Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 12:39 PM EDT

PDB ID	:	1ULQ
Title	:	Crystal structure of tt0182 from Thermus thermophilus HB8
Authors	:	Ago, H.; Hamada, K.; Ida, K.; Kanda, H.; Sugahara, M.; Yamamoto, M.; Kuroishi, C.; Kuramitsu, S.; Yokoyama, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-09-16
Resolution	:	3.00 Å(reported)

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

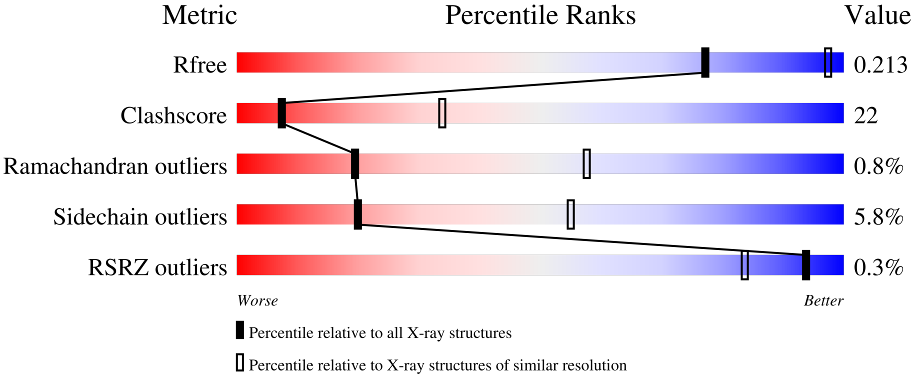
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	401	
1	B	401	
1	C	401	
1	D	401	
1	E	401	

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Mol	Chain	Length	Quality of chain
1	F	401	
1	G	401	
1	H	401	

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 23907 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 putative acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total 2984	C 1867	N 546	O 556	S 15	0	0	0
1	B	398	Total 2984	C 1867	N 546	O 556	S 15	0	0	0
1	C	399	Total 2991	C 1872	N 547	O 557	S 15	0	0	0
1	D	399	Total 2991	C 1872	N 547	O 557	S 15	0	0	0
1	E	399	Total 2991	C 1872	N 547	O 557	S 15	0	0	0
1	F	398	Total 2984	C 1867	N 546	O 556	S 15	0	0	0
1	G	399	Total 2991	C 1872	N 547	O 557	S 15	0	0	0
1	H	399	Total 2991	C 1872	N 547	O 557	S 15	0	0	0

3 Residue-property plots ⓘ

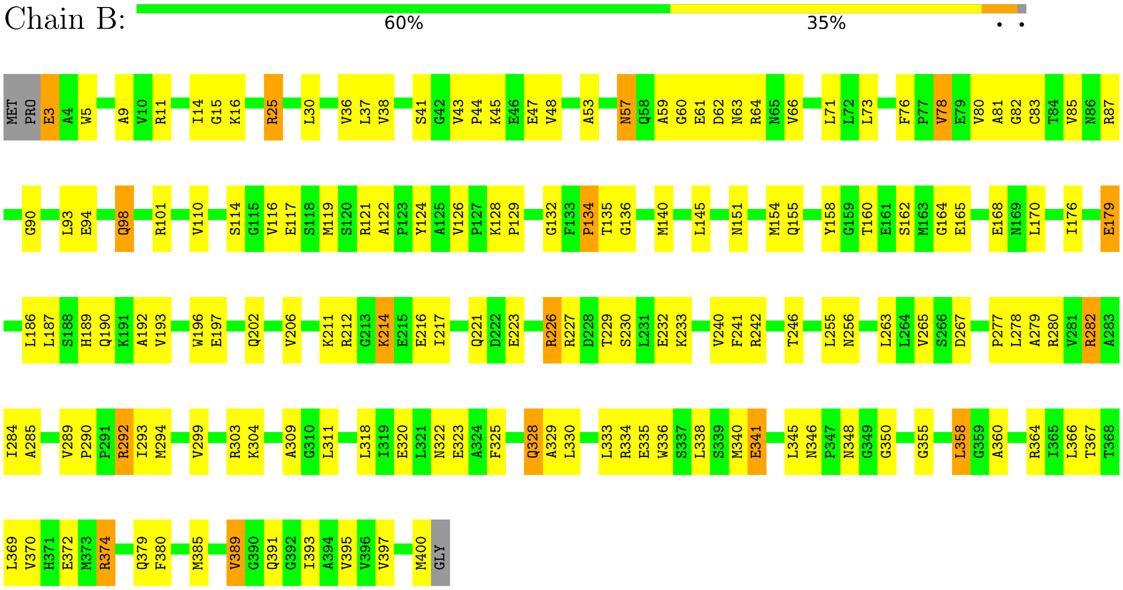
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: putative acetyl-CoA acetyltransferase

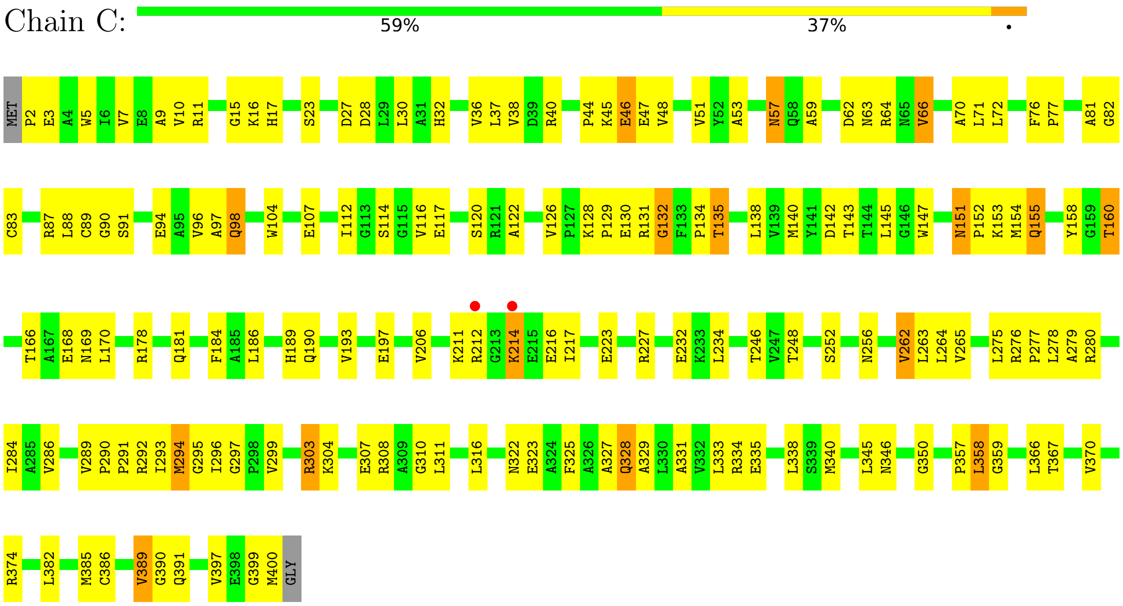
Chain A:

- Molecule 1: putative acetyl-CoA acetyltransferase

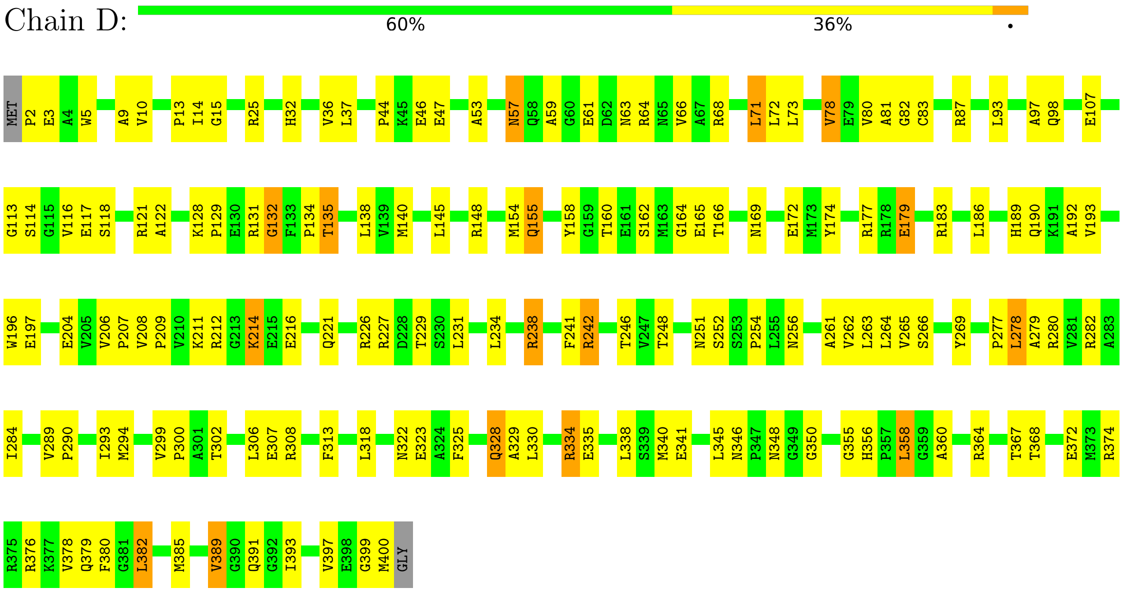
Chain B:



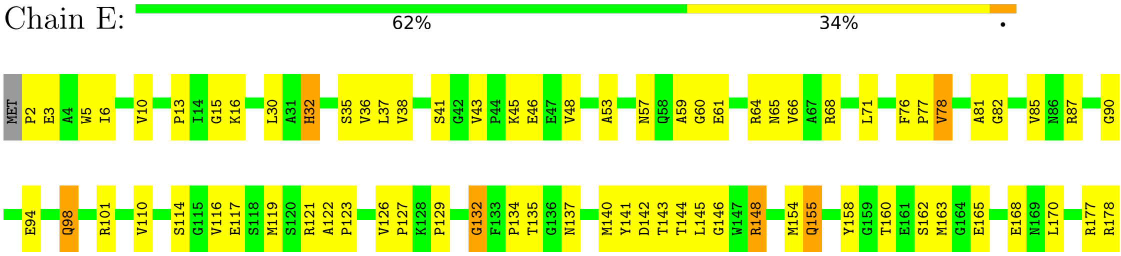
- Molecule 1: putative acetyl-CoA acetyltransferase

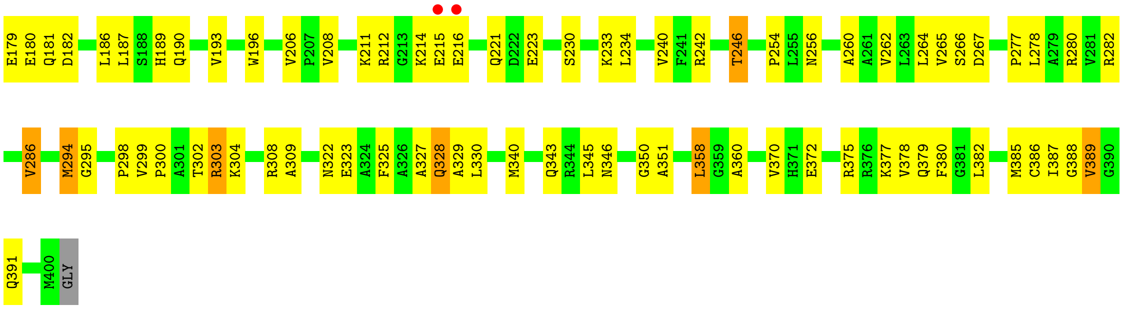


- Molecule 1: putative acetyl-CoA acetyltransferase

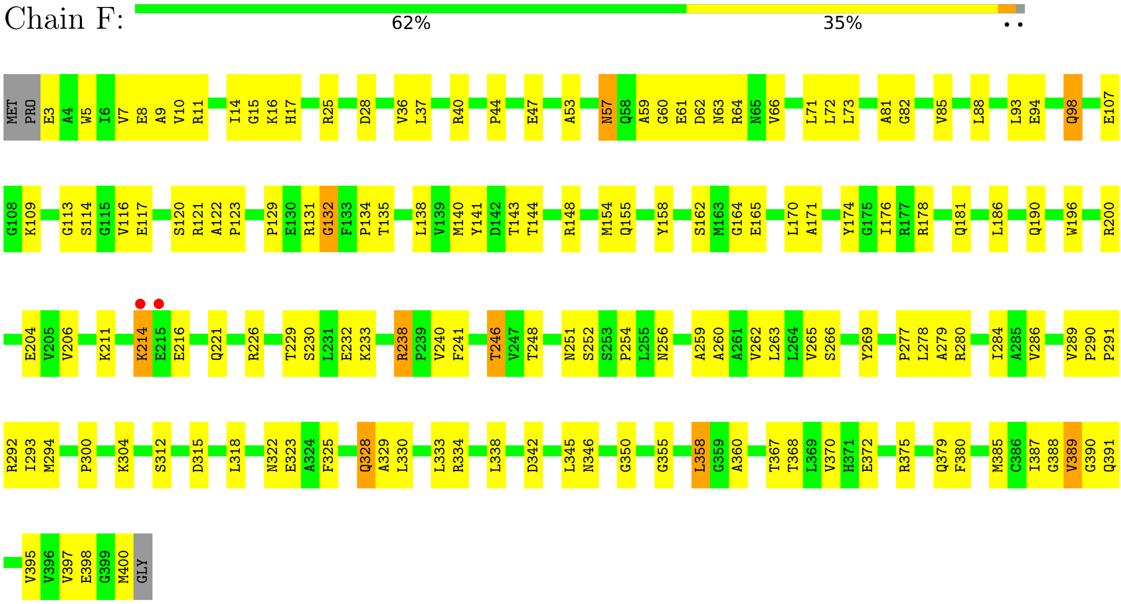


- Molecule 1: putative acetyl-CoA acetyltransferase

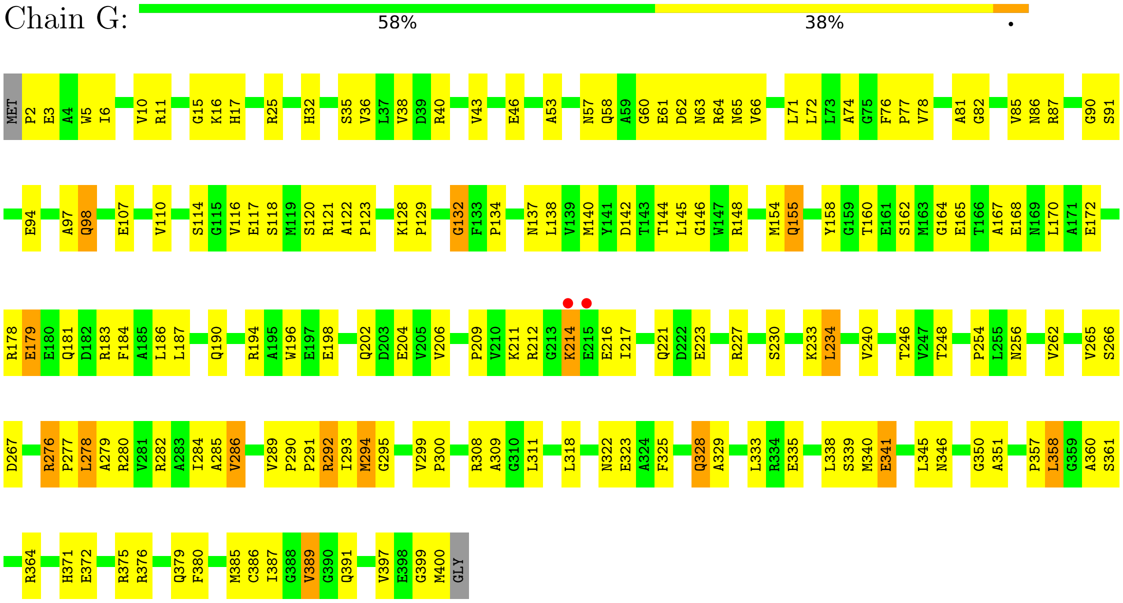




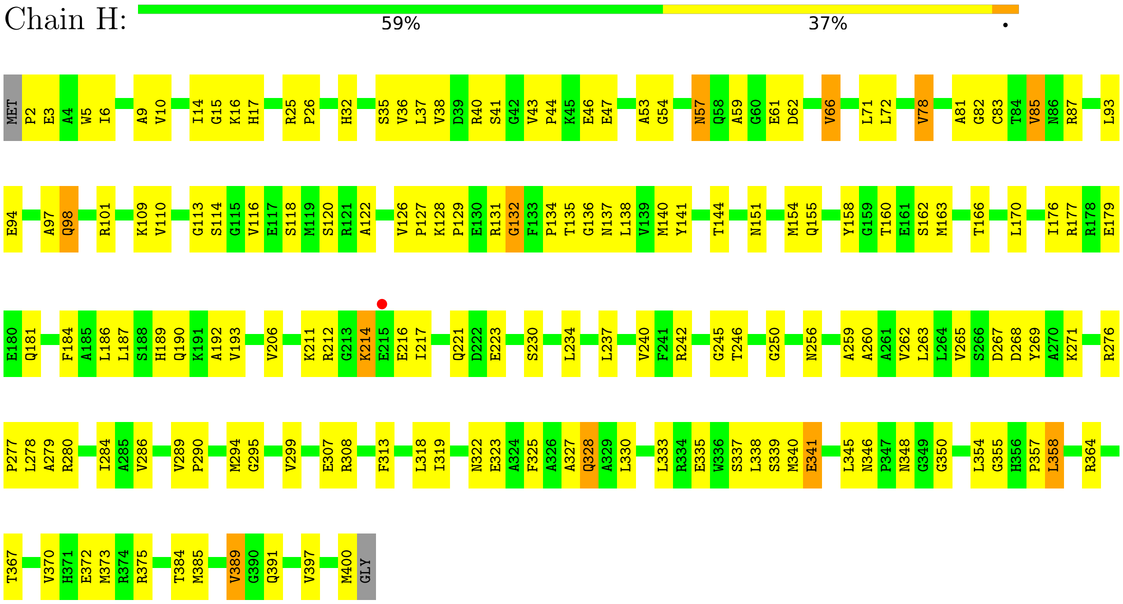
- Molecule 1: putative acetyl-CoA acetyltransferase



- Molecule 1: putative acetyl-CoA acetyltransferase



• Molecule 1: putative acetyl-CoA acetyltransferase



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.17Å 88.87Å 164.87Å 90.00° 100.45° 90.00°	Depositor
Resolution (Å)	48.50 – 3.00 48.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (48.50-3.00) 93.7 (48.52-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.275 0.219 , 0.213	Depositor DCC
R_{free} test set	3685 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23907	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2880e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.40	0/3036	0.66	0/4114
1	B	0.41	0/3036	0.69	0/4114
1	C	0.40	0/3044	0.66	0/4125
1	D	0.40	0/3044	0.66	0/4125
1	E	0.39	0/3044	0.66	0/4125
1	F	0.41	0/3036	0.67	0/4114
1	G	0.38	0/3044	0.66	0/4125
1	H	0.40	0/3044	0.67	0/4125
All	All	0.40	0/24328	0.67	0/32967

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 ⓘ

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	2984	0	3007	151	0
1	B	2984	0	3007	157	0
1	C	2991	0	3015	151	0
1	D	2991	0	3015	151	0
1	E	2991	0	3015	128	0
1	F	2984	0	3007	149	0
1	G	2991	0	3015	159	0
1	H	2991	0	3015	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23907	0	24096	1068	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 22.

All (1068) 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:F:129:PRO:HG2	1:H:129:PRO:HG2	1.18	1.15
1:H:36:VAL:HG11	1:H:206:VAL:HG11	1.25	1.10
1:G:2:PRO:HB2	1:G:5:TRP:HE1	1.17	1.09
1:A:36:VAL:HG21	1:A:206:VAL:HG21	1.37	1.06
1:B:129:PRO:HG2	1:D:129:PRO:HG2	1.09	1.06
1:A:212:ARG:HD2	1:A:217:ILE:HD12	1.35	1.05
1:F:174:TYR:HB2	1:F:176:ILE:HD11	1.41	1.03
1:G:214:LYS:H	1:G:214:LYS:HD3	1.20	1.03
1:F:36:VAL:HG21	1:F:206:VAL:HG21	1.42	1.01
1:B:374:ARG:HH11	1:B:374:ARG:HG3	1.28	0.98
1:G:36:VAL:HG21	1:G:206:VAL:HG21	1.45	0.98
1:H:2:PRO:HB2	1:H:5:TRP:HE1	1.25	0.97
1:E:36:VAL:HG21	1:E:206:VAL:HG21	1.49	0.95
1:H:280:ARG:HB2	1:H:400:MET:HE2	1.49	0.93
1:G:391:GLN:NE2	1:H:82:GLY:H	1.67	0.93
1:B:36:VAL:HG21	1:B:206:VAL:HG21	1.51	0.93
1:C:278:LEU:HG	1:C:370:VAL:HG12	1.50	0.92
1:A:391:GLN:NE2	1:B:82:GLY:H	1.67	0.92
1:D:2:PRO:HB3	1:D:280:ARG:HD2	1.49	0.91
1:G:230:SER:HB3	1:G:233:LYS:HG3	1.53	0.91
1:C:214:LYS:H	1:C:214:LYS:HD3	1.32	0.90
1:F:338:LEU:HD11	1:F:342:ASP:OD2	1.70	0.90
1:E:82:GLY:H	1:F:391:GLN:NE2	1.72	0.88
1:C:2:PRO:HB3	1:C:5:TRP:HE1	1.39	0.87
1:A:214:LYS:H	1:A:214:LYS:HD3	1.39	0.86
1:B:278:LEU:HD12	1:B:374:ARG:NH2	1.90	0.86
1:A:290:PRO:HA	1:B:78:VAL:HG21	1.57	0.85
1:E:2:PRO:O	1:E:267:ASP:HB3	1.76	0.85
1:B:44:PRO:HG2	1:B:47:GLU:HG2	1.58	0.85
1:A:212:ARG:HD2	1:A:217:ILE:CD1	2.07	0.84
1:B:129:PRO:HG2	1:D:129:PRO:CG	2.03	0.84
1:E:16:LYS:HG3	1:E:223:GLU:HG3	1.57	0.84
1:D:162:SER:OG	1:D:165:GLU:HG3	1.76	0.84

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G:391:GLN:HE22	1:H:82:GLY:H	1.25	0.83
1:C:16:LYS:HG3	1:C:223:GLU:HG3	1.58	0.83
1:F:230:SER:HB3	1:F:233:LYS:HG3	1.60	0.83
1:E:110:VAL:HG22	1:E:265:VAL:HG12	1.59	0.83
1:A:36:VAL:CG2	1:A:206:VAL:HG21	2.08	0.82
1:C:36:VAL:HG21	1:C:206:VAL:HG21	1.62	0.82
1:B:63:ASN:OD1	1:B:64:ARG:HG3	1.79	0.82
1:C:366:LEU:O	1:C:370:VAL:HG23	1.80	0.81
1:D:2:PRO:CB	1:D:280:ARG:HD2	2.10	0.81
1:F:211:LYS:HD2	1:F:216:GLU:HG2	1.61	0.81
1:C:186:LEU:O	1:C:190:GLN:HG3	1.79	0.81
1:B:336:TRP:HB3	1:B:338:LEU:HD13	1.62	0.81
1:E:2:PRO:CB	1:E:5:TRP:HE1	1.93	0.80
1:A:44:PRO:HG2	1:A:47:GLU:HG2	1.62	0.79
1:E:82:GLY:H	1:F:391:GLN:HE22	1.28	0.79
1:B:212:ARG:HD2	1:B:217:ILE:CD1	2.11	0.79
1:D:211:LYS:HD2	1:D:216:GLU:HG2	1.64	0.79
1:D:36:VAL:HG21	1:D:206:VAL:HG21	1.65	0.79
1:H:26:PRO:HG3	1:H:118:SER:HB3	1.65	0.79
1:B:16:LYS:HG3	1:B:223:GLU:HG3	1.63	0.79
1:C:214:LYS:HD3	1:C:214:LYS:N	1.96	0.79
1:F:129:PRO:HG2	1:H:129:PRO:CG	2.09	0.78
1:F:129:PRO:CG	1:H:129:PRO:HG2	2.09	0.78
1:D:9:ALA:HB1	1:D:367:THR:HG23	1.66	0.78
1:E:2:PRO:HB2	1:E:5:TRP:HE1	1.48	0.78
1:A:278:LEU:HG	1:A:370:VAL:HG12	1.67	0.77
1:D:323:GLU:CD	1:D:350:GLY:HA3	2.05	0.77
1:A:214:LYS:HD3	1:A:214:LYS:N	2.00	0.77
1:G:214:LYS:HD3	1:G:214:LYS:N	1.99	0.77
1:D:117:GLU:HG2	1:D:358:LEU:HB2	1.66	0.77
1:B:129:PRO:CG	1:D:129:PRO:HG2	2.03	0.77
1:G:32:HIS:O	1:G:36:VAL:HG23	1.85	0.77
1:E:129:PRO:CG	1:G:129:PRO:HG2	2.14	0.77
1:H:2:PRO:CB	1:H:5:TRP:HE1	1.98	0.77
1:D:44:PRO:HG2	1:D:47:GLU:HG2	1.67	0.76
1:D:238:ARG:CD	1:D:238:ARG:H	1.94	0.76
1:C:166:THR:HA	1:C:169:ASN:HD22	1.50	0.76
1:B:212:ARG:HD2	1:B:217:ILE:HD12	1.67	0.76
1:A:323:GLU:CD	1:A:350:GLY:HA3	2.06	0.75
1:D:238:ARG:H	1:D:238:ARG:HD2	1.51	0.75
1:H:372:GLU:OE1	1:H:375:ARG:HD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HG3	1:A:229:THR:OG1	1.87	0.75
1:D:131:ARG:HH12	1:D:135:THR:HG23	1.50	0.74
1:H:265:VAL:HG21	1:H:269:TYR:CD2	2.22	0.74
1:D:313:PHE:HE2	1:D:338:LEU:HD11	1.51	0.74
1:D:71:LEU:HD23	1:D:72:LEU:N	2.02	0.74
1:B:226:ARG:HH12	1:B:229:THR:HG23	1.53	0.73
1:F:214:LYS:HD3	1:F:214:LYS:N	2.03	0.73
1:G:16:LYS:HG3	1:G:223:GLU:HG3	1.70	0.73
1:A:155:GLN:HE21	1:A:160:THR:HG23	1.54	0.73
1:B:140:MET:HE3	1:C:138:LEU:HB2	1.70	0.73
1:A:183:ARG:HG3	1:A:340:MET:HE1	1.69	0.73
1:E:90:GLY:HA2	1:E:385:MET:CE	2.19	0.73
1:G:82:GLY:H	1:H:391:GLN:NE2	1.87	0.73
1:F:284:ILE:HG23	1:F:395:VAL:HG22	1.71	0.72
1:A:391:GLN:HE22	1:B:82:GLY:H	1.33	0.72
1:B:214:LYS:HD3	1:B:214:LYS:N	2.05	0.72
1:F:9:ALA:HB1	1:F:367:THR:HG23	1.71	0.72
1:A:122:ALA:O	1:B:128:LYS:HE2	1.89	0.72
1:D:279:ALA:HB1	1:D:397:VAL:CG1	2.19	0.72
1:G:36:VAL:CG2	1:G:206:VAL:HG21	2.19	0.72
1:H:318:LEU:HD23	1:H:373:MET:HG3	1.72	0.72
1:B:211:LYS:HG2	1:B:216:GLU:HG2	1.72	0.72
1:D:214:LYS:N	1:D:214:LYS:HD3	2.05	0.72
1:B:278:LEU:HD12	1:B:374:ARG:HH21	1.55	0.71
1:B:186:LEU:O	1:B:190:GLN:HG3	1.91	0.71
1:E:186:LEU:O	1:E:190:GLN:HG3	1.90	0.71
1:C:278:LEU:HD13	1:C:374:ARG:CZ	2.21	0.71
1:H:330:LEU:HD23	1:H:333:LEU:HD12	1.71	0.71
1:A:5:TRP:CE3	1:A:277:PRO:HG3	2.26	0.71
1:E:129:PRO:HG3	1:G:129:PRO:HG2	1.72	0.71
1:B:374:ARG:HG3	1:B:374:ARG:NH1	2.00	0.71
1:H:36:VAL:CG1	1:H:206:VAL:HG11	2.13	0.70
1:E:81:ALA:HB1	1:F:391:GLN:HE21	1.55	0.70
1:C:7:VAL:HG11	1:C:275:LEU:HB3	1.71	0.70
1:F:174:TYR:HB2	1:F:176:ILE:CD1	2.21	0.70
1:E:2:PRO:HG3	1:E:280:ARG:NH2	2.06	0.70
1:B:30:LEU:HD23	1:B:66:VAL:HG12	1.74	0.70
1:G:187:LEU:HD12	1:G:340:MET:HE3	1.73	0.70
1:F:254:PRO:HG2	1:F:256:ASN:OD1	1.91	0.69
1:C:391:GLN:NE2	1:D:82:GLY:H	1.90	0.69
1:F:171:ALA:HA	1:F:176:ILE:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HD2	1:B:122:ALA:O	1.92	0.69
1:H:26:PRO:HG3	1:H:118:SER:CB	2.21	0.69
1:H:16:LYS:HG3	1:H:223:GLU:HG3	1.74	0.69
1:C:328:GLN:HG3	1:C:329:ALA:N	2.07	0.69
1:C:323:GLU:CD	1:C:350:GLY:HA3	2.13	0.69
1:F:116:VAL:HG23	1:F:259:ALA:HB2	1.74	0.69
1:H:36:VAL:O	1:H:40:ARG:HG3	1.93	0.69
1:H:126:VAL:HG22	1:H:140:MET:HG2	1.74	0.68
1:C:90:GLY:HA2	1:C:385:MET:CE	2.24	0.68
1:F:62:ASP:O	1:F:66:VAL:HG22	1.92	0.68
1:H:299:VAL:HG21	1:H:335:GLU:HG3	1.74	0.68
1:D:209:PRO:HB2	1:D:216:GLU:OE1	1.94	0.68
1:C:38:VAL:HG11	1:C:45:LYS:HG3	1.74	0.67
1:F:323:GLU:CD	1:F:350:GLY:HA3	2.14	0.67
1:E:101:ARG:HH12	1:F:107:GLU:CD	1.98	0.67
1:G:85:VAL:HG11	1:G:94:GLU:HG3	1.77	0.67
1:C:126:VAL:HG22	1:C:140:MET:HG2	1.77	0.67
1:G:186:LEU:O	1:G:190:GLN:HG3	1.94	0.67
1:B:44:PRO:HG2	1:B:47:GLU:CG	2.25	0.67
1:C:87:ARG:HH11	1:C:391:GLN:NE2	1.93	0.67
1:B:292:ARG:HD3	1:B:293:ILE:HG23	1.77	0.67
1:E:15:GLY:O	1:E:256:ASN:HB3	1.95	0.67
1:G:279:ALA:HB1	1:G:397:VAL:HG13	1.76	0.67
1:A:322:ASN:HB2	1:A:385:MET:HG2	1.76	0.67
1:A:391:GLN:HE21	1:B:81:ALA:HB1	1.59	0.66
1:A:186:LEU:O	1:A:190:GLN:HG3	1.94	0.66
1:B:25:ARG:HB3	1:B:61:GLU:OE2	1.95	0.66
1:D:186:LEU:O	1:D:190:GLN:HG3	1.94	0.66
1:E:181:GLN:OE1	1:E:327:ALA:HB2	1.95	0.66
1:F:63:ASN:OD1	1:F:64:ARG:HG3	1.95	0.66
1:E:389:VAL:HG12	1:E:389:VAL:O	1.94	0.66
1:B:279:ALA:HB1	1:B:397:VAL:CG1	2.25	0.66
1:E:278:LEU:HG	1:E:370:VAL:HG13	1.78	0.66
1:A:107:GLU:CD	1:B:101:ARG:HH21	1.99	0.66
1:E:189:HIS:O	1:E:193:VAL:HG23	1.96	0.66
1:H:2:PRO:HB2	1:H:5:TRP:NE1	2.06	0.66
1:B:189:HIS:O	1:B:193:VAL:HG23	1.94	0.66
1:G:15:GLY:O	1:G:256:ASN:HB3	1.96	0.66
1:F:265:VAL:HG21	1:F:269:TYR:CD2	2.30	0.66
1:H:5:TRP:CE3	1:H:277:PRO:HG3	2.31	0.66
1:A:71:LEU:HD12	1:A:72:LEU:N	2.11	0.66

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:C:82:GLY:H	1:D:391:GLN:NE2	1.93	0.65
1:C:98:GLN:HG3	1:D:98:GLN:NE2	2.11	0.65
1:G:2:PRO:HB2	1:G:5:TRP:NE1	2.02	0.65
1:A:129:PRO:HG2	1:C:129:PRO:HG2	1.77	0.65
1:A:155:GLN:HE21	1:A:160:THR:CG2	2.08	0.65
1:B:3:GLU:HA	1:B:267:ASP:OD1	1.96	0.65
1:D:313:PHE:CE2	1:D:338:LEU:HD11	2.32	0.65
1:G:82:GLY:H	1:H:391:GLN:HE22	1.43	0.65
1:B:117:GLU:HG2	1:B:358:LEU:HB2	1.78	0.65
1:E:325:PHE:O	1:E:328:GLN:HG3	1.96	0.65
1:B:323:GLU:CD	1:B:350:GLY:HA3	2.16	0.65
1:C:90:GLY:HA2	1:C:385:MET:HE3	1.79	0.65
1:E:180:GLU:HG2	1:E:330:LEU:HD13	1.78	0.65
1:A:264:LEU:N	1:A:264:LEU:HD12	2.12	0.65
1:B:325:PHE:O	1:B:328:GLN:HG3	1.96	0.65
1:G:323:GLU:CD	1:G:350:GLY:HA3	2.17	0.65
1:D:379:GLN:HG2	1:D:380:PHE:CE1	2.32	0.65
1:F:289:VAL:HB	1:F:290:PRO:HD2	1.79	0.65
1:D:183:ARG:HG2	1:D:340:MET:HE1	1.79	0.64
1:C:36:VAL:CG2	1:C:206:VAL:HG21	2.26	0.64
1:F:214:LYS:HD3	1:F:214:LYS:H	1.62	0.64
1:A:110:VAL:HG22	1:A:265:VAL:HG23	1.79	0.64
1:C:389:VAL:HG12	1:C:389:VAL:O	1.98	0.64
1:H:162:SER:O	1:H:166:THR:HG23	1.97	0.64
1:D:87:ARG:HH11	1:D:391:GLN:HE22	1.46	0.64
1:F:36:VAL:CG2	1:F:206:VAL:HG21	2.24	0.64
1:F:85:VAL:HG11	1:F:94:GLU:CG	2.28	0.64
1:C:211:LYS:HG3	1:C:216:GLU:HG2	1.79	0.64
1:D:63:ASN:OD1	1:D:64:ARG:HG3	1.97	0.64
1:F:132:GLY:O	1:F:134:PRO:HD3	1.98	0.64
1:G:2:PRO:HB3	1:G:280:ARG:NE	2.12	0.64
1:G:36:VAL:O	1:G:40:ARG:HG2	1.98	0.64
1:C:2:PRO:HG3	1:C:280:ARG:CZ	2.28	0.64
1:C:71:LEU:HD12	1:C:72:LEU:N	2.13	0.64
1:A:183:ARG:HG3	1:A:340:MET:CE	2.28	0.63
1:F:138:LEU:HD12	1:G:140:MET:CE	2.28	0.63
1:A:117:GLU:HG2	1:A:358:LEU:HB2	1.80	0.63
1:G:196:TRP:CH2	1:G:221:GLN:HA	2.33	0.63
1:H:36:VAL:HG11	1:H:206:VAL:CG1	2.15	0.63
1:A:187:LEU:HD12	1:A:340:MET:HE3	1.78	0.63
1:F:372:GLU:OE1	1:F:375:ARG:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:LEU:HD11	1:H:295:GLY:HA3	1.79	0.63
1:G:17:HIS:CE1	1:G:120:SER:HA	2.32	0.63
1:A:290:PRO:HA	1:B:78:VAL:CG2	2.28	0.63
1:C:9:ALA:HB1	1:C:367:THR:HG23	1.78	0.63
1:C:128:LYS:HD2	1:D:122:ALA:O	1.97	0.63
1:E:178:ARG:HB2	1:E:246:THR:HG22	1.81	0.63
1:G:118:SER:OG	1:G:121:ARG:HG3	1.97	0.63
1:F:85:VAL:HG11	1:F:94:GLU:HG3	1.79	0.63
1:A:153:LYS:HD3	1:B:73:LEU:HD22	1.79	0.63
1:A:189:HIS:O	1:A:193:VAL:HG23	1.98	0.63
1:H:132:GLY:O	1:H:134:PRO:HD3	1.99	0.63
1:H:181:GLN:NE2	1:H:246:THR:HG21	2.13	0.63
1:D:376:ARG:HG3	1:D:378:VAL:HG23	1.81	0.62
1:G:318:LEU:HD13	1:G:376:ARG:HD2	1.81	0.62
1:B:196:TRP:CZ3	1:B:221:GLN:HG3	2.35	0.62
1:H:98:GLN:HE21	1:H:98:GLN:HA	1.65	0.62
1:H:279:ALA:HB1	1:H:397:VAL:CG1	2.29	0.62
1:C:53:ALA:HA	1:C:114:SER:O	2.00	0.62
1:D:57:ASN:HD21	1:D:59:ALA:HB3	1.65	0.62
1:F:290:PRO:HG2	1:F:293:ILE:CG1	2.30	0.62
1:F:322:ASN:HB2	1:F:385:MET:HG2	1.80	0.62
1:B:36:VAL:CG2	1:B:206:VAL:HG21	2.28	0.62
1:B:364:ARG:C	1:B:364:ARG:HD2	2.20	0.62
1:C:44:PRO:HG2	1:C:47:GLU:HG2	1.82	0.61
1:H:25:ARG:HB3	1:H:61:GLU:OE2	2.00	0.61
1:C:206:VAL:HG13	1:C:206:VAL:O	2.00	0.61
1:C:278:LEU:CD1	1:C:374:ARG:CZ	2.78	0.61
1:H:2:PRO:HG3	1:H:280:ARG:CZ	2.30	0.61
1:A:25:ARG:NH1	1:B:151:ASN:HB2	2.14	0.61
1:G:90:GLY:HA2	1:G:385:MET:CE	2.30	0.61
1:G:194:ARG:HG2	1:G:198:GLU:OE2	2.00	0.61
1:H:214:LYS:H	1:H:214:LYS:HD3	1.65	0.61
1:A:57:ASN:HD21	1:A:59:ALA:HB3	1.65	0.61
1:D:330:LEU:O	1:D:334:ARG:HG2	1.99	0.61
1:G:85:VAL:HG11	1:G:94:GLU:CG	2.30	0.61
1:C:184:PHE:HA	1:C:340:MET:HE3	1.83	0.61
1:D:44:PRO:HG2	1:D:47:GLU:CG	2.31	0.61
1:D:154:MET:HE1	1:D:158:TYR:HB2	1.82	0.61
1:C:57:ASN:ND2	1:C:59:ALA:H	1.98	0.61
1:G:322:ASN:HB2	1:G:385:MET:HG2	1.82	0.61
1:E:322:ASN:HB2	1:E:385:MET:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:OE1	1:B:101:ARG:NH2	2.32	0.60
1:A:372:GLU:O	1:A:376:ARG:HG2	2.00	0.60
1:D:196:TRP:CZ3	1:D:221:GLN:HG2	2.36	0.60
1:F:15:GLY:O	1:F:256:ASN:HB3	2.00	0.60
1:B:85:VAL:HG11	1:B:94:GLU:CG	2.31	0.60
1:D:36:VAL:CG2	1:D:206:VAL:HG21	2.29	0.60
1:E:132:GLY:O	1:E:134:PRO:HD3	2.01	0.60
1:H:122:ALA:HB3	1:H:144:THR:OG1	2.02	0.60
1:E:142:ASP:OD2	1:H:135:THR:HA	2.01	0.60
1:E:163:MET:HE1	1:E:294:MET:HG2	1.84	0.60
1:E:323:GLU:CD	1:E:350:GLY:HA3	2.22	0.60
1:G:107:GLU:HB3	1:H:308:ARG:NH1	2.16	0.60
1:C:299:VAL:HG21	1:C:335:GLU:HG3	1.84	0.60
1:A:291:PRO:HD3	1:B:78:VAL:CG2	2.31	0.60
1:G:170:LEU:HD21	1:G:293:ILE:HB	1.84	0.60
1:G:339:SER:OG	1:G:341:GLU:HG2	2.01	0.60
1:H:3:GLU:HA	1:H:267:ASP:OD1	2.02	0.60
1:D:71:LEU:HD11	1:D:80:VAL:HB	1.84	0.59
1:E:187:LEU:HD12	1:E:340:MET:HE3	1.83	0.59
1:B:212:ARG:HD2	1:B:217:ILE:HD11	1.83	0.59
1:C:30:LEU:HD23	1:C:70:ALA:CB	2.32	0.59
1:D:389:VAL:HG12	1:D:389:VAL:O	2.02	0.59
1:F:334:ARG:HG2	1:F:334:ARG:HH11	1.67	0.59
1:D:2:PRO:HB3	1:D:280:ARG:NH1	2.18	0.59
1:E:61:GLU:OE2	1:E:121:ARG:HD3	2.03	0.59
1:G:162:SER:OG	1:G:165:GLU:HG3	2.03	0.59
1:D:32:HIS:O	1:D:36:VAL:HG23	2.01	0.59
1:B:176:ILE:HD13	1:B:330:LEU:HB2	1.83	0.59
1:E:36:VAL:CG2	1:E:206:VAL:HG21	2.29	0.59
1:B:278:LEU:HD23	1:B:370:VAL:HG11	1.84	0.59
1:C:44:PRO:HG2	1:C:47:GLU:CG	2.33	0.59
1:F:204:GLU:OE1	1:F:368:THR:HA	2.02	0.59
1:H:187:LEU:HD12	1:H:340:MET:HE3	1.85	0.59
1:A:325:PHE:O	1:A:328:GLN:HG3	2.02	0.58
1:B:330:LEU:HD23	1:B:333:LEU:HD12	1.85	0.58
1:C:36:VAL:O	1:C:40:ARG:HG2	2.03	0.58
1:D:242:ARG:HH11	1:D:242:ARG:HB2	1.68	0.58
1:D:325:PHE:O	1:D:328:GLN:HG3	2.04	0.58
1:F:114:SER:HB2	1:F:260:ALA:O	2.04	0.58
1:G:71:LEU:HD12	1:G:72:LEU:N	2.19	0.58
1:C:117:GLU:HG2	1:C:358:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:LEU:HD11	1:H:136:GLY:HA2	1.85	0.58
1:F:280:ARG:HB2	1:F:400:MET:HE1	1.85	0.58
1:C:322:ASN:HB2	1:C:385:MET:HG2	1.85	0.58
1:E:129:PRO:HD2	1:G:134:PRO:HD2	1.85	0.58
1:D:132:GLY:O	1:D:134:PRO:HD3	2.04	0.58
1:E:65:ASN:ND2	1:E:68:ARG:HB2	2.18	0.58
1:A:182:ASP:HB3	1:A:234:LEU:HD23	1.84	0.58
1:B:119:MET:CE	1:B:255:LEU:HD23	2.33	0.58
1:C:151:ASN:HD22	1:C:152:PRO:HD2	1.69	0.58
1:D:189:HIS:O	1:D:193:VAL:HG23	2.04	0.58
1:C:289:VAL:HB	1:C:290:PRO:HD2	1.86	0.58
1:F:265:VAL:HG22	1:F:269:TYR:HB3	1.85	0.58
1:D:265:VAL:HG21	1:D:269:TYR:CD2	2.38	0.57
1:E:81:ALA:HB1	1:F:391:GLN:NE2	2.18	0.57
1:E:179:GLU:H	1:E:179:GLU:CD	2.06	0.57
1:B:110:VAL:HG22	1:B:265:VAL:HG12	1.85	0.57
1:D:278:LEU:HD22	1:D:374:ARG:NH2	2.20	0.57
1:A:168:GLU:OE1	1:A:246:THR:HG22	2.03	0.57
1:A:279:ALA:HB1	1:A:397:VAL:HG13	1.86	0.57
1:C:279:ALA:HB1	1:C:397:VAL:HG13	1.86	0.57
1:C:290:PRO:HA	1:D:78:VAL:HG21	1.87	0.57
1:D:254:PRO:HG2	1:D:256:ASN:OD1	2.04	0.57
1:F:278:LEU:HG	1:F:370:VAL:CG1	2.33	0.57
1:G:214:LYS:H	1:G:214:LYS:CD	2.06	0.57
1:C:290:PRO:HG2	1:C:293:ILE:HG12	1.86	0.57
1:F:135:THR:HG23	1:G:145:LEU:HD21	1.87	0.57
1:F:265:VAL:HG21	1:F:269:TYR:HD2	1.68	0.57
1:G:170:LEU:HD11	1:G:295:GLY:HA3	1.86	0.57
1:C:391:GLN:HE21	1:D:81:ALA:HB1	1.70	0.57
1:D:252:SER:HG	1:D:325:PHE:HD1	1.51	0.57
1:E:146:GLY:O	1:E:148:ARG:HD3	2.04	0.57
1:G:81:ALA:HB1	1:H:391:GLN:HE21	1.69	0.57
1:E:85:VAL:HG11	1:E:94:GLU:HG3	1.87	0.57
1:A:98:GLN:HG3	1:B:98:GLN:NE2	2.20	0.57
1:C:82:GLY:H	1:D:391:GLN:HE22	1.51	0.57
1:F:186:LEU:O	1:F:190:GLN:HG3	2.04	0.57
1:F:325:PHE:O	1:F:328:GLN:HG3	2.04	0.57
1:H:14:ILE:HG21	1:H:355:GLY:HA3	1.86	0.57
1:H:15:GLY:O	1:H:256:ASN:HB3	2.05	0.57
1:E:123:PRO:O	1:E:143:THR:HG23	2.04	0.56
1:H:179:GLU:H	1:H:179:GLU:CD	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:OD1	1:A:64:ARG:HG3	2.05	0.56
1:B:53:ALA:HA	1:B:114:SER:O	2.05	0.56
1:D:164:GLY:HA3	1:D:241:PHE:CE1	2.40	0.56
1:A:82:GLY:H	1:B:391:GLN:NE2	2.03	0.56
1:B:85:VAL:HG11	1:B:94:GLU:HG2	1.87	0.56
1:G:16:LYS:HG3	1:G:223:GLU:CG	2.35	0.56
1:G:187:LEU:HD12	1:G:340:MET:CE	2.35	0.56
1:H:2:PRO:HB3	1:H:280:ARG:NE	2.20	0.56
1:B:214:LYS:HD3	1:B:214:LYS:H	1.70	0.56
1:G:128:LYS:HG3	1:H:122:ALA:O	2.05	0.56
1:G:279:ALA:HB1	1:G:397:VAL:CG1	2.34	0.56
1:D:189:HIS:CB	1:D:229:THR:HG21	2.36	0.56
1:E:2:PRO:HB2	1:E:5:TRP:NE1	2.18	0.56
1:F:5:TRP:CE3	1:F:277:PRO:HG3	2.40	0.56
1:A:129:PRO:HG2	1:C:129:PRO:CG	2.36	0.56
1:A:330:LEU:HD23	1:A:333:LEU:HD12	1.87	0.56
1:E:90:GLY:HA2	1:E:385:MET:HE3	1.85	0.56
1:H:116:VAL:HG23	1:H:259:ALA:HB2	1.87	0.56
1:A:155:GLN:NE2	1:A:160:THR:HG23	2.19	0.56
1:A:254:PRO:HG2	1:A:256:ASN:OD1	2.06	0.56
1:A:135:THR:HG23	1:D:145:LEU:HD21	1.88	0.55
1:G:5:TRP:CE3	1:G:277:PRO:HG3	2.41	0.55
1:A:110:VAL:HG22	1:A:265:VAL:CG2	2.36	0.55
1:B:303:ARG:HG3	1:B:304:LYS:N	2.20	0.55
1:C:87:ARG:HH11	1:C:391:GLN:HE22	1.52	0.55
1:E:278:LEU:HG	1:E:370:VAL:CG1	2.36	0.55
1:H:187:LEU:HD12	1:H:340:MET:CE	2.37	0.55
1:D:37:LEU:HD21	1:D:263:LEU:HB2	1.87	0.55
1:E:129:PRO:HD2	1:G:134:PRO:CD	2.37	0.55
1:A:62:ASP:O	1:A:66:VAL:HG22	2.07	0.55
1:A:206:VAL:HG13	1:A:206:VAL:O	2.06	0.55
1:B:299:VAL:HG21	1:B:335:GLU:HG3	1.87	0.55
1:C:279:ALA:HB1	1:C:397:VAL:CG1	2.36	0.55
1:G:132:GLY:O	1:G:134:PRO:HD3	2.06	0.55
1:G:294:MET:HE3	1:G:295:GLY:HA2	1.88	0.55
1:C:328:GLN:HG3	1:C:329:ALA:H	1.71	0.55
1:G:282:ARG:NH1	1:G:309:ALA:O	2.39	0.55
1:H:2:PRO:O	1:H:267:ASP:HB3	2.06	0.55
1:H:322:ASN:HB2	1:H:385:MET:HG2	1.89	0.55
1:A:212:ARG:CD	1:A:217:ILE:HD12	2.23	0.55
1:D:214:LYS:HD3	1:D:214:LYS:H	1.71	0.55

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:32:HIS:O	1:A:36:VAL:HG23	2.06	0.55
1:B:290:PRO:HG2	1:B:293:ILE:CG1	2.36	0.55
1:G:399:GLY:O	1:G:400:MET:HG2	2.07	0.55
1:B:57:ASN:HD21	1:B:59:ALA:HB3	1.72	0.55
1:D:53:ALA:HA	1:D:114:SER:O	2.07	0.55
1:E:170:LEU:HD11	1:E:295:GLY:HA3	1.89	0.55
1:C:151:ASN:HD22	1:C:152:PRO:CD	2.20	0.54
1:G:290:PRO:HA	1:H:78:VAL:HG21	1.89	0.54
1:G:328:GLN:HG3	1:G:329:ALA:N	2.23	0.54
1:E:32:HIS:O	1:E:36:VAL:HG23	2.07	0.54
1:F:238:ARG:HE	1:F:238:ARG:N	2.06	0.54
1:H:131:ARG:HG2	1:H:132:GLY:H	1.71	0.54
1:D:248:THR:H	1:D:251:ASN:ND2	2.05	0.54
1:G:5:TRP:CZ3	1:G:277:PRO:HG3	2.41	0.54
1:H:265:VAL:HG22	1:H:269:TYR:HB3	1.89	0.54
1:F:140:MET:CE	1:G:138:LEU:HB2	2.37	0.54
1:G:372:GLU:OE1	1:G:375:ARG:HD2	2.08	0.54
1:A:290:PRO:HD3	1:B:78:VAL:HG11	1.89	0.54
1:C:5:TRP:CE3	1:C:277:PRO:HG3	2.42	0.54
1:F:113:GLY:O	1:F:262:VAL:HG12	2.08	0.54
1:G:391:GLN:HE21	1:H:81:ALA:HB1	1.72	0.54
1:C:184:PHE:HA	1:C:340:MET:CE	2.37	0.54
1:E:158:TYR:CZ	1:F:72:LEU:HD22	2.43	0.54
1:G:168:GLU:O	1:G:172:GLU:HG3	2.07	0.54
1:B:61:GLU:OE2	1:B:121:ARG:HD3	2.06	0.54
1:B:62:ASP:O	1:B:66:VAL:HG23	2.07	0.54
1:D:154:MET:CE	1:D:158:TYR:HB2	2.36	0.54
1:F:44:PRO:HG2	1:F:47:GLU:HG2	1.89	0.54
1:F:372:GLU:HA	1:F:375:ARG:HH11	1.73	0.54
1:G:38:VAL:HG13	1:G:43:VAL:O	2.07	0.54
1:A:238:ARG:CZ	1:A:238:ARG:H	2.21	0.54
1:G:63:ASN:OD1	1:G:64:ARG:HG3	2.08	0.54
1:A:173:MET:HE3	1:A:293:ILE:HG21	1.89	0.54
1:G:183:ARG:HG2	1:G:340:MET:HE1	1.89	0.54
1:F:322:ASN:CB	1:F:385:MET:HG2	2.38	0.53
1:G:184:PHE:HA	1:G:340:MET:CE	2.38	0.53
1:H:57:ASN:O	1:H:62:ASP:OD2	2.25	0.53
1:H:57:ASN:HD21	1:H:59:ALA:HB3	1.73	0.53
1:A:230:SER:OG	1:A:233:LYS:HG3	2.08	0.53
1:D:2:PRO:HB3	1:D:280:ARG:HH11	1.74	0.53
1:G:87:ARG:CZ	1:G:286:VAL:HG21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:LEU:HD21	1:H:263:LEU:N	2.23	0.53
1:B:90:GLY:HA2	1:B:385:MET:CE	2.38	0.53
1:D:322:ASN:HB2	1:D:385:MET:HG2	1.90	0.53
1:E:129:PRO:CG	1:G:129:PRO:CG	2.87	0.53
1:G:122:ALA:HB3	1:G:144:THR:OG1	2.09	0.53
1:A:44:PRO:HG2	1:A:47:GLU:CG	2.36	0.53
1:F:57:ASN:HD21	1:F:59:ALA:HB3	1.74	0.53
1:C:57:ASN:ND2	1:C:57:ASN:C	2.60	0.53
1:E:85:VAL:HG11	1:E:94:GLU:CG	2.39	0.53
1:F:226:ARG:HG3	1:F:229:THR:OG1	2.08	0.53
1:F:252:SER:HB3	1:F:325:PHE:HD1	1.74	0.53
1:F:290:PRO:HG2	1:F:293:ILE:HG13	1.90	0.53
1:H:278:LEU:HG	1:H:370:VAL:CG1	2.39	0.53
1:A:87:ARG:NE	1:A:94:GLU:OE1	2.41	0.53
1:E:196:TRP:CZ3	1:E:221:GLN:HG2	2.44	0.53
1:G:53:ALA:HA	1:G:114:SER:O	2.07	0.53
1:A:57:ASN:ND2	1:A:59:ALA:H	2.06	0.53
1:A:154:MET:CE	1:A:158:TYR:HB2	2.39	0.53
1:E:2:PRO:HB3	1:E:5:TRP:HE1	1.72	0.53
1:G:289:VAL:HB	1:G:290:PRO:HD2	1.91	0.53
1:G:292:ARG:HD3	1:G:293:ILE:HG23	1.91	0.53
1:A:128:LYS:HE3	1:C:134:PRO:O	2.09	0.53
1:A:140:MET:HE3	1:D:138:LEU:HD12	1.91	0.53
1:A:61:GLU:OE2	1:A:121:ARG:HD3	2.08	0.53
1:C:32:HIS:O	1:C:36:VAL:HG23	2.09	0.52
1:D:2:PRO:HB3	1:D:280:ARG:CD	2.32	0.52
1:E:3:GLU:O	1:E:266:SER:HA	2.10	0.52
1:F:117:GLU:HG2	1:F:358:LEU:HB2	1.91	0.52
1:A:196:TRP:CZ3	1:A:221:GLN:HG2	2.45	0.52
1:C:30:LEU:HD13	1:C:116:VAL:HB	1.90	0.52
1:D:113:GLY:O	1:D:262:VAL:HG12	2.09	0.52
1:D:155:GLN:NE2	1:D:160:THR:OG1	2.42	0.52
1:E:129:PRO:HG2	1:G:129:PRO:CG	2.39	0.52
1:H:17:HIS:CE1	1:H:120:SER:HA	2.43	0.52
1:B:279:ALA:HB1	1:B:397:VAL:HG12	1.91	0.52
1:D:379:GLN:HG2	1:D:380:PHE:CD1	2.44	0.52
1:F:176:ILE:HD12	1:F:176:ILE:H	1.73	0.52
1:H:325:PHE:O	1:H:328:GLN:HG3	2.09	0.52
1:B:278:LEU:HD23	1:B:370:VAL:CG1	2.38	0.52
1:B:345:LEU:O	1:B:346:ASN:C	2.48	0.52
1:C:83:CYS:HB2	1:D:87:ARG:CZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:SER:HG	1:D:165:GLU:HG3	1.74	0.52
1:G:227:ARG:HB2	1:G:227:ARG:NH1	2.25	0.52
1:H:323:GLU:CD	1:H:350:GLY:HA3	2.30	0.52
1:A:227:ARG:NH1	1:A:227:ARG:HB2	2.24	0.52
1:A:345:LEU:O	1:A:346:ASN:C	2.47	0.52
1:G:254:PRO:HG2	1:G:256:ASN:OD1	2.09	0.52
1:H:345:LEU:O	1:H:346:ASN:C	2.48	0.52
1:B:48:VAL:O	1:B:80:VAL:HG22	2.10	0.52
1:E:64:ARG:O	1:E:65:ASN:HB3	2.09	0.52
1:G:146:GLY:O	1:G:148:ARG:HG2	2.10	0.52
1:H:214:LYS:HD3	1:H:214:LYS:N	2.25	0.52
1:D:61:GLU:OE1	1:D:121:ARG:NH1	2.43	0.52
1:G:212:ARG:NE	1:G:217:ILE:HD12	2.24	0.52
1:E:57:ASN:HD21	1:E:59:ALA:HB3	1.75	0.52
1:E:117:GLU:HG2	1:E:358:LEU:HB2	1.91	0.52
1:G:110:VAL:HG22	1:G:265:VAL:HG12	1.91	0.52
1:G:387:ILE:HB	1:G:391:GLN:HB2	1.92	0.52
1:A:323:GLU:OE1	1:A:350:GLY:HA3	2.09	0.52
1:C:15:GLY:O	1:C:256:ASN:HB3	2.10	0.52
1:C:63:ASN:OD1	1:C:64:ARG:HG3	2.10	0.52
1:E:81:ALA:CB	1:F:391:GLN:HE21	2.22	0.52
1:E:391:GLN:NE2	1:F:82:GLY:H	2.07	0.52
1:F:389:VAL:HG12	1:F:389:VAL:O	2.10	0.52
1:G:58:GLN:HA	1:G:62:ASP:OD1	2.10	0.52
1:H:176:ILE:HD13	1:H:330:LEU:HB2	1.91	0.52
1:A:178:ARG:HH21	1:A:235:ALA:HA	1.74	0.52
1:E:122:ALA:HB1	1:E:143:THR:OG1	2.10	0.52
1:H:44:PRO:HG2	1:H:47:GLU:HG2	1.91	0.52
1:G:209:PRO:HB2	1:G:216:GLU:OE1	2.10	0.51
1:H:163:MET:HA	1:H:163:MET:CE	2.40	0.51
1:G:71:LEU:HD12	1:G:71:LEU:C	2.30	0.51
1:H:206:VAL:O	1:H:206:VAL:HG23	2.10	0.51
1:A:129:PRO:CG	1:C:129:PRO:HG2	2.40	0.51
1:A:187:LEU:HD12	1:A:340:MET:CE	2.39	0.51
1:C:232:GLU:HG3	1:E:378:VAL:HA	1.92	0.51
1:B:278:LEU:CD1	1:B:374:ARG:HH21	2.22	0.51
1:C:178:ARG:NH2	1:C:248:THR:HG21	2.25	0.51
1:D:226:ARG:O	1:D:229:THR:HG22	2.10	0.51
1:D:345:LEU:O	1:D:346:ASN:C	2.49	0.51
1:E:90:GLY:HA2	1:E:385:MET:HE1	1.91	0.51
1:G:291:PRO:HD3	1:H:78:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:PRO:HG2	1:H:47:GLU:CG	2.40	0.51
1:A:184:PHE:HA	1:A:340:MET:CE	2.41	0.51
1:B:145:LEU:HD21	1:C:135:THR:HG23	1.92	0.51
1:B:197:GLU:OE2	1:B:227:ARG:NH2	2.37	0.51
1:D:238:ARG:CD	1:D:238:ARG:N	2.66	0.51
1:E:98:GLN:NE2	1:F:98:GLN:HG3	2.26	0.51
1:G:90:GLY:HA2	1:G:385:MET:HE1	1.93	0.51
1:A:164:GLY:HA3	1:A:241:PHE:CD1	2.46	0.51
1:B:71:LEU:HD22	1:B:80:VAL:HG12	1.92	0.51
1:C:294:MET:HE3	1:C:386:CYS:HB2	1.93	0.51
1:F:53:ALA:HA	1:F:114:SER:O	2.11	0.51
1:H:181:GLN:NE2	1:H:246:THR:CG2	2.74	0.51
1:H:186:LEU:O	1:H:190:GLN:HG3	2.11	0.51
1:C:323:GLU:OE1	1:C:350:GLY:HA3	2.11	0.51
1:D:299:VAL:HG21	1:D:335:GLU:HG3	1.92	0.51
1:H:389:VAL:HG12	1:H:389:VAL:O	2.11	0.51
1:F:345:LEU:O	1:F:346:ASN:C	2.49	0.51
1:A:10:VAL:HG12	1:A:40:ARG:NH1	2.25	0.50
1:B:30:LEU:HD22	1:B:116:VAL:CG1	2.41	0.50
1:C:2:PRO:HG3	1:C:280:ARG:NH2	2.25	0.50
1:F:372:GLU:HA	1:F:375:ARG:HG2	1.93	0.50
1:A:287:ALA:HB2	1:A:304:LYS:HE2	1.92	0.50
1:D:15:GLY:O	1:D:256:ASN:HB3	2.10	0.50
1:E:16:LYS:HG3	1:E:223:GLU:CG	2.37	0.50
1:F:61:GLU:OE2	1:F:121:ARG:HD3	2.11	0.50
1:H:177:ARG:O	1:H:181:GLN:HG3	2.11	0.50
1:C:166:THR:HA	1:C:169:ASN:ND2	2.24	0.50
1:B:136:GLY:HA2	1:C:145:LEU:HD11	1.94	0.50
1:G:2:PRO:HB3	1:G:280:ARG:CD	2.42	0.50
1:G:25:ARG:NH2	1:H:151:ASN:HB2	2.26	0.50
1:G:196:TRP:CZ3	1:G:221:GLN:HG3	2.46	0.50
1:H:240:VAL:HG12	1:H:240:VAL:O	2.10	0.50
1:A:15:GLY:O	1:A:256:ASN:HB3	2.12	0.50
1:A:81:ALA:HB1	1:B:391:GLN:HE21	1.77	0.50
1:F:279:ALA:HB1	1:F:397:VAL:CG1	2.42	0.50
1:D:364:ARG:HD2	1:D:364:ARG:C	2.31	0.50
1:E:71:LEU:HD12	1:E:71:LEU:C	2.32	0.50
1:E:141:TYR:HA	1:H:137:ASN:OD1	2.12	0.50
1:H:337:SER:O	1:H:338:LEU:HD12	2.11	0.50
1:B:206:VAL:HG13	1:B:206:VAL:O	2.12	0.50
1:D:155:GLN:HE21	1:D:160:THR:CG2	2.25	0.50

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G:285:ALA:HA	1:G:308:ARG:NH1	2.27	0.50
1:A:389:VAL:HG12	1:A:389:VAL:O	2.12	0.49
1:E:119:MET:HG3	1:E:256:ASN:O	2.12	0.49
1:E:387:ILE:HB	1:E:391:GLN:HB2	1.94	0.49
1:F:248:THR:HG23	1:F:251:ASN:HD21	1.77	0.49
1:A:53:ALA:HA	1:A:114:SER:O	2.12	0.49
1:G:345:LEU:O	1:G:346:ASN:C	2.50	0.49
1:H:53:ALA:HA	1:H:114:SER:O	2.11	0.49
1:A:287:ALA:HB2	1:A:304:LYS:CE	2.42	0.49
1:B:5:TRP:CE3	1:B:277:PRO:HG3	2.47	0.49
1:B:311:LEU:HD11	1:B:380:PHE:CE2	2.48	0.49
1:D:279:ALA:HB1	1:D:397:VAL:HG12	1.94	0.49
1:E:5:TRP:CE3	1:E:277:PRO:HG3	2.47	0.49
1:F:25:ARG:NH1	1:F:61:GLU:HG2	2.27	0.49
1:G:333:LEU:HD22	1:G:338:LEU:HB3	1.93	0.49
1:C:345:LEU:O	1:C:346:ASN:C	2.50	0.49
1:G:6:ILE:O	1:G:278:LEU:HB2	2.12	0.49
1:G:107:GLU:CD	1:H:101:ARG:HH21	2.16	0.49
1:F:170:LEU:HD21	1:F:293:ILE:HB	1.94	0.49
1:G:10:VAL:HG12	1:G:11:ARG:N	2.28	0.49
1:H:265:VAL:CG2	1:H:269:TYR:CD2	2.94	0.49
1:D:248:THR:H	1:D:251:ASN:HD21	1.60	0.49
1:E:101:ARG:NH1	1:F:107:GLU:OE1	2.41	0.49
1:E:211:LYS:NZ	1:E:216:GLU:HB3	2.27	0.49
1:F:240:VAL:HG12	1:F:240:VAL:O	2.12	0.49
1:G:38:VAL:HG21	1:G:76:PHE:CZ	2.48	0.49
1:H:32:HIS:O	1:H:36:VAL:HG23	2.11	0.49
1:A:54:GLY:HA2	1:A:85:VAL:O	2.13	0.49
1:B:14:ILE:HG21	1:B:355:GLY:HA3	1.94	0.49
1:C:37:LEU:HD21	1:C:263:LEU:HB2	1.94	0.49
1:D:9:ALA:CB	1:D:367:THR:HG23	2.41	0.49
1:D:57:ASN:ND2	1:D:59:ALA:H	2.11	0.49
1:E:182:ASP:HB3	1:E:234:LEU:HD23	1.95	0.49
1:G:178:ARG:NH2	1:G:248:THR:HG21	2.28	0.49
1:G:181:GLN:HE22	1:G:246:THR:CG2	2.26	0.49
1:A:164:GLY:HA3	1:A:241:PHE:CE1	2.48	0.49
1:C:168:GLU:OE2	1:C:246:THR:N	2.28	0.49
1:C:308:ARG:NH1	1:D:107:GLU:HB3	2.27	0.49
1:G:170:LEU:CD1	1:G:295:GLY:HA3	2.42	0.49
1:B:85:VAL:HG11	1:B:94:GLU:HG3	1.95	0.49
1:G:364:ARG:C	1:G:364:ARG:HD2	2.32	0.49

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:H:131:ARG:HG2	1:H:132:GLY:N	2.27	0.49
1:A:286:VAL:HG13	1:B:81:ALA:CB	2.43	0.49
1:D:372:GLU:O	1:D:376:ARG:HG2	2.13	0.49
1:G:61:GLU:OE2	1:G:121:ARG:NH1	2.43	0.48
1:H:71:LEU:HD12	1:H:72:LEU:N	2.28	0.48
1:B:318:LEU:HD21	1:B:372:GLU:HG3	1.95	0.48
1:C:87:ARG:NE	1:C:94:GLU:OE1	2.45	0.48
1:E:114:SER:HB2	1:E:260:ALA:O	2.13	0.48
1:E:155:GLN:HE21	1:E:160:THR:HG23	1.77	0.48
1:F:181:GLN:NE2	1:F:246:THR:OG1	2.46	0.48
1:H:279:ALA:HB1	1:H:397:VAL:HG12	1.93	0.48
1:B:30:LEU:HD23	1:B:66:VAL:CG1	2.42	0.48
1:F:140:MET:HE2	1:G:138:LEU:HB2	1.94	0.48
1:H:189:HIS:O	1:H:193:VAL:HG23	2.12	0.48
1:H:339:SER:OG	1:H:341:GLU:HG2	2.13	0.48
1:A:146:GLY:O	1:A:148:ARG:HG3	2.13	0.48
1:A:336:TRP:HB3	1:A:338:LEU:HD13	1.96	0.48
1:D:14:ILE:HG21	1:D:355:GLY:HA3	1.95	0.48
1:D:189:HIS:HB3	1:D:229:THR:HG21	1.95	0.48
1:A:151:ASN:HB2	1:B:25:ARG:NH2	2.28	0.48
1:B:38:VAL:HG13	1:B:43:VAL:O	2.13	0.48
1:F:279:ALA:HB1	1:F:397:VAL:HG13	1.95	0.48
1:B:62:ASP:HB2	1:B:66:VAL:HG21	1.96	0.48
1:C:81:ALA:HB1	1:D:391:GLN:NE2	2.28	0.48
1:E:53:ALA:HA	1:E:114:SER:O	2.14	0.48
1:F:14:ILE:HG21	1:F:355:GLY:HA3	1.95	0.48
1:C:131:ARG:HG2	1:C:132:GLY:H	1.79	0.48
1:C:151:ASN:HD22	1:C:152:PRO:N	2.10	0.48
1:E:30:LEU:HD12	1:E:30:LEU:O	2.14	0.48
1:G:196:TRP:CE3	1:G:221:GLN:HG3	2.47	0.48
1:G:289:VAL:C	1:H:78:VAL:HG13	2.34	0.48
1:B:87:ARG:HH11	1:B:391:GLN:NE2	2.11	0.48
1:C:290:PRO:HG2	1:C:293:ILE:CG1	2.43	0.48
1:D:265:VAL:HG22	1:D:269:TYR:HB3	1.95	0.48
1:A:57:ASN:ND2	1:A:57:ASN:C	2.66	0.48
1:B:168:GLU:OE1	1:B:246:THR:HG22	2.14	0.48
1:C:155:GLN:NE2	1:C:160:THR:OG1	2.38	0.48
1:D:3:GLU:O	1:D:266:SER:HA	2.14	0.48
1:G:184:PHE:HA	1:G:340:MET:HE3	1.96	0.48
1:F:71:LEU:HD12	1:F:71:LEU:C	2.35	0.48
1:F:265:VAL:CG2	1:F:269:TYR:CD2	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:GLU:HB3	1:G:371:HIS:CD2	2.49	0.48
1:B:155:GLN:HE21	1:B:160:THR:CG2	2.27	0.47
1:D:97:ALA:CB	1:D:284:ILE:HD13	2.44	0.47
1:A:83:CYS:HB2	1:B:87:ARG:CZ	2.44	0.47
1:A:98:GLN:NE2	1:B:98:GLN:HG3	2.28	0.47
1:A:178:ARG:NH1	1:A:248:THR:HG21	2.30	0.47
1:D:97:ALA:HB1	1:D:284:ILE:HD13	1.96	0.47
1:D:252:SER:OG	1:D:325:PHE:HD1	1.97	0.47
1:F:37:LEU:HD21	1:F:263:LEU:HB2	1.96	0.47
1:F:176:ILE:HD12	1:F:176:ILE:N	2.28	0.47
1:G:3:GLU:O	1:G:266:SER:HA	2.13	0.47
1:C:51:VAL:HG22	1:C:112:ILE:HB	1.97	0.47
1:A:25:ARG:HD3	1:A:27:ASP:OD1	2.14	0.47
1:C:122:ALA:O	1:D:128:LYS:HE2	2.15	0.47
1:D:87:ARG:NH1	1:D:391:GLN:HE22	2.11	0.47
1:E:372:GLU:OE1	1:E:375:ARG:HD2	2.14	0.47
1:F:214:LYS:H	1:F:214:LYS:CD	2.24	0.47
1:C:126:VAL:CG2	1:C:140:MET:HG2	2.43	0.47
1:F:200:ARG:HG3	1:F:200:ARG:NH1	2.30	0.47
1:G:254:PRO:HG2	1:G:256:ASN:HD21	1.80	0.47
1:C:7:VAL:CG2	1:C:265:VAL:HG22	2.45	0.47
1:F:178:ARG:NH2	1:F:248:THR:HG21	2.29	0.47
1:A:90:GLY:HA2	1:A:385:MET:CE	2.44	0.47
1:B:116:VAL:HA	1:B:360:ALA:HB2	1.96	0.47
1:B:155:GLN:NE2	1:B:160:THR:OG1	2.48	0.47
1:B:328:GLN:HG3	1:B:329:ALA:N	2.29	0.47
1:B:328:GLN:HG3	1:B:329:ALA:H	1.79	0.47
1:C:252:SER:HB3	1:C:325:PHE:HD1	1.80	0.47
1:C:399:GLY:O	1:C:400:MET:HG2	2.15	0.47
1:F:36:VAL:O	1:F:40:ARG:HG2	2.15	0.47
1:G:46:GLU:HA	1:G:77:PRO:HG3	1.96	0.47
1:G:240:VAL:HG12	1:G:240:VAL:O	2.14	0.47
1:H:333:LEU:HD21	1:H:345:LEU:HD22	1.97	0.47
1:D:93:LEU:HB2	1:D:385:MET:CE	2.44	0.47
1:D:164:GLY:HA3	1:D:241:PHE:CD1	2.49	0.47
1:F:330:LEU:HD23	1:F:333:LEU:HD12	1.96	0.47
1:B:290:PRO:HG2	1:B:293:ILE:HG12	1.97	0.47
1:C:310:GLY:O	1:C:311:LEU:HD23	2.14	0.47
1:A:177:ARG:HB3	1:A:179:GLU:OE2	2.15	0.47
1:B:168:GLU:HB3	1:B:242:ARG:NH1	2.30	0.47
1:C:132:GLY:O	1:C:134:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:GLU:HA	1:F:375:ARG:NH1	2.30	0.47
1:G:107:GLU:OE1	1:H:101:ARG:NH2	2.47	0.47
1:G:391:GLN:NE2	1:H:82:GLY:N	2.50	0.47
1:B:140:MET:HE3	1:C:138:LEU:CB	2.44	0.46
1:D:87:ARG:HH11	1:D:391:GLN:NE2	2.10	0.46
1:E:98:GLN:HG3	1:F:98:GLN:NE2	2.29	0.46
1:H:155:GLN:NE2	1:H:160:THR:OG1	2.48	0.46
1:A:126:VAL:HG13	1:D:140:MET:HE2	1.96	0.46
1:B:389:VAL:O	1:B:389:VAL:HG12	2.15	0.46
1:C:81:ALA:HB1	1:D:391:GLN:HE21	1.80	0.46
1:E:60:GLY:CA	1:E:123:PRO:HG3	2.45	0.46
1:E:299:VAL:HB	1:E:300:PRO:CD	2.44	0.46
1:G:318:LEU:HD21	1:G:372:GLU:CG	2.45	0.46
1:E:170:LEU:CD1	1:E:295:GLY:HA3	2.45	0.46
1:F:116:VAL:HA	1:F:360:ALA:HB2	1.97	0.46
1:F:265:VAL:CG2	1:F:269:TYR:HB3	2.45	0.46
1:G:98:GLN:NE2	1:H:98:GLN:HG3	2.31	0.46
1:H:37:LEU:HD21	1:H:262:VAL:C	2.35	0.46
1:B:196:TRP:CH2	1:B:221:GLN:HG3	2.50	0.46
1:C:278:LEU:HG	1:C:370:VAL:CG1	2.32	0.46
1:D:116:VAL:HA	1:D:360:ALA:HB2	1.97	0.46
1:D:131:ARG:HG2	1:D:132:GLY:H	1.80	0.46
1:E:168:GLU:HB3	1:E:242:ARG:NH1	2.30	0.46
1:F:57:ASN:C	1:F:57:ASN:ND2	2.67	0.46
1:F:57:ASN:O	1:F:62:ASP:OD2	2.33	0.46
1:F:93:LEU:HB2	1:F:385:MET:CE	2.45	0.46
1:F:328:GLN:HG3	1:F:329:ALA:N	2.30	0.46
1:A:132:GLY:O	1:A:134:PRO:HD3	2.16	0.46
1:B:187:LEU:HD12	1:B:340:MET:CE	2.46	0.46
1:C:328:GLN:HE21	1:C:328:GLN:HB2	1.49	0.46
1:D:93:LEU:HB3	1:D:393:ILE:HD13	1.97	0.46
1:D:172:GLU:OE2	1:D:242:ARG:NH2	2.49	0.46
1:E:10:VAL:HG22	1:E:37:LEU:HD13	1.97	0.46
1:E:41:SER:OG	1:E:43:VAL:HG23	2.16	0.46
1:A:126:VAL:HB	1:B:124:TYR:HB2	1.97	0.46
1:B:284:ILE:HG22	1:B:285:ALA:N	2.31	0.46
1:E:345:LEU:O	1:E:346:ASN:C	2.53	0.46
1:H:181:GLN:OE1	1:H:327:ALA:HB2	2.16	0.46
1:A:16:LYS:HG3	1:A:223:GLU:HG3	1.96	0.46
1:A:122:ALA:HB3	1:A:144:THR:OG1	2.16	0.46
1:B:11:ARG:HD2	1:B:364:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ARG:HD2	1:B:364:ARG:O	2.15	0.46
1:B:379:GLN:NE2	1:B:380:PHE:CE1	2.84	0.46
1:B:189:HIS:CD2	1:B:229:THR:HG21	2.51	0.46
1:C:206:VAL:O	1:C:206:VAL:CG1	2.64	0.46
1:E:46:GLU:HA	1:E:77:PRO:HG3	1.97	0.46
1:F:238:ARG:H	1:F:238:ARG:NE	2.14	0.46
1:F:318:LEU:HD12	1:F:318:LEU:HA	1.78	0.46
1:H:289:VAL:HB	1:H:290:PRO:HD2	1.97	0.46
1:A:13:PRO:HD2	1:A:208:VAL:HG23	1.97	0.46
1:A:185:ALA:HB3	1:A:234:LEU:HD21	1.97	0.46
1:A:189:HIS:CE1	1:A:226:ARG:HG2	2.51	0.46
1:B:341:GLU:H	1:B:341:GLU:HG2	1.53	0.46
1:C:46:GLU:HA	1:C:77:PRO:HG3	1.98	0.46
1:D:264:LEU:N	1:D:264:LEU:HD12	2.31	0.46
1:G:16:LYS:HG3	1:G:223:GLU:CD	2.36	0.46
1:H:212:ARG:HD2	1:H:217:ILE:HD11	1.97	0.46
1:B:282:ARG:NH1	1:B:309:ALA:O	2.49	0.46
1:C:193:VAL:O	1:C:197:GLU:HB2	2.16	0.46
1:C:303:ARG:HG3	1:C:304:LYS:N	2.30	0.46
1:D:242:ARG:HH11	1:D:242:ARG:CB	2.28	0.46
1:E:212:ARG:HD3	1:E:212:ARG:HA	1.60	0.46
1:F:300:PRO:O	1:F:304:LYS:HG3	2.16	0.46
1:A:366:LEU:O	1:A:370:VAL:HG23	2.16	0.45
1:G:61:GLU:OE1	1:G:121:ARG:NH1	2.49	0.45
1:H:192:ALA:HB1	1:H:354:LEU:HD21	1.98	0.45
1:A:294:MET:HE3	1:A:295:GLY:N	2.32	0.45
1:A:322:ASN:CB	1:A:385:MET:HG2	2.46	0.45
1:A:328:GLN:HG3	1:A:329:ALA:N	2.31	0.45
1:A:357:PRO:O	1:A:358:LEU:C	2.55	0.45
1:B:16:LYS:HG3	1:B:223:GLU:CG	2.41	0.45
1:B:126:VAL:HG22	1:B:140:MET:HG2	1.99	0.45
1:B:230:SER:OG	1:B:233:LYS:HG3	2.16	0.45
1:B:289:VAL:HB	1:B:290:PRO:HD2	1.97	0.45
1:C:96:VAL:HG21	1:C:366:LEU:HD23	1.99	0.45
1:F:28:ASP:OD1	1:F:73:LEU:HD13	2.16	0.45
1:A:5:TRP:O	1:A:264:LEU:HA	2.15	0.45
1:B:37:LEU:HD21	1:B:263:LEU:HB2	1.96	0.45
1:B:57:ASN:ND2	1:B:59:ALA:H	2.14	0.45
1:C:325:PHE:O	1:C:328:GLN:HG3	2.17	0.45
1:D:299:VAL:HB	1:D:300:PRO:CD	2.46	0.45
1:G:211:LYS:HG2	1:G:216:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE1	1:A:294:MET:HG2	1.98	0.45
1:A:166:THR:HA	1:A:169:ASN:HD22	1.80	0.45
1:B:132:GLY:O	1:B:134:PRO:HD3	2.16	0.45
1:C:62:ASP:O	1:C:66:VAL:HG22	2.17	0.45
1:F:196:TRP:CH2	1:F:221:GLN:HA	2.52	0.45
1:H:62:ASP:O	1:H:66:VAL:HG22	2.17	0.45
1:H:98:GLN:HA	1:H:98:GLN:NE2	2.29	0.45
1:B:9:ALA:HB1	1:B:367:THR:HG23	1.98	0.45
1:B:322:ASN:HB2	1:B:385:MET:HG2	1.98	0.45
1:G:183:ARG:HG2	1:G:340:MET:CE	2.46	0.45
1:H:364:ARG:HD2	1:H:364:ARG:C	2.37	0.45
1:H:372:GLU:HA	1:H:375:ARG:HG2	1.99	0.45
1:B:379:GLN:CD	1:B:380:PHE:CE1	2.90	0.45
1:E:154:MET:CE	1:E:158:TYR:HB2	2.46	0.45
1:G:230:SER:HB3	1:G:233:LYS:CG	2.36	0.45
1:G:325:PHE:O	1:G:328:GLN:HG3	2.16	0.45
1:C:212:ARG:NE	1:C:217:ILE:HD12	2.31	0.45
1:D:197:GLU:OE2	1:D:227:ARG:NH2	2.47	0.45
1:E:78:VAL:HG11	1:F:290:PRO:N	2.31	0.45
1:F:44:PRO:HG2	1:F:47:GLU:CG	2.47	0.45
1:F:143:THR:HG22	1:F:148:ARG:NE	2.32	0.45
1:F:312:SER:N	1:F:315:ASP:OD2	2.38	0.45
1:A:299:VAL:HG21	1:A:335:GLU:HG3	1.99	0.45
1:C:357:PRO:O	1:C:358:LEU:C	2.54	0.45
1:D:57:ASN:ND2	1:D:57:ASN:C	2.70	0.45
1:E:303:ARG:HG3	1:E:304:LYS:N	2.30	0.45
1:E:379:GLN:HG2	1:E:380:PHE:CD1	2.52	0.45
1:F:131:ARG:HG2	1:F:132:GLY:N	2.32	0.45
1:B:37:LEU:HD21	1:B:263:LEU:N	2.32	0.45
1:C:153:LYS:HD3	1:D:73:LEU:HD22	1.98	0.45
1:C:181:GLN:OE1	1:C:327:ALA:HB2	2.17	0.45
1:D:131:ARG:HG2	1:D:132:GLY:N	2.32	0.45
1:D:328:GLN:HE21	1:D:328:GLN:HB2	1.64	0.45
1:G:311:LEU:HD11	1:G:380:PHE:CD2	2.52	0.45
1:E:181:GLN:HE22	1:E:246:THR:HB	1.82	0.45
1:H:38:VAL:HG13	1:H:43:VAL:O	2.16	0.45
1:B:62:ASP:HB2	1:B:66:VAL:CG2	2.47	0.44
1:F:328:GLN:HE21	1:F:328:GLN:HB2	1.52	0.44
1:G:276:ARG:HA	1:G:277:PRO:HD3	1.80	0.44
1:E:116:VAL:HG22	1:E:117:GLU:N	2.32	0.44
1:E:372:GLU:HA	1:E:375:ARG:NH1	2.31	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G:294:MET:CE	1:G:295:GLY:HA2	2.47	0.44
1:A:376:ARG:HG3	1:A:378:VAL:HG23	1.99	0.44
1:C:5:TRP:CZ3	1:C:277:PRO:HG3	2.52	0.44
1:C:391:GLN:HE22	1:D:82:GLY:H	1.64	0.44
1:E:240:VAL:O	1:E:240:VAL:HG12	2.18	0.44
1:F:122:ALA:HB3	1:F:144:THR:OG1	2.17	0.44
1:A:126:VAL:HG22	1:A:140:MET:HG2	1.99	0.44
1:B:179:GLU:OE2	1:B:179:GLU:N	2.46	0.44
1:C:48:VAL:HG21	1:C:76:PHE:HE2	1.83	0.44
1:D:179:GLU:CD	1:D:179:GLU:H	2.19	0.44
1:A:153:LYS:HE2	1:B:73:LEU:O	2.17	0.44
1:C:97:ALA:HB1	1:C:284:ILE:HD13	1.99	0.44
1:E:122:ALA:HB3	1:E:144:THR:OG1	2.17	0.44
1:F:379:GLN:HG2	1:F:380:PHE:CE1	2.53	0.44
1:A:279:ALA:HB1	1:A:397:VAL:CG1	2.47	0.44
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.90	0.44
1:B:176:ILE:HD13	1:B:330:LEU:CB	2.47	0.44
1:D:177:ARG:HB3	1:D:179:GLU:OE2	2.18	0.44
1:D:290:PRO:HG2	1:D:293:ILE:CG1	2.48	0.44
1:G:107:GLU:OE2	1:H:284:ILE:HB	2.18	0.44
1:B:280:ARG:HB2	1:B:400:MET:HE1	1.99	0.44
1:C:27:ASP:OD1	1:C:28:ASP:N	2.51	0.44
1:C:291:PRO:HD3	1:D:78:VAL:CG2	2.48	0.44
1:D:10:VAL:HG11	1:D:36:VAL:CG1	2.47	0.44
1:F:278:LEU:HG	1:F:370:VAL:HG13	2.00	0.44
1:G:323:GLU:O	1:G:351:ALA:HB3	2.17	0.44
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.83	0.44
1:B:320:GLU:HG3	1:B:369:LEU:HB2	2.00	0.44
1:C:333:LEU:HD21	1:C:345:LEU:CD2	2.48	0.44
1:D:318:LEU:HD21	1:D:372:GLU:HG3	2.00	0.44
1:E:6:ILE:HG23	1:E:262:VAL:HG23	2.00	0.44
1:E:308:ARG:NH1	1:F:107:GLU:HB3	2.33	0.44
1:F:206:VAL:O	1:F:206:VAL:HG13	2.18	0.44
1:A:25:ARG:HB3	1:A:61:GLU:OE2	2.18	0.43
1:C:212:ARG:CD	1:C:217:ILE:HD12	2.48	0.43
1:E:162:SER:OG	1:E:165:GLU:HG3	2.17	0.43
1:E:206:VAL:O	1:E:206:VAL:HG13	2.18	0.43
1:E:300:PRO:O	1:E:304:LYS:HG3	2.18	0.43
1:F:200:ARG:HG3	1:F:200:ARG:HH11	1.82	0.43
1:G:81:ALA:HB1	1:H:391:GLN:NE2	2.32	0.43
1:A:60:GLY:CA	1:A:123:PRO:HG3	2.48	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:328:GLN:HG3	1:A:329:ALA:H	1.82	0.43
1:B:212:ARG:CD	1:B:217:ILE:HD12	2.41	0.43
1:H:113:GLY:O	1:H:262:VAL:HG12	2.18	0.43
1:B:374:ARG:HH11	1:B:374:ARG:CG	2.13	0.43
1:C:7:VAL:HG12	1:C:7:VAL:O	2.19	0.43
1:D:131:ARG:CZ	1:D:134:PRO:HA	2.48	0.43
1:B:336:TRP:CB	1:B:338:LEU:HD13	2.40	0.43
1:E:143:THR:HA	1:E:148:ARG:NH1	2.34	0.43
1:F:57:ASN:ND2	1:F:59:ALA:H	2.16	0.43
1:A:82:GLY:H	1:B:391:GLN:HE22	1.67	0.43
1:B:284:ILE:HG23	1:B:395:VAL:HG22	2.00	0.43
1:D:322:ASN:HD21	1:D:356:HIS:CE1	2.36	0.43
1:E:154:MET:O	1:E:158:TYR:O	2.37	0.43
1:F:3:GLU:OE2	1:F:3:GLU:HA	2.19	0.43
1:F:88:LEU:HD12	1:F:388:GLY:O	2.17	0.43
1:H:9:ALA:HB1	1:H:367:THR:HG23	2.00	0.43
1:H:211:LYS:HG2	1:H:216:GLU:OE1	2.19	0.43
1:A:154:MET:O	1:A:158:TYR:O	2.36	0.43
1:A:385:MET:HE3	1:A:385:MET:HB2	1.98	0.43
1:C:130:GLU:CD	1:D:121:ARG:NH2	2.71	0.43
1:C:262:VAL:HG22	1:C:264:LEU:HD12	2.00	0.43
1:H:6:ILE:HG23	1:H:262:VAL:CG2	2.49	0.43
1:H:318:LEU:C	1:H:319:ILE:HG13	2.39	0.43
1:A:5:TRP:CE3	1:A:277:PRO:CG	3.01	0.43
1:A:87:ARG:CZ	1:B:83:CYS:HB2	2.48	0.43
1:A:278:LEU:HG	1:A:370:VAL:CG1	2.42	0.43
1:B:164:GLY:HA3	1:B:241:PHE:CE1	2.53	0.43
1:C:170:LEU:CD1	1:C:295:GLY:HA3	2.48	0.43
1:C:316:LEU:HD11	1:C:382:LEU:HD22	2.01	0.43
1:E:140:MET:HB2	1:H:138:LEU:HB2	2.00	0.43
1:E:140:MET:CE	1:H:138:LEU:HD12	2.48	0.43
1:F:71:LEU:HD12	1:F:72:LEU:N	2.34	0.43
1:G:299:VAL:HG21	1:G:335:GLU:HG3	2.01	0.43
1:G:328:GLN:HG3	1:G:329:ALA:H	1.82	0.43
1:E:68:ARG:NH2	1:F:390:GLY:O	2.51	0.43
1:F:7:VAL:O	1:F:7:VAL:CG1	2.66	0.43
1:F:387:ILE:HB	1:F:391:GLN:HB2	2.01	0.43
1:H:87:ARG:NH1	1:H:286:VAL:HG11	2.33	0.43
1:H:184:PHE:HA	1:H:340:MET:CE	2.48	0.43
1:A:302:THR:HG23	1:A:382:LEU:HD21	2.01	0.43
1:A:302:THR:HG23	1:A:382:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:VAL:HG12	1:C:11:ARG:N	2.33	0.43
1:D:61:GLU:OE2	1:D:121:ARG:HD3	2.19	0.43
1:D:154:MET:HE3	1:D:158:TYR:HD1	1.83	0.43
1:E:116:VAL:HA	1:E:360:ALA:HB2	2.00	0.43
1:F:162:SER:OG	1:F:165:GLU:HG3	2.18	0.43
1:H:126:VAL:HA	1:H:127:PRO:HD3	1.83	0.43
1:A:178:ARG:CZ	1:A:248:THR:HG21	2.49	0.43
1:B:119:MET:HE2	1:B:255:LEU:HD23	2.00	0.43
1:B:179:GLU:H	1:B:179:GLU:CD	2.21	0.43
1:E:5:TRP:CZ3	1:E:277:PRO:HG3	2.53	0.43
1:F:8:GLU:HB3	1:F:37:LEU:HD11	2.01	0.43
1:G:6:ILE:HG23	1:G:262:VAL:CG2	2.49	0.43
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.83	0.42
1:C:331:ALA:O	1:C:334:ARG:HB2	2.19	0.42
1:F:171:ALA:HA	1:F:176:ILE:CD1	2.44	0.42
1:G:328:GLN:HE21	1:G:328:GLN:HB2	1.57	0.42
1:H:87:ARG:HH21	1:H:94:GLU:CD	2.22	0.42
1:A:290:PRO:HA	1:A:291:PRO:HD3	1.83	0.42
1:C:17:HIS:CE1	1:C:120:SER:HA	2.54	0.42
1:C:151:ASN:HD22	1:C:151:ASN:C	2.21	0.42
1:C:154:MET:O	1:C:158:TYR:O	2.37	0.42
1:E:282:ARG:NH1	1:E:309:ALA:O	2.52	0.42
1:F:140:MET:HE3	1:G:138:LEU:HB2	2.00	0.42
1:D:328:GLN:HG3	1:D:329:ALA:N	2.33	0.42
1:E:126:VAL:HA	1:E:127:PRO:HD3	1.90	0.42
1:E:137:ASN:OD1	1:H:141:TYR:HA	2.18	0.42
1:F:164:GLY:HA3	1:F:241:PHE:CD1	2.54	0.42
1:F:265:VAL:HG22	1:F:266:SER:N	2.34	0.42
1:G:116:VAL:HA	1:G:360:ALA:HB2	2.01	0.42
1:G:154:MET:O	1:G:158:TYR:O	2.38	0.42
1:H:328:GLN:HE21	1:H:328:GLN:HB2	1.58	0.42
1:A:14:ILE:HG21	1:A:355:GLY:HA3	2.00	0.42
1:C:71:LEU:HD12	1:C:71:LEU:C	2.39	0.42
1:C:294:MET:CE	1:C:295:GLY:HA2	2.50	0.42
1:G:206:VAL:HG13	1:G:206:VAL:O	2.19	0.42
1:H:242:ARG:O	1:H:245:GLY:N	2.52	0.42
1:B:93:LEU:HB3	1:B:393:ILE:HD13	2.00	0.42
1:D:204:GLU:OE1	1:D:368:THR:HA	2.20	0.42
1:F:238:ARG:N	1:F:238:ARG:NE	2.67	0.42
1:H:93:LEU:HB2	1:H:385:MET:HE1	2.02	0.42
1:B:328:GLN:HE21	1:B:328:GLN:HB2	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:VAL:HG22	1:C:264:LEU:CD1	2.50	0.42
1:G:286:VAL:HG13	1:H:81:ALA:CB	2.50	0.42
1:H:114:SER:HB2	1:H:260:ALA:O	2.20	0.42
1:H:155:GLN:HE21	1:H:160:THR:CG2	2.33	0.42
1:B:192:ALA:HA	1:B:348:ASN:O	2.20	0.42
1:D:166:THR:HA	1:D:169:ASN:HD22	1.85	0.42
1:E:387:ILE:HB	1:E:391:GLN:CB	2.49	0.42
1:F:10:VAL:HG12	1:F:11:ARG:N	2.34	0.42
1:F:85:VAL:HG11	1:F:94:GLU:HG2	2.00	0.42
1:F:93:LEU:HB2	1:F:385:MET:HE2	2.01	0.42
1:F:252:SER:HB3	1:F:325:PHE:CD1	2.55	0.42
1:G:372:GLU:HA	1:G:375:ARG:HG2	2.02	0.42
1:H:192:ALA:HA	1:H:348:ASN:O	2.20	0.42
1:B:15:GLY:O	1:B:256:ASN:HB3	2.20	0.42
1:B:57:ASN:ND2	1:B:57:ASN:C	2.72	0.42
1:C:3:GLU:HG2	1:C:104:TRP:HA	2.01	0.42
1:C:30:LEU:HD23	1:C:70:ALA:HB3	2.01	0.42
1:D:36:VAL:HG11	1:D:206:VAL:HG21	2.02	0.42
1:D:192:ALA:HA	1:D:348:ASN:O	2.19	0.42
1:D:302:THR:HG23	1:D:382:LEU:HD11	2.01	0.42
1:D:364:ARG:HD2	1:D:364:ARG:O	2.20	0.42
1:E:323:GLU:O	1:E:351:ALA:HB3	2.20	0.42
1:F:154:MET:O	1:F:158:TYR:O	2.38	0.42
1:G:2:PRO:O	1:G:267:ASP:HB3	2.20	0.42
1:G:35:SER:OG	1:G:74:ALA:HB1	2.20	0.42
1:H:237:LEU:CD1	1:H:250:GLY:HA3	2.49	0.42
1:H:267:ASP:O	1:H:271:LYS:HD2	2.20	0.42
1:H:357:PRO:O	1:H:358:LEU:C	2.58	0.42
1:C:87:ARG:N	1:C:91:SER:OG	2.44	0.42
1:C:116:VAL:HG22	1:C:117:GLU:N	2.35	0.42
1:D:214:LYS:H	1:D:214:LYS:CD	2.31	0.42
1:D:306:LEU:HD23	1:D:306:LEU:HA	1.80	0.42
1:E:177:ARG:HB3	1:E:179:GLU:OE2	2.20	0.42
1:E:230:SER:OG	1:E:233:LYS:HG3	2.20	0.42
1:F:140:MET:CE	1:G:138:LEU:HD12	2.50	0.42
1:F:238:ARG:HE	1:F:238:ARG:H	1.68	0.42
1:G:294:MET:HE3	1:G:386:CYS:HB2	2.02	0.42
1:G:357:PRO:O	1:G:358:LEU:C	2.59	0.42
1:A:278:LEU:CG	1:A:370:VAL:HG12	2.45	0.42
1:A:280:ARG:HB2	1:A:400:MET:HE1	2.01	0.42
1:C:9:ALA:CB	1:C:367:THR:HG23	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:HIS:O	1:C:193:VAL:HG23	2.20	0.42
1:D:5:TRP:CE3	1:D:277:PRO:HG3	2.55	0.42
1:D:186:LEU:HD22	1:D:231:LEU:HD13	2.02	0.42
1:G:379:GLN:HG2	1:G:380:PHE:CD1	2.54	0.42
1:H:26:PRO:HG3	1:H:118:SER:HB2	1.99	0.42
1:A:296:ILE:O	1:A:296:ILE:HG23	2.18	0.41
1:A:328:GLN:HE21	1:A:328:GLN:HB2	1.54	0.41
1:B:154:MET:O	1:B:158:TYR:O	2.38	0.41
1:B:162:SER:OG	1:B:165:GLU:HG3	2.20	0.41
1:C:5:TRP:NE1	1:C:400:MET:HE1	2.35	0.41
1:C:87:ARG:CZ	1:D:83:CYS:HB2	2.50	0.41
1:C:147:TRP:CE3	1:C:160:THR:HG22	2.55	0.41
1:C:227:ARG:NH1	1:C:227:ARG:HB2	2.35	0.41
1:D:13:PRO:HD2	1:D:208:VAL:HG23	2.02	0.41
1:D:289:VAL:HB	1:D:290:PRO:HD2	2.01	0.41
1:E:264:LEU:HD12	1:E:264:LEU:N	2.35	0.41
1:G:179:GLU:H	1:G:179:GLU:HG2	1.52	0.41
1:G:291:PRO:HD3	1:H:78:VAL:HG22	2.02	0.41
1:A:184:PHE:HA	1:A:340:MET:HE3	2.01	0.41
1:D:174:TYR:N	1:D:174:TYR:CD1	2.89	0.41
1:E:298:PRO:HD3	1:E:386:CYS:HA	2.02	0.41
1:F:109:LYS:O	1:F:265:VAL:HG23	2.20	0.41
1:F:290:PRO:HA	1:F:291:PRO:HD3	1.99	0.41
1:G:64:ARG:O	1:G:65:ASN:HB3	2.19	0.41
1:G:97:ALA:HB1	1:G:284:ILE:HD13	2.02	0.41
1:C:88:LEU:HB3	1:C:89:CYS:H	1.58	0.41
1:D:118:SER:OG	1:D:121:ARG:HG3	2.20	0.41
1:D:206:VAL:O	1:D:206:VAL:HG13	2.20	0.41
1:D:242:ARG:CB	1:D:242:ARG:NH1	2.84	0.41
1:D:379:GLN:CG	1:D:380:PHE:CE1	3.03	0.41
1:E:302:THR:HG23	1:E:382:LEU:HD11	2.03	0.41
1:F:164:GLY:HA3	1:F:241:PHE:CE1	2.55	0.41
1:A:119:MET:CE	1:A:255:LEU:HD22	2.50	0.41
1:A:126:VAL:HA	1:A:127:PRO:HD3	1.91	0.41
1:E:328:GLN:HG3	1:E:329:ALA:N	2.35	0.41
1:E:372:GLU:OE1	1:E:375:ARG:NH1	2.40	0.41
1:F:178:ARG:CZ	1:F:248:THR:HG21	2.50	0.41
1:E:254:PRO:HG2	1:E:256:ASN:HD21	1.86	0.41
1:F:248:THR:HG23	1:F:251:ASN:ND2	2.36	0.41
1:G:212:ARG:CD	1:G:217:ILE:HD12	2.51	0.41
1:A:25:ARG:HH12	1:B:151:ASN:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:HA	1:C:277:PRO:HD3	1.81	0.41
1:E:87:ARG:HH11	1:E:391:GLN:NE2	2.19	0.41
1:F:5:TRP:CD1	1:F:400:MET:HE1	2.55	0.41
1:F:93:LEU:HD22	1:F:385:MET:CE	2.50	0.41
1:G:16:LYS:CG	1:G:223:GLU:HG3	2.46	0.41
1:G:36:VAL:HG11	1:G:206:VAL:HB	2.02	0.41
1:G:60:GLY:CA	1:G:123:PRO:HG3	2.50	0.41
1:H:54:GLY:HA2	1:H:85:VAL:O	2.20	0.41
1:A:116:VAL:HG22	1:A:117:GLU:N	2.34	0.41
1:A:364:ARG:HD2	1:A:364:ARG:C	2.41	0.41
1:B:60:GLY:C	1:B:62:ASP:H	2.24	0.41
1:C:7:VAL:HG21	1:C:265:VAL:HG22	2.01	0.41
1:C:294:MET:CE	1:C:386:CYS:SG	3.08	0.41
1:C:390:GLY:O	1:D:68:ARG:NH2	2.54	0.41
1:D:206:VAL:HA	1:D:207:PRO:HD3	1.93	0.41
1:D:399:GLY:O	1:D:400:MET:HG2	2.20	0.41
1:E:388:GLY:O	1:E:389:VAL:HB	2.21	0.41
1:G:290:PRO:HG2	1:G:293:ILE:CG1	2.51	0.41
1:H:276:ARG:HA	1:H:277:PRO:HD3	1.87	0.41
1:A:173:MET:HE1	1:A:293:ILE:HD13	2.03	0.41
1:A:182:ASP:CB	1:A:234:LEU:HD23	2.50	0.41
1:B:71:LEU:C	1:B:71:LEU:HD12	2.41	0.41
1:B:85:VAL:CG1	1:B:94:GLU:HG2	2.48	0.41
1:C:107:GLU:HB3	1:D:308:ARG:CZ	2.50	0.41
1:H:10:VAL:HG13	1:H:206:VAL:HG13	2.03	0.41
1:H:109:LYS:O	1:H:265:VAL:HG23	2.20	0.41
1:H:154:MET:HE3	1:H:158:TYR:HB2	2.03	0.41
1:E:78:VAL:HG13	1:F:289:VAL:C	2.41	0.41
1:G:86:ASN:HA	1:G:91:SER:OG	2.21	0.41
1:G:322:ASN:CB	1:G:385:MET:HG2	2.49	0.41
1:H:97:ALA:HB1	1:H:284:ILE:HD13	2.01	0.41
1:B:330:LEU:O	1:B:334:ARG:HG2	2.20	0.41
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.87	0.41
1:D:114:SER:HB3	1:D:261:ALA:CB	2.51	0.41
1:E:13:PRO:HD2	1:E:208:VAL:HG23	2.03	0.41
1:E:48:VAL:HG21	1:E:76:PHE:HE2	1.87	0.41
1:F:141:TYR:HA	1:G:137:ASN:OD1	2.21	0.41
1:G:389:VAL:HG12	1:G:389:VAL:O	2.21	0.41
1:A:71:LEU:HD12	1:A:71:LEU:C	2.41	0.40
1:A:238:ARG:H	1:A:238:ARG:NE	2.18	0.40
1:B:41:SER:OG	1:B:43:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD21	1:B:293:ILE:HB	2.02	0.40
1:B:240:VAL:O	1:B:240:VAL:CG1	2.68	0.40
1:C:7:VAL:HG21	1:C:265:VAL:CG2	2.52	0.40
1:C:122:ALA:HB1	1:C:143:THR:OG1	2.20	0.40
1:E:38:VAL:HG11	1:E:45:LYS:HG2	2.02	0.40
1:E:328:GLN:HE21	1:E:328:GLN:HB2	1.51	0.40
1:F:60:GLY:C	1:F:62:ASP:H	2.24	0.40
1:G:178:ARG:NH1	1:G:178:ARG:HG2	2.35	0.40
1:H:313:PHE:HE2	1:H:338:LEU:HD21	1.85	0.40
1:A:323:GLU:OE1	1:A:350:GLY:CA	2.69	0.40
1:C:328:GLN:HE22	1:C:386:CYS:HB3	1.86	0.40
1:E:372:GLU:HA	1:E:375:ARG:HH11	1.86	0.40
1:H:323:GLU:OE2	1:H:350:GLY:HA3	2.21	0.40
1:A:5:TRP:NE1	1:A:400:MET:HE1	2.37	0.40
1:B:45:LYS:HD3	1:B:76:PHE:HA	2.02	0.40
1:B:135:THR:HA	1:C:142:ASP:OD2	2.22	0.40
1:B:318:LEU:HD21	1:B:372:GLU:CG	2.52	0.40
1:C:44:PRO:HG2	1:C:47:GLU:HG3	2.03	0.40
1:F:16:LYS:HA	1:F:256:ASN:HD22	1.86	0.40
1:F:17:HIS:CE1	1:F:120:SER:HA	2.57	0.40
1:G:78:VAL:HG13	1:H:289:VAL:C	2.42	0.40
1:A:154:MET:HE3	1:A:158:TYR:HB2	2.02	0.40
1:B:196:TRP:CE3	1:B:221:GLN:HG3	2.56	0.40
1:B:334:ARG:HA	1:B:334:ARG:HD3	1.90	0.40
1:C:90:GLY:HA2	1:C:385:MET:HE1	2.01	0.40
1:C:128:LYS:HA	1:C:129:PRO:HD3	1.98	0.40
1:D:155:GLN:NE2	1:D:160:THR:HG23	2.37	0.40
1:D:211:LYS:HD2	1:D:216:GLU:CG	2.43	0.40
1:D:328:GLN:HG3	1:D:329:ALA:H	1.87	0.40
1:F:174:TYR:CB	1:F:176:ILE:HD11	2.30	0.40
1:G:142:ASP:OD1	1:H:128:LYS:HE2	2.22	0.40
1:G:164:GLY:O	1:G:167:ALA:HB3	2.21	0.40
1:H:110:VAL:HG22	1:H:265:VAL:HG23	2.04	0.40
1:H:176:ILE:HD13	1:H:330:LEU:CB	2.50	0.40
1:H:184:PHE:HA	1:H:340:MET:HE3	2.02	0.40
1:A:5:TRP:CZ3	1:A:277:PRO:HG3	2.55	0.40
1:A:93:LEU:HG	1:A:395:VAL:HG21	2.04	0.40
1:C:290:PRO:HA	1:C:291:PRO:HD3	1.88	0.40
1:C:296:ILE:O	1:C:297:GLY:C	2.59	0.40
1:D:93:LEU:HD23	1:D:393:ILE:HG23	2.04	0.40
1:D:155:GLN:HE21	1:D:160:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:VAL:HG13	1:F:81:ALA:CB	2.51	0.40
1:F:9:ALA:CB	1:F:367:THR:HG23	2.46	0.40
1:F:60:GLY:CA	1:F:123:PRO:HG3	2.51	0.40
1:F:379:GLN:O	1:F:398:GLU:HA	2.21	0.40
1:G:78:VAL:HG11	1:H:290:PRO:N	2.36	0.40
1:G:116:VAL:HG22	1:G:117:GLU:N	2.35	0.40
1:G:155:GLN:NE2	1:G:160:THR:OG1	2.54	0.40
1:G:234:LEU:HD12	1:G:234:LEU:HA	1.94	0.40
1:G:299:VAL:HB	1:G:300:PRO:CD	2.52	0.40
1:H:126:VAL:CG2	1:H:140:MET:HG2	2.46	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	396/401 (99%)	377 (95%)	15 (4%)	4 (1%)	15	53
1	B	396/401 (99%)	373 (94%)	20 (5%)	3 (1%)	19	57
1	C	397/401 (99%)	371 (94%)	22 (6%)	4 (1%)	15	53
1	D	397/401 (99%)	377 (95%)	17 (4%)	3 (1%)	19	57
1	E	397/401 (99%)	370 (93%)	24 (6%)	3 (1%)	19	57
1	F	396/401 (99%)	372 (94%)	21 (5%)	3 (1%)	19	57
1	G	397/401 (99%)	371 (94%)	23 (6%)	3 (1%)	19	57
1	H	397/401 (99%)	375 (94%)	19 (5%)	3 (1%)	19	57
All	All	3173/3208 (99%)	2986 (94%)	161 (5%)	26 (1%)	19	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LEU
1	B	358	LEU
1	C	358	LEU
1	D	358	LEU
1	E	358	LEU
1	F	358	LEU
1	G	358	LEU
1	H	358	LEU
1	A	132	GLY
1	E	389	VAL
1	B	389	VAL
1	C	389	VAL
1	F	389	VAL
1	E	132	GLY
1	D	389	VAL
1	G	132	GLY
1	G	389	VAL
1	H	389	VAL
1	A	389	VAL
1	C	359	GLY
1	D	132	GLY
1	A	254	PRO
1	B	134	PRO
1	F	132	GLY
1	H	132	GLY
1	C	132	GLY

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	302/304 (99%)	284 (94%)	18 (6%)	19	53
1	B	302/304 (99%)	286 (95%)	16 (5%)	22	58
1	C	303/304 (100%)	284 (94%)	19 (6%)	18	51
1	D	303/304 (100%)	279 (92%)	24 (8%)	12	41
1	E	303/304 (100%)	286 (94%)	17 (6%)	21	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	302/304 (99%)	291 (96%)	11 (4%)	35	70
1	G	303/304 (100%)	287 (95%)	16 (5%)	22	58
1	H	303/304 (100%)	284 (94%)	19 (6%)	18	51
All	All	2421/2432 (100%)	2281 (94%)	140 (6%)	20	55

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	57	ASN
1	A	78	VAL
1	A	98	GLN
1	A	135	THR
1	A	148	ARG
1	A	183	ARG
1	A	214	LYS
1	A	238	ARG
1	A	263	LEU
1	A	265	VAL
1	A	286	VAL
1	A	292	ARG
1	A	294	MET
1	A	296	ILE
1	A	307	GLU
1	A	328	GLN
1	A	334	ARG
1	B	3	GLU
1	B	25	ARG
1	B	57	ASN
1	B	78	VAL
1	B	98	GLN
1	B	179	GLU
1	B	202	GLN
1	B	214	LYS
1	B	226	ARG
1	B	232	GLU
1	B	282	ARG
1	B	292	ARG
1	B	294	MET
1	B	328	GLN
1	B	341	GLU

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Mol	Chain	Res	Type
1	B	374	ARG
1	C	23	SER
1	C	46	GLU
1	C	57	ASN
1	C	66	VAL
1	C	98	GLN
1	C	135	THR
1	C	151	ASN
1	C	155	GLN
1	C	160	THR
1	C	214	LYS
1	C	234	LEU
1	C	262	VAL
1	C	286	VAL
1	C	292	ARG
1	C	294	MET
1	C	303	ARG
1	C	307	GLU
1	C	328	GLN
1	C	338	LEU
1	D	25	ARG
1	D	46	GLU
1	D	57	ASN
1	D	66	VAL
1	D	71	LEU
1	D	78	VAL
1	D	135	THR
1	D	148	ARG
1	D	155	GLN
1	D	179	GLU
1	D	212	ARG
1	D	214	LYS
1	D	234	LEU
1	D	238	ARG
1	D	242	ARG
1	D	246	THR
1	D	278	LEU
1	D	282	ARG
1	D	294	MET
1	D	307	GLU
1	D	328	GLN
1	D	334	ARG

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Mol	Chain	Res	Type
1	D	341	GLU
1	D	382	LEU
1	E	32	HIS
1	E	35	SER
1	E	66	VAL
1	E	78	VAL
1	E	98	GLN
1	E	135	THR
1	E	148	ARG
1	E	155	GLN
1	E	214	LYS
1	E	215	GLU
1	E	246	THR
1	E	286	VAL
1	E	294	MET
1	E	303	ARG
1	E	328	GLN
1	E	343	GLN
1	E	377	LYS
1	F	57	ASN
1	F	98	GLN
1	F	155	GLN
1	F	214	LYS
1	F	232	GLU
1	F	238	ARG
1	F	246	THR
1	F	286	VAL
1	F	292	ARG
1	F	294	MET
1	F	328	GLN
1	G	57	ASN
1	G	66	VAL
1	G	98	GLN
1	G	155	GLN
1	G	179	GLU
1	G	202	GLN
1	G	214	LYS
1	G	234	LEU
1	G	276	ARG
1	G	278	LEU
1	G	286	VAL
1	G	292	ARG

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Mol	Chain	Res	Type
1	G	294	MET
1	G	328	GLN
1	G	341	GLU
1	G	361	SER
1	H	35	SER
1	H	41	SER
1	H	46	GLU
1	H	57	ASN
1	H	66	VAL
1	H	78	VAL
1	H	83	CYS
1	H	85	VAL
1	H	98	GLN
1	H	214	LYS
1	H	221	GLN
1	H	230	SER
1	H	234	LEU
1	H	268	ASP
1	H	294	MET
1	H	307	GLU
1	H	328	GLN
1	H	341	GLU
1	H	384	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	98	GLN
1	A	155	GLN
1	A	181	GLN
1	A	328	GLN
1	A	391	GLN
1	B	32	HIS
1	B	57	ASN
1	B	98	GLN
1	B	155	GLN
1	B	181	GLN
1	B	273	HIS
1	B	328	GLN
1	B	379	GLN
1	B	391	GLN

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Mol	Chain	Res	Type
1	C	57	ASN
1	C	98	GLN
1	C	151	ASN
1	C	155	GLN
1	C	169	ASN
1	C	328	GLN
1	C	391	GLN
1	D	57	ASN
1	D	98	GLN
1	D	155	GLN
1	D	169	ASN
1	D	251	ASN
1	D	273	HIS
1	D	322	ASN
1	D	328	GLN
1	D	391	GLN
1	E	57	ASN
1	E	98	GLN
1	E	155	GLN
1	E	328	GLN
1	E	391	GLN
1	F	32	HIS
1	F	57	ASN
1	F	98	GLN
1	F	155	GLN
1	F	181	GLN
1	F	251	ASN
1	F	273	HIS
1	F	391	GLN
1	G	17	HIS
1	G	57	ASN
1	G	98	GLN
1	G	155	GLN
1	G	181	GLN
1	G	328	GLN
1	G	391	GLN
1	H	17	HIS
1	H	32	HIS
1	H	57	ASN
1	H	98	GLN
1	H	155	GLN
1	H	273	HIS

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Mol	Chain	Res	Type
1	H	328	GLN
1	H	391	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	A	398/401 (99%)	-0.59	0	100	100	1, 10, 27, 58	0
1	B	398/401 (99%)	-0.60	0	100	100	1, 9, 23, 57	0
1	C	399/401 (99%)	-0.64	2 (0%)	91	75	1, 10, 26, 60	0
1	D	399/401 (99%)	-0.46	0	100	100	1, 14, 32, 57	0
1	E	399/401 (99%)	-0.59	2 (0%)	91	75	1, 13, 31, 64	0
1	F	398/401 (99%)	-0.50	2 (0%)	91	75	1, 13, 32, 61	0
1	G	399/401 (99%)	-0.56	2 (0%)	91	75	3, 14, 33, 65	0
1	H	399/401 (99%)	-0.54	1 (0%)	94	84	1, 11, 28, 61	0
All	All	3189/3208 (99%)	-0.56	9 (0%)	94	84	1, 12, 30, 65	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	215	GLU	3.2
1	G	214	LYS	2.6
1	E	215	GLU	2.5
1	F	215	GLU	2.4
1	E	216	GLU	2.4
1	C	214	LYS	2.4
1	H	215	GLU	2.2
1	F	214	LYS	2.2
1	C	212	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.