



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 AM GMT

PDB ID : 2ZQR  
Title : Crystal structure of AUH without RNA  
Authors : Kurimoto, K.; Kuwasako, K.; Muto, Y.; Nureki, O.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2008-08-16  
Resolution : 2.50 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

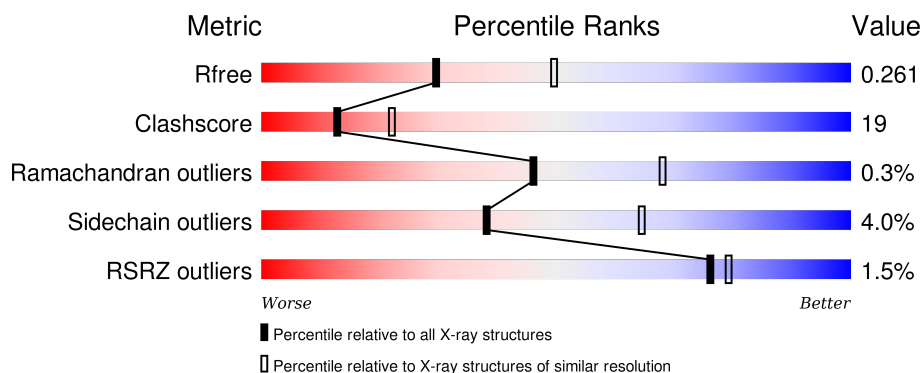
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	272	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>
1	B	272	<div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	C	272	<div> <div>%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	D	272	<div> <div>4%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
1	E	272	<div> <div>%</div> <div>63%</div> <div>31%</div> <div>..</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	272	<div><div><div>%</div><div><div></div></div><div>64%</div><div>32%</div><div><div></div><div></div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12354 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 Methylglutaconyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2000	1260	359	372	9			
1	B	265	Total	C	N	O	S	0	0	0
			1991	1255	358	369	9			
1	C	266	Total	C	N	O	S	0	0	0
			2000	1260	359	372	9			
1	D	265	Total	C	N	O	S	0	0	0
			1991	1255	358	369	9			
1	E	266	Total	C	N	O	S	0	0	0
			2000	1260	359	372	9			
1	F	265	Total	C	N	O	S	0	0	0
			1991	1255	358	369	9			

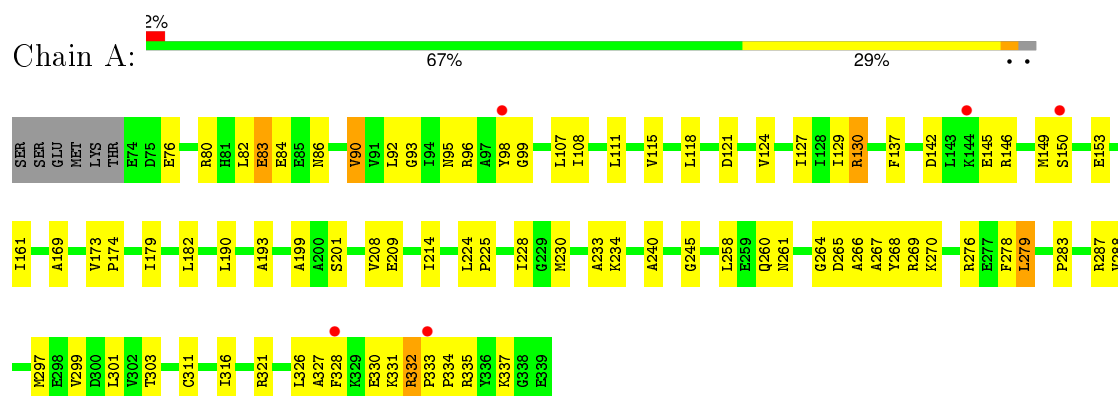
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	74	Total	O	0	0
			74	74		
2	C	57	Total	O	0	0
			57	57		
2	D	50	Total	O	0	0
			50	50		
2	E	62	Total	O	0	0
			62	62		
2	F	73	Total	O	0	0
			73	73		

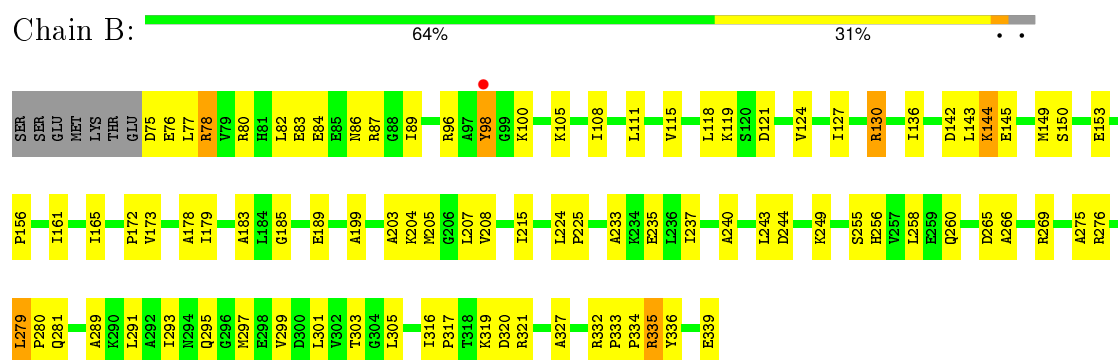
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

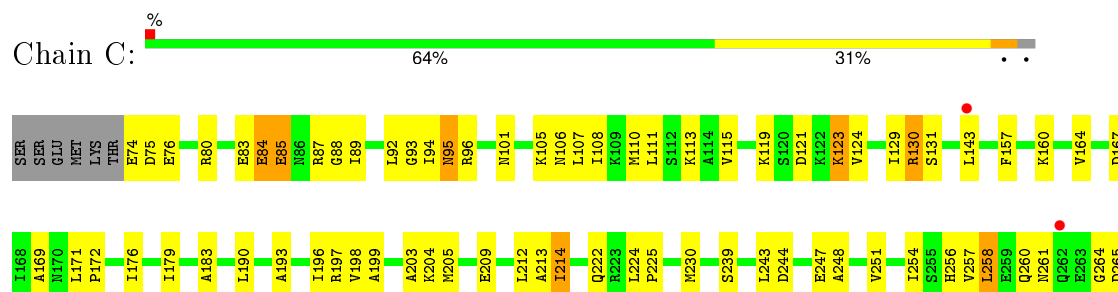
#### • Molecule 1: Methylglutaconyl-CoA hydratase



#### • Molecule 1: Methylglutaconyl-CoA hydratase

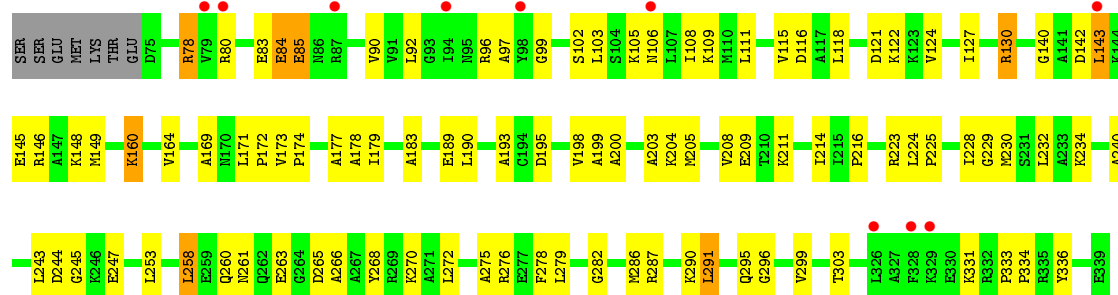


#### • Molecule 1: Methylglutaconyl-CoA hydratase

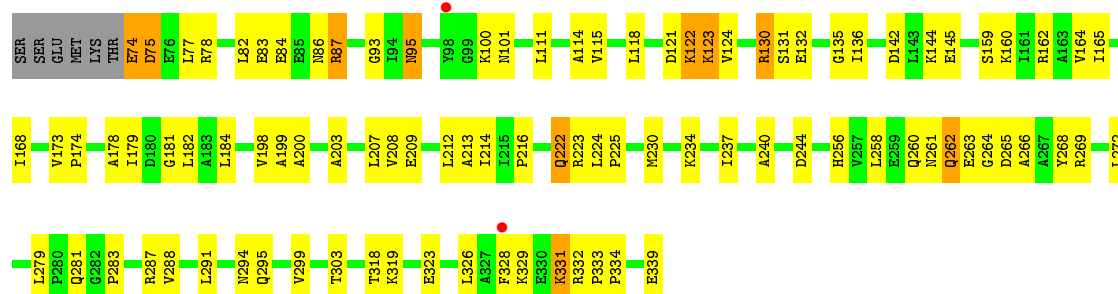




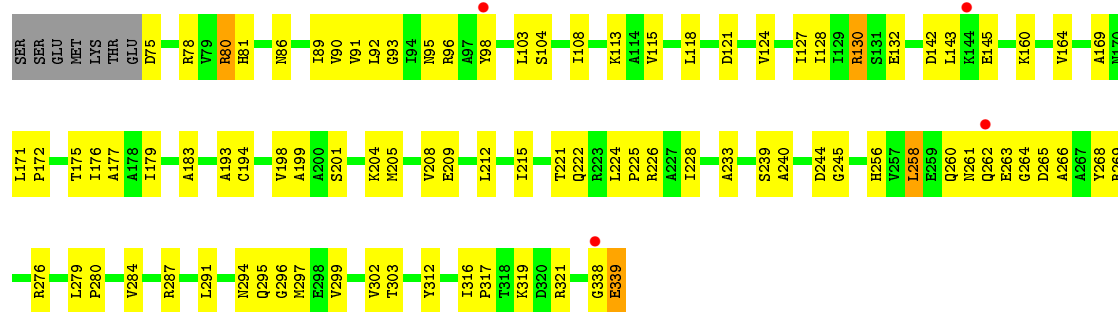
• Molecule 1: Methylglutaconyl-CoA hydratase



• Molecule 1: Methylglutaconyl-CoA hydratase



• Molecule 1: Methylglutaconyl-CoA hydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.21Å 132.43Å 80.04Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.50) 98.4 (39.21-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.263 0.196 , 0.261	Depositor DCC
$R_{free}$ test set	5420 reflections (10.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.7	EDS
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 53375 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/2021	0.58	0/2717
1	B	0.34	0/2012	0.59	0/2705
1	C	0.33	0/2021	0.60	0/2717
1	D	0.32	0/2012	0.59	0/2705
1	E	0.32	0/2021	0.58	0/2717
1	F	0.34	0/2012	0.59	0/2705
All	All	0.33	0/12099	0.59	0/16266

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2000	0	2116	72	0
1	B	1991	0	2110	80	0
1	C	2000	0	2116	85	0
1	D	1991	0	2110	87	0
1	E	2000	0	2116	84	0
1	F	1991	0	2110	91	0
2	A	65	0	0	2	0
2	B	74	0	0	2	0
2	C	57	0	0	1	0
2	D	50	0	0	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	62	0	0	3	0
2	F	73	0	0	5	0
All	All	12354	0	12678	474	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 19.

All (474) 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:78:ARG:HH11	1:B:78:ARG:HB2	1.22	1.03
1:D:291:LEU:HD13	1:D:295:GLN:HE22	1.25	1.00
1:D:276:ARG:HA	1:D:279:LEU:HD23	1.47	0.94
1:D:260:GLN:HE22	1:D:266:ALA:H	0.98	0.92
1:F:260:GLN:HE21	1:F:261:ASN:H	1.18	0.90
1:B:86:ASN:HD21	1:B:276:ARG:HH11	1.20	0.89
1:D:258:LEU:HD21	1:D:270:LYS:HB2	1.55	0.89
1:E:74:GLU:HG2	1:E:75:ASP:H	1.38	0.88
1:D:260:GLN:NE2	1:D:266:ALA:H	1.72	0.88
1:D:291:LEU:HD13	1:D:295:GLN:NE2	1.88	0.87
1:F:86:ASN:HD21	1:F:276:ARG:HH11	1.21	0.87
1:B:75:ASP:HB3	2:B:388:HOH:O	1.74	0.86
1:C:84:GLU:O	1:C:85:GLU:HB3	1.76	0.86
1:B:276:ARG:HA	1:B:279:LEU:HD22	1.56	0.86
1:C:260:GLN:HE21	1:C:261:ASN:H	1.26	0.84
1:D:105:LYS:O	1:D:109:LYS:HG3	1.77	0.83
1:D:143:LEU:H	1:D:143:LEU:HD12	1.42	0.82
1:A:230:MET:HG2	1:A:234:LYS:HE3	1.61	0.81
1:A:146:ARG:HE	1:A:149:MET:HE3	1.44	0.80
1:C:89:ILE:HD11	1:C:279:LEU:HD11	1.63	0.80
1:F:260:GLN:NE2	1:F:261:ASN:H	1.80	0.80
1:E:230:MET:HE3	1:F:297:MET:HG3	1.65	0.79
1:F:90:VAL:HB	1:F:127:ILE:HD13	1.65	0.79
1:E:260:GLN:NE2	1:E:261:ASN:H	1.82	0.78
1:B:291:LEU:HD22	1:B:295:GLN:NE2	1.99	0.78
1:D:276:ARG:HA	1:D:279:LEU:CD2	2.11	0.78
1:F:319:LYS:HD2	1:F:339:GLU:HG3	1.66	0.77
1:B:78:ARG:HB2	1:B:78:ARG:NH1	1.98	0.77
1:F:121:ASP:CG	1:F:124:VAL:HG23	2.04	0.77
1:D:105:LYS:HD2	1:D:109:LYS:HE3	1.66	0.76
1:B:260:GLN:HE22	1:B:266:ALA:H	1.33	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:GLN:HE21	1:E:261:ASN:H	1.31	0.76
1:A:276:ARG:HA	1:A:279:LEU:HD22	1.67	0.76
1:E:122:LYS:H	1:E:122:LYS:HE3	1.50	0.75
1:B:327:ALA:HA	1:B:332:ARG:NH1	2.01	0.74
1:E:160:LYS:O	1:E:164:VAL:HG23	1.88	0.74
1:C:260:GLN:HE22	1:C:266:ALA:H	1.35	0.73
1:A:230:MET:HE3	1:B:297:MET:HG3	1.70	0.73
1:E:182:LEU:HD21	1:E:184:LEU:HD12	1.69	0.73
1:D:230:MET:HG2	1:D:234:LYS:HE3	1.68	0.73
1:B:76:GLU:HB3	1:B:96:ARG:HG2	1.71	0.73
1:D:209:GLU:HB3	1:D:214:ILE:HG13	1.71	0.73
1:F:90:VAL:HG21	1:F:124:VAL:HG22	1.71	0.72
1:F:198:VAL:HG12	1:F:256:HIS:HB2	1.70	0.72
1:A:111:LEU:O	1:A:115:VAL:HG23	1.89	0.72
1:D:224:LEU:HB3	1:D:225:PRO:HD3	1.72	0.72
1:B:289:ALA:O	1:B:293:ILE:HG12	1.90	0.72
1:E:198:VAL:HG22	1:E:256:HIS:HB2	1.73	0.70
1:C:123:LYS:HG3	1:C:124:VAL:N	2.06	0.70
1:A:258:LEU:HD12	1:A:267:ALA:HA	1.73	0.70
1:B:142:ASP:OD2	1:B:145:GLU:HG3	1.91	0.69
1:C:80:ARG:HH11	1:C:80:ARG:HG2	1.55	0.69
1:F:316:ILE:HB	1:F:317:PRO:HD3	1.75	0.69
1:B:98:TYR:HD1	1:B:98:TYR:H	1.39	0.69
1:A:90:VAL:HG13	1:A:124:VAL:HG13	1.75	0.69
1:B:78:ARG:HG2	1:B:80:ARG:NH2	2.07	0.69
1:B:143:LEU:HD23	1:B:143:LEU:O	1.93	0.69
1:B:78:ARG:HG2	1:B:80:ARG:HH22	1.55	0.69
1:D:143:LEU:HD22	1:E:328:PHE:CE2	2.28	0.69
1:F:262:GLN:HG3	1:F:263:GLU:H	1.56	0.68
1:E:262:GLN:NE2	1:E:263:GLU:HG2	2.09	0.67
1:B:291:LEU:HD22	1:B:295:GLN:HE21	1.58	0.67
1:A:258:LEU:CD1	1:A:267:ALA:HA	2.25	0.67
1:E:260:GLN:HE22	1:E:266:ALA:H	1.40	0.67
1:D:258:LEU:HD12	1:D:258:LEU:N	2.10	0.67
1:D:263:GLU:HB2	1:D:265:ASP:OD1	1.95	0.66
1:E:222:GLN:OE1	1:F:296:GLY:HA3	1.95	0.66
1:C:76:GLU:OE1	1:C:96:ARG:HG2	1.95	0.66
1:D:208:VAL:HG12	1:D:240:ALA:O	1.95	0.65
1:D:260:GLN:HE22	1:D:266:ALA:N	1.82	0.65
1:F:260:GLN:NE2	1:F:264:GLY:HA2	2.12	0.65
1:D:336:TYR:HB2	2:D:365:HOH:O	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LYS:N	1:E:122:LYS:HE3	2.11	0.65
1:F:115:VAL:HG13	1:F:171:LEU:HD21	1.79	0.65
1:B:121:ASP:CG	1:B:124:VAL:HG23	2.17	0.65
1:F:78:ARG:HD2	1:F:132:GLU:OE1	1.97	0.64
1:D:103:LEU:HB3	1:D:108:ILE:HD11	1.79	0.64
1:D:90:VAL:HG11	1:D:124:VAL:HG12	1.80	0.64
1:D:179:ILE:HB	1:D:199:ALA:HB2	1.80	0.64
1:F:262:GLN:HG3	1:F:263:GLU:N	2.13	0.64
1:E:207:LEU:HD12	1:E:237:ILE:HD11	1.78	0.64
1:C:89:ILE:CD1	1:C:279:LEU:HD11	2.27	0.64
1:B:335:ARG:HH11	1:B:335:ARG:HG2	1.62	0.63
1:C:303:THR:HG21	1:E:299:VAL:HG11	1.80	0.63
1:A:260:GLN:HE22	1:A:266:ALA:H	1.46	0.63
1:F:127:ILE:C	1:F:128:ILE:HD12	2.19	0.63
1:F:78:ARG:HH12	1:F:95:ASN:ND2	1.97	0.63
1:A:260:GLN:HE21	1:A:261:ASN:H	1.46	0.63
1:F:312:TYR:CE2	1:F:316:ILE:HD11	2.34	0.63
1:D:203:ALA:O	1:D:244:ASP:HA	1.98	0.62
1:D:105:LYS:NZ	1:D:106:ASN:HB2	2.15	0.62
1:B:299:VAL:HG11	1:F:303:THR:HG21	1.80	0.62
1:D:121:ASP:CG	1:D:124:VAL:HG13	2.19	0.62
1:E:93:GLY:HA2	1:E:130:ARG:O	1.99	0.62
1:D:179:ILE:HB	1:D:199:ALA:CB	2.30	0.61
1:D:278:PHE:HE2	1:F:239:SER:HB3	1.66	0.61
1:C:84:GLU:HG3	1:C:84:GLU:O	2.01	0.61
1:B:332:ARG:HE	1:B:335:ARG:NE	1.96	0.61
1:F:262:GLN:HE21	1:F:263:GLU:HG2	1.64	0.61
1:D:142:ASP:OD2	1:D:145:GLU:HG3	2.01	0.61
1:D:84:GLU:HG3	1:D:84:GLU:O	2.01	0.61
1:A:146:ARG:HA	1:A:149:MET:HE3	1.83	0.61
1:E:328:PHE:O	1:E:331:LYS:HD3	2.01	0.61
1:E:122:LYS:CE	1:E:122:LYS:H	2.14	0.60
1:E:87:ARG:HG3	1:E:87:ARG:HH11	1.66	0.60
1:F:86:ASN:ND2	1:F:276:ARG:HD3	2.17	0.60
1:D:296:GLY:HA3	1:F:222:GLN:OE1	2.00	0.60
1:B:233:ALA:O	1:B:237:ILE:HG12	2.01	0.60
1:A:92:LEU:HD11	1:A:118:LEU:HD11	1.84	0.60
1:C:96:ARG:HB2	1:C:101:ASN:HA	1.83	0.60
1:D:291:LEU:CD1	1:D:295:GLN:HE22	2.06	0.60
1:A:146:ARG:NE	1:A:149:MET:HE3	2.16	0.60
1:F:90:VAL:CG2	1:F:124:VAL:HG22	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:H	1:C:101:ASN:ND2	2.00	0.60
1:B:161:ILE:O	1:B:165:ILE:HG12	2.02	0.59
1:A:129:ILE:HG21	1:A:190:LEU:HD21	1.82	0.59
1:D:244:ASP:OD1	1:D:247:GLU:HG3	2.02	0.59
1:C:84:GLU:O	1:C:85:GLU:CB	2.50	0.59
1:E:262:GLN:HE22	1:E:263:GLU:HG2	1.67	0.59
1:A:258:LEU:HD11	1:A:270:LYS:CB	2.33	0.58
1:A:93:GLY:HA2	1:A:130:ARG:O	2.04	0.58
1:D:223:ARG:HD2	2:D:342:HOH:O	2.02	0.58
1:A:76:GLU:HA	1:A:95:ASN:O	2.03	0.58
1:E:100:LYS:HD3	2:E:358:HOH:O	2.03	0.58
1:B:111:LEU:O	1:B:115:VAL:HG23	2.02	0.58
1:F:284:VAL:HG23	1:F:338:GLY:O	2.03	0.58
1:A:230:MET:CG	1:A:234:LYS:HE3	2.34	0.58
1:B:89:ILE:HD12	1:B:275:ALA:HB1	1.87	0.57
1:E:319:LYS:HE2	1:E:319:LYS:HA	1.85	0.57
1:F:92:LEU:HD11	1:F:118:LEU:HD11	1.84	0.57
1:D:230:MET:CG	1:D:234:LYS:HE3	2.34	0.57
1:C:74:GLU:HG2	1:C:75:ASP:N	2.19	0.57
1:E:230:MET:CG	1:E:234:LYS:HE3	2.34	0.57
1:C:129:ILE:HG21	1:C:190:LEU:HD21	1.86	0.57
1:A:288:VAL:HB	1:A:311:CYS:HB3	1.85	0.57
1:A:96:ARG:NH1	1:A:99:GLY:HA3	2.20	0.57
1:C:89:ILE:HD12	1:C:275:ALA:HB1	1.87	0.57
1:B:203:ALA:O	1:B:244:ASP:HA	2.04	0.57
1:A:179:ILE:HB	1:A:199:ALA:HB2	1.86	0.57
1:F:80:ARG:HG3	1:F:91:VAL:HB	1.85	0.57
1:B:145:GLU:O	1:B:149:MET:HG3	2.05	0.57
1:D:183:ALA:O	1:D:205:MET:HA	2.05	0.57
1:A:316:ILE:HA	1:A:321:ARG:HD3	1.84	0.57
1:A:150:SER:OG	1:A:153:GLU:HG3	2.05	0.56
1:A:258:LEU:HD11	1:A:270:LYS:HB3	1.86	0.56
1:A:327:ALA:CB	1:A:334:PRO:HG3	2.35	0.56
1:E:111:LEU:O	1:E:115:VAL:HG23	2.04	0.56
1:C:160:LYS:O	1:C:164:VAL:HG23	2.06	0.56
1:D:275:ALA:O	1:D:279:LEU:HD22	2.06	0.56
1:F:81:HIS:HE1	1:F:121:ASP:OD1	1.89	0.56
1:B:335:ARG:HG2	1:B:335:ARG:NH1	2.20	0.56
1:F:175:THR:O	1:F:176:ILE:HD13	2.06	0.56
1:F:183:ALA:O	1:F:205:MET:HA	2.06	0.56
1:E:230:MET:HE2	1:F:294:ASN:HA	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:VAL:HG11	1:E:303:THR:HG21	1.88	0.56
1:A:82:LEU:HB3	1:A:86:ASN:HB2	1.88	0.56
1:C:111:LEU:O	1:C:115:VAL:HG23	2.06	0.56
1:B:280:PRO:HB2	1:B:281:GLN:NE2	2.21	0.55
1:D:260:GLN:HE21	1:D:261:ASN:H	1.54	0.55
1:E:74:GLU:HG2	1:E:75:ASP:N	2.17	0.55
1:C:275:ALA:O	1:C:279:LEU:HD13	2.07	0.55
1:D:195:ASP:OD1	1:D:290:LYS:HE3	2.06	0.55
1:B:105:LYS:HG3	1:B:145:GLU:OE1	2.07	0.55
1:C:75:ASP:O	1:C:95:ASN:HB3	2.07	0.55
1:E:291:LEU:HD22	1:E:295:GLN:HE22	1.72	0.55
1:F:179:ILE:HB	1:F:199:ALA:HB2	1.89	0.55
1:C:203:ALA:O	1:C:244:ASP:HA	2.07	0.54
1:E:179:ILE:HB	1:E:199:ALA:HB2	1.88	0.54
1:A:327:ALA:HA	1:A:332:ARG:NH1	2.22	0.54
1:B:280:PRO:HB2	1:B:281:GLN:HE22	1.73	0.54
1:F:143:LEU:HD23	1:F:143:LEU:O	2.08	0.54
1:F:316:ILE:HB	1:F:317:PRO:CD	2.36	0.54
1:A:96:ARG:HH12	1:A:99:GLY:HA3	1.72	0.54
1:A:108:ILE:HG21	1:A:161:ILE:HD13	1.89	0.54
1:B:224:LEU:HB3	1:B:225:PRO:HD3	1.89	0.54
1:C:115:VAL:HG12	1:C:119:LYS:HE3	1.90	0.53
1:D:115:VAL:HG13	1:D:171:LEU:HD21	1.90	0.53
1:E:265:ASP:O	1:E:269:ARG:HG2	2.08	0.53
1:B:98:TYR:CD1	1:B:98:TYR:N	2.76	0.53
1:E:216:PRO:HG2	1:E:237:ILE:HD12	1.89	0.53
1:A:118:LEU:HD13	1:A:127:ILE:HD13	1.91	0.53
1:A:121:ASP:CG	1:A:124:VAL:HG23	2.29	0.53
1:C:302:VAL:HG21	1:F:302:VAL:HG11	1.90	0.53
1:D:105:LYS:CD	1:D:109:LYS:HE3	2.39	0.53
1:A:142:ASP:OD1	1:A:145:GLU:HG3	2.09	0.53
1:F:265:ASP:OD2	1:F:269:ARG:CZ	2.56	0.53
1:D:211:LYS:HG2	1:E:281:GLN:NE2	2.23	0.53
1:F:224:LEU:O	1:F:228:ILE:HG12	2.09	0.53
1:C:143:LEU:HD23	1:C:143:LEU:O	2.09	0.53
1:A:146:ARG:HE	1:A:149:MET:CE	2.17	0.52
1:A:121:ASP:OD1	1:A:124:VAL:HG23	2.09	0.52
1:E:82:LEU:O	1:E:87:ARG:HA	2.09	0.52
1:A:299:VAL:HG11	1:D:303:THR:HG21	1.90	0.52
1:F:164:VAL:HG23	2:F:409:HOH:O	2.09	0.52
1:B:316:ILE:HA	1:B:321:ARG:HD3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:GLY:C	2:F:391:HOH:O	2.47	0.52
1:D:145:GLU:O	1:D:149:MET:HG3	2.10	0.52
1:A:297:MET:HG3	1:C:230:MET:CE	2.40	0.52
1:A:260:GLN:NE2	1:A:264:GLY:HA2	2.24	0.52
1:A:326:LEU:O	1:A:330:GLU:HG3	2.10	0.52
1:E:224:LEU:HB3	1:E:225:PRO:HD3	1.92	0.52
1:D:90:VAL:CG1	1:D:124:VAL:HG12	2.40	0.52
1:B:185:GLY:O	1:B:189:GLU:HG3	2.09	0.51
1:E:261:ASN:OD1	1:E:264:GLY:N	2.43	0.51
1:D:169:ALA:HA	1:D:193:ALA:O	2.11	0.51
1:B:204:LYS:HA	1:B:243:LEU:O	2.10	0.51
1:B:78:ARG:HH11	1:B:78:ARG:CB	2.09	0.51
1:D:84:GLU:O	1:D:85:GLU:HB3	2.11	0.51
1:C:204:LYS:HA	1:C:243:LEU:O	2.10	0.51
1:C:121:ASP:CG	1:C:124:VAL:HG23	2.31	0.51
1:F:179:ILE:HB	1:F:199:ALA:CB	2.40	0.51
1:B:332:ARG:HE	1:B:335:ARG:HE	1.59	0.51
1:C:212:LEU:O	1:C:213:ALA:HB3	2.10	0.51
1:A:301:LEU:CD1	1:C:222:GLN:HB3	2.40	0.51
1:D:97:ALA:C	1:D:99:GLY:H	2.13	0.51
1:E:283:PRO:O	1:E:287:ARG:HG3	2.11	0.51
1:E:230:MET:CE	1:F:297:MET:HG3	2.39	0.51
1:D:92:LEU:HD21	1:D:118:LEU:HD11	1.92	0.51
1:A:330:GLU:HB2	1:A:332:ARG:HD3	1.92	0.51
1:C:198:VAL:HG23	1:C:198:VAL:O	2.11	0.51
1:E:77:LEU:HD12	1:E:93:GLY:O	2.11	0.50
1:B:316:ILE:HB	1:B:317:PRO:HD3	1.93	0.50
1:E:83:GLU:O	1:E:84:GLU:HB2	2.09	0.50
1:C:198:VAL:HG21	1:C:271:ALA:HB2	1.91	0.50
1:F:221:THR:O	1:F:225:PRO:HG2	2.10	0.50
1:F:209:GLU:HG2	1:F:215:ILE:O	2.12	0.50
1:C:291:LEU:O	1:C:295:GLN:HB2	2.11	0.50
1:F:319:LYS:N	1:F:339:GLU:O	2.41	0.50
1:E:78:ARG:HD2	1:E:132:GLU:OE1	2.12	0.50
1:C:93:GLY:HA2	1:C:130:ARG:O	2.12	0.50
1:F:201:SER:HA	1:F:245:GLY:HA3	1.94	0.50
1:F:260:GLN:HE22	1:F:266:ALA:H	1.59	0.50
1:F:319:LYS:HD2	1:F:339:GLU:CG	2.40	0.50
1:F:160:LYS:HB2	1:F:160:LYS:NZ	2.27	0.50
1:D:90:VAL:CG2	1:D:127:ILE:HG12	2.41	0.49
1:D:230:MET:O	1:D:234:LYS:HG3	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:SER:OG	1:B:153:GLU:HG3	2.11	0.49
1:D:160:LYS:O	1:D:164:VAL:HG23	2.11	0.49
1:B:119:LYS:HD3	1:B:172:PRO:HD3	1.94	0.49
1:A:297:MET:HG3	1:C:230:MET:HE3	1.93	0.49
1:B:179:ILE:O	1:B:199:ALA:HA	2.12	0.49
1:A:80:ARG:HD3	2:A:354:HOH:O	2.12	0.49
1:E:100:LYS:HG2	1:E:136:ILE:HD13	1.93	0.49
1:D:111:LEU:O	1:D:115:VAL:HG23	2.12	0.49
1:C:261:ASN:OD1	1:C:264:GLY:N	2.46	0.48
1:B:76:GLU:HB3	1:B:96:ARG:CG	2.43	0.48
1:B:235:GLU:HB2	1:C:196:ILE:HD12	1.95	0.48
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.76	0.48
1:B:100:LYS:HE3	1:B:136:ILE:HD11	1.94	0.48
1:F:90:VAL:HG21	1:F:124:VAL:CG2	2.42	0.48
1:F:169:ALA:HA	1:F:193:ALA:O	2.14	0.48
1:F:279:LEU:HB2	1:F:280:PRO:HD3	1.96	0.48
1:B:208:VAL:HG12	1:B:240:ALA:O	2.13	0.48
1:E:208:VAL:HG12	1:E:240:ALA:O	2.13	0.48
1:E:230:MET:HG2	1:E:234:LYS:HE3	1.96	0.48
1:C:96:ARG:NH1	1:C:96:ARG:HB3	2.29	0.48
1:E:159:SER:HA	1:E:162:ARG:NH1	2.29	0.48
1:A:169:ALA:HA	1:A:193:ALA:O	2.14	0.48
1:B:87:ARG:HG3	1:B:87:ARG:O	2.13	0.48
1:C:96:ARG:CD	1:C:107:LEU:HD22	2.44	0.48
1:C:130:ARG:HD3	1:C:131:SER:O	2.13	0.48
1:F:121:ASP:OD2	1:F:124:VAL:HG23	2.14	0.48
1:F:128:ILE:HD12	1:F:128:ILE:N	2.28	0.48
1:E:115:VAL:HG21	1:E:168:ILE:HD11	1.96	0.48
1:E:95:ASN:HB2	1:E:132:GLU:HG3	1.96	0.48
1:F:103:LEU:HB3	1:F:108:ILE:HD11	1.95	0.48
1:B:320:ASP:OD1	1:B:336:TYR:HA	2.14	0.47
1:F:228:ILE:HD11	1:F:233:ALA:HA	1.95	0.47
1:C:199:ALA:O	1:C:257:VAL:HA	2.14	0.47
1:C:169:ALA:HA	1:C:193:ALA:O	2.14	0.47
1:E:142:ASP:OD2	1:E:144:LYS:HB2	2.14	0.47
1:D:228:ILE:O	1:D:232:LEU:HD12	2.15	0.47
1:D:190:LEU:HD23	1:D:190:LEU:O	2.15	0.47
1:C:176:ILE:HG23	1:C:196:ILE:HB	1.96	0.47
1:C:83:GLU:HA	1:C:87:ARG:HA	1.97	0.47
1:C:318:THR:HB	1:C:339:GLU:OXT	2.15	0.47
1:C:298:GLU:HB2	2:E:387:HOH:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ASP:OD1	1:F:145:GLU:HG3	2.15	0.47
1:A:90:VAL:HG22	1:A:127:ILE:HG12	1.97	0.47
1:E:135:GLY:C	1:E:181:GLY:HA3	2.34	0.46
1:A:209:GLU:HB3	1:A:214:ILE:HG13	1.97	0.46
1:E:332:ARG:HH11	1:E:332:ARG:HG3	1.79	0.46
1:D:105:LYS:HZ2	1:D:106:ASN:HB2	1.79	0.46
1:C:89:ILE:HD11	1:C:279:LEU:CD1	2.40	0.46
1:D:198:VAL:O	1:D:198:VAL:HG23	2.15	0.46
1:E:114:ALA:O	1:E:118:LEU:HD13	2.16	0.46
1:B:118:LEU:HD13	1:B:127:ILE:HD13	1.97	0.46
1:E:326:LEU:HD12	1:E:332:ARG:HH21	1.81	0.46
1:A:173:VAL:HB	1:A:174:PRO:HD2	1.97	0.46
1:F:90:VAL:HB	1:F:127:ILE:CD1	2.42	0.46
1:C:80:ARG:HG2	1:C:80:ARG:NH1	2.28	0.46
1:B:207:LEU:HD12	1:B:237:ILE:HD11	1.96	0.46
1:F:208:VAL:HA	1:F:240:ALA:HB1	1.98	0.46
1:B:303:THR:HG21	1:F:299:VAL:HG11	1.98	0.46
1:A:201:SER:HA	1:A:245:GLY:HA3	1.97	0.46
1:D:200:ALA:O	1:D:245:GLY:HA3	2.16	0.46
1:C:74:GLU:CG	1:C:75:ASP:N	2.78	0.46
1:A:303:THR:HG21	1:D:299:VAL:HG11	1.97	0.46
1:A:83:GLU:HG3	1:A:84:GLU:H	1.81	0.46
1:A:137:PHE:HB3	1:A:182:LEU:O	2.15	0.46
1:E:268:TYR:CE2	1:E:272:LEU:HD11	2.51	0.46
1:F:209:GLU:HG2	1:F:215:ILE:C	2.36	0.45
1:A:301:LEU:N	1:C:298:GLU:OE1	2.49	0.45
1:D:78:ARG:HH11	1:D:78:ARG:HG2	1.82	0.45
1:A:146:ARG:HA	1:A:149:MET:CE	2.47	0.45
1:D:127:ILE:CD1	1:D:171:LEU:HD13	2.46	0.45
1:E:82:LEU:HB3	1:E:86:ASN:HB2	1.97	0.45
1:C:244:ASP:OD1	1:C:247:GLU:HG3	2.16	0.45
1:A:278:PHE:HE2	1:C:239:SER:HB3	1.80	0.45
1:F:130:ARG:HG2	1:F:268:TYR:CD1	2.52	0.45
1:C:209:GLU:O	1:C:214:ILE:HD13	2.17	0.45
1:C:209:GLU:HB3	1:C:214:ILE:HG12	1.97	0.45
1:D:336:TYR:OH	1:F:212:LEU:HA	2.17	0.45
1:E:288:VAL:HA	1:E:291:LEU:HD12	1.98	0.45
1:B:84:GLU:O	1:B:87:ARG:HG2	2.16	0.45
1:F:260:GLN:HE21	1:F:261:ASN:N	2.01	0.45
1:E:87:ARG:HG3	1:E:87:ARG:NH1	2.32	0.45
1:A:98:TYR:H	1:A:98:TYR:HD1	1.65	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ILE:N	1:E:181:GLY:HA3	2.31	0.45
1:F:222:GLN:O	1:F:226:ARG:HG3	2.16	0.45
1:C:179:ILE:HB	1:C:199:ALA:HB2	1.99	0.45
1:D:80:ARG:HG3	1:D:80:ARG:O	2.16	0.45
1:E:261:ASN:OD1	1:E:263:GLU:N	2.49	0.45
1:D:172:PRO:HB3	1:D:287:ARG:NH1	2.32	0.45
1:B:265:ASP:O	1:B:269:ARG:HG2	2.17	0.45
1:B:144:LYS:NZ	1:B:144:LYS:HA	2.32	0.45
1:B:130:ARG:HB2	2:B:355:HOH:O	2.16	0.45
1:C:80:ARG:HH11	1:C:80:ARG:CG	2.27	0.45
1:C:108:ILE:HG23	1:C:164:VAL:HG21	1.97	0.45
1:D:229:GLY:HA3	2:D:343:HOH:O	2.15	0.45
1:D:106:ASN:O	1:D:109:LYS:HB2	2.16	0.45
1:E:332:ARG:HG3	1:E:332:ARG:NH1	2.31	0.45
1:C:316:ILE:HB	1:C:317:PRO:HD3	1.99	0.45
1:C:183:ALA:O	1:C:205:MET:HA	2.17	0.45
1:D:253:LEU:O	1:D:253:LEU:HD12	2.16	0.44
1:E:207:LEU:HD12	1:E:237:ILE:CD1	2.46	0.44
1:A:260:GLN:NE2	1:A:266:ALA:H	2.12	0.44
1:B:179:ILE:HB	1:B:199:ALA:HB2	1.98	0.44
1:A:228:ILE:HD11	1:A:233:ALA:HA	1.98	0.44
1:B:332:ARG:HH11	1:B:332:ARG:HG2	1.83	0.44
1:F:78:ARG:HD2	1:F:132:GLU:CD	2.36	0.44
1:E:203:ALA:O	1:E:244:ASP:HA	2.18	0.44
1:D:96:ARG:HG2	1:D:96:ARG:HH11	1.83	0.44
1:E:173:VAL:HB	1:E:174:PRO:CD	2.47	0.44
1:D:282:GLY:O	1:D:286:MET:HG2	2.17	0.44
1:C:260:GLN:HE21	1:C:261:ASN:N	2.03	0.44
1:E:130:ARG:C	1:E:130:ARG:HD2	2.38	0.44
1:C:92:LEU:N	1:C:92:LEU:HD12	2.33	0.44
1:C:94:ILE:HG21	1:C:101:ASN:HB3	1.98	0.44
1:E:142:ASP:OD2	1:E:145:GLU:HG3	2.17	0.44
1:D:204:LYS:HA	1:D:243:LEU:O	2.17	0.44
1:B:333:PRO:HA	1:B:334:PRO:HD3	1.90	0.44
1:E:318:THR:HB	1:E:339:GLU:OXT	2.17	0.44
1:B:269:ARG:HG3	1:B:269:ARG:NH1	2.33	0.44
1:C:96:ARG:HD3	1:C:107:LEU:HD22	2.00	0.44
1:E:130:ARG:C	1:E:130:ARG:CD	2.86	0.44
1:F:284:VAL:CG2	1:F:338:GLY:O	2.66	0.44
1:F:260:GLN:NE2	1:F:264:GLY:CA	2.81	0.44
1:F:86:ASN:HD21	1:F:276:ARG:NH1	2.02	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASP:C	1:B:77:LEU:H	2.21	0.44
1:E:329:LYS:C	1:E:331:LYS:H	2.21	0.44
1:B:121:ASP:OD1	1:B:124:VAL:HG23	2.17	0.44
1:A:130:ARG:HG2	1:A:268:TYR:CD1	2.53	0.43
1:F:269:ARG:HA	1:F:269:ARG:HD3	1.84	0.43
1:B:260:GLN:NE2	1:B:266:ALA:H	2.10	0.43
1:B:153:GLU:O	1:B:156:PRO:HD2	2.18	0.43
1:D:84:GLU:O	1:D:85:GLU:CB	2.64	0.43
1:B:108:ILE:CD1	1:B:161:ILE:HG12	2.49	0.43
1:F:177:ALA:HB2	1:F:194:CYS:SG	2.59	0.43
1:C:260:GLN:NE2	1:C:261:ASN:H	2.06	0.43
1:D:90:VAL:HG22	1:D:127:ILE:HG12	2.01	0.43
1:D:189:GLU:OE1	1:D:216:PRO:HB3	2.18	0.43
1:F:130:ARG:HH11	1:F:130:ARG:HB2	1.83	0.43
1:A:328:PHE:O	1:A:331:LYS:HD3	2.18	0.43
1:C:260:GLN:CD	1:C:264:GLY:HA2	2.39	0.43
1:D:178:ALA:HA	1:D:198:VAL:HG23	2.00	0.43
1:E:200:ALA:HA	1:E:258:LEU:O	2.18	0.43
1:E:209:GLU:HB3	1:E:214:ILE:HG13	2.00	0.43
1:C:171:LEU:HA	1:C:172:PRO:HD3	1.84	0.43
1:B:316:ILE:HA	1:B:321:ARG:CD	2.48	0.43
1:E:212:LEU:O	1:E:213:ALA:HB3	2.19	0.43
1:B:183:ALA:O	1:B:205:MET:HA	2.18	0.43
1:C:273:ASP:HA	1:C:276:ARG:NH1	2.33	0.43
1:F:244:ASP:C	1:F:244:ASP:OD1	2.56	0.43
1:F:258:LEU:HD21	1:F:266:ALA:O	2.18	0.43
1:D:171:LEU:HA	1:D:172:PRO:HD3	1.84	0.43
1:A:316:ILE:HA	1:A:321:ARG:CD	2.49	0.43
1:A:265:ASP:O	1:A:269:ARG:HG2	2.19	0.43
1:D:177:ALA:O	1:D:198:VAL:HG22	2.19	0.42
1:F:172:PRO:HB2	1:F:287:ARG:NH1	2.33	0.42
1:E:333:PRO:HA	1:E:334:PRO:HD3	1.80	0.42
1:B:319:LYS:H	1:B:339:GLU:C	2.21	0.42
1:F:224:LEU:HB3	1:F:225:PRO:HD3	2.01	0.42
1:C:224:LEU:N	1:C:225:PRO:CD	2.82	0.42
1:D:102:SER:HA	1:D:140:GLY:O	2.18	0.42
1:E:291:LEU:CD2	1:E:295:GLN:HE22	2.33	0.42
1:B:130:ARG:HB3	1:B:178:ALA:HB3	2.01	0.42
1:D:118:LEU:HD13	1:D:127:ILE:HD13	2.00	0.42
1:C:123:LYS:NZ	1:C:124:VAL:HA	2.35	0.42
1:C:198:VAL:HG12	1:C:256:HIS:HB2	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LYS:HZ1	1:B:144:LYS:HA	1.84	0.42
1:C:248:ALA:HA	1:C:251:VAL:HG22	2.02	0.42
1:D:173:VAL:HB	1:D:174:PRO:CD	2.49	0.42
1:E:74:GLU:CD	1:E:74:GLU:N	2.73	0.42
1:F:78:ARG:HD2	1:F:132:GLU:OE2	2.20	0.42
1:C:130:ARG:HB2	2:C:379:HOH:O	2.19	0.42
1:B:75:ASP:C	1:B:77:LEU:N	2.71	0.42
1:C:190:LEU:C	1:C:190:LEU:HD23	2.40	0.42
1:B:215:ILE:HG13	1:C:312:TYR:HD1	1.84	0.42
1:D:103:LEU:N	1:D:140:GLY:O	2.38	0.42
1:F:89:ILE:HG23	1:F:128:ILE:HD13	2.01	0.41
1:C:157:PHE:O	1:C:160:LYS:HB3	2.20	0.41
1:A:108:ILE:HG21	1:A:161:ILE:CD1	2.49	0.41
1:E:123:LYS:NZ	1:E:123:LYS:HB3	2.35	0.41
1:C:74:GLU:N	1:C:110:MET:CE	2.83	0.41
1:F:130:ARG:NH1	2:F:343:HOH:O	2.50	0.41
1:E:121:ASP:CG	1:E:124:VAL:HG23	2.41	0.41
1:E:101:ASN:ND2	1:E:131:SER:OG	2.51	0.41
1:C:265:ASP:O	1:C:269:ARG:HG2	2.19	0.41
1:C:105:LYS:HG3	1:C:106:ASN:N	2.35	0.41
1:E:130:ARG:HB3	1:E:178:ALA:HB3	2.02	0.41
1:D:83:GLU:O	1:D:84:GLU:HG3	2.20	0.41
1:E:165:ILE:O	1:E:168:ILE:HB	2.20	0.41
1:E:262:GLN:O	1:E:262:GLN:HG2	2.20	0.41
1:A:337:LYS:HB2	1:A:337:LYS:HE2	1.90	0.41
1:D:146:ARG:C	1:D:148:LYS:H	2.24	0.41
1:F:124:VAL:HG11	1:F:127:ILE:HD11	2.03	0.41
1:C:88:GLY:HA2	1:C:123:LYS:NZ	2.35	0.41
1:F:104:SER:O	1:F:108:ILE:HG12	2.20	0.41
1:A:224:LEU:HB3	1:A:225:PRO:HD3	2.02	0.41
1:D:268:TYR:CZ	1:D:272:LEU:HD11	2.55	0.41
1:F:224:LEU:N	1:F:225:PRO:CD	2.84	0.41
1:E:258:LEU:HD23	1:E:258:LEU:N	2.35	0.41
1:C:272:LEU:O	1:C:276:ARG:HG3	2.21	0.41
1:D:333:PRO:HA	1:D:334:PRO:HD3	1.77	0.41
1:A:333:PRO:O	1:A:335:ARG:NH1	2.54	0.41
1:D:143:LEU:O	1:D:146:ARG:HB3	2.20	0.41
1:E:136:ILE:HA	1:E:182:LEU:H	1.86	0.41
1:A:173:VAL:HB	1:A:174:PRO:CD	2.51	0.41
1:E:173:VAL:HB	1:E:174:PRO:HD2	2.03	0.41
1:B:255:SER:HB2	1:B:256:HIS:CD2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ARG:CZ	2:F:358:HOH:O	2.69	0.41
1:F:96:ARG:NH2	2:F:358:HOH:O	2.52	0.41
1:B:332:ARG:NE	1:B:335:ARG:HE	2.19	0.41
1:D:230:MET:HE1	1:E:294:ASN:HA	2.03	0.41
1:A:107:LEU:O	1:A:111:LEU:HB2	2.20	0.41
1:F:316:ILE:HA	1:F:321:ARG:HD3	2.03	0.41
1:C:164:VAL:O	1:C:167:ASP:HB2	2.21	0.41
1:F:93:GLY:HA2	1:F:130:ARG:O	2.21	0.41
1:F:291:LEU:HD22	1:F:295:GLN:HE22	1.86	0.41
1:F:86:ASN:ND2	1:F:276:ARG:HH11	2.01	0.41
1:A:179:ILE:O	1:A:199:ALA:HA	2.20	0.41
1:A:283:PRO:O	1:A:287:ARG:HG3	2.21	0.41
1:E:223:ARG:HD2	2:E:364:HOH:O	2.21	0.41
1:A:208:VAL:HA	1:A:240:ALA:HB1	2.03	0.41
1:F:90:VAL:HG11	1:F:118:LEU:HD21	2.02	0.40
1:C:88:GLY:HA2	1:C:123:LYS:HZ3	1.85	0.40
1:F:78:ARG:HH12	1:F:95:ASN:HD22	1.67	0.40
1:B:82:LEU:O	1:B:87:ARG:HA	2.20	0.40
1:C:197:ARG:HB3	1:C:254:ILE:HG22	2.03	0.40
1:B:301:LEU:O	1:B:305:LEU:HG	2.20	0.40
1:D:173:VAL:HB	1:D:174:PRO:HD2	2.02	0.40
1:C:113:LYS:NZ	1:C:113:LYS:HB3	2.35	0.40
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.86	0.40
1:A:92:LEU:HD11	1:A:118:LEU:CD1	2.50	0.40
1:B:124:VAL:O	1:B:173:VAL:HG11	2.20	0.40
1:E:84:GLU:OE1	1:E:84:GLU:HA	2.20	0.40
1:A:224:LEU:N	1:A:225:PRO:CD	2.85	0.40
1:C:258:LEU:CD1	1:C:258:LEU:C	2.90	0.40
1:F:118:LEU:HD22	1:F:127:ILE:HD11	2.03	0.40
1:A:130:ARG:HB2	2:A:379:HOH:O	2.21	0.40
1:D:130:ARG:HH11	1:D:130:ARG:HB2	1.87	0.40
1:B:144:LYS:HA	1:B:144:LYS:CE	2.51	0.40
1:B:249:LYS:HE2	1:B:255:SER: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	264/272 (97%)	248 (94%)	16 (6%)	0	100	100
1	B	263/272 (97%)	249 (95%)	14 (5%)	0	100	100
1	C	264/272 (97%)	247 (94%)	15 (6%)	2 (1%)	24	41
1	D	263/272 (97%)	242 (92%)	20 (8%)	1 (0%)	39	61
1	E	264/272 (97%)	253 (96%)	10 (4%)	1 (0%)	39	61
1	F	263/272 (97%)	244 (93%)	19 (7%)	0	100	100
All	All	1581/1632 (97%)	1483 (94%)	94 (6%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	GLU
1	D	84	GLU
1	C	85	GLU
1	E	331	LYS

### 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	209/215 (97%)	204 (98%)	5 (2%)	57	82
1	B	208/215 (97%)	200 (96%)	8 (4%)	40	67
1	C	209/215 (97%)	201 (96%)	8 (4%)	40	67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	208/215 (97%)	198 (95%)	10 (5%)	31	55
1	E	209/215 (97%)	198 (95%)	11 (5%)	28	50
1	F	208/215 (97%)	200 (96%)	8 (4%)	40	67
All	All	1251/1290 (97%)	1201 (96%)	50 (4%)	38	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	90	VAL
1	A	130	ARG
1	A	279	LEU
1	A	332	ARG
1	B	78	ARG
1	B	83	GLU
1	B	98	TYR
1	B	130	ARG
1	B	144	LYS
1	B	258	LEU
1	B	279	LEU
1	B	335	ARG
1	C	95	ASN
1	C	123	LYS
1	C	130	ARG
1	C	214	ILE
1	C	258	LEU
1	C	272	LEU
1	C	295	GLN
1	C	326	LEU
1	D	78	ARG
1	D	85	GLU
1	D	116	ASP
1	D	122	LYS
1	D	130	ARG
1	D	143	LEU
1	D	160	LYS
1	D	258	LEU
1	D	291	LEU
1	D	331	LYS
1	E	74	GLU
1	E	75	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	87	ARG
1	E	95	ASN
1	E	122	LYS
1	E	123	LYS
1	E	130	ARG
1	E	222	GLN
1	E	262	GLN
1	E	279	LEU
1	E	323	GLU
1	F	75	ASP
1	F	80	ARG
1	F	98	TYR
1	F	113	LYS
1	F	130	ARG
1	F	204	LYS
1	F	258	LEU
1	F	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	281	GLN
1	B	81	HIS
1	B	86	ASN
1	B	95	ASN
1	B	260	GLN
1	B	281	GLN
1	B	295	GLN
1	C	95	ASN
1	C	101	ASN
1	C	260	GLN
1	C	281	GLN
1	D	95	ASN
1	D	260	GLN
1	D	281	GLN
1	D	295	GLN
1	E	95	ASN
1	E	260	GLN
1	E	262	GLN
1	E	281	GLN
1	E	295	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	81	HIS
1	F	86	ASN
1	F	95	ASN
1	F	260	GLN
1	F	262	GLN
1	F	281	GLN
1	F	295	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 ⓘ

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	266/272 (97%)	-0.16	5 (1%) 70 73	7, 24, 50, 61	0
1	B	265/272 (97%)	-0.25	1 (0%) 93 93	7, 21, 40, 50	0
1	C	266/272 (97%)	-0.14	2 (0%) 87 89	8, 25, 45, 56	0
1	D	265/272 (97%)	0.16	10 (3%) 44 49	11, 30, 52, 67	0
1	E	266/272 (97%)	-0.05	2 (0%) 87 89	7, 25, 46, 59	0
1	F	265/272 (97%)	-0.13	4 (1%) 76 79	7, 22, 43, 58	0
All	All	1593/1632 (97%)	-0.09	24 (1%) 76 79	7, 24, 48, 67	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	5.5
1	F	98	TYR	5.0
1	B	98	TYR	4.3
1	A	328	PHE	3.3
1	D	328	PHE	3.2
1	D	98	TYR	3.0
1	D	87	ARG	2.8
1	D	79	VAL	2.7
1	D	143	LEU	2.6
1	C	262	GLN	2.5
1	E	328	PHE	2.4
1	F	338	GLY	2.3
1	D	329	LYS	2.3
1	F	144	LYS	2.3
1	A	144	LYS	2.3
1	D	80	ARG	2.3
1	D	106	ASN	2.2
1	A	150	SER	2.1
1	E	98	TYR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	262	GLN	2.1
1	C	143	LEU	2.1
1	D	326	LEU	2.1
1	D	94	ILE	2.0
1	A	333	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.