230:GLU:HB2	1.94	0.49
1:F:260:THR:HG23	1:F:263:ASP:OD2	2.13	0.49
1:I:297:ILE:O	1:I:300:CYS:N	2.46	0.49
1:J:220:TRP:C	1:J:222:VAL:H	2.16	0.49
1:B:260:THR:HG23	1:B:263:ASP:OD2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:TYR:CE2	1:I:105:ARG:HD3	2.48	0.49
1:I:32:THR:HA	1:I:110:PHE:O	2.13	0.49
1:A:297:ILE:O	1:A:300:CYS:N	2.46	0.48
1:C:263:ASP:O	1:C:267:ILE:HG13	2.12	0.48
1:F:66:TRP:O	1:F:71:LEU:HB2	2.13	0.48
1:C:32:THR:HA	1:C:110:PHE:O	2.12	0.48
1:H:135:TYR:CB	1:H:138:GLN:HG2	2.43	0.48
1:H:168:THR:O	1:H:169:HIS:HB2	2.13	0.48
1:E:252:ILE:HG22	1:E:253:LEU:HD13	1.95	0.48
1:G:284:HIS:HD2	1:G:285:HIS:CE1	2.31	0.48
1:H:263:ASP:O	1:H:267:ILE:HG13	2.13	0.48
1:J:56:LEU:HA	1:J:56:LEU:HD23	1.64	0.48
1:A:119:PHE:CD2	1:A:120:PRO:HD3	2.49	0.48
1:D:32:THR:HA	1:D:110:PHE:O	2.14	0.48
1:B:174:ARG:HH22	1:I:13:ASP:CG	2.11	0.48
1:B:297:ILE:O	1:B:300:CYS:N	2.46	0.48
1:D:72:TRP:CZ3	1:D:135:TYR:CZ	3.01	0.48
1:F:235:SER:HB2	1:F:277:ILE:HD11	1.95	0.48
1:I:293:ASP:HB3	1:I:295:LEU:HD13	1.95	0.48
1:I:162:ILE:CD1	1:I:162:ILE:H	2.25	0.48
1:B:71:LEU:HD22	1:B:72:TRP:O	2.14	0.48
1:D:72:TRP:CD1	1:D:72:TRP:O	2.66	0.48
1:E:260:THR:HG23	1:E:263:ASP:OD2	2.14	0.48
1:F:294:ASP:C	1:F:296:LEU:H	2.14	0.48
1:H:99:ARG:HH21	1:I:180:SER:HB3	1.79	0.48
1:A:162:ILE:N	1:A:162:ILE:HD13	2.27	0.48
1:H:208:PHE:HE2	1:H:249:THR:HA	1.79	0.48
1:I:72:TRP:CZ3	1:I:135:TYR:CZ	3.02	0.48
1:B:26:VAL:HG21	1:B:160:TRP:HE1	1.78	0.48
1:D:119:PHE:C	1:D:121:PHE:N	2.65	0.48
1:G:119:PHE:CG	1:G:120:PRO:N	2.81	0.48
1:J:23:ILE:HG21	1:J:126:PHE:CD1	2.49	0.48
1:J:263:ASP:O	1:J:267:ILE:HG13	2.14	0.48
1:B:297:ILE:O	1:B:299:ARG:N	2.47	0.47
1:C:31:GLN:HG2	1:C:114:MET:HB2	1.96	0.47
1:F:114:MET:HE2	1:F:124:GLN:HG2	1.96	0.47
1:F:72:TRP:CD1	1:F:72:TRP:O	2.67	0.47
1:G:79:ILE:HD11	1:G:131:GLU:HB3	1.96	0.47
1:E:95:PHE:HE1	1:E:101:ILE:HD12	1.79	0.47
1:H:294:ASP:C	1:H:296:LEU:H	2.13	0.47
1:A:216:ILE:O	1:A:219:SER:HB3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:HZ	1:C:205:LEU:HD21	1.80	0.47
1:C:235:SER:HB2	1:C:277:ILE:HD11	1.95	0.47
1:E:135:TYR:CB	1:E:138:GLN:HG2	2.44	0.47
1:E:168:THR:O	1:E:169:HIS:HB2	2.14	0.47
1:G:15:SER:HB2	1:G:142:PHE:CZ	2.49	0.47
1:E:162:ILE:CD1	1:E:162:ILE:H	2.27	0.47
1:A:240:LEU:HD23	1:E:241:THR:HA	1.96	0.47
1:J:297:ILE:O	1:J:300:CYS:N	2.46	0.47
1:A:168:THR:O	1:A:169:HIS:HB2	2.15	0.47
1:D:95:PHE:HB2	1:D:99:ARG:O	2.15	0.47
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.64	0.47
1:B:220:TRP:C	1:B:222:VAL:H	2.18	0.47
1:F:119:PHE:CG	1:F:120:PRO:N	2.82	0.47
1:F:297:ILE:O	1:F:299:ARG:N	2.47	0.47
1:J:208:PHE:HE2	1:J:249:THR:HA	1.79	0.47
1:B:162:ILE:CD1	1:B:162:ILE:H	2.27	0.47
1:D:20:ILE:HD12	1:D:195:ILE:HD11	1.97	0.47
1:D:198:VAL:HG12	1:D:199:ARG:N	2.28	0.47
1:E:38:TYR:CE2	1:E:105:ARG:HD3	2.49	0.47
1:E:119:PHE:CG	1:E:120:PRO:N	2.83	0.47
1:G:28:THR:HA	1:G:116:PHE:CE1	2.50	0.47
1:H:297:ILE:O	1:H:300:CYS:N	2.46	0.47
1:C:119:PHE:C	1:C:121:PHE:N	2.68	0.47
1:C:26:VAL:HG21	1:C:160:TRP:HE1	1.80	0.47
1:C:97:ASP:OD1	1:C:99:ARG:NH1	2.47	0.47
1:D:72:TRP:CD1	1:D:72:TRP:C	2.88	0.47
1:E:63:ILE:HG12	1:E:92:LEU:HG	1.97	0.47
1:F:227:SER:O	1:F:231:ARG:NH1	2.47	0.47
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.81	0.47
1:I:20:ILE:HD12	1:I:195:ILE:HD11	1.96	0.47
1:I:66:TRP:O	1:I:71:LEU:HB2	2.14	0.47
1:J:162:ILE:CD1	1:J:162:ILE:H	2.26	0.47
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.49	0.47
1:D:252:ILE:HD13	1:D:252:ILE:HA	1.73	0.47
1:E:42:GLN:HA	1:E:100:VAL:O	2.14	0.47
1:H:32:THR:HA	1:H:110:PHE:O	2.14	0.47
1:I:263:ASP:O	1:I:267:ILE:HG13	2.15	0.47
1:A:135:TYR:CB	1:A:138:GLN:HG2	2.45	0.47
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.78	0.47
1:E:72:TRP:CZ3	1:E:135:TYR:CZ	3.03	0.47
1:G:241:THR:OG1	1:H:240:LEU:HD23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:VAL:HG12	1:I:199:ARG:N	2.29	0.47
1:A:234:THR:HG21	1:B:233:GLN:HG2	1.97	0.47
1:A:72:TRP:CZ3	1:A:135:TYR:CZ	3.03	0.47
1:B:168:THR:O	1:B:169:HIS:CB	2.63	0.47
1:C:247:LEU:HA	1:C:247:LEU:HD23	1.48	0.47
1:D:289:ASN:ND2	1:D:292:GLU:HB2	2.30	0.47
1:F:208:PHE:HE2	1:F:249:THR:HA	1.80	0.47
1:G:208:PHE:HE2	1:G:249:THR:HA	1.80	0.47
1:J:247:LEU:HA	1:J:247:LEU:HD23	1.48	0.47
1:A:77:GLU:O	1:A:130:LEU:HD23	2.15	0.46
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.67	0.46
1:D:119:PHE:CG	1:D:120:PRO:N	2.83	0.46
1:D:84:SER:HA	1:D:85:PRO:HD3	1.50	0.46
1:I:235:SER:HB2	1:I:277:ILE:HD11	1.96	0.46
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.50	0.46
1:G:97:ASP:OD1	1:G:99:ARG:NH1	2.48	0.46
1:I:119:PHE:C	1:I:121:PHE:N	2.67	0.46
1:A:314:VAL:HG12	1:A:315:LEU:HD23	1.96	0.46
1:B:264:GLN:O	1:B:267:ILE:N	2.49	0.46
1:B:140:LEU:HD22	1:B:191:ILE:HD11	1.96	0.46
1:C:119:PHE:CG	1:C:120:PRO:N	2.84	0.46
1:B:234:THR:HG21	1:C:233:GLN:HG2	1.96	0.46
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.41	0.46
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.42	0.46
1:E:220:TRP:C	1:E:222:VAL:H	2.18	0.46
1:F:284:HIS:HD2	1:F:285:HIS:CE1	2.34	0.46
1:G:252:ILE:HG22	1:G:253:LEU:HD13	1.96	0.46
1:A:26:VAL:HG21	1:A:160:TRP:HE1	1.80	0.46
1:A:204:TYR:O	1:A:209:ILE:HG12	2.15	0.46
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.51	0.46
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.44	0.46
1:G:247:LEU:HD23	1:G:247:LEU:HA	1.49	0.46
1:J:72:TRP:CD1	1:J:72:TRP:C	2.89	0.46
1:C:293:ASP:HB3	1:C:295:LEU:HD13	1.98	0.46
1:A:134:SER:OG	1:E:59:GLU:OE2	2.32	0.46
1:E:97:ASP:OD1	1:E:99:ARG:NH1	2.48	0.46
1:I:168:THR:O	1:I:169:HIS:HB2	2.16	0.46
1:I:63:ILE:HG12	1:I:92:LEU:HG	1.97	0.46
1:C:226:GLU:OE2	1:D:284:HIS:NE2	2.49	0.46
1:J:227:SER:OG	1:J:228:PHE:N	2.48	0.46
1:B:119:PHE:HE1	1:B:199:ARG:CZ	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:TYR:O	1:D:208:PHE:HB2	2.16	0.46
1:E:284:HIS:HD2	1:E:285:HIS:CE1	2.34	0.46
1:H:38:TYR:CE2	1:H:105:ARG:HD3	2.51	0.46
1:I:59:GLU:OE2	1:J:134:SER:OG	2.32	0.46
1:I:94:LEU:HD23	1:I:94:LEU:HA	1.68	0.46
1:A:99:ARG:HH21	1:B:180:SER:HB3	1.80	0.46
1:B:252:ILE:HG22	1:B:253:LEU:HD13	1.98	0.46
1:C:84:SER:HA	1:C:85:PRO:HD3	1.62	0.46
1:F:121:PHE:HZ	1:F:205:LEU:HD21	1.80	0.46
1:F:247:LEU:HD11	1:J:247:LEU:HD13	1.98	0.46
1:J:66:TRP:O	1:J:71:LEU:HB2	2.16	0.46
1:A:17:SER:O	1:A:40:VAL:HG23	2.16	0.46
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.51	0.46
1:E:162:ILE:N	1:E:162:ILE:HD13	2.31	0.46
1:I:95:PHE:HB2	1:I:99:ARG:O	2.16	0.46
1:J:114:MET:HE2	1:J:124:GLN:HG2	1.97	0.46
1:J:143:SER:HB3	1:J:168:THR:HG21	1.98	0.46
1:F:284:HIS:NE2	1:J:226:GLU:OE2	2.43	0.46
1:A:135:TYR:HB3	1:A:138:GLN:HG2	1.98	0.45
1:B:227:SER:O	1:B:231:ARG:NH1	2.49	0.45
1:E:255:ARG:O	1:E:256:LEU:HD23	2.16	0.45
1:F:252:ILE:HA	1:F:252:ILE:HD13	1.82	0.45
1:F:84:SER:HA	1:F:85:PRO:HD3	1.63	0.45
1:G:17:SER:O	1:G:40:VAL:HG23	2.16	0.45
1:A:84:SER:HA	1:A:85:PRO:HD3	1.63	0.45
1:E:38:TYR:CZ	1:E:105:ARG:HD3	2.52	0.45
1:F:234:THR:HG21	1:G:233:GLN:HG2	1.99	0.45
1:F:257:PRO:HG2	1:F:258:TYR:CD2	2.51	0.45
1:F:94:LEU:HD23	1:F:94:LEU:HA	1.69	0.45
1:G:168:THR:O	1:G:169:HIS:CB	2.64	0.45
1:G:298:GLN:O	1:G:301:ARG:HG3	2.16	0.45
1:A:220:TRP:C	1:A:222:VAL:H	2.20	0.45
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.50	0.45
1:C:314:VAL:HG12	1:C:315:LEU:HD23	1.99	0.45
1:E:264:GLN:O	1:E:267:ILE:N	2.50	0.45
1:H:162:ILE:H	1:H:162:ILE:CD1	2.29	0.45
1:H:220:TRP:C	1:H:222:VAL:H	2.19	0.45
1:G:241:THR:HA	1:H:240:LEU:CD2	2.46	0.45
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.50	0.45
1:A:298:GLN:O	1:A:301:ARG:HG3	2.17	0.45
1:B:107:LEU:HD12	1:B:108:GLY:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:N	1:B:162:ILE:HD13	2.31	0.45
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.51	0.45
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.51	0.45
1:H:227:SER:O	1:H:231:ARG:NH1	2.49	0.45
1:J:238:LEU:HB3	1:J:273:ILE:HD13	1.99	0.45
1:A:38:TYR:CE2	1:A:105:ARG:HD3	2.51	0.45
1:B:114:MET:HE2	1:B:124:GLN:HG2	1.97	0.45
1:B:150:GLU:HB2	1:B:153:ASP:OD1	2.16	0.45
1:C:38:TYR:CZ	1:C:105:ARG:HD3	2.51	0.45
1:D:208:PHE:HE2	1:D:249:THR:HA	1.81	0.45
1:E:84:SER:HA	1:E:85:PRO:HD3	1.65	0.45
1:H:63:ILE:HG12	1:H:92:LEU:HG	1.97	0.45
1:I:15:SER:HB2	1:I:142:PHE:CZ	2.52	0.45
1:A:119:PHE:CG	1:A:120:PRO:N	2.85	0.45
1:A:293:ASP:HB3	1:A:295:LEU:HD13	1.98	0.45
1:E:121:PHE:HZ	1:E:205:LEU:HD21	1.81	0.45
1:F:63:ILE:HG12	1:F:92:LEU:HG	1.99	0.45
1:G:42:GLN:HA	1:G:100:VAL:O	2.17	0.45
1:J:92:LEU:HA	1:J:92:LEU:HD23	1.72	0.45
1:B:38:TYR:CE2	1:B:105:ARG:HD3	2.51	0.45
1:B:216:ILE:O	1:B:219:SER:HB3	2.17	0.45
1:C:42:GLN:HA	1:C:100:VAL:O	2.16	0.45
1:C:202:SER:O	1:C:205:LEU:N	2.49	0.45
1:C:63:ILE:HG12	1:C:92:LEU:HG	1.97	0.45
1:D:247:LEU:HD23	1:D:247:LEU:HA	1.49	0.45
1:D:252:ILE:HG22	1:D:253:LEU:HD13	1.98	0.45
1:F:162:ILE:HD13	1:F:162:ILE:N	2.32	0.45
1:J:297:ILE:O	1:J:299:ARG:N	2.50	0.45
1:C:162:ILE:N	1:C:162:ILE:HD13	2.30	0.45
1:F:42:GLN:HA	1:F:100:VAL:O	2.17	0.45
1:G:72:TRP:CZ3	1:G:135:TYR:CZ	3.04	0.45
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.52	0.45
1:B:241:THR:HA	1:C:240:LEU:HD23	1.97	0.45
1:C:66:TRP:O	1:C:71:LEU:HB2	2.16	0.45
1:E:293:ASP:HB3	1:E:295:LEU:HD13	1.99	0.45
1:I:119:PHE:CG	1:I:120:PRO:N	2.85	0.45
1:F:134:SER:OG	1:J:59:GLU:OE2	2.35	0.45
1:A:133:PHE:CE2	1:E:91:ARG:HG2	2.52	0.45
1:D:128:LEU:HA	1:D:128:LEU:HD12	1.80	0.45
1:D:255:ARG:O	1:D:256:LEU:HD23	2.16	0.45
1:H:77:GLU:O	1:H:130:LEU:HD23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:O	1:A:256:LEU:HD23	2.17	0.44
1:A:97:ASP:OD1	1:A:99:ARG:NH1	2.50	0.44
1:C:72:TRP:CZ3	1:C:135:TYR:CZ	3.04	0.44
1:G:107:LEU:HD12	1:G:108:GLY:N	2.32	0.44
1:H:94:LEU:HA	1:H:94:LEU:HD23	1.71	0.44
1:J:224:TRP:CE2	1:J:301:ARG:HD3	2.52	0.44
1:E:181:VAL:CG2	1:E:185:GLN:HB2	2.48	0.44
1:F:72:TRP:CD1	1:F:72:TRP:C	2.91	0.44
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.82	0.44
1:G:216:ILE:O	1:G:219:SER:HB3	2.17	0.44
1:J:15:SER:HB2	1:J:142:PHE:CZ	2.52	0.44
1:J:284:HIS:HD2	1:J:285:HIS:CE1	2.35	0.44
1:A:140:LEU:HD22	1:A:191:ILE:HD11	2.00	0.44
1:E:135:TYR:HB3	1:E:138:GLN:HG2	1.99	0.44
1:G:202:SER:O	1:G:205:LEU:N	2.47	0.44
1:G:297:ILE:O	1:G:299:ARG:N	2.50	0.44
1:H:107:LEU:HD12	1:H:108:GLY:H	1.82	0.44
1:A:163:ARG:HB3	1:A:164:GLY:H	1.65	0.44
1:C:223:PHE:HE2	1:C:304:PHE:CE1	2.36	0.44
1:D:71:LEU:HD22	1:D:72:TRP:O	2.18	0.44
1:E:314:VAL:O	1:E:317:ILE:HG22	2.16	0.44
1:F:135:TYR:CB	1:F:138:GLN:HG2	2.47	0.44
1:F:233:GLN:HG2	1:J:234:THR:HG21	1.99	0.44
1:G:128:LEU:HA	1:G:128:LEU:HD12	1.72	0.44
1:F:240:LEU:CD2	1:J:241:THR:HA	2.47	0.44
1:B:31:GLN:HG2	1:B:114:MET:HB2	1.99	0.44
1:D:97:ASP:OD1	1:D:99:ARG:NH1	2.50	0.44
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.52	0.44
1:F:97:ASP:OD1	1:F:99:ARG:NH1	2.49	0.44
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.52	0.44
1:J:204:TYR:O	1:J:208:PHE:HB2	2.17	0.44
1:J:212:LEU:HA	1:J:212:LEU:HD23	1.82	0.44
1:J:84:SER:HA	1:J:85:PRO:HD3	1.65	0.44
1:B:289:ASN:ND2	1:B:292:GLU:HB2	2.30	0.44
1:E:252:ILE:HD13	1:E:252:ILE:HA	1.76	0.44
1:A:181:VAL:CG2	1:A:185:GLN:HB2	2.48	0.44
1:E:204:TYR:O	1:E:208:PHE:HB2	2.18	0.44
1:E:212:LEU:CD1	1:E:265:MET:HB3	2.45	0.44
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.74	0.44
1:I:205:LEU:HD23	1:I:205:LEU:HA	1.72	0.44
1:A:28:THR:HA	1:A:116:PHE:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ILE:H	1:E:145:ILE:HD12	1.83	0.44
1:A:233:GLN:HG2	1:E:234:THR:HG21	1.99	0.44
1:F:133:PHE:CE2	1:J:91:ARG:HG2	2.53	0.44
1:F:289:ASN:N	1:F:289:ASN:OD1	2.51	0.44
1:H:26:VAL:HG21	1:H:160:TRP:HE1	1.81	0.44
1:H:293:ASP:HB3	1:H:295:LEU:HD13	1.99	0.44
1:I:202:SER:O	1:I:204:TYR:N	2.51	0.44
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.86	0.43
1:B:238:LEU:HB3	1:B:273:ILE:HD13	2.00	0.43
1:C:220:TRP:C	1:C:222:VAL:H	2.21	0.43
1:D:316:VAL:CG2	1:D:317:ILE:HG12	2.46	0.43
1:E:15:SER:HB2	1:E:142:PHE:CZ	2.53	0.43
1:E:17:SER:O	1:E:40:VAL:HG23	2.18	0.43
1:F:20:ILE:HD12	1:F:195:ILE:HD11	2.00	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.53	0.43
1:I:257:PRO:HG2	1:I:258:TYR:CD2	2.53	0.43
1:I:243:VAL:HG22	1:I:270:TYR:OH	2.18	0.43
1:A:38:TYR:CZ	1:A:105:ARG:HD3	2.53	0.43
1:C:99:ARG:HH21	1:D:180:SER:HB3	1.83	0.43
1:F:59:GLU:OE2	1:G:134:SER:OG	2.34	0.43
1:H:238:LEU:HB3	1:H:273:ILE:HD13	1.99	0.43
1:I:225:LEU:HD13	1:I:230:GLU:HB3	1.99	0.43
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.73	0.43
1:D:253:LEU:HD12	1:D:253:LEU:HA	1.87	0.43
1:E:208:PHE:HE2	1:E:249:THR:HA	1.82	0.43
1:F:220:TRP:C	1:F:222:VAL:H	2.21	0.43
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.53	0.43
1:A:289:ASN:ND2	1:A:292:GLU:HB2	2.32	0.43
1:A:79:ILE:HD11	1:A:131:GLU:HB3	2.01	0.43
1:C:216:ILE:O	1:C:219:SER:HB3	2.18	0.43
1:C:255:ARG:O	1:C:256:LEU:HD23	2.18	0.43
1:C:284:HIS:HD2	1:C:285:HIS:CE1	2.36	0.43
1:D:121:PHE:HZ	1:D:205:LEU:HD21	1.83	0.43
1:G:248:TYR:HA	1:H:247:LEU:CD2	2.47	0.43
1:G:99:ARG:HH21	1:H:180:SER:HB3	1.83	0.43
1:C:72:TRP:C	1:C:72:TRP:CD1	2.91	0.43
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.52	0.43
1:G:84:SER:HA	1:G:85:PRO:HD3	1.56	0.43
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.86	0.43
1:B:59:GLU:OE2	1:C:134:SER:OG	2.36	0.43
1:D:145:ILE:H	1:D:145:ILE:HD12	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.54	0.43
1:F:155:GLU:HB2	1:F:161:TRP:CD1	2.53	0.43
1:G:314:VAL:HG12	1:G:315:LEU:HD23	2.00	0.43
1:H:122:ASP:N	1:H:122:ASP:OD2	2.52	0.43
1:H:19:PHE:CZ	1:H:146:GLN:HG3	2.52	0.43
1:I:220:TRP:C	1:I:222:VAL:H	2.22	0.43
1:A:241:THR:HA	1:B:240:LEU:HD23	2.00	0.43
1:A:32:THR:HA	1:A:110:PHE:O	2.18	0.43
1:B:15:SER:HB2	1:B:142:PHE:CZ	2.53	0.43
1:B:208:PHE:HE2	1:B:249:THR:HA	1.84	0.43
1:B:235:SER:HB2	1:B:277:ILE:HD11	2.00	0.43
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.75	0.43
1:C:163:ARG:HB3	1:C:164:GLY:H	1.57	0.43
1:C:298:GLN:O	1:C:301:ARG:HG3	2.17	0.43
1:D:162:ILE:HD13	1:D:162:ILE:N	2.31	0.43
1:D:220:TRP:C	1:D:222:VAL:H	2.22	0.43
1:F:15:SER:HB2	1:F:142:PHE:CZ	2.54	0.43
1:G:119:PHE:HE1	1:G:199:ARG:CZ	2.31	0.43
1:A:202:SER:O	1:A:205:LEU:N	2.49	0.43
1:B:97:ASP:OD1	1:B:99:ARG:NH1	2.52	0.43
1:C:20:ILE:HD12	1:C:195:ILE:HD11	2.00	0.43
1:F:92:LEU:HA	1:F:92:LEU:HD23	1.63	0.43
1:G:220:TRP:C	1:G:222:VAL:H	2.22	0.43
1:H:119:PHE:CG	1:H:120:PRO:N	2.87	0.43
1:J:162:ILE:HD13	1:J:162:ILE:N	2.34	0.43
1:A:227:SER:OG	1:A:228:PHE:N	2.52	0.43
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.70	0.43
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.54	0.43
1:B:255:ARG:O	1:B:256:LEU:HD23	2.18	0.43
1:F:31:GLN:HG2	1:F:114:MET:HB2	2.01	0.43
1:F:119:PHE:CD2	1:F:120:PRO:HD3	2.53	0.43
1:F:130:LEU:HD23	1:F:130:LEU:HA	1.89	0.43
1:G:162:ILE:HD13	1:G:162:ILE:N	2.30	0.43
1:G:224:TRP:N	1:G:224:TRP:CD1	2.86	0.43
1:I:216:ILE:O	1:I:219:SER:HB3	2.18	0.43
1:J:135:TYR:CB	1:J:138:GLN:HG2	2.48	0.43
1:J:257:PRO:HG2	1:J:258:TYR:CD2	2.53	0.43
1:A:316:VAL:HG23	1:A:317:ILE:HD12	2.00	0.43
1:C:141:ARG:HG2	1:C:142:PHE:HD2	1.84	0.43
1:F:32:THR:HA	1:F:110:PHE:O	2.18	0.43
1:G:31:GLN:HG2	1:G:114:MET:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:SER:HB3	1:G:168:THR:HG21	2.01	0.43
1:H:205:LEU:HD23	1:H:205:LEU:HA	1.83	0.43
1:H:84:SER:HA	1:H:85:PRO:HD3	1.63	0.43
1:I:135:TYR:CB	1:I:138:GLN:HG2	2.48	0.43
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.54	0.43
1:J:72:TRP:CZ3	1:J:135:TYR:CZ	3.07	0.43
1:D:294:ASP:C	1:D:296:LEU:H	2.14	0.42
1:E:20:ILE:HD12	1:E:195:ILE:HD11	2.01	0.42
1:H:31:GLN:HG2	1:H:114:MET:HB2	2.01	0.42
1:I:204:TYR:O	1:I:208:PHE:HB2	2.18	0.42
1:J:32:THR:HA	1:J:110:PHE:O	2.19	0.42
1:J:94:LEU:HD23	1:J:94:LEU:HA	1.71	0.42
1:B:72:TRP:CD1	1:B:72:TRP:O	2.72	0.42
1:G:163:ARG:HB3	1:G:164:GLY:H	1.60	0.42
1:G:72:TRP:C	1:G:72:TRP:CD1	2.92	0.42
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.01	0.42
1:B:99:ARG:HH21	1:C:180:SER:HB3	1.83	0.42
1:D:114:MET:HE2	1:D:124:GLN:HG2	2.01	0.42
1:D:225:LEU:HD13	1:D:230:GLU:HB3	2.01	0.42
1:G:119:PHE:CD2	1:G:120:PRO:HD3	2.54	0.42
1:H:252:ILE:HD13	1:H:252:ILE:HA	1.78	0.42
1:I:153:ASP:HB2	1:I:154:ASN:H	1.59	0.42
1:A:15:SER:HB2	1:A:142:PHE:CZ	2.54	0.42
1:B:38:TYR:CZ	1:B:105:ARG:HD3	2.54	0.42
1:C:252:ILE:HD13	1:C:252:ILE:HA	1.82	0.42
1:E:289:ASN:ND2	1:E:292:GLU:HB2	2.30	0.42
1:F:140:LEU:HD22	1:F:191:ILE:HD11	2.00	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.55	0.42
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.19	0.42
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.34	0.42
1:A:72:TRP:C	1:A:72:TRP:CD1	2.93	0.42
1:B:284:HIS:HD2	1:B:285:HIS:CE1	2.37	0.42
1:B:293:ASP:HB3	1:B:295:LEU:HD13	2.01	0.42
1:D:202:SER:O	1:D:205:LEU:N	2.51	0.42
1:E:216:ILE:O	1:E:219:SER:HB3	2.19	0.42
1:E:253:LEU:HD12	1:E:253:LEU:HA	1.91	0.42
1:F:95:PHE:HE1	1:F:101:ILE:HD12	1.85	0.42
1:B:119:PHE:CG	1:B:120:PRO:N	2.88	0.42
1:B:294:ASP:C	1:B:296:LEU:H	2.15	0.42
1:C:15:SER:HB2	1:C:142:PHE:CZ	2.55	0.42
1:D:135:TYR:CB	1:D:138:GLN:HG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:PHE:CD1	1:F:304:PHE:C	2.93	0.42
1:G:248:TYR:HA	1:H:247:LEU:HD21	2.02	0.42
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.86	0.42
1:H:114:MET:HE2	1:H:124:GLN:HG2	2.00	0.42
1:A:252:ILE:HD13	1:A:252:ILE:HA	1.85	0.42
1:B:202:SER:O	1:B:204:TYR:N	2.53	0.42
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.55	0.42
1:D:58:VAL:HB	1:D:92:LEU:HB2	2.02	0.42
1:D:81:VAL:HG21	1:D:85:PRO:HG3	2.02	0.42
1:E:298:GLN:O	1:E:301:ARG:HG3	2.20	0.42
1:E:78:PHE:O	1:E:81:VAL:HG12	2.19	0.42
1:F:56:LEU:HD23	1:F:56:LEU:HA	1.72	0.42
1:H:264:GLN:O	1:H:267:ILE:N	2.52	0.42
1:A:204:TYR:O	1:A:208:PHE:HB2	2.19	0.42
1:A:71:LEU:HD22	1:A:72:TRP:O	2.20	0.42
1:B:135:TYR:CB	1:B:138:GLN:HG2	2.50	0.42
1:D:316:VAL:HG23	1:D:317:ILE:CG1	2.47	0.42
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.79	0.42
1:E:94:LEU:HD23	1:E:94:LEU:HA	1.65	0.42
1:I:47:PRO:HA	1:I:98:GLY:HA2	2.01	0.42
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.77	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.77	0.42
1:B:95:PHE:HB2	1:B:99:ARG:O	2.20	0.42
1:D:209:ILE:H	1:D:209:ILE:HG12	1.67	0.42
1:D:227:SER:HB3	1:D:230:GLU:CB	2.49	0.42
1:D:297:ILE:O	1:D:299:ARG:N	2.53	0.42
1:E:294:ASP:C	1:E:296:LEU:H	2.13	0.42
1:G:140:LEU:HD13	1:G:191:ILE:CG1	2.46	0.42
1:F:241:THR:OG1	1:G:240:LEU:HD23	2.19	0.42
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.65	0.42
1:H:204:TYR:O	1:H:208:PHE:HB2	2.19	0.42
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.55	0.42
1:C:217:ALA:O	1:C:220:TRP:N	2.44	0.42
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.55	0.42
1:F:40:VAL:HA	1:F:102:TYR:O	2.20	0.42
1:F:204:TYR:O	1:F:209:ILE:HG12	2.19	0.42
1:F:212:LEU:HB3	1:F:265:MET:HE1	2.01	0.42
1:H:72:TRP:CD1	1:H:72:TRP:C	2.93	0.42
1:J:119:PHE:CG	1:J:120:PRO:N	2.88	0.42
1:J:20:ILE:HD12	1:J:195:ILE:HD11	2.02	0.42
1:C:294:ASP:C	1:C:296:LEU:H	2.17	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:TRP:CZ3	1:H:135:TYR:CZ	3.08	0.41
1:I:145:ILE:HD12	1:I:145:ILE:H	1.84	0.41
1:I:247:LEU:HA	1:I:247:LEU:HD23	1.56	0.41
1:A:227:SER:HB3	1:A:230:GLU:CB	2.50	0.41
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.68	0.41
1:B:204:TYR:O	1:B:208:PHE:HB2	2.20	0.41
1:F:107:LEU:HD12	1:F:108:GLY:N	2.35	0.41
1:F:202:SER:O	1:F:205:LEU:N	2.50	0.41
1:G:181:VAL:CG2	1:G:185:GLN:HB2	2.50	0.41
1:H:225:LEU:HD13	1:H:230:GLU:HB3	2.02	0.41
1:I:253:LEU:HD12	1:I:253:LEU:HA	1.85	0.41
1:I:284:HIS:HD2	1:I:285:HIS:CE1	2.36	0.41
1:I:58:VAL:HB	1:I:92:LEU:HB2	2.01	0.41
1:J:11:PRO:HB3	1:J:137:ASN:HB3	2.02	0.41
1:B:140:LEU:HD22	1:B:191:ILE:CD1	2.50	0.41
1:B:181:VAL:CG2	1:B:185:GLN:HB2	2.50	0.41
1:D:264:GLN:O	1:D:267:ILE:N	2.54	0.41
1:E:163:ARG:HB3	1:E:164:GLY:H	1.65	0.41
1:G:38:TYR:CE2	1:G:105:ARG:HD3	2.54	0.41
1:G:150:GLU:HB2	1:G:153:ASP:OD1	2.20	0.41
1:G:212:LEU:HD23	1:G:212:LEU:HA	1.82	0.41
1:H:224:TRP:CD1	1:H:224:TRP:N	2.88	0.41
1:I:162:ILE:N	1:I:162:ILE:HD13	2.30	0.41
1:J:141:ARG:HG2	1:J:142:PHE:HD2	1.84	0.41
1:B:153:ASP:HB2	1:B:154:ASN:H	1.59	0.41
1:C:202:SER:O	1:C:204:TYR:N	2.53	0.41
1:E:155:GLU:HB2	1:E:161:TRP:CD1	2.55	0.41
1:J:289:ASN:ND2	1:J:292:GLU:HB2	2.35	0.41
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.55	0.41
1:B:296:LEU:HD22	1:B:296:LEU:HA	1.90	0.41
1:C:253:LEU:HD12	1:C:253:LEU:HA	1.94	0.41
1:D:257:PRO:HG2	1:D:258:TYR:CD2	2.56	0.41
1:F:77:GLU:O	1:F:130:LEU:HD23	2.21	0.41
1:F:153:ASP:HB2	1:F:154:ASN:H	1.60	0.41
1:F:289:ASN:ND2	1:F:292:GLU:HB2	2.33	0.41
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.55	0.41
1:H:91:ARG:HD3	1:I:134:SER:CB	2.42	0.41
1:I:181:VAL:CG2	1:I:185:GLN:HB2	2.51	0.41
1:I:202:SER:O	1:I:205:LEU:N	2.50	0.41
1:I:227:SER:O	1:I:231:ARG:NH1	2.54	0.41
1:J:95:PHE:HB2	1:J:99:ARG:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:HE2	1:B:304:PHE:CE1	2.39	0.41
1:B:84:SER:HA	1:B:85:PRO:HD3	1.58	0.41
1:E:227:SER:O	1:E:231:ARG:NH1	2.53	0.41
1:E:225:LEU:HD13	1:E:230:GLU:HB3	2.02	0.41
1:E:81:VAL:HG21	1:E:85:PRO:HG3	2.03	0.41
1:F:26:VAL:HG21	1:F:160:TRP:HE1	1.86	0.41
1:H:135:TYR:HB2	1:H:138:GLN:HG2	2.02	0.41
1:J:42:GLN:HA	1:J:100:VAL:O	2.20	0.41
1:A:119:PHE:C	1:A:121:PHE:N	2.72	0.41
1:B:72:TRP:CD1	1:B:72:TRP:C	2.93	0.41
1:F:204:TYR:O	1:F:208:PHE:HB2	2.21	0.41
1:H:56:LEU:HA	1:H:56:LEU:HD23	1.73	0.41
1:I:314:VAL:HG12	1:I:315:LEU:HD23	2.01	0.41
1:J:252:ILE:HA	1:J:252:ILE:HD13	1.82	0.41
1:A:208:PHE:HE2	1:A:249:THR:HA	1.85	0.41
1:C:91:ARG:HD3	1:D:134:SER:CB	2.41	0.41
1:E:119:PHE:C	1:E:121:PHE:N	2.73	0.41
1:F:38:TYR:CZ	1:F:105:ARG:HD3	2.56	0.41
1:G:252:ILE:HD13	1:G:252:ILE:HA	1.82	0.41
1:G:289:ASN:N	1:G:289:ASN:OD1	2.53	0.41
1:H:119:PHE:C	1:H:121:PHE:N	2.71	0.41
1:J:119:PHE:CD2	1:J:120:PRO:HD3	2.56	0.41
1:A:31:GLN:HG2	1:A:114:MET:HB2	2.02	0.41
1:A:264:GLN:O	1:A:267:ILE:N	2.52	0.41
1:D:15:SER:HB2	1:D:142:PHE:CZ	2.55	0.41
1:G:71:LEU:HD22	1:G:72:TRP:O	2.21	0.41
1:H:130:LEU:HA	1:H:130:LEU:HD23	1.93	0.41
1:H:15:SER:HB2	1:H:142:PHE:CZ	2.56	0.41
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.46	0.41
1:H:59:GLU:OE2	1:I:134:SER:OG	2.36	0.41
1:B:42:GLN:HA	1:B:100:VAL:O	2.21	0.41
1:C:182:GLN:H	1:C:183:PRO:CD	2.30	0.41
1:C:227:SER:O	1:C:231:ARG:NH1	2.54	0.41
1:E:314:VAL:HG12	1:E:315:LEU:HD23	2.03	0.41
1:F:71:LEU:HD22	1:F:72:TRP:O	2.21	0.41
1:G:225:LEU:HD13	1:G:230:GLU:HB3	2.03	0.41
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.47	0.41
1:I:252:ILE:HD13	1:I:252:ILE:HA	1.79	0.41
1:I:92:LEU:HA	1:I:92:LEU:HD23	1.85	0.41
1:J:26:VAL:HG21	1:J:160:TRP:HE1	1.85	0.41
1:J:253:LEU:HA	1:J:253:LEU:HD12	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HB3	1:A:273:ILE:HD13	2.03	0.41
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.79	0.41
1:E:119:PHE:CD2	1:E:120:PRO:HD3	2.56	0.41
1:H:241:THR:OG1	1:I:240:LEU:HD23	2.20	0.41
1:H:256:LEU:HD13	1:H:258:TYR:CE1	2.56	0.41
1:H:38:TYR:CZ	1:H:105:ARG:HD3	2.56	0.41
1:D:59:GLU:OE2	1:E:134:SER:OG	2.38	0.40
1:E:176:ASP:O	1:E:178:LEU:N	2.54	0.40
1:F:128:LEU:HD12	1:F:128:LEU:HA	1.84	0.40
1:F:135:TYR:HB3	1:F:138:GLN:HG2	2.02	0.40
1:G:253:LEU:HD12	1:G:253:LEU:HA	1.90	0.40
1:H:314:VAL:HG12	1:H:315:LEU:HD23	2.02	0.40
1:I:42:GLN:HA	1:I:100:VAL:O	2.21	0.40
1:C:143:SER:HB3	1:C:168:THR:HG21	2.02	0.40
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.82	0.40
1:D:168:THR:O	1:D:169:HIS:HB2	2.21	0.40
1:E:257:PRO:HG2	1:E:258:TYR:CD2	2.56	0.40
1:F:287:GLN:HB2	1:F:288:ALA:H	1.53	0.40
1:G:157:ILE:HG22	1:H:31:GLN:HE22	1.86	0.40
1:I:114:MET:HE2	1:I:124:GLN:HG2	2.02	0.40
1:I:212:LEU:HD23	1:I:212:LEU:HA	1.85	0.40
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.90	0.40
1:C:72:TRP:HZ3	1:C:135:TYR:CE2	2.39	0.40
1:E:247:LEU:HD23	1:E:247:LEU:HA	1.51	0.40
1:E:32:THR:HA	1:E:110:PHE:O	2.21	0.40
1:G:140:LEU:HD22	1:G:191:ILE:HD11	2.02	0.40
1:G:176:ASP:O	1:G:178:LEU:N	2.55	0.40
1:H:66:TRP:O	1:H:71:LEU:HB2	2.22	0.40
1:J:242:VAL:O	1:J:245:TYR:N	2.54	0.40
1:J:256:LEU:HD13	1:J:258:TYR:CE1	2.56	0.40
1:B:224:TRP:N	1:B:224:TRP:CD1	2.89	0.40
1:F:278:LEU:HA	1:F:278:LEU:HD23	1.84	0.40
1:G:255:ARG:O	1:G:256:LEU:HD23	2.20	0.40
1:H:135:TYR:HB3	1:H:138:GLN:HG2	2.04	0.40
1:H:208:PHE:CD2	1:H:249:THR:HG22	2.56	0.40
1:J:209:ILE:HG12	1:J:209:ILE:H	1.73	0.40
1:J:255:ARG:O	1:J:256:LEU:HD23	2.21	0.40
1:C:135:TYR:CB	1:C:138:GLN:HG2	2.50	0.40
1:C:146:GLN:H	1:C:146:GLN:HG2	1.75	0.40
1:D:238:LEU:HB3	1:D:273:ILE:CD1	2.51	0.40
1:E:150:GLU:HB2	1:E:153:ASP:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:PHE:CD1	1:E:304:PHE:C	2.95	0.40
1:F:150:GLU:HB2	1:F:153:ASP:OD1	2.22	0.40
1:F:29:LEU:HA	1:F:29:LEU:HD23	1.84	0.40
1:F:314:VAL:HG12	1:F:315:LEU:HD23	2.03	0.40
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.56	0.40
1:I:210:LEU:HB3	1:I:211:PRO:HD3	2.02	0.40
1:J:130:LEU:HA	1:J:130:LEU:HD23	1.90	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	305/324 (94%)	248 (81%)	38 (12%)	19 (6%)	1	15
1	B	305/324 (94%)	249 (82%)	36 (12%)	20 (7%)	1	13
1	C	305/324 (94%)	250 (82%)	33 (11%)	22 (7%)	1	11
1	D	305/324 (94%)	249 (82%)	33 (11%)	23 (8%)	1	11
1	E	305/324 (94%)	249 (82%)	36 (12%)	20 (7%)	1	13
1	F	305/324 (94%)	249 (82%)	37 (12%)	19 (6%)	1	15
1	G	305/324 (94%)	249 (82%)	36 (12%)	20 (7%)	1	13
1	H	305/324 (94%)	253 (83%)	34 (11%)	18 (6%)	1	15
1	I	305/324 (94%)	255 (84%)	31 (10%)	19 (6%)	1	15
1	J	305/324 (94%)	247 (81%)	39 (13%)	19 (6%)	1	15
All	All	3050/3240 (94%)	2498 (82%)	353 (12%)	199 (6%)	1	14

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PRO
1	A	169	HIS
1	A	200	ASN
1	A	202	SER
1	B	120	PRO
1	B	138	GLN
1	B	169	HIS
1	B	200	ASN
1	B	202	SER
1	B	289	ASN
1	C	120	PRO
1	C	138	GLN
1	C	169	HIS
1	C	202	SER
1	D	120	PRO
1	D	138	GLN
1	D	169	HIS
1	D	200	ASN
1	D	202	SER
1	E	120	PRO
1	E	163	ARG
1	E	169	HIS
1	E	200	ASN
1	E	202	SER
1	E	289	ASN
1	F	120	PRO
1	F	138	GLN
1	F	169	HIS
1	F	202	SER
1	G	120	PRO
1	G	138	GLN
1	G	169	HIS
1	G	202	SER
1	H	120	PRO
1	H	138	GLN
1	H	169	HIS
1	H	202	SER
1	I	120	PRO
1	I	138	GLN
1	I	169	HIS
1	I	200	ASN
1	I	202	SER
1	J	120	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	138	GLN
1	J	169	HIS
1	J	200	ASN
1	J	202	SER
1	A	138	GLN
1	A	141	ARG
1	A	153	ASP
1	A	163	ARG
1	A	179	SER
1	A	295	LEU
1	A	298	GLN
1	B	153	ASP
1	B	179	SER
1	B	295	LEU
1	C	141	ARG
1	C	153	ASP
1	C	179	SER
1	C	200	ASN
1	D	153	ASP
1	D	163	ARG
1	D	179	SER
1	D	288	ALA
1	D	295	LEU
1	E	138	GLN
1	E	153	ASP
1	E	179	SER
1	E	295	LEU
1	E	298	GLN
1	F	153	ASP
1	F	163	ARG
1	F	179	SER
1	F	200	ASN
1	F	295	LEU
1	F	298	GLN
1	G	153	ASP
1	G	179	SER
1	G	295	LEU
1	H	153	ASP
1	H	163	ARG
1	H	179	SER
1	H	200	ASN
1	H	295	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	153	ASP
1	I	163	ARG
1	I	179	SER
1	I	295	LEU
1	I	298	GLN
1	J	153	ASP
1	J	163	ARG
1	J	179	SER
1	J	295	LEU
1	A	151	ASN
1	A	177	HIS
1	B	141	ARG
1	B	163	ARG
1	B	298	GLN
1	C	163	ARG
1	C	177	HIS
1	C	295	LEU
1	C	298	GLN
1	D	289	ASN
1	D	298	GLN
1	E	141	ARG
1	F	141	ARG
1	F	177	HIS
1	F	288	ALA
1	G	163	ARG
1	G	298	GLN
1	H	298	GLN
1	I	141	ARG
1	J	298	GLN
1	A	182	GLN
1	B	151	ASN
1	B	177	HIS
1	B	182	GLN
1	B	203	TYR
1	C	151	ASN
1	C	182	GLN
1	D	141	ARG
1	D	151	ASN
1	D	177	HIS
1	D	182	GLN
1	E	151	ASN
1	E	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	218	ALA
1	F	182	GLN
1	F	203	TYR
1	G	141	ARG
1	G	177	HIS
1	G	182	GLN
1	G	200	ASN
1	G	203	TYR
1	G	289	ASN
1	H	141	ARG
1	H	151	ASN
1	H	182	GLN
1	I	177	HIS
1	I	182	GLN
1	I	289	ASN
1	J	141	ARG
1	J	182	GLN
1	A	289	ASN
1	B	221	SER
1	B	257	PRO
1	C	203	TYR
1	C	221	SER
1	C	289	ASN
1	C	290	GLY
1	D	148	TYR
1	D	221	SER
1	D	290	GLY
1	E	257	PRO
1	E	290	GLY
1	F	151	ASN
1	G	148	TYR
1	G	151	ASN
1	G	257	PRO
1	H	177	HIS
1	H	221	SER
1	I	151	ASN
1	I	203	TYR
1	J	151	ASN
1	J	177	HIS
1	J	221	SER
1	J	257	PRO
1	A	257	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	GLY
1	C	176	ASP
1	C	257	PRO
1	D	203	TYR
1	E	177	HIS
1	F	257	PRO
1	F	290	GLY
1	G	290	GLY
1	H	257	PRO
1	H	290	GLY
1	I	257	PRO
1	I	290	GLY
1	J	148	TYR
1	J	290	GLY
1	D	183	PRO
1	D	257	PRO
1	E	47	PRO
1	E	183	PRO
1	F	183	PRO
1	J	183	PRO
1	A	183	PRO
1	B	183	PRO
1	D	47	PRO
1	G	183	PRO
1	I	183	PRO
1	A	47	PRO
1	C	119	PHE
1	C	183	PRO
1	H	183	PRO
1	B	290	GLY

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	275/285 (96%)	222 (81%)	53 (19%)	1 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	275/285 (96%)	220 (80%)	55 (20%)	1	7
1	C	275/285 (96%)	223 (81%)	52 (19%)	1	8
1	D	275/285 (96%)	221 (80%)	54 (20%)	1	7
1	E	275/285 (96%)	222 (81%)	53 (19%)	1	7
1	F	275/285 (96%)	222 (81%)	53 (19%)	1	7
1	G	275/285 (96%)	223 (81%)	52 (19%)	1	8
1	H	275/285 (96%)	224 (82%)	51 (18%)	1	8
1	I	275/285 (96%)	222 (81%)	53 (19%)	1	7
1	J	275/285 (96%)	224 (82%)	51 (18%)	1	8
All	All	2750/2850 (96%)	2223 (81%)	527 (19%)	1	7

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	15	SER
1	A	17	SER
1	A	22	LYS
1	A	26	VAL
1	A	29	LEU
1	A	32	THR
1	A	40	VAL
1	A	43	TRP
1	A	56	LEU
1	A	71	LEU
1	A	72	TRP
1	A	82	VAL
1	A	84	SER
1	A	87	THR
1	A	91	ARG
1	A	107	LEU
1	A	109	SER
1	A	118	LEU
1	A	124	GLN
1	A	128	LEU
1	A	130	LEU
1	A	134	SER
1	A	145	ILE
1	A	162	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	SER
1	A	172	ASP
1	A	178	LEU
1	A	182	GLN
1	A	194	ARG
1	A	202	SER
1	A	206	TRP
1	A	207	SER
1	A	212	LEU
1	A	219	SER
1	A	228	PHE
1	A	232	LEU
1	A	235	SER
1	A	238	LEU
1	A	240	LEU
1	A	250	SER
1	A	253	LEU
1	A	258	TYR
1	A	259	THR
1	A	260	THR
1	A	279	LEU
1	A	281	ILE
1	A	287	GLN
1	A	291	VAL
1	A	295	LEU
1	A	296	LEU
1	A	302	LEU
1	A	304	PHE
1	B	12	VAL
1	B	15	SER
1	B	17	SER
1	B	22	LYS
1	B	26	VAL
1	B	29	LEU
1	B	32	THR
1	B	40	VAL
1	B	56	LEU
1	B	71	LEU
1	B	72	TRP
1	B	78	PHE
1	B	82	VAL
1	B	84	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	87	THR
1	B	91	ARG
1	B	107	LEU
1	B	109	SER
1	B	118	LEU
1	B	124	GLN
1	B	128	LEU
1	B	130	LEU
1	B	134	SER
1	B	145	ILE
1	B	162	ILE
1	B	167	SER
1	B	168	THR
1	B	172	ASP
1	B	178	LEU
1	B	182	GLN
1	B	194	ARG
1	B	202	SER
1	B	206	TRP
1	B	207	SER
1	B	212	LEU
1	B	219	SER
1	B	228	PHE
1	B	232	LEU
1	B	235	SER
1	B	238	LEU
1	B	240	LEU
1	B	250	SER
1	B	253	LEU
1	B	258	TYR
1	B	259	THR
1	B	260	THR
1	B	279	LEU
1	B	281	ILE
1	B	287	GLN
1	B	291	VAL
1	B	295	LEU
1	B	296	LEU
1	B	302	LEU
1	B	304	PHE
1	B	315	LEU
1	C	12	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	15	SER
1	C	17	SER
1	C	22	LYS
1	C	26	VAL
1	C	29	LEU
1	C	32	THR
1	C	40	VAL
1	C	43	TRP
1	C	56	LEU
1	C	71	LEU
1	C	72	TRP
1	C	82	VAL
1	C	84	SER
1	C	87	THR
1	C	91	ARG
1	C	107	LEU
1	C	109	SER
1	C	118	LEU
1	C	124	GLN
1	C	128	LEU
1	C	130	LEU
1	C	134	SER
1	C	145	ILE
1	C	162	ILE
1	C	167	SER
1	C	172	ASP
1	C	178	LEU
1	C	182	GLN
1	C	194	ARG
1	C	202	SER
1	C	206	TRP
1	C	207	SER
1	C	212	LEU
1	C	219	SER
1	C	232	LEU
1	C	235	SER
1	C	238	LEU
1	C	240	LEU
1	C	250	SER
1	C	253	LEU
1	C	258	TYR
1	C	259	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	THR
1	C	279	LEU
1	C	281	ILE
1	C	287	GLN
1	C	291	VAL
1	C	295	LEU
1	C	296	LEU
1	C	302	LEU
1	C	304	PHE
1	D	12	VAL
1	D	15	SER
1	D	17	SER
1	D	22	LYS
1	D	26	VAL
1	D	29	LEU
1	D	32	THR
1	D	40	VAL
1	D	43	TRP
1	D	56	LEU
1	D	71	LEU
1	D	72	TRP
1	D	82	VAL
1	D	84	SER
1	D	87	THR
1	D	91	ARG
1	D	107	LEU
1	D	109	SER
1	D	118	LEU
1	D	124	GLN
1	D	128	LEU
1	D	130	LEU
1	D	134	SER
1	D	145	ILE
1	D	146	GLN
1	D	162	ILE
1	D	167	SER
1	D	168	THR
1	D	172	ASP
1	D	178	LEU
1	D	182	GLN
1	D	194	ARG
1	D	201	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	202	SER
1	D	206	TRP
1	D	207	SER
1	D	212	LEU
1	D	219	SER
1	D	232	LEU
1	D	235	SER
1	D	238	LEU
1	D	240	LEU
1	D	250	SER
1	D	253	LEU
1	D	259	THR
1	D	260	THR
1	D	279	LEU
1	D	281	ILE
1	D	287	GLN
1	D	291	VAL
1	D	295	LEU
1	D	296	LEU
1	D	302	LEU
1	D	304	PHE
1	E	12	VAL
1	E	15	SER
1	E	17	SER
1	E	22	LYS
1	E	26	VAL
1	E	29	LEU
1	E	32	THR
1	E	40	VAL
1	E	43	TRP
1	E	56	LEU
1	E	71	LEU
1	E	72	TRP
1	E	82	VAL
1	E	87	THR
1	E	91	ARG
1	E	107	LEU
1	E	109	SER
1	E	118	LEU
1	E	124	GLN
1	E	128	LEU
1	E	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	134	SER
1	E	145	ILE
1	E	162	ILE
1	E	167	SER
1	E	172	ASP
1	E	178	LEU
1	E	182	GLN
1	E	194	ARG
1	E	202	SER
1	E	206	TRP
1	E	207	SER
1	E	212	LEU
1	E	219	SER
1	E	228	PHE
1	E	232	LEU
1	E	235	SER
1	E	238	LEU
1	E	240	LEU
1	E	250	SER
1	E	253	LEU
1	E	259	THR
1	E	260	THR
1	E	262	ILE
1	E	279	LEU
1	E	281	ILE
1	E	287	GLN
1	E	291	VAL
1	E	295	LEU
1	E	296	LEU
1	E	302	LEU
1	E	304	PHE
1	E	317	ILE
1	F	12	VAL
1	F	15	SER
1	F	17	SER
1	F	22	LYS
1	F	26	VAL
1	F	29	LEU
1	F	32	THR
1	F	40	VAL
1	F	56	LEU
1	F	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	72	TRP
1	F	82	VAL
1	F	84	SER
1	F	87	THR
1	F	91	ARG
1	F	107	LEU
1	F	109	SER
1	F	118	LEU
1	F	124	GLN
1	F	128	LEU
1	F	130	LEU
1	F	134	SER
1	F	145	ILE
1	F	146	GLN
1	F	162	ILE
1	F	167	SER
1	F	172	ASP
1	F	178	LEU
1	F	182	GLN
1	F	194	ARG
1	F	202	SER
1	F	206	TRP
1	F	207	SER
1	F	212	LEU
1	F	219	SER
1	F	228	PHE
1	F	232	LEU
1	F	235	SER
1	F	238	LEU
1	F	240	LEU
1	F	250	SER
1	F	253	LEU
1	F	258	TYR
1	F	259	THR
1	F	260	THR
1	F	279	LEU
1	F	281	ILE
1	F	287	GLN
1	F	291	VAL
1	F	295	LEU
1	F	296	LEU
1	F	302	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	304	PHE
1	G	12	VAL
1	G	15	SER
1	G	17	SER
1	G	22	LYS
1	G	26	VAL
1	G	29	LEU
1	G	32	THR
1	G	40	VAL
1	G	43	TRP
1	G	56	LEU
1	G	71	LEU
1	G	72	TRP
1	G	82	VAL
1	G	87	THR
1	G	91	ARG
1	G	107	LEU
1	G	109	SER
1	G	118	LEU
1	G	124	GLN
1	G	128	LEU
1	G	130	LEU
1	G	134	SER
1	G	145	ILE
1	G	162	ILE
1	G	167	SER
1	G	168	THR
1	G	172	ASP
1	G	178	LEU
1	G	182	GLN
1	G	194	ARG
1	G	202	SER
1	G	206	TRP
1	G	207	SER
1	G	212	LEU
1	G	219	SER
1	G	232	LEU
1	G	235	SER
1	G	238	LEU
1	G	240	LEU
1	G	250	SER
1	G	253	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	259	THR
1	G	260	THR
1	G	279	LEU
1	G	281	ILE
1	G	287	GLN
1	G	291	VAL
1	G	295	LEU
1	G	296	LEU
1	G	299	ARG
1	G	302	LEU
1	G	304	PHE
1	H	12	VAL
1	H	15	SER
1	H	17	SER
1	H	22	LYS
1	H	26	VAL
1	H	29	LEU
1	H	32	THR
1	H	40	VAL
1	H	56	LEU
1	H	71	LEU
1	H	72	TRP
1	H	82	VAL
1	H	87	THR
1	H	91	ARG
1	H	107	LEU
1	H	109	SER
1	H	118	LEU
1	H	124	GLN
1	H	128	LEU
1	H	130	LEU
1	H	134	SER
1	H	145	ILE
1	H	162	ILE
1	H	167	SER
1	H	168	THR
1	H	172	ASP
1	H	178	LEU
1	H	182	GLN
1	H	194	ARG
1	H	202	SER
1	H	206	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	207	SER
1	H	212	LEU
1	H	219	SER
1	H	228	PHE
1	H	232	LEU
1	H	235	SER
1	H	238	LEU
1	H	240	LEU
1	H	250	SER
1	H	253	LEU
1	H	259	THR
1	H	260	THR
1	H	279	LEU
1	H	281	ILE
1	H	287	GLN
1	H	291	VAL
1	H	295	LEU
1	H	296	LEU
1	H	302	LEU
1	H	304	PHE
1	I	12	VAL
1	I	15	SER
1	I	17	SER
1	I	22	LYS
1	I	26	VAL
1	I	29	LEU
1	I	32	THR
1	I	40	VAL
1	I	56	LEU
1	I	71	LEU
1	I	72	TRP
1	I	82	VAL
1	I	84	SER
1	I	87	THR
1	I	91	ARG
1	I	107	LEU
1	I	109	SER
1	I	118	LEU
1	I	124	GLN
1	I	128	LEU
1	I	130	LEU
1	I	134	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	145	ILE
1	I	162	ILE
1	I	167	SER
1	I	168	THR
1	I	172	ASP
1	I	178	LEU
1	I	182	GLN
1	I	194	ARG
1	I	201	PRO
1	I	202	SER
1	I	206	TRP
1	I	207	SER
1	I	212	LEU
1	I	219	SER
1	I	232	LEU
1	I	235	SER
1	I	238	LEU
1	I	240	LEU
1	I	247	LEU
1	I	250	SER
1	I	253	LEU
1	I	259	THR
1	I	260	THR
1	I	279	LEU
1	I	281	ILE
1	I	287	GLN
1	I	291	VAL
1	I	295	LEU
1	I	296	LEU
1	I	302	LEU
1	I	304	PHE
1	J	12	VAL
1	J	15	SER
1	J	17	SER
1	J	22	LYS
1	J	26	VAL
1	J	29	LEU
1	J	32	THR
1	J	40	VAL
1	J	43	TRP
1	J	56	LEU
1	J	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	72	TRP
1	J	82	VAL
1	J	84	SER
1	J	87	THR
1	J	91	ARG
1	J	107	LEU
1	J	109	SER
1	J	118	LEU
1	J	124	GLN
1	J	128	LEU
1	J	130	LEU
1	J	134	SER
1	J	145	ILE
1	J	162	ILE
1	J	167	SER
1	J	172	ASP
1	J	178	LEU
1	J	182	GLN
1	J	194	ARG
1	J	202	SER
1	J	206	TRP
1	J	207	SER
1	J	212	LEU
1	J	219	SER
1	J	232	LEU
1	J	235	SER
1	J	238	LEU
1	J	240	LEU
1	J	250	SER
1	J	253	LEU
1	J	259	THR
1	J	260	THR
1	J	279	LEU
1	J	281	ILE
1	J	287	GLN
1	J	291	VAL
1	J	295	LEU
1	J	296	LEU
1	J	302	LEU
1	J	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	285	HIS
1	B	125	GLN
1	C	125	GLN
1	I	125	GLN
1	I	151	ASN
1	J	125	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	307/324 (94%)	-0.52	7 (2%) 60 54	57, 94, 173, 216	0
1	B	307/324 (94%)	-0.53	6 (1%) 65 60	59, 92, 176, 210	0
1	C	307/324 (94%)	-0.44	8 (2%) 56 49	56, 92, 174, 216	0
1	D	307/324 (94%)	-0.52	5 (1%) 72 66	57, 90, 172, 215	0
1	E	307/324 (94%)	-0.50	9 (2%) 51 45	57, 93, 177, 215	0
1	F	307/324 (94%)	-0.57	6 (1%) 65 60	59, 93, 173, 210	0
1	G	307/324 (94%)	-0.50	11 (3%) 42 38	57, 91, 175, 216	0
1	H	307/324 (94%)	-0.54	8 (2%) 56 49	57, 91, 174, 214	0
1	I	307/324 (94%)	-0.46	11 (3%) 42 38	56, 91, 174, 217	0
1	J	307/324 (94%)	-0.52	9 (2%) 51 45	56, 93, 174, 217	0
All	All	3070/3240 (94%)	-0.51	80 (2%) 56 49	56, 92, 176, 217	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	151	ASN	8.5
1	G	289	ASN	7.0
1	G	291	VAL	6.9
1	C	289	ASN	6.8
1	G	290	GLY	6.6
1	I	291	VAL	6.6
1	C	291	VAL	6.4
1	B	151	ASN	6.0
1	H	291	VAL	6.0
1	I	290	GLY	5.3
1	D	291	VAL	5.2
1	I	292	GLU	5.2
1	C	292	GLU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	288	ALA	5.1
1	I	289	ASN	4.9
1	I	288	ALA	4.7
1	J	291	VAL	4.6
1	H	289	ASN	4.5
1	D	290	GLY	4.5
1	A	152	ILE	4.5
1	I	153	ASP	4.5
1	A	151	ASN	4.4
1	B	315	LEU	4.3
1	J	152	ILE	4.1
1	E	152	ILE	4.1
1	F	151	ASN	4.1
1	C	180	SER	4.0
1	E	151	ASN	3.9
1	C	293	ASP	3.9
1	H	151	ASN	3.9
1	G	151	ASN	3.8
1	G	288	ALA	3.8
1	E	180	SER	3.7
1	G	179	SER	3.7
1	J	289	ASN	3.7
1	J	180	SER	3.5
1	I	287	GLN	3.5
1	H	288	ALA	3.5
1	H	290	GLY	3.5
1	E	291	VAL	3.5
1	G	292	GLU	3.4
1	J	290	GLY	3.4
1	A	291	VAL	3.4
1	G	180	SER	3.3
1	I	154	ASN	3.3
1	C	290	GLY	3.2
1	A	288	ALA	3.2
1	J	288	ALA	3.1
1	I	151	ASN	3.1
1	F	152	ILE	3.1
1	D	153	ASP	2.7
1	B	152	ILE	2.6
1	I	157	ILE	2.6
1	A	179	SER	2.6
1	H	152	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	314	VAL	2.6
1	E	306	LEU	2.6
1	J	157	ILE	2.5
1	G	287	GLN	2.5
1	H	292	GLU	2.5
1	B	180	SER	2.5
1	E	289	ASN	2.4
1	J	154	ASN	2.4
1	A	287	GLN	2.4
1	D	154	ASN	2.4
1	D	157	ILE	2.4
1	J	151	ASN	2.3
1	H	149	THR	2.3
1	A	286	ARG	2.2
1	E	290	GLY	2.2
1	F	287	GLN	2.2
1	G	152	ILE	2.1
1	I	152	ILE	2.1
1	B	313	CYS	2.1
1	F	313	CYS	2.1
1	E	157	ILE	2.1
1	E	288	ALA	2.1
1	F	156	GLU	2.1
1	F	154	ASN	2.0
1	G	293	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
2	NA	A	323	1/1	0.60	0.41	48,48,48,48	0
2	NA	F	323	1/1	0.70	0.36	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.