



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:15 PM UTC

PDB ID : 8EE8 / pdb_00008ee8
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ100-C in complex with ZIKV E glycoprotein
Authors : Sankhala, R.S.; Joyce, M.G.
Deposited on : 2022-09-06
Resolution : 2.80 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

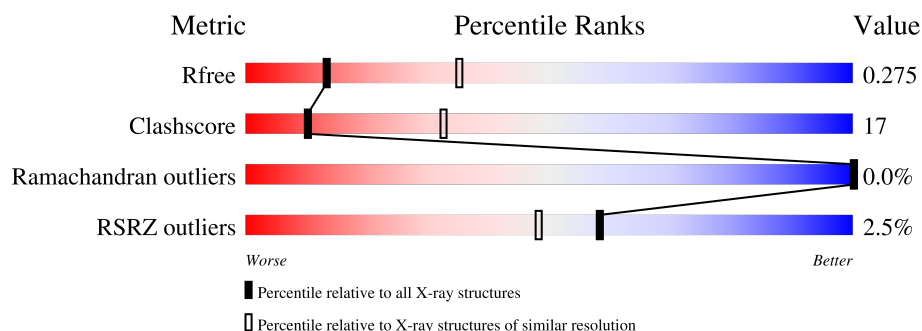
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	405	9% 70% 29% .
1	B	405	% 75% 25% .
1	E	405	2% 68% 30% .
1	Z	405	% 67% 33% .
2	D	222	5% 76% 21% ..
2	H	222	73% 26% .

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Mol	Chain	Length	Quality of chain
3	C	219	 79%20%.
3	L	219	 76%22%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18906 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Z	402	Total	C	N	O	S	0	0	0
			3068	1913	537	593	25			
1	E	403	Total	C	N	O	S	0	0	0
			3079	1921	538	594	26			
1	B	402	Total	C	N	O	S	0	0	0
			3071	1915	537	593	26			
1	A	403	Total	C	N	O	S	0	0	0
			3079	1921	538	594	26			

- Molecule 2 is a protein called rhMZ100-C antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1599	996	274	323	6			
2	D	217	Total	C	N	O	S	0	0	0
			1592	991	273	322	6			

- Molecule 3 is a protein called rhMZ100-C antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1632	1024	272	331	5			
3	C	217	Total	C	N	O	S	0	0	0
			1632	1024	272	331	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	13	Total	O	0	0
			13	13		
4	H	23	Total	O	0	0
			23	23		

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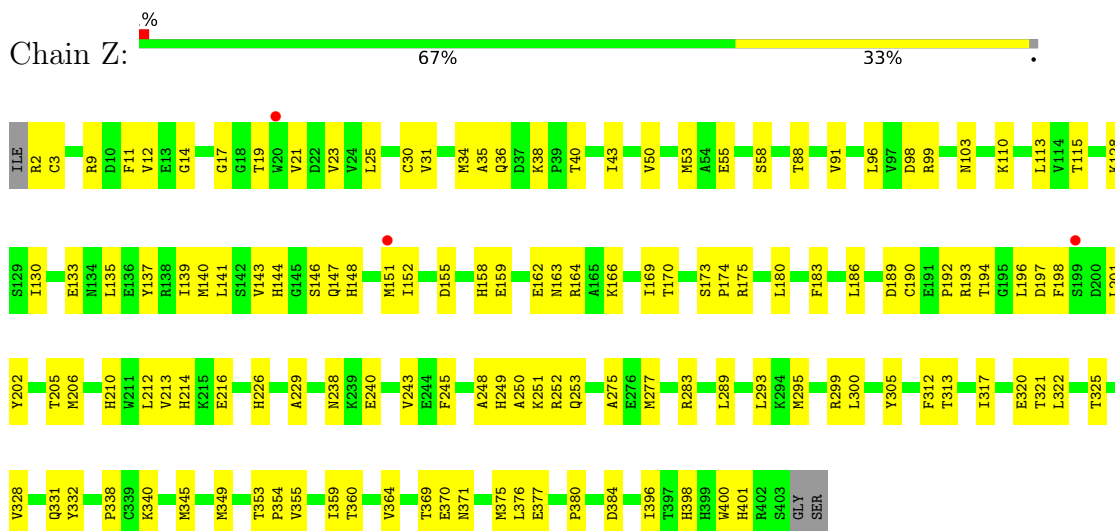
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	20	Total 20	O 20	0	0
4	E	18	Total 18	O 18	0	0
4	B	19	Total 19	O 19	0	0
4	C	27	Total 27	O 27	0	0
4	A	13	Total 13	O 13	0	0
4	D	21	Total 21	O 21	0	0

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.

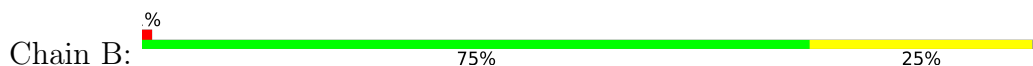
- Molecule 1: Envelope protein E

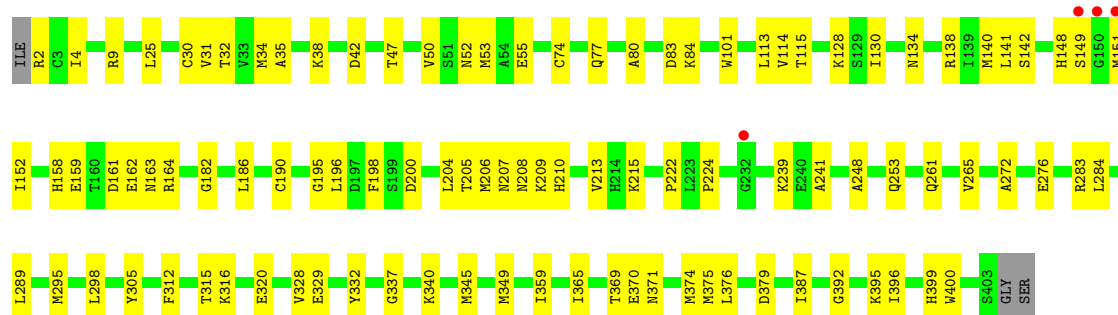


- Molecule 1: Envelope protein E

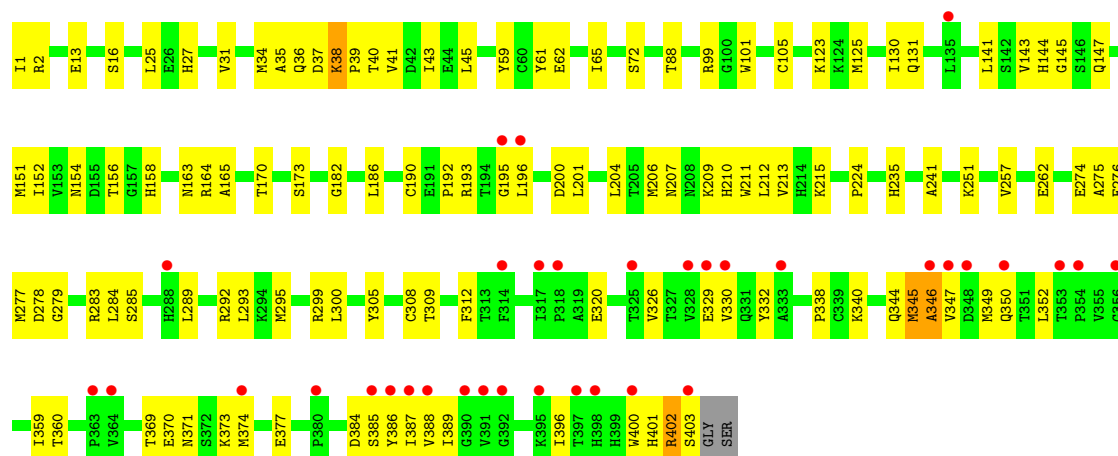


- Molecule 1: Envelope protein E

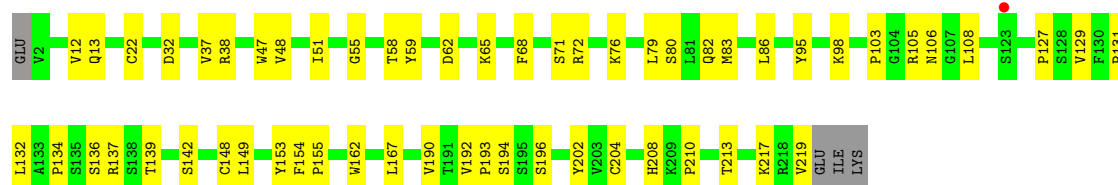




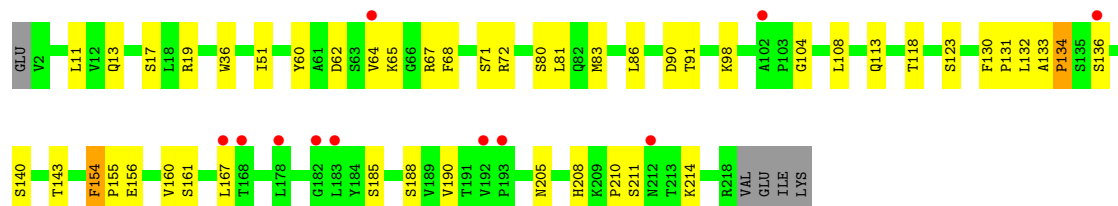
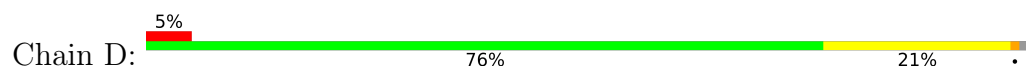
• Molecule 1: Envelope protein E



• Molecule 2: rhMZ100-C antibody heavy chain



• Molecule 2: rhMZ100-C antibody heavy chain



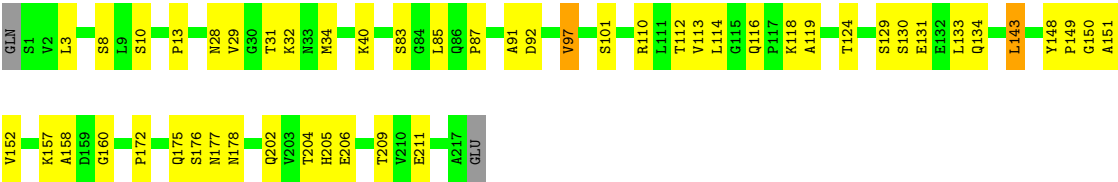
• Molecule 3: rhMZ100-C antibody light chain

Chain L:

76%

22%

..



● Molecule 3: rhMZ100-C antibody light chain

Chain C:

79%

20%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.84Å 126.68Å 140.48Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	14.98 – 2.80 14.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	61.2 (14.98-2.80) 61.2 (14.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.241 , 0.295 (Not available) , 0.275	Depositor DCC
R_{free} test set	2026 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 53569 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18906	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.22	0/3143	0.56	3/4257 (0.1%)
1	B	0.17	0/3136	0.45	0/4249
1	E	0.42	2/3144 (0.1%)	0.65	4/4260 (0.1%)
1	Z	0.23	1/3133 (0.0%)	0.49	1/4246 (0.0%)
2	D	0.26	1/1626 (0.1%)	0.56	2/2214 (0.1%)
2	H	0.22	0/1633	0.47	0/2224
3	C	0.18	0/1672	0.44	2/2281 (0.1%)
3	L	0.30	1/1672 (0.1%)	0.42	1/2281 (0.0%)
All	All	0.27	5/19159 (0.0%)	0.52	13/26012 (0.0%)

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	1
1	E	0	1
3	C	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	375	MET	C-O	-7.38	1.14	1.23
3	L	97	VAL	C-O	-7.23	1.16	1.23
1	Z	398	HIS	C-O	-6.06	1.17	1.23
2	D	154	PHE	N-CA	5.54	1.51	1.46
1	E	61	TYR	C-O	-5.08	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	346	ALA	N-CA-C	15.41	128.08	111.28
1	A	38	LYS	CA-C-N	13.56	133.97	119.87
1	A	38	LYS	C-N-CA	13.56	133.97	119.87
2	D	154	PHE	N-CA-C	11.89	128.28	112.35
1	A	38	LYS	N-CA-C	6.74	119.72	109.41
1	E	351	THR	CA-C-N	6.46	133.88	121.54
1	E	351	THR	C-N-CA	6.46	133.88	121.54
1	Z	193	ARG	N-CA-C	-5.72	98.61	110.80
3	L	143	LEU	N-CA-C	5.33	117.66	109.07
3	C	178	ASN	CB-CA-C	5.29	119.52	111.80
3	C	178	ASN	N-CA-CB	5.18	119.56	111.84
1	E	349	MET	N-CA-CB	-5.08	108.38	114.17
2	D	154	PHE	CB-CA-C	-5.05	104.80	113.04

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	GLY	Peptide
1	A	345	MET	Peptide
1	A	346	ALA	Peptide
1	A	402	ARG	Peptide
1	B	190	CYS	Peptide
3	C	148	TYR	Peptide
1	E	351	THR	Mainchain

5.2 Too-close contacts [i](#)

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	3079	0	3009	103	0
1	B	3071	0	2994	79	0
1	E	3079	0	3007	126	0
1	Z	3068	0	2987	122	4
2	D	1592	0	1558	49	3
2	H	1599	0	1565	58	0
3	C	1632	0	1582	35	0
3	L	1632	0	1581	81	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	0	0	0
4	B	19	0	0	6	0
4	C	27	0	0	4	0
4	D	21	0	0	1	0
4	E	18	0	0	3	0
4	H	23	0	0	0	0
4	L	20	0	0	3	0
4	Z	13	0	0	2	0
All	All	18906	0	18283	633	4

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 17.

All (633) 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:E:149:SER:HB3	1:E:375:MET:SD	1.42	1.57
1:E:149:SER:CB	1:E:375:MET:SD	2.21	1.28
3:L:124:THR:OG1	3:L:143:LEU:HD11	1.33	1.23
2:H:192:VAL:HG11	2:H:202:TYR:OH	1.42	1.17
1:Z:17:GLY:HA2	1:Z:36:GLN:OE1	1.49	1.12
1:E:357:ARG:O	1:E:378:LEU:HD12	1.48	1.12
1:E:25:LEU:HD21	1:E:45:LEU:HB2	1.17	1.11
3:L:119:ALA:O	3:L:148:TYR:HD2	1.31	1.11
3:L:157:LYS:CE	3:L:160:GLY:HA2	1.82	1.10
3:L:124:THR:O	3:L:143:LEU:CD1	2.00	1.10
2:D:154:PHE:CD2	2:D:155:PRO:HD3	1.88	1.09
2:H:12:VAL:HG11	2:H:86:LEU:CD1	1.82	1.07
1:Z:130:ILE:HG22	1:Z:198:PHE:HB3	1.27	1.07
2:D:123:SER:O	2:D:154:PHE:CE2	2.13	1.02
3:L:175:GLN:HG2	3:L:176:SER:H	1.23	1.02
1:E:62:GLU:OE1	1:E:122:SER:HB2	1.60	1.02
1:Z:205:THR:HG22	1:Z:210:HIS:ND1	1.75	1.02
3:L:148:TYR:CE1	3:L:205:HIS:CE1	2.47	1.02
2:D:154:PHE:CB	2:D:155:PRO:HD3	1.88	1.01
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.38	1.01
1:E:346:ALA:HB2	1:E:386:TYR:N	1.76	1.01
3:L:116:GLN:NE2	3:L:148:TYR:HA	1.76	1.00
1:E:341:VAL:HG21	1:E:374:MET:HE2	1.44	1.00
3:L:202:GLN:HG2	3:L:211:GLU:CD	1.83	0.99
1:Z:130:ILE:HG21	1:Z:198:PHE:HD1	1.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ALA:HB2	1:E:386:TYR:H	1.26	0.98
2:D:154:PHE:HB3	2:D:155:PRO:HD3	1.46	0.98
2:H:192:VAL:CG1	2:H:202:TYR:OH	2.12	0.97
1:E:3:CYS:SG	1:E:9:ARG:NH1	2.38	0.97
3:L:204:THR:HG22	3:L:209:THR:OG1	1.65	0.96
3:L:119:ALA:O	3:L:148:TYR:CD2	2.17	0.96
3:L:116:GLN:HE22	3:L:148:TYR:HA	1.26	0.96
1:E:25:LEU:CD2	1:E:45:LEU:HB2	1.95	0.96
1:A:13:GLU:OE1	1:A:34:MET:HE3	1.65	0.95
3:L:124:THR:OG1	3:L:143:LEU:CD1	2.15	0.95
1:B:148:HIS:HB2	1:B:375:MET:HG3	1.48	0.94
3:L:124:THR:O	3:L:143:LEU:HD13	1.65	0.93
1:A:38:LYS:HB3	1:A:39:PRO:HD2	1.51	0.92
3:C:121:PRO:HB2	3:C:144:ILE:HD11	1.51	0.92
3:L:148:TYR:HE1	3:L:206:GLU:HG3	1.32	0.92
3:L:157:LYS:HE3	3:L:160:GLY:HA2	1.49	0.91
1:B:53:MET:SD	1:B:283:ARG:NH2	2.43	0.91
1:E:149:SER:CA	1:E:375:MET:SD	2.59	0.90
2:D:123:SER:O	2:D:154:PHE:CD2	2.24	0.90
1:Z:96:LEU:HD12	1:Z:96:LEU:O	1.71	0.89
2:H:129:VAL:CG1	2:H:148:CYS:SG	2.60	0.89
1:A:38:LYS:CB	1:A:39:PRO:HD2	2.02	0.89
2:H:132:LEU:HD21	2:H:149:LEU:HD23	1.54	0.89
2:H:62:ASP:OD1	2:H:65:LYS:HE2	1.72	0.88
1:Z:130:ILE:HG21	1:Z:198:PHE:CD1	2.09	0.87
2:D:154:PHE:CG	2:D:155:PRO:HD3	2.09	0.87
1:Z:130:ILE:CG2	1:Z:198:PHE:HB3	2.03	0.87
1:E:308:CYS:SG	1:E:340:LYS:O	2.33	0.87
2:H:192:VAL:HG11	2:H:202:TYR:CZ	2.09	0.87
1:Z:170:THR:OG1	1:Z:173:SER:OG	1.91	0.87
1:E:345:MET:HG3	1:E:355:VAL:H	1.38	0.87
1:E:151:MET:O	1:E:164:ARG:NH2	2.09	0.85
3:L:148:TYR:CE1	3:L:205:HIS:ND1	2.44	0.85
1:E:357:ARG:O	1:E:378:LEU:CD1	2.23	0.85
3:L:119:ALA:H	3:L:148:TYR:HB3	1.42	0.84
1:E:346:ALA:CB	1:E:386:TYR:HB2	2.08	0.84
2:D:154:PHE:CD2	2:D:155:PRO:CD	2.61	0.83
1:Z:96:LEU:HD13	1:Z:110:LYS:HD2	1.61	0.83
1:Z:238:ASN:ND2	1:Z:240:GLU:CG	2.42	0.83
1:Z:35:ALA:HB2	1:Z:295:MET:HE2	1.61	0.82
1:Z:143:VAL:O	1:Z:147:GLN:NE2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ALA:HB2	1:E:386:TYR:HB2	1.61	0.82
2:D:154:PHE:HD2	2:D:155:PRO:HD3	1.38	0.82
1:E:25:LEU:HD21	1:E:45:LEU:CB	2.08	0.81
1:E:38:LYS:HD3	1:E:295:MET:HG3	1.61	0.81
1:Z:130:ILE:HG22	1:Z:130:ILE:O	1.80	0.81
1:Z:321:THR:HG1	1:Z:325:THR:HG1	1.27	0.81
1:B:55:GLU:HG3	1:B:128:LYS:HD3	1.63	0.81
2:H:154:PHE:HB3	2:H:155:PRO:HD3	1.63	0.81
1:Z:2:ARG:NH2	1:Z:155:ASP:OD1	2.14	0.80
2:H:208:HIS:HB3	2:H:213:THR:OG1	1.81	0.80
3:L:202:GLN:HG2	3:L:211:GLU:CG	2.10	0.80
1:E:346:ALA:CB	1:E:386:TYR:H	1.93	0.80
1:E:3:CYS:O	1:E:9:ARG:NH1	2.15	0.79
3:L:157:LYS:HE2	3:L:160:GLY:HA2	1.63	0.79
1:E:333:ALA:HA	1:E:371:ASN:OD1	1.83	0.78
1:Z:17:GLY:CA	1:Z:36:GLN:OE1	2.30	0.78
2:H:192:VAL:HG21	2:H:202:TYR:HE1	1.46	0.78
3:L:143:LEU:O	3:L:143:LEU:HD22	1.82	0.78
1:Z:96:LEU:CD1	1:Z:110:LYS:HD2	2.13	0.78
1:Z:238:ASN:ND2	1:Z:240:GLU:HG2	1.99	0.78
1:E:245:PHE:CD2	1:E:255:VAL:HG22	2.19	0.77
3:L:157:LYS:CE	3:L:160:GLY:CA	2.63	0.77
3:L:148:TYR:HD1	3:L:149:PRO:HD2	1.48	0.77
3:L:202:GLN:HG2	3:L:211:GLU:HG3	1.68	0.76
1:E:346:ALA:CB	1:E:386:TYR:N	2.48	0.76
1:E:344:GLN:HG2	1:E:345:MET:SD	2.25	0.76
2:H:129:VAL:HG12	2:H:148:CYS:SG	2.25	0.76
1:B:316:LYS:HG2	1:B:329:GLU:HB3	1.68	0.76
3:L:157:LYS:HE3	3:L:160:GLY:CA	2.16	0.75
3:C:154:VAL:HG12	3:C:203:VAL:HG12	1.69	0.75
2:D:154:PHE:HD2	2:D:155:PRO:CD	1.97	0.75
1:E:346:ALA:HB2	1:E:386:TYR:CA	2.17	0.74
3:L:175:GLN:CG	3:L:176:SER:H	2.00	0.74
3:L:92:ASP:OD1	3:L:110:ARG:HG3	1.90	0.72
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.71	0.71
1:E:345:MET:SD	1:E:354:PRO:HA	2.31	0.71
2:D:154:PHE:CB	2:D:155:PRO:CD	2.68	0.71
1:E:61:TYR:CE1	1:E:206:MET:CE	2.73	0.71
1:Z:192:PRO:CG	1:Z:194:THR:HG23	2.21	0.71
2:H:192:VAL:HG11	2:H:202:TYR:CE1	2.26	0.71
1:A:384:ASP:OD1	1:A:385:SER:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:129:SER:O	4:L:301:HOH:O	2.09	0.70
3:C:129:SER:OG	4:C:301:HOH:O	2.09	0.70
1:A:320:GLU:OE2	1:A:402:ARG:NH2	2.23	0.70
1:Z:251:LYS:NZ	4:Z:503:HOH:O	2.25	0.70
1:Z:30:CYS:SG	1:Z:31:VAL:N	2.65	0.69
3:L:143:LEU:CD1	3:L:143:LEU:H	2.05	0.69
1:A:72:SER:HB2	1:A:251:LYS:HA	1.74	0.69
2:H:13:GLN:HB3	1:B:195:GLY:HA3	1.75	0.69
1:B:208:ASN:O	4:B:501:HOH:O	2.09	0.69
1:B:30:CYS:SG	1:B:31:VAL:N	2.65	0.69
1:Z:19:THR:O	1:Z:21:VAL:HG23	1.92	0.69
3:L:148:TYR:CE1	3:L:206:GLU:HG3	2.23	0.69
3:L:3:LEU:HD21	3:L:97:VAL:HG23	1.75	0.69
1:E:61:TYR:CE1	1:E:206:MET:HE1	2.27	0.69
1:E:346:ALA:HB2	1:E:386:TYR:CB	2.22	0.68
2:D:154:PHE:CD2	2:D:155:PRO:HG3	2.28	0.68
2:H:129:VAL:HG13	2:H:148:CYS:SG	2.33	0.68
3:L:148:TYR:CD1	3:L:205:HIS:CE1	2.80	0.68
1:B:77:GLN:OE1	4:B:502:HOH:O	2.09	0.68
1:Z:192:PRO:HG2	1:Z:194:THR:HG23	1.76	0.68
2:H:192:VAL:HG21	2:H:202:TYR:CE1	2.28	0.68
1:E:245:PHE:CD2	1:E:255:VAL:CG2	2.77	0.68
3:L:175:GLN:HG2	3:L:176:SER:N	2.05	0.68
1:Z:96:LEU:HD13	1:Z:110:LYS:CD	2.24	0.68
1:B:149:SER:OG	1:B:375:MET:SD	2.47	0.68
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.75	0.67
1:E:305:TYR:HB2	1:E:340:LYS:HG3	1.75	0.67
1:B:4:ILE:O	4:B:503:HOH:O	2.11	0.67
1:E:25:LEU:HD11	1:E:45:LEU:H	1.58	0.67
1:B:161:ASP:O	4:B:504:HOH:O	2.12	0.67
1:A:2:ARG:HH21	1:A:154:ASN:N	1.92	0.67
1:Z:192:PRO:HB2	1:Z:194:THR:CG2	2.25	0.67
2:D:154:PHE:HD2	2:D:155:PRO:CG	2.08	0.66
1:Z:35:ALA:HB3	1:Z:38:LYS:HB2	1.77	0.66
2:H:137:ARG:HH11	2:H:139:THR:HG21	1.60	0.66
1:B:316:LYS:HZ2	1:A:101:TRP:CD1	2.13	0.66
1:Z:192:PRO:HB2	1:Z:194:THR:HG23	1.76	0.66
1:E:384:ASP:OD1	1:E:399:HIS:NE2	2.29	0.66
1:A:305:TYR:HB2	1:A:340:LYS:HG3	1.77	0.66
1:A:143:VAL:O	1:A:147:GLN:NE2	2.28	0.66
1:Z:384:ASP:OD1	1:Z:401:HIS:ND1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:13:PRO:HA	3:L:85:LEU:HB3	1.78	0.65
1:E:6:VAL:O	4:E:501:HOH:O	2.15	0.65
1:E:68:MET:SD	1:E:68:MET:N	2.69	0.65
1:B:9:ARG:NH1	1:B:32:THR:OG1	2.30	0.65
3:C:141:VAL:HG21	2:D:132:LEU:HD13	1.77	0.65
1:A:186:LEU:HD13	1:A:295:MET:HG3	1.79	0.65
3:L:114:LEU:HD21	3:L:118:LYS:HE3	1.77	0.65
3:L:124:THR:OG1	3:L:143:LEU:HD21	1.97	0.64
1:E:151:MET:SD	1:E:154:ASN:ND2	2.66	0.64
1:B:2:ARG:N	1:B:152:ILE:HA	2.11	0.64
1:A:400:TRP:CG	1:A:401:HIS:H	2.16	0.64
1:B:148:HIS:HE1	1:B:151:MET:HE3	1.63	0.64
2:D:154:PHE:HB3	2:D:155:PRO:CD	2.23	0.64
1:A:156:THR:O	1:A:164:ARG:NH2	2.30	0.63
1:E:200:ASP:HA	1:E:215:LYS:HE3	1.79	0.63
3:L:143:LEU:HD13	3:L:143:LEU:H	1.63	0.63
2:H:131:PRO:HB3	2:H:219:VAL:HA	1.80	0.63
1:Z:3:CYS:O	1:Z:9:ARG:NH1	2.32	0.63
1:A:170:THR:HG1	1:A:173:SER:HG	1.44	0.62
2:D:154:PHE:CD2	2:D:155:PRO:CG	2.82	0.62
2:H:155:PRO:HD2	2:H:208:HIS:HE2	1.63	0.62
3:L:124:THR:HG1	3:L:143:LEU:HD11	1.55	0.62
3:L:148:TYR:HE1	3:L:206:GLU:CG	2.07	0.62
1:B:130:ILE:HG21	1:B:198:PHE:CD1	2.35	0.62
1:A:182:GLY:O	1:A:299:ARG:NH1	2.32	0.62
1:A:204:LEU:HD21	1:A:206:MET:HE3	1.81	0.62
1:Z:189:ASP:OD1	1:Z:189:ASP:O	2.18	0.62
1:Z:144:HIS:CG	1:Z:360:THR:HG22	2.34	0.62
2:H:142:SER:HB2	2:H:194:SER:HB2	1.82	0.62
1:E:389:ILE:HG13	1:E:396:ILE:HB	1.81	0.62
1:E:99:ARG:O	1:E:108:PHE:HD1	1.83	0.62
1:Z:139:ILE:HD11	1:Z:169:ILE:HD12	1.81	0.61
3:L:119:ALA:N	3:L:148:TYR:HB3	2.14	0.61
1:E:61:TYR:CE1	1:E:206:MET:HE3	2.35	0.61
1:E:149:SER:HA	1:E:375:MET:SD	2.40	0.61
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.33	0.61
1:Z:238:ASN:HD22	1:Z:240:GLU:HG2	1.65	0.61
1:E:1:ILE:O	1:E:152:ILE:HA	2.01	0.61
1:E:170:THR:HG22	1:E:172:ASN:H	1.65	0.61
1:Z:345:MET:HB2	1:Z:355:VAL:O	2.00	0.61
1:A:344:GLN:HG2	1:A:345:MET:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ILE:HG22	1:E:141:LEU:HD22	1.83	0.61
1:A:38:LYS:HB3	1:A:39:PRO:CD	2.27	0.61
1:Z:140:MET:HE1	1:Z:166:LYS:HB3	1.83	0.61
1:A:312:PHE:HB3	1:A:330:VAL:HG11	1.82	0.61
1:Z:147:GLN:HB3	1:Z:151:MET:HG3	1.82	0.60
1:Z:192:PRO:CB	1:Z:194:THR:HG23	2.31	0.60
1:Z:370:GLU:N	1:Z:370:GLU:OE1	2.34	0.60
1:B:25:LEU:HB2	1:B:289:LEU:HB3	1.83	0.60
1:A:158:HIS:HB3	1:A:164:ARG:HG2	1.84	0.60
1:Z:17:GLY:H	1:Z:36:GLN:HB2	1.66	0.60
1:E:141:LEU:O	1:E:164:ARG:HA	2.01	0.60
3:L:124:THR:O	3:L:143:LEU:HD12	1.99	0.60
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.83	0.59
1:A:295:MET:N	1:A:295:MET:SD	2.75	0.59
3:L:157:LYS:HE2	3:L:160:GLY:CA	2.28	0.59
1:B:329:GLU:HG3	1:B:375:MET:HG2	1.84	0.59
1:E:345:MET:SD	1:E:354:PRO:HB3	2.42	0.59
1:B:345:MET:HG2	1:B:387:ILE:HD13	1.84	0.59
1:E:158:HIS:HB2	1:E:164:ARG:O	2.03	0.59
1:B:80:ALA:HB3	1:B:114:VAL:HG23	1.84	0.59
1:E:349:MET:HG3	1:B:399:HIS:CG	2.38	0.59
3:C:126:PHE:HB2	3:C:141:VAL:HG22	1.83	0.59
1:A:211:TRP:HB3	1:A:274:GLU:HG2	1.85	0.59
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.84	0.58
2:D:64:VAL:HG13	2:D:68:PHE:HB2	1.85	0.58
1:A:402:ARG:HE	1:A:402:ARG:HA	1.68	0.58
1:Z:88:THR:HG23	2:H:103:PRO:HB3	1.84	0.58
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.84	0.58
1:Z:202:TYR:N	1:Z:213:VAL:O	2.18	0.58
2:H:32:ASP:O	2:H:72:ARG:NH2	2.35	0.58
2:H:208:HIS:HB3	2:H:213:THR:HG1	1.69	0.58
1:E:212:LEU:HD11	1:E:284:LEU:HD22	1.84	0.58
3:L:148:TYR:HB2	3:L:149:PRO:HD3	1.86	0.58
1:Z:130:ILE:CG2	1:Z:198:PHE:HD1	2.06	0.58
1:A:37:ASP:O	1:A:300:LEU:HD21	2.04	0.58
2:H:37:VAL:HG23	2:H:95:TYR:HB2	1.86	0.57
2:H:59:TYR:CG	3:L:101:SER:HB2	2.38	0.57
1:Z:201:LEU:HD23	1:Z:212:LEU:HG	1.85	0.57
1:E:207:ASN:OD1	1:E:208:ASN:N	2.37	0.57
1:E:345:MET:CG	1:E:354:PRO:HA	2.34	0.57
1:Z:299:ARG:HE	1:Z:300:LEU:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:149:PRO:O	3:L:151:ALA:N	2.37	0.57
1:E:61:TYR:HD1	1:E:125:MET:HE2	1.69	0.57
3:C:214:VAL:HG23	2:D:136:SER:HB3	1.87	0.57
1:A:207:ASN:ND2	1:A:262:GLU:OE1	2.38	0.57
1:A:204:LEU:HD13	1:A:213:VAL:HG21	1.85	0.57
1:E:328:VAL:HG13	4:E:509:HOH:O	2.04	0.57
1:B:315:THR:OG1	1:B:329:GLU:HG2	2.05	0.57
1:Z:238:ASN:HD21	1:Z:240:GLU:CG	2.16	0.56
1:B:141:LEU:O	1:B:164:ARG:HA	2.06	0.56
1:Z:205:THR:CG2	1:Z:210:HIS:ND1	2.59	0.56
1:E:38:LYS:O	1:E:39:PRO:C	2.47	0.56
1:E:345:MET:SD	1:E:345:MET:N	2.76	0.56
1:E:62:GLU:OE1	1:E:122:SER:CB	2.45	0.56
3:C:10:SER:HB2	3:C:114:LEU:HD21	1.86	0.56
1:E:1:ILE:O	1:E:1:ILE:HG22	2.05	0.56
1:A:200:ASP:HA	1:A:215:LYS:HD2	1.87	0.56
1:A:16:SER:HA	1:A:36:GLN:HG2	1.88	0.56
2:D:140:SER:HB3	2:D:143:THR:HG21	1.87	0.56
1:B:148:HIS:CB	1:B:375:MET:HG3	2.29	0.56
3:L:148:TYR:CD1	3:L:149:PRO:HD2	2.36	0.56
3:L:124:THR:CB	3:L:143:LEU:HD11	2.34	0.55
1:Z:332:TYR:O	1:Z:371:ASN:HA	2.06	0.55
1:E:1:ILE:N	1:E:151:MET:O	2.39	0.55
1:Z:238:ASN:ND2	1:Z:240:GLU:OE2	2.39	0.55
1:B:101:TRP:HH2	1:A:329:GLU:HB2	1.69	0.55
1:B:276:GLU:OE2	4:B:501:HOH:O	2.17	0.55
2:D:91:THR:HG23	2:D:118:THR:HA	1.87	0.55
1:E:149:SER:OG	1:E:329:GLU:OE1	2.23	0.55
1:E:315:THR:OG1	1:E:329:GLU:HG3	2.06	0.55
1:E:346:ALA:O	1:E:347:VAL:C	2.49	0.55
2:H:217:LYS:HE2	3:L:131:GLU:OE1	2.07	0.55
1:E:91:VAL:HG11	1:E:243:VAL:HG11	1.89	0.55
1:Z:130:ILE:CG2	1:Z:198:PHE:CD1	2.87	0.54
1:Z:252:ARG:NH1	4:Z:506:HOH:O	2.40	0.54
1:E:180:LEU:HB2	1:E:184:GLY:O	2.07	0.54
1:A:31:VAL:HG13	1:A:43:ILE:HG23	1.88	0.54
1:A:320:GLU:HB2	1:A:400:TRP:HZ2	1.70	0.54
3:L:148:TYR:OH	3:L:205:HIS:O	2.25	0.54
1:Z:159:GLU:OE1	1:Z:159:GLU:N	2.39	0.54
1:A:158:HIS:HB2	1:A:164:ARG:O	2.07	0.54
1:A:344:GLN:HB3	1:A:388:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:PRO:HD2	2:H:208:HIS:NE2	2.23	0.54
1:E:147:GLN:O	1:E:375:MET:HB2	2.07	0.54
1:Z:130:ILE:CG2	1:Z:130:ILE:O	2.53	0.54
2:H:71:SER:HB2	2:H:80:SER:HB2	1.90	0.54
1:A:349:MET:C	1:A:352:LEU:HD23	2.32	0.54
2:D:123:SER:C	2:D:154:PHE:CD2	2.86	0.54
3:L:29:VAL:HG23	3:L:34:MET:HE3	1.90	0.54
1:Z:147:GLN:O	1:Z:375:MET:HB3	2.08	0.54
1:Z:293:LEU:O	1:Z:293:LEU:HD12	2.08	0.54
1:A:359:ILE:HG12	1:A:377:GLU:HB3	1.91	0.53
2:H:105:ARG:HG2	2:H:106:ASN:N	2.23	0.53
1:Z:169:ILE:HD13	1:Z:190:CYS:HB2	1.91	0.53
1:A:201:LEU:HD12	1:A:212:LEU:HG	1.89	0.53
3:C:125:LEU:C	3:C:126:PHE:HD1	2.16	0.53
1:B:206:MET:HE1	1:B:265:VAL:HG11	1.90	0.53
1:A:332:TYR:O	1:A:371:ASN:HA	2.09	0.53
1:Z:2:ARG:N	1:Z:152:ILE:HA	2.24	0.53
1:Z:55:GLU:HG3	1:Z:229:ALA:HB2	1.90	0.53
1:Z:140:MET:HE2	1:Z:164:ARG:NH2	2.24	0.53
1:Z:158:HIS:HB2	1:Z:164:ARG:HB3	1.91	0.53
1:E:61:TYR:CD1	1:E:206:MET:HE1	2.43	0.53
1:E:60:CYS:HB3	1:E:224:PRO:HG2	1.91	0.53
1:B:35:ALA:HB3	1:B:38:LYS:HB2	1.89	0.53
1:A:206:MET:O	1:A:209:LYS:HG3	2.09	0.53
2:D:51:ILE:HD13	2:D:72:ARG:HG3	1.91	0.53
1:Z:50:VAL:HB	1:Z:283:ARG:HG2	1.90	0.52
1:E:370:GLU:OE1	1:E:370:GLU:N	2.42	0.52
3:C:131:GLU:HB2	2:D:131:PRO:HG2	1.91	0.52
1:A:347:VAL:HB	1:A:352:LEU:HB3	1.91	0.52
1:Z:55:GLU:CD	1:Z:55:GLU:H	2.18	0.52
1:A:400:TRP:CG	1:A:401:HIS:N	2.77	0.52
1:E:25:LEU:HD11	1:E:45:LEU:N	2.23	0.52
3:C:127:PRO:HB3	3:C:214:VAL:HG21	1.91	0.52
1:B:148:HIS:CE1	1:B:151:MET:HE3	2.45	0.52
1:B:158:HIS:HB2	1:B:164:ARG:O	2.09	0.52
2:D:167:LEU:HD21	2:D:190:VAL:HG11	1.91	0.52
1:E:251:LYS:HE3	1:E:252:ARG:HD2	1.91	0.52
3:C:23:LEU:HD11	3:C:27:LEU:HD12	1.92	0.52
1:Z:360:THR:HG23	1:Z:377:GLU:HB3	1.92	0.52
1:E:30:CYS:SG	1:E:31:VAL:N	2.83	0.52
1:B:148:HIS:HB2	1:B:375:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HB	1:A:352:LEU:CG	2.39	0.52
2:D:13:GLN:H	2:D:13:GLN:CD	2.17	0.52
1:E:2:ARG:NH1	1:E:164:ARG:HD3	2.26	0.51
1:Z:345:MET:HE2	1:Z:380:PRO:HB3	1.93	0.51
2:H:162:TRP:HZ3	2:H:219:VAL:HG11	1.74	0.51
3:C:125:LEU:HD23	3:C:142:CYS:HB2	1.93	0.51
3:L:148:TYR:CZ	3:L:205:HIS:ND1	2.78	0.51
1:A:401:HIS:CG	1:A:403:SER:HA	2.46	0.51
1:B:140:MET:HE2	1:B:164:ARG:CZ	2.41	0.50
1:B:200:ASP:HA	1:B:215:LYS:HE3	1.93	0.50
1:B:115:THR:HG21	1:B:253:GLN:HB3	1.93	0.50
1:A:145:GLY:H	1:A:360:THR:HG23	1.77	0.50
3:L:157:LYS:HE3	3:L:160:GLY:C	2.36	0.50
1:E:142:SER:OG	1:E:164:ARG:HG3	2.12	0.50
1:A:141:LEU:HB2	1:A:165:ALA:HB3	1.93	0.50
1:Z:11:PHE:CZ	1:Z:325:THR:HG21	2.46	0.50
1:Z:141:LEU:O	1:Z:164:ARG:HA	2.12	0.50
3:L:148:TYR:CE1	3:L:206:GLU:CG	2.90	0.50
3:L:204:THR:HG22	3:L:209:THR:CB	2.40	0.50
1:A:329:GLU:OE2	1:A:373:LYS:HB3	2.12	0.50
2:D:60:TYR:HB2	2:D:65:LYS:HG2	1.93	0.50
1:A:158:HIS:CB	1:A:164:ARG:HG2	2.42	0.50
3:C:177:ASN:OD1	3:C:177:ASN:N	2.42	0.50
1:A:346:ALA:HA	1:A:386:TYR:H	1.76	0.50
1:Z:96:LEU:HD12	1:Z:110:LYS:HD2	1.92	0.50
1:E:238:ASN:HD22	1:E:241:ALA:HB2	1.77	0.50
1:A:387:ILE:HD11	1:A:400:TRP:HB2	1.94	0.50
1:Z:349:MET:HE2	1:Z:349:MET:HA	1.94	0.49
3:L:152:VAL:HG12	3:L:205:HIS:CD2	2.46	0.49
1:A:190:CYS:SG	1:A:289:LEU:HG	2.52	0.49
1:A:275:ALA:HB3	1:A:284:LEU:HD22	1.93	0.49
1:Z:214:HIS:NE2	1:Z:216:GLU:HB3	2.28	0.49
1:A:389:ILE:HG22	1:A:396:ILE:HB	1.95	0.49
1:Z:146:SER:HB2	1:Z:364:VAL:O	2.12	0.49
1:Z:238:ASN:ND2	1:Z:240:GLU:CD	2.70	0.49
3:C:128:PRO:HD3	3:C:140:LEU:HG	1.93	0.49
1:Z:25:LEU:HB2	1:Z:289:LEU:HB3	1.95	0.49
1:Z:186:LEU:HD11	1:Z:293:LEU:HD13	1.95	0.49
2:H:98:LYS:O	2:H:108:LEU:HA	2.13	0.49
2:H:155:PRO:HG2	2:H:210:PRO:HB2	1.95	0.49
1:E:307:LEU:HD22	1:E:342:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:THR:HG22	3:C:187:SER:HA	1.95	0.49
1:A:196:LEU:HD12	1:A:201:LEU:HG	1.95	0.48
1:A:350:GLN:O	1:A:352:LEU:HD22	2.13	0.48
1:A:293:LEU:HD12	1:A:295:MET:HE3	1.94	0.48
3:L:28:ASN:O	3:L:31:THR:HG22	2.13	0.48
1:A:61:TYR:CZ	1:A:123:LYS:HB3	2.49	0.48
1:Z:139:ILE:CD1	1:Z:169:ILE:HD12	2.43	0.48
1:B:149:SER:N	1:B:375:MET:SD	2.84	0.48
2:H:217:LYS:HD2	2:H:217:LYS:HA	1.50	0.48
1:E:378:LEU:HD23	1:E:387:ILE:CD1	2.43	0.48
1:Z:55:GLU:HA	1:Z:128:LYS:HG2	1.95	0.48
1:E:358:LEU:HD12	1:E:378:LEU:HD13	1.96	0.48
2:D:155:PRO:HB2	2:D:210:PRO:HG2	1.94	0.48
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.96	0.48
1:E:308:CYS:SG	1:E:340:LYS:C	2.96	0.48
1:E:345:MET:SD	1:E:354:PRO:CA	3.00	0.48
1:B:332:TYR:O	1:B:371:ASN:HA	2.14	0.48
1:Z:174:PRO:HG2	1:Z:175:ARG:HD2	1.96	0.48
3:L:87:PRO:HA	3:L:113:VAL:HG11	1.94	0.48
1:E:400:TRP:HE1	1:E:402:ARG:HB2	1.78	0.47
1:Z:113:LEU:HD23	1:Z:248:ALA:HB1	1.96	0.47
3:L:40:LYS:HG2	3:L:91:ALA:HB2	1.95	0.47
1:B:159:GLU:N	1:B:159:GLU:OE1	2.44	0.47
1:A:39:PRO:HD3	1:A:300:LEU:HD22	1.96	0.47
1:Z:293:LEU:HD12	1:Z:293:LEU:C	2.40	0.47
3:L:148:TYR:HB2	3:L:149:PRO:CD	2.44	0.47
1:E:385:SER:O	1:E:400:TRP:N	2.31	0.47
1:Z:135:LEU:HD11	1:Z:198:PHE:CE2	2.49	0.47
1:E:3:CYS:CB	1:E:9:ARG:HH12	2.27	0.47
1:E:232:GLY:HA2	1:E:233:THR:HA	1.61	0.47
1:A:278:ASP:HA	1:A:279:GLY:HA2	1.60	0.47
1:B:162:GLU:OE1	1:B:182:GLY:N	2.41	0.47
1:Z:17:GLY:N	1:Z:36:GLN:HB2	2.29	0.47
3:L:124:THR:OG1	3:L:143:LEU:CD2	2.62	0.47
3:C:158:ALA:N	4:C:302:HOH:O	2.26	0.47
1:A:275:ALA:HB3	1:A:284:LEU:HA	1.96	0.47
1:Z:210:HIS:CE1	1:Z:277:MET:HG2	2.49	0.47
1:Z:249:HIS:CG	1:Z:250:ALA:N	2.83	0.47
1:E:345:MET:SD	1:E:354:PRO:CB	3.03	0.47
1:E:350:GLN:HA	1:E:351:THR:HA	1.59	0.47
2:D:160:VAL:HG11	2:D:188:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:91:VAL:HG21	1:Z:243:VAL:HG11	1.96	0.47
1:A:35:ALA:CB	1:A:38:LYS:HB2	2.45	0.47
3:L:28:ASN:O	3:L:32:LYS:HG2	2.14	0.46
3:L:202:GLN:CG	3:L:211:GLU:HG3	2.43	0.46
1:E:14:GLY:N	1:E:34:MET:O	2.29	0.46
3:L:133:LEU:N	4:L:301:HOH:O	2.18	0.46
1:E:20:TRP:HD1	1:E:292:ARG:HH22	1.63	0.46
1:B:140:MET:HE2	1:B:164:ARG:NH2	2.31	0.46
1:A:2:ARG:HH21	1:A:154:ASN:H	1.62	0.46
1:A:62:GLU:HG2	1:A:123:LYS:HB2	1.97	0.46
1:A:210:HIS:O	1:A:211:TRP:HD1	1.98	0.46
2:D:208:HIS:ND1	2:D:211:SER:OG	2.39	0.46
1:Z:14:GLY:HA2	1:Z:21:VAL:HG21	1.96	0.46
1:B:53:MET:HE2	1:B:53:MET:HB3	1.75	0.46
1:Z:214:HIS:CE1	1:Z:216:GLU:HB3	2.51	0.46
1:Z:305:TYR:HB2	1:Z:340:LYS:HG3	1.98	0.46
1:Z:360:THR:OG1	1:Z:376:LEU:HD12	2.15	0.46
1:B:84:LYS:NZ	2:D:104:GLY:O	2.31	0.46
3:L:112:THR:HG21	3:L:149:PRO:HG3	1.97	0.46
1:A:25:LEU:HD13	1:A:45:LEU:HB2	1.96	0.46
1:A:292:ARG:NH1	1:A:293:LEU:O	2.48	0.46
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.30	0.46
2:H:142:SER:O	2:H:194:SER:N	2.45	0.46
2:H:162:TRP:CZ3	2:H:219:VAL:HG11	2.51	0.46
2:D:62:ASP:HA	2:D:65:LYS:HE2	1.98	0.46
1:B:392:GLY:O	1:B:395:LYS:HB2	2.15	0.46
1:E:25:LEU:HB3	1:E:289:LEU:HB2	1.96	0.46
1:E:47:THR:HB	1:E:138:ARG:HB3	1.97	0.46
1:E:224:PRO:HD3	1:E:241:ALA:HB3	1.96	0.46
1:E:378:LEU:HD23	1:E:387:ILE:HD12	1.96	0.46
1:A:224:PRO:HD3	1:A:241:ALA:HB3	1.98	0.46
1:Z:143:VAL:HG11	1:Z:183:PHE:CE1	2.52	0.46
1:Z:196:LEU:C	1:Z:196:LEU:HD12	2.41	0.46
1:Z:320:GLU:HB2	1:Z:400:TRP:HZ2	1.81	0.46
1:E:329:GLU:HB3	1:E:375:MET:HG3	1.98	0.46
1:B:224:PRO:HD3	1:B:241:ALA:HB3	1.97	0.46
1:A:369:THR:HA	1:A:370:GLU:HA	1.51	0.46
1:E:278:ASP:HA	1:E:279:GLY:HA2	1.55	0.45
1:B:74:CYS:N	4:B:502:HOH:O	2.32	0.45
3:C:129:SER:HB3	2:D:133:ALA:H	1.80	0.45
3:C:132:GLU:HB2	2:D:130:PHE:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.51	0.45
2:D:134:PRO:C	2:D:136:SER:H	2.25	0.45
1:Z:148:HIS:HA	1:Z:375:MET:N	2.32	0.45
3:L:124:THR:C	3:L:143:LEU:CD1	2.84	0.45
1:B:83:ASP:HB3	3:C:33:ASN:ND2	2.31	0.45
1:B:329:GLU:CG	1:B:375:MET:HG2	2.45	0.45
1:A:144:HIS:HB3	1:A:360:THR:HG23	1.97	0.45
1:E:2:ARG:HH11	1:E:164:ARG:HD3	1.82	0.45
1:Z:275:ALA:HB1	1:Z:283:ARG:O	2.17	0.45
2:H:12:VAL:HG22	2:H:13:GLN:H	1.82	0.45
1:B:370:GLU:HG3	1:B:371:ASN:N	2.31	0.45
3:C:17:ALA:HB3	3:C:82:ILE:HB	1.98	0.45
1:E:149:SER:N	1:E:375:MET:SD	2.89	0.45
1:E:295:MET:HB2	1:E:298:LEU:HD23	1.98	0.45
1:A:27:HIS:HE1	1:A:283:ARG:NH2	2.14	0.45
3:C:202:GLN:HG2	3:C:211:GLU:HG3	1.97	0.45
3:L:32:LYS:HB2	3:L:34:MET:HE2	1.99	0.45
1:E:197:ASP:H	1:E:201:LEU:CD1	2.30	0.45
1:B:101:TRP:HH2	1:A:329:GLU:CB	2.29	0.45
1:A:332:TYR:HB2	1:A:374:MET:HE1	1.99	0.45
2:D:161:SER:HB3	2:D:205:ASN:HB2	1.98	0.45
1:Z:162:GLU:HB2	1:Z:180:LEU:O	2.17	0.45
1:E:205:THR:HG23	1:E:210:HIS:CE1	2.52	0.45
1:E:252:ARG:HB2	4:E:516:HOH:O	2.17	0.45
1:B:305:TYR:HB2	1:B:340:LYS:HG3	1.99	0.45
1:A:308:CYS:SG	1:A:309:THR:N	2.90	0.45
1:Z:322:LEU:HB2	1:E:108:PHE:CE2	2.51	0.45
2:H:82:GLN:OE1	1:B:272:ALA:HA	2.17	0.45
1:B:337:GLY:HA3	1:B:365:ILE:HD11	1.99	0.45
1:B:349:MET:HA	1:B:349:MET:HE2	1.98	0.45
1:A:1:ILE:O	1:A:152:ILE:HA	2.17	0.45
1:Z:144:HIS:C	1:Z:147:GLN:HE21	2.24	0.44
1:A:401:HIS:NE2	1:A:403:SER:O	2.50	0.44
1:Z:115:THR:HG21	1:Z:253:GLN:HB3	1.98	0.44
1:E:332:TYR:O	1:E:371:ASN:HA	2.17	0.44
1:A:41:VAL:HA	1:A:143:VAL:HA	1.99	0.44
1:A:41:VAL:HG22	1:A:143:VAL:HG12	1.99	0.44
2:H:134:PRO:C	2:H:136:SER:H	2.26	0.44
3:L:143:LEU:CD1	3:L:143:LEU:N	2.72	0.44
3:L:157:LYS:HE2	3:L:160:GLY:N	2.33	0.44
1:E:125:MET:HB2	1:E:206:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:O	1:B:376:LEU:N	2.39	0.44
3:C:18:ARG:NH1	4:C:310:HOH:O	2.50	0.44
1:A:88:THR:HB	1:A:235:HIS:ND1	2.33	0.44
3:L:150:GLY:O	3:L:172:PRO:HG2	2.17	0.44
1:Z:137:TYR:HB2	1:Z:169:ILE:HB	1.99	0.44
1:Z:183:PHE:O	1:Z:299:ARG:N	2.43	0.44
1:Z:345:MET:HE3	1:Z:345:MET:HB3	1.90	0.44
1:B:113:LEU:HD23	1:B:248:ALA:HB1	1.99	0.44
2:D:71:SER:HB2	2:D:80:SER:HB2	1.98	0.44
1:Z:369:THR:HA	1:Z:370:GLU:HA	1.51	0.44
2:H:12:VAL:CG1	2:H:86:LEU:HD13	2.27	0.44
2:H:38:ARG:HD3	2:H:48:VAL:HG22	2.00	0.44
3:L:130:SER:O	3:L:134:GLN:HG2	2.18	0.44
3:L:177:ASN:O	3:L:178:ASN:OD1	2.35	0.44
1:E:162:GLU:HG2	1:E:182:GLY:H	1.83	0.44
1:Z:35:ALA:HB2	1:Z:295:MET:CE	2.38	0.44
1:E:144:HIS:CE1	1:E:359:ILE:HG22	2.53	0.44
1:B:369:THR:HA	1:B:370:GLU:HA	1.55	0.44
1:A:38:LYS:HA	1:A:300:LEU:HD21	1.99	0.44
1:Z:133:GLU:OE1	1:Z:133:GLU:HA	2.18	0.43
1:Z:143:VAL:HG12	1:Z:163:ASN:HA	1.99	0.43
1:B:42:ASP:O	1:B:141:LEU:HA	2.17	0.43
1:B:261:GLN:O	1:B:265:VAL:HG12	2.18	0.43
1:Z:312:PHE:C	1:Z:396:ILE:HD11	2.43	0.43
1:B:204:LEU:HD13	1:B:213:VAL:HG21	1.99	0.43
1:A:99:ARG:HB3	1:A:105:CYS:SG	2.58	0.43
2:D:17:SER:HB2	2:D:19:ARG:NH2	2.33	0.43
2:H:76:LYS:HE2	1:B:222:PRO:HG3	2.00	0.43
3:L:148:TYR:CE1	3:L:206:GLU:CD	2.97	0.43
1:Z:53:MET:CB	1:Z:283:ARG:HH22	2.31	0.43
2:H:142:SER:O	2:H:193:PRO:HA	2.19	0.43
2:H:162:TRP:HB3	2:H:167:LEU:HD23	2.01	0.43
3:C:49:LEU:HD13	3:C:59:LEU:HD23	2.01	0.43
1:A:276:GLU:HG2	1:A:277:MET:H	1.83	0.43
3:L:143:LEU:HD22	3:L:143:LEU:C	2.43	0.43
1:E:320:GLU:HB2	1:E:400:TRP:HZ2	1.82	0.43
1:E:143:VAL:HG23	1:E:163:ASN:O	2.19	0.43
3:C:27:LEU:HD13	3:C:32:LYS:HE2	2.01	0.43
3:C:28:ASN:O	3:C:32:LYS:HG2	2.18	0.43
1:Z:43:ILE:HG12	1:Z:141:LEU:HD22	2.00	0.43
2:H:37:VAL:HG12	2:H:47:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:VAL:O	1:E:40:THR:HG23	2.19	0.43
1:E:293:LEU:HD12	1:E:293:LEU:C	2.43	0.43
1:B:205:THR:HG23	1:B:210:HIS:CD2	2.54	0.43
3:C:126:PHE:HD1	3:C:126:PHE:N	2.16	0.43
1:A:206:MET:HG3	1:A:209:LYS:HE3	2.00	0.43
1:Z:353:THR:HA	1:Z:354:PRO:HD3	1.86	0.43
1:Z:12:VAL:HG11	1:Z:23:VAL:HG12	2.00	0.43
1:A:130:ILE:HG13	1:A:131:GLN:H	1.83	0.43
1:B:142:SER:HA	1:B:163:ASN:O	2.19	0.42
2:D:11:LEU:CD2	2:D:154:PHE:HZ	2.32	0.42
3:L:175:GLN:CG	3:L:176:SER:N	2.70	0.42
1:E:365:ILE:HD11	1:E:372:SER:HB2	2.01	0.42
1:B:141:LEU:HD23	1:B:186:LEU:HD23	2.00	0.42
1:A:209:LYS:HZ3	1:A:211:TRP:CG	2.37	0.42
1:Z:34:MET:HG2	1:Z:40:THR:HG23	2.01	0.42
1:Z:313:THR:OG1	1:Z:331:GLN:HG3	2.19	0.42
1:B:47:THR:HB	1:B:138:ARG:HB3	2.01	0.42
3:C:28:ASN:O	3:C:31:THR:HG22	2.19	0.42
3:C:40:LYS:HG2	3:C:91:ALA:HB2	2.01	0.42
3:C:126:PHE:N	3:C:126:PHE:CD1	2.87	0.42
1:A:1:ILE:N	1:A:151:MET:O	2.42	0.42
3:L:148:TYR:CZ	3:L:205:HIS:CG	3.08	0.42
3:C:44:ALA:HB2	2:D:113:GLN:HA	2.01	0.42
3:C:140:LEU:HD21	3:C:193:TRP:HZ3	1.84	0.42
1:A:164:ARG:HD3	1:A:164:ARG:N	2.35	0.42
1:A:312:PHE:HB3	1:A:330:VAL:CG1	2.49	0.42
1:A:326:VAL:HG21	1:A:400:TRP:NE1	2.34	0.42
1:E:204:LEU:HD21	1:E:206:MET:SD	2.59	0.42
1:E:369:THR:HA	1:E:370:GLU:HA	1.47	0.42
1:B:312:PHE:C	1:B:396:ILE:HD11	2.44	0.42
1:A:402:ARG:HE	1:A:402:ARG:CA	2.31	0.42
2:D:140:SER:HB3	2:D:143:THR:CG2	2.48	0.42
2:D:185:SER:OG	4:D:301:HOH:O	2.21	0.42
1:Z:321:THR:HG22	1:E:101:TRP:HH2	1.85	0.42
2:H:162:TRP:CZ3	2:H:204:CYS:HB2	2.55	0.42
3:L:129:SER:OG	3:L:130:SER:N	2.53	0.42
1:E:384:ASP:CG	1:E:399:HIS:HE2	2.28	0.42
1:B:148:HIS:HB2	1:B:375:MET:CG	2.35	0.42
1:B:320:GLU:HB2	1:B:400:TRP:HZ2	1.84	0.42
3:L:204:THR:CG2	3:L:209:THR:OG1	2.52	0.42
1:A:401:HIS:CE1	1:A:403:SER:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:MET:HE3	1:B:34:MET:HB3	1.96	0.42
1:A:39:PRO:O	1:A:40:THR:OG1	2.36	0.42
1:A:347:VAL:HB	1:A:352:LEU:CB	2.49	0.42
2:D:98:LYS:O	2:D:108:LEU:HA	2.20	0.42
2:H:155:PRO:HB2	2:H:210:PRO:HG2	2.00	0.42
1:B:329:GLU:CB	1:B:375:MET:HG2	2.49	0.42
3:C:205:HIS:C	3:C:206:GLU:HG3	2.45	0.42
1:A:59:TYR:HB2	1:A:125:MET:SD	2.60	0.42
1:A:143:VAL:HG22	1:A:163:ASN:HA	2.01	0.42
1:A:352:LEU:HD13	1:A:352:LEU:HA	1.55	0.42
1:Z:277:MET:HE2	1:Z:277:MET:HB2	1.96	0.42
3:L:8:SER:OG	4:L:302:HOH:O	2.22	0.42
3:L:157:LYS:HG2	3:L:158:ALA:N	2.35	0.42
3:C:161:SER:N	4:C:302:HOH:O	2.52	0.42
1:A:347:VAL:HB	1:A:352:LEU:HG	2.01	0.42
1:Z:158:HIS:HB2	1:Z:164:ARG:O	2.20	0.41
1:Z:305:TYR:CZ	1:Z:338:PRO:HB2	2.55	0.41
1:E:159:GLU:OE1	1:E:159:GLU:N	2.41	0.41
3:C:171:LYS:HB2	3:C:171:LYS:HE2	1.82	0.41
1:Z:99:ARG:NH2	1:Z:103:ASN:O	2.52	0.41
2:H:154:PHE:CB	2:H:155:PRO:HD3	2.42	0.41
1:E:320:GLU:HB2	1:E:400:TRP:CZ2	2.55	0.41
1:B:52:ASN:ND2	1:B:134:ASN:HB3	2.35	0.41
1:Z:91:VAL:HG23	1:Z:245:PHE:HZ	1.85	0.41
2:H:68:PHE:CE1	2:H:83:MET:HB3	2.56	0.41
1:E:183:PHE:O	1:E:299:ARG:N	2.51	0.41
1:B:38:LYS:NZ	1:B:298:LEU:O	2.40	0.41
1:B:196:LEU:HD11	1:B:198:PHE:CE2	2.55	0.41
1:Z:34:MET:HG2	1:Z:40:THR:CG2	2.50	0.41
3:L:10:SER:HB2	3:L:114:LEU:CD1	2.50	0.41
1:B:50:VAL:O	1:B:283:ARG:HD2	2.21	0.41
1:B:239:LYS:H	1:B:239:LYS:HG3	1.70	0.41
1:Z:206:MET:HE2	1:Z:206:MET:HB2	1.83	0.41
1:E:82:LEU:HD13	1:E:116:CYS:SG	2.60	0.41
1:E:154:ASN:H	1:E:164:ARG:NH1	2.18	0.41
3:C:116:GLN:HB3	3:C:148:TYR:CE1	2.55	0.41
1:A:193:ARG:HD3	1:A:193:ARG:HA	1.74	0.41
2:H:192:VAL:HG11	2:H:202:TYR:HH	1.72	0.41
3:L:148:TYR:O	3:L:149:PRO:C	2.63	0.41
1:E:88:THR:HB	1:E:235:HIS:ND1	2.36	0.41
1:B:329:GLU:HA	1:B:375:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ASP:H	1:E:201:LEU:HD11	1.85	0.41
1:E:245:PHE:CE2	1:E:255:VAL:HG21	2.55	0.41
1:A:65:ILE:HG13	1:A:257:VAL:HG13	2.03	0.41
1:E:341:VAL:HG11	1:E:374:MET:CE	2.51	0.41
1:B:359:ILE:HD11	1:B:379:ASP:HB2	2.02	0.41
2:D:155:PRO:HB2	2:D:210:PRO:CB	2.51	0.41
1:Z:50:VAL:CB	1:Z:283:ARG:HG2	2.51	0.41
2:H:51:ILE:HD11	2:H:55:GLY:HA2	2.02	0.41
1:E:344:GLN:NE2	1:E:352:LEU:O	2.53	0.41
1:E:378:LEU:HG	1:E:379:ASP:N	2.36	0.41
1:B:148:HIS:HB3	1:B:374:MET:HA	2.01	0.41
1:A:284:LEU:HD13	1:A:285:SER:N	2.35	0.41
1:A:320:GLU:HB2	1:A:400:TRP:CZ2	2.55	0.41
1:A:401:HIS:CD2	1:A:403:SER:HA	2.55	0.41
2:D:155:PRO:O	2:D:156:GLU:C	2.63	0.41
2:D:214:LYS:HE2	2:D:214:LYS:HB3	1.85	0.41
1:A:130:ILE:HG13	1:A:131:GLN:N	2.36	0.41
1:A:192:PRO:HD3	1:A:289:LEU:HD12	2.02	0.41
2:H:51:ILE:HD12	2:H:58:THR:HG22	2.03	0.40
1:Z:328:VAL:O	1:Z:376:LEU:N	2.42	0.40
2:H:155:PRO:HD2	2:H:208:HIS:CE1	2.56	0.40
2:H:196:SER:OG	2:H:202:TYR:OH	2.33	0.40
1:E:211:TRP:CZ2	1:E:274:GLU:HG2	2.56	0.40
1:B:207:ASN:C	1:B:209:LYS:H	2.28	0.40
1:B:295:MET:SD	1:B:295:MET:N	2.93	0.40
1:A:305:TYR:CZ	1:A:338:PRO:HB2	2.56	0.40
2:D:123:SER:C	2:D:154:PHE:CE2	2.95	0.40
1:Z:34:MET:SD	1:Z:359:ILE:HG23	2.61	0.40
2:H:192:VAL:HG12	2:H:202:TYR:OH	2.11	0.40
1:E:245:PHE:CD2	1:E:255:VAL:HG21	2.55	0.40
1:B:284:LEU:HD12	1:B:284:LEU:H	1.85	0.40
1:Z:58:SER:HB2	1:Z:226:HIS:CE1	2.56	0.40
1:Z:98:ASP:OD1	1:Z:110:LYS:CE	2.69	0.40
3:L:3:LEU:HD21	3:L:97:VAL:CG2	2.49	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:197:ASP:OD2	2:D:13:GLN:NE2[1_455]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:197:ASP:OD1	2:D:13:GLN:NE2[1_455]	2.00	0.20
1:Z:197:ASP:CG	2:D:13:GLN:NE2[1_455]	2.11	0.09
1:Z:317:ILE:CD1	3:L:83:SER:OG[2_445]	2.18	0.02

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	399/405 (98%)	359 (90%)	40 (10%)	0	100	100
1	B	400/405 (99%)	367 (92%)	33 (8%)	0	100	100
1	E	401/405 (99%)	368 (92%)	33 (8%)	0	100	100
1	Z	400/405 (99%)	361 (90%)	39 (10%)	0	100	100
2	D	215/222 (97%)	202 (94%)	12 (6%)	1 (0%)	24	55
2	H	216/222 (97%)	204 (94%)	12 (6%)	0	100	100
3	C	215/219 (98%)	201 (94%)	14 (6%)	0	100	100
3	L	215/219 (98%)	201 (94%)	14 (6%)	0	100	100
All	All	2461/2502 (98%)	2263 (92%)	197 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	134	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	163:ASN	C	164:ARG	N	3.09

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	403/405 (99%)	0.32	35 (8%) 16 11	18, 88, 137, 177	0
1	B	402/405 (99%)	-0.33	4 (0%) 79 72	25, 53, 97, 116	0
1	E	403/405 (99%)	-0.18	7 (1%) 69 60	16, 63, 102, 129	0
1	Z	402/405 (99%)	-0.19	3 (0%) 84 77	32, 61, 104, 132	0
2	D	217/222 (97%)	0.60	11 (5%) 33 25	37, 94, 161, 178	0
2	H	218/222 (98%)	-0.61	1 (0%) 87 82	20, 42, 79, 124	0
3	C	217/219 (99%)	-0.50	0 100 100	22, 46, 87, 105	0
3	L	217/219 (99%)	-0.51	0 100 100	19, 45, 87, 109	0
All	All	2479/2502 (99%)	-0.15	61 (2%) 58 48	16, 59, 126, 178	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	182	GLY	5.4
1	A	387	ILE	4.7
1	A	195	GLY	4.3
1	A	356	GLY	4.2
1	A	347	VAL	3.9
1	A	328	VAL	3.9
2	H	123	SER	3.8
1	Z	151	MET	3.5
1	A	390	GLY	3.5
1	B	149	SER	3.5
1	A	354	PRO	3.3
1	A	385	SER	3.3
2	D	136	SER	3.2
2	D	183	LEU	3.1
1	A	395	LYS	3.1
1	A	196	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	348	ASP	3.1
2	D	192	VAL	3.0
1	A	392	GLY	3.0
2	D	168	THR	3.0
1	E	351	THR	2.9
1	B	150	GLY	2.8
1	E	206	MET	2.8
2	D	193	PRO	2.8
1	E	76	THR	2.8
1	E	195	GLY	2.8
1	A	346	ALA	2.7
2	D	178	LEU	2.7
1	A	397	THR	2.7
1	A	363	PRO	2.7
2	D	212	ASN	2.7
1	A	330	VAL	2.7
1	Z	199	SER	2.7
1	A	386	TYR	2.6
1	A	380	PRO	2.6
1	A	364	VAL	2.6
1	E	146	SER	2.6
1	A	333	ALA	2.6
1	E	162	GLU	2.5
1	A	391	VAL	2.4
1	A	329	GLU	2.4
1	A	403	SER	2.4
1	A	388	VAL	2.3
2	D	64	VAL	2.3
1	A	350	GLN	2.3
1	A	135	LEU	2.3
1	A	400	TRP	2.3
1	A	325	THR	2.3
1	A	318	PRO	2.3
2	D	102	ALA	2.3
1	B	151	MET	2.2
1	A	314	PHE	2.2
1	A	374	MET	2.2
1	A	288	HIS	2.2
1	B	232	GLY	2.2
1	Z	20	TRP	2.1
1	A	317	ILE	2.1
1	A	353	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	67	ASP	2.0
1	A	398	HIS	2.0
2	D	167	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.