



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:25 PM UTC

PDB ID : 4HPQ / pdb_00004hpq
Title : Crystal Structure of the Atg17-Atg31-Atg29 Complex
Authors : Stanley, R.E.; Ragusa, M.J.; Hurley, J.H.
Deposited on : 2012-10-24
Resolution : 3.06 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 types of validation reports are described at

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

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

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

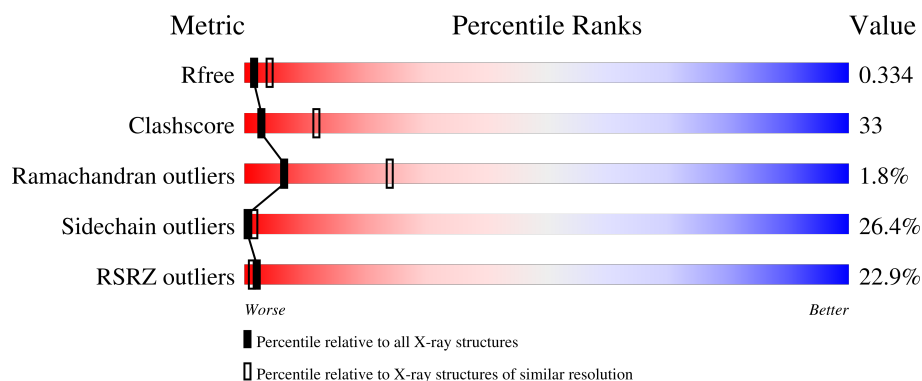
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	69	22% 65% 28% 6%
1	D	69	25% 62% 28% 9%
2	B	159	14% 39% 25% 9% 28%
2	E	159	14% 33% 30% 9% 28%
3	C	413	21% 35% 44% 16%

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Mol	Chain	Length	Quality of chain
3	F	413	21% 35% 45% 15% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9220 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 Atg29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			429	266	82	80	1			
1	D	69	Total	C	N	O	S	0	0	0
			429	266	82	80	1			

- Molecule 2 is a protein called Atg31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			932	587	156	185	4			
2	E	115	Total	C	N	O	S	0	0	0
			932	587	156	185	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MET	LEU	engineered mutation	UNP C5DEB9
B	110	MET	LEU	engineered mutation	UNP C5DEB9
B	146	ALA	-	expression tag	UNP C5DEB9
B	147	GLY	-	expression tag	UNP C5DEB9
B	148	GLN	-	expression tag	UNP C5DEB9
B	149	PHE	-	expression tag	UNP C5DEB9
B	150	TYR	-	expression tag	UNP C5DEB9
B	151	LEU	-	expression tag	UNP C5DEB9
B	152	ASN	-	expression tag	UNP C5DEB9
B	153	ALA	-	expression tag	UNP C5DEB9
B	154	HIS	-	expression tag	UNP C5DEB9
B	155	HIS	-	expression tag	UNP C5DEB9
B	156	HIS	-	expression tag	UNP C5DEB9
B	157	HIS	-	expression tag	UNP C5DEB9
B	158	HIS	-	expression tag	UNP C5DEB9
B	159	HIS	-	expression tag	UNP C5DEB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	87	MET	LEU	engineered mutation	UNP C5DEB9
E	110	MET	LEU	engineered mutation	UNP C5DEB9
E	146	ALA	-	expression tag	UNP C5DEB9
E	147	GLY	-	expression tag	UNP C5DEB9
E	148	GLN	-	expression tag	UNP C5DEB9
E	149	PHE	-	expression tag	UNP C5DEB9
E	150	TYR	-	expression tag	UNP C5DEB9
E	151	LEU	-	expression tag	UNP C5DEB9
E	152	ASN	-	expression tag	UNP C5DEB9
E	153	ALA	-	expression tag	UNP C5DEB9
E	154	HIS	-	expression tag	UNP C5DEB9
E	155	HIS	-	expression tag	UNP C5DEB9
E	156	HIS	-	expression tag	UNP C5DEB9
E	157	HIS	-	expression tag	UNP C5DEB9
E	158	HIS	-	expression tag	UNP C5DEB9
E	159	HIS	-	expression tag	UNP C5DEB9

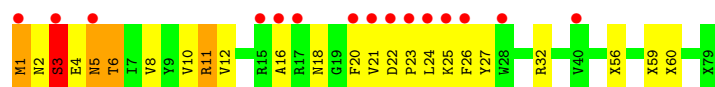
- Molecule 3 is a protein called Atg17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	396	Total	C	N	O	S	0	0	0
			3249	2036	565	635	13			
3	F	396	Total	C	N	O	S	0	0	0
			3249	2036	565	635	13			

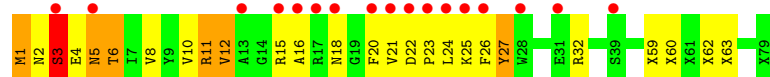
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

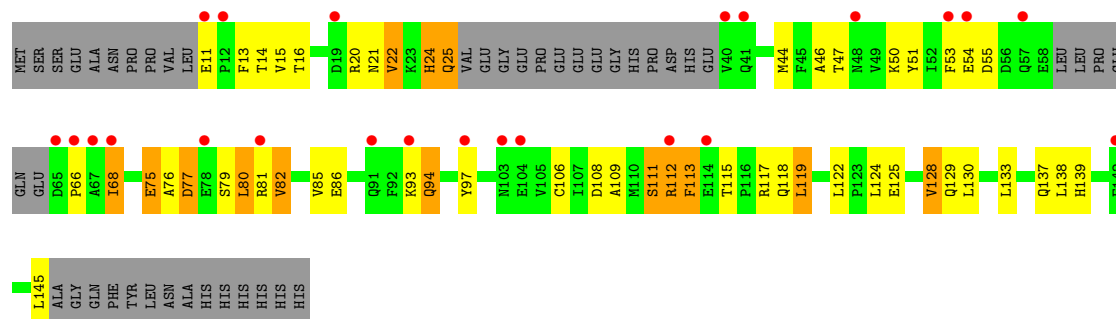
• Molecule 1: Atg29



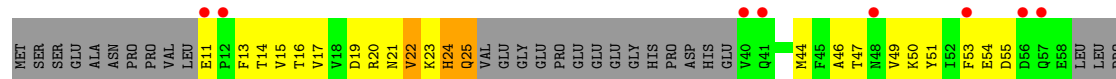
• Molecule 1: Atg29

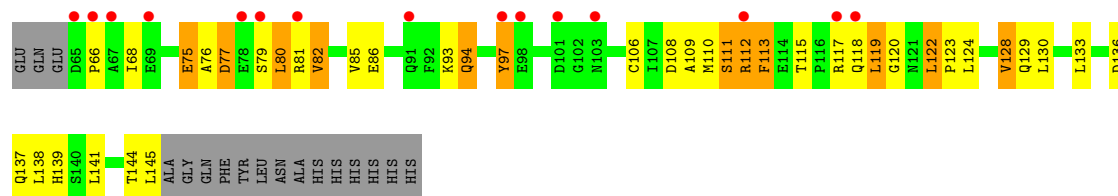


• Molecule 2: Atg31

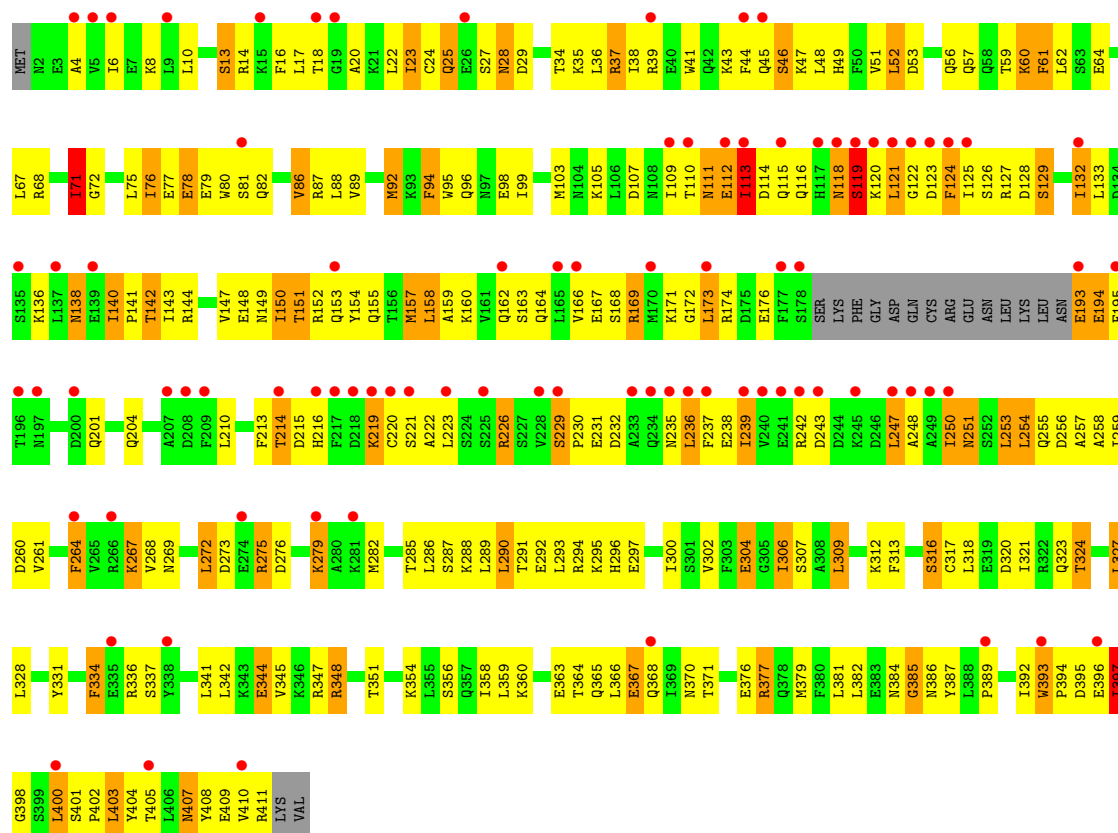


• Molecule 2: Atg31

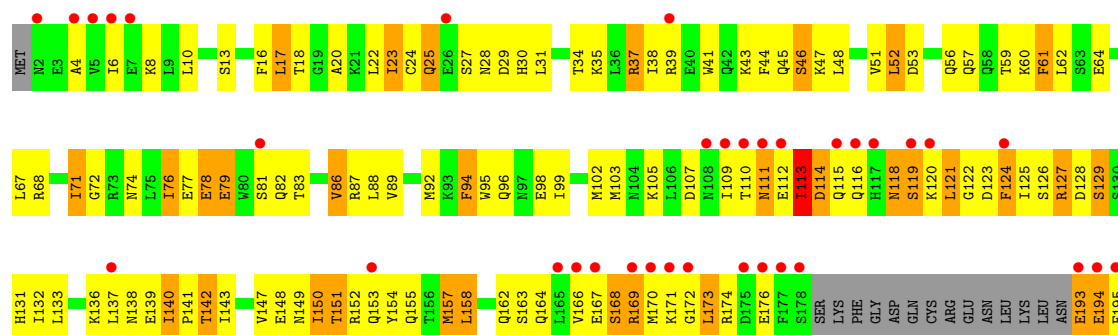


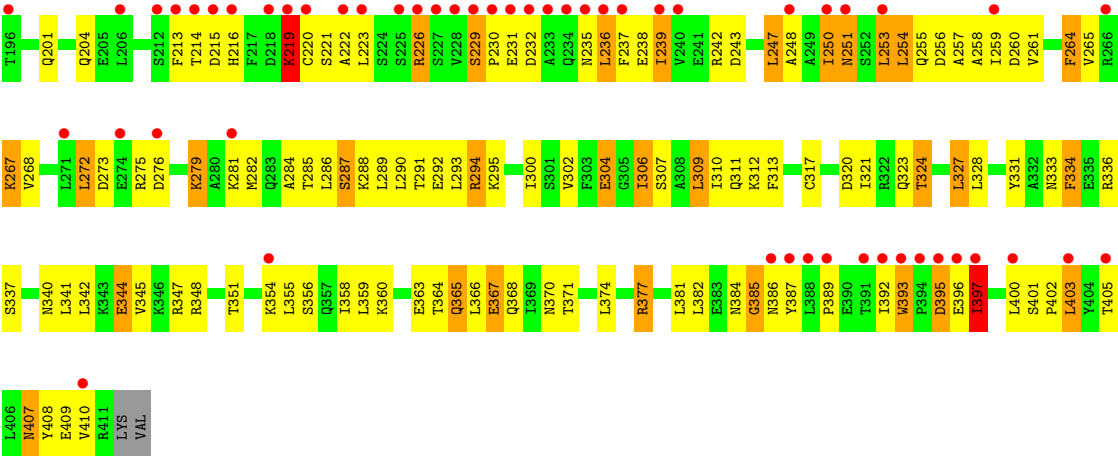


• Molecule 3: Atg17



• Molecule 3: Atg17





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	144.37Å 64.20Å 184.21Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	46.56 – 3.06 46.56 – 3.06	Depositor EDS
% Data completeness (in resolution range)	75.4 (46.56-3.06) 75.8 (46.56-3.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.303 , 0.336 0.302 , 0.334	Depositor DCC
R_{free} test set	3071 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9220	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/288	0.94	0/391
1	D	0.77	0/288	1.00	1/391 (0.3%)
2	B	0.71	0/944	0.99	2/1276 (0.2%)
2	E	0.96	0/944	1.10	3/1276 (0.2%)
3	C	0.73	0/3292	0.97	5/4426 (0.1%)
3	F	0.93	0/3292	1.03	4/4426 (0.1%)
All	All	0.83	0/9048	1.01	15/12186 (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
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	150	ILE	CB-CA-C	-6.28	103.84	111.88
2	B	112	ARG	N-CA-CB	-6.24	107.06	114.17
3	C	397	ILE	CB-CA-C	-6.03	104.25	111.97
3	F	219	LYS	N-CA-C	-5.80	104.87	111.07
3	F	397	ILE	CB-CA-C	-5.62	104.78	111.97
2	E	110	MET	N-CA-C	-5.52	100.96	109.52
3	F	150	ILE	CB-CA-C	-5.44	104.92	111.88
3	C	138	ASN	N-CA-C	5.24	116.99	111.28
3	C	385	GLY	N-CA-C	-5.23	100.78	113.18
2	B	112	ARG	N-CA-C	5.19	121.43	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	120	GLY	N-CA-C	-5.19	107.72	113.79
3	C	71	ILE	CB-CA-C	-5.18	105.11	111.94
1	D	27	TYR	N-CA-C	5.17	116.82	108.34
3	F	385	GLY	N-CA-C	-5.09	101.11	113.18
2	E	112	ARG	N-CA-CB	-5.01	106.05	114.27

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	SER	Peptide
2	E	111	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	429	0	278	38	0
1	D	429	0	280	42	0
2	B	932	0	911	62	0
2	E	932	0	911	65	0
3	C	3249	0	3253	248	0
3	F	3249	0	3253	238	0
All	All	9220	0	8886	595	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 33.

All (595) 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)
3:C:109:ILE:HG21	3:C:121:LEU:HD22	1.17	1.14
3:F:109:ILE:HG21	3:F:121:LEU:HD22	1.18	1.13
3:C:67:LEU:HD11	3:C:157:MET:HE2	1.51	0.91
3:F:67:LEU:HD11	3:F:157:MET:HE2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HB3	2:E:44:MET:SD	2.11	0.90
3:F:110:THR:O	3:F:111:ASN:CB	2.19	0.89
3:C:393:TRP:CZ2	3:F:345:VAL:HG23	2.08	0.88
3:C:109:ILE:HG21	3:C:121:LEU:CD2	2.04	0.88
3:F:109:ILE:HG21	3:F:121:LEU:CD2	2.02	0.88
3:C:110:THR:O	3:C:111:ASN:CB	2.21	0.87
3:F:109:ILE:HG22	3:F:120:LYS:HB3	1.57	0.86
2:E:22:VAL:HG11	2:E:130:LEU:HD22	1.56	0.86
3:C:110:THR:O	3:C:111:ASN:HB2	1.77	0.84
2:B:22:VAL:HG11	2:B:130:LEU:HD22	1.58	0.83
3:C:109:ILE:HG22	3:C:120:LYS:HB3	1.62	0.82
3:F:109:ILE:CG2	3:F:121:LEU:HD22	2.08	0.81
3:C:147:VAL:O	3:C:151:THR:HG22	1.79	0.81
3:F:193:GLU:OE2	3:F:193:GLU:N	2.12	0.81
3:F:110:THR:O	3:F:111:ASN:HB2	1.78	0.81
1:A:25:LYS:O	2:B:47:THR:HG21	1.80	0.80
3:F:57:GLN:HA	3:F:57:GLN:OE1	1.80	0.80
1:D:25:LYS:O	2:E:47:THR:HG21	1.82	0.79
3:C:193:GLU:OE2	3:C:193:GLU:N	2.16	0.78
3:C:334:PHE:CD1	3:C:334:PHE:C	2.61	0.78
3:C:44:PHE:HE2	3:C:279:LYS:CG	1.96	0.78
3:F:276:ASP:HA	3:F:279:LYS:HD3	1.65	0.78
3:F:147:VAL:O	3:F:151:THR:HG22	1.84	0.78
3:F:44:PHE:HE2	3:F:279:LYS:CG	1.97	0.78
3:C:57:GLN:OE1	3:C:57:GLN:HA	1.85	0.77
3:F:41:TRP:CD1	3:F:279:LYS:HZ3	2.03	0.76
3:C:359:LEU:HD21	3:F:366:LEU:HD11	1.66	0.76
3:C:393:TRP:HZ2	3:F:345:VAL:HG23	1.47	0.75
3:C:276:ASP:HA	3:C:279:LYS:HD3	1.68	0.75
1:D:5:ASN:O	1:D:5:ASN:ND2	2.19	0.75
2:B:93:LYS:HZ3	3:C:47:LYS:HD3	1.50	0.74
3:C:10:LEU:HA	3:C:220:CYS:SG	2.26	0.74
3:F:23:ILE:C	3:F:23:ILE:HD13	2.12	0.74
3:C:387:TYR:CD2	3:F:333:ASN:HB3	2.22	0.74
3:C:72:GLY:O	3:C:76:ILE:HB	1.87	0.74
3:F:334:PHE:CD1	3:F:334:PHE:C	2.65	0.73
3:F:119:SER:OG	3:F:123:ASP:HB2	1.88	0.73
3:F:223:LEU:HD21	3:F:236:LEU:HD12	1.69	0.73
1:D:16:ALA:HA	2:E:53:PHE:CD2	2.24	0.73
3:C:223:LEU:HD21	3:C:236:LEU:HD12	1.71	0.73
3:F:389:PRO:O	3:F:392:ILE:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:O	1:D:5:ASN:CG	2.33	0.71
1:A:1:MET:HB3	2:B:44:MET:SD	2.30	0.71
1:A:5:ASN:ND2	1:A:5:ASN:O	2.23	0.71
3:C:109:ILE:CG2	3:C:121:LEU:HD22	2.08	0.71
1:A:5:ASN:O	1:A:5:ASN:CG	2.33	0.70
1:D:1:MET:HB3	2:E:44:MET:CG	2.20	0.70
1:D:21:VAL:HG12	1:D:23:PRO:HD3	1.71	0.70
1:A:21:VAL:HG12	1:A:23:PRO:HD3	1.72	0.70
1:D:16:ALA:HA	2:E:53:PHE:HD2	1.56	0.70
3:F:10:LEU:HA	3:F:220:CYS:SG	2.31	0.70
3:C:41:TRP:CD1	3:C:279:LYS:HZ3	2.09	0.70
1:D:10:VAL:HG11	2:E:51:TYR:CD2	2.26	0.70
2:B:93:LYS:NZ	3:C:47:LYS:HD3	2.06	0.69
3:C:334:PHE:C	3:C:334:PHE:HD1	2.00	0.69
1:A:24:LEU:HD11	1:A:26:PHE:CE2	2.27	0.69
3:F:78:GLU:O	3:F:82:GLN:HG2	1.92	0.69
1:A:11:ARG:HB2	2:B:75:GLU:HG3	1.75	0.69
3:C:124:PHE:HD2	3:F:392:ILE:HD12	1.56	0.69
1:D:24:LEU:HD11	1:D:26:PHE:CE2	2.28	0.69
3:F:344:GLU:O	3:F:344:GLU:OE1	2.10	0.69
3:C:44:PHE:HE2	3:C:279:LYS:HG3	1.58	0.69
3:C:119:SER:OG	3:C:123:ASP:HB2	1.92	0.68
3:C:136:LYS:HE2	3:C:317:CYS:SG	2.33	0.68
3:F:72:GLY:O	3:F:76:ILE:HB	1.93	0.68
2:B:93:LYS:HZ2	3:C:47:LYS:HA	1.59	0.68
3:F:44:PHE:HE2	3:F:279:LYS:HG3	1.60	0.67
3:C:94:PHE:CD1	3:C:94:PHE:C	2.71	0.67
3:F:367:GLU:O	3:F:371:THR:HG23	1.94	0.67
3:C:78:GLU:O	3:C:82:GLN:HG2	1.95	0.66
2:B:15:VAL:HB	2:B:46:ALA:HB3	1.77	0.66
3:C:381:LEU:O	3:C:384:ASN:O	2.13	0.66
3:C:94:PHE:C	3:C:94:PHE:HD1	2.03	0.66
3:C:94:PHE:CE1	3:C:98:GLU:HG3	2.30	0.66
2:B:113:PHE:O	3:C:57:GLN:HG3	1.94	0.66
3:F:44:PHE:HE2	3:F:279:LYS:HG2	1.60	0.66
1:D:25:LYS:H	2:E:47:THR:CG2	2.09	0.65
3:C:23:ILE:C	3:C:23:ILE:HD13	2.22	0.65
3:C:99:ILE:HA	3:C:328:LEU:HD21	1.79	0.65
3:F:334:PHE:C	3:F:334:PHE:HD1	2.04	0.65
1:A:24:LEU:HD13	1:A:24:LEU:C	2.21	0.65
1:D:1:MET:CB	2:E:44:MET:SD	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:110:THR:O	3:F:111:ASN:HB3	1.96	0.65
1:A:27:TYR:OH	1:A:32:ARG:HA	1.96	0.65
3:F:111:ASN:OD1	3:F:118:ASN:ND2	2.28	0.65
3:F:136:LYS:HE2	3:F:317:CYS:SG	2.37	0.65
3:C:320:ASP:O	3:C:324:THR:OG1	2.14	0.65
1:D:27:TYR:OH	1:D:32:ARG:HA	1.96	0.64
3:C:162:GLN:O	3:C:166:VAL:HG22	1.98	0.64
3:C:44:PHE:HE2	3:C:279:LYS:HG2	1.60	0.64
1:D:24:LEU:HD13	1:D:24:LEU:C	2.23	0.64
1:A:20:PHE:CE1	2:B:53:PHE:CE2	2.86	0.64
2:B:93:LYS:NZ	3:C:46:SER:HB3	2.13	0.64
3:F:393:TRP:HB3	3:F:397:ILE:HG13	1.79	0.64
3:C:193:GLU:N	3:C:194:GLU:OE2	2.31	0.64
1:D:62:UNK:O	1:D:63:UNK:C	2.46	0.64
3:C:309:LEU:C	3:C:309:LEU:HD12	2.23	0.63
3:F:342:LEU:O	3:F:345:VAL:HG12	1.98	0.63
3:C:264:PHE:HE1	3:C:268:VAL:HG21	1.63	0.63
3:C:393:TRP:HB3	3:C:397:ILE:HG13	1.79	0.63
3:F:136:LYS:HD3	3:F:317:CYS:SG	2.39	0.63
3:C:136:LYS:HD3	3:C:317:CYS:SG	2.38	0.62
1:A:25:LYS:O	2:B:47:THR:CG2	2.47	0.62
3:F:24:CYS:O	3:F:25:GLN:C	2.40	0.62
3:F:162:GLN:O	3:F:166:VAL:HG22	1.99	0.62
2:E:112:ARG:O	2:E:113:PHE:C	2.42	0.62
3:C:384:ASN:C	3:C:385:GLY:O	2.41	0.62
3:C:238:GLU:O	3:C:242:ARG:HG3	2.00	0.62
1:A:10:VAL:HG11	2:B:51:TYR:CD2	2.35	0.61
1:D:2:ASN:O	1:D:3:SER:C	2.43	0.61
3:C:16:PHE:CE2	3:C:248:ALA:HA	2.34	0.61
3:C:342:LEU:O	3:C:345:VAL:HG12	2.00	0.61
3:F:264:PHE:CD1	3:F:264:PHE:C	2.79	0.61
1:A:2:ASN:O	1:A:3:SER:C	2.43	0.61
3:C:366:LEU:HD11	3:F:359:LEU:HD21	1.83	0.61
3:F:61:PHE:CD1	3:F:61:PHE:C	2.76	0.61
3:C:358:ILE:HG21	3:F:365:GLN:HG2	1.82	0.61
3:F:193:GLU:N	3:F:194:GLU:OE2	2.33	0.61
2:B:124:LEU:HD12	3:C:71:ILE:HG12	1.81	0.61
3:F:264:PHE:HE1	3:F:268:VAL:HG21	1.65	0.61
3:C:110:THR:O	3:C:111:ASN:HB3	2.01	0.60
3:F:264:PHE:O	3:F:267:LYS:HG2	2.00	0.60
3:C:344:GLU:O	3:C:344:GLU:OE1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:HA	2:B:53:PHE:CD2	2.36	0.60
2:E:15:VAL:HB	2:E:46:ALA:HB3	1.82	0.60
3:C:94:PHE:HE1	3:C:98:GLU:HG3	1.67	0.60
3:F:94:PHE:CE1	3:F:98:GLU:HG3	2.36	0.60
3:F:37:ARG:NH2	3:F:273:ASP:OD1	2.35	0.60
3:F:320:ASP:O	3:F:324:THR:OG1	2.20	0.60
3:F:359:LEU:HD12	3:F:410:VAL:CG2	2.32	0.60
2:E:85:VAL:HG21	2:E:97:TYR:CD1	2.37	0.60
3:C:61:PHE:CD1	3:C:61:PHE:C	2.78	0.59
2:B:115:THR:HG21	3:C:60:LYS:HD2	1.84	0.59
1:D:10:VAL:HG12	2:E:51:TYR:HA	1.83	0.59
2:E:75:GLU:O	2:E:82:VAL:HA	2.02	0.59
3:F:111:ASN:HA	3:F:120:LYS:HA	1.83	0.59
3:C:96:GLN:O	3:C:99:ILE:HG22	2.02	0.59
3:C:111:ASN:OD1	3:C:118:ASN:ND2	2.31	0.59
3:F:44:PHE:CE2	3:F:279:LYS:HG2	2.37	0.59
3:C:403:LEU:HB2	3:F:355:LEU:CD1	2.33	0.59
3:F:238:GLU:O	3:F:242:ARG:HG3	2.03	0.59
3:C:387:TYR:HB3	3:F:334:PHE:HA	1.86	0.58
3:F:16:PHE:CE2	3:F:248:ALA:HA	2.37	0.58
3:C:112:GLU:O	3:C:113:ILE:HG22	2.03	0.58
3:C:264:PHE:O	3:C:267:LYS:HG2	2.02	0.58
3:C:64:GLU:O	3:C:68:ARG:HB3	2.04	0.58
3:C:367:GLU:O	3:C:371:THR:HG23	2.03	0.58
2:E:21:ASN:OD1	2:E:22:VAL:N	2.36	0.58
3:F:99:ILE:HA	3:F:328:LEU:HD21	1.85	0.58
3:C:44:PHE:CE2	3:C:279:LYS:HG2	2.38	0.58
3:C:223:LEU:HD11	3:C:236:LEU:HD12	1.86	0.58
3:F:94:PHE:CD1	3:F:94:PHE:C	2.82	0.58
2:B:75:GLU:O	2:B:82:VAL:HA	2.03	0.58
3:C:387:TYR:CE2	3:F:333:ASN:HB3	2.39	0.58
3:F:313:PHE:CE1	3:F:317:CYS:SG	2.97	0.58
3:C:76:ILE:O	3:C:81:SER:HB2	2.04	0.57
3:F:41:TRP:CD1	3:F:279:LYS:NZ	2.72	0.57
3:F:138:ASN:O	3:F:141:PRO:HD2	2.04	0.57
2:B:124:LEU:CD1	3:C:71:ILE:HG12	2.34	0.57
3:C:389:PRO:O	3:C:392:ILE:HG22	2.03	0.57
3:C:359:LEU:HD12	3:C:410:VAL:CG2	2.35	0.57
3:C:393:TRP:CE3	3:C:396:GLU:HB3	2.39	0.57
2:E:85:VAL:CG2	2:E:97:TYR:CD1	2.88	0.57
3:C:111:ASN:HA	3:C:120:LYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:GLU:HG3	3:F:118:ASN:ND2	2.19	0.57
2:B:93:LYS:HZ1	3:C:46:SER:HB3	1.70	0.57
3:C:124:PHE:CD1	3:C:124:PHE:N	2.72	0.57
3:F:112:GLU:O	3:F:113:ILE:HG22	2.05	0.57
1:A:25:LYS:H	2:B:47:THR:CG2	2.18	0.56
3:C:344:GLU:OE1	3:C:344:GLU:C	2.48	0.56
3:C:96:GLN:HE21	3:C:133:LEU:HB2	1.68	0.56
2:E:93:LYS:HZ3	3:F:47:LYS:HD3	1.71	0.56
3:C:23:ILE:HD11	3:C:258:ALA:HB2	1.87	0.56
3:F:172:GLY:O	3:F:176:GLU:HG2	2.06	0.56
3:C:112:GLU:HG3	3:C:118:ASN:ND2	2.20	0.56
2:B:85:VAL:HG21	2:B:97:TYR:CD1	2.41	0.56
3:F:293:LEU:HD23	3:F:293:LEU:N	2.21	0.56
3:F:407:ASN:OD1	3:F:407:ASN:N	2.39	0.55
3:C:138:ASN:O	3:C:141:PRO:HD2	2.06	0.55
3:F:43:LYS:HB3	3:F:47:LYS:HE3	1.88	0.55
2:E:124:LEU:HD22	3:F:304:GLU:HG2	1.89	0.55
3:F:96:GLN:HE21	3:F:133:LEU:HB2	1.71	0.55
1:A:20:PHE:HE1	2:B:53:PHE:CE2	2.24	0.55
3:F:223:LEU:HD11	3:F:236:LEU:HD12	1.87	0.55
3:C:334:PHE:HD1	3:C:334:PHE:O	1.90	0.55
3:C:407:ASN:N	3:C:407:ASN:OD1	2.39	0.55
1:D:25:LYS:O	2:E:47:THR:CG2	2.54	0.55
3:F:61:PHE:O	3:F:62:LEU:C	2.49	0.55
3:F:384:ASN:C	3:F:385:GLY:O	2.45	0.55
3:C:128:ASP:O	3:C:129:SER:HB3	2.07	0.55
3:F:381:LEU:O	3:F:384:ASN:O	2.25	0.55
2:B:21:ASN:OD1	2:B:22:VAL:N	2.40	0.55
3:C:210:LEU:O	3:C:214:THR:OG1	2.25	0.55
3:F:109:ILE:O	3:F:120:LYS:HD2	2.06	0.55
3:C:354:LYS:O	3:C:358:ILE:HG12	2.07	0.54
1:A:10:VAL:HG12	2:B:51:TYR:HA	1.89	0.54
2:E:136:ASP:OD1	3:F:294:ARG:NH2	2.41	0.54
3:F:43:LYS:O	3:F:44:PHE:C	2.50	0.54
3:C:264:PHE:CD1	3:C:264:PHE:C	2.85	0.54
3:F:107:ASP:OD1	3:F:122:GLY:HA3	2.08	0.54
2:E:13:PHE:HB2	2:E:51:TYR:OH	2.09	0.53
2:E:124:LEU:CD2	3:F:304:GLU:HG2	2.38	0.53
3:F:94:PHE:C	3:F:94:PHE:HD1	2.16	0.53
2:B:85:VAL:CG2	2:B:97:TYR:CD1	2.91	0.53
3:C:215:ASP:O	3:C:219:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:34:THR:O	3:F:35:LYS:C	2.50	0.53
3:F:140:ILE:HG22	3:F:141:PRO:HD3	1.91	0.53
3:F:52:LEU:O	3:F:53:ASP:C	2.51	0.53
1:A:3:SER:HB2	2:B:47:THR:OG1	2.09	0.53
3:F:41:TRP:HD1	3:F:279:LYS:HZ3	1.53	0.53
3:F:96:GLN:O	3:F:99:ILE:HG22	2.07	0.53
3:F:267:LYS:HG3	3:F:268:VAL:N	2.23	0.53
3:C:111:ASN:O	3:C:112:GLU:C	2.52	0.53
3:C:124:PHE:CD2	3:F:392:ILE:HD12	2.41	0.53
3:F:17:LEU:HA	3:F:213:PHE:HD2	1.73	0.53
3:C:409:GLU:HB2	3:F:405:THR:OG1	2.09	0.53
3:F:23:ILE:HD11	3:F:258:ALA:HB2	1.91	0.53
3:F:393:TRP:CE3	3:F:396:GLU:HB3	2.44	0.53
3:C:41:TRP:CD1	3:C:279:LYS:NZ	2.76	0.52
2:B:112:ARG:O	2:B:113:PHE:C	2.50	0.52
3:C:44:PHE:CE2	3:C:279:LYS:CG	2.86	0.52
3:C:61:PHE:O	3:C:62:LEU:C	2.52	0.52
3:C:238:GLU:O	3:C:242:ARG:CG	2.58	0.52
3:F:64:GLU:O	3:F:68:ARG:HB3	2.09	0.52
3:F:154:TYR:O	3:F:158:LEU:HB2	2.09	0.52
1:A:1:MET:HB3	2:B:44:MET:CG	2.40	0.52
2:B:13:PHE:HB2	2:B:51:TYR:OH	2.10	0.52
3:C:313:PHE:CE1	3:C:317:CYS:SG	3.03	0.52
3:F:122:GLY:O	3:F:125:ILE:HG22	2.10	0.52
3:C:172:GLY:O	3:C:176:GLU:HG2	2.09	0.52
1:D:1:MET:N	1:D:6:THR:HG21	2.25	0.52
3:F:107:ASP:O	3:F:120:LYS:HG3	2.10	0.52
3:F:111:ASN:O	3:F:112:GLU:C	2.53	0.52
3:F:356:SER:OG	3:F:410:VAL:HG11	2.10	0.52
3:F:370:ASN:OD1	3:F:402:PRO:HB3	2.10	0.52
3:C:17:LEU:HA	3:C:213:PHE:HD2	1.75	0.52
3:C:148:GLU:HA	3:C:151:THR:CG2	2.39	0.52
3:C:215:ASP:OD1	3:C:216:HIS:N	2.43	0.52
3:C:291:THR:O	3:C:295:LYS:HG3	2.10	0.52
1:D:1:MET:SD	2:E:17:VAL:HG21	2.50	0.52
3:C:24:CYS:O	3:C:25:GLN:C	2.52	0.51
3:C:385:GLY:O	3:C:386:ASN:HB2	2.09	0.51
3:F:38:ILE:HG13	3:F:39:ARG:N	2.25	0.51
3:C:94:PHE:HD1	3:C:95:TRP:N	2.08	0.51
3:C:140:ILE:HG22	3:C:141:PRO:HD3	1.92	0.51
1:A:25:LYS:C	2:B:47:THR:HG21	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:UNK:O	1:A:60:UNK:N	2.43	0.51
3:C:405:THR:OG1	3:F:409:GLU:HB2	2.09	0.51
3:F:223:LEU:HD11	3:F:236:LEU:CD1	2.41	0.51
1:D:2:ASN:O	1:D:4:GLU:N	2.43	0.51
2:B:124:LEU:HD22	3:C:304:GLU:HG2	1.93	0.51
3:C:86:VAL:HG12	3:C:87:ARG:N	2.26	0.51
1:D:2:ASN:H	1:D:6:THR:HG21	1.74	0.51
3:F:41:TRP:CH2	3:F:45:GLN:HG3	2.46	0.51
3:F:124:PHE:N	3:F:124:PHE:CD1	2.75	0.51
3:F:167:GLU:O	3:F:171:LYS:HG2	2.10	0.51
3:F:285:THR:HA	3:F:288:LYS:HD3	1.93	0.51
3:F:385:GLY:O	3:F:386:ASN:HB2	2.10	0.51
1:D:10:VAL:CG1	2:E:51:TYR:CD2	2.94	0.51
3:F:302:VAL:O	3:F:306:ILE:HG23	2.11	0.51
1:D:1:MET:HB3	2:E:44:MET:CB	2.40	0.51
3:F:344:GLU:OE1	3:F:344:GLU:C	2.54	0.51
3:C:384:ASN:HD21	3:F:340:ASN:HB3	1.76	0.51
1:D:11:ARG:HB2	2:E:75:GLU:HG3	1.91	0.51
3:C:327:LEU:HD13	3:C:331:TYR:CE1	2.47	0.50
3:F:136:LYS:NZ	3:F:320:ASP:OD2	2.44	0.50
3:F:309:LEU:C	3:F:309:LEU:HD12	2.36	0.50
2:B:115:THR:HG22	3:C:61:PHE:HB2	1.92	0.50
3:C:89:VAL:CG2	3:C:140:ILE:HD12	2.41	0.50
3:C:285:THR:HA	3:C:288:LYS:HD3	1.92	0.50
3:F:94:PHE:HE1	3:F:98:GLU:HG3	1.77	0.50
3:C:174:ARG:HB2	3:C:174:ARG:CZ	2.40	0.50
3:F:86:VAL:HG12	3:F:87:ARG:N	2.27	0.50
1:A:2:ASN:H	1:A:6:THR:HG21	1.75	0.50
3:C:223:LEU:HD11	3:C:236:LEU:CD1	2.41	0.50
3:F:354:LYS:O	3:F:358:ILE:HG12	2.11	0.50
2:B:81:ARG:C	2:B:82:VAL:HG23	2.36	0.50
3:C:13:SER:OG	3:C:14:ARG:N	2.44	0.50
3:C:43:LYS:HB3	3:C:47:LYS:HE3	1.92	0.50
3:C:122:GLY:O	3:C:125:ILE:HG22	2.12	0.50
3:F:119:SER:OG	3:F:123:ASP:CB	2.59	0.50
3:F:128:ASP:O	3:F:129:SER:HB3	2.11	0.50
3:C:34:THR:O	3:C:35:LYS:C	2.54	0.49
3:C:403:LEU:HD22	3:C:403:LEU:N	2.27	0.49
3:F:257:ALA:O	3:F:260:ASP:N	2.45	0.49
3:C:107:ASP:OD1	3:C:122:GLY:HA3	2.12	0.49
3:C:356:SER:OG	3:C:410:VAL:HG11	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:ARG:HG3	3:F:347:ARG:HH22	1.77	0.49
2:E:19:ASP:OD2	2:E:111:SER:OG	2.31	0.49
3:C:229:SER:HB2	3:C:232:ASP:HB2	1.93	0.49
3:F:27:SER:HB3	3:F:261:VAL:HG11	1.95	0.49
3:F:223:LEU:HD13	3:F:237:PHE:CE1	2.48	0.49
3:F:344:GLU:OE2	3:F:347:ARG:NH2	2.46	0.49
2:E:145:LEU:CD2	3:F:47:LYS:HB2	2.43	0.49
3:F:76:ILE:O	3:F:81:SER:HB2	2.11	0.49
3:F:174:ARG:HB2	3:F:174:ARG:CZ	2.41	0.49
3:C:267:LYS:HG3	3:C:268:VAL:N	2.27	0.49
1:D:8:VAL:HG21	2:E:46:ALA:HB1	1.93	0.49
3:F:148:GLU:HA	3:F:151:THR:CG2	2.43	0.49
3:C:37:ARG:NH2	3:C:273:ASP:OD1	2.45	0.49
3:F:215:ASP:OD1	3:F:216:HIS:N	2.46	0.49
1:D:25:LYS:H	2:E:47:THR:HG23	1.78	0.49
3:C:23:ILE:HD12	3:C:254:LEU:HD11	1.95	0.49
3:C:119:SER:OG	3:C:123:ASP:N	2.46	0.49
1:D:2:ASN:O	1:D:4:GLU:O	2.30	0.49
3:F:403:LEU:N	3:F:403:LEU:HD22	2.28	0.49
3:F:89:VAL:CG2	3:F:140:ILE:HD12	2.43	0.49
3:C:230:PRO:HD2	3:C:232:ASP:OD2	2.12	0.48
3:F:230:PRO:HD2	3:F:232:ASP:OD2	2.13	0.48
2:E:24:HIS:C	2:E:24:HIS:CD2	2.91	0.48
2:E:124:LEU:CD2	3:F:304:GLU:CG	2.92	0.48
3:F:113:ILE:HG23	3:F:113:ILE:O	2.12	0.48
3:F:229:SER:HB2	3:F:232:ASP:HB2	1.95	0.48
1:A:16:ALA:HA	2:B:53:PHE:HD2	1.77	0.48
3:C:44:PHE:CD1	3:C:44:PHE:C	2.90	0.48
3:F:119:SER:OG	3:F:123:ASP:N	2.46	0.48
3:F:223:LEU:HD13	3:F:237:PHE:HE1	1.78	0.48
3:F:238:GLU:O	3:F:242:ARG:CG	2.61	0.48
3:C:167:GLU:O	3:C:171:LYS:HG2	2.14	0.48
3:C:216:HIS:C	3:C:216:HIS:CD2	2.91	0.48
1:A:1:MET:N	1:A:6:THR:HG21	2.27	0.48
3:C:119:SER:OG	3:C:119:SER:O	2.30	0.48
3:C:154:TYR:O	3:C:158:LEU:HB2	2.13	0.48
3:F:44:PHE:CE2	3:F:279:LYS:CG	2.87	0.48
3:C:27:SER:HB3	3:C:261:VAL:HG11	1.95	0.48
3:C:77:GLU:O	3:C:81:SER:HB3	2.14	0.48
3:F:89:VAL:HG22	3:F:140:ILE:HD12	1.96	0.48
3:F:152:ARG:HA	3:F:155:GLN:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:TRP:CH2	3:C:45:GLN:HG3	2.49	0.48
3:C:113:ILE:HG23	3:C:113:ILE:O	2.13	0.48
3:C:302:VAL:O	3:C:306:ILE:HG23	2.14	0.48
3:C:344:GLU:OE2	3:C:347:ARG:NH2	2.47	0.48
2:B:77:ASP:HB2	2:B:81:ARG:H	1.79	0.48
1:D:12:VAL:HG23	2:E:53:PHE:HA	1.96	0.48
1:D:25:LYS:C	2:E:47:THR:HG21	2.38	0.48
3:F:140:ILE:N	3:F:141:PRO:HD2	2.29	0.48
3:C:48:LEU:HG	3:C:52:LEU:CD2	2.44	0.48
3:C:141:PRO:O	3:C:142:THR:C	2.57	0.47
3:F:216:HIS:C	3:F:216:HIS:CD2	2.91	0.47
3:C:293:LEU:HD23	3:C:293:LEU:N	2.29	0.47
3:F:61:PHE:C	3:F:61:PHE:HD1	2.23	0.47
3:C:89:VAL:HG22	3:C:140:ILE:HD12	1.94	0.47
3:C:167:GLU:CG	3:C:168:SER:N	2.78	0.47
2:E:76:ALA:HB1	2:E:80:LEU:HA	1.96	0.47
3:F:167:GLU:CG	3:F:168:SER:N	2.77	0.47
1:A:8:VAL:HG21	2:B:46:ALA:HB1	1.96	0.47
3:C:44:PHE:CE2	3:C:279:LYS:HG3	2.44	0.47
3:F:359:LEU:HD12	3:F:410:VAL:HG21	1.95	0.47
1:A:59:UNK:O	1:A:60:UNK:CB	2.63	0.47
2:B:24:HIS:C	2:B:24:HIS:CD2	2.92	0.47
2:B:125:GLU:O	2:B:128:VAL:HG12	2.15	0.47
3:C:366:LEU:HD21	3:F:358:ILE:HB	1.96	0.47
1:D:8:VAL:CG2	2:E:46:ALA:HB1	2.44	0.47
2:B:124:LEU:CD2	3:C:304:GLU:HG2	2.43	0.47
3:C:223:LEU:HD13	3:C:237:PHE:HE1	1.80	0.47
3:C:393:TRP:CD2	3:C:396:GLU:HB3	2.50	0.47
2:E:77:ASP:HB2	2:E:81:ARG:H	1.78	0.47
1:A:2:ASN:O	1:A:4:GLU:N	2.47	0.47
1:A:25:LYS:H	2:B:47:THR:HG23	1.80	0.47
3:F:44:PHE:CE2	3:F:279:LYS:HG3	2.47	0.47
2:B:76:ALA:HB1	2:B:80:LEU:HA	1.97	0.46
2:B:138:LEU:O	2:B:139:HIS:C	2.58	0.46
3:C:141:PRO:O	3:C:144:ARG:N	2.48	0.46
3:C:223:LEU:HD13	3:C:237:PHE:CE1	2.50	0.46
3:F:385:GLY:C	3:F:387:TYR:N	2.73	0.46
3:C:152:ARG:HA	3:C:155:GLN:HG3	1.97	0.46
3:C:169:ARG:O	3:C:173:LEU:HD22	2.15	0.46
3:F:20:ALA:HA	3:F:23:ILE:HG22	1.97	0.46
3:F:48:LEU:HG	3:F:52:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:102:MET:HE3	3:F:331:TYR:HB3	1.97	0.46
2:E:20:ARG:HA	2:E:20:ARG:HD3	1.75	0.46
2:E:124:LEU:CD1	3:F:71:ILE:HG12	2.46	0.46
3:F:239:ILE:O	3:F:243:ASP:N	2.40	0.46
3:C:37:ARG:NH1	3:C:272:LEU:HB3	2.31	0.46
3:C:38:ILE:HG13	3:C:39:ARG:N	2.31	0.46
3:F:149:ASN:O	3:F:150:ILE:C	2.56	0.46
3:C:359:LEU:HD13	3:C:408:TYR:CG	2.51	0.46
2:E:122:LEU:HD23	2:E:122:LEU:N	2.31	0.46
2:E:81:ARG:C	2:E:82:VAL:HG23	2.41	0.46
2:E:124:LEU:HD12	3:F:71:ILE:HG12	1.96	0.46
2:E:53:PHE:N	2:E:53:PHE:CD1	2.84	0.46
3:F:94:PHE:HD1	3:F:95:TRP:N	2.12	0.46
3:F:310:ILE:O	3:F:311:GLN:C	2.58	0.46
3:F:213:PHE:HE1	3:F:250:ILE:HD11	1.80	0.46
2:B:145:LEU:HD22	3:C:44:PHE:CE1	2.51	0.45
3:C:148:GLU:HA	3:C:151:THR:HG22	1.98	0.45
3:C:384:ASN:HD21	3:F:340:ASN:CB	2.29	0.45
1:D:15:ARG:HG3	2:E:53:PHE:CE2	2.51	0.45
3:C:109:ILE:O	3:C:120:LYS:HD2	2.16	0.45
2:B:53:PHE:CD1	2:B:53:PHE:N	2.84	0.45
3:C:61:PHE:C	3:C:61:PHE:HD1	2.24	0.45
3:C:47:LYS:O	3:C:51:VAL:HG23	2.17	0.45
3:C:359:LEU:HD13	3:C:408:TYR:CB	2.47	0.45
3:F:23:ILE:HD12	3:F:254:LEU:HD11	1.99	0.45
3:F:113:ILE:C	3:F:114:ASP:OD1	2.60	0.45
3:C:118:ASN:O	3:C:120:LYS:N	2.49	0.45
3:F:291:THR:O	3:F:295:LYS:HG3	2.17	0.45
3:C:132:ILE:HD12	3:C:132:ILE:HA	1.90	0.45
3:F:119:SER:O	3:F:120:LYS:C	2.59	0.45
3:F:169:ARG:O	3:F:173:LEU:HD22	2.17	0.45
3:F:215:ASP:O	3:F:219:LYS:HG2	2.16	0.45
3:C:20:ALA:HA	3:C:23:ILE:HG22	1.99	0.45
3:C:159:ALA:O	3:C:160:LYS:C	2.60	0.45
3:C:317:CYS:O	3:C:318:LEU:C	2.60	0.45
1:D:10:VAL:CG1	2:E:51:TYR:HA	2.47	0.45
3:F:264:PHE:C	3:F:264:PHE:HD1	2.25	0.45
1:A:24:LEU:HD13	1:A:24:LEU:O	2.17	0.45
3:C:237:PHE:O	3:C:238:GLU:C	2.60	0.45
3:C:257:ALA:O	3:C:260:ASP:N	2.51	0.45
3:F:139:GLU:O	3:F:143:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:THR:HG21	3:C:60:LYS:CD	2.47	0.44
3:C:52:LEU:O	3:C:53:ASP:C	2.60	0.44
3:F:359:LEU:HD13	3:F:408:TYR:CG	2.53	0.44
3:F:385:GLY:C	3:F:387:TYR:H	2.24	0.44
2:B:77:ASP:OD2	2:B:81:ARG:HG3	2.17	0.44
3:F:222:ALA:HA	3:F:226:ARG:HG2	1.99	0.44
3:F:286:LEU:O	3:F:287:SER:C	2.60	0.44
3:F:258:ALA:O	3:F:261:VAL:HG12	2.17	0.44
2:B:93:LYS:NZ	3:C:46:SER:C	2.75	0.44
3:C:43:LYS:O	3:C:44:PHE:C	2.60	0.44
3:C:75:LEU:HB3	3:C:80:TRP:CH2	2.53	0.44
3:C:107:ASP:O	3:C:120:LYS:HG3	2.17	0.44
3:C:256:ASP:O	3:C:259:ILE:HB	2.17	0.44
3:C:231:GLU:O	3:C:231:GLU:HG2	2.18	0.44
3:C:286:LEU:O	3:C:289:LEU:N	2.49	0.44
3:C:327:LEU:HD22	3:C:327:LEU:HA	1.84	0.44
2:E:94:GLN:HA	2:E:109:ALA:HA	1.99	0.44
2:B:93:LYS:HZ2	3:C:47:LYS:CA	2.29	0.44
3:C:16:PHE:CZ	3:C:248:ALA:HA	2.53	0.44
3:C:366:LEU:HD21	3:F:358:ILE:CB	2.47	0.44
3:F:136:LYS:HE2	3:F:317:CYS:HA	1.99	0.44
1:A:2:ASN:O	1:A:4:GLU:O	2.35	0.44
1:D:4:GLU:OE2	1:D:4:GLU:HA	2.17	0.44
3:F:96:GLN:OE1	3:F:131:HIS:CD2	2.70	0.44
3:C:309:LEU:HD12	3:C:309:LEU:O	2.18	0.44
3:C:370:ASN:OD1	3:C:402:PRO:HB3	2.18	0.44
3:F:230:PRO:O	3:F:231:GLU:HB3	2.18	0.44
3:C:296:HIS:O	3:C:297:GLU:C	2.61	0.44
2:E:128:VAL:HG23	3:F:300:ILE:HG21	2.00	0.44
2:E:136:ASP:O	2:E:137:GLN:C	2.60	0.44
2:E:138:LEU:O	2:E:139:HIS:C	2.60	0.44
1:A:1:MET:CB	2:B:44:MET:SD	3.05	0.43
3:C:403:LEU:HB2	3:F:355:LEU:HD12	2.00	0.43
2:E:25:GLN:OE1	2:E:25:GLN:HA	2.18	0.43
3:F:74:ASN:N	3:F:74:ASN:HD22	2.16	0.43
3:C:169:ARG:C	3:C:173:LEU:HD22	2.42	0.43
3:C:376:GLU:OE2	3:C:379:MET:HE2	2.18	0.43
3:F:79:GLU:OE2	3:F:79:GLU:HA	2.17	0.43
3:C:76:ILE:O	3:C:81:SER:CB	2.66	0.43
3:C:286:LEU:O	3:C:287:SER:C	2.60	0.43
3:F:237:PHE:O	3:F:238:GLU:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:281:LYS:O	3:F:284:ALA:N	2.51	0.43
3:C:10:LEU:CA	3:C:220:CYS:SG	3.04	0.43
3:C:387:TYR:CE2	3:F:333:ASN:CB	3.01	0.43
3:C:393:TRP:O	3:C:394:PRO:C	2.61	0.43
2:E:85:VAL:HG22	2:E:97:TYR:CE1	2.54	0.43
3:F:125:ILE:HD12	3:F:125:ILE:HA	1.84	0.43
3:C:201:GLN:O	3:C:204:GLN:HB3	2.18	0.43
3:C:359:LEU:HD12	3:C:410:VAL:HG21	1.99	0.43
3:C:403:LEU:N	3:C:403:LEU:CD2	2.81	0.43
3:F:393:TRP:CD2	3:F:396:GLU:HB3	2.53	0.43
3:C:41:TRP:HD1	3:C:279:LYS:HZ3	1.59	0.43
3:C:163:SER:OG	3:C:164:GLN:N	2.51	0.43
3:C:313:PHE:CD1	3:C:313:PHE:C	2.96	0.43
3:C:119:SER:OG	3:C:123:ASP:CB	2.63	0.43
3:C:222:ALA:HA	3:C:226:ARG:HG2	2.00	0.43
3:C:247:LEU:O	3:C:248:ALA:C	2.60	0.43
2:E:115:THR:HG22	3:F:61:PHE:HB2	2.00	0.43
3:F:127:ARG:O	3:F:128:ASP:C	2.61	0.43
3:C:407:ASN:OD1	3:F:407:ASN:O	2.36	0.43
3:F:247:LEU:O	3:F:248:ALA:C	2.61	0.43
3:F:359:LEU:HD13	3:F:408:TYR:CB	2.49	0.43
3:F:327:LEU:HD13	3:F:331:TYR:CE1	2.53	0.43
3:C:48:LEU:HG	3:C:52:LEU:HD21	2.01	0.42
3:C:213:PHE:HE1	3:C:250:ILE:HD11	1.83	0.42
3:C:230:PRO:O	3:C:231:GLU:HB3	2.19	0.42
1:D:22:ASP:N	1:D:23:PRO:CD	2.82	0.42
3:F:247:LEU:HG	3:F:248:ALA:N	2.33	0.42
2:B:94:GLN:HA	2:B:109:ALA:HA	1.99	0.42
3:C:149:ASN:O	3:C:150:ILE:C	2.61	0.42
3:C:251:ASN:C	3:C:251:ASN:ND2	2.76	0.42
3:C:404:TYR:HA	3:F:410:VAL:HA	2.01	0.42
3:F:385:GLY:O	3:F:387:TYR:N	2.46	0.42
2:B:25:GLN:HA	2:B:25:GLN:OE1	2.20	0.42
2:B:117:ARG:O	2:B:119:LEU:O	2.37	0.42
3:C:94:PHE:CD1	3:C:95:TRP:N	2.87	0.42
3:C:239:ILE:O	3:C:243:ASP:N	2.43	0.42
3:F:44:PHE:O	3:F:45:GLN:C	2.61	0.42
3:F:118:ASN:O	3:F:120:LYS:N	2.51	0.42
3:C:75:LEU:HD13	3:C:80:TRP:CZ2	2.55	0.42
3:C:275:ARG:HD3	3:C:275:ARG:HA	1.81	0.42
1:D:8:VAL:HG21	2:E:46:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:ASP:O	3:F:259:ILE:HB	2.19	0.42
3:C:48:LEU:HD21	3:C:282:MET:HG2	2.01	0.42
3:C:136:LYS:HE2	3:C:317:CYS:CA	2.49	0.42
2:E:117:ARG:O	2:E:119:LEU:O	2.37	0.42
2:E:122:LEU:O	2:E:123:PRO:C	2.62	0.42
3:F:313:PHE:CD1	3:F:313:PHE:C	2.96	0.42
2:B:21:ASN:ND2	2:B:111:SER:O	2.53	0.42
3:C:411:ARG:NH1	3:F:396:GLU:OE1	2.53	0.42
1:D:24:LEU:HD13	1:D:24:LEU:O	2.20	0.42
3:F:4:ALA:O	3:F:8:LYS:HG3	2.20	0.42
3:F:264:PHE:O	3:F:265:VAL:C	2.61	0.42
1:A:10:VAL:CG1	2:B:51:TYR:CD2	3.03	0.42
3:F:20:ALA:HA	3:F:23:ILE:CG2	2.50	0.42
3:F:37:ARG:NH1	3:F:272:LEU:HB3	2.35	0.42
3:F:119:SER:CB	3:F:123:ASP:HB2	2.49	0.42
1:A:5:ASN:O	2:B:68:ILE:O	2.37	0.42
2:B:93:LYS:HZ3	3:C:46:SER:HB3	1.85	0.42
2:E:20:ARG:O	2:E:21:ASN:C	2.61	0.42
2:E:85:VAL:HG22	2:E:97:TYR:CD1	2.55	0.42
3:C:48:LEU:O	3:C:49:HIS:C	2.61	0.42
3:C:140:ILE:N	3:C:141:PRO:HD2	2.34	0.42
3:F:141:PRO:O	3:F:142:THR:C	2.62	0.42
3:F:344:GLU:OE1	3:F:344:GLU:CA	2.68	0.42
1:A:18:ASN:HA	1:A:20:PHE:CE1	2.55	0.42
3:F:31:LEU:HD23	3:F:31:LEU:HA	1.82	0.42
3:F:35:LYS:O	3:F:38:ILE:HG12	2.19	0.42
3:F:148:GLU:HA	3:F:151:THR:HG22	2.01	0.42
3:F:169:ARG:C	3:F:173:LEU:HD22	2.45	0.42
3:F:334:PHE:HD1	3:F:334:PHE:O	2.02	0.42
2:B:20:ARG:O	2:B:21:ASN:C	2.62	0.41
2:B:133:LEU:O	2:B:137:GLN:HG3	2.20	0.41
1:D:22:ASP:N	1:D:23:PRO:HD3	2.35	0.41
3:C:48:LEU:HD12	3:C:48:LEU:HA	1.92	0.41
3:C:194:GLU:CD	3:C:194:GLU:H	2.26	0.41
3:C:250:ILE:C	3:C:250:ILE:HD12	2.44	0.41
3:C:269:ASN:O	3:C:273:ASP:CG	2.64	0.41
1:D:59:UNK:O	1:D:60:UNK:CB	2.68	0.41
2:E:133:LEU:O	2:E:137:GLN:HG3	2.21	0.41
2:E:141:LEU:HD23	2:E:141:LEU:HA	1.94	0.41
3:F:48:LEU:HD21	3:F:282:MET:HG2	2.02	0.41
3:F:232:ASP:O	3:F:236:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:286:LEU:O	3:F:289:LEU:N	2.53	0.41
3:F:359:LEU:HD13	3:F:408:TYR:HB2	2.02	0.41
3:C:28:ASN:O	3:C:29:ASP:C	2.62	0.41
3:C:348:ARG:NH2	3:F:377:ARG:HG2	2.35	0.41
3:C:398:GLY:O	3:C:400:LEU:HB2	2.20	0.41
3:F:77:GLU:O	3:F:81:SER:HB3	2.20	0.41
3:F:231:GLU:O	3:F:231:GLU:HG2	2.20	0.41
1:A:22:ASP:N	1:A:23:PRO:CD	2.83	0.41
2:B:128:VAL:HG23	3:C:300:ILE:HG21	2.03	0.41
3:C:113:ILE:C	3:C:114:ASP:OD1	2.63	0.41
3:C:136:LYS:HE2	3:C:317:CYS:HA	2.01	0.41
3:C:385:GLY:C	3:C:387:TYR:N	2.78	0.41
3:F:47:LYS:O	3:F:51:VAL:HG23	2.20	0.41
3:F:137:LEU:O	3:F:140:ILE:HG22	2.19	0.41
1:D:2:ASN:ND2	1:D:4:GLU:O	2.54	0.41
3:F:251:ASN:ND2	3:F:251:ASN:C	2.78	0.41
2:E:51:TYR:HB3	2:E:53:PHE:HE1	1.86	0.41
3:C:136:LYS:CD	3:C:317:CYS:SG	3.08	0.41
2:E:139:HIS:C	2:E:139:HIS:ND1	2.79	0.41
3:F:82:GLN:CG	3:F:83:THR:N	2.84	0.41
3:F:136:LYS:HE2	3:F:317:CYS:CA	2.50	0.41
3:F:163:SER:OG	3:F:164:GLN:N	2.54	0.41
3:F:250:ILE:HD12	3:F:250:ILE:C	2.46	0.41
1:A:22:ASP:N	1:A:23:PRO:HD3	2.36	0.41
1:D:4:GLU:HB2	1:D:26:PHE:CE1	2.56	0.41
2:E:21:ASN:ND2	2:E:23:LYS:HD2	2.36	0.41
2:E:128:VAL:HG23	3:F:300:ILE:CG2	2.50	0.41
3:F:44:PHE:C	3:F:44:PHE:CD1	2.97	0.41
3:F:89:VAL:CG2	3:F:140:ILE:CD1	2.98	0.41
3:F:96:GLN:OE1	3:F:131:HIS:HD2	2.04	0.41
1:A:8:VAL:CG2	2:B:46:ALA:HB1	2.50	0.41
3:C:136:LYS:NZ	3:C:316:SER:OG	2.40	0.41
3:C:247:LEU:HG	3:C:248:ALA:N	2.36	0.41
3:C:289:LEU:O	3:C:290:LEU:C	2.64	0.41
3:F:393:TRP:O	3:F:395:ASP:N	2.54	0.41
3:C:251:ASN:C	3:C:251:ASN:HD22	2.28	0.40
1:D:18:ASN:HA	1:D:20:PHE:CE1	2.56	0.40
2:E:138:LEU:HD23	2:E:138:LEU:HA	1.98	0.40
3:F:403:LEU:N	3:F:403:LEU:CD2	2.84	0.40
2:B:20:ARG:HD3	2:B:20:ARG:HA	1.74	0.40
3:C:89:VAL:CG2	3:C:140:ILE:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:MET:HE3	3:C:136:LYS:HB2	2.03	0.40
3:C:123:ASP:HB3	3:C:124:PHE:CD1	2.56	0.40
3:C:250:ILE:HA	3:C:253:LEU:HD23	2.03	0.40
2:B:124:LEU:CD2	3:C:304:GLU:CG	2.99	0.40
3:C:136:LYS:CE	3:C:317:CYS:SG	3.05	0.40
2:E:93:LYS:NZ	3:F:46:SER:HB3	2.36	0.40
3:F:128:ASP:OD1	3:F:128:ASP:N	2.54	0.40
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.22	0.40
3:F:201:GLN:O	3:F:204:GLN:HB3	2.21	0.40
3:F:250:ILE:HA	3:F:253:LEU:HD23	2.03	0.40
3:F:251:ASN:C	3:F:251:ASN:HD22	2.29	0.40
3:C:4:ALA:O	3:C:8:LYS:HG3	2.21	0.40
3:C:143:ILE:O	3:C:147:VAL:HG23	2.21	0.40
3:C:359:LEU:HD13	3:C:408:TYR:HB2	2.03	0.40
3:C:393:TRP:CZ2	3:F:345:VAL:CG2	2.93	0.40
3:F:29:ASP:O	3:F:30:HIS:C	2.63	0.40
3:F:294:ARG:HD2	3:F:294:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	38/69 (55%)	31 (82%)	6 (16%)	1 (3%)	4	17
1	D	38/69 (55%)	30 (79%)	7 (18%)	1 (3%)	4	17
2	B	109/159 (69%)	94 (86%)	10 (9%)	5 (5%)	2	9
2	E	109/159 (69%)	94 (86%)	9 (8%)	6 (6%)	1	7
3	C	392/413 (95%)	339 (86%)	49 (12%)	4 (1%)	12	37
3	F	392/413 (95%)	340 (87%)	50 (13%)	2 (0%)	24	52
All	All	1078/1282 (84%)	928 (86%)	131 (12%)	19 (2%)	6	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	111	ASN
3	F	111	ASN
2	B	77	ASP
2	B	113	PHE
3	C	113	ILE
2	E	77	ASP
2	E	113	PHE
3	F	113	ILE
2	B	54	GLU
2	B	66	PRO
1	D	3	SER
2	E	54	GLU
2	E	66	PRO
1	A	3	SER
2	E	97	TYR
3	C	119	SER
3	C	112	GLU
2	B	82	VAL
2	E	82	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	23/36 (64%)	17 (74%)	6 (26%)	0	1
1	D	23/36 (64%)	17 (74%)	6 (26%)	0	1
2	B	107/145 (74%)	86 (80%)	21 (20%)	1	5
2	E	107/145 (74%)	84 (78%)	23 (22%)	1	4
3	C	367/383 (96%)	266 (72%)	101 (28%)	0	1
3	F	367/383 (96%)	262 (71%)	105 (29%)	0	1
All	All	994/1128 (88%)	732 (74%)	262 (26%)	0	1

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	SER
1	A	5	ASN
1	A	6	THR
1	A	11	ARG
1	A	12	VAL
2	B	11	GLU
2	B	14	THR
2	B	16	THR
2	B	22	VAL
2	B	24	HIS
2	B	25	GLN
2	B	50	LYS
2	B	55	ASP
2	B	68	ILE
2	B	75	GLU
2	B	79	SER
2	B	80	LEU
2	B	86	GLU
2	B	94	GLN
2	B	106	CYS
2	B	108	ASP
2	B	118	GLN
2	B	119	LEU
2	B	122	LEU
2	B	128	VAL
2	B	129	GLN
3	C	6	ILE
3	C	13	SER
3	C	18	THR
3	C	22	LEU
3	C	23	ILE
3	C	25	GLN
3	C	28	ASN
3	C	36	LEU
3	C	37	ARG
3	C	46	SER
3	C	52	LEU
3	C	56	GLN
3	C	59	THR
3	C	60	LYS
3	C	61	PHE
3	C	71	ILE

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Mol	Chain	Res	Type
3	C	76	ILE
3	C	78	GLU
3	C	79	GLU
3	C	86	VAL
3	C	88	LEU
3	C	92	MET
3	C	94	PHE
3	C	103	MET
3	C	105	LYS
3	C	113	ILE
3	C	115	GLN
3	C	116	GLN
3	C	118	ASN
3	C	119	SER
3	C	121	LEU
3	C	124	PHE
3	C	126	SER
3	C	127	ARG
3	C	129	SER
3	C	132	ILE
3	C	140	ILE
3	C	142	THR
3	C	151	THR
3	C	153	GLN
3	C	157	MET
3	C	158	LEU
3	C	169	ARG
3	C	173	LEU
3	C	193	GLU
3	C	194	GLU
3	C	195	PHE
3	C	214	THR
3	C	219	LYS
3	C	221	SER
3	C	226	ARG
3	C	229	SER
3	C	235	ASN
3	C	236	LEU
3	C	239	ILE
3	C	247	LEU
3	C	250	ILE
3	C	251	ASN

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Mol	Chain	Res	Type
3	C	253	LEU
3	C	254	LEU
3	C	255	GLN
3	C	264	PHE
3	C	267	LYS
3	C	272	LEU
3	C	275	ARG
3	C	279	LYS
3	C	290	LEU
3	C	292	GLU
3	C	294	ARG
3	C	304	GLU
3	C	306	ILE
3	C	307	SER
3	C	309	LEU
3	C	312	LYS
3	C	316	SER
3	C	321	ILE
3	C	323	GLN
3	C	324	THR
3	C	327	LEU
3	C	334	PHE
3	C	336	ARG
3	C	337	SER
3	C	341	LEU
3	C	344	GLU
3	C	348	ARG
3	C	351	THR
3	C	360	LYS
3	C	363	GLU
3	C	364	THR
3	C	365	GLN
3	C	367	GLU
3	C	368	GLN
3	C	377	ARG
3	C	382	LEU
3	C	393	TRP
3	C	395	ASP
3	C	397	ILE
3	C	400	LEU
3	C	401	SER
3	C	403	LEU

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Mol	Chain	Res	Type
3	C	407	ASN
1	D	1	MET
1	D	3	SER
1	D	5	ASN
1	D	6	THR
1	D	11	ARG
1	D	12	VAL
2	E	11	GLU
2	E	14	THR
2	E	16	THR
2	E	22	VAL
2	E	24	HIS
2	E	25	GLN
2	E	49	VAL
2	E	50	LYS
2	E	55	ASP
2	E	68	ILE
2	E	75	GLU
2	E	79	SER
2	E	80	LEU
2	E	86	GLU
2	E	94	GLN
2	E	106	CYS
2	E	108	ASP
2	E	118	GLN
2	E	119	LEU
2	E	122	LEU
2	E	128	VAL
2	E	129	GLN
2	E	144	THR
3	F	6	ILE
3	F	13	SER
3	F	17	LEU
3	F	18	THR
3	F	22	LEU
3	F	23	ILE
3	F	25	GLN
3	F	28	ASN
3	F	37	ARG
3	F	46	SER
3	F	52	LEU
3	F	56	GLN

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Mol	Chain	Res	Type
3	F	59	THR
3	F	60	LYS
3	F	61	PHE
3	F	71	ILE
3	F	76	ILE
3	F	78	GLU
3	F	79	GLU
3	F	86	VAL
3	F	88	LEU
3	F	92	MET
3	F	94	PHE
3	F	103	MET
3	F	105	LYS
3	F	113	ILE
3	F	114	ASP
3	F	115	GLN
3	F	116	GLN
3	F	118	ASN
3	F	119	SER
3	F	121	LEU
3	F	124	PHE
3	F	126	SER
3	F	127	ARG
3	F	129	SER
3	F	132	ILE
3	F	140	ILE
3	F	142	THR
3	F	151	THR
3	F	153	GLN
3	F	157	MET
3	F	158	LEU
3	F	168	SER
3	F	169	ARG
3	F	170	MET
3	F	173	LEU
3	F	193	GLU
3	F	194	GLU
3	F	195	PHE
3	F	214	THR
3	F	219	LYS
3	F	221	SER
3	F	226	ARG

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Mol	Chain	Res	Type
3	F	229	SER
3	F	235	ASN
3	F	236	LEU
3	F	239	ILE
3	F	247	LEU
3	F	250	ILE
3	F	251	ASN
3	F	253	LEU
3	F	254	LEU
3	F	255	GLN
3	F	264	PHE
3	F	267	LYS
3	F	272	LEU
3	F	275	ARG
3	F	279	LYS
3	F	287	SER
3	F	290	LEU
3	F	292	GLU
3	F	294	ARG
3	F	304	GLU
3	F	306	ILE
3	F	307	SER
3	F	309	LEU
3	F	312	LYS
3	F	321	ILE
3	F	323	GLN
3	F	324	THR
3	F	327	LEU
3	F	334	PHE
3	F	336	ARG
3	F	337	SER
3	F	341	LEU
3	F	344	GLU
3	F	348	ARG
3	F	351	THR
3	F	360	LYS
3	F	363	GLU
3	F	364	THR
3	F	365	GLN
3	F	367	GLU
3	F	368	GLN
3	F	374	LEU

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Mol	Chain	Res	Type
3	F	377	ARG
3	F	382	LEU
3	F	393	TRP
3	F	395	ASP
3	F	397	ILE
3	F	400	LEU
3	F	401	SER
3	F	403	LEU
3	F	407	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	5	ASN
1	A	18	ASN
2	B	84	GLN
2	B	91	GLN
2	B	118	GLN
3	C	25	GLN
3	C	56	GLN
3	C	74	ASN
3	C	82	GLN
3	C	96	GLN
3	C	117	HIS
3	C	131	HIS
3	C	149	ASN
3	C	162	GLN
3	C	204	GLN
3	C	216	HIS
3	C	235	ASN
3	C	251	ASN
3	C	283	GLN
3	C	311	GLN
3	C	326	ASN
3	C	333	ASN
1	D	2	ASN
1	D	5	ASN
1	D	18	ASN
2	E	24	HIS
2	E	84	GLN
2	E	91	GLN

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Mol	Chain	Res	Type
2	E	118	GLN
3	F	25	GLN
3	F	74	ASN
3	F	82	GLN
3	F	117	HIS
3	F	131	HIS
3	F	149	ASN
3	F	204	GLN
3	F	216	HIS
3	F	235	ASN
3	F	251	ASN
3	F	283	GLN
3	F	311	GLN
3	F	326	ASN
3	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	40:VAL	C	51:UNK	N	15.44
1	D	40:VAL	C	51:UNK	N	14.58

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	40/69 (57%)	1.95	15 (37%) 1 0	59, 94, 148, 158	0
1	D	40/69 (57%)	2.19	17 (42%) 0 0	53, 69, 117, 161	0
2	B	115/159 (72%)	1.24	23 (20%) 3 1	45, 78, 111, 126	0
2	E	115/159 (72%)	1.02	23 (20%) 3 1	23, 50, 94, 115	0
3	C	396/413 (95%)	1.29	86 (21%) 2 1	31, 72, 148, 189	0
3	F	396/413 (95%)	1.16	88 (22%) 2 1	22, 52, 126, 165	0
All	All	1102/1282 (85%)	1.27	252 (22%) 2 1	22, 67, 135, 189	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	233	ALA	8.9
3	F	110	THR	8.3
1	D	16	ALA	7.1
1	D	15	ARG	6.8
3	C	237	PHE	6.6
3	F	195	PHE	6.0
3	F	222	ALA	5.9
3	F	237	PHE	5.5
3	F	219	LYS	5.4
1	A	15	ARG	5.3
3	C	219	LYS	5.3
3	C	5	VAL	5.1
3	C	195	PHE	5.1
3	F	6	ILE	5.0
3	C	124	PHE	4.8
3	F	233	ALA	4.8
2	E	41	GLN	4.7
3	C	220	CYS	4.7
2	E	112	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
3	F	223	LEU	4.6
3	F	389	PRO	4.5
1	D	25	LYS	4.4
2	E	40	VAL	4.4
3	C	240	VAL	4.4
3	C	221	SER	4.4
1	D	3	SER	4.4
1	A	26	PHE	4.3
3	F	230	PRO	4.3
3	F	394	PRO	4.3
3	F	193	GLU	4.2
3	F	26	GLU	4.2
3	F	112	GLU	4.2
3	F	393	TRP	4.1
3	F	220	CYS	4.0
2	E	67	ALA	4.0
1	A	25	LYS	4.0
3	F	236	LEU	4.0
3	F	228	VAL	4.0
3	F	116	GLN	3.9
3	F	239	ILE	3.9
1	D	26	PHE	3.9
3	C	225	SER	3.9
3	C	45	GLN	3.9
1	D	23	PRO	3.8
2	B	40	VAL	3.8
3	C	177	PHE	3.7
3	C	335	GLU	3.7
3	F	215	ASP	3.7
1	A	23	PRO	3.7
3	C	200	ASP	3.7
2	B	57	GLN	3.7
3	F	216	HIS	3.7
3	C	9	LEU	3.7
3	F	5	VAL	3.6
2	B	48	ASN	3.5
3	C	178	SER	3.5
3	C	19	GLY	3.5
3	F	235	ASN	3.5
2	B	93	LYS	3.5
3	F	232	ASP	3.5
3	C	228	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	234	GLN	3.5
3	C	81	SER	3.5
3	C	266	ARG	3.5
3	F	177	PHE	3.4
1	D	5	ASN	3.4
3	F	166	VAL	3.4
1	D	28	TRP	3.4
2	E	65	ASP	3.4
3	C	139	GLU	3.4
3	F	178	SER	3.4
3	C	118	ASN	3.3
2	B	11	GLU	3.3
3	F	281	LYS	3.3
1	D	20	PHE	3.3
1	A	16	ALA	3.3
3	F	218	ASP	3.3
3	C	125	ILE	3.3
3	F	251	ASN	3.3
2	B	68	ILE	3.3
3	C	113	ILE	3.3
3	F	170	MET	3.3
3	C	248	ALA	3.2
3	C	218	ASP	3.2
1	D	24	LEU	3.2
1	A	20	PHE	3.2
1	A	1	MET	3.2
3	C	241	GLU	3.2
3	F	397	ILE	3.2
1	A	24	LEU	3.2
1	D	17	ARG	3.2
2	B	112	ARG	3.2
3	C	214	THR	3.2
3	F	4	ALA	3.2
3	F	120	LYS	3.1
2	E	117	ARG	3.1
3	C	109	ILE	3.1
2	B	19	ASP	3.1
3	C	26	GLU	3.1
2	E	118	GLN	3.1
3	F	234	GLN	3.1
3	C	236	LEU	3.1
3	F	391	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	266	ARG	3.1
3	C	15	LYS	3.1
3	C	239	ILE	3.1
2	B	91	GLN	3.1
2	E	48	ASN	3.0
2	E	66	PRO	3.0
1	D	22	ASP	3.0
2	B	41	GLN	3.0
3	C	112	GLU	3.0
3	C	274	GLU	3.0
3	F	231	GLU	3.0
3	F	227	SER	3.0
3	C	4	ALA	3.0
1	A	21	VAL	3.0
1	A	5	ASN	3.0
1	A	3	SER	3.0
3	C	166	VAL	3.0
3	C	216	HIS	3.0
1	D	31	GLU	2.9
3	C	193	GLU	2.9
3	F	229	SER	2.9
3	C	6	ILE	2.9
3	C	247	LEU	2.9
3	F	405	THR	2.9
2	B	114	GLU	2.9
1	D	21	VAL	2.9
1	D	13	ALA	2.9
3	F	396	GLU	2.9
2	E	97	TYR	2.9
3	C	207	ALA	2.9
2	B	103	ASN	2.9
2	E	11	GLU	2.9
2	E	78	GLU	2.9
3	F	117	HIS	2.8
2	B	81	ARG	2.8
3	C	162	GLN	2.8
3	C	132	ILE	2.8
3	C	223	LEU	2.8
3	F	137	LEU	2.8
1	A	17	ARG	2.8
3	F	81	SER	2.8
2	B	104	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	245	LYS	2.8
3	C	137	LEU	2.8
3	F	388	LEU	2.8
3	F	226	ARG	2.7
3	C	279	LYS	2.7
1	D	39	SER	2.7
3	F	167	GLU	2.7
3	C	209	PHE	2.7
3	C	135	SER	2.7
3	F	169	ARG	2.7
2	B	66	PRO	2.6
3	C	153	GLN	2.6
3	F	194	GLU	2.6
3	F	274	GLU	2.6
2	E	56	ASP	2.6
3	C	396	GLU	2.6
3	C	249	ALA	2.6
3	F	225	SER	2.6
3	F	175	ASP	2.6
3	F	392	ILE	2.6
3	F	115	GLN	2.6
3	F	165	LEU	2.6
3	F	119	SER	2.6
3	C	217	PHE	2.5
2	B	54	GLU	2.5
3	F	108	ASN	2.5
3	C	196	THR	2.5
3	F	410	VAL	2.5
1	D	18	ASN	2.5
3	F	248	ALA	2.5
2	E	98	GLU	2.5
1	A	22	ASP	2.5
3	C	18	THR	2.4
3	C	110	THR	2.4
3	F	276	ASP	2.4
3	C	165	LEU	2.4
3	F	109	ILE	2.4
3	F	259	ILE	2.4
3	C	170	MET	2.4
3	F	250	ILE	2.4
2	E	53	PHE	2.4
2	E	79	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	119	SER	2.4
3	C	123	ASP	2.4
3	C	117	HIS	2.4
3	F	171	LYS	2.4
2	E	12	PRO	2.4
3	C	235	ASN	2.3
2	B	53	PHE	2.3
3	F	124	PHE	2.3
3	F	253	LEU	2.3
3	F	214	THR	2.3
2	E	101	ASP	2.3
3	C	208	ASP	2.3
2	B	78	GLU	2.3
3	C	281	LYS	2.3
3	C	229	SER	2.3
3	C	338	TYR	2.3
3	C	121	LEU	2.3
3	F	7	GLU	2.3
3	F	240	VAL	2.3
3	F	354	LYS	2.3
3	F	196	THR	2.3
3	F	400	LEU	2.3
3	F	403	LEU	2.3
3	F	387	TYR	2.3
3	C	197	ASN	2.3
2	B	142	PHE	2.3
3	F	2	ASN	2.3
3	F	111	ASN	2.3
3	F	39	ARG	2.3
2	E	81	ARG	2.2
2	E	91	GLN	2.2
3	F	395	ASP	2.2
3	C	120	LYS	2.2
3	F	213	PHE	2.2
1	A	40	VAL	2.2
2	E	103	ASN	2.2
2	B	12	PRO	2.2
3	F	271	LEU	2.2
3	F	176	GLU	2.2
1	A	28	TRP	2.2
3	C	115	GLN	2.1
3	C	173	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	39	ARG	2.1
3	F	172	GLY	2.1
3	C	264	PHE	2.1
2	B	65	ASP	2.1
3	C	393	TRP	2.1
3	C	405	THR	2.1
2	E	57	GLN	2.1
3	F	212	SER	2.1
3	C	243	ASP	2.1
2	E	69	GLU	2.1
3	C	250	ILE	2.1
3	F	206	LEU	2.1
2	B	67	ALA	2.1
3	C	122	GLY	2.1
3	C	44	PHE	2.1
2	B	97	TYR	2.1
3	C	368	GLN	2.1
3	F	153	GLN	2.1
3	C	410	VAL	2.0
3	F	386	ASN	2.0
3	C	389	PRO	2.0
3	C	242	ARG	2.0
3	C	400	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.