



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:05 AM BST

PDB ID : 6KXG
Title : Crystal structure of caspase-11-CARD
Authors : Liu, M.Z.Y.; Jin, T.C.
Deposited on : 2019-09-11
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

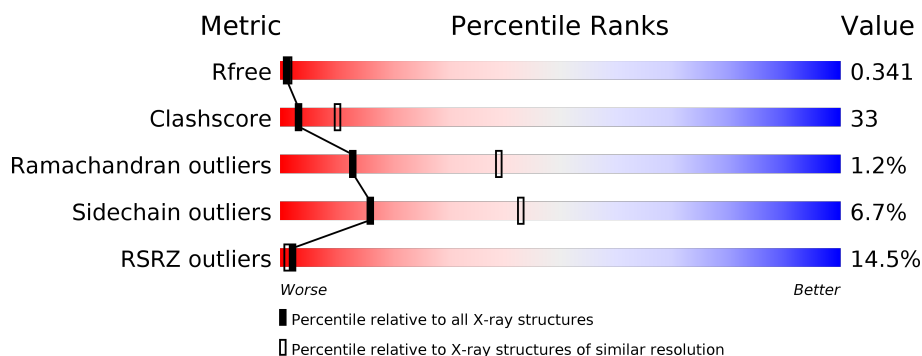
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	<div> <div>6%</div> <div>55%</div> <div>34%</div> <div>8%</div> </div>
1	B	462	<div> <div>20%</div> <div>47%</div> <div>34%</div> <div>5%</div> <div>14%</div> </div>
1	C	462	<div> <div>13%</div> <div>50%</div> <div>38%</div> <div>9%</div> </div>
1	D	462	<div> <div>13%</div> <div>48%</div> <div>35%</div> <div>5%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12882 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.

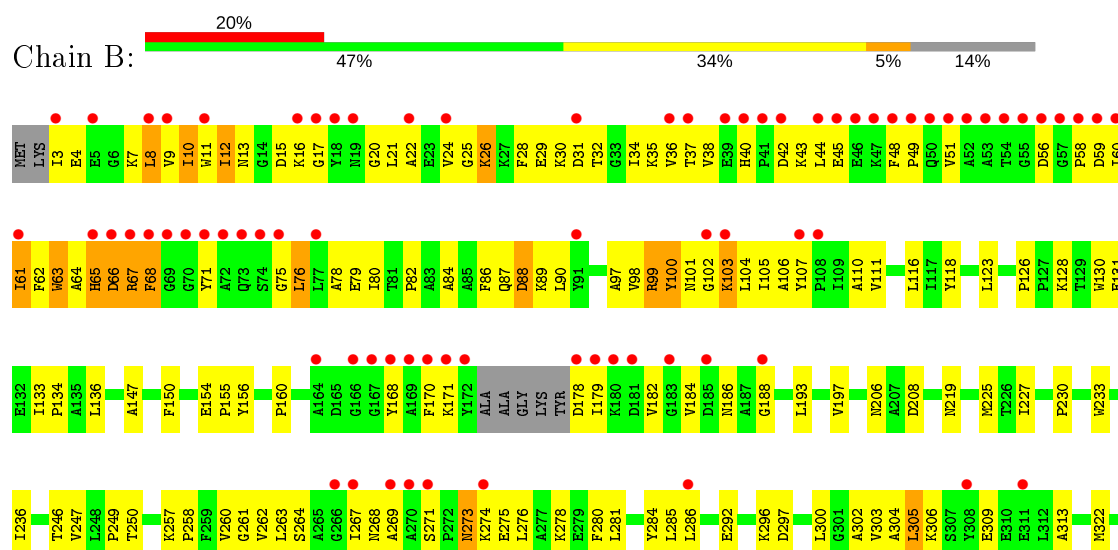
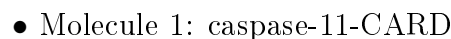
- Molecule 1 is a protein called caspase-11-CARD.

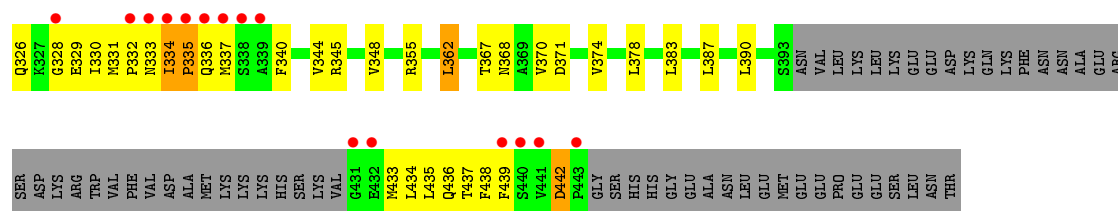
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3319	2140	541	630	8			
1	B	399	Total	C	N	O	S	0	0	0
			3079	1987	495	590	7			
1	C	419	Total	C	N	O	S	0	0	0
			3258	2096	534	620	8			
1	D	415	Total	C	N	O	S	0	0	0
			3223	2074	525	616	8			

- Molecule 2 is water.

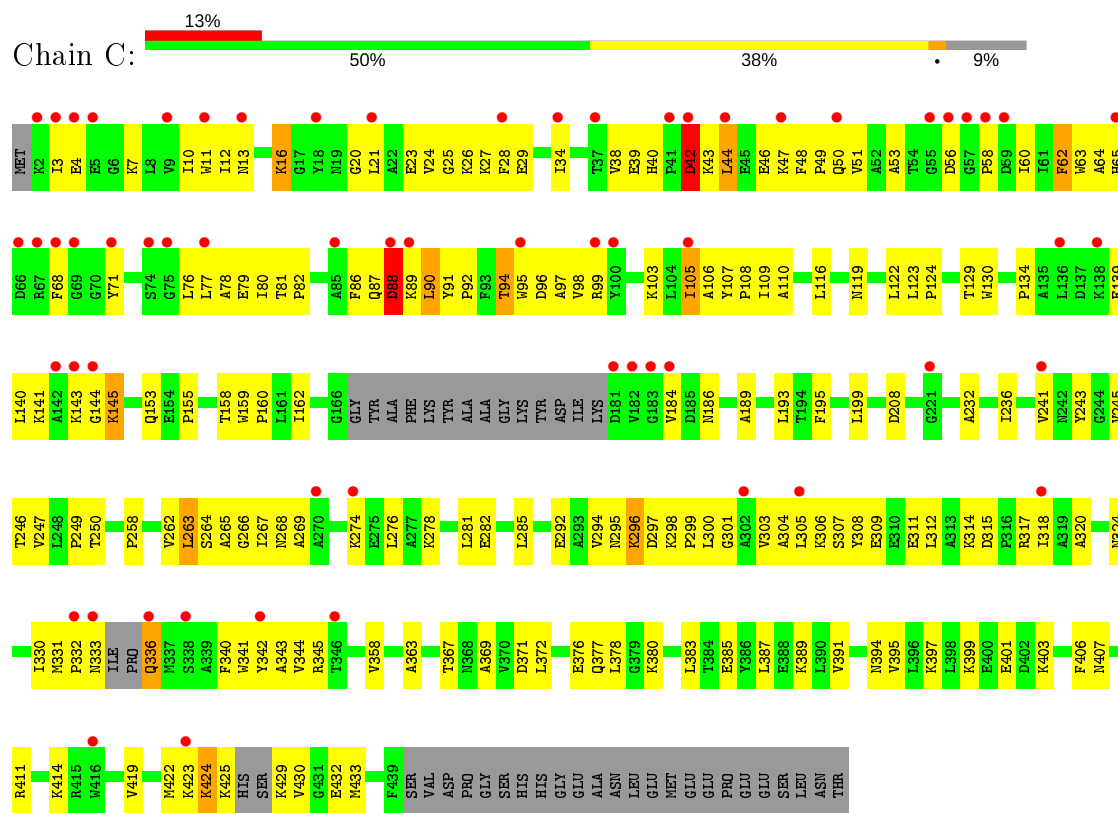
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		

- Molecule 1: caspase-11-CARD

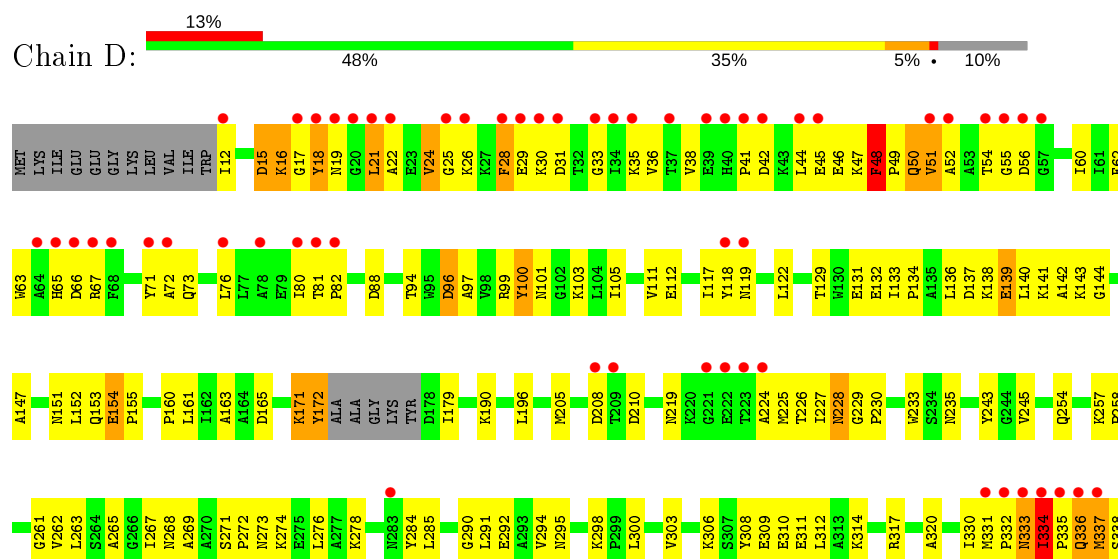


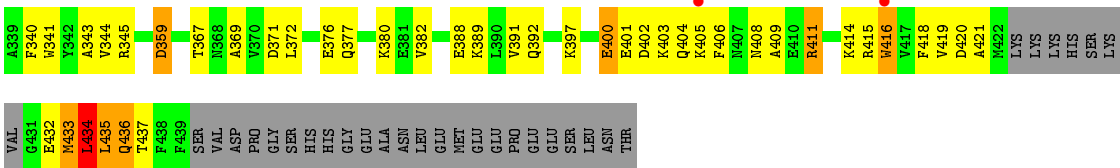


- Molecule 1: caspase-11-CARD



- Molecule 1: caspase-11-CARD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.31Å 145.16Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.67 – 2.81 40.40 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.67-2.81) 97.4 (40.40-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.305 , 0.340 0.305 , 0.341	Depositor DCC
R_{free} test set	2573 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.36	0/3394	0.55	0/4603
1	B	0.35	0/3149	0.58	0/4278
1	C	0.38	0/3326	0.53	0/4504
1	D	0.39	0/3294	0.58	0/4467
All	All	0.37	0/13163	0.56	0/17852

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3319	0	3306	177	0
1	B	3079	0	3055	256	0
1	C	3258	0	3257	218	0
1	D	3223	0	3198	215	0
2	A	3	0	0	0	0
All	All	12882	0	12816	848	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (848) 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:B:12:ILE:HD11	1:B:62:PHE:CD2	1.41	1.51
1:B:66:ASP:HB3	1:B:331:MET:SD	1.66	1.34
1:B:80:ILE:HD12	1:B:107:TYR:CZ	1.67	1.28
1:C:63:TRP:CD1	1:C:64:ALA:N	2.01	1.26
1:B:11:TRP:CB	1:B:61:ILE:HD11	1.65	1.26
1:B:11:TRP:CH2	1:B:58:PRO:HD3	1.70	1.25
1:D:24:VAL:CG2	1:D:28:PHE:HD2	1.51	1.23
1:D:334:ILE:HG22	1:D:335:PRO:CD	1.70	1.21
1:C:106:ALA:HB1	1:C:265:ALA:O	1.38	1.21
1:D:24:VAL:HG21	1:D:28:PHE:CD2	1.77	1.19
1:C:46:GLU:O	1:C:49:PRO:HD2	1.42	1.18
1:D:334:ILE:CG2	1:D:335:PRO:HD3	1.76	1.14
1:B:12:ILE:CD1	1:B:62:PHE:CD2	2.30	1.14
1:C:91:TYR:HB2	1:C:94:THR:HG22	1.27	1.14
1:D:48:PHE:N	1:D:49:PRO:HD3	1.63	1.14
1:C:305:LEU:HD21	1:C:307:SER:OG	1.47	1.13
1:B:11:TRP:HB2	1:B:61:ILE:HD11	1.12	1.12
1:D:24:VAL:HG22	1:D:29:GLU:HG3	1.16	1.11
1:B:8:LEU:HD22	1:B:273:ASN:HD22	1.13	1.11
1:D:334:ILE:CG2	1:D:335:PRO:CD	2.29	1.11
1:B:11:TRP:CA	1:B:61:ILE:HD11	1.80	1.10
1:A:107:TYR:OH	1:A:278:LYS:HE2	1.51	1.10
1:B:8:LEU:HD21	1:B:273:ASN:HB2	1.29	1.09
1:B:79:GLU:CD	1:B:103:LYS:HB3	1.71	1.09
1:D:334:ILE:HB	1:D:335:PRO:HD2	1.33	1.08
1:B:11:TRP:HB2	1:B:61:ILE:CD1	1.85	1.07
1:B:45:GLU:HG3	1:B:67:ARG:NH1	1.68	1.07
1:B:98:VAL:HG12	1:B:105:ILE:CG1	1.85	1.06
1:B:80:ILE:CD1	1:B:107:TYR:CZ	2.38	1.06
1:D:48:PHE:H	1:D:49:PRO:HD3	1.14	1.06
1:B:98:VAL:O	1:B:105:ILE:HG12	1.56	1.06
1:C:91:TYR:CD1	1:C:306:LYS:HE2	1.90	1.06
1:B:11:TRP:H	1:B:61:ILE:CD1	1.67	1.06
1:B:98:VAL:CG1	1:B:105:ILE:HG13	1.84	1.05
1:B:8:LEU:HD11	1:B:59:ASP:HB2	1.32	1.05
1:D:52:ALA:HB2	1:D:268:ASN:HD21	1.20	1.05
1:A:8:LEU:HB3	1:A:36:VAL:CG1	1.87	1.05
1:B:12:ILE:CD1	1:B:62:PHE:HD2	1.69	1.05
1:D:334:ILE:CB	1:D:335:PRO:CD	2.35	1.04
1:A:60:ILE:HD11	1:A:277:ALA:HB1	1.06	1.04
1:D:308:TYR:O	1:D:312:LEU:HD12	1.55	1.04
1:D:48:PHE:N	1:D:49:PRO:CD	2.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:CB	1:A:36:VAL:HG12	1.88	1.04
1:D:24:VAL:CG2	1:D:28:PHE:CD2	2.38	1.03
1:B:98:VAL:HG12	1:B:105:ILE:HG13	1.04	1.03
1:D:24:VAL:HG21	1:D:28:PHE:HD2	0.85	1.02
1:B:60:ILE:HG22	1:B:267:ILE:HG23	1.40	1.01
1:A:5:GLU:HB3	1:A:272:PRO:HB2	1.39	1.01
1:C:91:TYR:HA	1:C:306:LYS:HE3	1.41	1.01
1:A:284:TYR:O	1:A:287:THR:HG23	1.61	1.01
1:B:8:LEU:HD21	1:B:273:ASN:CB	1.91	1.01
1:B:8:LEU:CD2	1:B:273:ASN:HD22	1.73	1.00
1:C:91:TYR:HA	1:C:306:LYS:CE	1.92	1.00
1:B:63:TRP:HA	1:B:63:TRP:CE3	1.94	1.00
1:B:65:HIS:CE1	1:B:331:MET:HB3	1.95	1.00
1:A:8:LEU:HB3	1:A:36:VAL:HG12	1.03	0.99
1:C:48:PHE:HZ	1:C:77:LEU:HD11	1.26	0.99
1:C:87:GLN:O	1:C:88:ASP:HB2	1.58	0.99
1:D:24:VAL:HG23	1:D:28:PHE:HB3	1.39	0.99
1:B:219:ASN:OD1	1:B:236:ILE:HG22	1.62	0.99
1:D:334:ILE:CB	1:D:335:PRO:HD2	1.93	0.99
1:D:52:ALA:CB	1:D:268:ASN:HD21	1.77	0.97
1:A:81:THR:N	1:A:278:LYS:HZ1	1.63	0.97
1:A:5:GLU:HB2	1:A:273:ASN:ND2	1.79	0.96
1:B:8:LEU:CD1	1:B:59:ASP:HB2	1.95	0.96
1:A:268:ASN:HB3	1:A:271:SER:HB2	1.47	0.96
1:A:5:GLU:HB2	1:A:273:ASN:HD21	1.27	0.95
1:A:60:ILE:HD11	1:A:277:ALA:CB	1.96	0.95
1:B:12:ILE:HD11	1:B:62:PHE:CG	2.01	0.94
1:B:66:ASP:CB	1:B:331:MET:SD	2.56	0.94
1:A:81:THR:H	1:A:278:LYS:HZ1	0.96	0.94
1:C:91:TYR:CA	1:C:306:LYS:HE3	1.97	0.93
1:D:334:ILE:HB	1:D:335:PRO:CD	1.94	0.92
1:C:63:TRP:HD1	1:C:64:ALA:N	1.53	0.91
1:A:81:THR:H	1:A:278:LYS:NZ	1.69	0.91
1:B:12:ILE:HD11	1:B:62:PHE:HD2	1.11	0.91
1:D:137:ASP:OD1	1:D:141:LYS:HG2	1.70	0.91
1:B:11:TRP:N	1:B:61:ILE:CD1	2.34	0.91
1:C:98:VAL:HG13	1:C:105:ILE:HG23	1.54	0.90
1:D:21:LEU:HD23	1:D:38:VAL:HG11	1.54	0.90
1:D:24:VAL:CG2	1:D:29:GLU:HG3	2.02	0.89
1:D:179:ILE:HB	1:D:334:ILE:HD11	1.53	0.89
1:B:79:GLU:OE1	1:B:103:LYS:HG2	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:CD	1:B:103:LYS:CB	2.42	0.88
1:D:171:LYS:HG3	1:D:330:ILE:HG12	1.52	0.88
1:D:334:ILE:HG22	1:D:335:PRO:HD3	0.92	0.88
1:D:308:TYR:O	1:D:312:LEU:CD1	2.22	0.88
1:B:8:LEU:HD11	1:B:59:ASP:CB	2.03	0.87
1:B:80:ILE:HD13	1:B:107:TYR:CE2	2.08	0.87
1:C:46:GLU:O	1:C:49:PRO:CD	2.23	0.87
1:D:52:ALA:HB2	1:D:268:ASN:ND2	1.90	0.87
1:D:139:GLU:N	1:D:139:GLU:OE2	2.08	0.87
1:C:91:TYR:HB2	1:C:94:THR:CG2	2.03	0.87
1:C:65:HIS:HE1	1:C:330:ILE:HG23	1.39	0.87
1:D:24:VAL:HG23	1:D:28:PHE:CB	2.04	0.86
1:B:110:ALA:HB3	1:B:263:LEU:HD21	1.57	0.86
1:D:309:GLU:HA	1:D:312:LEU:HD13	1.55	0.86
1:B:11:TRP:CZ3	1:B:58:PRO:HD3	2.09	0.86
1:C:91:TYR:OH	1:C:309:GLU:HG2	1.75	0.86
1:D:401:GLU:HA	1:D:404:GLN:OE1	1.76	0.85
1:B:11:TRP:HZ3	1:B:51:VAL:HG11	1.42	0.85
1:B:63:TRP:HA	1:B:63:TRP:HE3	1.32	0.85
1:B:99:ARG:CZ	1:B:99:ARG:HB2	2.05	0.84
1:B:8:LEU:HD22	1:B:273:ASN:ND2	1.93	0.84
1:D:228:ASN:HD22	1:D:229:GLY:H	1.23	0.84
1:D:404:GLN:OE1	1:D:404:GLN:N	2.11	0.83
1:B:79:GLU:OE2	1:B:103:LYS:HB3	1.78	0.83
1:D:334:ILE:CG2	1:D:335:PRO:HD2	2.03	0.83
1:A:81:THR:N	1:A:278:LYS:NZ	2.26	0.83
1:D:331:MET:HG3	1:D:332:PRO:HD2	1.61	0.83
1:B:11:TRP:CZ3	1:B:51:VAL:HG11	2.14	0.82
1:D:24:VAL:HG22	1:D:29:GLU:CG	2.06	0.82
1:A:107:TYR:OH	1:A:278:LYS:CE	2.27	0.82
1:A:399:LYS:HA	1:A:403:LYS:HB2	1.58	0.82
1:C:92:PRO:HD3	1:C:306:LYS:NZ	1.94	0.82
1:B:80:ILE:CD1	1:B:107:TYR:CE2	2.62	0.81
1:B:9:VAL:C	1:B:10:ILE:HG13	1.99	0.81
1:A:413:ASP:OD1	1:A:416:TRP:HB2	1.80	0.81
1:B:103:LYS:HD2	1:B:103:LYS:H	1.46	0.80
1:C:21:LEU:HD23	1:C:38:VAL:HG23	1.63	0.80
1:C:90:LEU:HB2	1:C:95:TRP:CZ2	2.17	0.80
1:B:11:TRP:H	1:B:61:ILE:HD13	1.46	0.80
1:B:286:LEU:O	1:B:305:LEU:HD11	1.80	0.80
1:C:106:ALA:HB2	1:C:266:GLY:HA2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:CE1	1:B:260:VAL:O	2.35	0.80
1:B:45:GLU:HG3	1:B:67:ARG:HH11	1.46	0.80
1:C:48:PHE:CZ	1:C:77:LEU:HD11	2.14	0.80
1:D:434:LEU:H	1:D:434:LEU:CD2	1.96	0.79
1:C:424:LYS:HD2	1:C:425:LYS:HB2	1.64	0.79
1:B:98:VAL:O	1:B:105:ILE:CG1	2.29	0.79
1:B:11:TRP:N	1:B:61:ILE:HD11	1.96	0.79
1:C:91:TYR:CB	1:C:94:THR:HG22	2.12	0.79
1:B:387:LEU:HD21	1:B:434:LEU:HD21	1.65	0.79
1:B:45:GLU:HG3	1:B:67:ARG:HH12	1.45	0.79
1:B:42:ASP:HB3	1:B:43:LYS:HE3	1.64	0.79
1:B:32:THR:HG23	1:B:34:ILE:H	1.48	0.78
1:D:81:THR:HG22	1:D:278:LYS:HD3	1.66	0.78
1:C:106:ALA:CB	1:C:265:ALA:O	2.28	0.78
1:A:285:LEU:O	1:A:285:LEU:HD12	1.84	0.78
1:C:91:TYR:N	1:C:306:LYS:HE3	1.99	0.78
1:B:8:LEU:CD2	1:B:273:ASN:ND2	2.46	0.78
1:B:263:LEU:HD23	1:B:263:LEU:H	1.49	0.77
1:D:433:MET:O	1:D:433:MET:HE3	1.83	0.77
1:A:32:THR:O	1:A:34:ILE:HG12	1.85	0.77
1:B:110:ALA:HA	1:B:303:VAL:HA	1.67	0.77
1:B:66:ASP:OD1	1:B:66:ASP:N	2.18	0.77
1:B:11:TRP:CH2	1:B:58:PRO:CD	2.62	0.77
1:A:60:ILE:CD1	1:A:277:ALA:HB1	2.02	0.76
1:B:26:LYS:HZ2	1:B:30:LYS:HD3	1.50	0.76
1:D:133:ILE:HG13	1:D:134:PRO:HD3	1.66	0.76
1:C:89:LYS:O	1:C:306:LYS:HD2	1.86	0.76
1:B:179:ILE:HG13	1:B:334:ILE:HD12	1.67	0.75
1:B:80:ILE:HD12	1:B:107:TYR:OH	1.86	0.75
1:B:80:ILE:HD12	1:B:107:TYR:CE1	2.21	0.75
1:B:60:ILE:HG22	1:B:267:ILE:CG2	2.16	0.75
1:A:128:LYS:HE2	1:A:247:VAL:HG11	1.69	0.75
1:A:398:LEU:HD12	1:A:398:LEU:O	1.87	0.75
1:A:422:MET:O	1:A:423:LYS:HD3	1.86	0.74
1:B:11:TRP:CB	1:B:61:ILE:CD1	2.52	0.74
1:A:7:LYS:HD2	1:A:35:LYS:HE3	1.69	0.74
1:D:434:LEU:H	1:D:434:LEU:HD23	1.50	0.74
1:A:49:PRO:HA	1:A:76:LEU:HD13	1.67	0.74
1:B:48:PHE:HA	1:B:51:VAL:HG12	1.68	0.74
1:D:161:LEU:HD23	1:D:196:LEU:HD12	1.67	0.74
1:A:106:ALA:HB1	1:A:265:ALA:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:O	1:C:108:PRO:HG3	1.87	0.74
1:B:60:ILE:HA	1:B:267:ILE:HA	1.70	0.74
1:C:65:HIS:CD2	1:C:262:VAL:HG22	2.23	0.74
1:B:22:ALA:HB2	1:B:38:VAL:HG11	1.69	0.73
1:C:385:GLU:OE2	1:C:411:ARG:NH1	2.21	0.73
1:C:47:LYS:O	1:C:51:VAL:HG22	1.88	0.73
1:B:80:ILE:O	1:B:82:PRO:HD3	1.89	0.73
1:C:406:PHE:O	1:C:414:LYS:NZ	2.22	0.73
1:C:407:ASN:HA	1:C:414:LYS:HZ1	1.53	0.72
1:D:52:ALA:C	1:D:54:THR:H	1.93	0.72
1:C:63:TRP:CG	1:C:64:ALA:N	2.58	0.72
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.25	0.71
1:C:92:PRO:HD3	1:C:306:LYS:HZ1	1.53	0.71
1:C:143:LYS:H	1:C:143:LYS:HZ3	1.38	0.71
1:A:410:GLU:N	1:A:410:GLU:OE2	2.20	0.71
1:A:176:LYS:NZ	1:A:179:ILE:HG23	2.06	0.71
1:C:82:PRO:HB3	1:C:107:TYR:HE1	1.55	0.71
1:C:98:VAL:HG11	1:C:106:ALA:O	1.91	0.71
1:A:60:ILE:HA	1:A:266:GLY:O	1.91	0.70
1:C:21:LEU:HD23	1:C:38:VAL:CG2	2.21	0.70
1:C:80:ILE:CG2	1:C:107:TYR:CZ	2.75	0.70
1:D:42:ASP:O	1:D:47:LYS:NZ	2.21	0.70
1:D:24:VAL:HG23	1:D:28:PHE:CD2	2.25	0.70
1:C:63:TRP:HD1	1:C:64:ALA:CA	2.05	0.70
1:D:29:GLU:O	1:D:33:GLY:N	2.24	0.70
1:D:41:PRO:HB2	1:D:47:LYS:HZ1	1.57	0.70
1:B:329:GLU:HG3	1:B:330:ILE:H	1.57	0.70
1:C:298:LYS:NZ	1:C:300:LEU:HA	2.07	0.70
1:B:29:GLU:OE1	1:B:35:LYS:HA	1.93	0.69
1:A:186:ASN:OD1	1:A:187:ALA:N	2.26	0.69
1:B:16:LYS:HG2	1:B:300:LEU:HD23	1.73	0.69
1:B:11:TRP:HB2	1:B:61:ILE:CG1	2.22	0.69
1:C:77:LEU:HD23	1:C:105:ILE:HD11	1.74	0.69
1:D:60:ILE:HG12	1:D:267:ILE:HG22	1.74	0.69
1:D:435:LEU:O	1:D:437:THR:N	2.26	0.68
1:A:165:ASP:O	1:A:188:GLY:HA3	1.93	0.68
1:B:170:PHE:HE2	1:B:334:ILE:HG13	1.59	0.68
1:D:171:LYS:HG3	1:D:330:ILE:CG1	2.23	0.68
1:B:65:HIS:CE1	1:B:331:MET:CB	2.77	0.68
1:C:80:ILE:HD11	1:C:105:ILE:O	1.94	0.68
1:B:268:ASN:O	1:B:271:SER:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:VAL:CG2	1:D:28:PHE:HB3	2.19	0.67
1:D:101:ASN:O	1:D:103:LYS:HD2	1.94	0.67
1:C:79:GLU:OE2	1:C:103:LYS:HD2	1.94	0.67
1:D:228:ASN:HD22	1:D:229:GLY:N	1.91	0.67
1:B:12:ILE:HG22	1:B:13:ASN:N	2.10	0.67
1:B:273:ASN:OD1	1:B:273:ASN:N	2.23	0.67
1:C:377:GLN:HG2	1:C:380:LYS:HD2	1.76	0.67
1:A:389:LYS:HB3	1:D:372:LEU:HD12	1.77	0.67
1:C:308:TYR:HA	1:C:311:GLU:CD	2.15	0.66
1:A:80:ILE:HB	1:A:104:LEU:HB2	1.77	0.66
1:C:106:ALA:HB1	1:C:265:ALA:C	2.14	0.66
1:C:46:GLU:C	1:C:49:PRO:HD2	2.14	0.66
1:A:82:PRO:HG2	1:A:104:LEU:HD12	1.75	0.66
1:D:44:LEU:HA	1:D:47:LYS:HE2	1.76	0.66
1:B:103:LYS:HD2	1:B:103:LYS:N	2.09	0.66
1:B:99:ARG:HA	1:B:99:ARG:NH1	2.10	0.66
1:C:71:TYR:HB3	1:C:77:LEU:HD22	1.77	0.66
1:A:278:LYS:O	1:A:282:GLU:HG3	1.96	0.66
1:C:308:TYR:HA	1:C:311:GLU:OE1	1.96	0.66
1:A:89:LYS:NZ	1:A:307:SER:H	1.94	0.65
1:D:18:TYR:HD1	1:D:19:ASN:H	1.43	0.65
1:A:106:ALA:CB	1:A:265:ALA:O	2.45	0.65
1:A:399:LYS:HA	1:A:403:LYS:CB	2.27	0.65
1:A:8:LEU:CB	1:A:36:VAL:CG1	2.63	0.65
1:A:97:ALA:HA	1:A:330:ILE:HG21	1.78	0.65
1:D:88:ASP:O	1:D:306:LYS:NZ	2.29	0.65
1:C:95:TRP:O	1:C:98:VAL:N	2.30	0.65
1:D:119:ASN:HD21	1:D:122:LEU:HD23	1.61	0.65
1:A:45:GLU:OE2	1:A:45:GLU:N	2.29	0.65
1:D:16:LYS:NZ	1:D:63:TRP:HZ3	1.94	0.65
1:B:111:VAL:HG11	1:B:322:MET:SD	2.37	0.65
1:B:59:ASP:O	1:B:268:ASN:N	2.20	0.64
1:B:154:GLU:HG3	1:B:156:TYR:H	1.63	0.64
1:B:89:LYS:O	1:B:305:LEU:HD23	1.97	0.64
1:D:271:SER:OG	1:D:272:PRO:HD2	1.96	0.64
1:B:26:LYS:NZ	1:B:30:LYS:HD3	2.12	0.64
1:C:80:ILE:CG2	1:C:107:TYR:OH	2.45	0.64
1:D:376:GLU:OE2	1:D:377:GLN:NE2	2.30	0.64
1:A:29:GLU:HG2	1:A:29:GLU:O	1.96	0.64
1:A:395:VAL:HG13	1:A:396:LEU:HG	1.78	0.64
1:C:20:GLY:HA3	1:C:294:VAL:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ASP:OD1	1:D:254:GLN:NE2	2.30	0.64
1:D:81:THR:HG22	1:D:278:LYS:CD	2.28	0.64
1:A:285:LEU:C	1:A:285:LEU:HD12	2.16	0.64
1:D:273:ASN:HB3	1:D:276:LEU:HD23	1.79	0.64
1:B:60:ILE:CG2	1:B:267:ILE:HG23	2.23	0.64
1:C:78:ALA:HB2	1:C:269:ALA:HA	1.80	0.64
1:C:141:LYS:HD2	1:C:141:LYS:O	1.97	0.64
1:B:17:GLY:HA3	1:B:297:ASP:HB3	1.79	0.64
1:C:13:ASN:HD21	1:C:63:TRP:HZ3	1.45	0.64
1:C:295:ASN:OD1	1:C:300:LEU:N	2.28	0.63
1:C:10:ILE:HG12	1:C:60:ILE:HB	1.79	0.63
1:D:409:ALA:O	1:D:414:LYS:NZ	2.32	0.63
1:C:305:LEU:HD23	1:C:308:TYR:H	1.64	0.63
1:C:63:TRP:CD1	1:C:64:ALA:CA	2.81	0.63
1:B:100:TYR:C	1:B:102:GLY:H	2.02	0.63
1:B:367:THR:HA	1:B:370:VAL:HG12	1.81	0.63
1:D:19:ASN:HA	1:D:22:ALA:HB3	1.81	0.63
1:B:433:MET:HA	1:B:436:GLN:OE1	1.99	0.63
1:A:257:LYS:NZ	1:A:329:GLU:OE2	2.32	0.62
1:C:123:LEU:HD22	1:C:124:PRO:HD2	1.81	0.62
1:D:52:ALA:C	1:D:54:THR:N	2.49	0.62
1:A:201:LYS:NZ	1:A:352:ALA:O	2.20	0.62
1:C:91:TYR:CG	1:C:306:LYS:HE2	2.32	0.62
1:C:44:LEU:HD23	1:C:44:LEU:C	2.19	0.62
1:C:311:GLU:N	1:C:311:GLU:OE2	2.19	0.62
1:D:72:ALA:HB3	1:D:100:TYR:HE2	1.65	0.62
1:A:277:ALA:O	1:A:280:PHE:N	2.33	0.61
1:B:168:TYR:OH	1:B:171:LYS:NZ	2.26	0.61
1:C:245:VAL:HB	1:C:317:ARG:HA	1.82	0.61
1:B:335:PRO:C	1:B:337:MET:H	2.00	0.61
1:D:400:GLU:O	1:D:403:LYS:N	2.26	0.61
1:A:77:LEU:O	1:A:269:ALA:HB2	2.00	0.61
1:B:64:ALA:O	1:B:68:PHE:CD1	2.54	0.61
1:D:52:ALA:O	1:D:55:GLY:N	2.31	0.61
1:A:389:LYS:NZ	1:A:392:GLN:OE1	2.29	0.61
1:C:91:TYR:HA	1:C:306:LYS:NZ	2.14	0.61
1:B:100:TYR:O	1:B:102:GLY:N	2.34	0.61
1:B:79:GLU:OE1	1:B:103:LYS:CG	2.45	0.61
1:C:298:LYS:HD2	1:C:299:PRO:HD2	1.81	0.61
1:C:98:VAL:O	1:C:105:ILE:HG22	2.01	0.61
1:B:80:ILE:O	1:B:82:PRO:CD	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG3	1:D:258:PRO:HA	1.83	0.60
1:B:131:GLU:OE2	1:B:131:GLU:N	2.34	0.60
1:C:25:GLY:O	1:C:28:PHE:HB3	1.99	0.60
1:D:273:ASN:HB3	1:D:276:LEU:HB2	1.82	0.60
1:C:186:ASN:OD1	1:C:189:ALA:N	2.33	0.60
1:C:296:LYS:HE3	1:C:297:ASP:HB2	1.83	0.60
1:B:368:ASN:HD21	1:D:367:THR:HG21	1.65	0.60
1:C:65:HIS:CE1	1:C:97:ALA:HB1	2.36	0.60
1:D:219:ASN:HD21	1:D:235:ASN:HB3	1.66	0.60
1:B:87:GLN:HG2	1:B:87:GLN:O	2.01	0.60
1:A:77:LEU:HD12	1:A:105:ILE:HG23	1.83	0.60
1:D:411:ARG:HA	1:D:414:LYS:HE2	1.83	0.60
1:A:411:ARG:HA	1:A:414:LYS:HG3	1.84	0.59
1:A:5:GLU:HB2	1:A:273:ASN:CG	2.23	0.59
1:C:65:HIS:CD2	1:C:262:VAL:H	2.20	0.59
1:D:336:GLN:C	1:D:338:SER:H	2.05	0.59
1:A:11:TRP:HB2	1:A:61:ILE:HG22	1.84	0.59
1:D:285:LEU:O	1:D:291:LEU:HG	2.02	0.59
1:C:305:LEU:CD2	1:C:307:SER:OG	2.37	0.59
1:B:303:VAL:O	1:B:309:GLU:HB2	2.01	0.59
1:C:40:HIS:O	1:C:40:HIS:ND1	2.35	0.59
1:D:111:VAL:HG12	1:D:262:VAL:HG13	1.83	0.59
1:C:80:ILE:HG21	1:C:107:TYR:CZ	2.38	0.59
1:A:107:TYR:HE2	1:A:282:GLU:OE2	1.86	0.59
1:B:263:LEU:HD23	1:B:263:LEU:N	2.18	0.59
1:B:335:PRO:C	1:B:337:MET:N	2.56	0.59
1:C:119:ASN:HA	1:C:243:TYR:HA	1.84	0.59
1:D:15:ASP:N	1:D:15:ASP:OD1	2.31	0.58
1:A:273:ASN:HB3	1:A:276:LEU:HB2	1.85	0.58
1:A:423:LYS:NZ	1:A:433:MET:SD	2.76	0.58
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.38	0.58
1:A:6:GLY:H	1:A:273:ASN:HD21	1.49	0.58
1:D:434:LEU:C	1:D:436:GLN:H	2.05	0.58
1:B:98:VAL:O	1:B:98:VAL:HG12	2.03	0.58
1:A:10:ILE:HG21	1:A:21:LEU:HD23	1.84	0.58
1:D:16:LYS:NZ	1:D:63:TRP:CZ3	2.71	0.58
1:C:110:ALA:HA	1:C:303:VAL:HA	1.85	0.58
1:D:435:LEU:C	1:D:437:THR:H	2.05	0.58
1:B:13:ASN:HD21	1:B:15:ASP:CG	2.07	0.57
1:B:90:LEU:HG	1:B:305:LEU:HA	1.86	0.57
1:C:60:ILE:HG12	1:C:267:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HZ3	1:A:179:ILE:HG23	1.68	0.57
1:A:190:LYS:O	1:A:194:THR:HG23	2.05	0.57
1:A:194:THR:HG22	1:A:358:VAL:HG21	1.86	0.57
1:C:305:LEU:CD2	1:C:308:TYR:H	2.17	0.57
1:D:309:GLU:HA	1:D:312:LEU:CD1	2.33	0.57
1:A:117:ILE:HG23	1:A:245:VAL:HG12	1.86	0.57
1:C:86:PHE:CE2	1:C:282:GLU:HG2	2.39	0.57
1:D:433:MET:HE2	1:D:433:MET:N	2.19	0.57
1:D:117:ILE:HG12	1:D:245:VAL:HG12	1.87	0.57
1:A:28:PHE:CD2	1:A:32:THR:HG21	2.39	0.57
1:B:12:ILE:CG2	1:B:13:ASN:N	2.68	0.57
1:B:257:LYS:HB3	1:B:328:GLY:HA2	1.85	0.57
1:D:66:ASP:O	1:D:67:ARG:HG3	2.04	0.57
1:D:96:ASP:HA	1:D:99:ARG:HB3	1.86	0.57
1:B:11:TRP:C	1:B:61:ILE:HD11	2.25	0.57
1:C:407:ASN:HA	1:C:414:LYS:NZ	2.19	0.57
1:A:65:HIS:HE1	1:A:261:GLY:HA2	1.70	0.57
1:C:109:ILE:O	1:C:304:ALA:N	2.34	0.57
1:C:108:PRO:HA	1:C:264:SER:HA	1.87	0.57
1:A:32:THR:O	1:A:34:ILE:N	2.37	0.57
1:B:275:GLU:O	1:B:278:LYS:N	2.37	0.57
1:B:65:HIS:HE1	1:B:331:MET:CB	2.17	0.57
1:B:330:ILE:HD12	1:B:330:ILE:H	1.70	0.56
1:C:34:ILE:HG13	1:C:276:LEU:HD13	1.86	0.56
1:A:8:LEU:O	1:A:36:VAL:HA	2.04	0.56
1:A:81:THR:OG1	1:A:278:LYS:NZ	2.25	0.56
1:B:329:GLU:HG3	1:B:330:ILE:N	2.20	0.56
1:B:383:LEU:HD21	1:B:434:LEU:HD22	1.85	0.56
1:D:17:GLY:HA2	1:D:298:LYS:HE3	1.86	0.56
1:B:45:GLU:CG	1:B:67:ARG:HH12	2.16	0.56
1:B:76:LEU:O	1:B:269:ALA:HB2	2.06	0.56
1:C:90:LEU:HD22	1:C:304:ALA:C	2.26	0.56
1:A:118:TYR:CE1	1:A:126:PRO:HG3	2.41	0.56
1:A:6:GLY:O	1:A:34:ILE:HD12	2.05	0.56
1:C:141:LYS:O	1:C:144:GLY:N	2.39	0.56
1:D:172:TYR:N	1:D:172:TYR:CD1	2.73	0.56
1:B:12:ILE:CD1	1:B:62:PHE:CB	2.83	0.56
1:B:9:VAL:O	1:B:60:ILE:HG12	2.06	0.56
1:C:92:PRO:HD3	1:C:306:LYS:HZ3	1.68	0.56
1:D:308:TYR:CD2	1:D:312:LEU:HD11	2.40	0.56
1:B:390:LEU:H	1:B:390:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:HB3	1:B:262:VAL:O	2.06	0.56
1:C:119:ASN:HD21	1:C:122:LEU:HG	1.70	0.56
1:A:82:PRO:HG2	1:A:104:LEU:CD1	2.34	0.56
1:B:89:LYS:O	1:B:306:LYS:HG3	2.06	0.56
1:B:439:PHE:CE2	1:C:383:LEU:HD21	2.40	0.56
1:C:95:TRP:O	1:C:99:ARG:N	2.33	0.56
1:D:22:ALA:HB2	1:D:38:VAL:HG22	1.88	0.56
1:A:22:ALA:O	1:A:26:LYS:N	2.31	0.56
1:B:42:ASP:HB3	1:B:43:LYS:CE	2.36	0.56
1:B:90:LEU:C	1:B:306:LYS:HE3	2.27	0.55
1:B:186:ASN:OD1	1:B:188:GLY:N	2.28	0.55
1:D:434:LEU:O	1:D:436:GLN:N	2.39	0.55
1:D:52:ALA:CB	1:D:268:ASN:ND2	2.57	0.55
1:A:277:ALA:O	1:A:279:GLU:N	2.39	0.55
1:C:130:TRP:CD1	1:C:249:PRO:HB2	2.41	0.55
1:D:163:ALA:O	1:D:257:LYS:NZ	2.31	0.55
1:B:8:LEU:HD21	1:B:273:ASN:ND2	2.21	0.55
1:C:378:LEU:HD21	1:D:382:VAL:HG12	1.87	0.55
1:D:433:MET:O	1:D:433:MET:HG2	2.04	0.55
1:B:8:LEU:CD2	1:B:273:ASN:CB	2.78	0.55
1:B:179:ILE:CG1	1:B:334:ILE:HD12	2.33	0.55
1:B:90:LEU:HD23	1:B:304:ALA:HB3	1.88	0.54
1:C:143:LYS:H	1:C:143:LYS:NZ	2.05	0.54
1:C:90:LEU:HD22	1:C:304:ALA:O	2.07	0.54
1:B:434:LEU:HA	1:B:437:THR:HG22	1.89	0.54
1:C:50:GLN:HG3	1:C:423:LYS:CE	2.37	0.54
1:D:271:SER:OG	1:D:272:PRO:CD	2.55	0.54
1:D:312:LEU:H	1:D:312:LEU:HD12	1.72	0.54
1:B:292:GLU:OE2	1:B:296:LYS:HG3	2.08	0.54
1:C:109:ILE:N	1:C:109:ILE:HD12	2.22	0.54
1:C:21:LEU:HA	1:C:24:VAL:HG12	1.89	0.54
1:C:91:TYR:CZ	1:C:306:LYS:HG2	2.42	0.54
1:A:372:LEU:HD12	1:D:389:LYS:HG2	1.90	0.54
1:B:110:ALA:CB	1:B:263:LEU:HD21	2.34	0.54
1:B:160:PRO:HG3	1:B:258:PRO:HA	1.89	0.54
1:B:78:ALA:HB2	1:B:269:ALA:HA	1.88	0.54
1:B:99:ARG:HG3	1:B:99:ARG:O	2.08	0.54
1:C:308:TYR:HA	1:C:311:GLU:OE2	2.08	0.54
1:C:298:LYS:NZ	1:C:300:LEU:HD23	2.23	0.54
1:A:65:HIS:CE1	1:A:261:GLY:HA2	2.42	0.54
1:D:65:HIS:N	1:D:262:VAL:O	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:OD1	1:A:269:ALA:N	2.41	0.54
1:A:12:ILE:HG13	1:A:62:PHE:HB2	1.90	0.54
1:B:43:LYS:N	1:B:43:LYS:HE2	2.23	0.54
1:C:42:ASP:OD1	1:C:42:ASP:N	2.37	0.54
1:A:49:PRO:HA	1:A:76:LEU:CD1	2.36	0.53
1:B:31:ASP:OD1	1:B:284:TYR:OH	2.26	0.53
1:B:184:VAL:HG12	1:B:362:LEU:HD12	1.90	0.53
1:D:336:GLN:C	1:D:338:SER:N	2.61	0.53
1:B:206:ASN:OD1	1:B:208:ASP:N	2.22	0.53
1:A:394:ASN:OD1	1:A:403:LYS:NZ	2.42	0.53
1:B:71:TYR:CD1	1:B:71:TYR:N	2.75	0.53
1:C:232:ALA:O	1:C:236:ILE:HG13	2.09	0.53
1:B:65:HIS:HE1	1:B:260:VAL:O	1.87	0.53
1:B:79:GLU:OE1	1:B:103:LYS:CB	2.56	0.53
1:D:133:ILE:HA	1:D:136:LEU:HG	1.91	0.53
1:D:388:GLU:O	1:D:392:GLN:HG2	2.09	0.53
1:B:3:ILE:N	1:B:56:ASP:OD1	2.42	0.53
1:C:160:PRO:HG3	1:C:258:PRO:HA	1.91	0.53
1:D:433:MET:CE	1:D:433:MET:H	2.22	0.53
1:B:20:GLY:O	1:B:24:VAL:HG12	2.09	0.52
1:C:23:GLU:O	1:C:27:LYS:HG3	2.09	0.52
1:C:64:ALA:HA	1:C:263:LEU:HA	1.91	0.52
1:C:308:TYR:CG	1:C:308:TYR:O	2.62	0.52
1:D:268:ASN:OD1	1:D:269:ALA:N	2.42	0.52
1:A:60:ILE:HD13	1:A:281:LEU:HD11	1.90	0.52
1:B:99:ARG:NH1	1:B:99:ARG:CA	2.73	0.52
1:D:284:TYR:O	1:D:290:GLY:HA3	2.10	0.52
1:A:89:LYS:HZ3	1:A:307:SER:H	1.58	0.52
1:B:9:VAL:HG22	1:B:10:ILE:N	2.23	0.52
1:B:99:ARG:NH1	1:B:99:ARG:HB2	2.24	0.52
1:B:345:ARG:HH22	1:C:429:LYS:CD	2.22	0.52
1:C:89:LYS:NZ	1:C:305:LEU:HD11	2.24	0.52
1:C:89:LYS:O	1:C:306:LYS:CD	2.56	0.52
1:D:140:LEU:HD23	1:D:224:ALA:HB2	1.91	0.52
1:D:340:PHE:O	1:D:344:VAL:HG22	2.10	0.52
1:A:284:TYR:C	1:A:287:THR:HG23	2.26	0.52
1:B:48:PHE:HB3	1:B:49:PRO:HD3	1.91	0.52
1:C:430:VAL:HG22	1:C:432:GLU:H	1.74	0.52
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.91	0.52
1:A:176:LYS:HZ1	1:A:179:ILE:H	1.58	0.52
1:B:79:GLU:HG2	1:B:80:ILE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:VAL:HG23	1:D:320:ALA:HB3	1.91	0.52
1:D:25:GLY:O	1:D:30:LYS:HE3	2.09	0.52
1:B:45:GLU:CG	1:B:67:ARG:NH1	2.58	0.52
1:C:11:TRP:CE3	1:C:58:PRO:HD3	2.44	0.52
1:B:76:LEU:O	1:B:269:ALA:CB	2.58	0.52
1:B:286:LEU:O	1:B:305:LEU:CD1	2.55	0.52
1:C:419:VAL:HG23	1:C:422:MET:SD	2.50	0.52
1:D:24:VAL:HG23	1:D:28:PHE:CG	2.44	0.52
1:A:383:LEU:O	1:A:387:LEU:HD12	2.11	0.51
1:B:11:TRP:CA	1:B:61:ILE:CD1	2.66	0.51
1:D:119:ASN:ND2	1:D:122:LEU:HD23	2.26	0.51
1:D:81:THR:O	1:D:81:THR:HG23	2.10	0.51
1:A:81:THR:CB	1:A:278:LYS:HZ3	2.19	0.51
1:A:87:GLN:HG2	1:A:95:TRP:CE2	2.45	0.51
1:D:261:GLY:HA2	1:D:331:MET:HE3	1.92	0.51
1:A:288:ASP:OD1	1:A:307:SER:OG	2.27	0.51
1:C:184:VAL:HG21	1:C:344:VAL:HG22	1.91	0.51
1:D:41:PRO:HB2	1:D:47:LYS:NZ	2.26	0.51
1:D:433:MET:H	1:D:433:MET:HE2	1.75	0.51
1:A:278:LYS:O	1:A:282:GLU:CG	2.58	0.51
1:B:45:GLU:HB3	1:B:63:TRP:HE1	1.75	0.51
1:C:159:TRP:HZ3	1:C:184:VAL:HG23	1.75	0.51
1:C:90:LEU:HD23	1:C:305:LEU:HA	1.92	0.51
1:A:155:PRO:HD3	1:A:345:ARG:HB2	1.92	0.51
1:B:263:LEU:CD2	1:B:263:LEU:H	2.21	0.51
1:B:48:PHE:HA	1:B:51:VAL:CG1	2.39	0.51
1:B:322:MET:HG3	1:B:326:GLN:HE21	1.75	0.51
1:D:406:PHE:CE2	1:D:418:PHE:HB2	2.46	0.51
1:C:129:THR:HA	1:C:250:THR:H	1.76	0.51
1:B:103:LYS:N	1:B:103:LYS:CD	2.73	0.51
1:B:13:ASN:CG	1:B:15:ASP:H	2.14	0.51
1:B:370:VAL:O	1:B:374:VAL:HG13	2.11	0.51
1:A:389:LYS:CB	1:D:372:LEU:HD12	2.41	0.51
1:B:29:GLU:HA	1:B:32:THR:HG22	1.92	0.51
1:C:301:GLY:O	1:C:318:ILE:HD11	2.11	0.51
1:D:308:TYR:C	1:D:312:LEU:CD1	2.78	0.51
1:C:44:LEU:O	1:C:44:LEU:HG	2.10	0.50
1:D:48:PHE:CD1	1:D:48:PHE:C	2.85	0.50
1:B:434:LEU:HA	1:B:437:THR:CG2	2.42	0.50
1:C:311:GLU:CD	1:C:311:GLU:H	2.09	0.50
1:C:87:GLN:O	1:C:88:ASP:CB	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:CE2	1:A:120:LYS:HG2	2.46	0.50
1:A:398:LEU:HD12	1:A:398:LEU:C	2.30	0.50
1:D:405:LYS:NZ	1:D:420:ASP:OD2	2.43	0.50
1:A:68:PHE:HB3	1:A:105:ILE:HG21	1.93	0.50
1:B:331:MET:HG3	1:B:332:PRO:HD2	1.93	0.50
1:C:383:LEU:O	1:C:387:LEU:HD12	2.11	0.50
1:B:100:TYR:C	1:B:102:GLY:N	2.65	0.50
1:A:24:VAL:HG13	1:A:293:ALA:HB3	1.93	0.50
1:C:140:LEU:HA	1:C:143:LYS:CE	2.42	0.50
1:D:226:THR:HG22	1:D:227:ILE:H	1.76	0.50
1:D:419:VAL:HG12	1:D:419:VAL:O	2.12	0.50
1:D:435:LEU:C	1:D:437:THR:N	2.64	0.50
1:A:170:PHE:HB3	1:A:177:TYR:HB3	1.92	0.50
1:C:305:LEU:HD23	1:C:307:SER:N	2.27	0.50
1:C:343:ALA:HB2	1:C:369:ALA:HB2	1.93	0.50
1:B:9:VAL:HG23	1:B:37:THR:OG1	2.11	0.50
1:D:434:LEU:C	1:D:436:GLN:N	2.65	0.50
1:B:98:VAL:CG1	1:B:105:ILE:CG1	2.66	0.49
1:C:312:LEU:O	1:C:315:ASP:N	2.45	0.49
1:C:50:GLN:HG3	1:C:423:LYS:NZ	2.27	0.49
1:B:11:TRP:O	1:B:61:ILE:HD11	2.12	0.49
1:B:80:ILE:C	1:B:82:PRO:HD3	2.31	0.49
1:C:106:ALA:CB	1:C:266:GLY:HA2	2.36	0.49
1:C:48:PHE:HD2	1:C:71:TYR:CZ	2.30	0.49
1:D:138:LYS:O	1:D:139:GLU:C	2.48	0.49
1:D:52:ALA:HB1	1:D:268:ASN:HD21	1.72	0.49
1:B:59:ASP:HA	1:B:271:SER:HB2	1.95	0.49
1:A:28:PHE:CE1	1:A:280:PHE:HD1	2.30	0.49
1:A:232:ALA:O	1:A:236:ILE:HG13	2.12	0.49
1:B:387:LEU:HA	1:B:390:LEU:HD21	1.93	0.49
1:C:91:TYR:CA	1:C:306:LYS:CE	2.69	0.49
1:D:137:ASP:O	1:D:141:LYS:N	2.45	0.49
1:D:312:LEU:N	1:D:312:LEU:HD12	2.27	0.49
1:C:80:ILE:HG22	1:C:107:TYR:OH	2.12	0.49
1:A:305:LEU:HD21	1:A:307:SER:OG	2.12	0.49
1:C:98:VAL:HG13	1:C:105:ILE:CG2	2.36	0.49
1:D:47:LYS:N	1:D:49:PRO:HD3	2.28	0.49
1:D:52:ALA:O	1:D:54:THR:N	2.45	0.49
1:B:11:TRP:O	1:B:61:ILE:CD1	2.60	0.49
1:B:99:ARG:CZ	1:B:99:ARG:CB	2.85	0.49
1:A:440:SER:O	1:D:380:LYS:NZ	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:HB3	1:B:63:TRP:NE1	2.27	0.48
1:C:129:THR:HA	1:C:250:THR:N	2.28	0.48
1:C:333:ASN:OD1	1:C:333:ASN:O	2.31	0.48
1:D:51:VAL:O	1:D:56:ASP:C	2.51	0.48
1:B:345:ARG:NH2	1:C:395:VAL:O	2.46	0.48
1:C:158:THR:O	1:C:162:ILE:HG12	2.12	0.48
1:C:65:HIS:HD2	1:C:262:VAL:H	1.59	0.48
1:C:11:TRP:HA	1:C:39:GLU:O	2.13	0.48
1:A:171:LYS:O	1:A:178:ASP:N	2.37	0.48
1:B:8:LEU:O	1:B:36:VAL:HA	2.14	0.48
1:C:298:LYS:NZ	1:C:299:PRO:O	2.43	0.48
1:C:378:LEU:CD2	1:D:382:VAL:HG12	2.43	0.48
1:A:82:PRO:CG	1:A:104:LEU:HD12	2.43	0.48
1:A:60:ILE:HG12	1:A:267:ILE:HG13	1.95	0.48
1:B:11:TRP:CZ2	1:B:58:PRO:HD3	2.39	0.48
1:C:141:LYS:HD2	1:C:144:GLY:HA2	1.96	0.48
1:D:48:PHE:C	1:D:50:GLN:H	2.16	0.48
1:A:28:PHE:CZ	1:A:280:PHE:CD1	3.02	0.48
1:B:21:LEU:O	1:B:25:GLY:N	2.47	0.48
1:A:77:LEU:C	1:A:269:ALA:HB2	2.34	0.48
1:C:314:LYS:O	1:C:314:LYS:HD3	2.14	0.48
1:C:331:MET:SD	1:C:332:PRO:HD2	2.54	0.48
1:D:219:ASN:ND2	1:D:235:ASN:HB3	2.27	0.48
1:D:94:THR:HG22	1:D:111:VAL:HG11	1.96	0.48
1:B:99:ARG:NH1	1:B:99:ARG:CB	2.77	0.47
1:A:170:PHE:CB	1:A:177:TYR:HB3	2.43	0.47
1:B:79:GLU:CG	1:B:103:LYS:HB3	2.44	0.47
1:D:152:LEU:HD11	1:D:205:MET:SD	2.54	0.47
1:A:28:PHE:CE1	1:A:280:PHE:CD1	3.03	0.47
1:C:295:ASN:HA	1:C:298:LYS:O	2.14	0.47
1:D:433:MET:CE	1:D:433:MET:N	2.77	0.47
1:A:63:TRP:HA	1:A:63:TRP:CE3	2.50	0.47
1:C:53:ALA:HA	1:C:76:LEU:HD22	1.96	0.47
1:B:98:VAL:HG11	1:B:106:ALA:HB3	1.96	0.47
1:B:11:TRP:N	1:B:61:ILE:HD13	2.15	0.47
1:C:65:HIS:CE1	1:C:330:ILE:HG23	2.31	0.47
1:C:46:GLU:O	1:C:49:PRO:CG	2.61	0.47
1:C:86:PHE:CD2	1:C:282:GLU:HG2	2.50	0.47
1:A:154:GLU:HG3	1:A:156:TYR:H	1.80	0.47
1:C:245:VAL:HG12	1:C:320:ALA:HB3	1.96	0.47
1:D:274:LYS:O	1:D:278:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD13	1:A:108:PRO:HG2	1.97	0.47
1:B:59:ASP:O	1:B:267:ILE:HG22	2.15	0.47
1:A:80:ILE:HG22	1:A:82:PRO:HD3	1.97	0.47
1:B:178:ASP:N	1:B:334:ILE:HD11	2.30	0.47
1:C:193:LEU:HG	1:C:358:VAL:HG13	1.97	0.47
1:C:3:ILE:HG23	1:C:56:ASP:HA	1.97	0.47
1:B:9:VAL:O	1:B:10:ILE:HG13	2.13	0.47
1:A:440:SER:H	1:D:415:ARG:HH21	1.63	0.47
1:A:41:PRO:O	1:A:44:LEU:HB3	2.15	0.46
1:D:62:PHE:HB3	1:D:263:LEU:HD11	1.96	0.46
1:A:176:LYS:HZ1	1:A:179:ILE:N	2.12	0.46
1:A:90:LEU:HD13	1:A:108:PRO:CG	2.46	0.46
1:C:153:GLN:O	1:C:345:ARG:NH1	2.48	0.46
1:C:21:LEU:N	1:C:294:VAL:HG12	2.31	0.46
1:C:91:TYR:CG	1:C:306:LYS:CE	2.97	0.46
1:D:131:GLU:O	1:D:134:PRO:HD2	2.15	0.46
1:D:62:PHE:CE2	1:D:265:ALA:HB2	2.51	0.46
1:C:281:LEU:HA	1:C:285:LEU:HB3	1.97	0.46
1:D:65:HIS:CG	1:D:65:HIS:O	2.69	0.46
1:A:10:ILE:HD11	1:A:280:PHE:CE2	2.50	0.46
1:C:12:ILE:O	1:C:40:HIS:CB	2.64	0.46
1:A:10:ILE:HD11	1:A:280:PHE:HE2	1.80	0.46
1:B:86:PHE:HA	1:B:89:LYS:HZ2	1.80	0.46
1:B:8:LEU:HD21	1:B:273:ASN:CG	2.34	0.46
1:D:153:GLN:NE2	1:D:208:ASP:HA	2.31	0.46
1:D:411:ARG:HA	1:D:414:LYS:CE	2.46	0.46
1:B:98:VAL:HA	1:B:105:ILE:HD11	1.97	0.46
1:B:99:ARG:HH11	1:B:99:ARG:CA	2.29	0.46
1:C:16:LYS:HE2	1:C:263:LEU:HD13	1.98	0.46
1:C:90:LEU:HB2	1:C:95:TRP:HZ2	1.74	0.46
1:D:303:VAL:HG23	1:D:309:GLU:HB2	1.97	0.46
1:D:434:LEU:N	1:D:434:LEU:HD23	2.26	0.46
1:A:11:TRP:CD1	1:A:39:GLU:HB2	2.51	0.46
1:A:413:ASP:O	1:A:417:VAL:HG12	2.16	0.46
1:A:435:LEU:O	1:A:437:THR:N	2.49	0.46
1:A:48:PHE:CE2	1:A:61:ILE:HD13	2.51	0.46
1:B:150:PHE:CD1	1:B:227:ILE:HG13	2.51	0.46
1:C:208:ASP:OD1	1:C:208:ASP:N	2.39	0.46
1:D:72:ALA:HB3	1:D:100:TYR:CE2	2.46	0.46
1:C:389:LYS:NZ	1:D:371:ASP:OD2	2.44	0.46
1:B:335:PRO:O	1:B:337:MET:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD12	1:B:434:LEU:H	1.80	0.46
1:C:312:LEU:HB3	1:C:318:ILE:HD13	1.96	0.46
1:B:442:ASP:OD2	1:C:336:GLN:HG3	2.16	0.46
1:C:10:ILE:HG21	1:C:21:LEU:HD21	1.98	0.45
1:C:399:LYS:HZ2	1:C:401:GLU:HB2	1.81	0.45
1:B:344:VAL:O	1:B:348:VAL:HG23	2.16	0.45
1:B:437:THR:HG23	1:B:438:PHE:CD2	2.51	0.45
1:B:65:HIS:HD1	1:B:261:GLY:HA2	1.81	0.45
1:B:11:TRP:CH2	1:B:51:VAL:HG21	2.50	0.45
1:D:71:TYR:O	1:D:76:LEU:HB2	2.16	0.45
1:A:129:THR:HG23	1:A:132:GLU:H	1.81	0.45
1:B:236:ILE:HG21	1:B:236:ILE:HD13	1.76	0.45
1:B:89:LYS:O	1:B:305:LEU:CD2	2.63	0.45
1:D:141:LYS:HD3	1:D:141:LYS:HA	1.72	0.45
1:C:116:LEU:HD22	1:C:249:PRO:HG3	1.98	0.45
1:D:65:HIS:NE2	1:D:97:ALA:O	2.47	0.45
1:B:84:ALA:O	1:B:88:ASP:OD1	2.35	0.45
1:D:63:TRP:HA	1:D:63:TRP:CE3	2.51	0.45
1:A:101:ASN:C	1:A:103:LYS:HZ3	2.19	0.45
1:A:106:ALA:HA	1:A:265:ALA:O	2.17	0.45
1:A:398:LEU:C	1:A:398:LEU:CD1	2.85	0.45
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.49	0.45
1:C:26:LYS:O	1:C:29:GLU:HG2	2.17	0.45
1:C:363:ALA:O	1:C:367:THR:HG23	2.17	0.45
1:A:218:PHE:HE2	1:A:236:ILE:HD13	1.82	0.45
1:B:275:GLU:HA	1:B:278:LYS:HD3	1.99	0.45
1:D:97:ALA:HA	1:D:330:ILE:CG2	2.47	0.45
1:A:435:LEU:HB3	1:A:436:GLN:H	1.66	0.45
1:A:436:GLN:HB3	1:A:439:PHE:CD1	2.51	0.45
1:C:21:LEU:O	1:C:25:GLY:N	2.49	0.45
1:D:25:GLY:HA2	1:D:29:GLU:OE1	2.16	0.45
1:D:406:PHE:CZ	1:D:414:LYS:HG2	2.52	0.45
1:C:296:LYS:HD2	1:C:296:LYS:C	2.37	0.44
1:D:245:VAL:HG22	1:D:317:ARG:HB3	1.99	0.44
1:D:341:TRP:O	1:D:345:ARG:HB2	2.16	0.44
1:A:28:PHE:CZ	1:A:280:PHE:HD1	2.34	0.44
1:B:61:ILE:HD12	1:B:62:PHE:H	1.82	0.44
1:C:320:ALA:O	1:C:324:ASN:ND2	2.50	0.44
1:C:28:PHE:CE2	1:C:34:ILE:HB	2.53	0.44
1:D:48:PHE:O	1:D:48:PHE:CG	2.70	0.44
1:A:158:THR:O	1:A:162:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HG3	1:A:258:PRO:HA	1.98	0.44
1:A:77:LEU:O	1:A:269:ALA:CB	2.63	0.44
1:B:309:GLU:O	1:B:313:ALA:N	2.50	0.44
1:C:92:PRO:CD	1:C:306:LYS:NZ	2.75	0.44
1:A:10:ILE:HG21	1:A:21:LEU:CD2	2.46	0.44
1:D:118:TYR:O	1:D:243:TYR:HB2	2.18	0.44
1:D:52:ALA:C	1:D:55:GLY:H	2.21	0.44
1:A:236:ILE:O	1:A:239:SER:OG	2.28	0.44
1:B:97:ALA:HA	1:B:330:ILE:HG21	2.00	0.44
1:B:65:HIS:O	1:B:65:HIS:CG	2.70	0.44
1:C:399:LYS:NZ	1:C:401:GLU:HB2	2.33	0.44
1:D:16:LYS:N	1:D:16:LYS:HD2	2.33	0.44
1:D:418:PHE:CD1	1:D:418:PHE:C	2.91	0.44
1:A:7:LYS:CD	1:A:35:LYS:HE3	2.44	0.44
1:B:107:TYR:HB3	1:B:286:LEU:HD11	1.99	0.44
1:B:3:ILE:HG13	1:B:4:GLU:N	2.33	0.44
1:D:377:GLN:HA	1:D:380:LYS:HB2	1.98	0.44
1:A:184:VAL:HG11	1:A:344:VAL:HG22	2.00	0.44
1:A:60:ILE:CG2	1:A:265:ALA:HB1	2.48	0.44
1:B:182:VAL:HG13	1:B:340:PHE:HA	2.00	0.44
1:C:108:PRO:C	1:C:109:ILE:HD12	2.38	0.44
1:C:95:TRP:O	1:C:96:ASP:C	2.56	0.44
1:A:109:ILE:HG12	1:A:264:SER:HA	2.00	0.43
1:A:89:LYS:HZ1	1:A:307:SER:H	1.65	0.43
1:B:123:LEU:HD21	1:B:136:LEU:HD21	2.00	0.43
1:D:139:GLU:CD	1:D:139:GLU:N	2.71	0.43
1:D:402:ASP:OD2	1:D:421:ALA:HB2	2.18	0.43
1:A:176:LYS:HD2	1:A:177:TYR:N	2.32	0.43
1:A:90:LEU:HD12	1:A:95:TRP:CZ2	2.53	0.43
1:B:79:GLU:HG2	1:B:80:ILE:N	2.33	0.43
1:C:139:GLU:O	1:C:143:LYS:NZ	2.35	0.43
1:D:48:PHE:C	1:D:50:GLN:N	2.71	0.43
1:B:99:ARG:NH1	1:B:103:LYS:O	2.52	0.43
1:B:383:LEU:HD21	1:B:434:LEU:CD2	2.47	0.43
1:C:341:TRP:HZ3	1:C:342:TYR:CE1	2.35	0.43
1:C:376:GLU:O	1:C:380:LYS:HG3	2.17	0.43
1:C:43:LYS:H	1:C:43:LYS:HE2	1.83	0.43
1:C:63:TRP:O	1:C:264:SER:N	2.44	0.43
1:D:418:PHE:CD1	1:D:418:PHE:O	2.71	0.43
1:A:176:LYS:NZ	1:A:177:TYR:O	2.33	0.43
1:C:274:LYS:O	1:C:278:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:GLU:HG3	1:D:155:PRO:HD2	2.00	0.43
1:D:29:GLU:OE2	1:D:36:VAL:O	2.37	0.43
1:D:400:GLU:O	1:D:404:GLN:OE1	2.36	0.43
1:A:373:LYS:O	1:A:377:GLN:HG2	2.18	0.43
1:D:401:GLU:HA	1:D:404:GLN:CD	2.36	0.43
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.53	0.43
1:A:47:LYS:O	1:A:51:VAL:HG22	2.18	0.43
1:B:8:LEU:HD12	1:B:59:ASP:HB2	1.92	0.43
1:C:11:TRP:HB3	1:C:44:LEU:HD12	1.99	0.43
1:C:63:TRP:HD1	1:C:64:ALA:O	2.02	0.43
1:D:274:LYS:O	1:D:278:LYS:HG3	2.18	0.43
1:B:130:TRP:CD1	1:B:249:PRO:HB2	2.54	0.43
1:B:48:PHE:CA	1:B:51:VAL:HG12	2.45	0.43
1:C:377:GLN:HA	1:C:380:LYS:HG3	2.00	0.43
1:A:382:VAL:HG12	1:B:378:LEU:HD13	2.00	0.43
1:B:90:LEU:HD23	1:B:304:ALA:CB	2.49	0.43
1:C:246:THR:OG1	1:C:247:VAL:N	2.51	0.43
1:C:303:VAL:HG22	1:C:309:GLU:OE1	2.19	0.43
1:C:90:LEU:CB	1:C:95:TRP:CZ2	2.95	0.43
1:A:111:VAL:N	1:A:302:ALA:O	2.41	0.43
1:C:141:LYS:C	1:C:144:GLY:H	2.21	0.43
1:D:138:LYS:HD2	1:D:138:LYS:HA	1.61	0.43
1:D:26:LYS:O	1:D:26:LYS:HG2	2.19	0.43
1:B:133:ILE:HG13	1:B:134:PRO:HD3	2.01	0.43
1:B:7:LYS:HB2	1:B:35:LYS:O	2.19	0.43
1:C:92:PRO:CD	1:C:306:LYS:HZ3	2.30	0.43
1:D:336:GLN:O	1:D:338:SER:N	2.51	0.43
1:A:207:ALA:O	1:D:397:LYS:NZ	2.51	0.43
1:B:86:PHE:HA	1:B:89:LYS:NZ	2.34	0.42
1:D:18:TYR:HD1	1:D:19:ASN:N	2.14	0.42
1:D:29:GLU:OE1	1:D:35:LYS:HA	2.19	0.42
1:D:435:LEU:HD12	1:D:435:LEU:N	2.34	0.42
1:A:7:LYS:HD2	1:A:35:LYS:CG	2.48	0.42
1:B:267:ILE:HD11	1:B:281:LEU:HD12	2.01	0.42
1:B:64:ALA:HB1	1:B:66:ASP:OD1	2.19	0.42
1:D:96:ASP:N	1:D:96:ASP:OD1	2.52	0.42
1:A:106:ALA:CA	1:A:265:ALA:O	2.67	0.42
1:A:65:HIS:HB3	1:A:262:VAL:HG22	2.00	0.42
1:B:100:TYR:HB2	1:B:105:ILE:HG21	2.02	0.42
1:B:123:LEU:HA	1:B:123:LEU:HD12	1.94	0.42
1:B:21:LEU:HA	1:B:24:VAL:CG1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ASN:N	1:D:333:ASN:OD1	2.45	0.42
1:A:59:ASP:O	1:A:267:ILE:HA	2.19	0.42
1:A:278:LYS:O	1:A:282:GLU:HB2	2.19	0.42
1:A:98:VAL:HG21	1:A:106:ALA:HB3	2.01	0.42
1:D:142:ALA:O	1:D:144:GLY:N	2.52	0.42
1:B:193:LEU:O	1:B:197:VAL:HG13	2.19	0.42
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.71	0.42
1:D:142:ALA:C	1:D:144:GLY:H	2.22	0.42
1:A:21:LEU:HA	1:A:24:VAL:CG2	2.50	0.42
1:A:278:LYS:O	1:A:282:GLU:CB	2.67	0.42
1:A:32:THR:C	1:A:34:ILE:H	2.22	0.42
1:A:32:THR:C	1:A:34:ILE:N	2.73	0.42
1:A:78:ALA:HB2	1:A:269:ALA:HA	2.01	0.42
1:C:98:VAL:O	1:C:105:ILE:CG2	2.66	0.42
1:D:147:ALA:O	1:D:225:MET:HG2	2.19	0.42
1:A:80:ILE:HD11	1:A:105:ILE:O	2.20	0.42
1:B:147:ALA:O	1:B:225:MET:N	2.53	0.42
1:B:281:LEU:HA	1:B:285:LEU:HB3	2.00	0.42
1:C:308:TYR:C	1:C:311:GLU:OE2	2.58	0.42
1:A:63:TRP:HB3	1:A:68:PHE:CE1	2.54	0.42
1:C:298:LYS:HZ2	1:C:300:LEU:HD23	1.83	0.42
1:C:62:PHE:HZ	1:C:285:LEU:CD2	2.33	0.42
1:D:105:ILE:H	1:D:105:ILE:HG13	1.71	0.42
1:D:80:ILE:O	1:D:82:PRO:HD3	2.20	0.42
1:A:129:THR:OG1	1:A:131:GLU:OE1	2.38	0.42
1:B:435:LEU:O	1:B:439:PHE:HB2	2.19	0.42
1:D:151:ASN:OD1	1:D:210:ASP:HA	2.20	0.42
1:A:305:LEU:HD23	1:A:306:LYS:N	2.35	0.41
1:B:12:ILE:O	1:B:40:HIS:HA	2.19	0.41
1:B:128:LYS:O	1:B:250:THR:HG22	2.20	0.41
1:A:267:ILE:HG12	1:A:277:ALA:CB	2.50	0.41
1:A:400:GLU:HB2	1:A:401:GLU:HG3	2.01	0.41
1:B:155:PRO:HG3	1:B:345:ARG:HB2	2.01	0.41
1:B:110:ALA:HB1	1:B:302:ALA:O	2.21	0.41
1:B:110:ALA:CA	1:B:303:VAL:HA	2.46	0.41
1:B:355:ARG:HH21	1:C:397:LYS:NZ	2.18	0.41
1:C:76:LEU:O	1:C:77:LEU:HD12	2.19	0.41
1:C:90:LEU:CD2	1:C:305:LEU:HA	2.49	0.41
1:D:230:PRO:HA	1:D:233:TRP:CD2	2.54	0.41
1:A:108:PRO:O	1:A:286:LEU:HD21	2.20	0.41
1:B:12:ILE:CG2	1:B:13:ASN:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:O	1:C:40:HIS:HA	2.20	0.41
1:C:40:HIS:O	1:C:40:HIS:CG	2.72	0.41
1:D:73:GLN:HB2	1:D:100:TYR:OH	2.21	0.41
1:D:45:GLU:O	1:D:45:GLU:HG3	2.21	0.41
1:A:147:ALA:O	1:A:225:MET:N	2.54	0.41
1:D:292:GLU:O	1:D:295:ASN:N	2.52	0.41
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.95	0.41
1:C:153:GLN:HB3	1:C:345:ARG:HH12	1.85	0.41
1:D:12:ILE:HD12	1:D:62:PHE:HB2	2.02	0.41
1:A:129:THR:HG1	1:A:131:GLU:H	1.68	0.41
1:B:59:ASP:OD1	1:B:271:SER:HA	2.20	0.41
1:B:275:GLU:O	1:B:276:LEU:C	2.58	0.41
1:B:80:ILE:CD1	1:B:107:TYR:CE1	2.93	0.41
1:D:97:ALA:HA	1:D:330:ILE:HG21	2.02	0.41
1:B:116:LEU:HD22	1:B:249:PRO:HD3	2.02	0.41
1:B:118:TYR:CE1	1:B:126:PRO:HG3	2.56	0.41
1:C:391:VAL:HG12	1:C:403:LYS:HG3	2.03	0.41
1:C:50:GLN:HG3	1:C:423:LYS:HE3	2.02	0.41
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.21	0.41
1:D:153:GLN:HG3	1:D:210:ASP:HB3	2.03	0.41
1:D:377:GLN:HE22	1:D:380:LYS:CE	2.34	0.41
1:D:80:ILE:HD11	1:D:267:ILE:HG12	2.02	0.41
1:A:305:LEU:HD23	1:A:307:SER:N	2.36	0.41
1:B:3:ILE:HB	1:B:56:ASP:HA	2.03	0.41
1:C:4:GLU:OE1	1:C:7:LYS:N	2.44	0.41
1:D:179:ILE:HB	1:D:334:ILE:CD1	2.37	0.41
1:A:389:LYS:HE2	1:B:371:ASP:OD1	2.20	0.41
1:C:134:PRO:HG3	1:C:199:LEU:HD21	2.03	0.41
1:C:3:ILE:H	1:C:3:ILE:HG13	1.68	0.41
1:C:63:TRP:CD1	1:C:64:ALA:HB3	2.56	0.41
1:D:17:GLY:HA3	1:D:294:VAL:HG23	2.03	0.41
1:D:46:GLU:CG	1:D:416:TRP:HH2	2.34	0.41
1:B:110:ALA:HB2	1:B:303:VAL:HG12	2.03	0.41
1:C:81:THR:HG22	1:C:278:LYS:NZ	2.36	0.41
1:C:424:LYS:HD2	1:C:425:LYS:CB	2.42	0.41
1:C:91:TYR:CB	1:C:94:THR:CG2	2.87	0.41
1:D:294:VAL:HG13	1:D:300:LEU:HD11	2.03	0.41
1:D:331:MET:HG3	1:D:332:PRO:CD	2.40	0.41
1:D:414:LYS:HE2	1:D:414:LYS:HB2	1.71	0.41
1:A:246:THR:OG1	1:A:247:VAL:N	2.53	0.41
1:A:394:ASN:ND2	1:A:398:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HA	1:B:104:LEU:HD13	1.94	0.41
1:C:371:ASP:CG	1:D:389:LYS:HZ1	2.24	0.41
1:D:343:ALA:HB2	1:D:369:ALA:HB2	2.02	0.41
1:C:315:ASP:OD2	1:C:317:ARG:NH1	2.54	0.40
1:C:372:LEU:HD23	1:C:372:LEU:HA	1.92	0.40
1:D:71:TYR:HA	1:D:76:LEU:HD23	2.03	0.40
1:A:309:GLU:O	1:A:313:ALA:N	2.49	0.40
1:B:130:TRP:O	1:B:133:ILE:HG12	2.21	0.40
1:B:28:PHE:O	1:B:32:THR:HG22	2.21	0.40
1:C:268:ASN:OD1	1:C:269:ALA:N	2.53	0.40
1:B:107:TYR:O	1:B:264:SER:HA	2.21	0.40
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.57	0.40
1:B:280:PHE:O	1:B:284:TYR:HB2	2.20	0.40
1:B:7:LYS:HE3	1:B:37:THR:HG23	2.03	0.40
1:C:144:GLY:C	1:C:145:LYS:HE2	2.42	0.40
1:C:63:TRP:HD1	1:C:64:ALA:C	2.25	0.40
1:D:47:LYS:H	1:D:49:PRO:HD3	1.85	0.40
1:A:364:ALA:O	1:A:368:ASN:HB2	2.21	0.40
1:B:246:THR:OG1	1:B:247:VAL:N	2.55	0.40
1:C:130:TRP:HB3	1:C:195:PHE:CE2	2.56	0.40
1:C:155:PRO:HD2	1:C:341:TRP:CZ2	2.55	0.40
1:D:190:LYS:HD2	1:D:359:ASP:OD1	2.21	0.40
1:D:112:GLU:N	1:D:261:GLY:O	2.52	0.40
1:D:30:LYS:HA	1:D:30:LYS:HE2	2.04	0.40
1:D:314:LYS:HE2	1:D:314:LYS:HB3	1.92	0.40
1:A:178:ASP:HB3	1:A:181:ASP:HB3	2.02	0.40
1:D:388:GLU:O	1:D:391:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/462 (92%)	393 (93%)	26 (6%)	4 (1%)	17	46
1	B	393/462 (85%)	357 (91%)	32 (8%)	4 (1%)	15	44
1	C	411/462 (89%)	389 (95%)	19 (5%)	3 (1%)	22	53
1	D	409/462 (88%)	365 (89%)	36 (9%)	8 (2%)	7	24
All	All	1636/1848 (88%)	1504 (92%)	113 (7%)	19 (1%)	13	39

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	399	LYS
1	A	400	GLU
1	B	335	PRO
1	C	241	VAL
1	D	334	ILE
1	D	436	GLN
1	A	33	GLY
1	B	75	GLY
1	B	101	ASN
1	C	42	ASP
1	D	435	LEU
1	D	143	LYS
1	D	411	ARG
1	B	336	GLN
1	D	434	LEU
1	D	337	MET
1	C	88	ASP
1	D	48	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/373 (92%)	323 (94%)	19 (6%)	21	51
1	B	318/373 (85%)	296 (93%)	22 (7%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	338/373 (91%)	320 (95%)	18 (5%)	22	54
1	D	333/373 (89%)	303 (91%)	30 (9%)	9	28
All	All	1331/1492 (89%)	1242 (93%)	89 (7%)	16	43

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	31	ASP
1	A	103	LYS
1	A	172	TYR
1	A	256	SER
1	A	257	LYS
1	A	276	LEU
1	A	278	LYS
1	A	282	GLU
1	A	285	LEU
1	A	287	THR
1	A	333	ASN
1	A	372	LEU
1	A	387	LEU
1	A	398	LEU
1	A	399	LYS
1	A	400	GLU
1	A	401	GLU
1	A	423	LYS
1	B	8	LEU
1	B	10	ILE
1	B	12	ILE
1	B	26	LYS
1	B	61	ILE
1	B	63	TRP
1	B	65	HIS
1	B	66	ASP
1	B	67	ARG
1	B	68	PHE
1	B	76	LEU
1	B	88	ASP
1	B	99	ARG
1	B	100	TYR
1	B	103	LYS

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Mol	Chain	Res	Type
1	B	273	ASN
1	B	274	LYS
1	B	305	LEU
1	B	333	ASN
1	B	334	ILE
1	B	362	LEU
1	B	442	ASP
1	C	16	LYS
1	C	42	ASP
1	C	44	LEU
1	C	62	PHE
1	C	68	PHE
1	C	88	ASP
1	C	90	LEU
1	C	94	THR
1	C	105	ILE
1	C	145	LYS
1	C	263	LEU
1	C	292	GLU
1	C	296	LYS
1	C	336	GLN
1	C	340	PHE
1	C	394	ASN
1	C	424	LYS
1	C	433	MET
1	D	15	ASP
1	D	16	LYS
1	D	18	TYR
1	D	21	LEU
1	D	24	VAL
1	D	28	PHE
1	D	31	ASP
1	D	48	PHE
1	D	50	GLN
1	D	51	VAL
1	D	96	ASP
1	D	100	TYR
1	D	139	GLU
1	D	154	GLU
1	D	171	LYS
1	D	172	TYR
1	D	228	ASN

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Mol	Chain	Res	Type
1	D	310	GLU
1	D	311	GLU
1	D	333	ASN
1	D	334	ILE
1	D	336	GLN
1	D	337	MET
1	D	359	ASP
1	D	400	GLU
1	D	408	ASN
1	D	416	TRP
1	D	432	GLU
1	D	433	MET
1	D	434	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	B	65	HIS
1	B	326	GLN
1	B	333	ASN
1	C	65	HIS
1	C	73	GLN
1	C	356	GLN
1	C	377	GLN
1	D	50	GLN
1	D	228	ASN
1	D	377	GLN
1	D	408	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/462 (92%)	0.56	28 (6%) 18 11	54, 108, 184, 260	0
1	B	399/462 (86%)	1.23	92 (23%) 0 0	58, 114, 222, 270	0
1	C	419/462 (90%)	0.90	62 (14%) 2 1	58, 116, 221, 264	0
1	D	415/462 (89%)	0.86	59 (14%) 2 1	60, 115, 222, 331	0
All	All	1660/1848 (89%)	0.88	241 (14%) 2 1	54, 114, 220, 331	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	ASP	11.7
1	B	18	TYR	9.6
1	B	57	GLY	7.6
1	C	56	ASP	7.6
1	B	58	PRO	7.4
1	B	172	TYR	7.3
1	A	433	MET	7.0
1	D	26	LYS	7.0
1	B	74	SER	6.5
1	B	55	GLY	6.5
1	B	40	HIS	6.5
1	B	54	THR	6.4
1	B	71	TYR	6.2
1	C	182	VAL	6.1
1	D	19	ASN	6.1
1	C	183	GLY	6.1
1	D	337	MET	6.1
1	D	42	ASP	5.9
1	B	9	VAL	5.7
1	C	59	ASP	5.5
1	D	416	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	24	VAL	5.5
1	B	441	VAL	5.4
1	C	75	GLY	5.4
1	A	31	ASP	5.2
1	B	75	GLY	5.1
1	B	8	LEU	5.1
1	B	66	ASP	5.1
1	B	269	ALA	5.0
1	C	68	PHE	4.9
1	C	66	ASP	4.9
1	C	55	GLY	4.9
1	C	74	SER	4.7
1	B	67	ARG	4.7
1	B	274	LYS	4.7
1	B	168	TYR	4.7
1	C	336	GLN	4.7
1	D	57	GLY	4.7
1	B	334	ILE	4.7
1	D	333	ASN	4.6
1	B	56	ASP	4.6
1	D	223	THR	4.5
1	C	2	LYS	4.5
1	B	179	ILE	4.5
1	B	53	ALA	4.4
1	C	67	ARG	4.4
1	B	51	VAL	4.4
1	A	398	LEU	4.3
1	B	65	HIS	4.3
1	B	70	GLY	4.3
1	D	56	ASP	4.3
1	B	49	PRO	4.3
1	C	3	ILE	4.1
1	B	37	THR	4.1
1	B	170	PHE	4.1
1	B	169	ALA	4.1
1	D	40	HIS	4.1
1	B	17	GLY	4.1
1	B	178	ASP	4.0
1	B	68	PHE	4.0
1	B	77	LEU	4.0
1	B	3	ILE	4.0
1	C	65	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	266	GLY	3.9
1	B	69	GLY	3.8
1	D	335	PRO	3.8
1	B	267	ILE	3.8
1	D	18	TYR	3.7
1	D	28	PHE	3.7
1	B	167	GLY	3.6
1	C	69	GLY	3.6
1	B	41	PRO	3.6
1	D	222	GLU	3.6
1	B	180	LYS	3.6
1	D	64	ALA	3.6
1	C	58	PRO	3.5
1	B	271	SER	3.5
1	A	59	ASP	3.5
1	B	337	MET	3.5
1	C	333	ASN	3.5
1	B	36	VAL	3.5
1	C	144	GLY	3.4
1	D	224	ALA	3.4
1	B	183	GLY	3.4
1	B	336	GLN	3.4
1	D	33	GLY	3.4
1	C	105	ILE	3.4
1	D	31	ASP	3.4
1	B	73	GLN	3.3
1	D	334	ILE	3.3
1	D	118	TYR	3.3
1	D	119	ASN	3.3
1	B	11	TRP	3.3
1	D	67	ARG	3.2
1	D	71	TYR	3.2
1	C	138	LYS	3.2
1	B	39	GLU	3.2
1	D	41	PRO	3.2
1	D	80	ILE	3.2
1	B	50	GLN	3.1
1	B	16	LYS	3.1
1	D	68	PHE	3.1
1	D	65	HIS	3.1
1	B	332	PRO	3.1
1	C	57	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLN	3.1
1	B	335	PRO	3.0
1	A	412	SER	3.0
1	C	332	PRO	3.0
1	A	404	GLN	3.0
1	A	5	GLU	3.0
1	A	399	LYS	2.9
1	B	181	ASP	2.9
1	D	221	GLY	2.9
1	D	34	ILE	2.9
1	C	5	GLU	2.9
1	C	95	TRP	2.9
1	A	54	THR	2.9
1	B	44	LEU	2.9
1	C	34	ILE	2.8
1	D	30	LYS	2.8
1	C	270	ALA	2.8
1	D	37	THR	2.8
1	C	28	PHE	2.8
1	B	185	ASP	2.8
1	C	88	ASP	2.8
1	A	8	LEU	2.8
1	A	269	ALA	2.8
1	B	60	ILE	2.8
1	C	100	TYR	2.8
1	D	21	LEU	2.7
1	A	32	THR	2.7
1	C	416	TRP	2.7
1	B	59	ASP	2.7
1	B	338	SER	2.7
1	B	432	GLU	2.7
1	A	76	LEU	2.7
1	A	78	ALA	2.7
1	B	440	SER	2.7
1	D	52	ALA	2.7
1	B	443	PRO	2.7
1	B	270	ALA	2.7
1	D	17	GLY	2.7
1	B	171	LYS	2.6
1	C	42	ASP	2.6
1	A	406	PHE	2.6
1	C	89	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	143	LYS	2.6
1	B	286	LEU	2.6
1	C	9	VAL	2.6
1	B	108	PRO	2.6
1	C	44	LEU	2.6
1	D	66	ASP	2.6
1	D	76	LEU	2.6
1	B	102	GLY	2.6
1	C	71	TYR	2.6
1	D	45	GLU	2.6
1	D	44	LEU	2.6
1	B	5	GLU	2.6
1	D	39	GLU	2.6
1	B	52	ALA	2.6
1	D	35	LYS	2.6
1	D	405	LYS	2.5
1	C	142	ALA	2.5
1	D	51	VAL	2.5
1	D	29	GLU	2.5
1	B	42	ASP	2.5
1	D	81	THR	2.5
1	B	166	GLY	2.5
1	D	22	ALA	2.5
1	A	177	TYR	2.5
1	D	20	GLY	2.5
1	D	209	THR	2.4
1	A	405	LYS	2.4
1	A	279	GLU	2.4
1	D	208	ASP	2.4
1	B	45	GLU	2.4
1	B	107	TYR	2.4
1	B	19	ASN	2.4
1	C	13	ASN	2.4
1	C	47	LYS	2.4
1	C	21	LEU	2.4
1	B	61	ILE	2.4
1	B	328	GLY	2.3
1	D	54	THR	2.3
1	B	48	PHE	2.3
1	C	221	GLY	2.3
1	A	98	VAL	2.3
1	C	41	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	332	PRO	2.3
1	D	82	PRO	2.3
1	B	164	ALA	2.3
1	C	77	LEU	2.3
1	C	342	TYR	2.3
1	B	439	PHE	2.3
1	C	318	ILE	2.3
1	D	12	ILE	2.3
1	B	47	LYS	2.2
1	C	302	ALA	2.2
1	B	31	ASP	2.2
1	A	99	ARG	2.2
1	C	338	SER	2.2
1	C	184	VAL	2.2
1	B	188	GLY	2.2
1	A	332	PRO	2.2
1	C	85	ALA	2.2
1	D	331	MET	2.2
1	D	72	ALA	2.2
1	C	241	VAL	2.2
1	B	46	GLU	2.2
1	A	414	LYS	2.2
1	C	11	TRP	2.2
1	B	311	GLU	2.2
1	D	25	GLY	2.2
1	A	359	ASP	2.2
1	B	22	ALA	2.2
1	B	308	TYR	2.2
1	C	136	LEU	2.1
1	B	72	ALA	2.1
1	B	339	ALA	2.1
1	D	78	ALA	2.1
1	C	4	GLU	2.1
1	B	91	TYR	2.1
1	A	407	ASN	2.1
1	D	55	GLY	2.1
1	A	77	LEU	2.1
1	C	18	TYR	2.1
1	B	333	ASN	2.1
1	C	99	ARG	2.1
1	A	60	ILE	2.1
1	A	106	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	2.1
1	C	274	LYS	2.1
1	C	423	LYS	2.1
1	C	346	THR	2.1
1	B	431	GLY	2.0
1	B	103	LYS	2.0
1	D	336	GLN	2.0
1	A	108	PRO	2.0
1	D	283	ASN	2.0
1	C	37	THR	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.