



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:41 pm BST

PDB ID : 1HTZ  
Title : CRYSTAL STRUCTURE OF TEM52 BETA-LACTAMASE  
Authors : Stevens, R.C.; Orenica, M.C.  
Deposited on : 2001-01-03  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

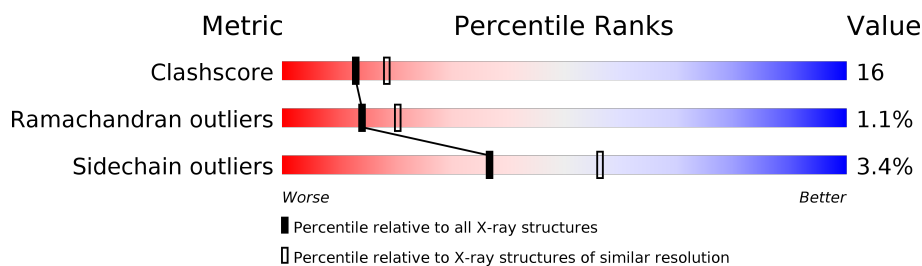
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	263	83% 15% .
1	B	263	77% 21% .
1	C	263	80% 17% .
1	D	263	81% 17% .
1	E	263	78% 21% .
1	F	263	35% 60% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12753 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 BETA-LACTAMASE MUTANT TEM52.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			
1	B	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			
1	C	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			
1	D	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			
1	E	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			
1	F	263	Total	C	N	O	S	0	0	0
			2028	1266	361	391	10			

- Molecule 2 is water.

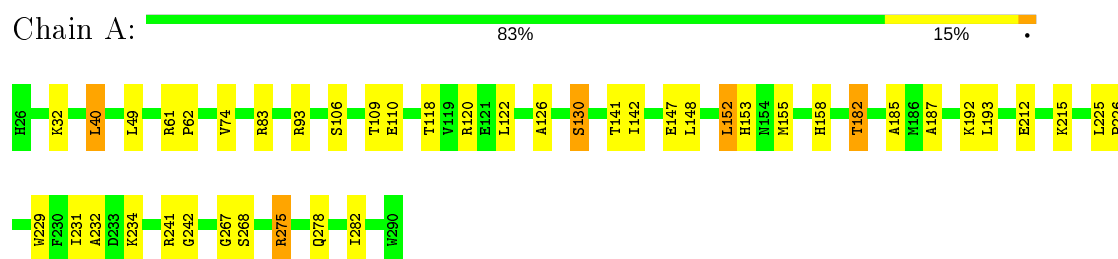
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		
2	B	65	Total	O	0	0
			65	65		
2	C	106	Total	O	0	0
			106	106		
2	D	109	Total	O	0	0
			109	109		
2	E	146	Total	O	0	0
			146	146		
2	F	26	Total	O	0	0
			26	26		

### 3 Residue-property plots [i](#)

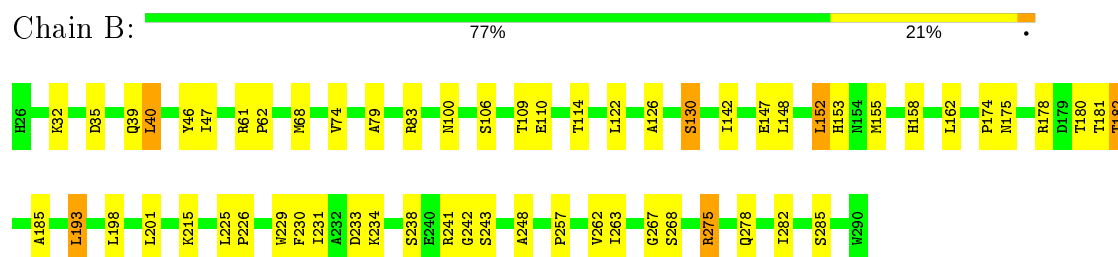
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

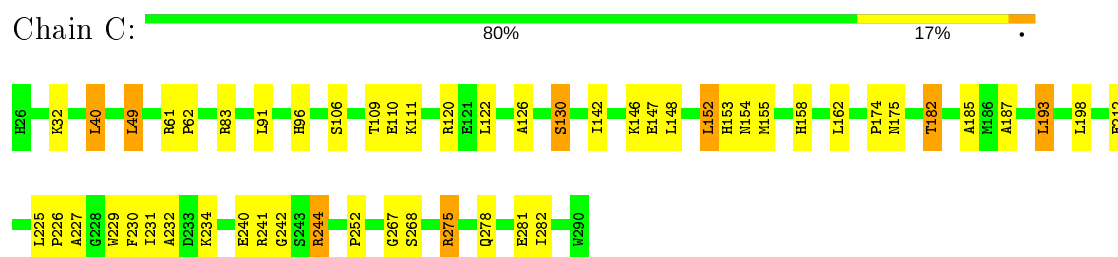
#### • Molecule 1: BETA-LACTAMASE MUTANT TEM52



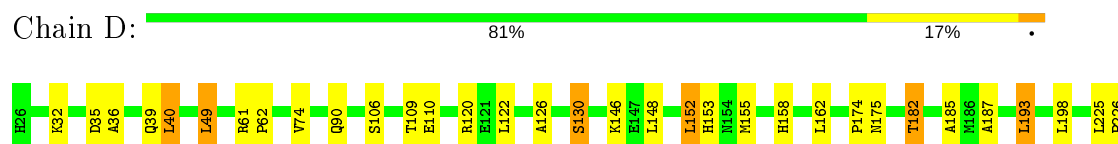
#### • Molecule 1: BETA-LACTAMASE MUTANT TEM52

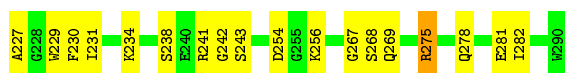


#### • Molecule 1: BETA-LACTAMASE MUTANT TEM52



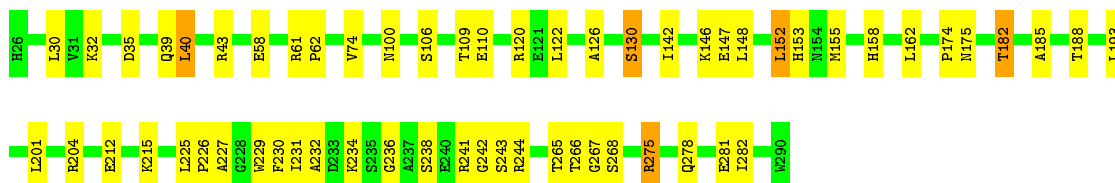
#### • Molecule 1: BETA-LACTAMASE MUTANT TEM52





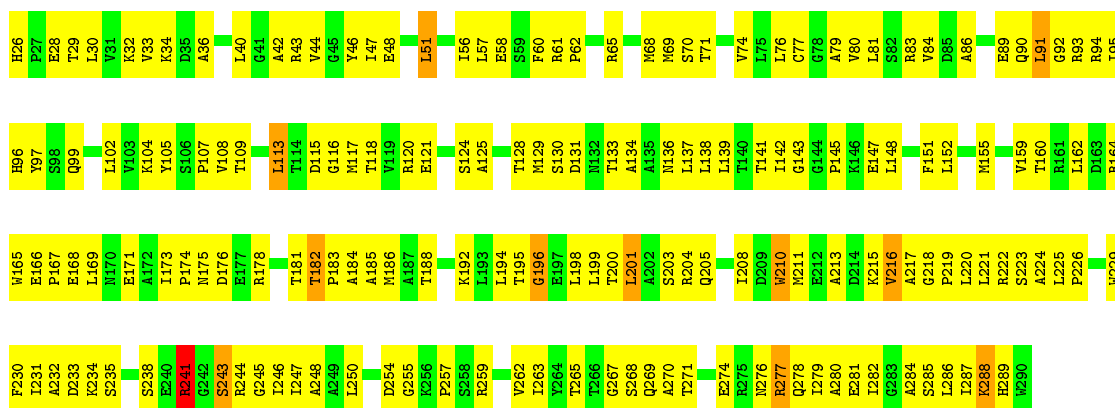
• Molecule 1: BETA-LACTAMASE MUTANT TEM52

Chain E: 78% 21% .



• Molecule 1: BETA-LACTAMASE MUTANT TEM52

Chain F: 35% 60% .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.38 Å 88.38 Å 500.39 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	91.0 (20.00-2.40)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.217 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 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	0.35	0/2062	0.61	0/2792
1	B	0.31	0/2062	0.60	0/2792
1	C	0.34	0/2062	0.61	0/2792
1	D	0.34	0/2062	0.61	0/2792
1	E	0.35	0/2062	0.62	0/2792
1	F	0.35	0/2062	0.58	0/2792
All	All	0.34	0/12372	0.60	0/16752

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	2028	0	2041	35	0
1	B	2028	0	2041	46	0
1	C	2028	0	2041	49	0
1	D	2028	0	2041	48	0
1	E	2028	0	2041	51	0
1	F	2028	0	2041	175	0
2	A	133	0	0	5	0
2	B	65	0	0	5	0
2	C	106	0	0	6	0
2	D	109	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	146	0	0	10	0
2	F	26	0	0	20	0
All	All	12753	0	12246	400	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 16.

All (400) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:HG22	1:B:185:ALA:H	1.24	1.01
1:A:182:THR:HG22	1:A:185:ALA:H	1.25	1.00
1:C:182:THR:HG22	1:C:185:ALA:H	1.23	0.98
1:D:182:THR:HG22	1:D:185:ALA:H	1.24	0.98
1:E:182:THR:HG22	1:E:185:ALA:H	1.25	0.97
1:F:203:SER:HB2	2:F:512:HOH:O	1.70	0.90
1:F:241:ARG:HB2	1:F:241:ARG:HH11	1.36	0.89
1:F:40:LEU:HD11	1:F:278:GLN:HG3	1.55	0.89
1:C:241:ARG:HB3	1:C:241:ARG:HH11	1.37	0.86
1:E:62:PRO:O	1:E:182:THR:HG23	1.76	0.84
1:F:217:ALA:O	1:F:222:ARG:HG3	1.77	0.84
1:D:226:PRO:HG2	1:D:229:TRP:CD1	2.13	0.83
1:F:62:PRO:O	1:F:182:THR:HG23	1.77	0.83
1:C:226:PRO:HG2	1:C:229:TRP:CD1	2.15	0.82
1:E:226:PRO:HG2	1:E:229:TRP:CD1	2.13	0.82
1:F:225:LEU:HG	1:F:226:PRO:HD2	1.62	0.81
1:B:62:PRO:O	1:B:182:THR:HG23	1.82	0.80
1:F:218:GLY:H	1:F:219:PRO:HD2	1.45	0.80
1:F:117:MET:HB3	2:F:444:HOH:O	1.81	0.79
1:F:269:GLN:HG3	2:F:513:HOH:O	1.83	0.79
1:D:90:GLN:HG3	2:D:375:HOH:O	1.83	0.78
1:F:159:VAL:HG11	1:F:182:THR:HB	1.66	0.77
1:B:226:PRO:HG2	1:B:229:TRP:CD1	2.19	0.77
1:A:226:PRO:HG2	1:A:229:TRP:CD1	2.20	0.77
1:A:62:PRO:O	1:A:182:THR:HG23	1.84	0.77
1:C:62:PRO:O	1:C:182:THR:HG23	1.85	0.76
1:D:62:PRO:O	1:D:182:THR:HG23	1.86	0.75
1:F:40:LEU:CD1	1:F:278:GLN:HG3	2.17	0.73
1:F:270:ALA:HB1	1:F:274:GLU:CG	2.17	0.73
1:F:270:ALA:HB1	1:F:274:GLU:HG2	1.70	0.72
1:F:224:ALA:O	1:F:287:ILE:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:NH1	1:C:241:ARG:HB3	2.03	0.71
1:D:40:LEU:HD13	1:D:278:GLN:HG3	1.73	0.71
1:F:137:LEU:O	1:F:141:THR:HG23	1.91	0.71
1:F:286:LEU:HD13	2:F:582:HOH:O	1.91	0.71
1:F:48:GLU:HB2	1:F:57:LEU:HB2	1.73	0.71
1:D:90:GLN:NE2	2:D:348:HOH:O	2.24	0.70
1:F:32:LYS:HE2	1:F:281:GLU:HB3	1.73	0.69
1:F:148:LEU:HD23	1:F:162:LEU:HD22	1.73	0.69
1:F:131:ASP:HB3	1:F:134:ALA:HB3	1.75	0.69
1:D:32:LYS:NZ	2:D:377:HOH:O	2.25	0.69
1:F:164:ARG:NH1	1:F:171:GLU:HG3	2.06	0.69
1:F:107:PRO:HG3	2:F:515:HOH:O	1.94	0.68
1:F:124:SER:HB2	1:F:210:TRP:HE1	1.59	0.68
1:F:238:SER:OG	1:F:243:SER:HB2	1.94	0.68
1:E:182:THR:HG21	2:E:433:HOH:O	1.94	0.68
1:B:106:SER:O	1:B:110:GLU:HG2	1.93	0.68
1:D:241:ARG:HB3	1:D:241:ARG:NH1	2.08	0.68
1:F:225:LEU:HD12	1:F:287:ILE:HD11	1.75	0.67
1:F:65:ARG:HA	1:F:181:THR:O	1.94	0.67
1:F:69:MET:SD	1:F:238:SER:HB3	2.36	0.66
1:F:230:PHE:HB3	2:F:511:HOH:O	1.95	0.66
1:F:182:THR:HG22	1:F:185:ALA:H	1.60	0.65
1:F:225:LEU:HD11	1:F:229:TRP:HB3	1.78	0.65
1:F:244:ARG:HB2	2:F:441:HOH:O	1.97	0.65
1:F:44:VAL:HG22	1:F:265:THR:HG22	1.78	0.65
1:F:164:ARG:HH12	1:F:171:GLU:HG3	1.62	0.64
1:F:48:GLU:CD	1:F:58:GLU:HB3	2.19	0.64
1:F:117:MET:HE2	2:F:444:HOH:O	1.98	0.63
1:B:242:GLY:HA2	1:B:275:ARG:NH1	2.13	0.63
1:F:74:VAL:HG23	1:F:234:LYS:HG2	1.80	0.63
1:E:106:SER:O	1:E:110:GLU:HG2	1.98	0.63
1:D:242:GLY:HA2	1:D:275:ARG:NH1	2.15	0.62
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.63	0.62
1:E:242:GLY:HA2	1:E:275:ARG:NH1	2.14	0.62
1:C:275:ARG:HH11	1:C:275:ARG:HG2	1.65	0.62
1:A:148:LEU:O	1:A:152:LEU:HD22	2.01	0.61
1:F:243:SER:N	1:F:267:GLY:HA2	2.14	0.61
1:F:99:GLN:N	1:F:113:LEU:HD21	2.15	0.61
1:C:146:LYS:HG3	2:C:323:HOH:O	2.00	0.61
1:F:40:LEU:O	1:F:268:SER:HB2	2.00	0.61
1:C:242:GLY:HA2	1:C:275:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ARG:HG2	1:E:275:ARG:HH11	1.64	0.60
1:C:40:LEU:HD13	1:C:278:GLN:HG3	1.84	0.60
1:F:47:ILE:HG22	1:F:262:VAL:HB	1.84	0.59
1:A:40:LEU:O	1:A:268:SER:HB2	2.02	0.59
1:D:153:HIS:CE1	1:D:158:HIS:HD1	2.19	0.59
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.66	0.59
1:F:33:VAL:O	1:F:36:ALA:HB3	2.03	0.59
1:E:40:LEU:O	1:E:268:SER:HB2	2.03	0.59
1:F:225:LEU:HG	1:F:226:PRO:CD	2.31	0.58
1:D:36:ALA:N	2:D:377:HOH:O	2.36	0.58
1:A:241:ARG:HB3	1:A:241:ARG:NH1	2.19	0.58
1:D:148:LEU:O	1:D:152:LEU:HD22	2.04	0.58
1:B:148:LEU:O	1:B:152:LEU:HD22	2.03	0.58
1:F:241:ARG:HB2	1:F:241:ARG:NH1	2.14	0.58
1:C:142:ILE:O	1:C:147:GLU:HG3	2.04	0.57
1:A:83:ARG:NH2	1:D:227:ALA:O	2.37	0.57
1:D:40:LEU:CD1	1:D:278:GLN:HG3	2.33	0.57
1:D:35:ASP:O	1:D:39:GLN:HG2	2.04	0.57
1:B:40:LEU:HD13	1:B:278:GLN:HG3	1.86	0.57
1:D:32:LYS:CE	2:D:377:HOH:O	2.53	0.57
1:E:120:ARG:NH2	2:E:410:HOH:O	2.28	0.57
1:C:148:LEU:O	1:C:152:LEU:HD22	2.05	0.57
1:F:32:LYS:HE2	1:F:281:GLU:CB	2.34	0.57
1:C:96:HIS:HD2	2:C:374:HOH:O	1.87	0.57
1:C:241:ARG:HH11	1:C:241:ARG:CB	2.15	0.56
1:C:40:LEU:O	1:C:268:SER:HB2	2.04	0.56
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.71	0.56
1:F:143:GLY:HA3	1:F:147:GLU:HG3	1.87	0.56
1:F:77:CYS:O	1:F:81:LEU:HG	2.04	0.56
1:C:182:THR:HG21	2:C:346:HOH:O	2.05	0.56
1:A:182:THR:HG22	1:A:185:ALA:N	2.08	0.56
1:F:48:GLU:OE1	1:F:58:GLU:HB3	2.05	0.56
1:F:46:TYR:HD1	1:F:263:ILE:HG12	1.70	0.56
1:F:199:LEU:HB3	2:F:512:HOH:O	2.06	0.56
1:D:242:GLY:HA3	1:D:268:SER:H	1.71	0.56
1:D:36:ALA:CA	2:D:377:HOH:O	2.54	0.55
1:E:241:ARG:NH1	1:E:241:ARG:HB3	2.22	0.55
1:F:51:LEU:H	1:F:259:ARG:HA	1.72	0.55
1:B:182:THR:HG22	1:B:185:ALA:N	2.08	0.55
1:E:120:ARG:NE	2:E:410:HOH:O	2.26	0.55
1:F:186:MET:HE3	1:F:247:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:HB	2:B:332:HOH:O	2.07	0.55
1:C:242:GLY:HA2	1:C:275:ARG:NH1	2.21	0.55
1:B:148:LEU:HD23	1:B:162:LEU:HD22	1.89	0.55
1:E:241:ARG:HB3	1:E:241:ARG:HH11	1.72	0.55
1:F:171:GLU:HG2	2:F:464:HOH:O	2.06	0.55
1:E:106:SER:HB3	1:E:109:THR:OG1	2.07	0.55
1:E:242:GLY:HA2	1:E:275:ARG:HH12	1.72	0.54
1:F:26:HIS:CE1	1:F:28:GLU:HB2	2.43	0.54
2:C:380:HOH:O	1:D:269:GLN:HB3	2.07	0.54
1:D:32:LYS:HE3	2:D:377:HOH:O	2.08	0.54
1:F:220:LEU:HD12	1:F:246:ILE:HD12	1.89	0.54
1:F:224:ALA:HB2	1:F:280:ALA:HA	1.89	0.54
1:C:83:ARG:NH2	1:E:227:ALA:O	2.40	0.54
1:F:36:ALA:O	1:F:40:LEU:HD13	2.07	0.54
1:D:182:THR:HG22	1:D:185:ALA:N	2.08	0.54
1:E:182:THR:HG22	1:E:185:ALA:N	2.09	0.54
1:C:49:LEU:HD22	1:C:187:ALA:HB1	1.90	0.53
1:F:174:PRO:O	1:F:175:ASN:HB2	2.08	0.53
1:F:40:LEU:HB3	1:F:268:SER:HB3	1.88	0.53
1:C:182:THR:HG22	1:C:185:ALA:N	2.07	0.53
1:D:49:LEU:HD22	1:D:187:ALA:HB1	1.90	0.53
1:E:148:LEU:HD23	1:E:162:LEU:HD22	1.91	0.53
1:F:104:LYS:HG2	1:F:105:TYR:N	2.24	0.53
1:C:83:ARG:NE	2:C:342:HOH:O	2.24	0.53
1:E:215:LYS:HE2	2:E:360:HOH:O	2.09	0.53
1:E:30:LEU:HD11	1:E:58:GLU:OE2	2.08	0.53
1:B:242:GLY:HA2	1:B:275:ARG:HH12	1.72	0.52
1:C:40:LEU:O	1:C:268:SER:CB	2.56	0.52
1:E:40:LEU:HD13	1:E:278:GLN:HG3	1.90	0.52
1:F:142:ILE:O	1:F:147:GLU:HG3	2.10	0.52
1:F:182:THR:HG22	1:F:184:ALA:H	1.75	0.52
1:F:102:LEU:HD21	1:F:109:THR:O	2.09	0.52
1:A:106:SER:HB3	1:A:109:THR:OG1	2.10	0.52
1:A:242:GLY:C	1:A:267:GLY:HA2	2.30	0.52
1:D:126:ALA:O	1:D:130:SER:HA	2.08	0.52
1:F:203:SER:C	1:F:205:GLN:H	2.12	0.52
1:F:231:ILE:HD13	1:F:250:LEU:HB3	1.91	0.52
1:A:40:LEU:O	1:A:268:SER:CB	2.58	0.52
1:C:32:LYS:HE2	1:C:281:GLU:CB	2.40	0.51
1:F:130:SER:HB2	1:F:234:LYS:NZ	2.25	0.51
1:F:219:PRO:O	1:F:276:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:THR:OG1	1:F:274:GLU:HB2	2.10	0.51
1:F:79:ALA:O	1:F:83:ARG:HG3	2.10	0.51
1:E:238:SER:OG	1:E:243:SER:HB2	2.10	0.51
1:F:173:ILE:O	1:F:176:ASP:HB3	2.11	0.51
1:A:83:ARG:NE	2:A:377:HOH:O	2.27	0.51
1:A:275:ARG:NH1	1:A:275:ARG:HG2	2.24	0.51
1:A:215:LYS:CE	2:A:404:HOH:O	2.59	0.51
1:B:275:ARG:NH1	1:B:275:ARG:HG2	2.26	0.51
1:C:275:ARG:HG2	1:C:275:ARG:NH1	2.26	0.51
1:D:238:SER:OG	1:D:243:SER:HB2	2.10	0.51
1:E:153:HIS:CE1	1:E:158:HIS:ND1	2.79	0.50
1:B:193:LEU:HD12	1:B:198:LEU:HD23	1.93	0.50
1:F:133:THR:HA	1:F:136:ASN:HD22	1.75	0.50
1:F:204:ARG:HG3	2:F:458:HOH:O	2.11	0.50
1:E:148:LEU:O	1:E:152:LEU:HD22	2.11	0.50
1:E:188:THR:HG23	2:E:425:HOH:O	2.10	0.50
1:E:268:SER:HB2	2:E:411:HOH:O	2.11	0.50
1:C:229:TRP:CZ2	1:C:252:PRO:HB3	2.47	0.50
1:E:61:ARG:N	1:E:62:PRO:CD	2.74	0.50
1:F:148:LEU:O	1:F:152:LEU:HD13	2.10	0.50
1:D:106:SER:O	1:D:110:GLU:HG2	2.12	0.50
1:D:242:GLY:C	1:D:267:GLY:HA2	2.31	0.50
1:E:275:ARG:NH1	1:E:275:ARG:HG2	2.26	0.50
1:F:80:VAL:O	1:F:84:VAL:HG23	2.11	0.50
1:A:242:GLY:HA2	1:A:275:ARG:HH12	1.76	0.50
1:B:35:ASP:O	1:B:39:GLN:HG2	2.12	0.50
1:F:284:ALA:O	1:F:288:LYS:HB2	2.12	0.50
1:E:126:ALA:O	1:E:130:SER:HA	2.12	0.50
1:F:234:LYS:HB3	1:F:247:ILE:CG1	2.42	0.50
1:B:215:LYS:CE	2:B:334:HOH:O	2.59	0.49
1:B:61:ARG:N	1:B:62:PRO:CD	2.75	0.49
1:F:130:SER:CB	1:F:234:LYS:HZ1	2.25	0.49
1:D:242:GLY:O	1:D:275:ARG:NH1	2.45	0.49
1:A:61:ARG:N	1:A:62:PRO:CD	2.75	0.49
1:F:182:THR:HG22	1:F:184:ALA:N	2.27	0.49
1:F:94:ARG:HA	1:F:118:THR:HA	1.92	0.49
1:C:193:LEU:HD12	1:C:198:LEU:HD23	1.93	0.49
1:A:106:SER:O	1:A:110:GLU:HG2	2.12	0.49
1:D:61:ARG:N	1:D:62:PRO:CD	2.76	0.49
1:F:51:LEU:CD2	1:F:257:PRO:HB2	2.42	0.49
1:B:46:TYR:CD1	1:B:263:ILE:HG12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:THR:O	1:F:196:GLY:O	2.31	0.49
1:F:211:MET:HB2	1:F:232:ALA:HB1	1.95	0.49
1:F:271:THR:O	1:F:274:GLU:N	2.41	0.49
1:F:99:GLN:HB2	1:F:113:LEU:HD11	1.95	0.49
1:C:61:ARG:N	1:C:62:PRO:CD	2.75	0.49
1:D:241:ARG:HH11	1:D:241:ARG:HB3	1.74	0.49
1:F:99:GLN:HG3	2:F:498:HOH:O	2.12	0.49
1:F:128:THR:HG22	1:F:210:TRP:O	2.13	0.48
1:F:42:ALA:HB2	1:F:267:GLY:O	2.13	0.48
1:B:242:GLY:C	1:B:267:GLY:HA2	2.33	0.48
1:E:74:VAL:HG23	1:E:234:LYS:HG2	1.96	0.48
1:A:142:ILE:O	1:A:147:GLU:HG3	2.13	0.48
1:F:61:ARG:N	1:F:62:PRO:CD	2.77	0.48
1:F:71:THR:HG22	1:F:235:SER:O	2.12	0.48
1:F:128:THR:HB	1:F:213:ALA:O	2.13	0.48
1:F:79:ALA:HB2	1:F:151:PHE:CD2	2.49	0.48
1:F:47:ILE:HD13	1:F:184:ALA:HA	1.95	0.48
1:F:200:THR:N	2:F:512:HOH:O	2.47	0.48
1:F:278:GLN:O	1:F:282:ILE:HG13	2.14	0.48
1:A:40:LEU:HD13	1:A:278:GLN:HG3	1.95	0.48
1:B:126:ALA:O	1:B:130:SER:HA	2.12	0.48
1:C:153:HIS:CE1	1:C:158:HIS:ND1	2.81	0.48
1:F:201:LEU:HD13	1:F:201:LEU:C	2.33	0.48
1:B:230:PHE:CD1	1:B:257:PRO:HB3	2.48	0.48
1:F:201:LEU:HD13	1:F:201:LEU:O	2.13	0.48
1:A:215:LYS:HE3	2:A:404:HOH:O	2.14	0.48
1:F:218:GLY:H	1:F:219:PRO:CD	2.21	0.48
1:B:152:LEU:O	1:B:155:MET:HG3	2.14	0.47
1:F:125:ALA:O	1:F:131:ASP:HB2	2.14	0.47
1:B:83:ARG:NH2	1:C:227:ALA:O	2.47	0.47
1:F:159:VAL:HG11	1:F:182:THR:CB	2.42	0.47
1:F:109:THR:HG23	1:F:131:ASP:OD2	2.14	0.47
1:F:174:PRO:HD3	1:F:241:ARG:HH22	1.79	0.47
1:E:242:GLY:C	1:E:267:GLY:HA2	2.35	0.47
1:A:242:GLY:HA2	1:A:275:ARG:NH1	2.29	0.47
1:A:153:HIS:CE1	1:A:158:HIS:ND1	2.83	0.47
1:D:278:GLN:O	1:D:282:ILE:HG13	2.15	0.47
1:A:126:ALA:O	1:A:130:SER:HA	2.13	0.47
1:D:153:HIS:CE1	1:D:158:HIS:ND1	2.82	0.47
1:D:241:ARG:HH11	1:D:241:ARG:CB	2.28	0.47
1:A:152:LEU:O	1:A:155:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:NH1	2:B:337:HOH:O	2.35	0.47
1:B:215:LYS:HE3	2:B:334:HOH:O	2.15	0.47
1:C:126:ALA:O	1:C:130:SER:HA	2.14	0.47
1:E:40:LEU:O	1:E:268:SER:CB	2.63	0.47
1:F:211:MET:CB	1:F:232:ALA:HB1	2.44	0.47
1:F:108:VAL:HB	1:F:131:ASP:OD2	2.15	0.46
1:F:194:LEU:HD22	1:F:208:ILE:HB	1.97	0.46
1:D:120:ARG:NH2	2:D:343:HOH:O	2.33	0.46
1:E:241:ARG:CB	1:E:241:ARG:HH11	2.28	0.46
1:F:270:ALA:HB1	1:F:274:GLU:HB3	1.96	0.46
1:B:74:VAL:HG23	1:B:234:LYS:HG2	1.97	0.46
1:B:285:SER:HB2	2:B:305:HOH:O	2.15	0.46
1:D:106:SER:HB3	1:D:109:THR:OG1	2.16	0.46
1:D:193:LEU:HD12	1:D:198:LEU:HD23	1.98	0.46
1:F:257:PRO:HA	2:F:511:HOH:O	2.16	0.46
1:D:275:ARG:HG2	1:D:275:ARG:NH1	2.31	0.46
1:B:46:TYR:HD1	1:B:263:ILE:HG12	1.80	0.46
1:D:152:LEU:O	1:D:155:MET:HG3	2.16	0.46
1:F:233:ASP:CB	1:F:248:ALA:HB2	2.46	0.46
1:F:270:ALA:HB1	1:F:274:GLU:CB	2.45	0.46
1:C:148:LEU:HD23	1:C:162:LEU:HD22	1.98	0.45
1:A:192:LYS:NZ	2:A:399:HOH:O	2.46	0.45
1:C:32:LYS:HE2	1:C:281:GLU:HB3	1.99	0.45
1:F:226:PRO:HD2	1:F:287:ILE:HD12	1.98	0.45
1:F:169:LEU:O	1:F:169:LEU:HD12	2.16	0.45
1:F:171:GLU:HB3	1:F:173:ILE:HG13	1.97	0.45
1:F:243:SER:HA	1:F:265:THR:O	2.15	0.45
1:F:40:LEU:HB3	1:F:268:SER:CB	2.46	0.45
1:A:141:THR:HG22	1:D:254:ASP:OD1	2.15	0.45
1:E:236:GLY:O	1:E:244:ARG:HD3	2.16	0.45
1:F:76:LEU:HD21	1:F:138:LEU:HB2	1.98	0.45
1:F:89:GLU:OE1	1:F:90:GLN:N	2.48	0.45
1:B:106:SER:HB3	1:B:109:THR:OG1	2.16	0.45
1:C:230:PHE:CD1	1:C:230:PHE:C	2.90	0.45
1:B:47:ILE:HG22	1:B:262:VAL:HB	1.99	0.45
1:F:109:THR:OG1	1:F:133:THR:HB	2.17	0.45
1:F:71:THR:O	1:F:186:MET:HE1	2.15	0.45
1:F:277:ARG:HG2	1:F:281:GLU:OE2	2.17	0.45
1:B:153:HIS:CE1	1:B:158:HIS:ND1	2.85	0.45
1:E:120:ARG:HD2	2:E:322:HOH:O	2.17	0.45
1:B:40:LEU:O	1:B:268:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:HD23	1:D:162:LEU:HD22	1.99	0.45
1:F:130:SER:HB2	1:F:234:LYS:HZ1	1.82	0.45
1:C:106:SER:HB3	1:C:109:THR:OG1	2.17	0.45
1:F:120:ARG:N	2:F:568:HOH:O	2.50	0.45
1:B:174:PRO:HD3	1:B:241:ARG:NH1	2.32	0.44
1:E:278:GLN:O	1:E:282:ILE:HG13	2.17	0.44
1:B:142:ILE:O	1:B:147:GLU:HG3	2.17	0.44
1:C:91:LEU:HB3	1:C:120:ARG:HB2	1.99	0.44
1:F:47:ILE:HG21	1:F:183:PRO:O	2.17	0.44
1:F:121:GLU:HG3	2:F:574:HOH:O	2.17	0.44
1:F:95:ILE:HG22	1:F:96:HIS:N	2.32	0.44
1:C:240:GLU:C	1:C:242:GLY:H	2.21	0.44
1:F:213:ALA:O	1:F:215:LYS:HE3	2.18	0.44
1:F:220:LEU:HD11	1:F:244:ARG:NH1	2.33	0.44
1:A:74:VAL:HG23	1:A:234:LYS:HG2	2.00	0.44
1:F:84:VAL:C	1:F:86:ALA:H	2.20	0.44
1:C:242:GLY:CA	1:C:275:ARG:NH1	2.81	0.44
1:C:32:LYS:HE2	1:C:281:GLU:HB2	1.99	0.44
1:B:225:LEU:HD22	1:B:231:ILE:HB	1.99	0.44
1:C:152:LEU:O	1:C:155:MET:HG3	2.18	0.44
1:D:242:GLY:HA2	1:D:275:ARG:HH12	1.83	0.44
1:F:136:ASN:HD21	1:F:166:GLU:HB2	1.82	0.44
1:F:28:GLU:HB2	1:F:289:HIS:CD2	2.53	0.44
1:A:49:LEU:HD22	1:A:187:ALA:HB1	1.98	0.44
1:E:204:ARG:HD2	2:E:394:HOH:O	2.18	0.44
1:F:43:ARG:HH11	1:F:43:ARG:CB	2.30	0.44
1:A:120:ARG:NH1	2:A:329:HOH:O	2.34	0.43
1:D:74:VAL:HG23	1:D:234:LYS:HG2	2.00	0.43
1:F:220:LEU:CD1	1:F:246:ILE:HD12	2.48	0.43
1:F:218:GLY:C	1:F:220:LEU:H	2.22	0.43
1:F:224:ALA:HB2	1:F:280:ALA:CB	2.48	0.43
1:F:68:MET:SD	1:F:160:THR:HG23	2.58	0.43
1:F:84:VAL:HG21	1:F:91:LEU:HG	1.99	0.43
1:A:278:GLN:O	1:A:282:ILE:HG13	2.19	0.43
1:C:242:GLY:C	1:C:267:GLY:HA2	2.39	0.43
1:F:223:SER:HA	2:F:539:HOH:O	2.18	0.43
1:F:30:LEU:CD2	1:F:34:LYS:HE3	2.48	0.43
1:B:278:GLN:O	1:B:282:ILE:HG13	2.18	0.43
1:C:244:ARG:HD3	1:C:244:ARG:HA	1.87	0.43
1:D:174:PRO:O	1:D:175:ASN:HB2	2.18	0.43
1:F:129:MET:O	2:F:515:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LYS:HG3	2:E:379:HOH:O	2.18	0.43
1:F:229:TRP:O	1:F:230:PHE:C	2.56	0.43
1:B:230:PHE:CE1	1:B:257:PRO:HB3	2.54	0.43
1:F:195:THR:OG1	1:F:196:GLY:N	2.50	0.43
1:F:241:ARG:CB	1:F:241:ARG:HH11	2.19	0.43
1:C:278:GLN:O	1:C:282:ILE:HG13	2.19	0.43
1:C:154:ASN:HB2	2:C:317:HOH:O	2.18	0.43
1:A:93:ARG:O	1:A:118:THR:HA	2.19	0.42
1:B:178:ARG:O	1:B:180:THR:HG23	2.19	0.42
1:D:32:LYS:HE2	1:D:281:GLU:HB3	2.01	0.42
1:F:139:LEU:HD23	1:F:139:LEU:HA	1.90	0.42
1:F:62:PRO:O	1:F:183:PRO:HD2	2.19	0.42
1:A:225:LEU:HD22	1:A:231:ILE:HB	2.01	0.42
1:E:242:GLY:O	1:E:275:ARG:NH1	2.52	0.42
1:F:30:LEU:O	1:F:34:LYS:HG3	2.19	0.42
1:B:68:MET:HG2	1:B:181:THR:CG2	2.50	0.42
1:F:234:LYS:HA	1:F:234:LYS:HD2	1.76	0.42
1:C:234:LYS:HD2	1:C:234:LYS:HA	1.85	0.42
1:F:166:GLU:HA	1:F:167:PRO:HA	1.83	0.42
1:F:188:THR:O	1:F:192:LYS:HG3	2.20	0.42
1:F:194:LEU:HB3	2:F:443:HOH:O	2.20	0.42
1:F:250:LEU:HD23	1:F:250:LEU:H	1.84	0.42
1:A:212:GLU:HA	1:A:232:ALA:HA	2.02	0.42
1:C:110:GLU:HG3	1:C:111:LYS:HG3	2.02	0.42
1:E:152:LEU:O	1:E:155:MET:HG3	2.20	0.42
1:F:164:ARG:NH1	1:F:178:ARG:NH2	2.68	0.42
1:F:285:SER:O	1:F:288:LYS:HB3	2.20	0.42
1:F:76:LEU:O	1:F:80:VAL:HG23	2.20	0.42
1:F:97:TYR:OH	1:F:117:MET:HG3	2.20	0.42
1:E:174:PRO:O	1:E:175:ASN:HB2	2.19	0.42
1:E:215:LYS:CE	2:E:360:HOH:O	2.65	0.42
1:B:174:PRO:O	1:B:175:ASN:HB2	2.20	0.41
1:B:230:PHE:C	1:B:230:PHE:CD1	2.93	0.41
1:D:230:PHE:CD1	1:D:230:PHE:C	2.93	0.41
1:E:201:LEU:HD13	1:E:201:LEU:C	2.40	0.41
1:F:145:PRO:HD3	1:F:165:TRP:CZ2	2.55	0.41
1:F:198:LEU:O	1:F:199:LEU:HD23	2.20	0.41
1:F:220:LEU:HD22	1:F:279:ILE:HG13	2.01	0.41
1:F:130:SER:CB	1:F:234:LYS:NZ	2.82	0.41
1:F:69:MET:O	1:F:71:THR:N	2.48	0.41
1:B:233:ASP:HB3	1:B:248:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:O	1:B:83:ARG:HG3	2.20	0.41
1:F:220:LEU:O	1:F:222:ARG:N	2.49	0.41
1:F:231:ILE:HG23	1:F:231:ILE:O	2.20	0.41
1:F:47:ILE:CD1	1:F:184:ALA:HA	2.50	0.41
1:F:89:GLU:OE2	1:F:93:ARG:NH2	2.51	0.41
1:D:225:LEU:HD22	1:D:231:ILE:HB	2.01	0.41
1:E:230:PHE:C	1:E:230:PHE:CD1	2.93	0.41
1:F:288:LYS:HE2	1:F:289:HIS:CE1	2.55	0.41
1:F:56:ILE:HB	2:F:528:HOH:O	2.20	0.41
1:C:174:PRO:O	1:C:175:ASN:HB2	2.21	0.41
1:F:280:ALA:O	1:F:284:ALA:N	2.53	0.41
1:C:225:LEU:HD22	1:C:231:ILE:HB	2.01	0.41
1:E:43:ARG:HB2	1:E:266:THR:CG2	2.50	0.41
1:B:238:SER:OG	1:B:243:SER:HB2	2.21	0.41
1:C:146:LYS:HE3	1:C:146:LYS:HB2	1.85	0.41
1:F:29:THR:O	1:F:33:VAL:HG23	2.21	0.41
1:E:142:ILE:O	1:E:147:GLU:HG3	2.20	0.41
1:F:43:ARG:O	1:F:265:THR:HA	2.20	0.41
1:F:81:LEU:HD23	1:F:91:LEU:HD21	2.02	0.41
1:D:146:LYS:HE3	1:D:146:LYS:HB2	1.85	0.41
1:F:99:GLN:CD	1:F:102:LEU:HD12	2.40	0.41
1:E:212:GLU:HA	1:E:232:ALA:HA	2.03	0.41
1:E:32:LYS:HE2	1:E:281:GLU:HB3	2.03	0.41
1:F:244:ARG:HD3	1:F:245:GLY:H	1.86	0.41
1:C:32:LYS:HD2	1:C:32:LYS:HA	1.85	0.40
1:F:204:ARG:O	1:F:204:ARG:HG2	2.20	0.40
1:B:201:LEU:HD13	1:B:201:LEU:C	2.41	0.40
1:E:225:LEU:HD22	1:E:231:ILE:HB	2.03	0.40
1:F:233:ASP:HB3	1:F:248:ALA:HB2	2.02	0.40
1:F:90:GLN:C	1:F:92:GLY:H	2.25	0.40
1:B:32:LYS:HD2	1:B:32:LYS:HA	1.82	0.40
1:E:43:ARG:O	1:E:265:THR:HA	2.20	0.40
1:E:32:LYS:HE2	1:E:281:GLU:CB	2.51	0.40
1:E:35:ASP:O	1:E:39:GLN:HG2	2.20	0.40
1:F:182:THR:CG2	1:F:184:ALA:H	2.35	0.40
1:F:203:SER:C	1:F:205:GLN:N	2.74	0.40
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.82	0.40
1:C:212:GLU:HA	1:C:232:ALA:HA	2.03	0.40
1:D:256:LYS:HG2	2:D:374:HOH:O	2.20	0.40
1:F:99:GLN:NE2	1:F:102:LEU:HD12	2.36	0.40
1:F:167:PRO:O	1:F:169:LEU:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/263 (99%)	251 (96%)	10 (4%)	0	100	100
1	B	261/263 (99%)	251 (96%)	10 (4%)	0	100	100
1	C	261/263 (99%)	249 (95%)	12 (5%)	0	100	100
1	D	261/263 (99%)	250 (96%)	11 (4%)	0	100	100
1	E	261/263 (99%)	250 (96%)	11 (4%)	0	100	100
1	F	261/263 (99%)	197 (76%)	46 (18%)	18 (7%)	1	0
All	All	1566/1578 (99%)	1448 (92%)	100 (6%)	18 (1%)	14	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	91	LEU
1	F	288	LYS
1	F	70	SER
1	F	168	GLU
1	F	196	GLY
1	F	221	LEU
1	F	241	ARG
1	F	277	ARG
1	F	155	MET
1	F	201	LEU
1	F	216	VAL
1	F	243	SER
1	F	254	ASP
1	F	115	ASP
1	F	116	GLY
1	F	255	GLY
1	F	51	LEU

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Mol	Chain	Res	Type
1	F	60	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/218 (100%)	211 (97%)	7 (3%)	39	59
1	B	218/218 (100%)	210 (96%)	8 (4%)	34	53
1	C	218/218 (100%)	209 (96%)	9 (4%)	30	48
1	D	218/218 (100%)	210 (96%)	8 (4%)	34	53
1	E	218/218 (100%)	210 (96%)	8 (4%)	34	53
1	F	218/218 (100%)	213 (98%)	5 (2%)	50	70
All	All	1308/1308 (100%)	1263 (97%)	45 (3%)	37	56

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	122	LEU
1	A	130	SER
1	A	152	LEU
1	A	182	THR
1	A	193	LEU
1	A	275	ARG
1	B	40	LEU
1	B	100	ASN
1	B	122	LEU
1	B	130	SER
1	B	152	LEU
1	B	182	THR
1	B	193	LEU
1	B	275	ARG
1	C	40	LEU
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	122	LEU
1	C	130	SER
1	C	152	LEU
1	C	182	THR
1	C	193	LEU
1	C	244	ARG
1	C	275	ARG
1	D	40	LEU
1	D	49	LEU
1	D	122	LEU
1	D	130	SER
1	D	152	LEU
1	D	182	THR
1	D	193	LEU
1	D	275	ARG
1	E	40	LEU
1	E	100	ASN
1	E	122	LEU
1	E	130	SER
1	E	152	LEU
1	E	182	THR
1	E	193	LEU
1	E	275	ARG
1	F	113	LEU
1	F	182	THR
1	F	210	TRP
1	F	216	VAL
1	F	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	132	ASN
1	A	153	HIS
1	A	269	GLN
1	B	99	GLN
1	B	132	ASN
1	B	153	HIS
1	B	269	GLN
1	C	132	ASN
1	C	153	HIS

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Mol	Chain	Res	Type
1	C	269	GLN
1	D	132	ASN
1	D	153	HIS
1	D	269	GLN
1	E	132	ASN
1	E	153	HIS
1	E	269	GLN
1	F	132	ASN
1	F	153	HIS
1	F	269	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.