



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 02:13 PM EDT

PDB ID : 8EE8
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

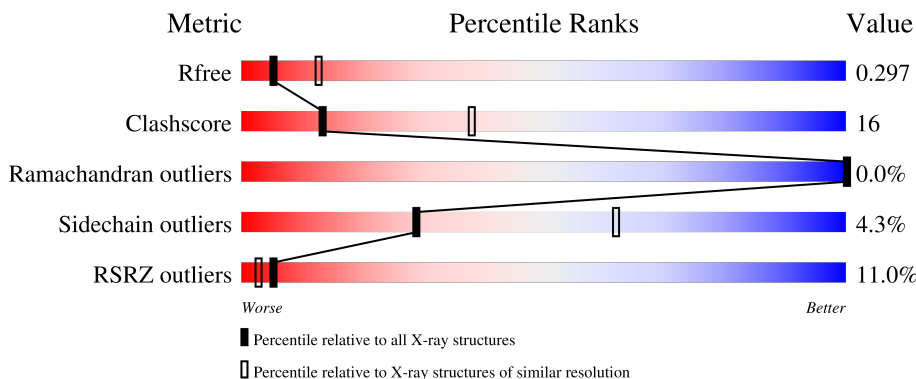
1 Overall quality at a glance

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.



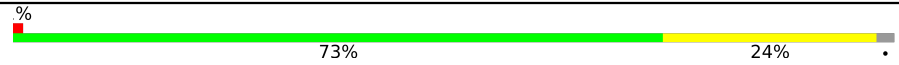

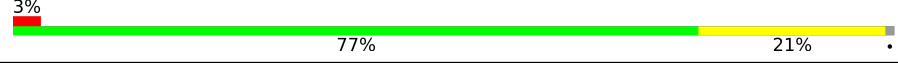
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	 26% 66% 27% 6%
1	B	405	 5% 74% 22% ..
1	E	405	 9% 68% 30% .
1	Z	405	 7% 69% 30% .
2	D	222	 30% 76% 21% ..

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Mol	Chain	Length	Quality of chain
2	H	222	 <p>73% 24% 3%</p>
3	C	219	 <p>77% 21% 2%</p>
3	L	219	 <p>77% 21% 3%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	Z	402	Total 3068	C 1913	N 537	O 593	S 25	0	0	0
1	E	403	Total 3079	C 1921	N 538	O 594	S 26	0	0	0
1	B	402	Total 3071	C 1915	N 537	O 593	S 26	0	0	0
1	A	403	Total 3079	C 1921	N 538	O 594	S 26	0	0	0

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

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

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

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

- Molecule 4 is water.

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

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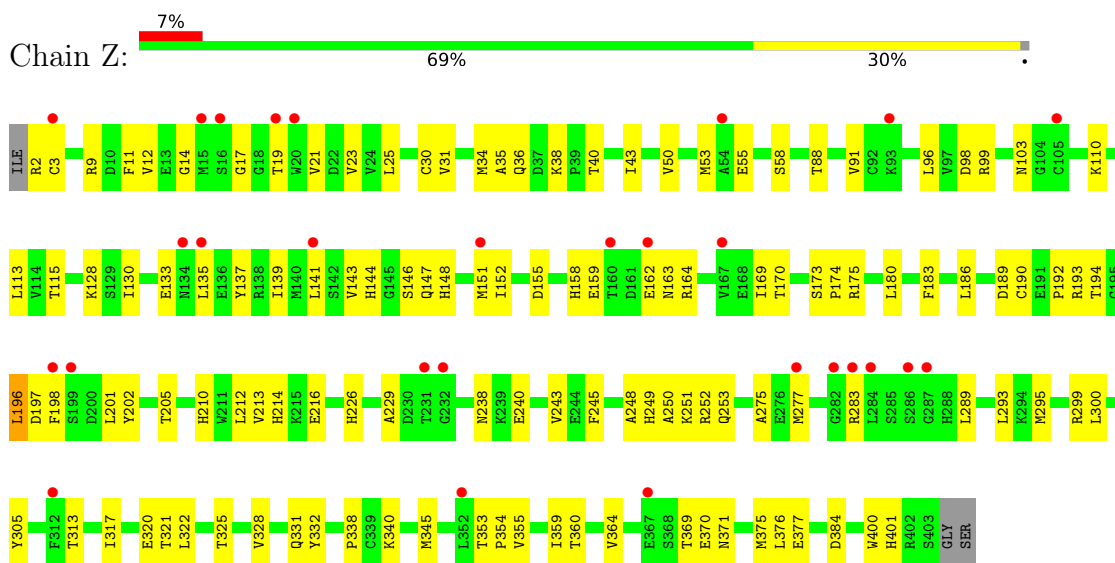
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	20	Total O 20 20	0	0
4	E	18	Total O 18 18	0	0
4	B	19	Total O 19 19	0	0
4	C	27	Total O 27 27	0	0
4	A	13	Total O 13 13	0	0
4	D	21	Total O 21 21	0	0

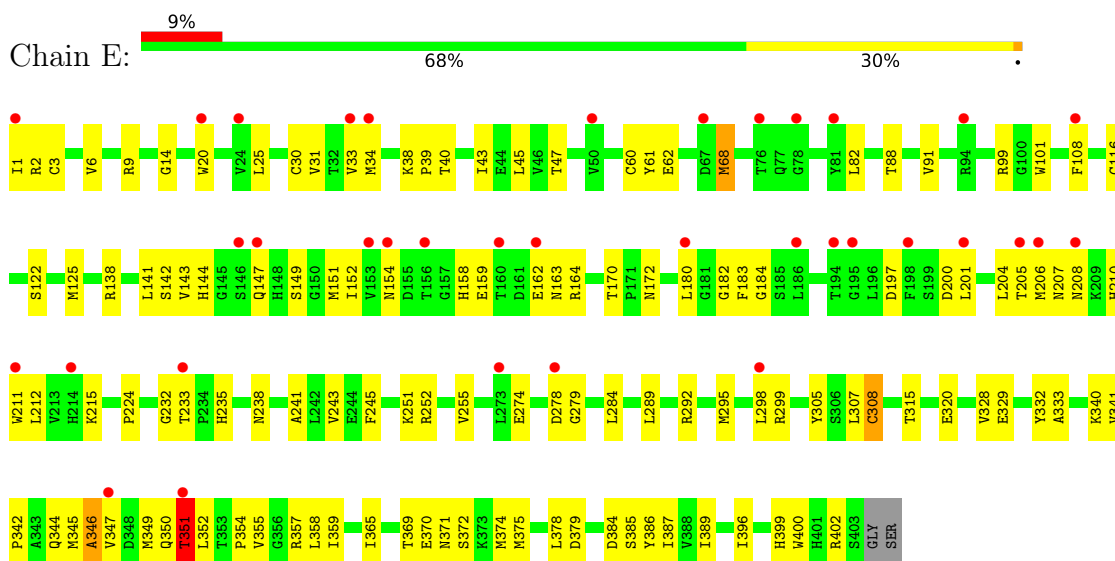
3 Residue-property plots [i](#)

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.

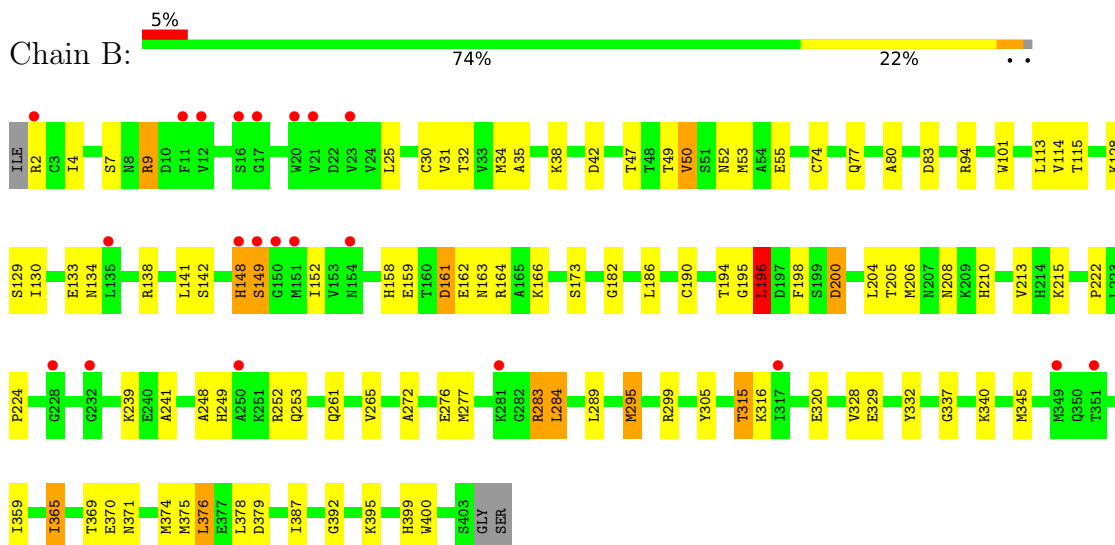
- Molecule 1: Envelope protein E



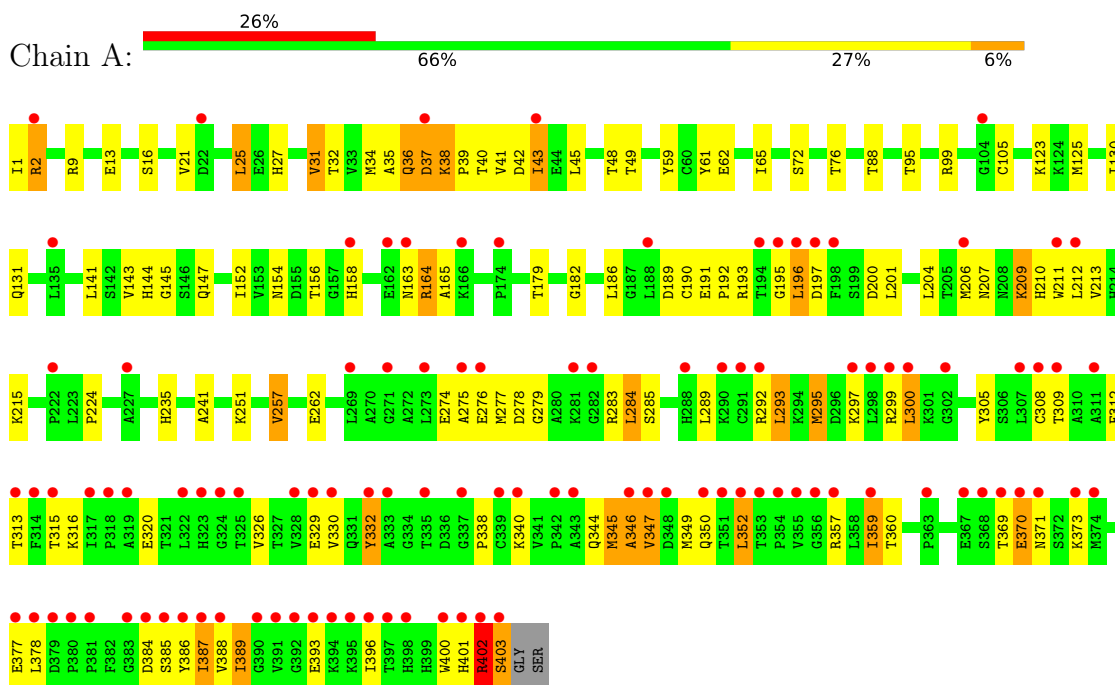
- Molecule 1: Envelope protein E



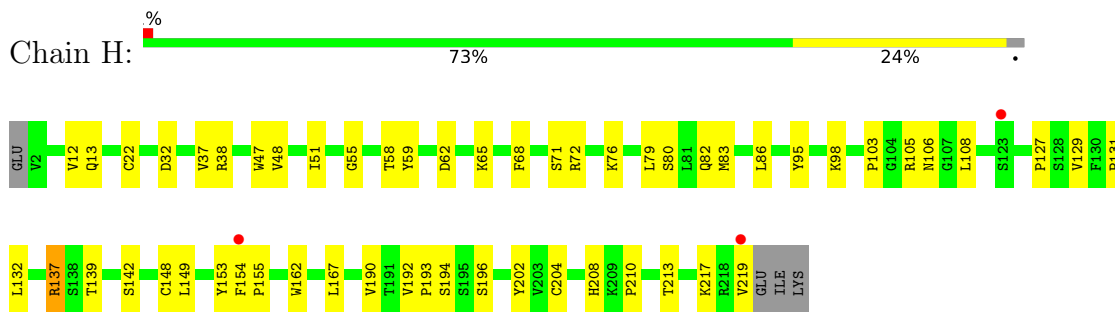
- Molecule 1: Envelope protein E



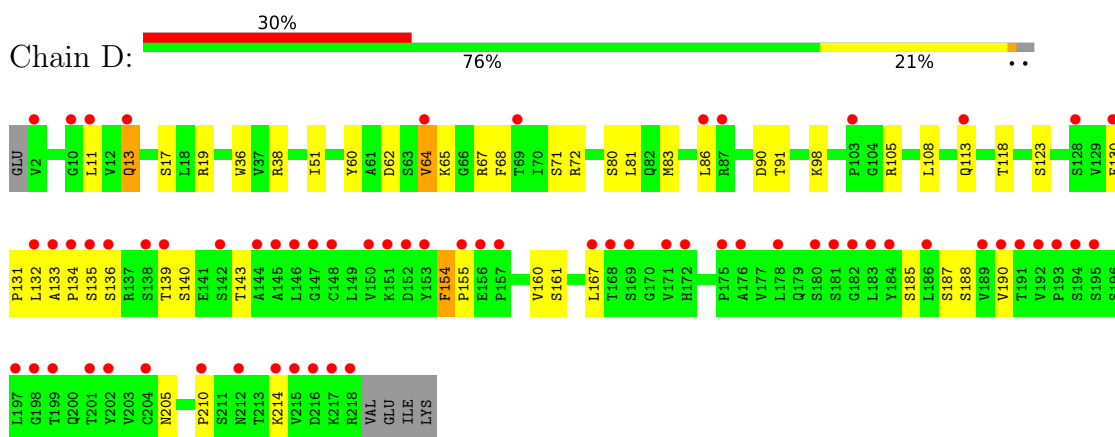
- Molecule 1: Envelope protein E



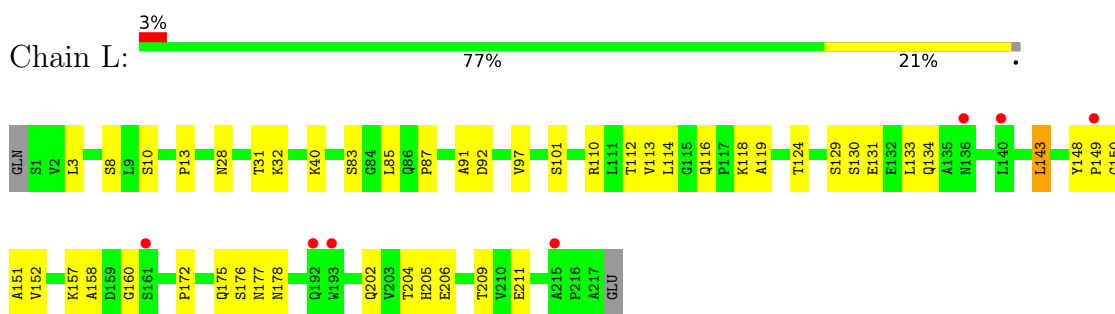
- Molecule 2: rhMZ100-C antibody heavy chain



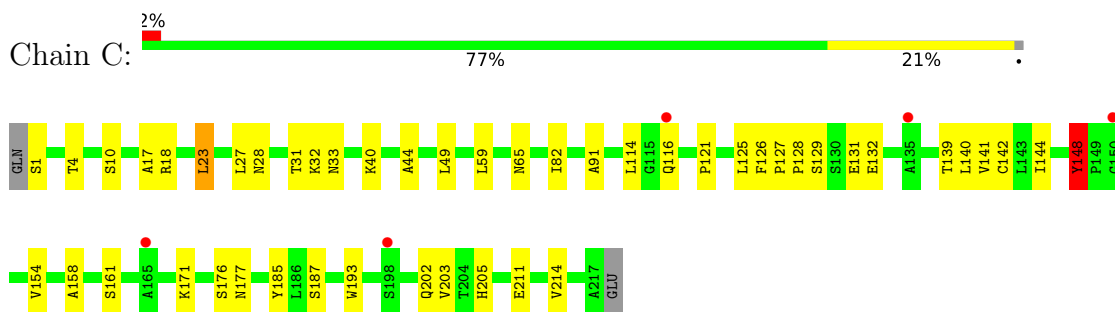
- Molecule 2: rhMZ100-C antibody heavy chain



- Molecule 3: rhMZ100-C antibody light chain



- Molecule 3: rhMZ100-C antibody light chain



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 47.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	61.2 (14.98-2.80) 61.2 (47.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.241 , 0.295 0.244 , 0.297	Depositor DCC
R_{free} test set	2026 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtrriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	0 of 53569 reflections	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18906	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage'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	0.28	0/3143	0.53	0/4257
1	B	0.27	0/3136	0.54	1/4249 (0.0%)
1	E	0.38	0/3144	0.60	2/4260 (0.0%)
1	Z	0.28	0/3133	0.53	0/4246
2	D	0.30	0/1626	0.57	2/2214 (0.1%)
2	H	0.30	0/1633	0.57	0/2224
3	C	0.28	0/1672	0.51	0/2281
3	L	0.32	0/1672	0.51	0/2281
All	All	0.31	0/19159	0.55	5/26012 (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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	LEU	CA-CB-CG	7.73	133.08	115.30
2	D	154	PHE	N-CA-C	6.40	128.28	111.00
1	E	346	ALA	N-CA-C	6.33	128.08	111.00
1	E	351	THR	CA-C-N	-5.98	104.05	117.20
2	D	154	PHE	C-N-CD	-5.61	108.26	120.60

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	96	0
1	B	3071	0	2994	65	0
1	E	3079	0	3007	125	0
1	Z	3068	0	2987	115	4
2	D	1592	0	1558	45	3
2	H	1599	0	1565	57	0
3	C	1632	0	1582	35	0
3	L	1632	0	1581	76	1
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	595	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 16.

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)
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:Z:130:ILE:HG21	1:Z:198:PHE:HD1	1.23	0.99
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
3:L:202:GLN:HG2	3:L:211:GLU:CD	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:VAL:O	1:Z:147:GLN:NE2	2.12	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:124:THR:HG1	3:L:143:LEU:HD11	1.47	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
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:HE3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:O	1:A:299:ARG:NH1	2.32	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:61:TYR:CE1	1:E:206:MET:HE1	2.34	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: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
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: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:H:208:HIS:HB3	2:H:213:THR:HG1	1.68	0.58
2:D:64:VAL:HG13	2:D:68:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:L:149:PRO:O	3:L:151:ALA:N	2.37	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: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
1:A:13:GLU:OE1	1:A:34:MET:HE3	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:THR:OG1	1:E:329:GLU:HG3	2.06	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
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: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
1:Z:35:ALA:HB2	1:Z:295:MET:CE	2.38	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
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:158:HIS:HB2	1:Z:164:ARG:HB3	1.91	0.53
1:A:13:GLU:OE1	1:A:34:MET:CE	2.56	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: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:158:HIS:HB2	1:B:164:ARG:O	2.09	0.52
1:E:341:VAL:HG21	1:E:374:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:347:VAL:HB	1:A:352:LEU:CG	2.39	0.52
1:E:38:LYS:O	1:E:39:PRO:C	2.47	0.52
1:E:2:ARG:NH1	1:E:164:ARG:HD3	2.26	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: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
1:E:142:SER:OG	1:E:164:ARG:HG3	2.12	0.50
1:E:346:ALA:O	1:E:347:VAL:C	2.49	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
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:349:MET:C	1:A:352:LEU:HD23	2.32	0.49
1:A:389:ILE:HG22	1:A:396:ILE:HB	1.95	0.49
2:D:123:SER:C	2:D:154:PHE:CD2	2.86	0.49
1:Z:146:SER:HB2	1:Z:364:VAL:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:TYR:CD1	1:E:206:MET:HE1	2.47	0.49
1:E:307:LEU:HD22	1:E:342:PRO:HG3	1.94	0.49
3:C:125:LEU:C	3:C:126:PHE:HD1	2.16	0.49
3:C:139:THR:HG22	3:C:187:SER:HA	1.95	0.49
3:C:185:TYR:HE2	2:D:187:SER:HG	1.61	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
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: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:Z:55:GLU:CD	1:Z:55:GLU:H	2.18	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:249:HIS:CG	1:Z:250:ALA:N	2.83	0.47
2:D:13:GLN:H	2:D:13:GLN:CD	2.17	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
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: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
1:Z:14:GLY:HA2	1:Z:21:VAL:HG21	1.96	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
3:L:112:THR:HG21	3:L:149:PRO:HG3	1.97	0.46
1:E:341:VAL:HG21	1:E:374:MET:HE2	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:E:341:VAL:HG11	1:E:374:MET:HE1	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:36:TRP:CE2	2:D:81:LEU:HB2	2.51	0.45
1:Z:35:ALA:HB2	1:Z:295:MET:HE2	1.98	0.45
1:Z:148:HIS:HA	1:Z:375:MET:N	2.32	0.45
3:L:157:LYS:HE3	3:L:160:GLY:C	2.36	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
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
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
1:Z:359:ILE:O	1:Z:360:THR:OG1	2.34	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:A:1:ILE:O	1:A:152:ILE:HA	2.17	0.45
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:ASN:ND2	1:Z:240:GLU:CD	2.70	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: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: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
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
1:E:308:CYS:SG	1:E:340:LYS:C	2.96	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
1:E:33:VAL:O	1:E:40:THR:HG23	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Z:293:LEU:HD12	1:Z:293:LEU:C	2.40	0.42
1:E:1:ILE:N	1:E:151:MET:O	2.39	0.42
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: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
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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:ALA:HB2	1:Z:295:MET:HE1	2.02	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: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: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
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
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:Z:196:LEU:C	1:Z:196:LEU:HD12	2.41	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
3:L:124:THR:C	3:L:143:LEU:CD1	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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%)	29	61
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](#)

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	337/338 (100%)	294 (87%)	43 (13%)	4	13
1	B	336/338 (99%)	308 (92%)	28 (8%)	11	32
1	E	337/338 (100%)	335 (99%)	2 (1%)	86	96
1	Z	335/338 (99%)	333 (99%)	2 (1%)	86	96
2	D	181/186 (97%)	175 (97%)	6 (3%)	38	72
2	H	182/186 (98%)	181 (100%)	1 (0%)	88	96
3	C	182/184 (99%)	175 (96%)	7 (4%)	33	67
3	L	182/184 (99%)	181 (100%)	1 (0%)	88	96
All	All	2072/2092 (99%)	1982 (96%)	90 (4%)	29	62

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	193	ARG
1	Z	196	LEU
2	H	137	ARG
3	L	143	LEU
1	E	68	MET
1	E	308	CYS
1	B	7	SER
1	B	9	ARG
1	B	34	MET
1	B	49	THR
1	B	50	VAL
1	B	94	ARG
1	B	129	SER
1	B	133	GLU
1	B	148	HIS
1	B	149	SER
1	B	161	ASP
1	B	166	LYS
1	B	173	SER
1	B	194	THR
1	B	196	LEU
1	B	200	ASP
1	B	206	MET
1	B	249	HIS
1	B	252	ARG
1	B	277	MET
1	B	283	ARG
1	B	284	LEU
1	B	295	MET
1	B	299	ARG
1	B	315	THR
1	B	365	ILE
1	B	376	LEU
1	B	378	LEU
3	C	1	SER
3	C	4	THR
3	C	23	LEU
3	C	65	ASN
3	C	148	TYR
3	C	176	SER
3	C	205	HIS
1	A	2	ARG
1	A	9	ARG

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Mol	Chain	Res	Type
1	A	21	VAL
1	A	25	LEU
1	A	31	VAL
1	A	32	THR
1	A	36	GLN
1	A	37	ASP
1	A	38	LYS
1	A	42	ASP
1	A	43	ILE
1	A	48	THR
1	A	49	THR
1	A	76	THR
1	A	95	THR
1	A	164	ARG
1	A	179	THR
1	A	189	ASP
1	A	191	GLU
1	A	196	LEU
1	A	197	ASP
1	A	209	LYS
1	A	257	VAL
1	A	284	LEU
1	A	293	LEU
1	A	295	MET
1	A	297	LYS
1	A	300	LEU
1	A	313	THR
1	A	315	THR
1	A	316	LYS
1	A	332	TYR
1	A	347	VAL
1	A	352	LEU
1	A	357	ARG
1	A	359	ILE
1	A	370	GLU
1	A	378	LEU
1	A	387	ILE
1	A	389	ILE
1	A	393	GLU
1	A	402	ARG
1	A	403	SER
2	D	13	GLN

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Mol	Chain	Res	Type
2	D	38	ARG
2	D	64	VAL
2	D	105	ARG
2	D	135	SER
2	D	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	144	HIS
1	Z	238	ASN
1	Z	398	HIS
2	H	179	GLN
3	L	116	GLN
1	E	147	GLN
1	B	253	GLN
1	A	27	HIS
1	A	36	GLN
1	A	207	ASN

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 monosaccharides 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%)	1.40	107 (26%) 0 0	18, 88, 137, 177	0
1	B	402/405 (99%)	0.36	21 (5%) 27 18	25, 53, 97, 116	0
1	E	403/405 (99%)	0.56	36 (8%) 9 5	16, 63, 102, 129	0
1	Z	402/405 (99%)	0.53	28 (6%) 16 9	32, 61, 104, 132	0
2	D	217/222 (97%)	1.87	66 (30%) 0 0	37, 94, 161, 178	0
2	H	218/222 (98%)	0.10	3 (1%) 75 70	20, 42, 79, 124	0
3	C	217/219 (99%)	0.21	5 (2%) 60 51	22, 46, 87, 105	0
3	L	217/219 (99%)	0.22	7 (3%) 47 37	19, 45, 87, 109	0
All	All	2479/2502 (99%)	0.67	273 (11%) 5 3	16, 59, 126, 178	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	182	GLY	11.3
1	A	195	GLY	10.9
2	D	198	GLY	10.9
2	D	133	ALA	10.9
1	A	386	TYR	10.8
2	D	168	THR	10.7
1	A	387	ILE	10.3
1	A	403	SER	9.9
1	A	196	LEU	9.1
2	D	183	LEU	9.0
1	A	391	VAL	8.8
2	D	138	SER	8.4
1	A	350	GLN	8.2
2	D	192	VAL	8.0
1	A	390	GLY	8.0
2	D	178	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
2	D	167	LEU	7.5
2	D	214	LYS	7.4
2	D	199	THR	7.3
1	A	333	ALA	7.3
2	D	136	SER	7.2
2	D	201	THR	7.1
2	D	190	VAL	7.0
2	D	212	ASN	6.9
2	D	197	LEU	6.9
1	A	363	PRO	6.6
1	E	146	SER	6.6
2	D	169	SER	6.5
1	A	356	GLY	6.3
2	D	193	PRO	6.1
1	A	347	VAL	6.1
1	A	395	LYS	6.0
2	D	130	PHE	6.0
1	A	354	PRO	5.9
1	A	379	ASP	5.9
1	Z	151	MET	5.7
2	D	176	ALA	5.7
1	A	197	ASP	5.6
1	A	353	THR	5.6
1	A	400	TRP	5.5
2	D	218	ARG	5.5
1	A	380	PRO	5.5
1	A	318	PRO	5.4
1	A	322	LEU	5.4
1	A	369	THR	5.4
2	D	204	CYS	5.3
1	E	195	GLY	5.2
1	A	314	PHE	5.2
2	D	139	THR	5.2
1	A	368	SER	5.2
1	A	194	THR	5.1
3	C	198	SER	5.1
2	D	215	VAL	5.1
1	A	309	THR	5.1
2	D	184	TYR	5.1
1	A	392	GLY	5.1
2	D	132	LEU	5.0
1	E	198	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	Z	20	TRP	4.9
1	A	385	SER	4.9
2	D	128	SER	4.9
2	D	181	SER	4.8
2	H	154	PHE	4.8
1	A	290	LYS	4.8
1	A	329	GLU	4.8
1	A	351	THR	4.8
1	Z	199	SER	4.7
1	B	349	MET	4.7
1	A	328	VAL	4.6
1	E	160	THR	4.6
2	D	146	LEU	4.6
1	E	67	ASP	4.6
1	A	324	GLY	4.5
1	A	352	LEU	4.5
2	D	134	PRO	4.4
1	A	288	HIS	4.4
1	A	166	LYS	4.4
2	H	123	SER	4.3
1	A	281	LYS	4.3
1	A	393	GLU	4.3
1	A	397	THR	4.3
1	B	228	GLY	4.3
1	B	149	SER	4.1
1	A	371	ASN	4.1
1	A	396	ILE	4.1
1	A	292	ARG	4.1
1	A	163	ASN	4.1
1	A	325	THR	4.1
1	E	76	THR	4.0
1	A	355	VAL	4.0
1	A	359	ILE	4.0
1	A	346	ALA	4.0
2	D	153	TYR	3.9
1	A	332	TYR	3.9
1	B	351	THR	3.8
1	A	315	THR	3.8
3	L	193	TRP	3.8
1	E	351	THR	3.8
1	A	311	ALA	3.8
1	E	1	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	162	GLU	3.7
2	D	216	ASP	3.7
2	D	172	HIS	3.6
1	A	335	THR	3.6
1	A	308	CYS	3.6
1	A	330	VAL	3.6
2	D	156	GLU	3.6
1	A	394	LYS	3.5
1	B	17	GLY	3.5
1	A	357	ARG	3.5
2	D	186	LEU	3.5
1	B	281	LYS	3.5
1	E	180	LEU	3.5
1	A	313	THR	3.5
2	D	142	SER	3.5
2	D	210	PRO	3.5
1	B	21	VAL	3.5
2	H	219	VAL	3.5
1	Z	284	LEU	3.4
1	Z	141	LEU	3.4
1	A	323	HIS	3.4
2	D	157	PRO	3.4
1	A	377	GLU	3.4
1	E	278	ASP	3.4
2	D	180	SER	3.4
2	D	152	ASP	3.4
2	D	195	SER	3.3
1	A	402	ARG	3.3
1	Z	16	SER	3.3
1	A	135	LEU	3.3
1	A	388	VAL	3.3
1	Z	134	ASN	3.3
1	B	23	VAL	3.3
1	Z	15	MET	3.3
1	B	148	HIS	3.2
1	Z	160	THR	3.2
1	E	108	PHE	3.2
1	A	319	ALA	3.2
1	A	307	LEU	3.2
1	B	2	ARG	3.1
1	A	401	HIS	3.1
1	Z	277	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	Z	135	LEU	3.1
1	A	317	ILE	3.1
1	E	205	THR	3.1
1	E	206	MET	3.0
1	A	212	LEU	3.0
2	D	145	ALA	3.0
1	E	156	THR	3.0
2	D	150	VAL	3.0
1	B	11	PHE	3.0
1	A	273	LEU	3.0
1	A	378	LEU	2.9
1	Z	162	GLU	2.9
1	A	340	LYS	2.9
1	A	373	LYS	2.9
2	D	64	VAL	2.9
3	L	149	PRO	2.9
3	L	215	ALA	2.9
1	A	374	MET	2.9
1	B	232	GLY	2.8
2	D	191	THR	2.8
2	D	147	GLY	2.8
1	Z	352	LEU	2.8
1	E	94	ARG	2.8
1	A	398	HIS	2.8
1	Z	283	ARG	2.7
1	A	282	GLY	2.7
1	A	299	ARG	2.7
1	Z	282	GLY	2.7
1	E	81	TYR	2.7
1	A	339	CYS	2.7
2	D	202	TYR	2.7
2	D	69	THR	2.7
1	A	383	GLY	2.7
1	E	33	VAL	2.7
1	E	50	VAL	2.7
3	L	140	LEU	2.7
1	A	198	PHE	2.6
1	A	162	GLU	2.6
1	E	20	TRP	2.6
1	E	186	LEU	2.6
1	E	34	MET	2.6
1	B	16	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	222	PRO	2.6
1	E	78	GLY	2.6
1	Z	198	PHE	2.6
1	Z	105	CYS	2.5
1	B	20	TRP	2.5
1	A	158	HIS	2.5
1	E	211	TRP	2.5
1	E	347	VAL	2.5
1	Z	232	GLY	2.5
1	Z	367	GLU	2.5
1	E	208	ASN	2.5
2	D	87	ARG	2.5
1	B	150	GLY	2.5
1	A	43	ILE	2.5
2	D	175	PRO	2.4
1	E	154	ASN	2.4
1	A	337	GLY	2.4
2	D	13	GLN	2.4
1	B	317	ILE	2.4
1	A	22	ASP	2.4
1	Z	54	ALA	2.4
2	D	171	VAL	2.4
1	E	147	GLN	2.4
2	D	113	GLN	2.4
2	D	144	ALA	2.4
2	D	103	PRO	2.4
1	B	151	MET	2.4
1	Z	286	SER	2.4
1	Z	93	LYS	2.3
1	E	273	LEU	2.3
2	D	10	GLY	2.3
1	A	2	ARG	2.3
1	A	275	ALA	2.3
1	Z	19	THR	2.3
1	Z	3	CYS	2.3
2	D	217	LYS	2.3
1	A	348	ASP	2.3
1	E	24	VAL	2.3
1	A	302	GLY	2.3
1	A	342	PRO	2.3
1	A	271	GLY	2.3
2	D	151	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	150	GLY	2.3
1	A	370	GLU	2.3
1	E	201	LEU	2.2
1	A	104	GLY	2.2
1	A	384	ASP	2.2
1	A	188	LEU	2.2
2	D	155	PRO	2.2
1	Z	312	PHE	2.2
1	A	37	ASP	2.2
1	Z	231	THR	2.2
1	E	233	THR	2.2
1	A	206	MET	2.2
2	D	189	VAL	2.2
1	B	250	ALA	2.2
2	D	148	CYS	2.2
3	L	161	SER	2.2
1	A	343	ALA	2.2
1	A	381	PRO	2.2
2	D	194	SER	2.2
1	E	153	VAL	2.2
2	D	2	VAL	2.2
1	A	227	ALA	2.1
1	A	300	LEU	2.1
3	C	165	ALA	2.1
2	D	135	SER	2.1
1	B	135	LEU	2.1
1	A	269	LEU	2.1
1	A	298	LEU	2.1
1	A	367	GLU	2.1
1	Z	287	GLY	2.1
1	A	211	TRP	2.1
1	E	194	THR	2.1
1	A	291	CYS	2.1
2	D	86	LEU	2.1
3	C	116	GLN	2.1
1	E	298	LEU	2.0
1	Z	167	VAL	2.0
2	D	11	LEU	2.0
1	E	214	HIS	2.0
3	L	192	GLN	2.0
3	C	135	ALA	2.0
3	L	136	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	297	LYS	2.0
1	B	154	ASN	2.0
1	A	174	PRO	2.0
1	A	276	GLU	2.0
1	B	12	VAL	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 monosaccharides 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.