



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:41 pm GMT

PDB ID : 1IZN  
Title : Crystal Structure of Actin Filament Capping Protein CapZ  
Authors : Yamashita, A.; Maeda, K.; Maeda, Y.  
Deposited on : 2002-10-10  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

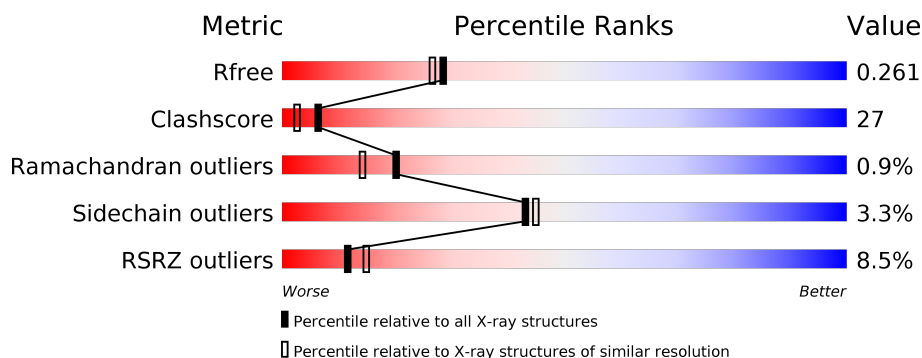
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	<div> <div>15%</div> <div>50%</div> <div>42%</div> <div>• •</div> </div>
1	C	286	<div> <div>10%</div> <div>57%</div> <div>34%</div> <div>5% 5%</div> </div>
2	B	277	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>
2	D	277	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	B	1002	-	-	X	X
3	NO3	B	1003	-	-	-	X
3	NO3	D	1001	-	-	-	X
3	NO3	D	1004	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9272 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.

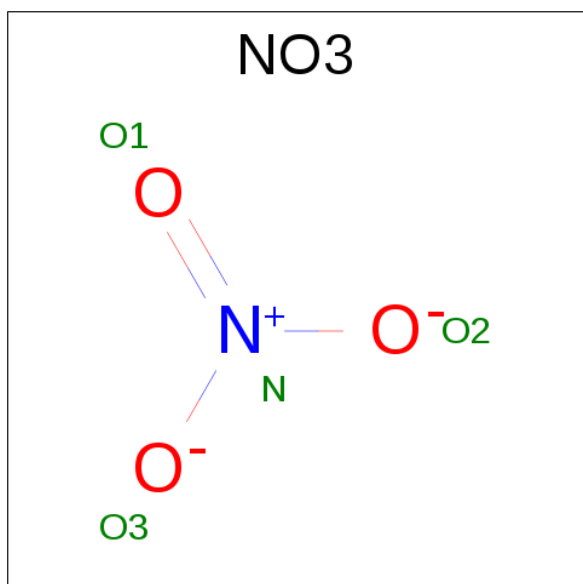
- Molecule 1 is a protein called CapZ alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2238	1413	392	428	5			
1	C	273	Total	C	N	O	S	0	0	0
			2225	1402	388	430	5			

- Molecule 2 is a protein called CapZ beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2140	1334	374	422	10			
2	D	270	Total	C	N	O	S	0	0	0
			2140	1334	374	422	10			

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	D	1	Total N O 4 1 3	0	0

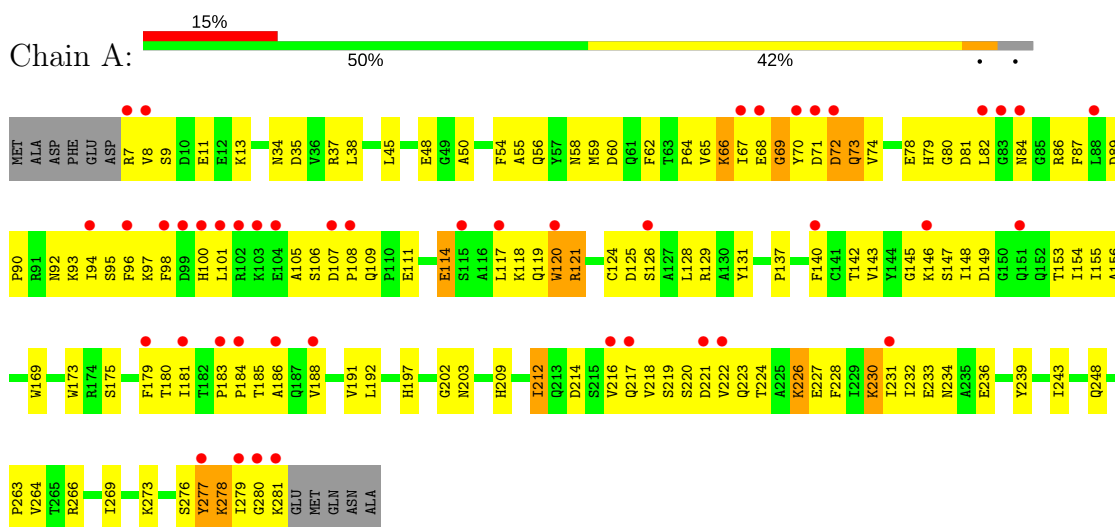
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	175	Total O 175 175	0	0
4	C	83	Total O 83 83	0	0
4	D	177	Total O 177 177	0	0

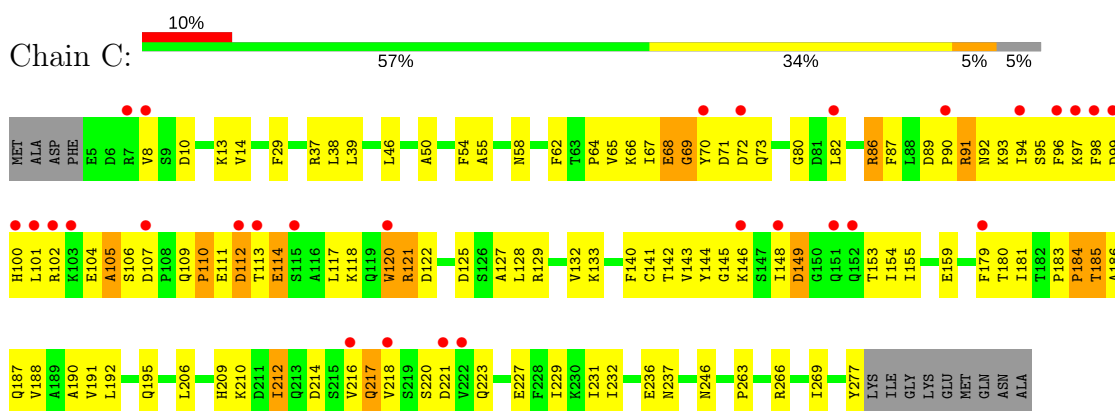
### 3 Residue-property plots [i](#)

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 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 ( $\text{RSRZ} > 2$ ). 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.

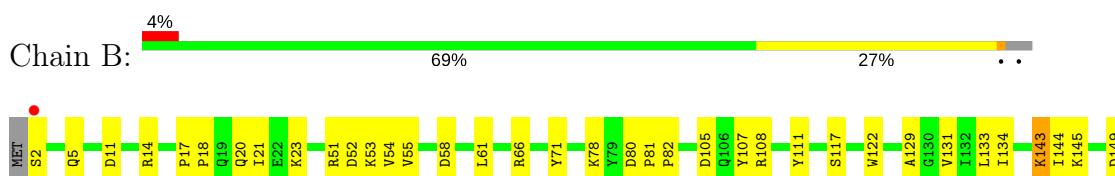
#### • Molecule 1: CapZ alpha-1 subunit

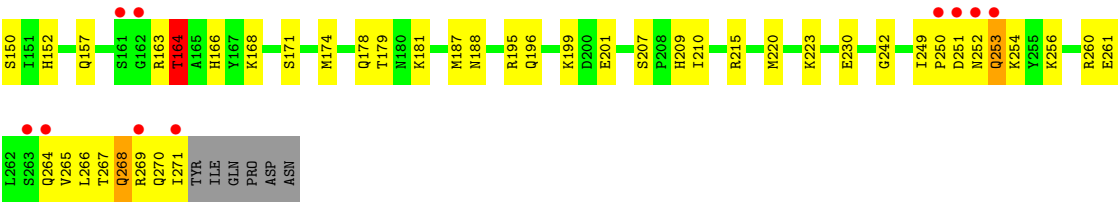


#### • Molecule 1: CapZ alpha-1 subunit

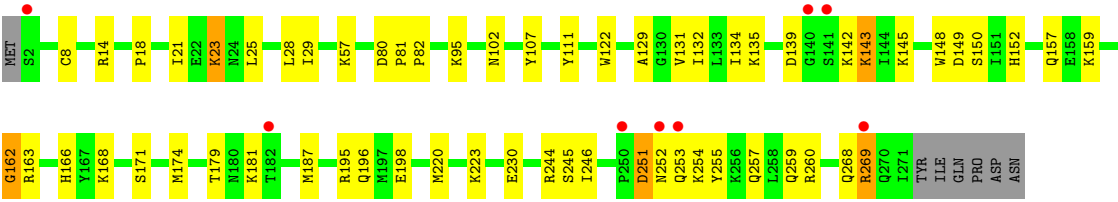


#### • Molecule 2: CapZ beta-1 subunit





• Molecule 2: CapZ beta-1 subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.20Å 57.20Å 99.20Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.10) 100.0 (49.25-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.222 , 0.262 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	2970 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

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	0/2290	0.68	1/3102 (0.0%)
1	C	0.39	0/2277	0.69	1/3087 (0.0%)
2	B	0.36	0/2175	0.63	1/2936 (0.0%)
2	D	0.36	0/2175	0.61	0/2936
All	All	0.37	0/8917	0.66	3/12061 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	164	THR	N-CA-C	-7.08	91.87	111.00
1	A	72	ASP	N-CA-C	5.80	126.67	111.00
1	C	105	ALA	N-CA-C	-5.33	96.61	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2166	175	0
1	C	2225	0	2136	173	0
2	B	2140	0	2128	75	0
2	D	2140	0	2128	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	0	5	0
3	D	8	0	0	2	0
4	A	78	0	0	5	0
4	B	175	0	0	10	0
4	C	83	0	0	5	0
4	D	177	0	0	11	0
All	All	9272	0	8558	463	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 27.

All (463) 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)
3:D:1001:NO3:O3	3:D:1001:NO3:N	1.58	1.37
3:B:1003:NO3:O3	3:B:1003:NO3:N	1.60	1.31
3:B:1002:NO3:O3	3:B:1002:NO3:N	1.58	1.30
3:D:1004:NO3:O3	3:D:1004:NO3:N	1.60	1.30
1:C:70:TYR:HB3	1:C:72:ASP:HB3	1.27	1.11
1:C:82:LEU:HD12	1:C:86:ARG:HB2	1.33	1.11
1:C:86:ARG:HH11	1:C:86:ARG:HB3	1.21	1.06
1:A:281:LYS:HD3	1:C:277:TYR:HB2	1.35	1.05
1:C:70:TYR:CB	1:C:72:ASP:HB3	1.87	1.04
2:D:139:ASP:HB2	2:D:142:LYS:HE2	1.39	1.04
1:C:220:SER:HB3	1:C:223:GLN:HB3	1.43	1.01
1:A:278:LYS:H	1:A:278:LYS:HD3	1.32	0.94
1:A:67:ILE:HG22	1:A:72:ASP:CG	1.88	0.93
1:C:96:PHE:HE2	1:C:98:PHE:HB2	1.33	0.93
1:C:120:TRP:CZ3	1:C:221:ASP:HA	2.05	0.92
2:B:163:ARG:HD2	4:D:1050:HOH:O	1.69	0.92
2:B:265:VAL:O	2:B:269:ARG:HB2	1.72	0.89
1:C:70:TYR:CE2	1:C:92:ASN:HB3	2.07	0.88
1:A:202:GLY:O	2:B:14:ARG:HD2	1.75	0.87
1:C:97:LYS:HB3	1:C:107:ASP:HB2	1.57	0.87
1:C:181:ILE:HG22	1:C:183:PRO:HD3	1.58	0.86
1:A:82:LEU:HD12	1:A:86:ARG:HB2	1.56	0.85
1:C:90:PRO:O	1:C:93:LYS:HG3	1.77	0.84
1:A:98:PHE:HD2	1:A:105:ALA:HB2	1.42	0.84
1:C:86:ARG:CB	1:C:86:ARG:HH11	1.90	0.84
1:C:120:TRP:HZ3	1:C:221:ASP:HA	1.42	0.84
2:B:268:GLN:HE21	2:B:268:GLN:N	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HA	1:C:121:ARG:NH2	1.93	0.84
2:D:143:LYS:HD3	2:D:143:LYS:H	1.43	0.84
1:C:96:PHE:CE2	1:C:98:PHE:HB2	2.12	0.83
2:D:257:GLN:O	2:D:260:ARG:HG2	1.78	0.83
2:B:143:LYS:N	2:B:143:LYS:HD3	1.94	0.83
2:B:143:LYS:HG2	2:B:144:ILE:HG13	1.61	0.83
1:C:82:LEU:HD12	1:C:86:ARG:CB	2.08	0.82
1:C:237:ASN:ND2	2:D:246:ILE:HG23	1.95	0.82
1:A:281:LYS:HD3	1:C:277:TYR:CB	2.10	0.82
1:C:153:THR:HG22	1:C:180:THR:HA	1.63	0.81
2:D:269:ARG:HE	2:D:269:ARG:HA	1.46	0.81
1:C:67:ILE:HB	1:C:72:ASP:CG	2.02	0.80
1:C:102:ARG:HG2	1:C:102:ARG:HH11	1.46	0.79
1:A:219:SER:H	1:A:224:THR:HG22	1.46	0.79
1:C:91:ARG:HA	1:C:121:ARG:HH21	1.47	0.78
1:A:273:LYS:HA	1:A:277:TYR:CD1	2.18	0.77
1:A:181:ILE:HG22	1:A:183:PRO:HD3	1.67	0.77
1:A:72:ASP:HA	4:A:330:HOH:O	1.84	0.75
2:B:266:LEU:O	2:B:270:GLN:HG3	1.86	0.74
1:C:86:ARG:CD	1:C:97:LYS:HB2	2.18	0.74
1:A:67:ILE:HD13	1:A:96:PHE:HB2	1.67	0.74
1:A:120:TRP:CZ3	1:A:221:ASP:HA	2.23	0.73
1:A:70:TYR:CB	1:A:72:ASP:HB3	2.19	0.73
1:A:277:TYR:H	1:A:277:TYR:HD1	1.35	0.73
1:A:276:SER:O	1:A:278:LYS:HD2	1.90	0.71
2:B:157:GLN:HB2	2:B:166:HIS:HB3	1.70	0.71
1:A:278:LYS:HD3	1:A:278:LYS:N	2.04	0.71
1:C:86:ARG:HB3	1:C:86:ARG:NH1	2.02	0.71
1:C:91:ARG:CA	1:C:121:ARG:HH21	2.03	0.71
2:B:195:ARG:NH1	2:B:223:LYS:HB3	2.06	0.71
2:B:268:GLN:NE2	2:B:268:GLN:N	2.39	0.71
1:A:185:THR:HG23	1:A:216:VAL:C	2.11	0.71
1:C:67:ILE:N	1:C:72:ASP:OD1	2.23	0.70
1:C:97:LYS:O	1:C:106:SER:N	2.23	0.70
1:A:266:ARG:HH11	1:A:266:ARG:HG3	1.54	0.70
1:A:58:ASN:HD22	1:A:100:HIS:HD2	1.36	0.70
1:A:227:GLU:O	1:A:231:ILE:HG13	1.93	0.69
1:C:120:TRP:HB3	1:C:154:ILE:HD11	1.73	0.69
1:A:153:THR:CG2	1:A:180:THR:HG22	2.22	0.69
1:C:95:SER:HB2	1:C:111:GLU:CB	2.23	0.69
1:A:125:ASP:HA	1:A:143:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LYS:HD3	1:C:155:ILE:HD12	1.75	0.68
1:A:220:SER:HB3	1:A:223:GLN:HB2	1.74	0.68
1:A:121:ARG:HG3	1:A:145:GLY:CA	2.23	0.68
1:A:121:ARG:HG3	1:A:145:GLY:HA3	1.76	0.68
1:C:95:SER:H	1:C:111:GLU:HB3	1.59	0.68
1:C:89:ASP:O	1:C:93:LYS:HA	1.94	0.67
2:B:54:VAL:HG23	2:B:55:VAL:HG23	1.76	0.67
1:C:94:ILE:HG12	1:C:110:PRO:HA	1.77	0.67
1:C:86:ARG:HH22	1:C:109:GLN:HB2	1.59	0.67
1:A:55:ALA:HA	1:A:100:HIS:NE2	2.10	0.67
1:A:34:ASN:O	1:A:38:LEU:HD23	1.95	0.67
1:A:67:ILE:N	1:A:72:ASP:OD2	2.27	0.67
1:A:58:ASN:HD22	1:A:100:HIS:CD2	2.12	0.67
2:D:135:LYS:HE2	4:D:1020:HOH:O	1.93	0.67
2:B:134:ILE:HB	2:B:150:SER:HB2	1.77	0.66
2:D:195:ARG:HD2	2:D:220:MET:SD	2.35	0.66
1:A:82:LEU:HD12	1:A:86:ARG:CB	2.24	0.66
1:A:185:THR:HG23	1:A:216:VAL:O	1.95	0.66
1:C:127:ALA:C	1:C:229:ILE:HD11	2.15	0.66
1:A:153:THR:HG22	1:A:180:THR:HG22	1.78	0.66
1:C:129:ARG:O	1:C:133:LYS:HE2	1.95	0.66
2:B:264:GLN:HA	2:B:267:THR:OG1	1.96	0.66
1:A:95:SER:HB3	1:A:109:GLN:O	1.96	0.65
2:D:143:LYS:HD3	2:D:143:LYS:N	2.11	0.65
2:B:178:GLN:HG2	2:B:188:ASN:ND2	2.12	0.65
1:C:70:TYR:HB2	1:C:72:ASP:HB3	1.75	0.65
1:A:66:LYS:HA	1:A:72:ASP:OD2	1.96	0.65
1:C:70:TYR:CB	1:C:72:ASP:CB	2.71	0.65
1:C:93:LYS:NZ	1:C:93:LYS:HB2	2.11	0.65
1:C:277:TYR:HE1	2:D:102:ASN:HD21	1.45	0.65
1:A:70:TYR:HB2	1:A:72:ASP:HB3	1.79	0.65
1:A:153:THR:HG22	1:A:180:THR:HA	1.79	0.65
1:A:98:PHE:CD2	1:A:105:ALA:HB2	2.29	0.65
2:D:143:LYS:H	2:D:143:LYS:CD	2.09	0.65
1:A:106:SER:O	1:A:107:ASP:OD2	2.13	0.64
1:A:243:ILE:HG23	2:B:187:MET:CE	2.27	0.64
2:D:253:GLN:N	2:D:253:GLN:CD	2.50	0.64
1:C:8:VAL:HG13	1:C:13:LYS:HE3	1.79	0.64
2:B:252:ASN:ND2	4:B:1113:HOH:O	2.29	0.64
1:A:114:GLU:H	1:A:114:GLU:CD	2.00	0.64
1:C:97:LYS:N	1:C:106:SER:O	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HA	1:A:277:TYR:CE1	2.32	0.63
2:D:253:GLN:HA	4:D:1161:HOH:O	1.98	0.63
1:C:97:LYS:CB	1:C:107:ASP:HB2	2.26	0.63
1:A:90:PRO:O	1:A:121:ARG:NH1	2.32	0.63
1:C:87:PHE:HB2	1:C:96:PHE:CZ	2.33	0.63
1:A:59:MET:CE	1:A:78:GLU:HA	2.29	0.62
2:B:268:GLN:HE21	2:B:268:GLN:CA	2.12	0.62
1:C:54:PHE:CD2	1:C:101:LEU:HD23	2.34	0.62
1:C:70:TYR:HB2	1:C:72:ASP:OD2	2.00	0.62
1:A:70:TYR:HB3	1:A:72:ASP:HB3	1.81	0.62
1:A:120:TRP:HB3	1:A:154:ILE:HD11	1.82	0.62
1:A:243:ILE:HG23	2:B:187:MET:HE1	1.81	0.62
1:A:67:ILE:CG2	1:A:70:TYR:HB2	2.29	0.62
2:B:14:ARG:HG2	4:B:1169:HOH:O	1.98	0.62
1:C:232:ILE:O	1:C:236:GLU:HG3	2.00	0.62
1:A:278:LYS:CD	1:A:278:LYS:N	2.61	0.62
1:A:278:LYS:CD	1:A:278:LYS:H	2.10	0.61
1:A:281:LYS:HA	1:C:277:TYR:HB2	1.82	0.61
2:B:253:GLN:N	2:B:253:GLN:CD	2.54	0.61
1:C:54:PHE:CE2	1:C:101:LEU:HD23	2.35	0.61
2:D:252:ASN:ND2	4:D:1111:HOH:O	2.34	0.61
1:C:113:THR:HG23	1:C:113:THR:O	2.01	0.61
1:C:121:ARG:NH1	1:C:122:ASP:HA	2.15	0.61
1:A:72:ASP:O	1:A:73:GLN:C	2.37	0.61
1:C:102:ARG:NH1	1:C:102:ARG:HG2	2.15	0.60
1:C:93:LYS:HZ2	1:C:93:LYS:HB2	1.67	0.60
2:D:134:ILE:HB	2:D:150:SER:HB2	1.82	0.60
1:A:67:ILE:HD12	1:A:105:ALA:O	2.02	0.60
1:C:91:ARG:N	1:C:121:ARG:HH21	2.00	0.60
2:B:149:ASP:HB2	2:B:174:MET:HB2	1.83	0.60
1:C:192:LEU:O	1:C:209:HIS:HA	2.02	0.59
2:D:223:LYS:HD2	4:D:1162:HOH:O	2.00	0.59
1:C:192:LEU:HD11	1:C:212:ILE:HD11	1.84	0.59
2:B:195:ARG:CZ	2:B:223:LYS:HD3	2.33	0.58
1:A:277:TYR:N	1:A:277:TYR:CD1	2.70	0.58
1:A:70:TYR:O	1:A:71:ASP:HB3	2.02	0.58
1:A:279:ILE:HG13	1:A:280:GLY:N	2.18	0.58
1:C:70:TYR:CD2	1:C:92:ASN:HB3	2.38	0.58
2:D:162:GLY:HA3	4:D:1123:HOH:O	2.02	0.58
1:A:137:PRO:HG2	2:B:242:GLY:O	2.04	0.58
1:A:37:ARG:HD3	4:A:328:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:OG	1:A:11:GLU:HG2	2.04	0.58
2:B:143:LYS:H	2:B:143:LYS:HD3	1.67	0.57
2:B:195:ARG:NH1	2:B:223:LYS:HD3	2.18	0.57
2:B:163:ARG:NH1	4:B:1099:HOH:O	2.24	0.57
2:D:157:GLN:HG3	4:D:1062:HOH:O	2.03	0.57
1:A:8:VAL:O	1:A:8:VAL:HG13	2.04	0.57
1:C:70:TYR:OH	1:C:94:ILE:HD12	2.05	0.57
1:A:67:ILE:HG22	1:A:72:ASP:CB	2.35	0.57
1:A:266:ARG:HG3	1:A:266:ARG:NH1	2.19	0.57
2:B:52:ASP:OD2	2:B:54:VAL:HG22	2.04	0.57
1:C:86:ARG:HH11	1:C:86:ARG:CG	2.18	0.57
1:A:72:ASP:O	1:A:74:VAL:N	2.38	0.56
1:A:87:PHE:HB2	1:A:96:PHE:CZ	2.40	0.56
1:C:90:PRO:O	1:C:93:LYS:CG	2.49	0.56
1:A:73:GLN:HG3	1:A:140:PHE:CE1	2.41	0.56
1:C:128:LEU:N	1:C:229:ILE:HD11	2.20	0.56
1:C:121:ARG:HH12	1:C:125:ASP:HB3	1.69	0.56
1:A:232:ILE:O	1:A:236:GLU:HG3	2.05	0.56
1:A:119:GLN:OE1	1:A:221:ASP:HB2	2.05	0.56
1:C:70:TYR:HB2	1:C:72:ASP:CB	2.35	0.56
1:C:73:GLN:NE2	1:C:140:PHE:CZ	2.74	0.56
1:A:230:LYS:HD2	1:A:230:LYS:O	2.05	0.56
2:B:270:GLN:O	2:B:271:ILE:C	2.43	0.56
1:A:90:PRO:O	1:A:93:LYS:HG2	2.05	0.56
2:B:252:ASN:OD1	2:B:254:LYS:HB3	2.06	0.56
1:C:188:VAL:HB	1:C:214:ASP:HB3	1.88	0.56
1:C:67:ILE:HB	1:C:72:ASP:OD2	2.06	0.56
2:B:145:LYS:N	2:B:145:LYS:HD2	2.21	0.55
1:C:102:ARG:HB3	1:C:104:GLU:H	1.71	0.55
1:A:89:ASP:O	1:A:93:LYS:HA	2.06	0.55
1:C:183:PRO:HG2	4:C:343:HOH:O	2.06	0.55
1:A:220:SER:OG	1:A:221:ASP:N	2.38	0.55
1:A:80:GLY:O	1:A:87:PHE:HA	2.07	0.55
2:D:18:PRO:O	2:D:21:ILE:HG13	2.06	0.55
2:B:80:ASP:HA	2:B:81:PRO:C	2.26	0.55
1:A:188:VAL:N	1:A:214:ASP:O	2.29	0.55
2:B:267:THR:C	2:B:268:GLN:HE21	2.10	0.55
1:A:186:ALA:N	1:A:216:VAL:O	2.37	0.55
1:A:121:ARG:HG3	1:A:145:GLY:N	2.21	0.54
1:A:56:GLN:O	1:A:60:ASP:OD2	2.23	0.54
1:A:120:TRP:CZ3	1:A:221:ASP:CA	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:GLN:HB2	2:D:166:HIS:HB3	1.90	0.54
2:B:230:GLU:HG3	4:B:1036:HOH:O	2.07	0.54
1:A:120:TRP:NE1	1:A:181:ILE:HD13	2.23	0.54
1:A:54:PHE:HB3	1:A:100:HIS:HB3	1.90	0.54
2:B:2:SER:HA	2:B:5:GLN:HG3	1.90	0.54
1:A:59:MET:HE3	1:A:78:GLU:HA	1.88	0.54
1:A:219:SER:H	1:A:224:THR:CG2	2.16	0.54
1:A:223:GLN:O	1:A:226:LYS:HG3	2.08	0.54
1:C:121:ARG:C	1:C:121:ARG:HH11	2.10	0.54
2:B:195:ARG:NH2	2:B:223:LYS:HD3	2.22	0.54
1:C:8:VAL:O	1:C:8:VAL:HG13	2.08	0.54
1:C:125:ASP:HA	1:C:143:VAL:HG21	1.90	0.53
2:D:251:ASP:OD1	2:D:251:ASP:N	2.38	0.53
1:A:248:GLN:NE2	1:A:248:GLN:HA	2.23	0.53
1:A:86:ARG:NH1	1:A:97:LYS:HB2	2.24	0.53
1:A:120:TRP:CD1	1:A:181:ILE:HD13	2.42	0.53
2:B:53:LYS:HE2	4:B:1123:HOH:O	2.08	0.53
1:A:153:THR:HG21	1:A:180:THR:HG22	1.91	0.53
1:A:67:ILE:O	1:A:69:GLY:N	2.41	0.53
1:A:101:LEU:C	1:A:101:LEU:HD23	2.28	0.53
1:A:55:ALA:HA	1:A:100:HIS:CD2	2.43	0.53
1:A:66:LYS:HE3	1:A:72:ASP:OD1	2.10	0.53
1:A:95:SER:O	1:A:108:PRO:HA	2.09	0.53
1:C:93:LYS:NZ	1:C:93:LYS:CB	2.72	0.53
1:A:62:PHE:O	1:A:64:PRO:HD3	2.09	0.52
1:C:86:ARG:NH2	1:C:107:ASP:O	2.42	0.52
1:A:58:ASN:ND2	1:A:100:HIS:HD2	2.06	0.52
1:A:192:LEU:HD12	1:A:192:LEU:N	2.25	0.52
1:C:68:GLU:CG	1:C:105:ALA:O	2.57	0.52
1:A:192:LEU:O	1:A:209:HIS:HA	2.09	0.52
1:C:50:ALA:O	1:C:54:PHE:HD1	1.92	0.52
2:D:139:ASP:CB	2:D:142:LYS:HE2	2.27	0.52
1:C:86:ARG:HD2	1:C:97:LYS:HB2	1.90	0.52
1:A:124:CYS:SG	1:A:154:ILE:HD13	2.50	0.52
2:B:80:ASP:OD2	2:B:81:PRO:HA	2.10	0.52
1:C:95:SER:HB2	1:C:111:GLU:HB3	1.92	0.52
1:A:50:ALA:O	1:A:54:PHE:HD1	1.92	0.52
1:C:93:LYS:O	1:C:111:GLU:O	2.28	0.52
1:C:86:ARG:NE	1:C:97:LYS:HB2	2.25	0.52
1:A:180:THR:O	1:A:186:ALA:HB1	2.10	0.51
1:C:93:LYS:HE2	1:C:118:LYS:NZ	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:HG2	1:C:121:ARG:NH1	2.24	0.51
1:A:70:TYR:C	1:A:72:ASP:N	2.64	0.51
1:C:10:ASP:O	1:C:14:VAL:HG23	2.11	0.51
1:A:128:LEU:HD22	1:A:156:ALA:HB1	1.91	0.51
1:A:273:LYS:HG3	1:A:277:TYR:CG	2.46	0.51
1:C:114:GLU:H	1:C:114:GLU:CD	2.14	0.51
1:A:192:LEU:HD11	1:A:212:ILE:HD11	1.93	0.51
1:A:280:GLY:O	1:A:281:LYS:HB2	2.11	0.51
1:C:121:ARG:HH12	1:C:125:ASP:CB	2.23	0.51
1:C:148:ILE:O	1:C:149:ASP:OD1	2.28	0.51
1:C:37:ARG:HD3	4:C:338:HOH:O	2.09	0.51
1:C:62:PHE:O	1:C:64:PRO:HD3	2.11	0.51
1:A:126:SER:HA	1:A:129:ARG:HB2	1.92	0.51
1:C:109:GLN:O	1:C:111:GLU:N	2.44	0.51
2:D:82:PRO:HA	4:D:1106:HOH:O	2.10	0.51
1:C:227:GLU:O	1:C:231:ILE:HG13	2.10	0.50
1:A:114:GLU:OE2	1:A:118:LYS:HG2	2.11	0.50
1:C:190:ALA:HB3	1:C:212:ILE:HG13	1.93	0.50
1:A:221:ASP:OD1	1:A:222:VAL:HG23	2.11	0.50
1:A:243:ILE:HD12	2:B:187:MET:HE3	1.92	0.50
1:A:67:ILE:HD13	1:A:96:PHE:CB	2.36	0.50
2:D:131:VAL:HA	2:D:152:HIS:O	2.12	0.50
1:A:8:VAL:HG13	1:A:13:LYS:HE3	1.93	0.50
1:A:279:ILE:HG13	1:A:280:GLY:H	1.77	0.50
2:B:199:LYS:NZ	4:B:1174:HOH:O	2.45	0.50
1:C:86:ARG:HD2	1:C:97:LYS:HA	1.93	0.50
2:D:269:ARG:NE	2:D:269:ARG:HA	2.21	0.50
1:A:120:TRP:HE1	1:A:181:ILE:HD13	1.76	0.50
1:A:273:LYS:HB2	1:A:273:LYS:NZ	2.26	0.50
1:A:184:PRO:O	1:A:218:VAL:HB	2.12	0.49
2:D:145:LYS:HD2	2:D:145:LYS:N	2.27	0.49
2:D:230:GLU:HG3	4:D:1011:HOH:O	2.13	0.49
1:C:86:ARG:NH1	1:C:95:SER:OG	2.45	0.49
1:A:248:GLN:HE21	1:A:248:GLN:HA	1.78	0.49
1:C:105:ALA:N	4:C:348:HOH:O	2.46	0.49
1:C:246:ASN:ND2	2:D:179:THR:HG21	2.27	0.49
1:C:263:PRO:HG3	2:D:111:TYR:CE1	2.48	0.49
2:D:253:GLN:H	2:D:253:GLN:CD	2.15	0.49
1:A:86:ARG:CZ	1:A:97:LYS:HB2	2.43	0.49
1:C:120:TRP:HA	1:C:120:TRP:CE3	2.48	0.49
1:C:70:TYR:N	1:C:72:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:GLN:H	2:D:253:GLN:NE2	2.10	0.49
1:A:120:TRP:HZ3	1:A:221:ASP:CA	2.26	0.49
1:A:45:LEU:O	1:A:48:GLU:HB2	2.12	0.49
2:B:143:LYS:N	2:B:143:LYS:CD	2.70	0.49
1:C:80:GLY:O	1:C:87:PHE:HA	2.13	0.48
1:C:181:ILE:HG23	1:C:218:VAL:HG21	1.94	0.48
2:D:179:THR:HG22	2:D:187:MET:HB3	1.95	0.48
1:A:125:ASP:HA	1:A:143:VAL:CG2	2.42	0.48
2:D:162:GLY:O	2:D:163:ARG:HB2	2.13	0.48
2:D:252:ASN:ND2	2:D:255:TYR:CE1	2.81	0.48
2:B:265:VAL:O	2:B:269:ARG:CB	2.55	0.48
1:C:269:ILE:HD12	2:D:107:TYR:HD1	1.79	0.48
1:A:120:TRP:CD1	1:A:181:ILE:CD1	2.96	0.48
1:A:59:MET:HE2	1:A:78:GLU:HA	1.93	0.48
1:C:99:ASP:HB3	1:C:102:ARG:HB2	1.95	0.48
1:C:216:VAL:HG22	1:C:217:GLN:N	2.28	0.48
2:D:252:ASN:OD1	2:D:254:LYS:HB2	2.13	0.48
2:D:139:ASP:HB2	2:D:142:LYS:CE	2.26	0.48
1:A:263:PRO:HG3	2:B:111:TYR:CE1	2.48	0.48
1:C:102:ARG:NH1	1:C:102:ARG:CG	2.77	0.48
1:A:217:GLN:HG3	1:A:227:GLU:OE2	2.14	0.48
1:C:121:ARG:HH12	1:C:122:ASP:HA	1.78	0.47
1:C:99:ASP:CG	1:C:102:ARG:CG	2.83	0.47
1:A:121:ARG:HH21	1:A:125:ASP:CB	2.27	0.47
2:B:143:LYS:HB2	2:B:181:LYS:HD3	1.96	0.47
1:C:98:PHE:HA	1:C:105:ALA:HA	1.95	0.47
2:D:143:LYS:HG3	2:D:181:LYS:HE2	1.96	0.47
1:A:120:TRP:HZ3	1:A:221:ASP:CB	2.27	0.47
1:C:129:ARG:O	1:C:133:LYS:HG3	2.13	0.47
1:C:87:PHE:HB2	1:C:96:PHE:CE1	2.49	0.47
2:D:195:ARG:HG2	2:D:196:GLN:N	2.30	0.47
2:B:17:PRO:HB2	2:B:20:GLN:NE2	2.29	0.47
2:D:25:LEU:O	2:D:29:ILE:HG13	2.15	0.47
2:B:249:ILE:O	2:B:251:ASP:N	2.46	0.47
2:B:61:LEU:HD22	2:B:71:TYR:CG	2.50	0.47
1:C:277:TYR:HE1	2:D:102:ASN:ND2	2.10	0.47
2:D:257:GLN:HA	2:D:260:ARG:NE	2.30	0.47
1:C:95:SER:HB2	1:C:111:GLU:HG2	1.96	0.47
1:A:120:TRP:HZ3	1:A:221:ASP:HB3	1.79	0.47
1:C:86:ARG:HD2	1:C:97:LYS:CA	2.45	0.47
1:C:118:LYS:HG2	1:C:122:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:SER:OG	1:C:221:ASP:N	2.48	0.47
1:C:70:TYR:CB	1:C:72:ASP:OD2	2.63	0.47
1:A:95:SER:N	1:A:109:GLN:O	2.48	0.46
1:A:128:LEU:CD2	1:A:156:ALA:HB1	2.45	0.46
1:C:153:THR:HA	1:C:179:PHE:O	2.15	0.46
1:C:70:TYR:O	1:C:71:ASP:HB3	2.14	0.46
3:B:1002:NO3:O2	2:D:95:LYS:HG2	2.15	0.46
1:C:192:LEU:CD1	1:C:192:LEU:N	2.78	0.46
1:C:266:ARG:HH11	1:C:266:ARG:HG3	1.80	0.46
1:C:98:PHE:CE1	1:C:100:HIS:HA	2.51	0.46
2:D:163:ARG:HG3	2:D:163:ARG:NH1	2.31	0.46
1:A:243:ILE:HG23	2:B:187:MET:HE3	1.96	0.46
2:B:171:SER:OG	2:B:220:MET:HG2	2.16	0.46
1:C:142:THR:HA	4:C:306:HOH:O	2.15	0.46
1:A:67:ILE:CD1	1:A:96:PHE:HB2	2.41	0.46
1:C:86:ARG:HH21	1:C:109:GLN:HG3	1.80	0.45
1:C:86:ARG:NH2	1:C:109:GLN:CG	2.79	0.45
1:C:89:ASP:OD1	1:C:92:ASN:ND2	2.37	0.45
1:A:95:SER:HB2	1:A:111:GLU:CG	2.46	0.45
1:A:82:LEU:HB2	1:A:86:ARG:O	2.15	0.45
2:B:105:ASP:OD1	2:B:108:ARG:NH1	2.45	0.45
2:B:179:THR:HG22	2:B:187:MET:HB3	1.97	0.45
1:C:192:LEU:HD12	1:C:192:LEU:N	2.31	0.45
2:B:267:THR:OG1	2:B:268:GLN:NE2	2.49	0.45
1:C:55:ALA:HA	1:C:100:HIS:CE1	2.51	0.45
2:D:23:LYS:HA	2:D:23:LYS:HE2	1.98	0.45
1:A:191:VAL:O	1:A:191:VAL:HG13	2.16	0.45
1:A:131:TYR:HE1	1:A:233:GLU:HG3	1.82	0.45
1:C:95:SER:CB	1:C:111:GLU:CB	2.93	0.45
1:A:183:PRO:HA	1:A:184:PRO:C	2.35	0.45
2:B:21:ILE:HD11	4:B:1072:HOH:O	2.16	0.45
1:C:112:ASP:N	1:C:112:ASP:OD1	2.49	0.45
1:C:117:LEU:HD23	1:C:145:GLY:CA	2.47	0.45
1:C:29:PHE:HE2	1:C:54:PHE:CE2	2.35	0.45
1:A:146:LYS:HG2	1:A:147:SER:N	2.32	0.45
1:A:56:GLN:NE2	4:A:337:HOH:O	2.49	0.45
2:B:256:LYS:O	2:B:260:ARG:HG3	2.16	0.45
1:C:120:TRP:HA	1:C:120:TRP:HE3	1.81	0.45
2:D:259:GLN:HA	2:D:259:GLN:NE2	2.31	0.45
1:A:81:ASP:HA	1:A:87:PHE:CD1	2.52	0.45
2:B:143:LYS:H	2:B:143:LYS:CD	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ASP:HB2	2:D:174:MET:HB2	1.99	0.45
2:B:131:VAL:HA	2:B:152:HIS:O	2.17	0.44
1:C:114:GLU:O	1:C:114:GLU:HG2	2.17	0.44
1:A:107:ASP:O	1:A:107:ASP:OD2	2.35	0.44
1:A:70:TYR:OH	1:A:94:ILE:HG21	2.16	0.44
1:C:8:VAL:CG1	1:C:13:LYS:HE3	2.46	0.44
1:C:91:ARG:HD3	1:C:129:ARG:HH11	1.82	0.44
1:A:117:LEU:HD23	1:A:146:LYS:H	1.82	0.44
1:C:132:VAL:HG21	1:C:141:CYS:HB3	1.99	0.44
1:C:95:SER:HB2	1:C:111:GLU:CG	2.47	0.44
1:A:218:VAL:HG13	1:A:224:THR:HG21	1.98	0.44
1:A:67:ILE:HG22	1:A:72:ASP:OD1	2.18	0.44
1:C:191:VAL:O	1:C:191:VAL:HG13	2.17	0.44
1:A:95:SER:HB2	1:A:111:GLU:HG2	2.00	0.44
1:A:219:SER:N	1:A:224:THR:CG2	2.81	0.44
1:C:70:TYR:C	1:C:72:ASP:N	2.66	0.44
1:C:86:ARG:NH2	1:C:109:GLN:HG3	2.32	0.44
1:A:89:ASP:O	1:A:93:LYS:N	2.48	0.44
2:B:82:PRO:HA	4:B:1132:HOH:O	2.18	0.44
2:D:132:ILE:HB	2:D:152:HIS:HB2	1.99	0.44
2:B:122:TRP:CE2	2:B:129:ALA:HB3	2.53	0.43
1:C:125:ASP:HA	1:C:143:VAL:CG2	2.48	0.43
2:D:80:ASP:HA	2:D:81:PRO:C	2.38	0.43
1:A:95:SER:HB3	1:A:109:GLN:HB2	1.99	0.43
2:B:210:ILE:HG13	3:B:1002:NO3:O1	2.17	0.43
2:B:261:GLU:O	2:B:265:VAL:HG23	2.18	0.43
1:C:99:ASP:CG	1:C:102:ARG:HG3	2.39	0.43
1:C:90:PRO:HG3	1:C:144:TYR:CD2	2.53	0.43
1:C:38:LEU:HD12	2:D:8:CYS:SG	2.58	0.43
2:B:164:THR:HA	2:B:201:GLU:O	2.19	0.43
2:B:23:LYS:HG3	4:B:1018:HOH:O	2.17	0.43
1:C:86:ARG:HD2	1:C:97:LYS:CB	2.49	0.43
2:D:244:ARG:HG2	2:D:245:SER:N	2.33	0.43
1:A:117:LEU:HD11	1:A:120:TRP:HD1	1.84	0.43
1:A:97:LYS:HD2	1:A:97:LYS:C	2.39	0.43
2:D:57:LYS:NZ	4:D:1175:HOH:O	2.51	0.43
1:C:97:LYS:HB3	1:C:106:SER:O	2.19	0.43
1:A:107:ASP:N	1:A:108:PRO:HD3	2.34	0.43
1:C:186:ALA:HB2	1:C:218:VAL:HG13	2.01	0.43
1:A:37:ARG:NH1	4:A:328:HOH:O	2.49	0.43
1:A:65:VAL:HG22	1:A:66:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HE2	1:A:78:GLU:CA	2.48	0.42
1:C:89:ASP:OD1	1:C:92:ASN:HB2	2.19	0.42
1:A:173:TRP:HE1	1:A:175:SER:HB2	1.84	0.42
1:A:70:TYR:CE2	1:A:92:ASN:HB3	2.54	0.42
2:B:78:LYS:HD2	4:B:1104:HOH:O	2.20	0.42
1:C:121:ARG:HH11	1:C:121:ARG:HG2	1.82	0.42
1:C:266:ARG:NH1	1:C:266:ARG:HG3	2.34	0.42
2:D:163:ARG:HH11	2:D:163:ARG:HG3	1.83	0.42
1:A:79:HIS:CD2	1:A:155:ILE:HG21	2.54	0.42
2:B:51:ARG:HD3	2:B:58:ASP:OD1	2.18	0.42
1:C:120:TRP:HB3	1:C:154:ILE:CD1	2.45	0.42
1:C:89:ASP:O	1:C:93:LYS:CA	2.66	0.42
1:C:58:ASN:HD22	1:C:100:HIS:CD2	2.37	0.42
1:A:35:ASP:OD1	2:B:11:ASP:OD2	2.37	0.42
1:C:70:TYR:HB2	1:C:72:ASP:CG	2.40	0.42
1:A:153:THR:HA	1:A:179:PHE:O	2.20	0.42
1:A:219:SER:OG	1:A:220:SER:N	2.52	0.42
1:C:210:LYS:HE2	1:C:212:ILE:HG23	2.01	0.42
1:C:67:ILE:O	1:C:69:GLY:N	2.52	0.42
1:A:58:ASN:ND2	1:A:100:HIS:CD2	2.83	0.42
2:B:268:GLN:NE2	2:B:268:GLN:CA	2.81	0.42
2:B:55:VAL:HG12	2:B:55:VAL:O	2.20	0.42
1:A:281:LYS:CD	1:C:277:TYR:HB2	2.26	0.42
1:C:64:PRO:HG3	1:C:159:GLU:OE2	2.20	0.42
2:B:18:PRO:O	2:B:21:ILE:HG13	2.20	0.42
1:C:183:PRO:HA	1:C:185:THR:N	2.35	0.42
1:A:118:LYS:HA	1:A:118:LYS:HD3	1.86	0.41
1:A:87:PHE:HB2	1:A:96:PHE:CE1	2.55	0.41
1:C:216:VAL:HG22	1:C:217:GLN:H	1.84	0.41
2:D:168:LYS:HG3	2:D:198:GLU:HG2	2.01	0.41
2:D:171:SER:OG	2:D:220:MET:HG2	2.21	0.41
1:C:37:ARG:HG3	1:C:46:LEU:HD22	2.01	0.41
1:A:142:THR:HA	4:A:331:HOH:O	2.19	0.41
1:C:91:ARG:CZ	1:C:129:ARG:HD3	2.50	0.41
1:C:66:LYS:NZ	1:C:71:ASP:H	2.18	0.41
1:A:101:LEU:CD2	1:A:101:LEU:C	2.89	0.41
1:A:269:ILE:HD12	2:B:107:TYR:HD1	1.85	0.41
1:C:109:GLN:O	1:C:110:PRO:C	2.58	0.41
1:C:29:PHE:CE2	1:C:54:PHE:CE2	3.08	0.41
1:A:119:GLN:OE1	1:A:221:ASP:CB	2.68	0.41
1:A:192:LEU:CD1	1:A:192:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:CE3	1:A:221:ASP:HA	2.55	0.41
1:C:183:PRO:HA	1:C:184:PRO:C	2.37	0.41
1:C:70:TYR:CA	1:C:72:ASP:OD2	2.69	0.41
1:C:65:VAL:O	1:C:73:GLN:HA	2.21	0.41
1:C:195:GLN:HA	1:C:206:LEU:O	2.21	0.41
1:A:203:ASN:HB2	2:B:14:ARG:HD3	2.03	0.41
2:B:117:SER:HA	2:B:133:LEU:O	2.21	0.41
1:C:72:ASP:HA	4:C:344:HOH:O	2.21	0.41
2:D:14:ARG:HG2	4:D:1129:HOH:O	2.20	0.41
2:D:159:LYS:HZ1	2:D:166:HIS:HB2	1.86	0.41
2:B:207:SER:OG	2:B:215:ARG:NH2	2.54	0.41
1:C:39:LEU:HD13	2:D:28:LEU:HD11	2.03	0.41
1:A:264:VAL:O	1:A:266:ARG:NH1	2.54	0.40
2:B:2:SER:O	2:B:5:GLN:HB2	2.21	0.40
1:C:269:ILE:HD12	2:D:107:TYR:CD1	2.56	0.40
1:C:82:LEU:HB2	1:C:86:ARG:O	2.21	0.40
1:A:228:PHE:HA	1:A:231:ILE:HD12	2.03	0.40
1:A:239:TYR:O	1:A:243:ILE:HG12	2.20	0.40
1:C:68:GLU:OE2	1:C:105:ALA:HB3	2.21	0.40
2:B:209:HIS:HB2	3:B:1002:NO3:O1	2.21	0.40
2:D:122:TRP:CE2	2:D:129:ALA:HB3	2.57	0.40
1:A:148:ILE:O	1:A:149:ASP:OD1	2.40	0.40
1:A:169:TRP:HA	1:A:197:HIS:O	2.22	0.40
1:A:66:LYS:HB2	1:A:73:GLN:OE1	2.22	0.40
2:B:168:LYS:HE3	2:B:196:GLN:OE1	2.21	0.40
2:B:66:ARG:HB2	2:B:71:TYR:CE2	2.56	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	273/286 (96%)	248 (91%)	21 (8%)	4 (2%)	12	6
1	C	271/286 (95%)	245 (90%)	22 (8%)	4 (2%)	12	6
2	B	268/277 (97%)	258 (96%)	9 (3%)	1 (0%)	38	35
2	D	268/277 (97%)	262 (98%)	5 (2%)	1 (0%)	38	35
All	All	1080/1126 (96%)	1013 (94%)	57 (5%)	10 (1%)	20	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	C	68	GLU
2	D	162	GLY
1	A	73	GLN
1	C	91	ARG
1	A	277	TYR
2	B	250	PRO
1	C	69	GLY
1	C	110	PRO
1	A	69	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/252 (96%)	232 (96%)	11 (4%)	32	30
1	C	242/252 (96%)	231 (96%)	11 (4%)	32	30
2	B	241/248 (97%)	237 (98%)	4 (2%)	66	72
2	D	241/248 (97%)	235 (98%)	6 (2%)	53	57
All	All	967/1000 (97%)	935 (97%)	32 (3%)	43	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG

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Mol	Chain	Res	Type
1	A	66	LYS
1	A	84	ASN
1	A	114	GLU
1	A	120	TRP
1	A	121	ARG
1	A	212	ILE
1	A	226	LYS
1	A	230	LYS
1	A	234	ASN
1	A	278	LYS
2	B	143	LYS
2	B	164	THR
2	B	253	GLN
2	B	268	GLN
1	C	86	ARG
1	C	112	ASP
1	C	114	GLU
1	C	120	TRP
1	C	121	ARG
1	C	149	ASP
1	C	184	PRO
1	C	185	THR
1	C	187	GLN
1	C	212	ILE
1	C	217	GLN
2	D	23	LYS
2	D	143	LYS
2	D	148	TRP
2	D	251	ASP
2	D	268	GLN
2	D	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	100	HIS
1	A	135	HIS
1	A	167	ASN
1	A	234	ASN
1	A	248	GLN
2	B	20	GLN

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Mol	Chain	Res	Type
2	B	157	GLN
2	B	166	HIS
2	B	178	GLN
2	B	259	GLN
2	B	264	GLN
2	B	268	GLN
1	C	30	ASN
1	C	34	ASN
1	C	41	ASN
1	C	73	GLN
1	C	100	HIS
1	C	162	GLN
1	C	217	GLN
1	C	234	ASN
2	D	4	GLN
2	D	102	ASN
2	D	166	HIS
2	D	259	GLN
2	D	264	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NO3	B	1002	-	1,3,3	5.48	1 (100%)	0,3,3	0.00	-
3	NO3	B	1003	-	1,3,3	6.02	1 (100%)	0,3,3	0.00	-
3	NO3	D	1001	-	1,3,3	5.93	1 (100%)	0,3,3	0.00	-
3	NO3	D	1004	-	1,3,3	5.93	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NO3	B	1002	-	-	0/0/0/0	0/0/0/0
3	NO3	B	1003	-	-	0/0/0/0	0/0/0/0
3	NO3	D	1001	-	-	0/0/0/0	0/0/0/0
3	NO3	D	1004	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	NO3	O1-N	5.48	1.44	1.23
3	D	1001	NO3	O1-N	5.93	1.46	1.23
3	D	1004	NO3	O1-N	5.93	1.46	1.23
3	B	1003	NO3	O1-N	6.02	1.46	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	NO3	4	0
3	B	1003	NO3	1	0
3	D	1001	NO3	1	0
3	D	1004	NO3	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/286 (96%)	0.75	44 (16%) <b>2</b> <b>3</b>	20, 52, 88, 92	0
1	C	273/286 (95%)	0.59	29 (10%) <b>7</b> <b>8</b>	20, 52, 85, 92	0
2	B	270/277 (97%)	-0.10	11 (4%) 38 45	13, 29, 64, 87	0
2	D	270/277 (97%)	-0.14	8 (2%) 51 58	14, 29, 62, 81	0
All	All	1088/1126 (96%)	0.28	92 (8%) <b>11</b> <b>15</b>	13, 40, 81, 92	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	GLY	10.6
1	A	277	TYR	6.7
1	A	70	TYR	6.5
1	C	94	ILE	5.4
1	A	100	HIS	4.8
2	B	269	ARG	4.8
1	A	98	PHE	4.7
2	D	2	SER	4.5
1	C	82	LEU	4.3
1	A	102	ARG	4.2
1	C	98	PHE	4.2
1	A	120	TRP	4.0
1	A	67	ILE	4.0
1	A	72	ASP	3.9
1	C	97	LYS	3.8
1	C	148	ILE	3.6
1	C	103	LYS	3.5
1	C	102	ARG	3.5
2	B	2	SER	3.4
1	A	231	ILE	3.4
1	A	71	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	3.3
1	A	7	ARG	3.3
1	C	101	LEU	3.2
1	A	216	VAL	3.2
1	C	72	ASP	3.1
1	A	96	PHE	3.1
1	A	221	ASP	3.0
1	C	96	PHE	3.0
1	A	151	GLN	3.0
1	C	70	TYR	3.0
1	A	88	LEU	3.0
1	A	103	LYS	2.9
1	A	115	SER	2.9
1	C	120	TRP	2.9
2	B	250	PRO	2.9
1	A	140	PHE	2.8
2	D	269	ARG	2.8
1	C	99	ASP	2.8
1	A	188	VAL	2.8
1	A	183	PRO	2.8
2	D	250	PRO	2.7
1	C	216	VAL	2.7
1	A	107	ASP	2.7
2	B	252	ASN	2.7
1	A	186	ALA	2.7
2	D	141	SER	2.6
1	A	184	PRO	2.6
1	A	217	GLN	2.6
1	C	107	ASP	2.6
1	C	151	GLN	2.5
2	B	271	ILE	2.5
1	A	108	PRO	2.5
1	A	101	LEU	2.5
1	C	222	VAL	2.4
1	C	90	PRO	2.4
1	C	100	HIS	2.4
1	A	146	LYS	2.4
1	A	8	VAL	2.4
1	A	99	ASP	2.4
1	C	146	LYS	2.3
1	C	112	ASP	2.3
2	B	162	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	251	ASP	2.3
1	C	115	SER	2.3
1	C	152	GLN	2.2
2	D	182	THR	2.2
1	A	82	LEU	2.2
1	A	281	LYS	2.2
1	A	104	GLU	2.2
1	C	8	VAL	2.2
1	C	113	THR	2.2
1	A	83	GLY	2.2
2	B	264	GLN	2.1
2	D	253	GLN	2.1
1	C	221	ASP	2.1
2	B	263	SER	2.1
1	A	68	GLU	2.1
1	C	179	PHE	2.1
1	A	126	SER	2.1
1	A	181	ILE	2.1
1	A	279	ILE	2.1
2	D	140	GLY	2.1
1	A	94	ILE	2.1
1	C	218	VAL	2.1
2	B	253	GLN	2.1
1	A	84	ASN	2.0
1	A	179	PHE	2.0
1	C	7	ARG	2.0
2	B	161	SER	2.0
1	A	117	LEU	2.0
2	D	252	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO3	B	1003	4/4	0.88	0.35	8.09	53,54,54,56	0
3	NO3	D	1004	4/4	0.92	0.20	5.37	43,44,46,47	0
3	NO3	D	1001	4/4	0.94	0.17	3.62	24,28,30,31	0
3	NO3	B	1002	4/4	0.98	0.17	3.51	22,26,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.