



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:36 PM GMT

PDB ID : 5A9V
Title : Structure of apo BipA
Authors : Kumar, V.; Chen, Y.; Ero, R.; Li, Z.; Gao, Y.
Deposited on : 2015-07-23
Resolution : 3.31 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

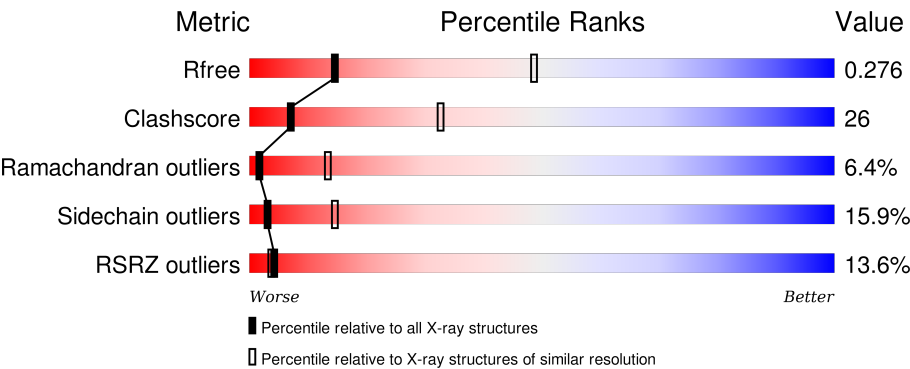
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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	607	<div><div>12%</div><div>59%</div><div>25%</div><div>5%</div><div>9%</div></div>
1	B	607	<div><div>13%</div><div>58%</div><div>26%</div><div>6%</div><div>9%</div></div>
1	C	607	<div><div>14%</div><div>59%</div><div>25%</div><div>6%</div><div>9%</div></div>
1	D	607	<div><div>12%</div><div>58%</div><div>25%</div><div>6%</div><div>9%</div></div>
1	E	607	<div><div>13%</div><div>59%</div><div>25%</div><div>5%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	607	<div><div></div><div>12%</div><div>58%</div><div>25%</div><div>6%</div><div>•</div><div>9%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25398 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.

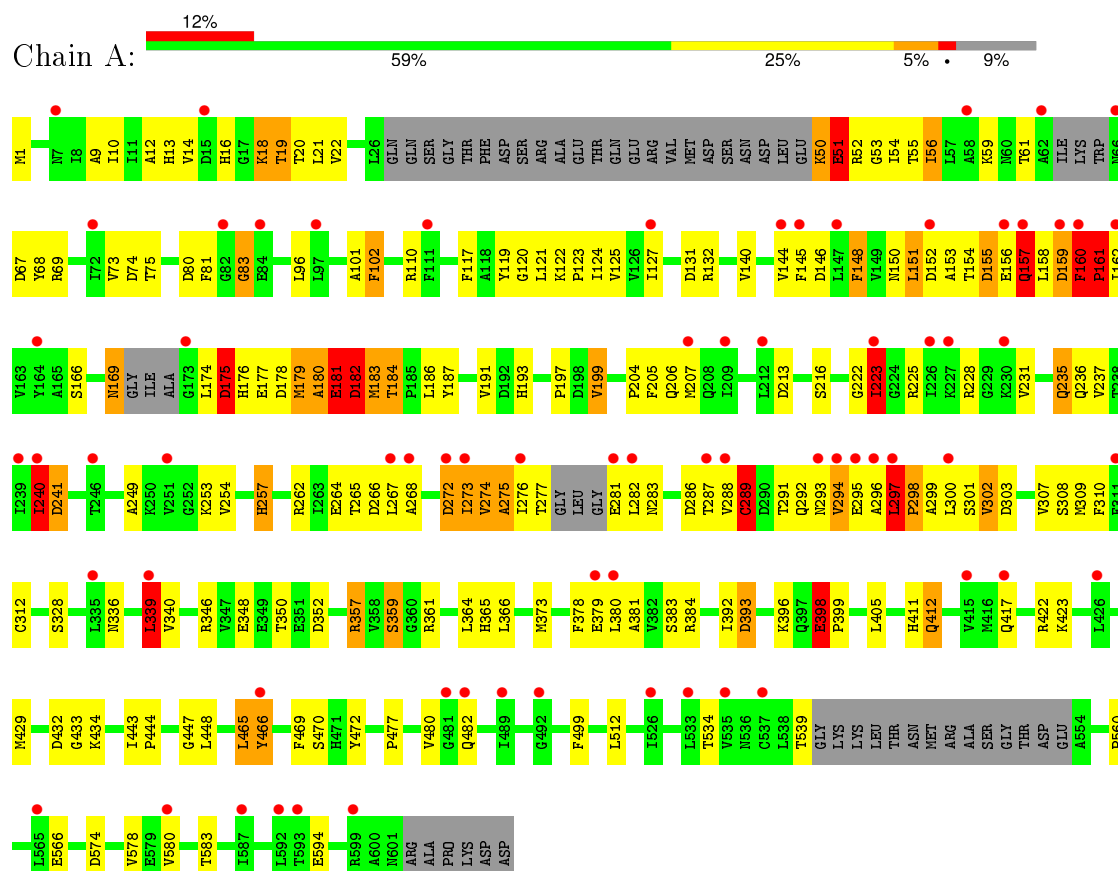
- Molecule 1 is a protein called GTP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	B	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	C	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	D	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	E	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	F	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			

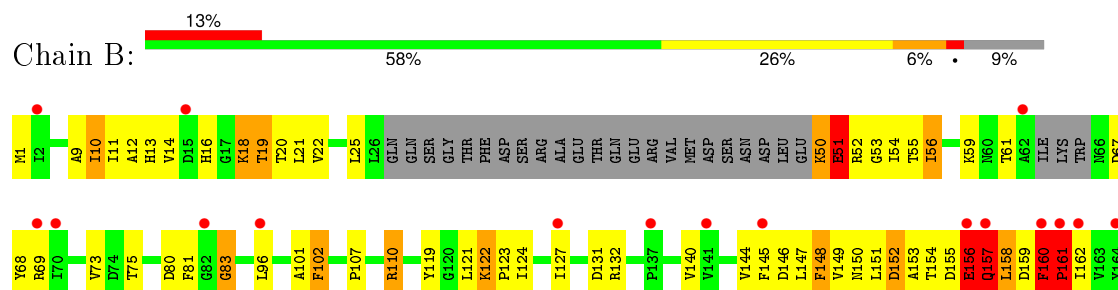
3 Residue-property plots

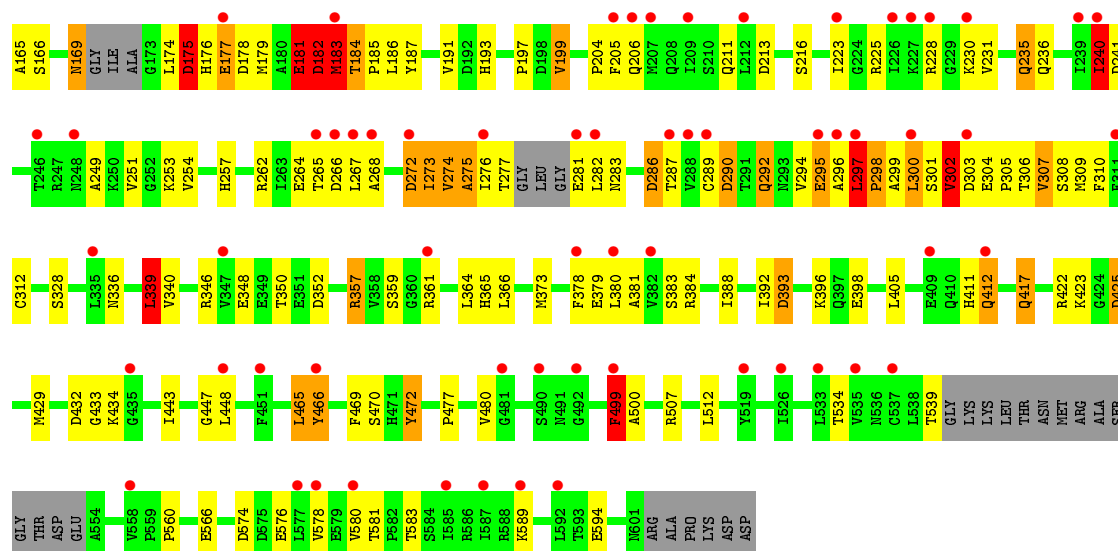
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GTP-BINDING PROTEIN

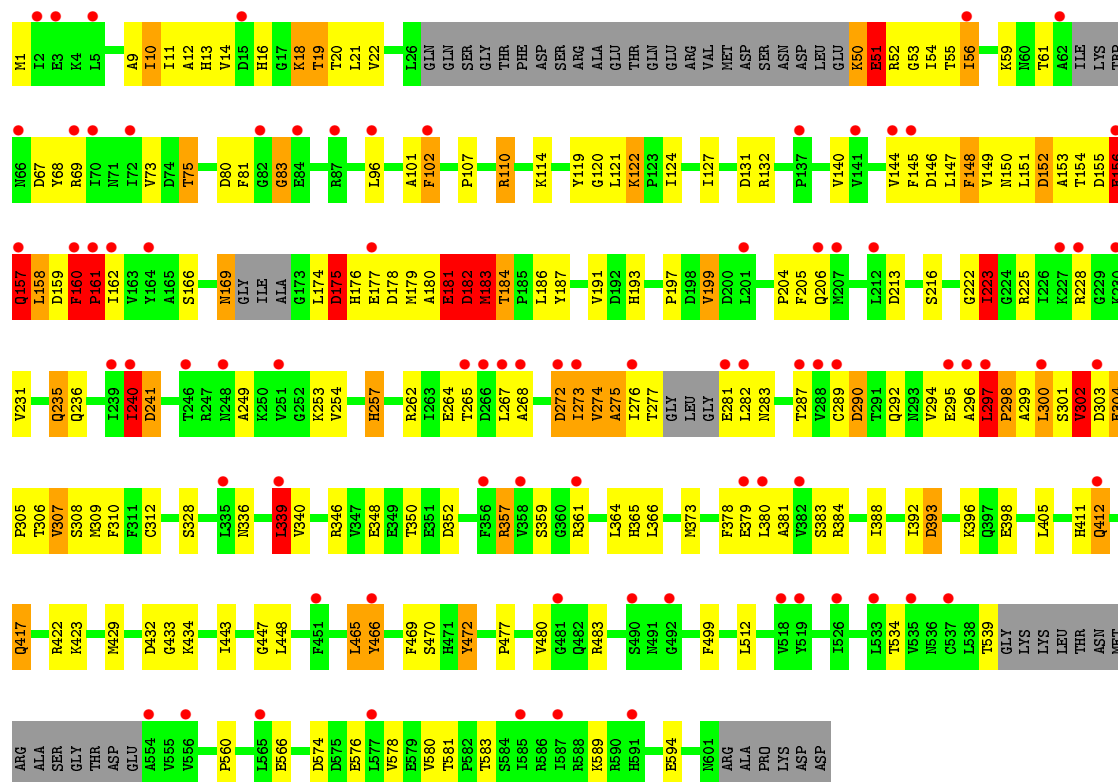


• Molecule 1: GTP-BINDING PROTEIN

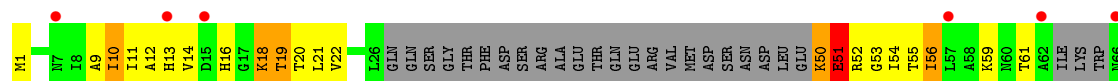


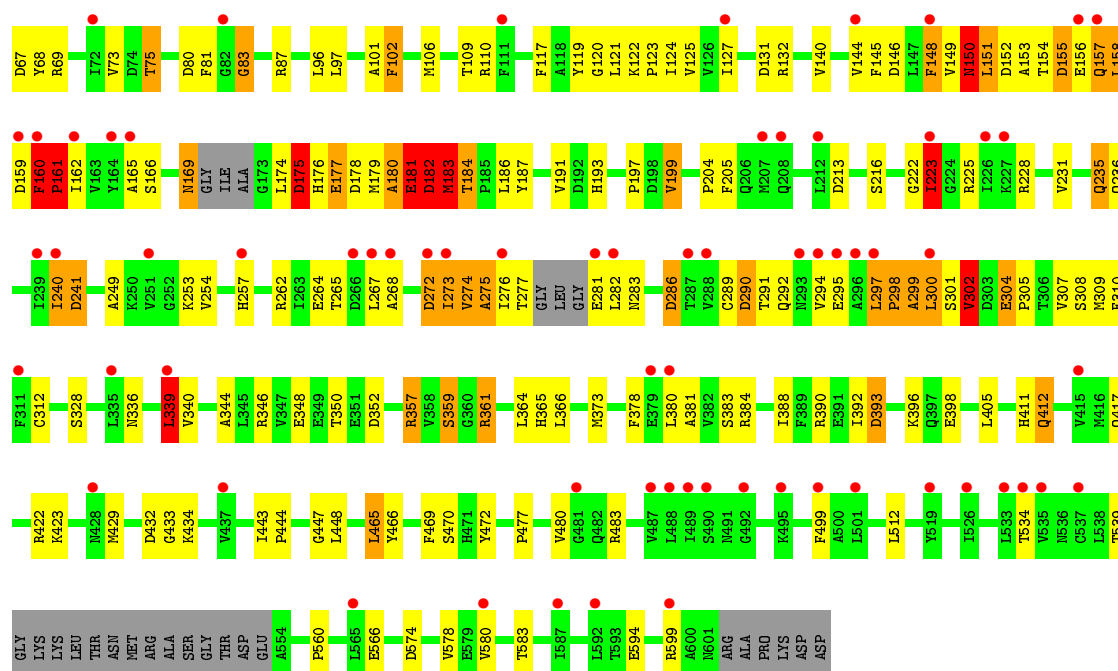


• Molecule 1: GTP-BINDING PROTEIN

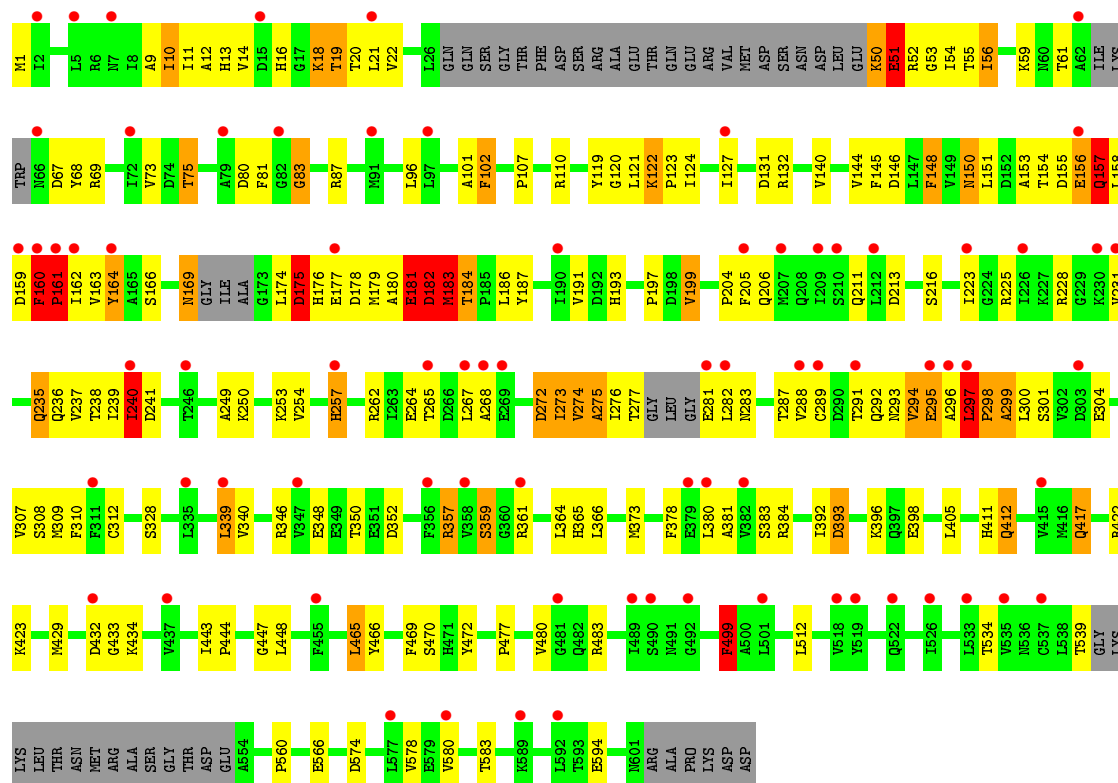


• Molecule 1: GTP-BINDING PROTEIN



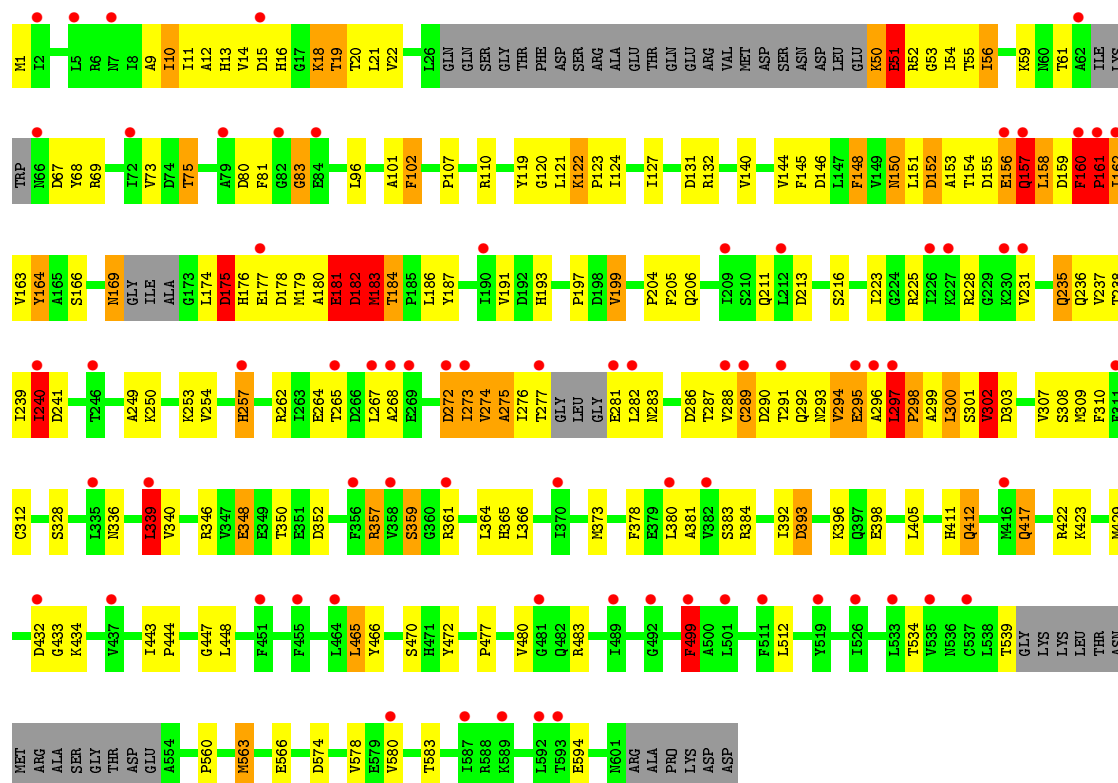


- Molecule 1: GTP-BINDING PROTEIN



- Molecule 1: GTP-BINDING PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	241.95Å 241.95Å 241.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.31 49.39 – 3.31	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.39-3.31) 91.9 (49.39-3.31)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.263 , 0.288 0.280 , 0.276	Depositor DCC
R_{free} test set	9472 reflections (11.14%)	DCC
Wilson B-factor (Å ²)	114.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 132.6	EDS
Estimated twinning fraction	0.429 for l,-k,h 0.429 for -l,-k,-h 0.429 for -h,-l,-k 0.429 for -h,l,k 0.439 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	120 of 94684 reflections (0.127%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25398	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.61	1/4292 (0.0%)	0.91	6/5786 (0.1%)
1	B	0.60	0/4292	0.91	8/5786 (0.1%)
1	C	0.59	0/4292	0.89	6/5786 (0.1%)
1	D	0.59	0/4292	0.89	6/5786 (0.1%)
1	E	0.58	0/4292	0.89	5/5786 (0.1%)
1	F	0.59	1/4292 (0.0%)	0.93	9/5786 (0.2%)
All	All	0.59	2/25752 (0.0%)	0.90	40/34716 (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	4
1	B	0	4
1	C	0	4
1	D	0	5
1	E	0	4
1	F	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	GLU	CD-OE2	-8.25	1.16	1.25
1	F	348	GLU	CD-OE2	-5.46	1.19	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	15	ASP	CB-CG-OD2	14.00	130.90	118.30
1	A	266	ASP	CB-CG-OD2	11.71	128.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	15	ASP	CB-CG-OD1	-11.48	107.97	118.30
1	A	398	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	F	563	MET	CA-CB-CG	-8.02	99.66	113.30
1	B	499	PHE	CB-CG-CD1	7.05	125.74	120.80
1	F	499	PHE	CB-CG-CD1	6.62	125.44	120.80
1	E	499	PHE	CB-CG-CD1	6.45	125.32	120.80
1	B	500	ALA	CB-CA-C	-6.18	100.83	110.10
1	B	161	PRO	N-CA-CB	5.98	110.48	103.30
1	F	161	PRO	N-CA-CB	5.98	110.47	103.30
1	A	161	PRO	N-CA-CB	5.97	110.46	103.30
1	C	161	PRO	N-CA-CB	5.94	110.43	103.30
1	E	161	PRO	N-CA-CB	5.93	110.42	103.30
1	D	161	PRO	N-CA-CB	5.92	110.41	103.30
1	A	69	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	69	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	69	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	E	69	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	F	69	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	69	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	466	TYR	CA-CB-CG	5.18	123.25	113.40
1	B	466	TYR	CA-CB-CG	5.18	123.24	113.40
1	F	348	GLU	CG-CD-OE1	5.18	128.66	118.30
1	C	466	TYR	CA-CB-CG	5.14	123.17	113.40
1	D	483	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	483	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	483	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	304	GLU	C-N-CD	5.08	139.07	128.40
1	E	297	LEU	C-N-CD	5.08	139.06	128.40
1	C	297	LEU	C-N-CD	5.07	139.05	128.40
1	F	297	LEU	C-N-CD	5.06	139.03	128.40
1	A	297	LEU	C-N-CD	5.06	139.02	128.40
1	D	304	GLU	C-N-CD	5.06	139.02	128.40
1	C	304	GLU	C-N-CD	5.05	139.01	128.40
1	D	297	LEU	C-N-CD	5.05	139.00	128.40
1	B	297	LEU	C-N-CD	5.04	138.99	128.40
1	B	286	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	C	483	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	286	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Peptide
1	A	19	THR	Peptide
1	A	240	ILE	Peptide
1	A	465	LEU	Peptide
1	B	132	ARG	Peptide
1	B	19	THR	Peptide
1	B	240	ILE	Peptide
1	B	465	LEU	Peptide
1	C	132	ARG	Peptide
1	C	19	THR	Peptide
1	C	240	ILE	Peptide
1	C	465	LEU	Peptide
1	D	132	ARG	Peptide
1	D	19	THR	Peptide
1	D	240	ILE	Peptide
1	D	291	THR	Peptide
1	D	465	LEU	Peptide
1	E	132	ARG	Peptide
1	E	19	THR	Peptide
1	E	240	ILE	Peptide
1	E	465	LEU	Peptide
1	F	132	ARG	Peptide
1	F	19	THR	Peptide
1	F	240	ILE	Peptide
1	F	465	LEU	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	4233	0	4156	217	0
1	B	4233	0	4156	238	0
1	C	4233	0	4156	240	0
1	D	4233	0	4155	213	0
1	E	4233	0	4156	218	0
1	F	4233	0	4156	221	0
All	All	25398	0	24935	1329	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 26.

All (1329) 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:287:THR:HB	1:A:297:LEU:CD1	1.13	1.55
1:B:169:ASN:HD21	1:B:182:ASP:N	1.09	1.48
1:A:287:THR:CB	1:A:297:LEU:CD1	1.94	1.45
1:C:287:THR:CB	1:C:297:LEU:HD11	1.53	1.39
1:D:169:ASN:OD1	1:D:182:ASP:CB	1.70	1.38
1:B:169:ASN:CG	1:B:182:ASP:HB2	1.02	1.37
1:B:287:THR:CB	1:B:297:LEU:HD11	1.56	1.33
1:C:287:THR:HB	1:C:297:LEU:CD1	1.57	1.32
1:B:169:ASN:CG	1:B:182:ASP:CB	1.98	1.31
1:A:287:THR:OG1	1:A:297:LEU:HG	1.22	1.30
1:B:287:THR:HB	1:B:297:LEU:CD1	1.59	1.30
1:E:123:PRO:HG2	1:E:156:GLU:OE2	1.14	1.29
1:B:289:CYS:CB	1:B:294:VAL:HG11	1.66	1.25
1:A:287:THR:CB	1:A:297:LEU:CG	2.15	1.25
1:C:289:CYS:CB	1:C:294:VAL:HG11	1.66	1.24
1:A:287:THR:CB	1:A:297:LEU:HG	1.65	1.24
1:B:169:ASN:OD1	1:B:182:ASP:HB2	1.28	1.24
1:F:123:PRO:CG	1:F:156:GLU:OE2	1.85	1.24
1:A:287:THR:CG2	1:A:297:LEU:HD12	1.69	1.22
1:C:287:THR:CB	1:C:297:LEU:CD1	2.15	1.21
1:B:169:ASN:ND2	1:B:182:ASP:N	1.90	1.19
1:D:289:CYS:SG	1:D:294:VAL:HG11	1.83	1.18
1:A:178:ASP:HB2	1:A:179:MET:HB2	1.19	1.17
1:B:183:MET:O	1:B:187:TYR:CD2	1.98	1.17
1:B:169:ASN:ND2	1:B:182:ASP:HB2	1.60	1.16
1:A:398:GLU:OE1	1:A:399:PRO:HD2	1.45	1.16
1:F:156:GLU:HG2	1:F:159:ASP:HB2	1.23	1.15
1:B:169:ASN:OD1	1:B:182:ASP:CB	1.93	1.15
1:F:239:ILE:CD1	1:F:288:VAL:HG13	1.75	1.15
1:B:287:THR:CB	1:B:297:LEU:CD1	2.18	1.14
1:E:289:CYS:HB2	1:E:294:VAL:HG11	1.30	1.13
1:A:287:THR:HB	1:A:297:LEU:HD12	1.27	1.13
1:B:289:CYS:HB2	1:B:294:VAL:HG11	1.13	1.13
1:C:289:CYS:SG	1:C:294:VAL:HG11	1.89	1.12
1:C:287:THR:CG2	1:C:297:LEU:HD12	1.79	1.12
1:C:178:ASP:HB2	1:C:179:MET:HB2	1.25	1.12
1:D:169:ASN:OD1	1:D:182:ASP:HB2	0.96	1.11
1:F:123:PRO:HG2	1:F:156:GLU:OE2	0.94	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:CYS:SG	1:B:294:VAL:HG11	1.91	1.10
1:C:289:CYS:HB2	1:C:294:VAL:HG11	1.16	1.10
1:A:156:GLU:HG3	1:A:159:ASP:HB2	1.22	1.10
1:F:239:ILE:HD13	1:F:288:VAL:HG13	1.26	1.09
1:C:287:THR:HG21	1:C:297:LEU:HD12	1.33	1.09
1:E:178:ASP:HB2	1:E:179:MET:HB2	1.26	1.09
1:D:178:ASP:HB2	1:D:179:MET:HB2	1.34	1.09
1:B:287:THR:CG2	1:B:297:LEU:HD12	1.82	1.09
1:E:123:PRO:CG	1:E:156:GLU:OE2	1.99	1.09
1:A:287:THR:HB	1:A:297:LEU:CG	1.81	1.08
1:A:287:THR:HG21	1:A:297:LEU:HB2	1.23	1.08
1:D:97:LEU:CD2	1:D:148:PHE:HZ	1.65	1.08
1:F:178:ASP:HB2	1:F:179:MET:HB2	1.25	1.08
1:B:178:ASP:HB2	1:B:179:MET:HB2	1.27	1.08
1:A:289:CYS:HB2	1:A:294:VAL:HG11	1.20	1.08
1:A:123:PRO:HG2	1:A:156:GLU:OE1	1.54	1.07
1:F:289:CYS:HB2	1:F:294:VAL:HG11	1.35	1.07
1:E:156:GLU:HG2	1:E:159:ASP:HB2	1.07	1.07
1:C:287:THR:CG2	1:C:297:LEU:CD1	2.32	1.07
1:B:287:THR:CG2	1:B:297:LEU:CD1	2.34	1.05
1:B:169:ASN:HD21	1:B:182:ASP:CA	1.68	1.05
1:C:305:PRO:HG3	1:C:346:ARG:HG3	1.33	1.05
1:B:305:PRO:HG3	1:B:346:ARG:HG3	1.30	1.05
1:D:160:PHE:CE2	1:D:162:ILE:HD12	1.91	1.04
1:D:123:PRO:HG2	1:D:156:GLU:OE1	1.56	1.04
1:A:287:THR:CB	1:A:297:LEU:HD12	1.71	1.04
1:C:156:GLU:HG2	1:C:159:ASP:HB2	1.38	1.04
1:B:287:THR:HG21	1:B:297:LEU:HD12	1.35	1.03
1:C:157:GLN:HG2	1:D:599:ARG:HD3	1.41	1.03
1:B:156:GLU:HG2	1:B:159:ASP:HB2	1.37	1.02
1:F:287:THR:HG21	1:F:297:LEU:HG	1.41	1.01
1:B:289:CYS:SG	1:B:294:VAL:CG1	2.49	1.00
1:F:160:PHE:CE2	1:F:162:ILE:HD12	1.96	1.00
1:C:156:GLU:HA	1:C:158:LEU:N	1.77	1.00
1:B:156:GLU:HA	1:B:158:LEU:N	1.77	1.00
1:A:287:THR:HG21	1:A:297:LEU:CB	1.89	1.00
1:A:124:ILE:HA	1:A:161:PRO:CB	1.90	1.00
1:E:156:GLU:HA	1:E:158:LEU:N	1.77	1.00
1:C:289:CYS:SG	1:C:294:VAL:CG1	2.48	1.00
1:F:156:GLU:HA	1:F:158:LEU:N	1.77	1.00
1:A:178:ASP:CB	1:A:179:MET:HB2	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:HG3	1:A:159:ASP:CB	1.92	1.00
1:C:156:GLU:CG	1:C:159:ASP:HB2	1.92	0.99
1:B:156:GLU:CG	1:B:159:ASP:HB2	1.92	0.99
1:D:156:GLU:HA	1:D:158:LEU:N	1.78	0.99
1:B:169:ASN:ND2	1:B:182:ASP:CB	2.18	0.99
1:A:156:GLU:HA	1:A:158:LEU:N	1.77	0.99
1:B:160:PHE:CD2	1:B:162:ILE:HD12	1.98	0.99
1:A:160:PHE:CE2	1:A:162:ILE:HD12	1.97	0.99
1:A:240:ILE:HD12	1:A:296:ALA:HB1	1.43	0.98
1:D:124:ILE:HA	1:D:161:PRO:CB	1.93	0.98
1:C:289:CYS:HB2	1:C:294:VAL:CG1	1.94	0.98
1:B:289:CYS:HB2	1:B:294:VAL:CG1	1.92	0.98
1:E:160:PHE:CE2	1:E:162:ILE:HD12	1.99	0.98
1:F:289:CYS:CB	1:F:294:VAL:HG11	1.92	0.98
1:C:169:ASN:ND2	1:C:182:ASP:O	1.97	0.97
1:B:294:VAL:HG12	1:B:295:GLU:H	1.26	0.97
1:B:169:ASN:ND2	1:B:182:ASP:CA	2.25	0.97
1:C:294:VAL:HG12	1:C:295:GLU:H	1.24	0.97
1:B:306:THR:CA	1:B:388:ILE:HD12	1.94	0.97
1:C:160:PHE:CD2	1:C:162:ILE:HD12	1.99	0.97
1:E:294:VAL:HG12	1:E:295:GLU:H	1.27	0.97
1:D:124:ILE:HG23	1:D:161:PRO:HA	1.46	0.97
1:E:289:CYS:CB	1:E:294:VAL:HG11	1.94	0.96
1:D:156:GLU:CG	1:D:159:ASP:HB2	1.95	0.96
1:D:156:GLU:HG3	1:D:159:ASP:HB2	1.47	0.96
1:E:169:ASN:ND2	1:E:182:ASP:O	1.97	0.96
1:F:169:ASN:ND2	1:F:182:ASP:O	1.97	0.96
1:A:124:ILE:HG23	1:A:161:PRO:HA	1.48	0.96
1:A:287:THR:HB	1:A:297:LEU:HD11	0.97	0.95
1:D:169:ASN:CG	1:D:182:ASP:CB	2.34	0.95
1:A:176:HIS:CG	1:A:177:GLU:HA	2.02	0.95
1:B:166:SER:N	1:B:182:ASP:OD2	2.00	0.95
1:D:97:LEU:CD2	1:D:148:PHE:CZ	2.49	0.95
1:C:160:PHE:CD1	1:C:162:ILE:HB	2.03	0.94
1:F:160:PHE:CD2	1:F:162:ILE:HD12	2.03	0.94
1:C:287:THR:HG21	1:C:297:LEU:CD1	1.95	0.94
1:B:160:PHE:CD1	1:B:162:ILE:HB	2.02	0.94
1:D:160:PHE:CD1	1:D:162:ILE:HB	2.02	0.93
1:B:287:THR:HG21	1:B:297:LEU:CD1	1.97	0.93
1:C:306:THR:CA	1:C:388:ILE:HD12	1.98	0.93
1:A:160:PHE:CD1	1:A:162:ILE:HB	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:GLU:CG	1:E:159:ASP:HB2	1.99	0.93
1:B:122:LYS:NZ	1:B:158:LEU:O	2.00	0.93
1:A:50:LYS:HE3	1:A:51:GLU:HG3	1.50	0.93
1:C:122:LYS:NZ	1:C:158:LEU:O	2.01	0.92
1:D:97:LEU:HD23	1:D:148:PHE:HZ	1.30	0.92
1:F:156:GLU:CG	1:F:159:ASP:HB2	1.97	0.92
1:D:305:PRO:HD2	1:D:390:ARG:CZ	1.99	0.92
1:E:160:PHE:CD2	1:E:162:ILE:HD12	2.05	0.92
1:D:160:PHE:CD2	1:D:162:ILE:HD12	2.05	0.91
1:A:287:THR:HG1	1:A:297:LEU:HG	1.22	0.91
1:E:156:GLU:HA	1:E:158:LEU:H	1.35	0.91
1:C:160:PHE:CE2	1:C:162:ILE:HD12	2.06	0.90
1:E:156:GLU:HG2	1:E:159:ASP:CB	2.01	0.90
1:C:178:ASP:CB	1:C:179:MET:HB2	2.02	0.90
1:A:289:CYS:CB	1:A:294:VAL:HG11	2.02	0.90
1:A:287:THR:CG2	1:A:297:LEU:CD1	2.39	0.90
1:F:178:ASP:CB	1:F:179:MET:HB2	2.02	0.90
1:B:183:MET:O	1:B:187:TYR:HD2	1.42	0.89
1:D:160:PHE:CE1	1:D:162:ILE:HB	2.07	0.89
1:F:52:ARG:HB3	1:F:53:GLY:HA3	1.55	0.89
1:E:178:ASP:CB	1:E:179:MET:HB2	2.02	0.89
1:E:52:ARG:HB3	1:E:53:GLY:HA3	1.55	0.89
1:B:169:ASN:HD21	1:B:182:ASP:H	1.17	0.89
1:B:160:PHE:CE2	1:B:162:ILE:HD12	2.07	0.89
1:B:178:ASP:CB	1:B:179:MET:HB2	2.03	0.88
1:F:294:VAL:HG12	1:F:295:GLU:H	1.37	0.88
1:F:239:ILE:HD12	1:F:288:VAL:HG22	1.54	0.88
1:F:287:THR:HB	1:F:297:LEU:HD11	1.52	0.88
1:E:160:PHE:CD1	1:E:162:ILE:HB	2.08	0.88
1:D:156:GLU:HA	1:D:158:LEU:H	1.38	0.88
1:C:147:LEU:HA	1:C:150:ASN:OD1	1.74	0.88
1:F:160:PHE:CD1	1:F:162:ILE:HB	2.09	0.88
1:B:52:ARG:HB3	1:B:53:GLY:HA3	1.55	0.88
1:A:160:PHE:CD2	1:A:162:ILE:HD12	2.09	0.88
1:C:50:LYS:HE3	1:C:51:GLU:HG3	1.56	0.88
1:D:169:ASN:ND2	1:D:182:ASP:O	2.07	0.87
1:A:156:GLU:HA	1:A:158:LEU:H	1.39	0.87
1:A:169:ASN:HD21	1:A:182:ASP:C	1.78	0.87
1:D:169:ASN:CG	1:D:182:ASP:HB2	1.94	0.86
1:C:289:CYS:CB	1:C:294:VAL:CG1	2.51	0.86
1:A:54:ILE:CG2	1:A:55:THR:HG22	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HA	1:B:150:ASN:OD1	1.75	0.86
1:C:54:ILE:CG2	1:C:55:THR:HG22	2.06	0.86
1:D:54:ILE:CG2	1:D:55:THR:HG22	2.06	0.86
1:F:239:ILE:CD1	1:F:288:VAL:CG1	2.53	0.86
1:A:287:THR:HG22	1:A:297:LEU:HD12	1.58	0.86
1:C:156:GLU:HA	1:C:158:LEU:H	1.40	0.86
1:A:160:PHE:CE1	1:A:162:ILE:HB	2.11	0.86
1:A:169:ASN:ND2	1:A:182:ASP:O	2.09	0.86
1:B:169:ASN:ND2	1:B:182:ASP:H	1.69	0.85
1:B:289:CYS:CB	1:B:294:VAL:CG1	2.50	0.85
1:A:287:THR:CG2	1:A:297:LEU:CG	2.53	0.85
1:D:97:LEU:HD23	1:D:148:PHE:CZ	2.11	0.85
1:B:156:GLU:HA	1:B:158:LEU:H	1.40	0.85
1:B:160:PHE:CE1	1:B:162:ILE:HB	2.12	0.85
1:D:178:ASP:HB2	1:D:179:MET:CB	2.06	0.85
1:D:294:VAL:HG12	1:D:295:GLU:H	1.39	0.85
1:F:123:PRO:HG2	1:F:156:GLU:CD	1.96	0.84
1:C:174:LEU:HG	1:C:175:ASP:OD2	1.77	0.84
1:B:61:THR:OG1	1:B:67:ASP:HA	1.78	0.84
1:D:289:CYS:CB	1:D:294:VAL:HG11	2.07	0.84
1:D:156:GLU:N	1:D:157:GLN:HB2	1.92	0.84
1:A:61:THR:OG1	1:A:67:ASP:HA	1.78	0.84
1:F:156:GLU:HA	1:F:158:LEU:H	1.40	0.84
1:C:22:VAL:CG1	1:C:56:ILE:HG21	2.08	0.84
1:D:61:THR:OG1	1:D:67:ASP:HA	1.78	0.84
1:A:181:GLU:O	1:A:183:MET:N	2.11	0.83
1:F:174:LEU:HG	1:F:175:ASP:OD2	1.77	0.83
1:C:160:PHE:CE1	1:C:162:ILE:HB	2.12	0.83
1:A:294:VAL:HG12	1:A:295:GLU:H	1.42	0.83
1:F:61:THR:OG1	1:F:67:ASP:HA	1.77	0.83
1:C:61:THR:OG1	1:C:67:ASP:HA	1.78	0.83
1:A:287:THR:HG21	1:A:297:LEU:CG	2.08	0.83
1:D:289:CYS:SG	1:D:294:VAL:CG1	2.67	0.83
1:A:176:HIS:NE2	1:A:177:GLU:OE1	2.12	0.83
1:B:25:LEU:HD23	1:B:183:MET:SD	2.18	0.83
1:A:153:ALA:HB3	1:A:154:THR:C	1.99	0.83
1:D:22:VAL:CG1	1:D:56:ILE:HG21	2.08	0.83
1:E:160:PHE:CE1	1:E:162:ILE:HB	2.14	0.82
1:F:160:PHE:CE1	1:F:162:ILE:HB	2.14	0.82
1:E:296:ALA:C	1:E:297:LEU:HD23	1.98	0.82
1:E:61:THR:OG1	1:E:67:ASP:HA	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASN:HD21	1:D:182:ASP:CA	1.92	0.82
1:F:178:ASP:HB2	1:F:179:MET:CB	2.09	0.82
1:E:178:ASP:HB2	1:E:179:MET:CB	2.09	0.82
1:D:153:ALA:HB3	1:D:154:THR:C	2.00	0.82
1:D:157:GLN:HB3	1:D:158:LEU:HD12	1.61	0.82
1:F:169:ASN:HD21	1:F:182:ASP:C	1.83	0.82
1:E:300:LEU:HB2	1:E:301:SER:HA	1.61	0.82
1:E:169:ASN:HD21	1:E:182:ASP:C	1.83	0.82
1:A:169:ASN:HD21	1:A:182:ASP:CA	1.88	0.82
1:A:289:CYS:HB2	1:A:294:VAL:CG1	2.08	0.81
1:A:287:THR:OG1	1:A:297:LEU:CG	2.15	0.81
1:D:169:ASN:OD1	1:D:182:ASP:HB3	1.78	0.81
1:F:160:PHE:CZ	1:F:162:ILE:HD12	2.14	0.81
1:D:157:GLN:O	1:D:159:ASP:HB3	1.80	0.81
1:F:153:ALA:HB3	1:F:154:THR:C	2.00	0.81
1:E:174:LEU:HG	1:E:175:ASP:OD2	1.79	0.81
1:E:153:ALA:HB3	1:E:154:THR:C	2.00	0.81
1:D:178:ASP:CB	1:D:179:MET:HB2	2.11	0.81
1:C:169:ASN:HD21	1:C:182:ASP:CA	1.93	0.81
1:D:50:LYS:HE3	1:D:51:GLU:HG3	1.63	0.81
1:B:169:ASN:OD1	1:B:182:ASP:CG	2.19	0.81
1:C:169:ASN:HD21	1:C:182:ASP:C	1.83	0.80
1:A:177:GLU:N	1:A:178:ASP:HA	1.96	0.80
1:D:169:ASN:CG	1:D:182:ASP:HB3	2.02	0.80
1:E:157:GLN:O	1:E:159:ASP:HB3	1.80	0.80
1:B:176:HIS:CG	1:B:177:GLU:HA	2.17	0.80
1:B:153:ALA:HB3	1:B:154:THR:C	2.02	0.80
1:E:156:GLU:N	1:E:157:GLN:HB2	1.96	0.80
1:F:239:ILE:HD11	1:F:288:VAL:HG13	1.63	0.80
1:A:240:ILE:CD1	1:A:296:ALA:HB1	2.11	0.79
1:C:153:ALA:HB3	1:C:154:THR:C	2.02	0.79
1:F:156:GLU:N	1:F:157:GLN:HB2	1.97	0.79
1:B:178:ASP:HB2	1:B:179:MET:CB	2.11	0.79
1:E:169:ASN:HD21	1:E:182:ASP:CA	1.93	0.79
1:E:160:PHE:CZ	1:E:162:ILE:HD12	2.17	0.79
1:F:157:GLN:O	1:F:159:ASP:HB3	1.81	0.79
1:E:123:PRO:HG2	1:E:156:GLU:CD	2.01	0.79
1:F:169:ASN:HD21	1:F:182:ASP:CA	1.93	0.79
1:E:287:THR:HG21	1:E:297:LEU:HG	1.64	0.78
1:B:287:THR:OG1	1:B:297:LEU:HG	1.83	0.78
1:B:177:GLU:H	1:B:179:MET:HG3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ILE:CG2	1:D:161:PRO:HA	2.14	0.78
1:F:176:HIS:HA	1:F:177:GLU:C	2.05	0.78
1:B:306:THR:HA	1:B:388:ILE:HD12	1.67	0.77
1:D:169:ASN:HD21	1:D:182:ASP:C	1.88	0.77
1:F:287:THR:CG2	1:F:297:LEU:HG	2.14	0.77
1:C:178:ASP:HB2	1:C:179:MET:CB	2.09	0.77
1:C:287:THR:OG1	1:C:297:LEU:HG	1.84	0.77
1:B:306:THR:N	1:B:388:ILE:HD12	1.99	0.77
1:C:158:LEU:HA	1:C:159:ASP:HB3	1.67	0.77
1:D:176:HIS:HA	1:D:177:GLU:C	2.05	0.77
1:D:174:LEU:HG	1:D:175:ASP:OD2	1.85	0.77
1:A:156:GLU:CG	1:A:159:ASP:HB2	2.09	0.77
1:D:156:GLU:H	1:D:157:GLN:HB2	1.49	0.77
1:A:117:PHE:CD2	1:A:152:ASP:O	2.37	0.77
1:C:176:HIS:HA	1:C:177:GLU:C	2.05	0.76
1:B:158:LEU:HA	1:B:159:ASP:HB3	1.66	0.76
1:E:239:ILE:CD1	1:E:288:VAL:HG13	2.15	0.76
1:E:300:LEU:HB2	1:E:301:SER:CA	2.16	0.76
1:A:50:LYS:CE	1:A:51:GLU:HG3	2.15	0.76
1:A:124:ILE:CG2	1:A:161:PRO:HA	2.15	0.76
1:A:157:GLN:O	1:A:159:ASP:HB3	1.86	0.75
1:D:180:ALA:O	1:D:182:ASP:N	2.19	0.75
1:C:306:THR:N	1:C:388:ILE:HD12	2.01	0.75
1:E:300:LEU:HB3	1:E:304:GLU:HG3	1.67	0.75
1:D:158:LEU:HA	1:D:159:ASP:HB3	1.69	0.74
1:B:181:GLU:O	1:B:183:MET:N	2.20	0.74
1:E:176:HIS:HA	1:E:177:GLU:C	2.08	0.74
1:B:160:PHE:HA	1:B:161:PRO:C	2.08	0.74
1:D:156:GLU:CA	1:D:157:GLN:HB2	2.17	0.74
1:B:176:HIS:HA	1:B:177:GLU:C	2.06	0.74
1:C:289:CYS:SG	1:C:294:VAL:HG12	2.27	0.74
1:A:174:LEU:HG	1:A:175:ASP:OD2	1.86	0.74
1:A:22:VAL:CG1	1:A:56:ILE:HG21	2.18	0.73
1:E:287:THR:HB	1:E:297:LEU:CD1	2.19	0.73
1:F:163:VAL:HG13	1:F:176:HIS:CD2	2.24	0.73
1:F:297:LEU:N	1:F:297:LEU:HD23	2.03	0.73
1:C:294:VAL:HG12	1:C:295:GLU:N	2.03	0.73
1:F:160:PHE:HA	1:F:161:PRO:C	2.08	0.73
1:D:117:PHE:HZ	1:D:148:PHE:CD1	2.07	0.73
1:A:54:ILE:HG22	1:A:55:THR:HG22	1.69	0.73
1:B:289:CYS:SG	1:B:294:VAL:HG12	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PHE:O	1:B:193:HIS:NE2	2.22	0.73
1:E:297:LEU:N	1:E:297:LEU:HD23	2.03	0.73
1:E:160:PHE:HA	1:E:161:PRO:C	2.08	0.72
1:C:54:ILE:HG22	1:C:55:THR:HG22	1.70	0.72
1:E:153:ALA:HB3	1:E:154:THR:CA	2.20	0.72
1:D:106:MET:O	1:D:109:THR:OG1	2.06	0.72
1:C:160:PHE:HA	1:C:161:PRO:C	2.08	0.72
1:F:287:THR:HB	1:F:297:LEU:CD1	2.19	0.72
1:D:289:CYS:HB2	1:D:294:VAL:HG11	1.69	0.72
1:D:54:ILE:HG22	1:D:55:THR:HG22	1.70	0.72
1:E:287:THR:HG21	1:E:297:LEU:CG	2.19	0.72
1:C:306:THR:HA	1:C:388:ILE:HB	1.72	0.72
1:A:240:ILE:CD1	1:A:296:ALA:CB	2.67	0.72
1:C:156:GLU:N	1:C:157:GLN:HB2	2.05	0.71
1:F:240:ILE:HD12	1:F:287:THR:OG1	1.89	0.71
1:A:297:LEU:HD23	1:A:297:LEU:N	2.04	0.71
1:F:158:LEU:HA	1:F:159:ASP:HB3	1.71	0.71
1:B:183:MET:O	1:B:187:TYR:CE2	2.43	0.71
1:B:177:GLU:N	1:B:178:ASP:HA	2.04	0.71
1:D:156:GLU:HG2	1:D:159:ASP:HB2	1.70	0.71
1:E:87:ARG:NH2	1:E:300:LEU:O	2.23	0.71
1:F:153:ALA:HB3	1:F:154:THR:CA	2.21	0.71
1:D:22:VAL:CG1	1:D:56:ILE:HD13	2.21	0.71
1:C:22:VAL:CG1	1:C:56:ILE:HD13	2.21	0.71
1:C:160:PHE:O	1:C:193:HIS:NE2	2.22	0.71
1:A:160:PHE:HA	1:A:161:PRO:C	2.10	0.71
1:B:300:LEU:CB	1:B:301:SER:HA	2.19	0.71
1:C:287:THR:CB	1:C:297:LEU:CG	2.69	0.70
1:E:294:VAL:C	1:E:295:GLU:HG2	2.10	0.70
1:A:22:VAL:CG1	1:A:56:ILE:HD13	2.21	0.70
1:F:277:THR:HB	1:F:281:GLU:N	2.06	0.70
1:A:237:VAL:HA	1:A:291:THR:HG23	1.72	0.70
1:A:178:ASP:CA	1:A:179:MET:HB2	2.20	0.70
1:C:222:GLY:O	1:C:223:ILE:O	2.09	0.70
1:C:300:LEU:CB	1:C:301:SER:HA	2.19	0.70
1:C:306:THR:HA	1:C:388:ILE:HD12	1.71	0.70
1:B:150:ASN:ND2	1:B:151:LEU:HD22	2.06	0.70
1:C:157:GLN:O	1:C:159:ASP:HB3	1.92	0.70
1:C:150:ASN:ND2	1:C:151:LEU:HD22	2.06	0.70
1:B:306:THR:HB	1:B:472:TYR:OH	1.91	0.70
1:B:52:ARG:CB	1:B:53:GLY:HA3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ALA:HB3	1:D:154:THR:CA	2.22	0.70
1:C:301:SER:O	1:C:302:VAL:HG13	1.92	0.70
1:C:153:ALA:HB3	1:C:154:THR:CA	2.21	0.70
1:B:306:THR:HA	1:B:388:ILE:HB	1.72	0.70
1:B:156:GLU:N	1:B:157:GLN:HB2	2.06	0.70
1:F:52:ARG:CB	1:F:53:GLY:HA3	2.21	0.70
1:E:158:LEU:HA	1:E:159:ASP:HB3	1.74	0.70
1:B:153:ALA:HB3	1:B:154:THR:CA	2.21	0.70
1:C:277:THR:HB	1:C:281:GLU:N	2.07	0.70
1:F:13:HIS:O	1:F:16:HIS:CE1	2.45	0.70
1:B:294:VAL:HG12	1:B:295:GLU:N	2.05	0.70
1:E:52:ARG:CB	1:E:53:GLY:HA3	2.21	0.70
1:C:13:HIS:O	1:C:16:HIS:CE1	2.45	0.70
1:D:169:ASN:HD21	1:D:182:ASP:N	1.89	0.69
1:F:239:ILE:CD1	1:F:288:VAL:HG22	2.21	0.69
1:A:169:ASN:ND2	1:A:182:ASP:C	2.45	0.69
1:B:287:THR:CB	1:B:297:LEU:CG	2.70	0.69
1:B:294:VAL:C	1:B:295:GLU:HG2	2.13	0.69
1:F:287:THR:HG21	1:F:297:LEU:CG	2.20	0.69
1:C:54:ILE:HG23	1:C:55:THR:HG22	1.75	0.69
1:B:13:HIS:O	1:B:16:HIS:CE1	2.46	0.69
1:E:13:HIS:O	1:E:16:HIS:CE1	2.45	0.69
1:C:50:LYS:CE	1:C:51:GLU:HG3	2.23	0.69
1:D:13:HIS:O	1:D:16:HIS:CE1	2.45	0.69
1:A:54:ILE:HG22	1:A:55:THR:CG2	2.23	0.69
1:D:22:VAL:HG12	1:D:56:ILE:HG21	1.75	0.69
1:E:239:ILE:HD13	1:E:288:VAL:HG13	1.73	0.69
1:B:301:SER:O	1:B:302:VAL:HG13	1.93	0.69
1:B:157:GLN:O	1:B:159:ASP:HB3	1.93	0.69
1:D:54:ILE:HG22	1:D:55:THR:CG2	2.23	0.69
1:E:50:LYS:HE3	1:E:51:GLU:HG3	1.75	0.68
1:D:22:VAL:HG11	1:D:56:ILE:HD13	1.76	0.68
1:F:300:LEU:CB	1:F:301:SER:HA	2.23	0.68
1:C:292:GLN:O	1:C:294:VAL:HG23	1.94	0.68
1:D:277:THR:HB	1:D:281:GLU:N	2.07	0.68
1:C:54:ILE:HG22	1:C:55:THR:CG2	2.23	0.68
1:C:294:VAL:C	1:C:295:GLU:HG2	2.14	0.68
1:E:287:THR:CB	1:E:297:LEU:HG	2.23	0.68
1:A:160:PHE:CZ	1:A:162:ILE:HD12	2.28	0.68
1:C:22:VAL:HG11	1:C:56:ILE:HD13	1.75	0.68
1:F:160:PHE:CG	1:F:162:ILE:HD12	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:VAL:HG12	1:E:295:GLU:N	2.07	0.68
1:A:13:HIS:O	1:A:16:HIS:CE1	2.46	0.68
1:E:150:ASN:ND2	1:E:151:LEU:HD22	2.07	0.68
1:E:277:THR:HB	1:E:281:GLU:N	2.09	0.68
1:F:239:ILE:HD13	1:F:288:VAL:CG1	2.13	0.67
1:E:160:PHE:CG	1:E:162:ILE:HD12	2.30	0.67
1:A:398:GLU:OE1	1:A:399:PRO:CD	2.34	0.67
1:A:153:ALA:HB3	1:A:154:THR:CA	2.24	0.67
1:A:145:PHE:O	1:A:148:PHE:HB3	1.94	0.67
1:D:290:ASP:O	1:D:294:VAL:HG21	1.94	0.67
1:D:301:SER:O	1:D:302:VAL:HG13	1.94	0.67
1:B:150:ASN:O	1:C:423:LYS:NZ	2.27	0.67
1:B:160:PHE:O	1:B:193:HIS:CE1	2.48	0.67
1:A:156:GLU:N	1:A:157:GLN:HB2	2.10	0.67
1:B:145:PHE:O	1:B:148:PHE:HB3	1.95	0.67
1:B:297:LEU:HD23	1:B:297:LEU:N	2.10	0.67
1:B:277:THR:HB	1:B:281:GLU:N	2.09	0.67
1:E:287:THR:HB	1:E:297:LEU:HD11	1.76	0.67
1:A:176:HIS:HA	1:A:177:GLU:C	2.15	0.66
1:C:160:PHE:CG	1:C:162:ILE:HD12	2.30	0.66
1:D:300:LEU:CB	1:D:301:SER:HA	2.22	0.66
1:A:54:ILE:HG23	1:A:55:THR:HG22	1.75	0.66
1:D:54:ILE:HG23	1:D:55:THR:HG22	1.75	0.66
1:F:50:LYS:HE3	1:F:51:GLU:HG3	1.77	0.66
1:C:22:VAL:HG12	1:C:56:ILE:HG21	1.75	0.66
1:B:50:LYS:HE3	1:B:51:GLU:HG3	1.75	0.66
1:F:240:ILE:CD1	1:F:287:THR:OG1	2.43	0.66
1:A:240:ILE:HD13	1:A:296:ALA:HB2	1.78	0.66
1:B:292:GLN:O	1:B:294:VAL:HG23	1.96	0.66
1:D:160:PHE:HA	1:D:161:PRO:C	2.15	0.66
1:E:300:LEU:HD12	1:E:300:LEU:N	2.11	0.66
1:A:22:VAL:HG11	1:A:56:ILE:HD13	1.78	0.66
1:C:306:THR:HB	1:C:472:TYR:OH	1.95	0.66
1:B:300:LEU:HB2	1:B:301:SER:HA	1.77	0.66
1:D:117:PHE:HZ	1:D:148:PHE:CE1	2.13	0.65
1:B:160:PHE:CG	1:B:162:ILE:HD12	2.31	0.65
1:C:160:PHE:O	1:C:193:HIS:CE1	2.48	0.65
1:C:145:PHE:O	1:C:148:PHE:HB3	1.94	0.65
1:A:277:THR:HB	1:A:281:GLU:N	2.10	0.65
1:F:181:GLU:O	1:F:183:MET:N	2.30	0.65
1:F:373:MET:O	1:F:378:PHE:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:THR:CG2	1:E:297:LEU:HG	2.25	0.65
1:E:163:VAL:HG13	1:E:176:HIS:CD2	2.32	0.65
1:F:294:VAL:C	1:F:295:GLU:HG2	2.16	0.65
1:A:174:LEU:H	1:A:174:LEU:HD23	1.62	0.65
1:E:181:GLU:O	1:E:183:MET:N	2.30	0.65
1:C:300:LEU:HB2	1:C:301:SER:HA	1.77	0.65
1:B:165:ALA:HA	1:B:182:ASP:OD2	1.97	0.65
1:C:373:MET:O	1:C:378:PHE:HB2	1.97	0.65
1:E:373:MET:O	1:E:378:PHE:HB2	1.97	0.65
1:B:287:THR:HG21	1:B:297:LEU:CG	2.27	0.64
1:F:239:ILE:HD11	1:F:288:VAL:CG1	2.24	0.64
1:A:123:PRO:CG	1:A:156:GLU:OE1	2.40	0.64
1:B:158:LEU:CA	1:B:159:ASP:HB3	2.27	0.64
1:A:300:LEU:CB	1:A:301:SER:HA	2.25	0.64
1:C:297:LEU:HD23	1:C:297:LEU:N	2.12	0.64
1:C:177:GLU:N	1:C:178:ASP:HA	2.13	0.64
1:F:150:ASN:ND2	1:F:151:LEU:HD22	2.12	0.64
1:D:373:MET:O	1:D:378:PHE:HB2	1.97	0.64
1:A:249:ALA:HB3	1:A:275:ALA:HB2	1.80	0.64
1:D:177:GLU:CB	1:D:178:ASP:HA	2.25	0.64
1:A:176:HIS:ND1	1:A:177:GLU:HA	2.12	0.64
1:B:176:HIS:NE2	1:B:177:GLU:OE1	2.31	0.64
1:D:249:ALA:HB3	1:D:275:ALA:HB2	1.80	0.64
1:C:287:THR:HG21	1:C:297:LEU:CG	2.27	0.64
1:E:177:GLU:N	1:E:178:ASP:HA	2.12	0.64
1:D:169:ASN:ND2	1:D:182:ASP:CB	2.61	0.64
1:F:296:ALA:C	1:F:297:LEU:HD23	2.18	0.64
1:B:249:ALA:HB3	1:B:275:ALA:HB2	1.80	0.64
1:F:249:ALA:HB3	1:F:275:ALA:HB2	1.80	0.64
1:A:151:LEU:O	1:A:152:ASP:HB2	1.97	0.63
1:C:181:GLU:O	1:C:183:MET:N	2.30	0.63
1:B:373:MET:O	1:B:378:PHE:HB2	1.97	0.63
1:A:22:VAL:HG12	1:A:56:ILE:HG21	1.80	0.63
1:F:169:ASN:ND2	1:F:182:ASP:C	2.47	0.63
1:A:373:MET:O	1:A:378:PHE:HB2	1.98	0.63
1:E:249:ALA:HB3	1:E:275:ALA:HB2	1.80	0.63
1:E:177:GLU:H	1:E:179:MET:HG3	1.64	0.63
1:D:155:ASP:O	1:D:156:GLU:HB3	1.98	0.63
1:B:423:LYS:NZ	1:C:150:ASN:O	2.32	0.63
1:A:22:VAL:HG11	1:A:56:ILE:CD1	2.29	0.63
1:F:177:GLU:N	1:F:178:ASP:HA	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:CA	1:C:159:ASP:HB3	2.28	0.63
1:E:123:PRO:HG3	1:E:148:PHE:HZ	1.63	0.63
1:C:249:ALA:HB3	1:C:275:ALA:HB2	1.80	0.63
1:E:169:ASN:ND2	1:E:182:ASP:C	2.47	0.62
1:F:160:PHE:HA	1:F:162:ILE:HG13	1.81	0.62
1:D:181:GLU:O	1:D:183:MET:N	2.31	0.62
1:F:180:ALA:O	1:F:182:ASP:N	2.32	0.62
1:B:432:ASP:O	1:B:434:LYS:N	2.33	0.62
1:C:287:THR:OG1	1:C:297:LEU:CG	2.47	0.62
1:C:180:ALA:O	1:C:182:ASP:N	2.32	0.62
1:E:180:ALA:O	1:E:182:ASP:N	2.32	0.62
1:F:432:ASP:O	1:F:434:LYS:N	2.32	0.62
1:B:287:THR:OG1	1:B:297:LEU:CG	2.47	0.62
1:E:432:ASP:O	1:E:434:LYS:N	2.32	0.62
1:A:287:THR:CG2	1:A:297:LEU:HG	2.23	0.62
1:A:300:LEU:HB2	1:A:301:SER:HA	1.80	0.62
1:E:123:PRO:CB	1:E:156:GLU:OE2	2.47	0.61
1:A:50:LYS:HD3	1:A:51:GLU:HB2	1.81	0.61
1:D:300:LEU:HB2	1:D:301:SER:HA	1.81	0.61
1:C:50:LYS:HD3	1:C:51:GLU:HB2	1.81	0.61
1:A:117:PHE:HD2	1:A:152:ASP:O	1.83	0.61
1:F:157:GLN:HB3	1:F:158:LEU:HD12	1.83	0.61
1:D:22:VAL:HG11	1:D:56:ILE:CD1	2.31	0.61
1:A:287:THR:CB	1:A:297:LEU:HD11	1.93	0.61
1:E:160:PHE:HA	1:E:162:ILE:HG13	1.82	0.61
1:A:176:HIS:CD2	1:A:177:GLU:HA	2.35	0.61
1:A:155:ASP:O	1:A:156:GLU:HB3	2.00	0.61
1:A:432:ASP:O	1:A:434:LYS:N	2.32	0.61
1:D:432:ASP:O	1:D:434:LYS:N	2.33	0.61
1:B:169:ASN:CB	1:B:182:ASP:HB2	2.19	0.61
1:F:123:PRO:HG3	1:F:148:PHE:HZ	1.65	0.61
1:D:169:ASN:ND2	1:D:182:ASP:CA	2.63	0.61
1:F:289:CYS:SG	1:F:294:VAL:HG11	2.41	0.61
1:A:294:VAL:C	1:A:295:GLU:HG2	2.20	0.60
1:A:296:ALA:C	1:A:297:LEU:HD23	2.20	0.60
1:C:160:PHE:HD1	1:C:161:PRO:O	1.85	0.60
1:E:162:ILE:O	1:E:162:ILE:HG22	2.02	0.60
1:C:22:VAL:HG11	1:C:56:ILE:CD1	2.30	0.60
1:C:432:ASP:O	1:C:434:LYS:N	2.32	0.60
1:F:162:ILE:O	1:F:162:ILE:HG22	2.02	0.60
1:C:160:PHE:HA	1:C:162:ILE:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:ILE:HD12	1:E:287:THR:OG1	2.01	0.60
1:B:160:PHE:HA	1:B:162:ILE:HG13	1.84	0.60
1:B:107:PRO:HB2	1:C:417:GLN:HG3	1.83	0.60
1:D:169:ASN:ND2	1:D:182:ASP:C	2.50	0.60
1:C:174:LEU:H	1:C:174:LEU:HD23	1.66	0.60
1:F:174:LEU:H	1:F:174:LEU:HD23	1.66	0.60
1:A:153:ALA:N	1:A:154:THR:HA	2.16	0.60
1:D:176:HIS:HA	1:D:177:GLU:O	2.02	0.60
1:E:160:PHE:HD1	1:E:161:PRO:O	1.85	0.60
1:E:22:VAL:CG1	1:E:56:ILE:HG21	2.32	0.60
1:B:287:THR:HB	1:B:297:LEU:HD11	0.71	0.59
1:B:156:GLU:HG3	1:B:159:ASP:HB2	1.79	0.59
1:D:153:ALA:H	1:D:154:THR:HA	1.67	0.59
1:D:156:GLU:HG3	1:D:159:ASP:CB	2.25	0.59
1:C:156:GLU:HG3	1:C:159:ASP:HB2	1.80	0.59
1:A:160:PHE:CE1	1:A:162:ILE:CB	2.86	0.59
1:F:160:PHE:CE1	1:F:162:ILE:CB	2.86	0.59
1:F:22:VAL:CG1	1:F:56:ILE:HG21	2.32	0.59
1:C:177:GLU:H	1:C:179:MET:HG3	1.67	0.59
1:C:157:GLN:C	1:C:159:ASP:HB3	2.23	0.59
1:B:160:PHE:HD1	1:B:161:PRO:O	1.85	0.59
1:E:160:PHE:CE1	1:E:162:ILE:CB	2.86	0.59
1:F:160:PHE:HD1	1:F:161:PRO:O	1.86	0.59
1:A:177:GLU:H	1:A:179:MET:HG3	1.66	0.59
1:C:169:ASN:ND2	1:C:182:ASP:C	2.48	0.59
1:D:153:ALA:N	1:D:154:THR:HA	2.18	0.59
1:F:153:ALA:H	1:F:154:THR:HA	1.68	0.59
1:F:160:PHE:CE1	1:F:162:ILE:HD12	2.38	0.59
1:D:50:LYS:CE	1:D:51:GLU:HG3	2.32	0.59
1:B:22:VAL:CG1	1:B:56:ILE:HG21	2.33	0.59
1:C:162:ILE:O	1:C:162:ILE:HG22	2.02	0.59
1:A:197:PRO:O	1:A:199:VAL:HG22	2.03	0.59
1:B:417:GLN:HG3	1:C:107:PRO:HB2	1.85	0.59
1:A:158:LEU:HA	1:A:159:ASP:HB3	1.85	0.58
1:D:197:PRO:O	1:D:199:VAL:HG22	2.03	0.58
1:E:156:GLU:HG3	1:E:159:ASP:N	2.18	0.58
1:D:160:PHE:CE1	1:D:162:ILE:CB	2.86	0.58
1:B:162:ILE:O	1:B:162:ILE:HG22	2.02	0.58
1:F:177:GLU:H	1:F:179:MET:HG3	1.68	0.58
1:F:174:LEU:N	1:F:174:LEU:HD23	2.18	0.58
1:A:169:ASN:ND2	1:A:182:ASP:CA	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ALA:N	1:F:154:THR:HA	2.19	0.58
1:D:290:ASP:O	1:D:294:VAL:CG2	2.51	0.58
1:B:307:VAL:N	1:B:388:ILE:HD12	2.18	0.58
1:E:153:ALA:H	1:E:154:THR:HA	1.68	0.58
1:F:300:LEU:HB2	1:F:301:SER:HA	1.85	0.58
1:E:197:PRO:O	1:E:199:VAL:HG22	2.03	0.58
1:F:123:PRO:CB	1:F:156:GLU:OE2	2.49	0.58
1:A:158:LEU:HA	1:A:159:ASP:CB	2.33	0.58
1:F:169:ASN:ND2	1:F:182:ASP:CA	2.65	0.58
1:E:169:ASN:ND2	1:E:182:ASP:CA	2.65	0.58
1:C:197:PRO:O	1:C:199:VAL:HG22	2.03	0.58
1:F:197:PRO:O	1:F:199:VAL:HG22	2.03	0.58
1:A:287:THR:HG21	1:A:297:LEU:CD1	2.31	0.58
1:E:160:PHE:CE1	1:E:162:ILE:HD12	2.39	0.58
1:B:157:GLN:C	1:B:159:ASP:HB3	2.24	0.58
1:B:153:ALA:N	1:B:154:THR:HA	2.18	0.58
1:F:169:ASN:HD21	1:F:182:ASP:N	2.02	0.58
1:E:169:ASN:HD21	1:E:182:ASP:N	2.02	0.58
1:B:197:PRO:O	1:B:199:VAL:HG22	2.03	0.58
1:A:240:ILE:HD13	1:A:296:ALA:CB	2.32	0.57
1:B:169:ASN:CG	1:B:182:ASP:H	2.07	0.57
1:C:307:VAL:N	1:C:388:ILE:HD12	2.19	0.57
1:B:131:ASP:OD2	1:B:166:SER:OG	2.20	0.57
1:C:153:ALA:N	1:C:154:THR:HA	2.18	0.57
1:F:239:ILE:HD12	1:F:288:VAL:CG2	2.30	0.57
1:C:169:ASN:HD21	1:C:182:ASP:N	2.02	0.57
1:D:178:ASP:HB2	1:D:179:MET:CG	2.34	0.57
1:E:157:GLN:HB3	1:E:158:LEU:HD12	1.86	0.57
1:C:174:LEU:N	1:C:174:LEU:HD23	2.19	0.57
1:A:178:ASP:HB2	1:A:179:MET:CB	2.13	0.57
1:C:160:PHE:CD1	1:C:162:ILE:CB	2.86	0.57
1:E:153:ALA:N	1:E:154:THR:HA	2.20	0.57
1:E:176:HIS:CG	1:E:177:GLU:HA	2.40	0.56
1:D:97:LEU:HD21	1:D:148:PHE:CZ	2.39	0.56
1:F:176:HIS:CG	1:F:177:GLU:HA	2.40	0.56
1:F:52:ARG:HB3	1:F:53:GLY:CA	2.33	0.56
1:F:298:PRO:O	1:F:299:ALA:HB3	2.05	0.56
1:F:156:GLU:HG2	1:F:159:ASP:CB	2.16	0.56
1:F:158:LEU:HA	1:F:159:ASP:CB	2.31	0.56
1:A:176:HIS:CG	1:A:177:GLU:CA	2.86	0.56
1:C:176:HIS:CG	1:C:177:GLU:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ILE:HG22	1:D:162:ILE:O	2.05	0.56
1:A:180:ALA:O	1:A:182:ASP:N	2.38	0.56
1:D:298:PRO:O	1:D:299:ALA:HB3	2.05	0.56
1:A:123:PRO:HG2	1:A:156:GLU:CD	2.24	0.56
1:E:175:ASP:O	1:E:178:ASP:HB3	2.05	0.56
1:D:158:LEU:CA	1:D:159:ASP:HB3	2.35	0.56
1:E:52:ARG:HB3	1:E:53:GLY:CA	2.33	0.56
1:E:157:GLN:C	1:E:159:ASP:HB3	2.24	0.56
1:E:174:LEU:HD23	1:E:174:LEU:H	1.70	0.56
1:F:289:CYS:SG	1:F:294:VAL:CG1	2.94	0.56
1:E:237:VAL:HA	1:E:291:THR:HG23	1.86	0.56
1:C:160:PHE:CZ	1:C:162:ILE:HD12	2.41	0.56
1:E:153:ALA:HB3	1:E:154:THR:HA	1.87	0.56
1:E:131:ASP:OD2	1:E:166:SER:OG	2.20	0.56
1:D:179:MET:O	1:D:180:ALA:HB2	2.05	0.56
1:E:287:THR:CG2	1:E:297:LEU:HD12	2.36	0.56
1:B:177:GLU:N	1:B:179:MET:HG3	2.18	0.56
1:E:107:PRO:HB2	1:F:417:GLN:HG3	1.87	0.56
1:D:131:ASP:OD2	1:D:166:SER:OG	2.21	0.56
1:D:12:ALA:HB3	1:D:18:LYS:HG3	1.88	0.56
1:E:350:THR:OG1	1:E:352:ASP:O	2.23	0.56
1:E:160:PHE:CD1	1:E:162:ILE:CB	2.87	0.56
1:C:157:GLN:CG	1:D:599:ARG:HD3	2.27	0.56
1:F:213:ASP:HA	1:F:340:VAL:HG22	1.88	0.56
1:F:131:ASP:OD2	1:F:166:SER:OG	2.21	0.56
1:F:240:ILE:HD12	1:F:296:ALA:HB1	1.88	0.55
1:D:150:ASN:ND2	1:D:151:LEU:HD22	2.19	0.55
1:A:131:ASP:OD2	1:A:166:SER:OG	2.21	0.55
1:C:287:THR:HB	1:C:297:LEU:HD11	0.68	0.55
1:C:175:ASP:O	1:C:178:ASP:HB3	2.07	0.55
1:F:238:THR:OG1	1:F:291:THR:HG22	2.07	0.55
1:D:158:LEU:HA	1:D:159:ASP:C	2.26	0.55
1:E:300:LEU:HB2	1:E:301:SER:O	2.06	0.55
1:B:124:ILE:HG23	1:B:161:PRO:CB	2.36	0.55
1:F:206:GLN:CG	1:F:297:LEU:HD22	2.37	0.55
1:B:176:HIS:ND1	1:B:177:GLU:HA	2.22	0.55
1:E:213:ASP:HA	1:E:340:VAL:HG22	1.89	0.55
1:C:350:THR:OG1	1:C:352:ASP:O	2.23	0.55
1:C:298:PRO:O	1:C:299:ALA:HB3	2.07	0.55
1:F:175:ASP:O	1:F:178:ASP:HB3	2.06	0.55
1:B:306:THR:HA	1:B:388:ILE:CD1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HA	1:C:159:ASP:CB	2.31	0.55
1:E:417:GLN:HG3	1:F:107:PRO:HB2	1.88	0.55
1:A:175:ASP:O	1:A:178:ASP:HB3	2.07	0.55
1:D:50:LYS:HD3	1:D:51:GLU:HB2	1.88	0.55
1:B:153:ALA:HB3	1:B:154:THR:HA	1.88	0.55
1:A:213:ASP:HA	1:A:340:VAL:HG22	1.89	0.55
1:E:156:GLU:CA	1:E:157:GLN:CB	2.85	0.54
1:B:294:VAL:CG1	1:B:295:GLU:H	2.10	0.54
1:F:158:LEU:CA	1:F:159:ASP:HB3	2.37	0.54
1:B:153:ALA:H	1:B:154:THR:HA	1.72	0.54
1:A:53:GLY:O	1:A:74:ASP:HB2	2.08	0.54
1:F:12:ALA:HB3	1:F:18:LYS:HG3	1.88	0.54
1:C:124:ILE:HG23	1:C:161:PRO:CB	2.37	0.54
1:C:153:ALA:H	1:C:154:THR:HA	1.71	0.54
1:B:277:THR:OG1	1:B:282:LEU:N	2.40	0.54
1:D:213:ASP:HA	1:D:340:VAL:HG22	1.89	0.54
1:F:156:GLU:CA	1:F:157:GLN:CB	2.86	0.54
1:B:174:LEU:HG	1:B:175:ASP:N	2.22	0.54
1:D:157:GLN:C	1:D:159:ASP:HB3	2.27	0.54
1:A:158:LEU:CA	1:A:159:ASP:CB	2.86	0.54
1:C:158:LEU:HA	1:C:159:ASP:C	2.28	0.54
1:F:277:THR:OG1	1:F:282:LEU:N	2.40	0.54
1:A:350:THR:OG1	1:A:352:ASP:O	2.23	0.54
1:B:213:ASP:HA	1:B:340:VAL:HG22	1.89	0.54
1:F:160:PHE:CD1	1:F:162:ILE:CB	2.88	0.54
1:E:87:ARG:CZ	1:E:300:LEU:O	2.55	0.54
1:F:300:LEU:CB	1:F:301:SER:CA	2.86	0.54
1:C:12:ALA:HB3	1:C:18:LYS:HG3	1.88	0.54
1:B:298:PRO:O	1:B:299:ALA:HB3	2.08	0.54
1:F:240:ILE:HD13	1:F:296:ALA:HB2	1.88	0.54
1:C:156:GLU:CA	1:C:157:GLN:CB	2.86	0.54
1:C:158:LEU:CA	1:C:159:ASP:CB	2.86	0.54
1:B:158:LEU:CA	1:B:159:ASP:CB	2.86	0.54
1:C:277:THR:OG1	1:C:282:LEU:N	2.40	0.54
1:B:287:THR:CB	1:B:297:LEU:HG	2.36	0.54
1:A:158:LEU:HA	1:A:159:ASP:C	2.27	0.54
1:E:277:THR:OG1	1:E:282:LEU:N	2.40	0.54
1:D:350:THR:OG1	1:D:352:ASP:O	2.23	0.54
1:D:176:HIS:ND1	1:D:177:GLU:HA	2.22	0.54
1:F:239:ILE:CD1	1:F:288:VAL:CG2	2.86	0.54
1:A:277:THR:OG1	1:A:282:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ALA:HA	1:C:73:VAL:O	2.08	0.54
1:E:158:LEU:CA	1:E:159:ASP:CB	2.86	0.54
1:E:158:LEU:CA	1:E:159:ASP:HB3	2.38	0.54
1:B:306:THR:CA	1:B:388:ILE:HB	2.38	0.54
1:F:153:ALA:HB3	1:F:154:THR:HA	1.89	0.54
1:D:277:THR:OG1	1:D:282:LEU:N	2.40	0.54
1:F:158:LEU:CA	1:F:159:ASP:CB	2.86	0.54
1:A:178:ASP:CA	1:A:179:MET:CB	2.86	0.54
1:B:307:VAL:N	1:B:388:ILE:CD1	2.70	0.54
1:B:156:GLU:CA	1:B:157:GLN:CB	2.86	0.54
1:A:9:ALA:HA	1:A:73:VAL:O	2.07	0.54
1:A:300:LEU:CB	1:A:301:SER:CA	2.86	0.54
1:E:238:THR:OG1	1:E:291:THR:HG22	2.08	0.54
1:C:213:ASP:HA	1:C:340:VAL:HG22	1.89	0.54
1:E:158:LEU:HA	1:E:159:ASP:C	2.28	0.53
1:A:156:GLU:CA	1:A:157:GLN:CB	2.86	0.53
1:C:158:LEU:HD21	1:D:599:ARG:HH12	1.73	0.53
1:B:300:LEU:CB	1:B:301:SER:CA	2.86	0.53
1:A:153:ALA:H	1:A:154:THR:HA	1.73	0.53
1:B:9:ALA:HA	1:B:73:VAL:O	2.08	0.53
1:C:145:PHE:O	1:C:146:ASP:C	2.47	0.53
1:F:157:GLN:C	1:F:159:ASP:HB3	2.28	0.53
1:D:156:GLU:HG3	1:D:159:ASP:N	2.24	0.53
1:F:164:TYR:CD1	1:F:164:TYR:N	2.77	0.53
1:B:158:LEU:HA	1:B:159:ASP:C	2.28	0.53
1:E:140:VAL:O	1:E:144:VAL:HG23	2.08	0.53
1:F:140:VAL:O	1:F:144:VAL:HG23	2.08	0.53
1:D:178:ASP:HB2	1:D:179:MET:SD	2.49	0.53
1:F:160:PHE:O	1:F:193:HIS:CE1	2.61	0.53
1:B:174:LEU:HG	1:B:175:ASP:OD2	2.09	0.53
1:B:306:THR:C	1:B:388:ILE:HD12	2.29	0.53
1:F:158:LEU:HA	1:F:159:ASP:C	2.28	0.53
1:A:156:GLU:HA	1:A:157:GLN:C	2.26	0.53
1:A:156:GLU:H	1:A:157:GLN:HB2	1.73	0.53
1:E:174:LEU:HD23	1:E:174:LEU:N	2.23	0.53
1:F:163:VAL:HG13	1:F:176:HIS:HD2	1.71	0.53
1:F:199:VAL:HB	1:F:267:LEU:HD11	1.91	0.53
1:D:140:VAL:O	1:D:144:VAL:HG23	2.08	0.53
1:C:307:VAL:N	1:C:388:ILE:CD1	2.72	0.53
1:A:169:ASN:HD21	1:A:182:ASP:N	2.05	0.53
1:A:140:VAL:O	1:A:144:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:VAL:HB	1:E:267:LEU:HD11	1.91	0.53
1:E:9:ALA:HA	1:E:73:VAL:O	2.08	0.53
1:C:140:VAL:O	1:C:144:VAL:HG23	2.08	0.52
1:E:300:LEU:H	1:E:301:SER:HA	1.74	0.52
1:A:145:PHE:O	1:A:146:ASP:C	2.47	0.52
1:D:10:ILE:O	1:D:75:THR:OG1	2.20	0.52
1:A:288:VAL:HG12	1:A:289:CYS:H	1.74	0.52
1:F:160:PHE:CD1	1:F:162:ILE:HD12	2.44	0.52
1:F:287:THR:CB	1:F:297:LEU:HG	2.40	0.52
1:D:153:ALA:HB3	1:D:154:THR:HA	1.91	0.52
1:D:174:LEU:H	1:D:174:LEU:HD23	1.74	0.52
1:E:156:GLU:CA	1:E:157:GLN:HB2	2.40	0.52
1:A:160:PHE:HD1	1:A:161:PRO:O	1.92	0.52
1:D:9:ALA:HA	1:D:73:VAL:O	2.08	0.52
1:F:350:THR:OG1	1:F:352:ASP:O	2.23	0.52
1:D:160:PHE:CZ	1:D:162:ILE:HD12	2.43	0.52
1:D:300:LEU:CB	1:D:301:SER:CA	2.86	0.52
1:C:153:ALA:HB3	1:C:154:THR:HA	1.89	0.52
1:F:9:ALA:HA	1:F:73:VAL:O	2.09	0.52
1:A:145:PHE:O	1:A:148:PHE:CB	2.58	0.52
1:B:350:THR:OG1	1:B:352:ASP:O	2.23	0.52
1:E:145:PHE:O	1:E:146:ASP:C	2.47	0.52
1:D:310:PHE:HB2	1:D:357:ARG:NH2	2.24	0.52
1:A:205:PHE:O	1:A:289:CYS:HA	2.10	0.52
1:C:300:LEU:CB	1:C:301:SER:CA	2.86	0.52
1:C:276:ILE:HG22	1:C:277:THR:HG23	1.92	0.52
1:E:276:ILE:HG22	1:E:277:THR:HG23	1.92	0.52
1:E:160:PHE:CD1	1:E:162:ILE:HD12	2.44	0.52
1:E:160:PHE:N	1:E:161:PRO:CB	2.73	0.52
1:B:306:THR:HA	1:B:388:ILE:CB	2.40	0.52
1:C:158:LEU:HD21	1:D:599:ARG:NH1	2.24	0.52
1:B:160:PHE:N	1:B:161:PRO:CB	2.73	0.52
1:C:150:ASN:ND2	1:C:151:LEU:CD2	2.73	0.52
1:E:300:LEU:HB2	1:E:301:SER:C	2.30	0.52
1:F:145:PHE:O	1:F:146:ASP:C	2.48	0.52
1:D:117:PHE:CZ	1:D:148:PHE:CD1	2.94	0.52
1:B:160:PHE:CD1	1:B:162:ILE:CB	2.86	0.52
1:B:150:ASN:ND2	1:B:151:LEU:CD2	2.73	0.52
1:F:310:PHE:HB2	1:F:357:ARG:NH2	2.25	0.52
1:E:310:PHE:HB2	1:E:357:ARG:NH2	2.25	0.52
1:F:160:PHE:N	1:F:161:PRO:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:GLU:CB	1:F:178:ASP:HA	2.39	0.52
1:B:160:PHE:CE1	1:B:162:ILE:CB	2.91	0.52
1:D:305:PRO:HG2	1:D:388:ILE:CD1	2.39	0.52
1:F:276:ILE:HG22	1:F:277:THR:HG23	1.92	0.52
1:C:199:VAL:HB	1:C:267:LEU:HD11	1.91	0.52
1:C:287:THR:CB	1:C:297:LEU:HG	2.37	0.51
1:C:160:PHE:N	1:C:161:PRO:CB	2.73	0.51
1:D:199:VAL:HB	1:D:267:LEU:HD11	1.91	0.51
1:C:310:PHE:HB2	1:C:357:ARG:NH2	2.25	0.51
1:A:294:VAL:HG12	1:A:295:GLU:N	2.20	0.51
1:F:156:GLU:CA	1:F:157:GLN:HB2	2.40	0.51
1:C:177:GLU:CB	1:C:178:ASP:HA	2.39	0.51
1:A:199:VAL:HB	1:A:267:LEU:HD11	1.91	0.51
1:C:131:ASP:OD2	1:C:166:SER:OG	2.21	0.51
1:A:207:MET:O	1:A:297:LEU:HD11	2.10	0.51
1:A:287:THR:HG21	1:A:297:LEU:HD12	1.81	0.51
1:B:140:VAL:O	1:B:144:VAL:HG23	2.09	0.51
1:A:117:PHE:HD2	1:A:153:ALA:HA	1.74	0.51
1:C:294:VAL:CG1	1:C:295:GLU:H	2.08	0.51
1:E:164:TYR:N	1:E:164:TYR:CD1	2.79	0.51
1:D:150:ASN:ND2	1:D:151:LEU:CD2	2.73	0.51
1:D:160:PHE:N	1:D:161:PRO:CB	2.73	0.51
1:D:304:GLU:CD	1:D:390:ARG:CZ	2.79	0.51
1:E:239:ILE:HD11	1:E:288:VAL:HG13	1.91	0.51
1:B:199:VAL:HB	1:B:267:LEU:HD11	1.91	0.51
1:B:54:ILE:HG23	1:B:73:VAL:HG13	1.91	0.51
1:E:160:PHE:HA	1:E:161:PRO:O	2.10	0.51
1:E:159:ASP:O	1:E:162:ILE:HD11	2.11	0.51
1:F:156:GLU:N	1:F:157:GLN:CB	2.73	0.51
1:F:160:PHE:HA	1:F:161:PRO:O	2.09	0.51
1:D:300:LEU:H	1:D:301:SER:HA	1.76	0.51
1:D:304:GLU:HB3	1:D:390:ARG:CZ	2.40	0.51
1:B:276:ILE:HG22	1:B:277:THR:HG23	1.92	0.51
1:A:276:ILE:HG22	1:A:277:THR:HG23	1.92	0.51
1:C:296:ALA:C	1:C:297:LEU:HD23	2.31	0.51
1:E:300:LEU:CD1	1:E:300:LEU:N	2.74	0.51
1:D:276:ILE:HG22	1:D:277:THR:HG23	1.92	0.51
1:F:184:THR:HA	1:F:187:TYR:HD2	1.76	0.51
1:E:184:THR:HA	1:E:187:TYR:HD2	1.76	0.51
1:B:174:LEU:H	1:B:174:LEU:HD23	1.75	0.51
1:D:158:LEU:HA	1:D:159:ASP:CB	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LYS:HD3	1:E:51:GLU:HB2	1.93	0.51
1:C:184:THR:HA	1:C:187:TYR:HD2	1.76	0.51
1:B:310:PHE:HB2	1:B:357:ARG:NH2	2.25	0.51
1:C:306:THR:CA	1:C:388:ILE:HB	2.39	0.51
1:D:158:LEU:CA	1:D:159:ASP:CB	2.88	0.51
1:A:160:PHE:N	1:A:161:PRO:CB	2.73	0.51
1:D:301:SER:OG	1:D:302:VAL:HG22	2.11	0.51
1:D:179:MET:HE3	1:D:182:ASP:OD1	2.11	0.51
1:F:176:HIS:HA	1:F:177:GLU:O	2.11	0.51
1:C:145:PHE:O	1:C:148:PHE:CB	2.57	0.51
1:B:160:PHE:CZ	1:B:162:ILE:HD12	2.45	0.50
1:F:50:LYS:HD3	1:F:51:GLU:HB2	1.93	0.50
1:E:289:CYS:SG	1:E:294:VAL:HG11	2.51	0.50
1:C:176:HIS:HA	1:C:177:GLU:O	2.10	0.50
1:D:145:PHE:O	1:D:146:ASP:C	2.47	0.50
1:C:156:GLU:N	1:C:157:GLN:CB	2.73	0.50
1:B:145:PHE:O	1:B:146:ASP:C	2.47	0.50
1:E:160:PHE:O	1:E:193:HIS:CE1	2.64	0.50
1:B:50:LYS:HD3	1:B:51:GLU:HB2	1.93	0.50
1:F:156:GLU:HG3	1:F:159:ASP:N	2.26	0.50
1:E:206:GLN:CD	1:E:297:LEU:HD22	2.31	0.50
1:C:169:ASN:ND2	1:C:182:ASP:CA	2.65	0.50
1:D:13:HIS:C	1:D:16:HIS:CE1	2.85	0.50
1:D:184:THR:HA	1:D:187:TYR:HD2	1.75	0.50
1:F:159:ASP:O	1:F:162:ILE:HD11	2.12	0.50
1:B:165:ALA:C	1:B:182:ASP:OD2	2.50	0.50
1:B:157:GLN:HB3	1:B:158:LEU:HD12	1.94	0.50
1:B:145:PHE:O	1:B:148:PHE:CB	2.58	0.50
1:C:287:THR:HG1	1:C:297:LEU:HG	1.73	0.50
1:C:13:HIS:C	1:C:16:HIS:CE1	2.85	0.50
1:B:309:MET:HG2	1:B:366:LEU:HD13	1.94	0.50
1:B:25:LEU:CD2	1:B:183:MET:SD	2.96	0.50
1:E:177:GLU:CB	1:E:178:ASP:HA	2.41	0.50
1:C:306:THR:HA	1:C:388:ILE:CD1	2.38	0.50
1:C:157:GLN:HB3	1:C:158:LEU:HD12	1.93	0.50
1:E:309:MET:HG2	1:E:366:LEU:HD13	1.94	0.50
1:F:176:HIS:NE2	1:F:177:GLU:OE1	2.45	0.50
1:F:160:PHE:CD2	1:F:162:ILE:CD1	2.86	0.49
1:F:287:THR:CG2	1:F:297:LEU:CD1	2.90	0.49
1:A:160:PHE:O	1:A:193:HIS:CE1	2.65	0.49
1:F:153:ALA:CB	1:F:154:THR:CA	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:HD12	1:C:296:ALA:HB1	1.94	0.49
1:D:176:HIS:CE1	1:D:177:GLU:CD	2.86	0.49
1:F:160:PHE:O	1:F:193:HIS:NE2	2.45	0.49
1:A:162:ILE:HG22	1:A:162:ILE:O	2.12	0.49
1:F:13:HIS:C	1:F:16:HIS:CE1	2.85	0.49
1:F:309:MET:HG2	1:F:366:LEU:HD13	1.94	0.49
1:A:310:PHE:HB2	1:A:357:ARG:NH2	2.26	0.49
1:C:253:LYS:HG2	1:C:254:VAL:N	2.28	0.49
1:E:123:PRO:HB2	1:E:156:GLU:OE2	2.12	0.49
1:C:22:VAL:HG12	1:C:56:ILE:HD13	1.94	0.49
1:A:309:MET:HG2	1:A:366:LEU:HD13	1.94	0.49
1:B:296:ALA:C	1:B:297:LEU:HD23	2.32	0.49
1:C:158:LEU:HG	1:D:599:ARG:NH1	2.27	0.49
1:C:52:ARG:CB	1:C:53:GLY:HA3	2.42	0.49
1:D:174:LEU:N	1:D:174:LEU:HD23	2.27	0.49
1:F:50:LYS:HA	1:F:51:GLU:CB	2.41	0.49
1:A:176:HIS:CE1	1:A:177:GLU:CD	2.86	0.49
1:F:206:GLN:CD	1:F:297:LEU:HD22	2.33	0.49
1:C:156:GLU:HA	1:C:157:GLN:C	2.27	0.49
1:A:125:VAL:H	1:A:161:PRO:CB	2.25	0.49
1:E:54:ILE:HG23	1:E:73:VAL:HG13	1.93	0.49
1:A:12:ALA:HB3	1:A:18:LYS:HG3	1.95	0.49
1:E:176:HIS:CE1	1:E:177:GLU:CD	2.86	0.49
1:F:176:HIS:CE1	1:F:177:GLU:CD	2.86	0.49
1:C:306:THR:C	1:C:388:ILE:HD12	2.32	0.49
1:B:156:GLU:N	1:B:157:GLN:CB	2.73	0.49
1:D:177:GLU:N	1:D:178:ASP:HA	2.27	0.49
1:E:150:ASN:ND2	1:E:151:LEU:CD2	2.76	0.49
1:C:309:MET:HG2	1:C:366:LEU:HD13	1.95	0.49
1:B:287:THR:HG21	1:B:297:LEU:HG	1.95	0.49
1:E:160:PHE:CD2	1:E:162:ILE:CD1	2.88	0.49
1:E:176:HIS:NE2	1:E:177:GLU:OE1	2.46	0.49
1:E:300:LEU:N	1:E:301:SER:HA	2.26	0.49
1:D:309:MET:HG2	1:D:366:LEU:HD13	1.95	0.49
1:E:287:THR:CG2	1:E:297:LEU:CD1	2.91	0.49
1:E:287:THR:CG2	1:E:297:LEU:CG	2.88	0.49
1:C:178:ASP:CA	1:C:179:MET:HB2	2.43	0.49
1:D:305:PRO:HG2	1:D:388:ILE:HD13	1.94	0.49
1:E:253:LYS:HG2	1:E:254:VAL:N	2.27	0.49
1:F:122:LYS:NZ	1:F:158:LEU:O	2.39	0.49
1:D:156:GLU:HA	1:D:157:GLN:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:HA	1:B:51:GLU:CB	2.42	0.49
1:E:153:ALA:CB	1:E:154:THR:CA	2.87	0.49
1:E:13:HIS:C	1:E:16:HIS:CE1	2.86	0.49
1:E:205:PHE:CE1	1:E:231:VAL:HG22	2.48	0.49
1:B:240:ILE:HD12	1:B:296:ALA:HB1	1.95	0.48
1:E:287:THR:CB	1:E:297:LEU:CD1	2.91	0.48
1:C:176:HIS:NE2	1:C:177:GLU:OE1	2.46	0.48
1:B:176:HIS:CE1	1:B:177:GLU:CD	2.86	0.48
1:B:178:ASP:CA	1:B:179:MET:HB2	2.42	0.48
1:D:124:ILE:HG23	1:D:161:PRO:CA	2.30	0.48
1:D:160:PHE:O	1:D:193:HIS:CE1	2.66	0.48
1:A:22:VAL:HG12	1:A:56:ILE:HD13	1.93	0.48
1:E:50:LYS:HA	1:E:51:GLU:CB	2.42	0.48
1:B:205:PHE:CE1	1:B:231:VAL:HG22	2.48	0.48
1:F:240:ILE:HD13	1:F:296:ALA:CB	2.42	0.48
1:D:160:PHE:CZ	1:D:162:ILE:HG21	2.48	0.48
1:A:124:ILE:HG23	1:A:161:PRO:CA	2.31	0.48
1:B:12:ALA:HB3	1:B:18:LYS:HG3	1.94	0.48
1:A:205:PHE:CE1	1:A:231:VAL:HG22	2.48	0.48
1:C:176:HIS:CE1	1:C:177:GLU:CD	2.86	0.48
1:F:205:PHE:CE1	1:F:231:VAL:HG22	2.49	0.48
1:A:13:HIS:C	1:A:16:HIS:CE1	2.87	0.48
1:F:253:LYS:HG2	1:F:254:VAL:N	2.28	0.48
1:C:159:ASP:O	1:C:162:ILE:HD11	2.14	0.48
1:A:300:LEU:N	1:A:301:SER:HA	2.28	0.48
1:F:54:ILE:HG23	1:F:73:VAL:HG13	1.94	0.48
1:D:294:VAL:HG12	1:D:295:GLU:N	2.18	0.48
1:F:240:ILE:HD12	1:F:287:THR:HG1	1.77	0.48
1:B:159:ASP:O	1:B:162:ILE:HG13	2.13	0.48
1:C:306:THR:HA	1:C:388:ILE:CB	2.41	0.48
1:D:87:ARG:NH2	1:D:301:SER:HB3	2.29	0.48
1:B:54:ILE:HG21	1:B:211:GLN:OE1	2.13	0.48
1:C:205:PHE:CE1	1:C:231:VAL:HG22	2.48	0.48
1:A:50:LYS:CE	1:A:51:GLU:CG	2.90	0.48
1:E:52:ARG:CB	1:E:53:GLY:CA	2.91	0.48
1:D:22:VAL:HG12	1:D:56:ILE:HD13	1.94	0.48
1:F:249:ALA:HB3	1:F:275:ALA:CB	2.44	0.48
1:E:12:ALA:HB3	1:E:18:LYS:HG3	1.95	0.48
1:F:52:ARG:CB	1:F:53:GLY:CA	2.91	0.48
1:B:165:ALA:CA	1:B:182:ASP:OD2	2.61	0.48
1:C:160:PHE:CD2	1:C:162:ILE:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB3	1:A:154:THR:HA	1.95	0.48
1:B:13:HIS:C	1:B:16:HIS:CE1	2.87	0.48
1:F:300:LEU:N	1:F:301:SER:HA	2.29	0.48
1:E:249:ALA:HB3	1:E:275:ALA:CB	2.44	0.48
1:D:253:LYS:HG2	1:D:254:VAL:N	2.28	0.48
1:E:293:ASN:O	1:E:294:VAL:HG22	2.14	0.47
1:A:55:THR:HB	1:A:73:VAL:HA	1.94	0.47
1:E:122:LYS:NZ	1:E:158:LEU:O	2.38	0.47
1:B:178:ASP:CA	1:B:179:MET:CB	2.92	0.47
1:D:290:ASP:HB3	1:D:292:GLN:HB3	1.95	0.47
1:F:240:ILE:CD1	1:F:296:ALA:HB1	2.43	0.47
1:E:310:PHE:CG	1:E:383:SER:HB3	2.49	0.47
1:F:10:ILE:O	1:F:75:THR:OG1	2.20	0.47
1:F:287:THR:CB	1:F:297:LEU:CD1	2.92	0.47
1:F:178:ASP:CA	1:F:179:MET:HB2	2.43	0.47
1:A:50:LYS:CD	1:A:51:GLU:HB2	2.44	0.47
1:A:253:LYS:HG2	1:A:254:VAL:N	2.29	0.47
1:A:176:HIS:CE1	1:A:177:GLU:HA	2.50	0.47
1:B:177:GLU:N	1:B:178:ASP:CA	2.76	0.47
1:C:305:PRO:O	1:C:306:THR:HG22	2.15	0.47
1:B:305:PRO:O	1:B:306:THR:HG22	2.15	0.47
1:B:159:ASP:O	1:B:162:ILE:HD11	2.15	0.47
1:D:205:PHE:CE1	1:D:231:VAL:HG22	2.49	0.47
1:D:423:LYS:HG3	1:D:480:VAL:HG11	1.96	0.47
1:E:10:ILE:O	1:E:75:THR:OG1	2.20	0.47
1:D:176:HIS:CG	1:D:177:GLU:HA	2.49	0.47
1:E:240:ILE:HD12	1:E:296:ALA:HB1	1.96	0.47
1:E:163:VAL:HG13	1:E:176:HIS:HD2	1.77	0.47
1:E:178:ASP:CA	1:E:179:MET:HB2	2.44	0.47
1:F:293:ASN:O	1:F:294:VAL:HG22	2.15	0.47
1:B:423:LYS:HG3	1:B:480:VAL:HG11	1.97	0.47
1:E:54:ILE:HG21	1:E:211:GLN:OE1	2.14	0.47
1:F:54:ILE:HG21	1:F:211:GLN:OE1	2.14	0.47
1:B:253:LYS:HG2	1:B:254:VAL:N	2.29	0.47
1:D:156:GLU:CA	1:D:157:GLN:CB	2.86	0.47
1:C:423:LYS:HG3	1:C:480:VAL:HG11	1.97	0.47
1:B:301:SER:OG	1:B:302:VAL:HG22	2.15	0.47
1:F:423:LYS:HG3	1:F:480:VAL:HG11	1.97	0.47
1:F:150:ASN:ND2	1:F:151:LEU:CD2	2.78	0.47
1:A:222:GLY:O	1:A:223:ILE:C	2.51	0.47
1:B:52:ARG:CB	1:B:53:GLY:CA	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:LYS:HG3	1:E:480:VAL:HG11	1.97	0.47
1:A:293:ASN:O	1:A:294:VAL:HG22	2.15	0.47
1:E:160:PHE:O	1:E:193:HIS:NE2	2.48	0.47
1:E:289:CYS:SG	1:E:294:VAL:CG1	3.03	0.47
1:F:164:TYR:HD1	1:F:164:TYR:H	1.63	0.47
1:C:206:GLN:CG	1:C:297:LEU:HD22	2.46	0.46
1:E:176:HIS:ND1	1:E:177:GLU:HA	2.30	0.46
1:F:294:VAL:HG12	1:F:295:GLU:N	2.16	0.46
1:C:301:SER:OG	1:C:302:VAL:HG22	2.15	0.46
1:B:249:ALA:HB3	1:B:275:ALA:CB	2.44	0.46
1:E:10:ILE:HG22	1:E:11:ILE:N	2.30	0.46
1:A:423:LYS:HG3	1:A:480:VAL:HG11	1.97	0.46
1:D:294:VAL:O	1:D:295:GLU:HB2	2.14	0.46
1:E:176:HIS:HA	1:E:177:GLU:O	2.14	0.46
1:D:117:PHE:CZ	1:D:148:PHE:CE1	2.99	0.46
1:A:249:ALA:HB3	1:A:275:ALA:CB	2.44	0.46
1:C:249:ALA:HB3	1:C:275:ALA:CB	2.44	0.46
1:E:22:VAL:HG12	1:E:56:ILE:HG21	1.96	0.46
1:B:160:PHE:CD2	1:B:162:ILE:CD1	2.86	0.46
1:C:146:ASP:O	1:C:150:ASN:OD1	2.33	0.46
1:C:55:THR:O	1:C:56:ILE:HB	2.16	0.46
1:D:52:ARG:CB	1:D:53:GLY:HA3	2.44	0.46
1:C:240:ILE:HD13	1:C:296:ALA:HB2	1.98	0.46
1:C:176:HIS:ND1	1:C:177:GLU:HA	2.31	0.46
1:D:148:PHE:N	1:D:150:ASN:OD1	2.48	0.46
1:A:144:VAL:O	1:A:148:PHE:CD2	2.69	0.46
1:D:249:ALA:HB3	1:D:275:ALA:CB	2.44	0.46
1:E:283:ASN:OD1	1:E:346:ARG:HA	2.16	0.46
1:A:156:GLU:N	1:A:157:GLN:CB	2.78	0.46
1:D:151:LEU:O	1:D:152:ASP:HB2	2.16	0.46
1:C:160:PHE:CE1	1:C:162:ILE:CB	2.90	0.46
1:E:239:ILE:HD12	1:E:288:VAL:HG22	1.97	0.46
1:A:283:ASN:OD1	1:A:346:ARG:HA	2.16	0.46
1:C:159:ASP:O	1:C:162:ILE:HG13	2.15	0.46
1:A:101:ALA:HB2	1:A:127:ILE:HG22	1.98	0.46
1:B:274:VAL:O	1:B:275:ALA:HB3	2.16	0.46
1:A:422:ARG:NH1	1:A:447:GLY:O	2.48	0.46
1:E:287:THR:HG21	1:E:297:LEU:HB2	1.98	0.46
1:D:156:GLU:HA	1:D:157:GLN:HB2	1.97	0.46
1:B:156:GLU:HA	1:B:157:GLN:C	2.27	0.46
1:C:101:ALA:HB2	1:C:127:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:O	1:C:148:PHE:CD2	2.69	0.46
1:B:22:VAL:HG12	1:B:56:ILE:HG21	1.98	0.46
1:F:283:ASN:OD1	1:F:346:ARG:HA	2.16	0.46
1:D:55:THR:O	1:D:56:ILE:HB	2.16	0.46
1:B:273:ILE:HD11	1:B:276:ILE:HD11	1.98	0.46
1:A:310:PHE:CG	1:A:383:SER:HB3	2.51	0.46
1:D:283:ASN:OD1	1:D:346:ARG:HA	2.16	0.46
1:C:287:THR:HG21	1:C:297:LEU:HG	1.97	0.46
1:F:287:THR:CG2	1:F:297:LEU:CG	2.88	0.46
1:F:176:HIS:ND1	1:F:177:GLU:HA	2.31	0.46
1:A:237:VAL:HA	1:A:291:THR:CG2	2.44	0.46
1:F:22:VAL:HG12	1:F:56:ILE:HG21	1.97	0.46
1:D:222:GLY:O	1:D:223:ILE:C	2.52	0.46
1:E:156:GLU:H	1:E:157:GLN:HB2	1.76	0.46
1:C:283:ASN:OD1	1:C:346:ARG:HA	2.16	0.46
1:A:182:ASP:O	1:A:183:MET:HE1	2.16	0.46
1:B:146:ASP:O	1:B:150:ASN:OD1	2.34	0.46
1:F:156:GLU:H	1:F:157:GLN:HB2	1.76	0.45
1:E:273:ILE:HD11	1:E:276:ILE:HD11	1.98	0.45
1:E:274:VAL:O	1:E:275:ALA:HB3	2.16	0.45
1:D:101:ALA:HB2	1:D:127:ILE:HG22	1.98	0.45
1:D:422:ARG:NH1	1:D:447:GLY:O	2.48	0.45
1:A:206:GLN:HG2	1:A:297:LEU:HD22	1.99	0.45
1:C:160:PHE:CA	1:C:162:ILE:HG13	2.47	0.45
1:A:124:ILE:CA	1:A:161:PRO:CB	2.80	0.45
1:B:144:VAL:O	1:B:148:PHE:CD2	2.69	0.45
1:F:273:ILE:HD11	1:F:276:ILE:HD11	1.98	0.45
1:C:273:ILE:HD11	1:C:276:ILE:HD11	1.98	0.45
1:F:274:VAL:O	1:F:275:ALA:HB3	2.16	0.45
1:D:101:ALA:HA	1:D:140:VAL:HG21	1.98	0.45
1:B:175:ASP:O	1:B:178:ASP:HB3	2.16	0.45
1:C:274:VAL:O	1:C:275:ALA:HB3	2.16	0.45
1:E:96:LEU:HA	1:E:96:LEU:HD23	1.74	0.45
1:C:422:ARG:NH1	1:C:447:GLY:O	2.49	0.45
1:B:290:ASP:O	1:B:294:VAL:HG21	2.16	0.45
1:E:240:ILE:HD13	1:E:296:ALA:HB2	1.98	0.45
1:E:177:GLU:N	1:E:178:ASP:CA	2.79	0.45
1:B:300:LEU:N	1:B:301:SER:HA	2.32	0.45
1:A:101:ALA:HA	1:A:140:VAL:HG21	1.99	0.45
1:D:274:VAL:O	1:D:275:ALA:HB3	2.16	0.45
1:C:12:ALA:HB3	1:C:18:LYS:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG12	1:A:289:CYS:N	2.32	0.45
1:B:294:VAL:O	1:B:295:GLU:HG2	2.16	0.45
1:F:239:ILE:HA	1:F:287:THR:O	2.16	0.45
1:B:176:HIS:CG	1:B:177:GLU:CA	2.95	0.45
1:F:301:SER:OG	1:F:302:VAL:HG22	2.16	0.45
1:F:237:VAL:HA	1:F:291:THR:HG23	1.98	0.45
1:B:310:PHE:CG	1:B:383:SER:HB3	2.51	0.45
1:E:54:ILE:HA	1:E:55:THR:HA	1.47	0.45
1:C:534:THR:HG21	1:C:594:GLU:HB2	1.99	0.45
1:B:289:CYS:HG	1:B:294:VAL:CG1	2.26	0.45
1:B:283:ASN:OD1	1:B:346:ARG:HA	2.17	0.45
1:F:54:ILE:HA	1:F:55:THR:HA	1.47	0.45
1:E:534:THR:HG21	1:E:594:GLU:HB2	1.99	0.45
1:B:425:ASP:CG	1:C:114:LYS:HE2	2.36	0.45
1:A:178:ASP:HA	1:A:179:MET:CB	2.45	0.45
1:D:61:THR:HG1	1:D:67:ASP:HA	1.79	0.45
1:C:222:GLY:O	1:C:223:ILE:C	2.50	0.45
1:A:273:ILE:HD11	1:A:276:ILE:HD11	1.98	0.45
1:F:534:THR:HG21	1:F:594:GLU:HB2	1.99	0.45
1:F:124:ILE:HA	1:F:161:PRO:CB	2.47	0.45
1:C:178:ASP:CA	1:C:179:MET:CB	2.95	0.45
1:D:146:ASP:O	1:D:150:ASN:OD1	2.34	0.45
1:F:164:TYR:CE1	1:F:175:ASP:HB2	2.51	0.45
1:A:160:PHE:CG	1:A:162:ILE:HD12	2.51	0.45
1:C:50:LYS:HA	1:C:51:GLU:CB	2.46	0.45
1:B:101:ALA:HB2	1:B:127:ILE:HG22	1.98	0.45
1:C:61:THR:HG1	1:C:67:ASP:HA	1.76	0.45
1:E:300:LEU:CB	1:E:304:GLU:HG3	2.43	0.45
1:D:50:LYS:HA	1:D:51:GLU:CB	2.47	0.45
1:A:274:VAL:O	1:A:275:ALA:HB3	2.17	0.45
1:C:10:ILE:O	1:C:75:THR:OG1	2.20	0.45
1:B:119:TYR:O	1:B:121:LEU:N	2.50	0.45
1:B:534:THR:HG21	1:B:594:GLU:HB2	1.99	0.45
1:B:206:GLN:CG	1:B:297:LEU:HD22	2.46	0.44
1:E:237:VAL:CA	1:E:291:THR:HG23	2.46	0.44
1:A:12:ALA:HB3	1:A:18:LYS:CG	2.48	0.44
1:F:119:TYR:O	1:F:121:LEU:N	2.50	0.44
1:C:158:LEU:CD2	1:D:599:ARG:HH12	2.30	0.44
1:B:101:ALA:HA	1:B:140:VAL:HG21	1.98	0.44
1:B:149:VAL:C	1:B:151:LEU:H	2.21	0.44
1:C:153:ALA:CB	1:C:154:THR:CA	2.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:N	1:C:301:SER:HA	2.32	0.44
1:E:287:THR:HG21	1:E:297:LEU:CB	2.46	0.44
1:C:305:PRO:C	1:C:306:THR:CG2	2.86	0.44
1:B:12:ALA:HB3	1:B:18:LYS:CG	2.46	0.44
1:B:204:PRO:O	1:B:228:ARG:HB3	2.17	0.44
1:C:290:ASP:O	1:C:294:VAL:HG21	2.17	0.44
1:B:305:PRO:C	1:B:306:THR:CG2	2.86	0.44
1:D:12:ALA:HB3	1:D:18:LYS:CG	2.47	0.44
1:E:101:ALA:HB2	1:E:127:ILE:HG22	1.98	0.44
1:F:101:ALA:HA	1:F:140:VAL:HG21	1.99	0.44
1:E:119:TYR:O	1:E:121:LEU:N	2.51	0.44
1:E:272:ASP:N	1:E:272:ASP:OD1	2.50	0.44
1:A:293:ASN:C	1:A:294:VAL:CG2	2.86	0.44
1:F:12:ALA:HB3	1:F:18:LYS:CG	2.47	0.44
1:F:272:ASP:N	1:F:272:ASP:OD1	2.50	0.44
1:C:287:THR:CG2	1:C:297:LEU:CG	2.89	0.44
1:D:165:ALA:HA	1:D:182:ASP:OD2	2.17	0.44
1:B:240:ILE:HD13	1:B:296:ALA:HB2	1.99	0.44
1:D:160:PHE:CA	1:D:161:PRO:CB	2.95	0.44
1:D:160:PHE:HD1	1:D:161:PRO:O	2.01	0.44
1:F:301:SER:O	1:F:302:VAL:HG13	2.17	0.44
1:A:267:LEU:HG	1:A:268:ALA:N	2.33	0.44
1:A:174:LEU:N	1:A:174:LEU:HD23	2.32	0.44
1:A:156:GLU:H	1:A:157:GLN:CB	2.31	0.44
1:A:54:ILE:HA	1:A:55:THR:HA	1.71	0.44
1:E:150:ASN:HB2	1:F:423:LYS:NZ	2.33	0.44
1:E:273:ILE:HD11	1:E:276:ILE:CD1	2.48	0.44
1:B:273:ILE:HD11	1:B:276:ILE:CD1	2.48	0.44
1:D:534:THR:HG21	1:D:594:GLU:HB2	1.99	0.44
1:D:289:CYS:HB2	1:D:294:VAL:CG1	2.43	0.44
1:A:61:THR:HG1	1:A:67:ASP:HA	1.80	0.44
1:D:273:ILE:HD11	1:D:276:ILE:HD11	1.98	0.44
1:C:267:LEU:HG	1:C:268:ALA:N	2.33	0.44
1:E:101:ALA:HA	1:E:140:VAL:HG21	1.99	0.44
1:F:101:ALA:HB2	1:F:127:ILE:HG22	1.98	0.44
1:E:160:PHE:CD1	1:E:162:ILE:CG1	3.01	0.44
1:F:160:PHE:CD1	1:F:162:ILE:CG1	3.01	0.44
1:E:293:ASN:C	1:E:294:VAL:CG2	2.86	0.44
1:C:174:LEU:O	1:C:178:ASP:HB3	2.18	0.44
1:F:178:ASP:CA	1:F:179:MET:CB	2.95	0.44
1:D:124:ILE:CA	1:D:161:PRO:CB	2.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ILE:HD11	1:F:276:ILE:CD1	2.48	0.44
1:E:267:LEU:HG	1:E:268:ALA:N	2.33	0.44
1:D:310:PHE:CG	1:D:383:SER:HB3	2.53	0.44
1:B:425:ASP:OD1	1:C:114:LYS:HD3	2.17	0.44
1:C:204:PRO:O	1:C:228:ARG:HB3	2.18	0.44
1:C:411:HIS:O	1:C:412:GLN:C	2.56	0.44
1:D:272:ASP:N	1:D:272:ASP:OD1	2.51	0.44
1:A:272:ASP:N	1:A:272:ASP:OD1	2.51	0.44
1:F:156:GLU:HA	1:F:157:GLN:C	2.27	0.43
1:F:240:ILE:CD1	1:F:296:ALA:CB	2.95	0.43
1:E:178:ASP:CA	1:E:179:MET:CB	2.95	0.43
1:D:149:VAL:O	1:D:151:LEU:N	2.51	0.43
1:F:177:GLU:N	1:F:178:ASP:CA	2.80	0.43
1:F:293:ASN:C	1:F:294:VAL:CG2	2.86	0.43
1:B:159:ASP:O	1:B:160:PHE:HB2	2.18	0.43
1:F:310:PHE:CG	1:F:383:SER:HB3	2.53	0.43
1:B:272:ASP:N	1:B:272:ASP:OD1	2.51	0.43
1:C:240:ILE:HD13	1:C:296:ALA:CB	2.49	0.43
1:B:287:THR:CG2	1:B:297:LEU:HG	2.48	0.43
1:C:160:PHE:CG	1:C:162:ILE:CD1	3.01	0.43
1:C:110:ARG:NH2	1:C:151:LEU:HD11	2.33	0.43
1:C:101:ALA:HA	1:C:140:VAL:HG21	1.99	0.43
1:A:273:ILE:HD11	1:A:276:ILE:CD1	2.48	0.43
1:E:12:ALA:HB3	1:E:18:LYS:CG	2.47	0.43
1:F:422:ARG:NH1	1:F:447:GLY:O	2.48	0.43
1:A:156:GLU:HG2	1:A:156:GLU:O	2.18	0.43
1:D:117:PHE:HZ	1:D:148:PHE:HD1	1.62	0.43
1:B:177:GLU:CB	1:B:178:ASP:HA	2.48	0.43
1:D:344:ALA:HB1	1:D:361:ARG:HB2	2.00	0.43
1:A:204:PRO:O	1:A:228:ARG:HB3	2.17	0.43
1:A:160:PHE:CD1	1:A:162:ILE:CB	2.91	0.43
1:B:54:ILE:HA	1:B:55:THR:HA	1.46	0.43
1:F:204:PRO:O	1:F:228:ARG:HB3	2.18	0.43
1:A:534:THR:HG21	1:A:594:GLU:HB2	1.99	0.43
1:C:119:TYR:O	1:C:121:LEU:N	2.50	0.43
1:B:176:HIS:HA	1:B:177:GLU:O	2.18	0.43
1:C:158:LEU:CD2	1:D:599:ARG:NH1	2.81	0.43
1:C:348:GLU:HB2	1:C:357:ARG:HB3	2.01	0.43
1:B:348:GLU:HB2	1:B:357:ARG:HB3	2.00	0.43
1:E:380:LEU:O	1:E:580:VAL:HG22	2.18	0.43
1:D:204:PRO:O	1:D:228:ARG:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ASP:N	1:F:152:ASP:OD1	2.52	0.43
1:F:160:PHE:CG	1:F:162:ILE:CD1	3.00	0.43
1:D:300:LEU:N	1:D:301:SER:HA	2.29	0.43
1:B:50:LYS:CE	1:B:51:GLU:HG3	2.46	0.43
1:B:267:LEU:HG	1:B:268:ALA:N	2.33	0.43
1:E:204:PRO:O	1:E:228:ARG:HB3	2.18	0.43
1:B:184:THR:HB	1:B:185:PRO:HD3	2.01	0.43
1:E:156:GLU:N	1:E:157:GLN:CB	2.73	0.43
1:C:144:VAL:O	1:C:144:VAL:HG12	2.19	0.43
1:F:144:VAL:HG12	1:F:144:VAL:O	2.19	0.43
1:E:422:ARG:NH1	1:E:447:GLY:O	2.48	0.43
1:A:177:GLU:N	1:A:178:ASP:CA	2.73	0.43
1:E:287:THR:CB	1:E:297:LEU:CG	2.95	0.43
1:A:157:GLN:C	1:A:159:ASP:HB3	2.39	0.43
1:C:149:VAL:C	1:C:151:LEU:H	2.22	0.43
1:C:273:ILE:HD11	1:C:276:ILE:CD1	2.48	0.43
1:D:273:ILE:HD11	1:D:276:ILE:CD1	2.49	0.43
1:F:19:THR:HG22	1:F:22:VAL:HB	2.01	0.43
1:E:144:VAL:O	1:E:144:VAL:HG12	2.19	0.43
1:F:348:GLU:HB2	1:F:357:ARG:HB3	2.01	0.43
1:B:411:HIS:O	1:B:412:GLN:C	2.57	0.43
1:E:411:HIS:O	1:E:412:GLN:C	2.57	0.43
1:F:411:HIS:O	1:F:412:GLN:C	2.57	0.43
1:E:160:PHE:CG	1:E:162:ILE:CD1	3.01	0.43
1:C:294:VAL:O	1:C:295:GLU:HG2	2.18	0.43
1:C:19:THR:HG22	1:C:22:VAL:HB	2.01	0.43
1:C:240:ILE:CD1	1:C:296:ALA:HB1	2.49	0.43
1:C:289:CYS:HG	1:C:294:VAL:CG1	2.29	0.42
1:E:297:LEU:N	1:E:297:LEU:CD2	2.73	0.42
1:C:177:GLU:N	1:C:178:ASP:CA	2.81	0.42
1:D:158:LEU:N	1:D:158:LEU:HD12	2.33	0.42
1:B:144:VAL:HG12	1:B:144:VAL:O	2.19	0.42
1:D:267:LEU:HG	1:D:268:ALA:N	2.34	0.42
1:A:292:GLN:O	1:A:294:VAL:HG23	2.18	0.42
1:B:240:ILE:HD13	1:B:296:ALA:CB	2.50	0.42
1:F:174:LEU:O	1:F:178:ASP:HB3	2.19	0.42
1:C:54:ILE:HA	1:C:55:THR:HA	1.71	0.42
1:C:300:LEU:HG	1:C:304:GLU:OE1	2.19	0.42
1:F:267:LEU:HG	1:F:268:ALA:N	2.34	0.42
1:E:298:PRO:O	1:E:299:ALA:HB3	2.18	0.42
1:F:380:LEU:O	1:F:580:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:HIS:O	1:A:412:GLN:C	2.57	0.42
1:E:124:ILE:HA	1:E:161:PRO:CB	2.49	0.42
1:D:125:VAL:H	1:D:161:PRO:CB	2.32	0.42
1:E:348:GLU:HB2	1:E:357:ARG:HB3	2.01	0.42
1:E:87:ARG:NH1	1:E:300:LEU:O	2.52	0.42
1:E:423:LYS:NZ	1:F:150:ASN:HB2	2.35	0.42
1:D:348:GLU:HB2	1:D:357:ARG:HB3	2.01	0.42
1:A:119:TYR:O	1:A:121:LEU:N	2.50	0.42
1:E:19:THR:HG22	1:E:22:VAL:HB	2.01	0.42
1:B:10:ILE:HG22	1:B:11:ILE:N	2.35	0.42
1:D:307:VAL:O	1:D:359:SER:HA	2.20	0.42
1:A:156:GLU:HA	1:A:157:GLN:CB	2.49	0.42
1:E:164:TYR:O	1:E:179:MET:CE	2.67	0.42
1:C:159:ASP:O	1:C:160:PHE:HB2	2.19	0.42
1:B:160:PHE:CA	1:B:162:ILE:HG13	2.47	0.42
1:E:61:THR:HG1	1:E:67:ASP:HA	1.80	0.42
1:D:444:PRO:O	1:D:447:GLY:N	2.53	0.42
1:D:119:TYR:O	1:D:121:LEU:N	2.50	0.42
1:A:380:LEU:O	1:A:580:VAL:HG22	2.19	0.42
1:A:298:PRO:O	1:A:299:ALA:HB3	2.19	0.42
1:F:307:VAL:O	1:F:359:SER:HA	2.20	0.42
1:F:205:PHE:O	1:F:289:CYS:HB3	2.20	0.42
1:D:54:ILE:HA	1:D:55:THR:HA	1.71	0.42
1:C:68:TYR:CZ	1:C:191:VAL:HG11	2.55	0.42
1:D:81:PHE:O	1:D:83:GLY:N	2.53	0.42
1:A:307:VAL:O	1:A:359:SER:HA	2.20	0.42
1:D:380:LEU:O	1:D:580:VAL:HG22	2.19	0.42
1:A:240:ILE:HD11	1:A:289:CYS:SG	2.60	0.42
1:B:306:THR:C	1:B:307:VAL:HG23	2.41	0.42
1:C:160:PHE:CD1	1:C:161:PRO:O	2.70	0.42
1:A:160:PHE:CE1	1:A:162:ILE:CG2	3.03	0.42
1:A:144:VAL:HG12	1:A:144:VAL:O	2.19	0.42
1:E:381:ALA:HA	1:E:578:VAL:O	2.20	0.42
1:D:411:HIS:O	1:D:412:GLN:C	2.57	0.42
1:B:152:ASP:OD1	1:B:152:ASP:N	2.52	0.42
1:C:272:ASP:N	1:C:272:ASP:OD1	2.51	0.42
1:B:110:ARG:NH2	1:B:151:LEU:HD11	2.34	0.42
1:B:19:THR:HG22	1:B:22:VAL:HB	2.01	0.42
1:D:10:ILE:HG22	1:D:11:ILE:N	2.33	0.42
1:C:81:PHE:O	1:C:83:GLY:N	2.53	0.42
1:B:307:VAL:N	1:B:388:ILE:HG13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:CA	1:C:157:GLN:HB2	2.49	0.42
1:E:182:ASP:O	1:E:183:MET:HE2	2.20	0.42
1:D:144:VAL:O	1:D:144:VAL:HG12	2.19	0.42
1:B:205:PHE:CE1	1:B:231:VAL:CG2	3.03	0.42
1:E:307:VAL:O	1:E:359:SER:HA	2.20	0.42
1:B:380:LEU:O	1:B:580:VAL:HG22	2.19	0.42
1:A:469:PHE:CD1	1:A:469:PHE:C	2.93	0.42
1:A:81:PHE:O	1:A:83:GLY:N	2.53	0.42
1:C:380:LEU:O	1:C:580:VAL:HG22	2.19	0.42
1:C:50:LYS:CD	1:C:51:GLU:HB2	2.49	0.41
1:E:50:LYS:CE	1:E:51:GLU:HG3	2.47	0.41
1:C:205:PHE:CE1	1:C:231:VAL:CG2	3.03	0.41
1:C:306:THR:C	1:C:307:VAL:HG23	2.41	0.41
1:B:51:GLU:HB3	1:B:52:ARG:H	1.69	0.41
1:A:184:THR:HA	1:A:187:TYR:HD2	1.85	0.41
1:B:422:ARG:NH1	1:B:447:GLY:O	2.48	0.41
1:B:381:ALA:HA	1:B:578:VAL:O	2.20	0.41
1:D:469:PHE:CD1	1:D:469:PHE:C	2.93	0.41
1:E:175:ASP:HB2	1:E:176:HIS:H	1.71	0.41
1:A:237:VAL:CA	1:A:291:THR:CG2	2.98	0.41
1:D:187:TYR:O	1:D:191:VAL:HG23	2.20	0.41
1:A:348:GLU:HB2	1:A:357:ARG:HB3	2.02	0.41
1:F:10:ILE:HG22	1:F:11:ILE:N	2.35	0.41
1:F:381:ALA:HA	1:F:578:VAL:O	2.20	0.41
1:D:381:ALA:HA	1:D:578:VAL:O	2.20	0.41
1:A:205:PHE:CE1	1:A:231:VAL:CG2	3.03	0.41
1:D:169:ASN:ND2	1:D:182:ASP:N	2.64	0.41
1:D:160:PHE:CE1	1:D:162:ILE:CG2	3.03	0.41
1:A:19:THR:HG22	1:A:22:VAL:HB	2.01	0.41
1:A:237:VAL:C	1:A:291:THR:HG22	2.41	0.41
1:C:310:PHE:CG	1:C:383:SER:HB3	2.55	0.41
1:A:68:TYR:CZ	1:A:191:VAL:HG11	2.55	0.41
1:C:469:PHE:C	1:C:469:PHE:CD1	2.93	0.41
1:D:169:ASN:ND2	1:D:182:ASP:HB3	2.32	0.41
1:F:160:PHE:CE2	1:F:162:ILE:CD1	2.86	0.41
1:A:156:GLU:CA	1:A:157:GLN:HB2	2.49	0.41
1:D:19:THR:HG22	1:D:22:VAL:HB	2.01	0.41
1:F:68:TYR:CZ	1:F:191:VAL:HG11	2.55	0.41
1:C:187:TYR:O	1:C:191:VAL:HG23	2.21	0.41
1:D:68:TYR:CZ	1:D:191:VAL:HG11	2.55	0.41
1:A:444:PRO:O	1:A:447:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:PRO:O	1:E:447:GLY:N	2.54	0.41
1:B:469:PHE:C	1:B:469:PHE:CD1	2.93	0.41
1:B:81:PHE:O	1:B:83:GLY:N	2.53	0.41
1:E:240:ILE:CD1	1:E:287:THR:OG1	2.67	0.41
1:A:157:GLN:HB3	1:A:158:LEU:H	1.70	0.41
1:C:307:VAL:H	1:C:388:ILE:HD12	1.85	0.41
1:E:205:PHE:CE1	1:E:231:VAL:CG2	3.03	0.41
1:E:81:PHE:O	1:E:83:GLY:N	2.53	0.41
1:B:68:TYR:CZ	1:B:191:VAL:HG11	2.56	0.41
1:F:336:ASN:HA	1:F:339:LEU:HB2	2.03	0.41
1:B:251:VAL:HG12	1:B:273:ILE:HB	2.03	0.41
1:E:174:LEU:O	1:E:178:ASP:HB3	2.20	0.41
1:F:290:ASP:O	1:F:294:VAL:HG21	2.21	0.41
1:F:444:PRO:O	1:F:447:GLY:N	2.54	0.41
1:C:576:GLU:HG2	1:C:589:LYS:HD3	2.03	0.41
1:B:240:ILE:CD1	1:B:296:ALA:HB1	2.50	0.41
1:F:156:GLU:CG	1:F:159:ASP:CB	2.86	0.41
1:E:287:THR:HB	1:E:297:LEU:CG	2.51	0.41
1:E:295:GLU:HA	1:E:296:ALA:HA	1.81	0.41
1:E:164:TYR:H	1:E:164:TYR:HD1	1.69	0.41
1:F:205:PHE:CE1	1:F:231:VAL:CG2	3.03	0.41
1:D:310:PHE:HB2	1:D:357:ARG:HH22	1.85	0.41
1:E:68:TYR:CZ	1:E:191:VAL:HG11	2.55	0.41
1:D:336:ASN:HA	1:D:339:LEU:HB2	2.02	0.41
1:E:469:PHE:C	1:E:469:PHE:CD1	2.93	0.41
1:C:152:ASP:N	1:C:152:ASP:OD1	2.52	0.41
1:A:288:VAL:C	1:A:289:CYS:SG	3.00	0.41
1:D:148:PHE:O	1:D:151:LEU:HD22	2.21	0.41
1:B:306:THR:CA	1:B:388:ILE:CD1	2.82	0.41
1:A:52:ARG:CB	1:A:53:GLY:HA3	2.50	0.41
1:C:10:ILE:HG22	1:C:11:ILE:N	2.36	0.41
1:B:576:GLU:HG2	1:B:589:LYS:HD3	2.03	0.41
1:A:381:ALA:HA	1:A:578:VAL:O	2.21	0.41
1:F:81:PHE:O	1:F:83:GLY:N	2.53	0.41
1:C:381:ALA:HA	1:C:578:VAL:O	2.20	0.41
1:B:287:THR:HG22	1:B:297:LEU:HD12	1.91	0.40
1:B:123:PRO:O	1:B:124:ILE:HD13	2.21	0.40
1:D:177:GLU:CB	1:D:178:ASP:CA	2.96	0.40
1:F:174:LEU:CD2	1:F:174:LEU:N	2.84	0.40
1:F:179:MET:HE3	1:F:182:ASP:OD1	2.20	0.40
1:C:158:LEU:CG	1:D:599:ARG:NH1	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PHE:CE1	1:F:156:GLU:OE1	2.75	0.40
1:F:175:ASP:HB2	1:F:176:HIS:H	1.70	0.40
1:B:176:HIS:CD2	1:B:177:GLU:HA	2.55	0.40
1:F:187:TYR:O	1:F:191:VAL:HG23	2.21	0.40
1:B:336:ASN:HA	1:B:339:LEU:HB2	2.03	0.40
1:B:230:LYS:HG2	1:B:266:ASP:HB3	2.04	0.40
1:C:174:LEU:CD2	1:C:174:LEU:N	2.84	0.40
1:C:19:THR:HG21	1:C:52:ARG:O	2.22	0.40
1:F:50:LYS:CE	1:F:51:GLU:HG3	2.48	0.40
1:B:310:PHE:HB2	1:B:357:ARG:HH22	1.86	0.40
1:C:379:GLU:HG2	1:C:581:THR:HA	2.04	0.40
1:C:336:ASN:HA	1:C:339:LEU:HB2	2.03	0.40
1:F:123:PRO:O	1:F:124:ILE:HD13	2.22	0.40
1:D:149:VAL:C	1:D:151:LEU:N	2.74	0.40
1:D:300:LEU:HG	1:D:304:GLU:OE1	2.21	0.40
1:A:237:VAL:CA	1:A:291:THR:HG23	2.45	0.40
1:E:22:VAL:CG1	1:E:56:ILE:HD13	2.52	0.40
1:E:187:TYR:O	1:E:191:VAL:HG23	2.22	0.40
1:B:379:GLU:HG2	1:B:581:THR:HA	2.04	0.40
1:A:336:ASN:HA	1:A:339:LEU:HB2	2.02	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	543/607 (90%)	421 (78%)	85 (16%)	37 (7%)	1	12
1	B	543/607 (90%)	420 (77%)	89 (16%)	34 (6%)	2	14
1	C	543/607 (90%)	418 (77%)	89 (16%)	36 (7%)	1	13
1	D	543/607 (90%)	419 (77%)	87 (16%)	37 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	543/607 (90%)	425 (78%)	86 (16%)	32 (6%)	2	16
1	F	543/607 (90%)	424 (78%)	85 (16%)	34 (6%)	2	14
All	All	3258/3642 (90%)	2527 (78%)	521 (16%)	210 (6%)	2	13

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	A	181	GLU
1	A	182	ASP
1	A	223	ILE
1	A	393	ASP
1	A	477	PRO
1	B	161	PRO
1	B	182	ASP
1	B	302	VAL
1	B	393	ASP
1	B	477	PRO
1	C	161	PRO
1	C	181	GLU
1	C	182	ASP
1	C	223	ILE
1	C	302	VAL
1	C	393	ASP
1	C	477	PRO
1	D	161	PRO
1	D	181	GLU
1	D	182	ASP
1	D	223	ILE
1	D	302	VAL
1	D	393	ASP
1	D	477	PRO
1	E	161	PRO
1	E	181	GLU
1	E	182	ASP
1	E	393	ASP
1	E	477	PRO
1	F	161	PRO
1	F	181	GLU
1	F	182	ASP
1	F	393	ASP

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Mol	Chain	Res	Type
1	F	477	PRO
1	A	18	LYS
1	A	20	THR
1	A	80	ASP
1	A	148	PHE
1	A	179	MET
1	A	180	ALA
1	A	286	ASP
1	A	294	VAL
1	A	396	LYS
1	A	433	GLY
1	B	18	LYS
1	B	20	THR
1	B	51	GLU
1	B	56	ILE
1	B	80	ASP
1	B	148	PHE
1	B	181	GLU
1	B	286	ASP
1	B	396	LYS
1	B	433	GLY
1	C	18	LYS
1	C	20	THR
1	C	80	ASP
1	C	148	PHE
1	C	396	LYS
1	C	433	GLY
1	D	18	LYS
1	D	20	THR
1	D	51	GLU
1	D	180	ALA
1	D	286	ASP
1	D	396	LYS
1	D	433	GLY
1	E	18	LYS
1	E	20	THR
1	E	51	GLU
1	E	56	ILE
1	E	80	ASP
1	E	148	PHE
1	E	294	VAL
1	E	396	LYS

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Mol	Chain	Res	Type
1	E	433	GLY
1	F	18	LYS
1	F	20	THR
1	F	51	GLU
1	F	80	ASP
1	F	148	PHE
1	F	286	ASP
1	F	294	VAL
1	F	302	VAL
1	F	396	LYS
1	F	433	GLY
1	A	51	GLU
1	A	83	GLY
1	A	175	ASP
1	A	257	HIS
1	A	275	ALA
1	A	298	PRO
1	A	302	VAL
1	A	412	GLN
1	B	83	GLY
1	B	160	PHE
1	B	175	ASP
1	B	183	MET
1	B	257	HIS
1	B	275	ALA
1	B	298	PRO
1	B	412	GLN
1	C	51	GLU
1	C	83	GLY
1	C	102	PHE
1	C	160	PHE
1	C	183	MET
1	C	257	HIS
1	C	275	ALA
1	C	298	PRO
1	C	412	GLN
1	D	80	ASP
1	D	83	GLY
1	D	150	ASN
1	D	175	ASP
1	D	183	MET
1	D	257	HIS

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Mol	Chain	Res	Type
1	D	275	ALA
1	D	298	PRO
1	D	412	GLN
1	E	83	GLY
1	E	160	PHE
1	E	183	MET
1	E	257	HIS
1	E	275	ALA
1	E	412	GLN
1	F	56	ILE
1	F	83	GLY
1	F	102	PHE
1	F	183	MET
1	F	257	HIS
1	F	275	ALA
1	F	298	PRO
1	F	412	GLN
1	A	102	PHE
1	A	155	ASP
1	A	160	PHE
1	A	289	CYS
1	A	339	LEU
1	B	102	PHE
1	B	155	ASP
1	B	156	GLU
1	B	290	ASP
1	B	339	LEU
1	C	155	ASP
1	C	156	GLU
1	C	290	ASP
1	C	339	LEU
1	D	102	PHE
1	D	160	PHE
1	D	290	ASP
1	D	339	LEU
1	E	102	PHE
1	E	155	ASP
1	E	157	GLN
1	E	299	ALA
1	E	339	LEU
1	F	160	PHE
1	F	339	LEU

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Mol	Chain	Res	Type
1	A	157	GLN
1	A	241	ASP
1	A	499	PHE
1	A	560	PRO
1	B	157	GLN
1	B	235	GLN
1	B	499	PHE
1	B	560	PRO
1	C	56	ILE
1	C	157	GLN
1	C	175	ASP
1	C	235	GLN
1	C	499	PHE
1	C	560	PRO
1	D	56	ILE
1	D	157	GLN
1	D	499	PHE
1	D	560	PRO
1	E	175	ASP
1	E	235	GLN
1	E	298	PRO
1	E	499	PHE
1	E	560	PRO
1	F	155	ASP
1	F	157	GLN
1	F	175	ASP
1	F	499	PHE
1	F	560	PRO
1	A	56	ILE
1	A	235	GLN
1	C	241	ASP
1	D	155	ASP
1	D	235	GLN
1	D	241	ASP
1	D	299	ALA
1	F	235	GLN
1	B	307	VAL
1	C	307	VAL
1	A	14	VAL
1	B	14	VAL
1	C	14	VAL
1	D	14	VAL

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Mol	Chain	Res	Type
1	E	14	VAL
1	F	14	VAL
1	D	120	GLY
1	E	120	GLY
1	F	120	GLY
1	A	120	GLY
1	C	120	GLY
1	F	162	ILE

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	450/519 (87%)	379 (84%)	71 (16%)	3	15
1	B	450/519 (87%)	376 (84%)	74 (16%)	3	13
1	C	450/519 (87%)	381 (85%)	69 (15%)	3	16
1	D	450/519 (87%)	382 (85%)	68 (15%)	3	17
1	E	450/519 (87%)	381 (85%)	69 (15%)	3	16
1	F	450/519 (87%)	373 (83%)	77 (17%)	2	12
All	All	2700/3114 (87%)	2272 (84%)	428 (16%)	3	14

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ILE
1	A	21	LEU
1	A	50	LYS
1	A	51	GLU
1	A	59	LYS
1	A	75	THR
1	A	96	LEU
1	A	102	PHE
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	150	ASN
1	A	151	LEU
1	A	157	GLN
1	A	159	ASP
1	A	160	PHE
1	A	169	ASN
1	A	175	ASP
1	A	181	GLU
1	A	182	ASP
1	A	183	MET
1	A	184	THR
1	A	186	LEU
1	A	199	VAL
1	A	216	SER
1	A	223	ILE
1	A	225	ARG
1	A	235	GLN
1	A	236	GLN
1	A	240	ILE
1	A	241	ASP
1	A	257	HIS
1	A	262	ARG
1	A	264	GLU
1	A	265	THR
1	A	272	ASP
1	A	273	ILE
1	A	274	VAL
1	A	289	CYS
1	A	297	LEU
1	A	302	VAL
1	A	303	ASP
1	A	308	SER
1	A	312	CYS
1	A	328	SER
1	A	339	LEU
1	A	357	ARG
1	A	359	SER
1	A	361	ARG
1	A	364	LEU
1	A	365	HIS
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	384	ARG
1	A	392	ILE
1	A	393	ASP
1	A	398	GLU
1	A	405	LEU
1	A	417	GLN
1	A	429	MET
1	A	443	ILE
1	A	448	LEU
1	A	465	LEU
1	A	466	TYR
1	A	470	SER
1	A	472	TYR
1	A	482	GLN
1	A	512	LEU
1	A	539	THR
1	A	566	GLU
1	A	574	ASP
1	A	583	THR
1	B	1	MET
1	B	10	ILE
1	B	21	LEU
1	B	50	LYS
1	B	51	GLU
1	B	59	LYS
1	B	75	THR
1	B	96	LEU
1	B	102	PHE
1	B	110	ARG
1	B	122	LYS
1	B	152	ASP
1	B	156	GLU
1	B	157	GLN
1	B	158	LEU
1	B	160	PHE
1	B	169	ASN
1	B	175	ASP
1	B	177	GLU
1	B	181	GLU
1	B	182	ASP
1	B	183	MET
1	B	184	THR

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Mol	Chain	Res	Type
1	B	186	LEU
1	B	199	VAL
1	B	216	SER
1	B	223	ILE
1	B	225	ARG
1	B	235	GLN
1	B	236	GLN
1	B	240	ILE
1	B	241	ASP
1	B	262	ARG
1	B	264	GLU
1	B	265	THR
1	B	272	ASP
1	B	273	ILE
1	B	274	VAL
1	B	292	GLN
1	B	295	GLU
1	B	297	LEU
1	B	300	LEU
1	B	302	VAL
1	B	303	ASP
1	B	308	SER
1	B	312	CYS
1	B	328	SER
1	B	339	LEU
1	B	357	ARG
1	B	359	SER
1	B	361	ARG
1	B	364	LEU
1	B	365	HIS
1	B	384	ARG
1	B	392	ILE
1	B	393	ASP
1	B	398	GLU
1	B	405	LEU
1	B	417	GLN
1	B	425	ASP
1	B	429	MET
1	B	443	ILE
1	B	448	LEU
1	B	465	LEU
1	B	466	TYR

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Mol	Chain	Res	Type
1	B	470	SER
1	B	472	TYR
1	B	499	PHE
1	B	507	ARG
1	B	512	LEU
1	B	539	THR
1	B	566	GLU
1	B	574	ASP
1	B	583	THR
1	C	1	MET
1	C	10	ILE
1	C	21	LEU
1	C	50	LYS
1	C	51	GLU
1	C	59	LYS
1	C	75	THR
1	C	96	LEU
1	C	102	PHE
1	C	110	ARG
1	C	122	LYS
1	C	152	ASP
1	C	156	GLU
1	C	157	GLN
1	C	158	LEU
1	C	160	PHE
1	C	169	ASN
1	C	175	ASP
1	C	181	GLU
1	C	182	ASP
1	C	183	MET
1	C	184	THR
1	C	186	LEU
1	C	199	VAL
1	C	216	SER
1	C	223	ILE
1	C	225	ARG
1	C	235	GLN
1	C	236	GLN
1	C	240	ILE
1	C	241	ASP
1	C	257	HIS
1	C	262	ARG

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Mol	Chain	Res	Type
1	C	264	GLU
1	C	265	THR
1	C	272	ASP
1	C	273	ILE
1	C	274	VAL
1	C	297	LEU
1	C	300	LEU
1	C	302	VAL
1	C	303	ASP
1	C	308	SER
1	C	312	CYS
1	C	328	SER
1	C	339	LEU
1	C	357	ARG
1	C	359	SER
1	C	361	ARG
1	C	364	LEU
1	C	365	HIS
1	C	384	ARG
1	C	392	ILE
1	C	393	ASP
1	C	398	GLU
1	C	405	LEU
1	C	417	GLN
1	C	429	MET
1	C	443	ILE
1	C	448	LEU
1	C	465	LEU
1	C	466	TYR
1	C	470	SER
1	C	472	TYR
1	C	512	LEU
1	C	539	THR
1	C	566	GLU
1	C	574	ASP
1	C	583	THR
1	D	1	MET
1	D	10	ILE
1	D	21	LEU
1	D	50	LYS
1	D	51	GLU
1	D	59	LYS

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Mol	Chain	Res	Type
1	D	75	THR
1	D	96	LEU
1	D	102	PHE
1	D	110	ARG
1	D	122	LYS
1	D	148	PHE
1	D	150	ASN
1	D	151	LEU
1	D	158	LEU
1	D	160	PHE
1	D	169	ASN
1	D	175	ASP
1	D	177	GLU
1	D	181	GLU
1	D	182	ASP
1	D	183	MET
1	D	184	THR
1	D	186	LEU
1	D	199	VAL
1	D	216	SER
1	D	223	ILE
1	D	225	ARG
1	D	235	GLN
1	D	236	GLN
1	D	240	ILE
1	D	241	ASP
1	D	262	ARG
1	D	264	GLU
1	D	265	THR
1	D	272	ASP
1	D	273	ILE
1	D	274	VAL
1	D	297	LEU
1	D	300	LEU
1	D	302	VAL
1	D	308	SER
1	D	312	CYS
1	D	328	SER
1	D	339	LEU
1	D	357	ARG
1	D	359	SER
1	D	361	ARG

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Mol	Chain	Res	Type
1	D	364	LEU
1	D	365	HIS
1	D	384	ARG
1	D	392	ILE
1	D	393	ASP
1	D	398	GLU
1	D	405	LEU
1	D	417	GLN
1	D	429	MET
1	D	443	ILE
1	D	448	LEU
1	D	465	LEU
1	D	466	TYR
1	D	470	SER
1	D	472	TYR
1	D	512	LEU
1	D	539	THR
1	D	566	GLU
1	D	574	ASP
1	D	583	THR
1	E	1	MET
1	E	10	ILE
1	E	21	LEU
1	E	50	LYS
1	E	51	GLU
1	E	59	LYS
1	E	75	THR
1	E	102	PHE
1	E	110	ARG
1	E	122	LYS
1	E	150	ASN
1	E	156	GLU
1	E	157	GLN
1	E	160	PHE
1	E	164	TYR
1	E	169	ASN
1	E	175	ASP
1	E	181	GLU
1	E	182	ASP
1	E	183	MET
1	E	184	THR
1	E	186	LEU

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Mol	Chain	Res	Type
1	E	199	VAL
1	E	216	SER
1	E	223	ILE
1	E	225	ARG
1	E	235	GLN
1	E	236	GLN
1	E	240	ILE
1	E	241	ASP
1	E	250	LYS
1	E	257	HIS
1	E	262	ARG
1	E	264	GLU
1	E	265	THR
1	E	272	ASP
1	E	273	ILE
1	E	274	VAL
1	E	292	GLN
1	E	295	GLU
1	E	297	LEU
1	E	308	SER
1	E	312	CYS
1	E	328	SER
1	E	339	LEU
1	E	357	ARG
1	E	359	SER
1	E	361	ARG
1	E	364	LEU
1	E	365	HIS
1	E	384	ARG
1	E	392	ILE
1	E	393	ASP
1	E	398	GLU
1	E	405	LEU
1	E	417	GLN
1	E	429	MET
1	E	443	ILE
1	E	448	LEU
1	E	465	LEU
1	E	466	TYR
1	E	470	SER
1	E	472	TYR
1	E	499	PHE

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Mol	Chain	Res	Type
1	E	512	LEU
1	E	539	THR
1	E	566	GLU
1	E	574	ASP
1	E	583	THR
1	F	1	MET
1	F	10	ILE
1	F	21	LEU
1	F	50	LYS
1	F	51	GLU
1	F	59	LYS
1	F	75	THR
1	F	96	LEU
1	F	102	PHE
1	F	110	ARG
1	F	122	LYS
1	F	150	ASN
1	F	152	ASP
1	F	156	GLU
1	F	157	GLN
1	F	158	LEU
1	F	160	PHE
1	F	164	TYR
1	F	169	ASN
1	F	175	ASP
1	F	181	GLU
1	F	182	ASP
1	F	183	MET
1	F	184	THR
1	F	186	LEU
1	F	199	VAL
1	F	216	SER
1	F	223	ILE
1	F	225	ARG
1	F	235	GLN
1	F	236	GLN
1	F	240	ILE
1	F	241	ASP
1	F	250	LYS
1	F	257	HIS
1	F	262	ARG
1	F	264	GLU

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Mol	Chain	Res	Type
1	F	265	THR
1	F	272	ASP
1	F	273	ILE
1	F	274	VAL
1	F	289	CYS
1	F	292	GLN
1	F	295	GLU
1	F	297	LEU
1	F	300	LEU
1	F	302	VAL
1	F	303	ASP
1	F	308	SER
1	F	312	CYS
1	F	328	SER
1	F	339	LEU
1	F	357	ARG
1	F	359	SER
1	F	361	ARG
1	F	364	LEU
1	F	365	HIS
1	F	384	ARG
1	F	392	ILE
1	F	393	ASP
1	F	398	GLU
1	F	405	LEU
1	F	417	GLN
1	F	429	MET
1	F	443	ILE
1	F	448	LEU
1	F	465	LEU
1	F	466	TYR
1	F	470	SER
1	F	472	TYR
1	F	499	PHE
1	F	512	LEU
1	F	539	THR
1	F	563	MET
1	F	566	GLU
1	F	574	ASP
1	F	583	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	169	ASN
1	A	193	HIS
1	A	211	GLN
1	A	292	GLN
1	A	482	GLN
1	B	16	HIS
1	B	169	ASN
1	B	292	GLN
1	B	482	GLN
1	C	16	HIS
1	C	169	ASN
1	C	292	GLN
1	C	482	GLN
1	D	16	HIS
1	D	157	GLN
1	D	169	ASN
1	D	193	HIS
1	D	482	GLN
1	E	16	HIS
1	E	157	GLN
1	E	169	ASN
1	E	292	GLN
1	E	482	GLN
1	F	16	HIS
1	F	157	GLN
1	F	169	ASN
1	F	176	HIS
1	F	292	GLN
1	F	482	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/607 (91%)	0.84	71 (12%) 5 4	79, 130, 184, 219	0
1	B	555/607 (91%)	0.84	79 (14%) 4 3	80, 129, 184, 221	0
1	C	555/607 (91%)	0.88	82 (14%) 3 3	82, 130, 183, 216	0
1	D	555/607 (91%)	0.85	73 (13%) 4 4	85, 131, 183, 218	0
1	E	555/607 (91%)	0.83	76 (13%) 4 4	83, 131, 183, 225	0
1	F	555/607 (91%)	0.84	72 (12%) 5 4	83, 131, 182, 218	0
All	All	3330/3642 (91%)	0.84	453 (13%) 4 4	79, 131, 184, 225	0

All (453) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	160	PHE	7.3
1	F	295	GLU	6.8
1	D	297	LEU	5.5
1	C	82	GLY	5.4
1	B	295	GLU	5.3
1	A	157	GLN	5.2
1	A	62	ALA	5.2
1	A	481	GLY	5.1
1	F	492	GLY	5.0
1	C	62	ALA	4.8
1	D	481	GLY	4.8
1	F	160	PHE	4.8
1	E	295	GLU	4.8
1	C	157	GLN	4.8
1	A	160	PHE	4.7
1	F	526	ILE	4.7
1	C	481	GLY	4.6
1	D	240	ILE	4.6
1	A	240	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	537	CYS	4.5
1	D	300	LEU	4.5
1	F	296	ALA	4.5
1	D	62	ALA	4.5
1	C	230	LYS	4.4
1	E	268	ALA	4.3
1	B	533	LEU	4.3
1	D	159	ASP	4.3
1	E	281	GLU	4.3
1	E	257	HIS	4.2
1	C	267	LEU	4.2
1	D	268	ALA	4.2
1	F	297	LEU	4.1
1	F	66	ASN	4.1
1	C	295	GLU	4.1
1	D	15	ASP	4.1
1	F	265	THR	4.1
1	C	160	PHE	4.1
1	D	227	LYS	4.1
1	F	288	VAL	4.1
1	E	288	VAL	4.0
1	C	297	LEU	4.0
1	C	281	GLU	4.0
1	B	481	GLY	4.0
1	D	281	GLU	3.9
1	A	156	GLU	3.9
1	D	160	PHE	3.9
1	B	281	GLU	3.9
1	E	296	ALA	3.9
1	E	161	PRO	3.8
1	F	281	GLU	3.8
1	B	160	PHE	3.8
1	A	268	ALA	3.8
1	A	276	ILE	3.8
1	A	159	ASP	3.8
1	A	300	LEU	3.7
1	D	82	GLY	3.7
1	E	526	ILE	3.7
1	B	161	PRO	3.6
1	A	82	GLY	3.6
1	A	281	GLU	3.6
1	A	15	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	240	ILE	3.6
1	F	537	CYS	3.5
1	E	592	LEU	3.5
1	A	297	LEU	3.5
1	B	537	CYS	3.5
1	E	205	PHE	3.5
1	B	288	VAL	3.5
1	B	205	PHE	3.5
1	B	492	GLY	3.5
1	C	554	ALA	3.5
1	D	379	GLU	3.4
1	D	157	GLN	3.4
1	F	268	ALA	3.4
1	D	492	GLY	3.4
1	C	526	ILE	3.4
1	C	268	ALA	3.4
1	E	265	THR	3.4
1	F	481	GLY	3.4
1	D	296	ALA	3.4
1	F	282	LEU	3.4
1	B	230	LYS	3.4
1	D	276	ILE	3.3
1	A	227	LYS	3.3
1	A	294	VAL	3.3
1	E	535	VAL	3.3
1	E	297	LEU	3.3
1	B	164	TYR	3.3
1	D	490	SER	3.3
1	A	287	THR	3.2
1	C	288	VAL	3.2
1	B	157	GLN	3.2
1	A	267	LEU	3.2
1	F	5	LEU	3.2
1	F	177	GLU	3.2
1	C	66	ASN	3.1
1	A	339	LEU	3.1
1	F	339	LEU	3.1
1	E	580	VAL	3.1
1	F	592	LEU	3.1
1	D	537	CYS	3.1
1	D	293	ASN	3.1
1	C	161	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	266	ASP	3.1
1	B	177	GLU	3.1
1	C	137	PRO	3.1
1	E	481	GLY	3.1
1	C	206	GLN	3.1
1	B	207	MET	3.1
1	C	287	THR	3.0
1	D	339	LEU	3.0
1	F	580	VAL	3.0
1	A	296	ALA	3.0
1	F	257	HIS	3.0
1	D	499	PHE	3.0
1	D	535	VAL	3.0
1	B	268	ALA	3.0
1	C	533	LEU	3.0
1	E	207	MET	3.0
1	F	62	ALA	3.0
1	F	289	CYS	3.0
1	E	382	VAL	3.0
1	D	380	LEU	3.0
1	B	240	ILE	3.0
1	E	226	ILE	2.9
1	C	565	LEU	2.9
1	D	267	LEU	2.9
1	A	295	GLU	2.9
1	E	432	ASP	2.9
1	F	269	GLU	2.9
1	C	492	GLY	2.9
1	C	273	ILE	2.9
1	C	207	MET	2.9
1	B	361	ARG	2.9
1	B	227	LYS	2.9
1	A	592	LEU	2.9
1	E	289	CYS	2.9
1	B	297	LEU	2.9
1	A	164	TYR	2.9
1	A	380	LEU	2.9
1	E	339	LEU	2.9
1	C	466	TYR	2.9
1	E	501	LEU	2.9
1	B	82	GLY	2.8
1	E	162	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	206	GLN	2.8
1	E	311	PHE	2.8
1	E	209	ILE	2.8
1	F	272	ASP	2.8
1	F	311	PHE	2.8
1	F	157	GLN	2.8
1	E	533	LEU	2.8
1	F	267	LEU	2.8
1	F	82	GLY	2.8
1	B	267	LEU	2.8
1	D	164	TYR	2.8
1	C	412	GLN	2.8
1	E	177	GLU	2.8
1	C	156	GLU	2.8
1	D	295	GLU	2.8
1	C	335	LEU	2.8
1	F	587	ILE	2.8
1	B	380	LEU	2.8
1	A	535	VAL	2.8
1	D	294	VAL	2.8
1	E	437	VAL	2.8
1	F	231	VAL	2.8
1	C	282	LEU	2.8
1	E	5	LEU	2.8
1	C	556	VAL	2.8
1	A	580	VAL	2.7
1	F	226	ILE	2.7
1	E	380	LEU	2.7
1	A	599	ARG	2.7
1	E	282	LEU	2.7
1	A	293	ASN	2.7
1	D	580	VAL	2.7
1	B	226	ILE	2.7
1	C	239	ILE	2.7
1	C	490	SER	2.7
1	A	593	THR	2.7
1	D	272	ASP	2.7
1	F	161	PRO	2.7
1	C	303	ASP	2.7
1	C	535	VAL	2.7
1	D	288	VAL	2.7
1	F	501	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	296	ALA	2.7
1	D	156	GLU	2.7
1	D	489	ILE	2.7
1	E	267	LEU	2.7
1	C	591	HIS	2.7
1	B	62	ALA	2.7
1	C	379	GLU	2.7
1	C	72	ILE	2.7
1	E	240	ILE	2.7
1	D	282	LEU	2.7
1	B	378	PHE	2.7
1	E	347	VAL	2.7
1	E	66	ASN	2.7
1	F	212	LEU	2.7
1	D	257	HIS	2.7
1	E	291	THR	2.6
1	B	15	ASP	2.6
1	D	144	VAL	2.6
1	F	593	THR	2.6
1	D	335	LEU	2.6
1	E	210	SER	2.6
1	F	156	GLU	2.6
1	F	432	ASP	2.6
1	D	311	PHE	2.6
1	B	303	ASP	2.6
1	B	535	VAL	2.6
1	F	240	ILE	2.6
1	E	519	TYR	2.6
1	B	412	GLN	2.6
1	D	526	ILE	2.6
1	A	282	LEU	2.6
1	B	282	LEU	2.6
1	E	335	LEU	2.6
1	B	435	GLY	2.6
1	A	226	ILE	2.6
1	F	2	ILE	2.6
1	F	209	ILE	2.6
1	F	15	ASP	2.6
1	F	499	PHE	2.6
1	A	239	ILE	2.6
1	A	311	PHE	2.6
1	C	339	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	533	LEU	2.6
1	D	212	LEU	2.5
1	C	56	ILE	2.5
1	C	289	CYS	2.5
1	F	190	ILE	2.5
1	C	577	LEU	2.5
1	C	162	ILE	2.5
1	A	492	GLY	2.5
1	A	207	MET	2.5
1	E	303	ASP	2.5
1	E	577	LEU	2.5
1	F	335	LEU	2.5
1	A	162	ILE	2.5
1	E	492	GLY	2.5
1	B	311	PHE	2.5
1	F	356	PHE	2.5
1	C	164	TYR	2.5
1	D	208	GLN	2.5
1	E	212	LEU	2.5
1	D	534	THR	2.5
1	D	495	LYS	2.5
1	A	533	LEU	2.5
1	C	537	CYS	2.5
1	D	519	TYR	2.5
1	A	246	THR	2.5
1	D	239	ILE	2.5
1	B	409	GLU	2.5
1	E	415	VAL	2.5
1	E	518	VAL	2.5
1	B	137	PRO	2.5
1	B	183	MET	2.5
1	D	148	PHE	2.5
1	D	533	LEU	2.5
1	D	273	ILE	2.5
1	E	127	ILE	2.5
1	A	84	GLU	2.4
1	A	288	VAL	2.4
1	F	227	LYS	2.4
1	D	287	THR	2.4
1	A	209	ILE	2.4
1	A	272	ASP	2.4
1	F	230	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	592	LEU	2.4
1	F	464	LEU	2.4
1	F	535	VAL	2.4
1	A	273	ILE	2.4
1	D	127	ILE	2.4
1	E	159	ASP	2.4
1	B	519	TYR	2.4
1	D	207	MET	2.4
1	A	58	ALA	2.4
1	C	69	ARG	2.4
1	E	522	GLN	2.4
1	C	265	THR	2.4
1	B	162	ILE	2.4
1	F	511	PHE	2.4
1	A	489	ILE	2.4
1	E	589	LYS	2.4
1	F	437	VAL	2.4
1	C	587	ILE	2.4
1	E	15	ASP	2.4
1	B	289	CYS	2.4
1	B	589	LYS	2.4
1	D	437	VAL	2.4
1	C	361	ARG	2.4
1	B	209	ILE	2.4
1	C	300	LEU	2.4
1	A	251	VAL	2.4
1	B	466	TYR	2.4
1	D	7	ASN	2.4
1	D	428	ASN	2.4
1	D	415	VAL	2.4
1	B	145	PHE	2.4
1	D	251	VAL	2.3
1	B	265	THR	2.3
1	C	228	ARG	2.3
1	B	335	LEU	2.3
1	F	162	ILE	2.3
1	C	15	ASP	2.3
1	E	269	GLU	2.3
1	A	212	LEU	2.3
1	B	526	ILE	2.3
1	C	382	VAL	2.3
1	E	231	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	356	PHE	2.3
1	C	272	ASP	2.3
1	C	519	TYR	2.3
1	F	380	LEU	2.3
1	C	276	ILE	2.3
1	C	177	GLU	2.3
1	E	156	GLU	2.3
1	E	379	GLU	2.3
1	D	13	HIS	2.3
1	C	3	GLU	2.3
1	A	127	ILE	2.3
1	A	587	ILE	2.3
1	B	558	VAL	2.3
1	E	455	PHE	2.3
1	B	223	ILE	2.3
1	D	587	ILE	2.3
1	B	141	VAL	2.3
1	A	526	ILE	2.3
1	D	162	ILE	2.3
1	B	347	VAL	2.3
1	A	426	LEU	2.3
1	E	97	LEU	2.3
1	C	227	LYS	2.3
1	C	356	PHE	2.3
1	F	291	THR	2.2
1	C	87	ARG	2.2
1	B	212	LEU	2.2
1	D	223	ILE	2.2
1	D	226	ILE	2.2
1	F	358	VAL	2.2
1	E	490	SER	2.2
1	A	230	LYS	2.2
1	B	451	PHE	2.2
1	A	537	CYS	2.2
1	B	382	VAL	2.2
1	E	246	THR	2.2
1	B	69	ARG	2.2
1	E	164	TYR	2.2
1	B	127	ILE	2.2
1	A	145	PHE	2.2
1	B	228	ARG	2.2
1	F	361	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	62	ALA	2.2
1	F	7	ASN	2.2
1	D	565	LEU	2.2
1	B	499	PHE	2.2
1	A	173	GLY	2.2
1	B	272	ASP	2.2
1	D	266	ASP	2.2
1	C	451	PHE	2.2
1	A	379	GLU	2.2
1	B	266	ASP	2.2
1	E	230	LYS	2.2
1	F	277	THR	2.2
1	F	382	VAL	2.2
1	F	416	MET	2.2
1	F	489	ILE	2.2
1	B	490	SER	2.2
1	A	97	LEU	2.2
1	D	488	LEU	2.2
1	A	7	ASN	2.2
1	B	287	THR	2.2
1	C	145	PHE	2.2
1	A	144	VAL	2.2
1	C	201	LEU	2.2
1	D	57	LEU	2.2
1	B	239	ILE	2.2
1	C	144	VAL	2.2
1	F	370	ILE	2.2
1	A	415	VAL	2.2
1	F	246	THR	2.2
1	A	335	LEU	2.1
1	C	518	VAL	2.1
1	D	599	ARG	2.1
1	E	190	ILE	2.1
1	E	223	ILE	2.1
1	A	147	LEU	2.1
1	C	102	PHE	2.1
1	A	482	GLN	2.1
1	E	358	VAL	2.1
1	B	577	LEU	2.1
1	D	165	ALA	2.1
1	F	589	LYS	2.1
1	E	21	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	ASP	2.1
1	F	79	ALA	2.1
1	B	156	GLU	2.1
1	B	580	VAL	2.1
1	C	2	ILE	2.1
1	A	223	ILE	2.1
1	B	448	LEU	2.1
1	D	501	LEU	2.1
1	E	361	ARG	2.1
1	B	296	ALA	2.1
1	C	84	GLU	2.1
1	B	2	ILE	2.1
1	B	585	ILE	2.1
1	B	592	LEU	2.1
1	C	141	VAL	2.1
1	D	72	ILE	2.1
1	C	380	LEU	2.1
1	A	417	GLN	2.1
1	B	587	ILE	2.1
1	C	70	ILE	2.1
1	E	72	ILE	2.1
1	F	273	ILE	2.1
1	B	246	THR	2.1
1	B	248	ASN	2.1
1	E	79	ALA	2.1
1	F	519	TYR	2.1
1	B	578	VAL	2.1
1	A	565	LEU	2.1
1	B	96	LEU	2.1
1	C	585	ILE	2.1
1	E	489	ILE	2.1
1	A	466	TYR	2.0
1	F	84	GLU	2.0
1	C	246	THR	2.0
1	E	82	GLY	2.0
1	D	111	PHE	2.0
1	D	487	VAL	2.0
1	C	5	LEU	2.0
1	F	72	ILE	2.0
1	F	455	PHE	2.0
1	C	251	VAL	2.0
1	B	276	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	300	LEU	2.0
1	E	2	ILE	2.0
1	A	111	PHE	2.0
1	D	66	ASN	2.0
1	F	451	PHE	2.0
1	C	358	VAL	2.0
1	A	72	ILE	2.0
1	A	66	ASN	2.0
1	C	248	ASN	2.0
1	E	7	ASN	2.0
1	E	91	MET	2.0
1	B	70	ILE	2.0
1	C	96	LEU	2.0
1	C	212	LEU	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.