Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:57 AM EST

PDB ID	:	3OW7
Title	:	Crystal structure of the membrane fusion protein CusB from Escherichia coli.
Authors	:	Su, C.-C.
Deposited on	:	2010-09-17
Resolution	:	3.78 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
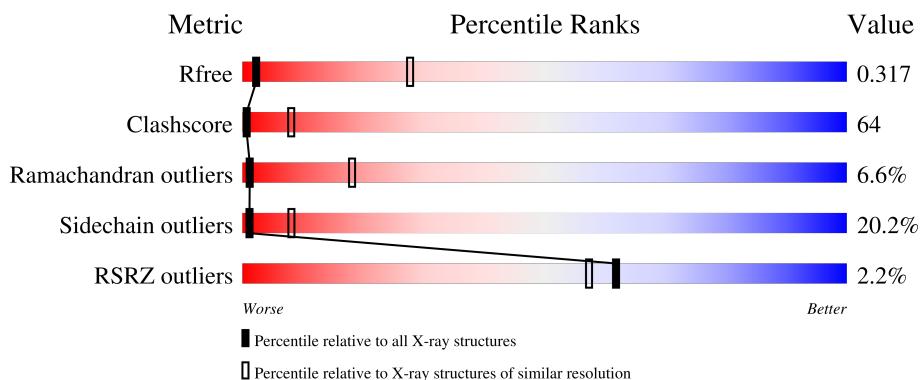
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
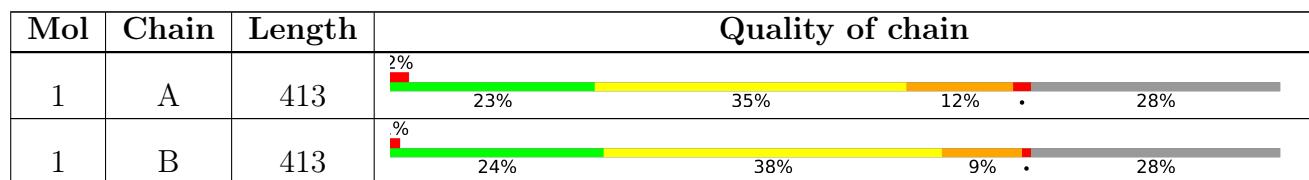
The reported resolution of this entry is 3.78 Å.

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	Percentile Ranks	Value
Rfree		0.317
Clashscore		64
Ramachandran outliers		6.6%
Sidechain outliers		20.2%
RSRZ outliers		2.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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	413	2% · 23% · 35% · 12% · · 28%
1	B	413	% · 24% · 38% · 9% · · 28%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4545 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2267	1444	391	427	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	expression tag	UNP P77239
A	409	HIS	-	expression tag	UNP P77239
A	410	HIS	-	expression tag	UNP P77239
A	411	HIS	-	expression tag	UNP P77239
A	412	HIS	-	expression tag	UNP P77239
A	413	HIS	-	expression tag	UNP P77239
B	408	HIS	-	expression tag	UNP P77239
B	409	HIS	-	expression tag	UNP P77239
B	410	HIS	-	expression tag	UNP P77239
B	411	HIS	-	expression tag	UNP P77239
B	412	HIS	-	expression tag	UNP P77239
B	413	HIS	-	expression tag	UNP P77239
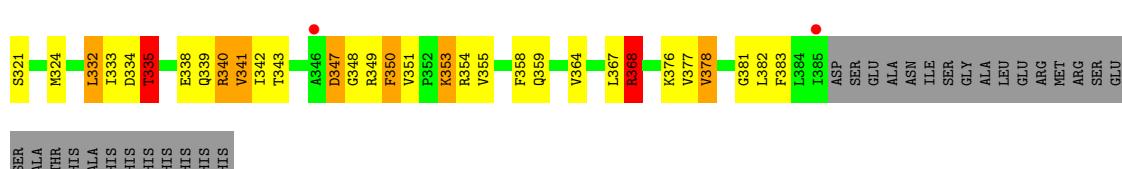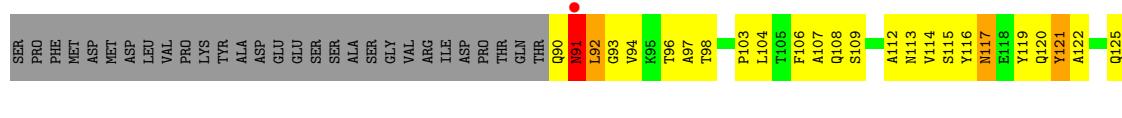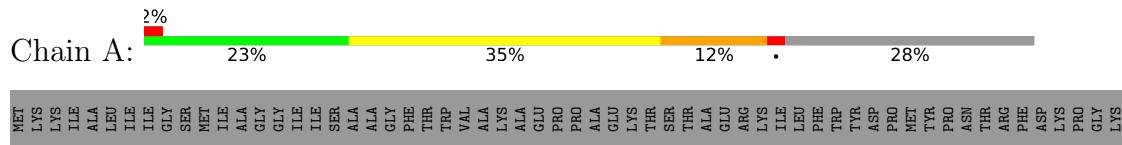
- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
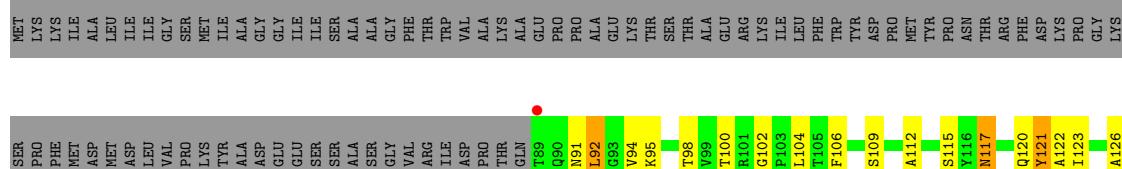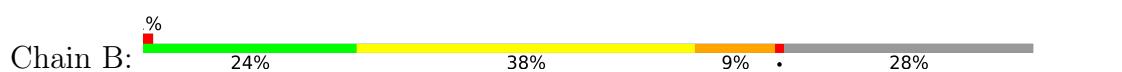
3   Residue-property plots ⓘ
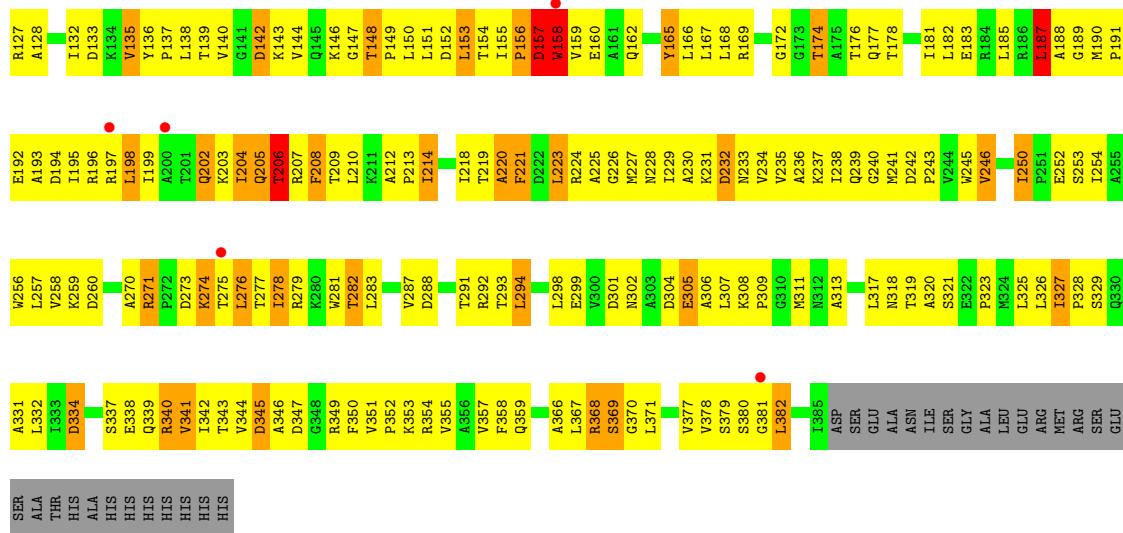
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cation efflux system protein cusB

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R127 A128 I132 D133 K134 V135 Y136 P137 L138 T139 V140 G141 D142 K143 V144 Q145 K146 G147 T148 P149 L150 L151 D152 L153 T154 I155 P156 D157 W158 V159 E160 A161 Q162 Y165 L166 L167 L168 R169 G172 G173 T174 A175 T176 Q177 T178 I181 L182 E183 R184 L185 R186 L187 A188 G189 M190 P191

E192 A193 D194 I195 R196 R197 L198 I199 A200 T201 Q202 K203 I204 Q205 T206 R207 F208 T209 L210 K211 A212 P213 I214 I218 T219 A220 F221 D222 L223 R224 A225 G226 M227 N228 I229 A230 K231 D232 N233 V234 V235 A236 K237 I238 Q239 G240 M241 D242 P243 V244 W245 V246 I250 P251 E252 S253 I254 A255

W256 L257 V258 K259 D260 A270 R271 P272 D273 K274 T275 L276 T277 I278 R279 K280 W281 T282 L283 V287 D288 T291 R292 T293 L294 L298 E299 V300 D301 N302 A303 D304 E305 A306 L307 K308 P309 G310 M311 N312 A313 L317 N318 T319 A320 S321 E322 P323 M324 L325 L326 I327 P328 S329 Q330

A331 L332 I333 D334 S337 E338 Q339 R340 V341 I342 T343 V344 D345 A346 D347 G348 R349 F350 V351 P352 K353 R354 V355 A356 V357 F358 Q359 A366 L367 R368 S369 G370 L371 V377 V378 S379 S380 G381 L382 I385 ASP SER GLU ALA ASN ILE SER GLY ALA LEU GLU ARG MET ARG SER GLU

SER ALA THR HIS ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	84.24Å 111.01Å 258.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.63 – 3.78 36.63 – 3.71	Depositor EDS
% Data completeness (in resolution range)	82.8 (36.63-3.78) 91.7 (36.63-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.20 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.324 0.285 , 0.317	Depositor DCC
R_{free} test set	588 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å²)	148.8	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 194.4	EDS
L-test for twinning [2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å²)	227.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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	0/2306	0.67	4/3142 (0.1%)
1	B	0.34	0/2313	0.62	1/3152 (0.0%)
All	All	0.35	0/4619	0.65	5/6294 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	368	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	231	LYS	N-CA-C	5.82	126.71	111.00
1	A	251	PRO	N-CA-C	-5.37	98.13	112.10
1	B	187	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	368	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	2267	0	2336	338	0
1	B	2274	0	2341	267	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4545	0	4677	592	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 64.

All (592) 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:A:250:ILE:CG2	1:A:255:ALA:HB2	1.57	1.34
1:A:256:TRP:CH2	1:A:257:LEU:HD22	1.64	1.32
1:A:251:PRO:HG2	1:A:254:ILE:CG2	1.66	1.23
1:A:256:TRP:CZ3	1:A:257:LEU:HD22	1.75	1.20
1:A:257:LEU:O	1:A:259:LYS:HD3	1.42	1.19
1:A:368:ARG:HA	1:A:368:ARG:NE	1.52	1.18
1:A:256:TRP:CH2	1:A:257:LEU:CD2	2.30	1.15
1:A:256:TRP:CZ2	1:A:257:LEU:CD2	2.30	1.15
1:B:120:GLN:HG2	1:B:240:GLY:HA3	1.27	1.14
1:B:146:LYS:HD3	1:B:147:GLY:H	1.04	1.13
1:A:148:THR:HB	1:A:149:PRO:HD3	1.31	1.13
1:A:251:PRO:CG	1:A:254:ILE:CG2	2.30	1.08
1:A:228:ASN:C	1:A:229:ILE:HD12	1.74	1.08
1:A:250:ILE:HG23	1:A:251:PRO:HD2	1.28	1.08
1:A:251:PRO:HG2	1:A:254:ILE:HG22	1.29	1.07
1:A:250:ILE:HG21	1:A:255:ALA:CB	1.83	1.07
1:B:132:ILE:HB	1:B:226:GLY:HA2	1.35	1.04
1:A:250:ILE:HG21	1:A:255:ALA:HB2	1.05	1.04
1:A:251:PRO:HD2	1:A:254:ILE:CG2	1.87	1.04
1:A:251:PRO:CG	1:A:254:ILE:HG21	1.89	1.03
1:A:251:PRO:CD	1:A:254:ILE:CG2	2.38	1.01
1:A:256:TRP:CZ2	1:A:257:LEU:HD22	1.89	1.01
1:B:154:THR:HG22	1:B:207:ARG:HB3	1.41	1.00
1:B:331:ALA:O	1:B:341:VAL:HG11	1.61	0.99
1:A:136:TYR:HB3	1:A:138:LEU:HD21	1.44	0.98
1:B:341:VAL:HG12	1:B:342:ILE:H	1.23	0.98
1:A:368:ARG:HA	1:A:368:ARG:CZ	1.93	0.98
1:B:258:VAL:HG13	1:B:259:LYS:H	1.26	0.98
1:B:146:LYS:HD3	1:B:147:GLY:N	1.79	0.97
1:A:235:VAL:HG22	1:A:235:VAL:O	1.61	0.97
1:B:241:MET:HE1	1:B:305:GLU:HG3	1.46	0.96
1:B:166:LEU:HD21	1:B:202:GLN:NE2	1.82	0.95
1:A:256:TRP:CZ2	1:A:257:LEU:HD21	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:CB	1:A:230:ALA:HA	1.99	0.93
1:A:251:PRO:CG	1:A:254:ILE:HG22	1.94	0.92
1:B:241:MET:CE	1:B:305:GLU:HG3	1.99	0.92
1:A:231:LYS:O	1:A:232:ASP:HB2	1.66	0.92
1:A:246:VAL:HG22	1:A:298:LEU:HB2	1.51	0.92
1:A:106:PHE:CD2	1:B:253:SER:HA	2.04	0.92
1:A:368:ARG:NE	1:A:368:ARG:CA	2.29	0.90
1:B:205:GLN:HA	1:B:205:GLN:OE1	1.70	0.90
1:A:256:TRP:CE3	1:A:257:LEU:HA	2.07	0.90
1:A:229:ILE:HD12	1:A:229:ILE:N	1.84	0.89
1:B:331:ALA:O	1:B:341:VAL:CG1	2.20	0.89
1:A:221:PHE:O	1:A:222:ASP:HB3	1.72	0.89
1:A:229:ILE:N	1:A:229:ILE:CD1	2.34	0.89
1:B:142:ASP:O	1:B:218:ILE:CD1	2.21	0.88
1:A:284:LEU:HD21	1:A:297:ARG:HD2	1.52	0.87
1:A:132:ILE:HG23	1:A:227:MET:H	1.40	0.87
1:A:358:PHE:HD2	1:A:368:ARG:NE	1.72	0.87
1:A:250:ILE:HG22	1:A:255:ALA:HB2	1.53	0.86
1:A:256:TRP:CE3	1:A:257:LEU:HD22	2.09	0.86
1:A:235:VAL:O	1:A:236:ALA:CB	2.20	0.86
1:B:368:ARG:HE	1:B:368:ARG:HA	1.40	0.86
1:B:192:GLU:O	1:B:196:ARG:HG3	1.76	0.85
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.58	0.85
1:A:153:LEU:HD21	1:A:208:PHE:HD1	1.41	0.85
1:A:250:ILE:O	1:A:293:THR:HA	1.76	0.85
1:A:251:PRO:CD	1:A:254:ILE:HG21	2.05	0.85
1:A:332:LEU:HA	1:A:341:VAL:CG1	2.07	0.84
1:B:344:VAL:HG12	1:B:346:ALA:H	1.41	0.84
1:A:129:ALA:HB2	1:A:230:ALA:HA	1.59	0.83
1:A:368:ARG:HA	1:A:368:ARG:HE	1.43	0.83
1:B:305:GLU:O	1:B:305:GLU:HG2	1.78	0.83
1:A:256:TRP:CZ3	1:A:257:LEU:HA	2.14	0.83
1:B:340:ARG:HB3	1:B:353:LYS:O	1.79	0.82
1:A:153:LEU:HD23	1:A:155:ILE:HG13	1.61	0.82
1:B:132:ILE:HD11	1:B:229:ILE:HD11	1.61	0.82
1:A:219:THR:HG23	1:A:237:LYS:HB3	1.61	0.82
1:A:256:TRP:CE3	1:A:256:TRP:C	2.53	0.82
1:A:256:TRP:CE2	1:A:257:LEU:HD22	2.15	0.81
1:A:250:ILE:CG2	1:A:251:PRO:HD2	2.10	0.81
1:A:358:PHE:CD2	1:A:368:ARG:NE	2.49	0.81
1:A:250:ILE:HG23	1:A:251:PRO:CD	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HG2	1:B:354:ARG:HA	1.61	0.81
1:A:256:TRP:CE2	1:A:257:LEU:CD2	2.64	0.80
1:B:120:GLN:HG2	1:B:240:GLY:CA	2.09	0.80
1:A:165:TYR:HB2	1:A:181:ILE:HG21	1.62	0.80
1:B:252:GLU:OE1	1:B:292:ARG:HB3	1.82	0.80
1:B:142:ASP:O	1:B:218:ILE:HD13	1.83	0.79
1:A:90:GLN:HG2	1:A:383:PHE:CE1	2.17	0.79
1:B:144:VAL:O	1:B:144:VAL:CG2	2.30	0.79
1:A:308:LYS:HB3	1:A:309:PRO:CD	2.13	0.79
1:A:136:TYR:HB3	1:A:138:LEU:CD2	2.12	0.78
1:A:166:LEU:HD12	1:A:204:ILE:HG13	1.65	0.78
1:B:162:GLN:HE21	1:B:185:LEU:HD21	1.46	0.78
1:A:153:LEU:HD21	1:A:208:PHE:CD1	2.19	0.78
1:A:147:GLY:HA3	1:A:212:ALA:O	1.83	0.78
1:A:340:ARG:HB2	1:A:353:LYS:O	1.84	0.76
1:B:223:LEU:HD23	1:B:223:LEU:H	1.50	0.76
1:A:153:LEU:HD11	1:A:208:PHE:HB2	1.67	0.76
1:A:242:ASP:HB3	1:A:243:PRO:HD3	1.67	0.76
1:B:327:ILE:HD12	1:B:328:PRO:O	1.86	0.76
1:A:148:THR:HB	1:A:149:PRO:CD	2.14	0.75
1:B:148:THR:HB	1:B:149:PRO:HD2	1.66	0.75
1:B:150:LEU:HD11	1:B:212:ALA:HB2	1.66	0.75
1:A:219:THR:HG21	1:A:239:GLN:HG2	1.66	0.75
1:B:120:GLN:CG	1:B:240:GLY:HA3	2.14	0.75
1:A:244:VAL:HG11	1:A:307:LEU:HG	1.68	0.75
1:A:108:GLN:O	1:A:316:GLN:HA	1.87	0.75
1:A:255:ALA:O	1:A:258:VAL:HG23	1.86	0.74
1:A:251:PRO:HD2	1:A:254:ILE:HG22	1.69	0.74
1:A:190:MET:SD	2:A:414:CU1:CU	1.76	0.74
1:B:339:GLN:HE21	1:B:339:GLN:HA	1.51	0.73
1:B:144:VAL:O	1:B:144:VAL:HG23	1.86	0.73
1:A:256:TRP:CE3	1:A:257:LEU:N	2.56	0.73
1:A:319:THR:HG22	1:A:320:ALA:H	1.52	0.73
1:B:142:ASP:O	1:B:218:ILE:HD12	1.88	0.73
1:B:334:ASP:HB2	1:B:338:GLU:O	1.89	0.73
1:A:103:PRO:HB3	1:A:321:SER:O	1.89	0.73
1:A:165:TYR:HE2	1:A:178:THR:HG1	1.36	0.72
1:A:129:ALA:CA	1:A:230:ALA:HA	2.19	0.72
1:A:235:VAL:O	1:A:235:VAL:CG2	2.35	0.72
1:A:251:PRO:HG2	1:A:254:ILE:HG21	1.53	0.72
1:A:284:LEU:HD21	1:A:297:ARG:CD	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CZ	1:A:228:ASN:OD1	2.43	0.71
1:A:148:THR:CB	1:A:149:PRO:HD3	2.16	0.71
1:B:223:LEU:HD23	1:B:223:LEU:N	2.05	0.71
1:A:285:PRO:HG2	1:B:357:VAL:HG23	1.72	0.71
1:A:235:VAL:O	1:A:236:ALA:HB2	1.89	0.71
1:B:198:LEU:O	1:B:202:GLN:HA	1.89	0.71
1:B:92:LEU:HD22	1:B:92:LEU:H	1.54	0.71
1:B:122:ALA:HB3	1:B:214:ILE:HD12	1.71	0.71
1:A:256:TRP:CD2	1:A:257:LEU:HD22	2.26	0.70
1:B:146:LYS:CD	1:B:147:GLY:H	1.95	0.70
1:B:368:ARG:HA	1:B:368:ARG:NE	2.04	0.70
1:A:158:TRP:O	1:A:162:GLN:HG2	1.89	0.70
1:A:153:LEU:CD1	1:A:208:PHE:HB2	2.22	0.70
1:A:256:TRP:C	1:A:256:TRP:HE3	1.93	0.70
1:A:131:PHE:CE2	1:A:228:ASN:OD1	2.44	0.70
1:B:135:VAL:HG21	1:B:224:ARG:HA	1.74	0.69
1:B:377:VAL:HG22	1:B:378:VAL:H	1.58	0.69
1:A:256:TRP:HE3	1:A:256:TRP:O	1.76	0.69
1:B:214:ILE:HD11	1:B:238:ILE:HB	1.74	0.69
1:A:129:ALA:HA	1:A:230:ALA:HA	1.74	0.69
1:A:256:TRP:CE3	1:A:257:LEU:CA	2.76	0.69
1:B:270:ALA:C	1:B:271:ARG:HG3	2.13	0.69
1:B:302:ASN:ND2	1:B:307:LEU:HG	2.08	0.68
1:B:340:ARG:CG	1:B:354:ARG:HA	2.22	0.68
1:B:166:LEU:HD21	1:B:202:GLN:HE22	1.57	0.68
1:A:251:PRO:CD	1:A:254:ILE:HG22	2.13	0.68
1:B:132:ILE:HG13	1:B:227:MET:H	1.59	0.68
1:B:278:ILE:HD12	1:B:298:LEU:HD21	1.75	0.68
1:B:343:THR:HB	1:B:351:VAL:HG13	1.75	0.68
1:A:129:ALA:HB2	1:A:230:ALA:CA	2.24	0.68
1:A:227:MET:O	1:A:229:ILE:HD13	1.94	0.68
1:A:219:THR:CG2	1:A:239:GLN:HG2	2.23	0.67
1:A:284:LEU:N	1:A:284:LEU:HD22	2.09	0.67
1:A:296:LEU:HD23	1:A:296:LEU:O	1.95	0.67
1:A:368:ARG:CA	1:A:368:ARG:HE	1.97	0.67
1:B:250:ILE:O	1:B:293:THR:HA	1.93	0.67
1:B:258:VAL:HG13	1:B:259:LYS:N	2.04	0.67
1:B:152:ASP:C	1:B:153:LEU:HD13	2.15	0.67
1:B:121:TYR:CZ	1:B:237:LYS:HD2	2.30	0.66
1:A:257:LEU:O	1:A:259:LYS:CD	2.34	0.66
1:B:377:VAL:HG22	1:B:378:VAL:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HB2	1:B:380:SER:HB2	1.78	0.65
1:B:142:ASP:OD1	1:B:142:ASP:N	2.30	0.65
1:A:166:LEU:CD1	1:A:204:ILE:HG13	2.26	0.65
1:A:358:PHE:HD2	1:A:368:ARG:CD	2.10	0.65
1:B:358:PHE:HB2	1:B:368:ARG:HB2	1.80	0.64
1:A:107:ALA:O	1:A:108:GLN:HG3	1.97	0.64
1:A:132:ILE:CG2	1:A:227:MET:H	2.08	0.64
1:A:174:THR:HB	1:A:177:GLN:HE21	1.61	0.64
1:A:94:VAL:HG13	1:A:381:GLY:HA3	1.78	0.64
1:A:235:VAL:O	1:A:236:ALA:HB3	1.97	0.64
1:A:129:ALA:HA	1:A:229:ILE:O	1.98	0.64
1:B:347:ASP:HB2	1:B:349:ARG:CD	2.27	0.64
1:A:256:TRP:CH2	1:A:257:LEU:HD21	2.22	0.64
1:A:165:TYR:HE2	1:A:178:THR:OG1	1.81	0.64
1:A:167:LEU:O	1:A:171:THR:HG23	1.98	0.64
1:A:218:ILE:HD12	1:A:218:ILE:H	1.62	0.63
1:A:91:ASN:ND2	1:A:93:GLY:H	1.97	0.63
1:B:117:ASN:OD1	1:B:117:ASN:N	2.27	0.63
1:A:347:ASP:O	1:A:349:ARG:HG2	1.99	0.63
1:B:341:VAL:HG12	1:B:342:ILE:N	2.04	0.63
1:A:153:LEU:HD13	1:A:153:LEU:H	1.64	0.63
1:B:132:ILE:CG1	1:B:227:MET:H	2.11	0.63
1:B:298:LEU:HD23	1:B:299:GLU:H	1.63	0.63
1:A:251:PRO:CD	1:A:251:PRO:O	2.47	0.62
1:A:174:THR:HG22	1:A:176:THR:H	1.64	0.62
1:A:307:LEU:HD12	1:A:308:LYS:O	1.99	0.62
1:A:119:TYR:CE1	1:A:245:TRP:HH2	2.16	0.62
1:A:332:LEU:HA	1:A:341:VAL:HG11	1.80	0.62
1:B:355:VAL:HG11	1:B:371:LEU:HG	1.81	0.62
1:B:228:ASN:C	1:B:229:ILE:HD12	2.19	0.62
1:B:278:ILE:CG1	1:B:298:LEU:HD21	2.30	0.61
1:B:332:LEU:HA	1:B:341:VAL:CG2	2.30	0.61
1:A:129:ALA:CB	1:A:230:ALA:CA	2.76	0.61
1:A:321:SER:HA	1:B:256:TRP:CE2	2.35	0.61
1:A:153:LEU:C	1:A:153:LEU:HD22	2.21	0.61
1:A:284:LEU:HD23	1:A:295:GLN:HB3	1.82	0.61
1:B:214:ILE:HD13	1:B:214:ILE:H	1.64	0.61
1:A:250:ILE:CG2	1:A:255:ALA:CB	2.52	0.61
1:A:250:ILE:HG22	1:A:251:PRO:O	2.00	0.61
1:A:256:TRP:CZ3	1:A:257:LEU:CD2	2.67	0.61
1:A:307:LEU:HD12	1:A:308:LYS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLN:C	1:B:340:ARG:HG3	2.21	0.61
1:A:253:SER:HA	1:B:106:PHE:CE2	2.36	0.61
1:A:253:SER:HB3	1:B:106:PHE:CD2	2.36	0.61
1:A:122:ALA:HB2	1:A:214:ILE:HD11	1.83	0.60
1:A:266:LEU:HD23	1:A:278:ILE:HD11	1.83	0.60
1:A:167:LEU:HD12	1:A:167:LEU:C	2.21	0.60
1:B:279:ARG:HD2	1:B:301:ASP:OD1	2.01	0.60
1:A:245:TRP:HE1	1:A:299:GLU:HG2	1.65	0.60
1:B:339:GLN:HA	1:B:339:GLN:NE2	2.16	0.60
1:B:343:THR:OG1	1:B:353:LYS:HB2	2.01	0.60
1:A:149:PRO:C	1:A:150:LEU:HD12	2.21	0.60
1:A:213:PRO:O	1:A:214:ILE:HG12	2.02	0.60
1:B:319:THR:HG22	1:B:320:ALA:H	1.67	0.60
1:B:166:LEU:HD12	1:B:204:ILE:HG12	1.84	0.60
1:B:168:LEU:HD23	1:B:178:THR:HG22	1.84	0.60
1:A:150:LEU:HD21	1:A:212:ALA:HB2	1.83	0.60
1:B:208:PHE:CD1	1:B:208:PHE:N	2.67	0.60
1:B:183:GLU:O	1:B:187:LEU:HB3	2.02	0.59
1:A:165:TYR:CE1	1:A:198:LEU:HD21	2.37	0.59
1:A:165:TYR:OH	1:A:199:ILE:HG13	2.02	0.59
1:A:278:ILE:HD13	1:A:298:LEU:CD1	2.32	0.59
1:A:308:LYS:HB3	1:A:309:PRO:HD3	1.84	0.59
1:B:331:ALA:HB2	1:B:379:SER:HA	1.83	0.59
1:A:287:VAL:HG12	1:A:294:LEU:HD21	1.84	0.59
1:A:228:ASN:C	1:A:229:ILE:CD1	2.59	0.59
1:B:355:VAL:CG1	1:B:371:LEU:HG	2.32	0.59
1:A:284:LEU:HD21	1:A:297:ARG:HG3	1.83	0.59
1:B:153:LEU:HD13	1:B:153:LEU:N	2.17	0.59
1:A:251:PRO:O	1:A:254:ILE:HG22	2.03	0.59
1:B:288:ASP:HB2	1:B:293:THR:HB	1.85	0.59
1:A:340:ARG:HD3	1:A:354:ARG:HG3	1.85	0.59
1:B:154:THR:HG22	1:B:207:ARG:CB	2.26	0.59
1:A:382:LEU:HD23	1:A:383:PHE:N	2.17	0.59
1:B:229:ILE:HG23	1:B:233:ASN:OD1	2.03	0.59
1:A:117:ASN:ND2	1:A:243:PRO:HB2	2.18	0.58
1:B:104:LEU:O	1:B:320:ALA:HA	2.04	0.58
1:A:150:LEU:O	1:A:151:LEU:O	2.21	0.58
1:B:122:ALA:CB	1:B:214:ILE:HD12	2.34	0.58
1:A:137:PRO:O	1:A:138:LEU:HD13	2.02	0.58
1:B:256:TRP:CE2	1:B:257:LEU:HD22	2.37	0.58
1:B:258:VAL:CG1	1:B:259:LYS:H	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLN:OE1	1:B:205:GLN:CA	2.47	0.58
1:A:126:ALA:O	1:A:232:ASP:N	2.37	0.58
1:A:129:ALA:HB2	1:A:230:ALA:CB	2.34	0.58
1:A:358:PHE:HD1	1:A:359:GLN:HG3	1.67	0.58
1:A:127:ARG:HA	1:A:232:ASP:OD1	2.03	0.58
1:A:148:THR:CB	1:A:149:PRO:CD	2.80	0.58
1:A:246:VAL:CG2	1:A:298:LEU:HB2	2.31	0.57
1:B:288:ASP:CB	1:B:293:THR:HB	2.33	0.57
1:A:333:ILE:HD12	1:A:334:ASP:H	1.69	0.57
1:B:94:VAL:HG12	1:B:381:GLY:HA2	1.86	0.57
1:B:319:THR:HG22	1:B:320:ALA:N	2.20	0.57
1:A:162:GLN:HE22	1:A:190:MET:CE	2.17	0.57
1:A:280:LYS:HA	1:A:280:LYS:HE3	1.87	0.57
1:A:251:PRO:HD2	1:A:251:PRO:O	2.03	0.57
1:A:358:PHE:CD2	1:A:368:ARG:CD	2.87	0.57
1:B:347:ASP:HB2	1:B:349:ARG:HD3	1.87	0.57
1:A:104:LEU:O	1:A:320:ALA:HA	2.04	0.56
1:B:198:LEU:O	1:B:202:GLN:CA	2.52	0.56
1:A:90:GLN:HG2	1:A:383:PHE:HE1	1.68	0.56
1:A:307:LEU:HD12	1:A:307:LEU:C	2.24	0.56
1:B:132:ILE:CD1	1:B:227:MET:H	2.17	0.56
1:A:148:THR:O	1:A:211:LYS:HA	2.04	0.56
1:B:221:PHE:CG	1:B:221:PHE:O	2.58	0.56
1:B:156:PRO:O	1:B:158:TRP:N	2.38	0.56
1:A:250:ILE:CG2	1:A:251:PRO:CD	2.79	0.56
1:A:296:LEU:HD23	1:A:296:LEU:C	2.26	0.56
1:B:278:ILE:CD1	1:B:298:LEU:HD21	2.35	0.56
1:B:152:ASP:CG	1:B:209:THR:HG22	2.27	0.56
1:B:288:ASP:HB3	1:B:291:THR:O	2.06	0.56
1:B:332:LEU:HA	1:B:341:VAL:HG22	1.88	0.56
1:A:125:GLN:HB2	1:A:232:ASP:O	2.06	0.56
1:A:91:ASN:O	1:A:92:LEU:HB2	2.06	0.55
1:A:134:LYS:O	1:A:135:VAL:HB	2.06	0.55
1:A:256:TRP:HD1	1:B:106:PHE:HE2	1.54	0.55
1:B:306:ALA:C	1:B:307:LEU:HD23	2.26	0.55
1:A:358:PHE:CD2	1:A:368:ARG:HD2	2.41	0.55
1:A:94:VAL:HG22	1:A:382:LEU:H	1.72	0.55
1:B:178:THR:O	1:B:181:ILE:HG22	2.06	0.55
1:B:178:THR:O	1:B:182:LEU:HD13	2.06	0.55
1:A:283:LEU:O	1:A:285:PRO:HD3	2.06	0.55
1:B:106:PHE:HZ	1:B:359:GLN:HE22	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:TYR:H	1:B:136:TYR:HD2	1.52	0.55
1:B:146:LYS:CD	1:B:147:GLY:N	2.62	0.55
1:A:97:ALA:HB3	1:A:377:VAL:HG13	1.88	0.55
1:A:253:SER:HB3	1:B:106:PHE:HD2	1.72	0.55
1:A:162:GLN:O	1:A:165:TYR:HB3	2.07	0.55
1:A:138:LEU:HB2	1:A:221:PHE:HE1	1.71	0.55
1:A:285:PRO:CG	1:B:357:VAL:HG23	2.36	0.55
1:A:114:VAL:HG21	1:A:307:LEU:HD13	1.89	0.54
1:A:256:TRP:HD1	1:B:106:PHE:CE2	2.25	0.54
1:B:95:LYS:O	1:B:378:VAL:HG23	2.07	0.54
1:A:284:LEU:HD21	1:A:297:ARG:CG	2.36	0.54
1:A:142:ASP:HB2	1:A:218:ILE:HD13	1.90	0.54
1:A:319:THR:HG22	1:A:320:ALA:N	2.22	0.54
1:B:274:LYS:H	1:B:274:LYS:HD2	1.72	0.54
1:A:92:LEU:O	1:A:92:LEU:HD22	2.08	0.54
1:A:317:LEU:C	1:A:317:LEU:HD12	2.28	0.54
1:B:298:LEU:HD23	1:B:299:GLU:N	2.23	0.54
1:B:340:ARG:NH2	1:B:354:ARG:HH22	2.06	0.54
1:A:114:VAL:HB	1:A:307:LEU:HD11	1.90	0.54
1:A:332:LEU:HA	1:A:341:VAL:HG12	1.88	0.54
1:A:146:LYS:O	1:A:146:LYS:HG2	2.08	0.53
1:A:332:LEU:HG	1:A:333:ILE:N	2.23	0.53
1:B:144:VAL:CG1	1:B:218:ILE:HD11	2.38	0.53
1:B:187:LEU:HD12	1:B:187:LEU:C	2.29	0.53
1:B:194:ASP:OD2	1:B:208:PHE:HB3	2.07	0.53
1:B:305:GLU:O	1:B:305:GLU:CG	2.54	0.53
1:A:121:TYR:HD1	1:A:121:TYR:H	1.56	0.53
1:A:251:PRO:HD2	1:A:254:ILE:HG23	1.81	0.53
1:B:283:LEU:HD23	1:B:294:LEU:HD12	1.90	0.53
1:B:241:MET:HE3	1:B:305:GLU:HG3	1.87	0.53
1:A:283:LEU:HD11	1:A:296:LEU:HD12	1.91	0.53
1:B:327:ILE:HD12	1:B:327:ILE:C	2.29	0.53
1:B:342:ILE:HB	1:B:378:VAL:HG12	1.90	0.53
1:A:91:ASN:CG	1:A:92:LEU:N	2.60	0.53
1:A:260:ASP:O	1:A:263:GLN:HG2	2.09	0.53
1:B:156:PRO:O	1:B:157:ASP:C	2.47	0.53
1:B:202:GLN:O	1:B:203:LYS:C	2.47	0.53
1:B:347:ASP:HB2	1:B:349:ARG:HD2	1.90	0.53
1:A:218:ILE:HD12	1:A:218:ILE:N	2.23	0.52
1:B:140:VAL:HG13	1:B:220:ALA:H	1.72	0.52
1:B:148:THR:CB	1:B:149:PRO:HD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LEU:HD12	1:B:318:ASN:H	1.75	0.52
1:A:249:ALA:HB1	1:A:293:THR:OG1	2.10	0.52
1:A:284:LEU:O	1:A:286:GLY:N	2.43	0.52
1:B:193:ALA:O	1:B:197:ARG:HG3	2.09	0.52
1:B:198:LEU:HD12	1:B:198:LEU:C	2.30	0.52
1:B:302:ASN:ND2	1:B:305:GLU:HA	2.25	0.52
1:A:94:VAL:HG22	1:A:382:LEU:N	2.25	0.52
1:A:114:VAL:HG21	1:A:311:MET:HB2	1.90	0.52
1:B:126:ALA:HB3	1:B:231:LYS:O	2.09	0.52
1:A:305:GLU:O	1:A:306:ALA:HB3	2.10	0.52
1:A:315:LEU:HG	1:A:315:LEU:O	2.10	0.52
1:B:230:ALA:O	1:B:231:LYS:HG3	2.10	0.52
1:A:115:SER:N	1:A:245:TRP:O	2.43	0.52
1:A:244:VAL:HG11	1:A:307:LEU:CG	2.38	0.52
1:A:250:ILE:CG2	1:A:251:PRO:O	2.58	0.52
1:B:147:GLY:HA3	1:B:212:ALA:O	2.10	0.52
1:B:112:ALA:HB3	1:B:313:ALA:O	2.10	0.51
1:B:165:TYR:CD2	1:B:182:LEU:HD11	2.45	0.51
1:B:221:PHE:O	1:B:221:PHE:CD1	2.64	0.51
1:A:117:ASN:N	1:A:117:ASN:OD1	2.42	0.51
1:B:106:PHE:HZ	1:B:359:GLN:NE2	2.08	0.51
1:A:284:LEU:CD2	1:A:297:ARG:HD2	2.35	0.51
1:A:284:LEU:HD11	1:A:297:ARG:HD2	1.92	0.51
1:A:304:ASP:O	1:A:305:GLU:HB2	2.09	0.51
1:B:229:ILE:HD12	1:B:229:ILE:N	2.26	0.51
1:B:174:THR:HG23	1:B:177:GLN:HB3	1.93	0.51
1:B:198:LEU:HD12	1:B:199:ILE:N	2.26	0.51
1:B:223:LEU:HB3	1:B:227:MET:SD	2.51	0.51
1:A:119:TYR:CE1	1:A:245:TRP:CH2	2.99	0.51
1:B:148:THR:HB	1:B:149:PRO:CD	2.39	0.51
1:A:135:VAL:HG12	1:A:136:TYR:O	2.11	0.51
1:B:271:ARG:NH1	1:B:306:ALA:HB1	2.26	0.51
1:B:281:TRP:HZ3	1:B:283:LEU:CD1	2.23	0.51
1:A:231:LYS:O	1:A:232:ASP:CB	2.44	0.51
1:A:334:ASP:HB2	1:A:338:GLU:O	2.11	0.51
1:B:218:ILE:HD12	1:B:218:ILE:H	1.76	0.51
1:A:122:ALA:HB3	1:A:238:ILE:HB	1.91	0.50
1:A:144:VAL:HG13	1:A:218:ILE:HD11	1.93	0.50
1:B:152:ASP:HA	1:B:209:THR:HG22	1.93	0.50
1:A:358:PHE:HD2	1:A:368:ARG:HD2	1.76	0.50
1:A:129:ALA:CB	1:A:230:ALA:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:O	1:A:222:ASP:CB	2.52	0.50
1:A:126:ALA:O	1:A:232:ASP:HA	2.11	0.50
1:A:129:ALA:CA	1:A:229:ILE:O	2.60	0.50
1:A:334:ASP:O	1:A:335:THR:HG23	2.12	0.50
1:B:132:ILE:HG13	1:B:227:MET:N	2.27	0.50
1:B:122:ALA:HB3	1:B:214:ILE:CD1	2.39	0.50
1:B:158:TRP:CH2	1:B:188:ALA:HB1	2.47	0.50
1:B:380:SER:O	1:B:382:LEU:HD23	2.11	0.50
1:A:221:PHE:CG	1:A:222:ASP:N	2.79	0.50
1:A:244:VAL:HG23	1:A:302:ASN:HB3	1.93	0.50
1:A:266:LEU:HD22	1:A:315:LEU:HD13	1.92	0.50
1:A:377:VAL:HG22	1:A:378:VAL:N	2.26	0.50
1:B:198:LEU:O	1:B:202:GLN:N	2.43	0.50
1:B:345:ASP:O	1:B:346:ALA:HB3	2.12	0.50
1:B:341:VAL:CG1	1:B:342:ILE:H	2.04	0.50
1:A:150:LEU:HD12	1:A:150:LEU:N	2.27	0.49
1:A:114:VAL:HG11	1:A:307:LEU:HD22	1.95	0.49
1:A:316:GLN:O	1:A:316:GLN:HG3	2.12	0.49
1:A:368:ARG:HA	1:A:368:ARG:NH2	2.24	0.49
1:B:308:LYS:O	1:B:311:MET:HG3	2.12	0.49
1:B:337:SER:O	1:B:339:GLN:HG2	2.12	0.49
1:B:340:ARG:HA	1:B:355:VAL:HG22	1.95	0.49
1:B:345:ASP:OD1	1:B:345:ASP:N	2.45	0.49
1:A:119:TYR:HE1	1:A:245:TRP:HH2	1.56	0.49
1:A:214:ILE:HG13	1:A:215:ASP:O	2.12	0.49
1:B:135:VAL:HG12	1:B:135:VAL:O	2.12	0.49
1:B:136:TYR:O	1:B:138:LEU:N	2.44	0.49
1:A:278:ILE:HG21	1:A:298:LEU:HD13	1.95	0.49
1:A:121:TYR:HA	1:A:238:ILE:O	2.12	0.49
1:A:256:TRP:CD1	1:B:106:PHE:HE2	2.30	0.49
1:B:121:TYR:CE2	1:B:237:LYS:HD2	2.48	0.49
1:B:230:ALA:O	1:B:233:ASN:OD1	2.30	0.49
1:A:135:VAL:O	1:A:136:TYR:CB	2.59	0.49
1:B:206:THR:HG23	1:B:207:ARG:H	1.77	0.49
1:B:169:ARG:NH1	1:B:202:GLN:HG2	2.27	0.49
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.13	0.49
1:A:265:THR:HB	1:A:316:GLN:HG2	1.94	0.49
1:A:229:ILE:N	1:A:229:ILE:HD13	2.27	0.48
1:B:106:PHE:CZ	1:B:359:GLN:NE2	2.81	0.48
1:A:145:GLN:HG3	1:A:146:LYS:N	2.28	0.48
1:A:227:MET:O	1:A:229:ILE:CD1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:O	1:B:366:ALA:HA	2.14	0.48
1:B:139:THR:N	1:B:142:ASP:OD2	2.39	0.48
1:B:192:GLU:HA	1:B:195:ILE:HD11	1.95	0.48
1:B:342:ILE:O	1:B:377:VAL:HG23	2.13	0.48
1:A:267:THR:HG23	1:A:314:TRP:HB2	1.95	0.48
1:A:307:LEU:CD1	1:A:308:LYS:O	2.61	0.48
1:A:91:ASN:O	1:A:92:LEU:CB	2.62	0.48
1:A:117:ASN:C	1:A:119:TYR:H	2.17	0.48
1:A:273:ASP:HB3	1:A:274:LYS:H	1.47	0.48
1:A:302:ASN:OD1	1:A:302:ASN:C	2.52	0.48
1:B:136:TYR:CZ	1:B:149:PRO:HB2	2.49	0.48
1:A:112:ALA:HB3	1:A:313:ALA:O	2.13	0.47
1:A:358:PHE:CD1	1:A:359:GLN:HG3	2.48	0.47
1:A:106:PHE:HD2	1:B:253:SER:HA	1.67	0.47
1:B:203:LYS:O	1:B:204:ILE:C	2.53	0.47
1:B:278:ILE:O	1:B:278:ILE:HG12	2.11	0.47
1:B:377:VAL:CG2	1:B:378:VAL:H	2.23	0.47
1:B:117:ASN:HD21	1:B:243:PRO:HG2	1.79	0.47
1:B:254:ILE:O	1:B:254:ILE:HG22	2.14	0.47
1:A:237:LYS:HG2	1:A:238:ILE:N	2.30	0.47
1:B:339:GLN:HB3	1:B:355:VAL:O	2.14	0.47
1:A:232:ASP:O	1:A:233:ASN:C	2.52	0.47
1:A:291:THR:CG2	1:A:293:THR:HB	2.45	0.47
1:B:308:LYS:H	1:B:311:MET:HE3	1.79	0.47
1:A:150:LEU:C	1:A:151:LEU:HD23	2.35	0.47
1:A:136:TYR:CD1	1:A:137:PRO:HD2	2.50	0.47
1:A:245:TRP:CZ3	1:A:297:ARG:NH2	2.82	0.47
1:B:210:LEU:HD12	1:B:210:LEU:C	2.36	0.47
1:A:91:ASN:CB	1:A:382:LEU:HD22	2.45	0.46
1:A:96:THR:OG1	1:A:376:LYS:HD3	2.15	0.46
1:A:122:ALA:HB2	1:A:214:ILE:CD1	2.45	0.46
1:A:150:LEU:N	1:A:150:LEU:CD1	2.78	0.46
1:A:224:ARG:HG2	1:A:225:ALA:N	2.30	0.46
1:A:227:MET:C	1:A:229:ILE:CD1	2.83	0.46
1:A:358:PHE:CD2	1:A:368:ARG:CZ	2.97	0.46
1:A:120:GLN:HG2	1:A:240:GLY:HA3	1.97	0.46
1:A:260:ASP:OD1	1:A:262:SER:N	2.36	0.46
1:A:343:THR:O	1:A:350:PHE:HA	2.15	0.46
1:B:112:ALA:HB3	1:B:313:ALA:HB3	1.96	0.46
1:B:112:ALA:HB1	1:B:246:VAL:HG23	1.97	0.46
1:B:327:ILE:HD11	1:B:332:LEU:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HG23	1:A:227:MET:N	2.20	0.46
1:B:235:VAL:CG2	1:B:236:ALA:N	2.78	0.46
1:A:104:LEU:HD12	1:A:324:MET:HE1	1.96	0.46
1:A:284:LEU:HD22	1:A:284:LEU:H	1.78	0.46
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.71	0.46
1:B:219:THR:O	1:B:220:ALA:HB3	2.15	0.46
1:B:271:ARG:HB2	1:B:273:ASP:OD1	2.16	0.46
1:B:327:ILE:CD1	1:B:328:PRO:O	2.61	0.46
1:B:377:VAL:CG2	1:B:378:VAL:N	2.77	0.46
1:A:156:PRO:O	1:A:159:VAL:HG22	2.15	0.46
1:A:190:MET:HA	1:A:191:PRO:HD2	1.78	0.46
1:B:332:LEU:HA	1:B:341:VAL:HG21	1.96	0.46
1:B:127:ARG:O	1:B:128:ALA:HB2	2.16	0.46
1:B:274:LYS:HD2	1:B:274:LYS:N	2.31	0.46
1:B:275:THR:HG23	1:B:277:THR:HG23	1.97	0.46
1:B:132:ILE:HG13	1:B:227:MET:O	2.16	0.46
1:B:132:ILE:HD12	1:B:227:MET:H	1.80	0.46
1:B:153:LEU:HD22	1:B:208:PHE:O	2.15	0.46
1:A:253:SER:HA	1:B:106:PHE:HE2	1.81	0.45
1:A:382:LEU:HD23	1:A:382:LEU:C	2.37	0.45
1:B:302:ASN:HD21	1:B:307:LEU:HG	1.79	0.45
1:B:166:LEU:CD1	1:B:204:ILE:HG12	2.47	0.45
1:A:367:LEU:O	1:A:368:ARG:NH2	2.49	0.45
1:B:282:THR:OG1	1:B:283:LEU:N	2.49	0.45
1:A:266:LEU:CD2	1:A:315:LEU:HD13	2.46	0.45
1:B:304:ASP:O	1:B:305:GLU:HB3	2.17	0.45
1:A:135:VAL:O	1:A:136:TYR:HB2	2.15	0.45
1:A:259:LYS:HE2	1:A:259:LYS:HB2	1.75	0.45
1:B:132:ILE:HG22	1:B:133:ASP:N	2.32	0.45
1:A:339:GLN:O	1:A:340:ARG:HB3	2.15	0.45
1:B:254:ILE:O	1:B:254:ILE:CG2	2.64	0.45
1:B:115:SER:N	1:B:245:TRP:O	2.50	0.45
1:A:142:ASP:OD2	1:A:142:ASP:N	2.51	0.44
1:A:153:LEU:C	1:A:153:LEU:CD2	2.85	0.44
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.62	0.44
1:B:210:LEU:HD12	1:B:210:LEU:O	2.17	0.44
1:B:302:ASN:CG	1:B:305:GLU:HA	2.36	0.44
1:B:368:ARG:O	1:B:369:SER:CB	2.65	0.44
1:A:167:LEU:HD12	1:A:168:LEU:N	2.32	0.44
1:A:250:ILE:HG21	1:A:255:ALA:CA	2.44	0.44
1:A:297:ARG:O	1:A:298:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HB	1:A:378:VAL:HG12	1.98	0.44
1:A:132:ILE:HD12	1:A:151:LEU:HD12	1.98	0.44
1:A:253:SER:HA	1:A:256:TRP:CD1	2.52	0.44
1:B:156:PRO:O	1:B:159:VAL:N	2.34	0.44
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.16	0.44
1:B:246:VAL:HG13	1:B:298:LEU:HB3	1.99	0.44
1:B:327:ILE:HD12	1:B:328:PRO:C	2.38	0.44
1:B:92:LEU:HD22	1:B:92:LEU:N	2.28	0.44
1:B:102:GLY:O	1:B:323:PRO:HA	2.17	0.44
1:B:132:ILE:HG22	1:B:133:ASP:H	1.82	0.44
1:A:144:VAL:HG22	1:A:216:GLY:O	2.18	0.44
1:A:201:THR:C	1:A:203:LYS:H	2.21	0.44
1:B:159:VAL:HG23	1:B:160:GLU:N	2.32	0.44
1:A:91:ASN:HB2	1:A:382:LEU:HD22	2.00	0.44
1:A:213:PRO:C	1:A:214:ILE:HG12	2.38	0.44
1:A:291:THR:HG22	1:A:293:THR:HB	2.00	0.44
1:B:133:ASP:HB3	1:B:152:ASP:HB2	1.99	0.44
1:B:147:GLY:CA	1:B:212:ALA:O	2.66	0.43
1:B:155:ILE:HG13	1:B:208:PHE:HE1	1.82	0.43
1:B:155:ILE:O	1:B:159:VAL:HG13	2.18	0.43
1:B:157:ASP:O	1:B:158:TRP:C	2.56	0.43
1:B:190:MET:HA	1:B:191:PRO:HD2	1.79	0.43
1:B:307:LEU:HD23	1:B:307:LEU:N	2.33	0.43
1:A:258:VAL:HA	1:A:263:GLN:OE1	2.18	0.43
1:B:104:LEU:HD12	1:B:104:LEU:HA	1.74	0.43
1:B:136:TYR:CD2	1:B:136:TYR:N	2.86	0.43
1:B:139:THR:O	1:B:142:ASP:OD1	2.36	0.43
1:B:271:ARG:HE	1:B:311:MET:HE1	1.82	0.43
1:B:345:ASP:C	1:B:347:ASP:H	2.21	0.43
1:B:165:TYR:CD1	1:B:165:TYR:C	2.92	0.43
1:B:256:TRP:CE2	1:B:257:LEU:CD2	3.00	0.43
1:A:120:GLN:CG	1:A:240:GLY:HA3	2.49	0.43
1:A:196:ARG:O	1:A:199:ILE:HG22	2.18	0.43
1:B:231:LYS:CG	1:B:232:ASP:H	2.31	0.43
1:B:234:VAL:HG13	1:B:234:VAL:O	2.19	0.43
1:A:198:LEU:C	1:A:198:LEU:HD23	2.39	0.43
1:A:340:ARG:CD	1:A:354:ARG:HG3	2.47	0.43
1:B:144:VAL:O	1:B:144:VAL:HG22	2.15	0.43
1:B:340:ARG:HH21	1:B:354:ARG:HH22	1.66	0.43
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.36	0.43
1:B:339:GLN:O	1:B:340:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HG23	1:B:350:PHE:HB3	2.00	0.43
1:A:134:LYS:O	1:A:135:VAL:CB	2.67	0.43
1:A:256:TRP:HA	1:B:358:PHE:HZ	1.83	0.43
1:A:270:ALA:O	1:A:272:PRO:HD2	2.18	0.43
1:A:114:VAL:HG12	1:A:246:VAL:HG12	2.01	0.43
1:A:153:LEU:O	1:A:207:ARG:HA	2.19	0.43
1:A:250:ILE:HD13	1:A:250:ILE:HA	1.88	0.43
1:A:130:GLY:HA3	1:A:155:ILE:HG12	2.01	0.42
1:A:155:ILE:HG22	1:A:157:ASP:H	1.84	0.42
1:B:256:TRP:CD2	1:B:257:LEU:HD22	2.54	0.42
1:B:331:ALA:O	1:B:341:VAL:HG13	2.12	0.42
1:A:231:LYS:HD2	1:A:231:LYS:HA	1.63	0.42
1:B:152:ASP:CG	1:B:209:THR:CG2	2.88	0.42
1:B:275:THR:HG23	1:B:277:THR:OG1	2.18	0.42
1:A:174:THR:N	1:A:177:GLN:HG3	2.34	0.42
1:A:244:VAL:HG12	1:A:245:TRP:N	2.35	0.42
1:A:297:ARG:C	1:A:298:LEU:HD23	2.39	0.42
1:A:284:LEU:HD23	1:A:295:GLN:CB	2.49	0.42
1:B:224:ARG:O	1:B:225:ALA:HB3	2.20	0.42
1:A:132:ILE:HG13	1:A:133:ASP:N	2.35	0.42
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.92	0.42
1:B:232:ASP:OD1	1:B:232:ASP:N	2.53	0.42
1:B:317:LEU:HD12	1:B:318:ASN:N	2.35	0.42
1:A:138:LEU:HB2	1:A:221:PHE:CE1	2.53	0.42
1:A:264:PHE:HE1	1:A:281:TRP:CG	2.37	0.42
1:A:244:VAL:HG12	1:A:245:TRP:H	1.85	0.42
1:A:130:GLY:N	1:A:229:ILE:O	2.52	0.41
1:A:150:LEU:CD2	1:A:212:ALA:HB2	2.50	0.41
1:A:287:VAL:HG12	1:A:294:LEU:CD2	2.49	0.41
1:B:250:ILE:HG22	1:B:294:LEU:HB2	2.02	0.41
1:B:351:VAL:HA	1:B:352:PRO:HD3	1.94	0.41
1:A:159:VAL:HG23	1:A:160:GLU:N	2.36	0.41
1:A:182:LEU:HD21	1:A:199:ILE:HD12	2.01	0.41
1:A:91:ASN:ND2	1:A:93:GLY:N	2.66	0.41
1:A:177:GLN:H	1:A:177:GLN:HG2	1.63	0.41
1:A:250:ILE:HG23	1:A:254:ILE:HG23	2.02	0.41
1:A:284:LEU:N	1:A:284:LEU:CD2	2.79	0.41
1:B:278:ILE:HG13	1:B:298:LEU:HD21	2.03	0.41
1:A:167:LEU:C	1:A:167:LEU:CD1	2.88	0.41
1:A:241:MET:SD	1:A:305:GLU:OE1	2.78	0.41
1:A:244:VAL:HG21	1:A:302:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PRO:C	1:A:138:LEU:HD13	2.41	0.41
1:A:174:THR:HG22	1:A:176:THR:N	2.34	0.41
1:B:144:VAL:HG12	1:B:218:ILE:HD11	2.02	0.41
1:B:174:THR:O	1:B:178:THR:HG23	2.20	0.41
1:A:168:LEU:HD12	1:A:173:GLY:HA3	2.03	0.41
1:B:95:LYS:HB2	1:B:379:SER:O	2.21	0.41
1:A:155:ILE:HA	1:A:156:PRO:HD3	1.71	0.41
1:B:331:ALA:HB2	1:B:379:SER:CA	2.49	0.41
1:B:140:VAL:CG1	1:B:220:ALA:H	2.34	0.41
1:B:288:ASP:HB3	1:B:293:THR:HB	2.00	0.41
1:A:162:GLN:HE22	1:A:190:MET:HE3	1.84	0.40
1:A:254:ILE:HG23	1:A:255:ALA:N	2.36	0.40
1:A:342:ILE:CG2	1:A:350:PHE:HB3	2.51	0.40
1:B:128:ALA:CB	1:B:158:TRP:CZ3	3.04	0.40
1:B:275:THR:HG23	1:B:277:THR:CG2	2.51	0.40
1:A:91:ASN:HD21	1:A:93:GLY:H	1.67	0.40
1:A:237:LYS:HG2	1:A:238:ILE:H	1.86	0.40
1:B:276:LEU:HA	1:B:276:LEU:HD13	1.83	0.40
1:B:347:ASP:N	1:B:347:ASP:OD1	2.55	0.40
1:A:104:LEU:HD21	1:A:364:VAL:HG23	2.01	0.40
1:A:159:VAL:CG2	1:A:160:GLU:N	2.85	0.40
1:A:311:MET:HB3	1:A:312:ASN:H	1.66	0.40
1:B:104:LEU:N	1:B:321:SER:OG	2.55	0.40
1:B:223:LEU:N	1:B:223:LEU:CD2	2.75	0.40
1:B:230:ALA:O	1:B:231:LYS:CG	2.70	0.40
1:B:287:VAL:HA	1:B:293:THR:O	2.22	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	294/413 (71%)	227 (77%)	44 (15%)	23 (8%)	1	14
1	B	295/413 (71%)	240 (81%)	39 (13%)	16 (5%)	2	22
All	All	589/826 (71%)	467 (79%)	83 (14%)	39 (7%)	1	18

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	151	LEU
1	A	204	ILE
1	A	214	ILE
1	A	236	ALA
1	B	156	PRO
1	B	157	ASP
1	B	221	PHE
1	A	91	ASN
1	A	92	LEU
1	A	148	THR
1	A	222	ASP
1	A	272	PRO
1	A	311	MET
1	A	335	THR
1	A	341	VAL
1	A	348	GLY
1	B	135	VAL
1	B	172	GLY
1	A	270	ALA
1	A	273	ASP
1	A	305	GLU
1	A	308	LYS
1	B	158	TRP
1	B	206	THR
1	A	221	PHE
1	A	225	ALA
1	A	285	PRO
1	A	290	ALA
1	B	369	SER
1	A	340	ARG
1	B	137	PRO
1	B	189	GLY
1	B	213	PRO
1	B	220	ALA

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Mol	Chain	Res	Type
1	B	341	VAL
1	B	204	ILE
1	B	309	PRO
1	B	370	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	242/338 (72%)	192 (79%)	50 (21%)	1	7
1	B	243/338 (72%)	195 (80%)	48 (20%)	1	8
All	All	485/676 (72%)	387 (80%)	98 (20%)	1	8

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	98	THR
1	A	109	SER
1	A	113	ASN
1	A	116	TYR
1	A	117	ASN
1	A	121	TYR
1	A	132	ILE
1	A	134	LYS
1	A	136	TYR
1	A	138	LEU
1	A	142	ASP
1	A	150	LEU
1	A	153	LEU
1	A	167	LEU
1	A	168	LEU
1	A	178	THR
1	A	198	LEU
1	A	204	ILE

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Mol	Chain	Res	Type
1	A	206	THR
1	A	207	ARG
1	A	210	LEU
1	A	215	ASP
1	A	219	THR
1	A	222	ASP
1	A	224	ARG
1	A	229	ILE
1	A	231	LYS
1	A	235	VAL
1	A	256	TRP
1	A	258	VAL
1	A	260	ASP
1	A	271	ARG
1	A	273	ASP
1	A	276	LEU
1	A	280	LYS
1	A	282	THR
1	A	292	ARG
1	A	298	LEU
1	A	307	LEU
1	A	316	GLN
1	A	332	LEU
1	A	335	THR
1	A	347	ASP
1	A	350	PHE
1	A	351	VAL
1	A	353	LYS
1	A	355	VAL
1	A	368	ARG
1	A	378	VAL
1	B	91	ASN
1	B	92	LEU
1	B	98	THR
1	B	100	THR
1	B	109	SER
1	B	117	ASN
1	B	121	TYR
1	B	123	ILE
1	B	142	ASP
1	B	143	LYS
1	B	148	THR

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Mol	Chain	Res	Type
1	B	151	LEU
1	B	153	LEU
1	B	157	ASP
1	B	158	TRP
1	B	165	TYR
1	B	167	LEU
1	B	174	THR
1	B	176	THR
1	B	187	LEU
1	B	198	LEU
1	B	202	GLN
1	B	205	GLN
1	B	206	THR
1	B	208	PHE
1	B	214	ILE
1	B	223	LEU
1	B	232	ASP
1	B	239	GLN
1	B	246	VAL
1	B	250	ILE
1	B	260	ASP
1	B	271	ARG
1	B	274	LYS
1	B	276	LEU
1	B	278	ILE
1	B	282	THR
1	B	294	LEU
1	B	305	GLU
1	B	326	LEU
1	B	327	ILE
1	B	329	SER
1	B	334	ASP
1	B	340	ARG
1	B	345	ASP
1	B	367	LEU
1	B	368	ARG
1	B	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	177	GLN
1	A	228	ASN
1	A	330	GLN
1	A	339	GLN
1	A	359	GLN
1	B	145	GLN
1	B	239	GLN
1	B	263	GLN
1	B	302	ASN
1	B	318	ASN
1	B	339	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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	296/413 (71%)	0.01	7 (2%)	59	54	133, 211, 301, 394	0
1	B	297/413 (71%)	0.11	6 (2%)	65	61	135, 224, 341, 582	0
All	All	593/826 (71%)	0.06	13 (2%)	62	57	133, 218, 329, 582	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	4.8
1	B	197	ARG	3.4
1	B	89	THR	3.0
1	B	158	TRP	2.9
1	B	275	THR	2.9
1	A	91	ASN	2.5
1	B	200	ALA	2.4
1	A	157	ASP	2.4
1	A	346	ALA	2.4
1	A	213	PRO	2.4
1	B	381	GLY	2.2
1	A	211	LYS	2.1
1	A	300	VAL	2.0

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	CU1	A	415	1/1	0.73	0.31	247,247,247,247	0
2	CU1	B	415	1/1	0.86	2.40	547,547,547,547	0
2	CU1	A	414	1/1	0.90	0.59	452,452,452,452	0
2	CU1	B	414	1/1	0.97	0.42	296,296,296,296	0

6.5 Other polymers ⓘ

There are no such residues in this entry.