



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:02 AM GMT

PDB ID : 3NVA  
Title : Dimeric form of CTP synthase from *Sulfolobus solfataricus*  
Authors : Harris, P.; Willemoes, M.; Lauritsen, I.; Johansson, E.; Jensen, K.F.  
Deposited on : 2010-07-08  
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

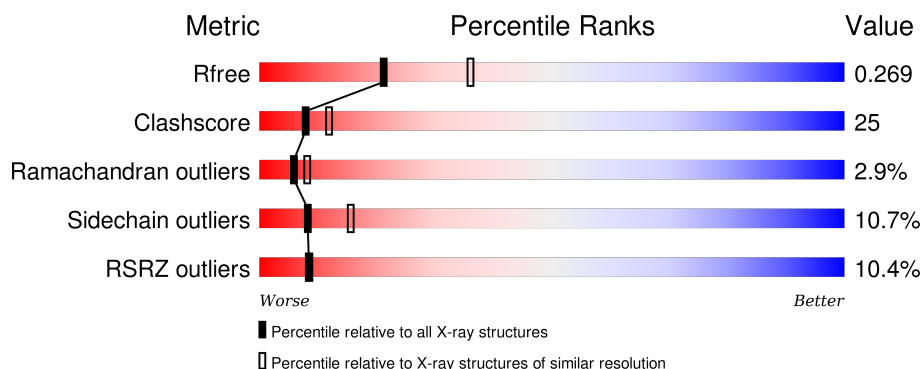
# 1 Overall quality at a glance

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	535	<div> <div>8%</div> <div>61%</div> <div>32%</div> <div>6%</div> </div>
1	B	535	<div> <div>13%</div> <div>53%</div> <div>39%</div> <div>8%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8529 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 CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	1	0	0
			4191	2685	708	790	8			
1	B	533	Total	C	N	O	S	2	0	0
			4191	2685	708	790	8			

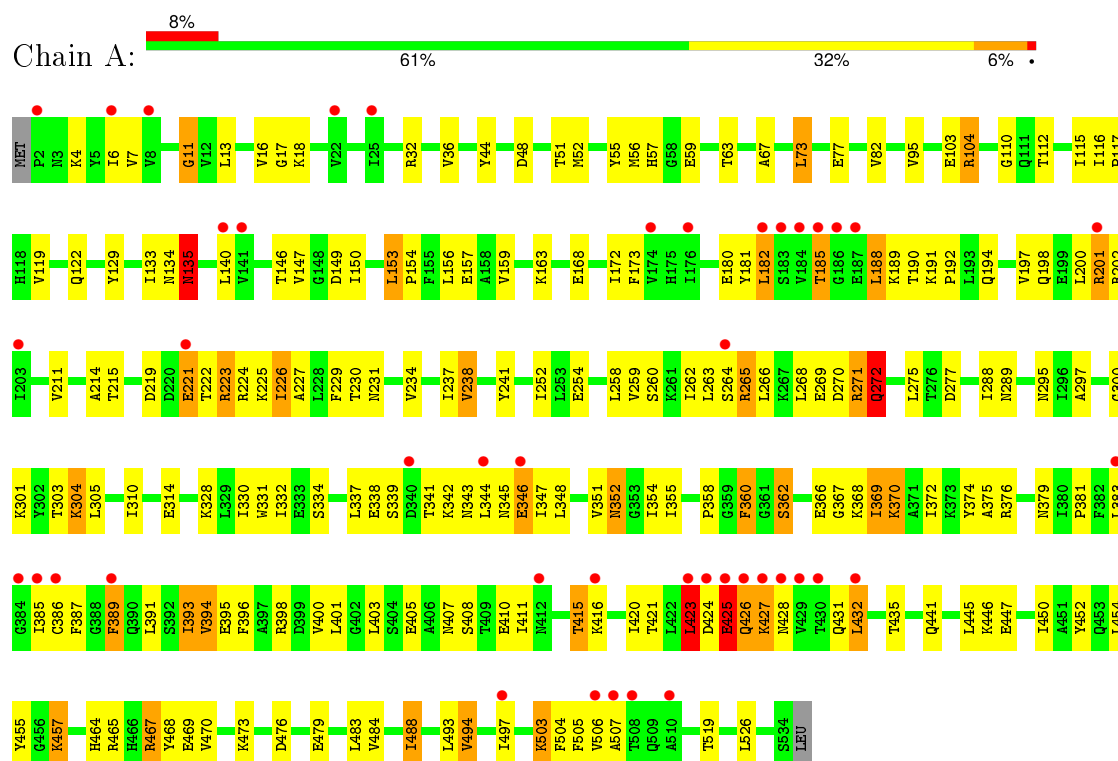
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	72	Total	O	0	0
			72	72		

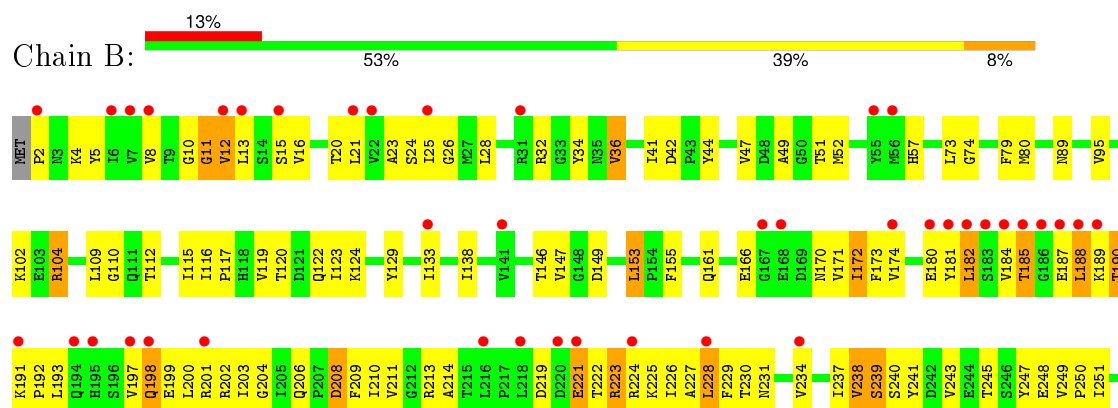
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: CTP synthase



#### • Molecule 1: CTP synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.45Å 76.78Å 98.87Å 100.99° 95.36° 108.42°	Depositor
Resolution (Å)	27.39 – 2.50 28.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (27.39-2.50) 89.1 (28.74-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, $R_{free}$	0.207 , 0.282 0.191 , 0.269	Depositor DCC
$R_{free}$ test set	1948 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 39001 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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	0.44	0/4265	0.61	2/5773 (0.0%)
1	B	0.42	0/4265	0.59	1/5773 (0.0%)
All	All	0.43	0/8530	0.60	3/11546 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	LEU	CA-CB-CG	5.58	128.15	115.30
1	B	432	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	73	LEU	CA-CB-CG	5.03	126.87	115.30

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	4191	0	4288	206	0
1	B	4191	0	4288	230	0
2	A	75	0	0	3	0
2	B	72	0	0	9	0
All	All	8529	0	8576	422	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 25.

All (422) 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:304:LYS:HZ2	1:B:304:LYS:H	1.06	1.00
1:A:52:MET:SD	1:B:112:THR:HG22	2.07	0.95
1:B:401:LEU:HD23	1:B:403:LEU:HD11	1.48	0.94
1:A:181:TYR:HA	1:A:188:LEU:HA	1.48	0.93
1:B:401:LEU:HD13	1:B:478:LEU:HD23	1.48	0.93
1:B:432:LEU:HD12	1:B:433:GLY:H	1.32	0.92
1:B:360:PHE:HE1	1:B:386:CYS:HG	1.18	0.89
1:A:467:ARG:HG2	1:A:467:ARG:HH11	1.36	0.88
1:B:271:ARG:HG3	1:B:272:GLN:H	1.39	0.88
1:B:457:LYS:HE3	1:B:460:VAL:HG12	1.54	0.88
1:A:197:VAL:HG21	1:A:230:THR:HA	1.57	0.86
1:A:181:TYR:HE1	1:A:222:THR:HG21	1.39	0.86
1:A:483:LEU:HD21	1:A:497:ILE:HB	1.60	0.83
1:A:344:LEU:HD11	1:A:374:TYR:CD2	2.14	0.82
1:B:345:ASN:ND2	1:B:378:HIS:HE1	1.77	0.82
1:A:467:ARG:CG	1:A:467:ARG:HH11	1.92	0.82
1:A:369:ILE:HD11	1:A:394:VAL:HG11	1.61	0.82
1:B:239:SER:HA	2:B:543:HOH:O	1.80	0.81
1:A:470:VAL:HB	1:A:494:VAL:CG1	2.10	0.81
1:A:369:ILE:HD11	1:A:394:VAL:CG1	2.10	0.81
1:A:344:LEU:C	1:A:346:GLU:H	1.84	0.80
1:A:393:ILE:HD12	1:A:497:ILE:HD13	1.63	0.80
1:B:304:LYS:NZ	1:B:304:LYS:H	1.79	0.80
1:B:493:LEU:HD12	2:B:586:HOH:O	1.80	0.80
1:A:271:ARG:HG3	1:A:272:GLN:H	1.47	0.79
1:B:4:LYS:HE2	1:B:266:LEU:HB3	1.65	0.79
1:A:221:GLU:O	1:A:224:ARG:HG2	1.83	0.78
1:A:7:VAL:HG11	1:A:159:VAL:HG11	1.64	0.77
1:B:424:ASP:HB3	1:B:432:LEU:HD21	1.67	0.77
1:B:360:PHE:CD1	1:B:387:PHE:HB2	2.19	0.77
1:B:181:TYR:HA	1:B:188:LEU:HA	1.68	0.76
1:A:344:LEU:HD12	1:A:344:LEU:C	2.06	0.76
1:A:11:GLY:HA2	1:A:16:VAL:HG11	1.66	0.76
1:B:180:GLU:HB3	1:B:189:LYS:HE2	1.68	0.76
1:A:426:GLN:O	1:A:427:LYS:HB2	1.86	0.75
1:A:57:HIS:HE1	1:B:110:GLY:O	1.66	0.75
1:B:360:PHE:HD1	1:B:387:PHE:HB2	1.50	0.74
1:A:410:GLU:HB2	1:A:468:TYR:CZ	2.23	0.74
1:A:396:PHE:O	1:A:400:VAL:HG22	1.87	0.74
1:A:360:PHE:CD1	1:A:387:PHE:HB2	2.23	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HB3	1:A:192:PRO:HD3	1.71	0.72
1:A:112:THR:HG22	1:B:57:HIS:CE1	2.24	0.72
1:B:432:LEU:HD12	1:B:433:GLY:N	2.07	0.70
1:B:313:LYS:HE2	1:B:331:TRP:HZ2	1.57	0.69
1:B:239:SER:HB2	2:B:552:HOH:O	1.92	0.69
1:A:405:GLU:HG3	1:A:416:LYS:HD3	1.73	0.69
1:A:470:VAL:HB	1:A:494:VAL:HG11	1.74	0.69
1:B:432:LEU:CD1	1:B:433:GLY:H	2.04	0.69
1:A:360:PHE:HD1	1:A:387:PHE:HB2	1.57	0.69
1:A:181:TYR:CE1	1:A:222:THR:HG21	2.27	0.68
1:A:425:GLU:O	1:A:426:GLN:HG3	1.93	0.67
1:B:12:VAL:O	1:B:13:LEU:HD12	1.95	0.67
1:A:393:ILE:CD1	1:A:497:ILE:HD13	2.24	0.67
1:A:344:LEU:O	1:A:344:LEU:HD12	1.96	0.66
1:B:197:VAL:HG21	1:B:230:THR:HA	1.78	0.66
1:A:334:SER:O	1:A:367:GLY:HA3	1.95	0.66
1:A:352:ASN:OD1	1:A:352:ASN:N	2.30	0.65
1:A:300:GLY:HA2	1:A:368:LYS:HE2	1.78	0.65
1:A:358:PRO:HG3	1:A:385:ILE:HG22	1.77	0.65
1:B:115:ILE:HG22	1:B:116:ILE:HD12	1.77	0.65
1:B:403:LEU:HD12	1:B:403:LEU:N	2.12	0.65
1:A:159:VAL:CG1	1:A:173:PHE:HE2	2.09	0.64
1:B:407:ASN:HB2	1:B:415:THR:HG21	1.79	0.64
1:B:32:ARG:NH1	1:B:259:VAL:HG12	2.13	0.64
1:B:345:ASN:HD21	1:B:378:HIS:HE1	1.44	0.63
1:A:221:GLU:HG2	1:A:222:THR:N	2.13	0.63
1:A:344:LEU:O	1:A:346:GLU:N	2.31	0.63
1:B:32:ARG:HH11	1:B:263:LEU:HD11	1.63	0.63
1:A:180:GLU:O	1:A:189:LYS:HG2	1.98	0.63
1:A:197:VAL:O	1:A:201:ARG:HG2	1.99	0.63
1:A:483:LEU:HD23	1:A:484:VAL:N	2.13	0.63
1:A:223:ARG:HG3	1:A:224:ARG:N	2.14	0.62
1:A:344:LEU:C	1:A:346:GLU:N	2.53	0.62
1:A:129:TYR:OH	1:A:133:ILE:HD12	1.99	0.62
1:B:304:LYS:N	1:B:304:LYS:HZ2	1.89	0.62
1:B:214:ALA:O	1:B:241:TYR:HA	1.99	0.62
1:A:360:PHE:CD1	1:A:360:PHE:N	2.66	0.61
1:B:313:LYS:HG2	1:B:317:TYR:CE2	2.36	0.61
1:A:297:ALA:HB2	1:A:351:VAL:HG11	1.83	0.61
1:B:305:LEU:HD23	1:B:307:ASP:H	1.64	0.61
1:A:387:PHE:HZ	1:A:411:ILE:HD11	1.65	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PHE:CZ	1:A:411:ILE:HD11	2.35	0.61
1:B:307:ASP:OD1	1:B:310:ILE:HD12	2.00	0.60
1:B:227:ALA:HA	1:B:237:ILE:HD11	1.83	0.60
1:A:159:VAL:CG1	1:A:173:PHE:CE2	2.84	0.60
1:B:264:SER:O	1:B:267:LYS:N	2.32	0.60
1:A:455:TYR:OH	2:A:568:HOH:O	2.16	0.60
1:B:275:LEU:O	1:B:278:TRP:N	2.34	0.60
1:B:5:TYR:HB2	1:B:171:VAL:HG22	1.84	0.60
1:B:129:TYR:OH	1:B:133:ILE:HD12	2.01	0.60
1:B:190:THR:HG21	1:B:229:PHE:CZ	2.37	0.60
1:B:310:ILE:O	1:B:314:GLU:HG2	2.02	0.60
1:B:271:ARG:CG	1:B:272:GLN:H	2.03	0.60
1:B:124:LYS:NZ	1:B:161:GLN:OE1	2.34	0.59
1:A:77:GLU:HG2	1:A:82:VAL:O	2.02	0.59
1:B:422:LEU:CD2	1:B:467:ARG:HH21	2.15	0.59
1:A:146:THR:HB	1:A:149:ASP:OD2	2.03	0.59
1:A:56:MET:HB3	1:A:57:HIS:CD2	2.38	0.59
1:B:334:SER:O	1:B:367:GLY:HA3	2.03	0.59
1:A:338:GLU:HG2	1:A:366:GLU:HB2	1.85	0.58
1:B:379:ASN:HD21	1:B:503:LYS:H	1.50	0.58
1:A:354:ILE:HD12	1:A:375:ALA:HB2	1.86	0.58
1:B:447:GLU:H	1:B:447:GLU:CD	2.06	0.57
1:A:394:VAL:HG21	1:A:407:ASN:HA	1.86	0.57
1:A:115:ILE:HD13	1:A:119:VAL:HG21	1.86	0.57
1:A:304:LYS:H	1:A:304:LYS:HZ2	1.50	0.57
1:B:219:ASP:OD2	1:B:222:THR:N	2.37	0.57
1:A:441:GLN:HB2	1:A:464:HIS:CE1	2.39	0.57
1:A:379:ASN:HD21	1:A:503:LYS:H	1.51	0.57
1:B:271:ARG:NE	1:B:271:ARG:HA	2.20	0.57
1:B:224:ARG:HH12	1:B:228:LEU:CD1	2.17	0.57
1:B:271:ARG:HA	1:B:271:ARG:HE	1.70	0.57
1:B:393:ILE:CD1	1:B:497:ILE:HD13	2.34	0.57
1:A:55:TYR:CE2	1:A:56:MET:HG3	2.40	0.57
1:B:470:VAL:HB	1:B:494:VAL:HG13	1.86	0.57
1:A:51:THR:O	1:B:110:GLY:HA2	2.05	0.57
1:A:57:HIS:CE1	1:B:110:GLY:O	2.55	0.57
1:A:467:ARG:NH1	1:A:467:ARG:HG2	2.13	0.56
1:B:260:SER:OG	1:B:271:ARG:NH1	2.38	0.56
1:B:243:VAL:HG22	1:B:248:GLU:OE1	2.04	0.56
1:A:426:GLN:O	1:A:427:LYS:CB	2.52	0.56
1:B:191:LYS:HB3	1:B:192:PRO:HD3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:CG1	1:A:395:GLU:N	2.68	0.56
1:A:427:LYS:HB3	1:A:428:ASN:HA	1.86	0.56
1:A:214:ALA:O	1:A:241:TYR:HA	2.05	0.56
1:B:423:LEU:O	1:B:434:GLY:HA2	2.06	0.56
1:B:269:GLU:HB3	2:B:575:HOH:O	2.05	0.56
1:A:55:TYR:HE2	1:A:56:MET:HE2	1.71	0.56
1:B:403:LEU:HD12	1:B:403:LEU:H	1.71	0.56
1:A:396:PHE:CE1	1:A:400:VAL:HG21	2.41	0.56
1:B:266:LEU:O	1:B:267:LYS:HB2	2.06	0.56
1:B:95:VAL:HG13	1:B:122:GLN:HG2	1.88	0.55
1:B:73:LEU:HD11	1:B:89:ASN:HB2	1.87	0.55
1:A:265:ARG:HG3	1:A:265:ARG:HH11	1.71	0.55
1:A:344:LEU:HA	1:A:347:ILE:HG13	1.89	0.55
1:A:344:LEU:HD11	1:A:374:TYR:CE2	2.41	0.55
1:B:479:GLU:HA	1:B:483:LEU:O	2.06	0.55
1:A:48:ASP:CG	1:B:104:ARG:HH22	2.10	0.55
1:B:291:LYS:O	1:B:292:LYS:HB2	2.07	0.55
1:A:328:LYS:HE3	1:A:330:ILE:HD11	1.89	0.54
1:A:401:LEU:HD23	1:A:403:LEU:HG	1.88	0.54
1:A:6:ILE:HB	1:A:140:LEU:HD23	1.88	0.54
1:B:345:ASN:HD21	1:B:378:HIS:CE1	2.25	0.54
1:A:150:ILE:HA	1:A:153:LEU:HD22	1.89	0.54
1:A:424:ASP:HB3	1:A:432:LEU:HD12	1.90	0.54
1:B:427:LYS:N	1:B:428:ASN:HA	2.22	0.54
1:B:422:LEU:HD21	1:B:467:ARG:HH21	1.73	0.54
1:A:6:ILE:N	1:A:6:ILE:HD12	2.23	0.54
1:A:494:VAL:HG12	2:A:558:HOH:O	2.07	0.54
1:B:32:ARG:HH12	1:B:259:VAL:HG12	1.72	0.53
1:B:224:ARG:HH12	1:B:228:LEU:HD11	1.72	0.53
1:B:410:GLU:HB2	1:B:468:TYR:CZ	2.44	0.53
1:A:103:GLU:OE2	1:A:104:ARG:HD3	2.09	0.53
1:B:297:ALA:HB2	1:B:351:VAL:HG11	1.89	0.53
1:A:310:ILE:O	1:A:314:GLU:HG2	2.08	0.53
1:A:446:LYS:O	1:A:452:TYR:HB2	2.09	0.53
1:A:470:VAL:HB	1:A:494:VAL:HG13	1.87	0.53
1:B:305:LEU:HB3	1:B:308:SER:OG	2.08	0.53
1:B:281:PHE:CZ	1:B:518:PRO:HB3	2.44	0.52
1:A:396:PHE:O	1:A:400:VAL:CG2	2.55	0.52
1:A:163:LYS:HD2	1:A:173:PHE:HE1	1.74	0.52
1:B:407:ASN:CB	1:B:415:THR:HG21	2.38	0.52
1:B:344:LEU:C	1:B:346:GLU:H	2.13	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:HG2	1:B:201:ARG:HH11	1.75	0.52
1:B:300:GLY:HA3	1:B:357:LEU:HD12	1.92	0.52
1:A:368:LYS:O	1:A:372:ILE:HG13	2.10	0.52
1:B:172:ILE:CG1	1:B:173:PHE:N	2.72	0.52
1:B:401:LEU:CD2	1:B:403:LEU:HD11	2.31	0.52
1:A:355:ILE:HG12	1:A:383:LEU:HB3	1.92	0.52
1:B:338:GLU:OE2	1:B:364:GLY:HA2	2.10	0.52
1:B:190:THR:HG21	1:B:229:PHE:CE1	2.45	0.51
1:B:313:LYS:HE2	1:B:331:TRP:CZ2	2.43	0.51
1:B:36:VAL:HG13	1:B:138:ILE:HB	1.91	0.51
1:A:115:ILE:HA	1:A:119:VAL:CG2	2.40	0.51
1:A:32:ARG:NH1	1:A:259:VAL:HG12	2.25	0.51
1:A:410:GLU:HB2	1:A:468:TYR:CE1	2.46	0.51
1:B:115:ILE:HA	1:B:119:VAL:CG2	2.41	0.51
1:B:226:ILE:HD11	1:B:237:ILE:HD13	1.93	0.51
1:B:16:VAL:HA	1:B:213:ARG:HG2	1.93	0.51
1:B:172:ILE:HG13	1:B:173:PHE:N	2.25	0.51
1:B:182:LEU:HG	1:B:187:GLU:O	2.11	0.51
1:A:221:GLU:O	1:A:225:LYS:HG3	2.10	0.50
1:A:391:LEU:O	1:A:394:VAL:HG12	2.11	0.50
1:A:394:VAL:CG2	1:A:407:ASN:HA	2.40	0.50
1:A:424:ASP:OD1	1:A:426:GLN:O	2.28	0.50
1:A:339:SER:C	1:A:341:THR:H	2.15	0.50
1:A:396:PHE:CD1	1:A:400:VAL:HG21	2.45	0.50
1:B:238:VAL:HG21	1:B:258:LEU:HB2	1.92	0.50
1:B:341:THR:O	1:B:342:LYS:C	2.49	0.50
1:A:295:ASN:OD1	1:A:328:LYS:HE2	2.11	0.50
1:B:401:LEU:HD23	1:B:403:LEU:CD1	2.31	0.50
1:B:270:ASP:OD1	1:B:271:ARG:N	2.44	0.50
1:A:225:LYS:O	1:A:229:PHE:HD2	1.95	0.50
1:A:159:VAL:HG12	1:A:173:PHE:CE2	2.46	0.50
1:A:6:ILE:HG13	1:A:172:ILE:HD11	1.94	0.50
1:A:303:THR:HB	1:A:331:TRP:HB3	1.94	0.50
1:B:344:LEU:HD23	1:B:344:LEU:H	1.77	0.50
1:B:211:VAL:HG22	1:B:238:VAL:HG12	1.94	0.50
1:A:227:ALA:HA	1:A:237:ILE:HD11	1.94	0.49
1:A:301:LYS:HG2	2:A:601:HOH:O	2.12	0.49
1:B:358:PRO:HG3	1:B:385:ILE:HG22	1.94	0.49
1:B:325:VAL:O	1:B:327:PRO:HD3	2.13	0.49
1:A:221:GLU:HG2	1:A:222:THR:H	1.76	0.49
1:A:394:VAL:HG12	1:A:395:GLU:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:CB	1:A:494:VAL:HG11	2.43	0.49
1:A:201:ARG:HH22	1:A:231:ASN:HB3	1.77	0.49
1:A:300:GLY:HA2	1:A:368:LYS:CE	2.42	0.49
1:B:441:GLN:HB2	1:B:464:HIS:CE1	2.47	0.49
1:A:344:LEU:HD13	1:A:348:LEU:HD12	1.95	0.49
1:B:104:ARG:HD2	1:B:104:ARG:HA	1.42	0.49
1:B:291:LYS:NZ	1:B:324:GLY:HA3	2.26	0.49
1:B:271:ARG:CG	1:B:272:GLN:N	2.74	0.49
1:A:159:VAL:HG11	1:A:173:PHE:HE2	1.77	0.49
1:A:57:HIS:CD2	1:B:112:THR:HG23	2.48	0.48
1:A:57:HIS:CE1	1:B:112:THR:HG23	2.48	0.48
1:B:300:GLY:HA2	1:B:368:LYS:HE2	1.95	0.48
1:A:194:GLN:OE1	1:A:229:PHE:HD1	1.96	0.48
1:B:370:LYS:HE3	1:B:373:LYS:HD3	1.95	0.48
1:B:26:GLY:HA3	1:B:80:MET:HE2	1.93	0.48
1:A:182:LEU:HG	1:A:189:LYS:HB3	1.94	0.48
1:B:26:GLY:HA3	1:B:80:MET:CE	2.43	0.48
1:A:389:PHE:HA	1:A:507:ALA:HB1	1.94	0.48
1:A:398:ARG:HA	1:A:403:LEU:H	1.79	0.48
1:A:271:ARG:HG3	1:A:272:GLN:N	2.22	0.48
1:B:427:LYS:H	1:B:428:ASN:HA	1.77	0.48
1:B:2:PRO:CD	1:B:166:GLU:OE1	2.61	0.48
1:A:425:GLU:C	1:A:426:GLN:HG3	2.33	0.48
1:B:23:ALA:HB1	1:B:79:PHE:HB2	1.95	0.48
1:B:401:LEU:HB3	1:B:403:LEU:CD1	2.44	0.48
1:B:352:ASN:OD1	1:B:352:ASN:N	2.47	0.48
1:B:231:ASN:CG	1:B:231:ASN:O	2.52	0.48
1:A:479:GLU:HA	1:A:483:LEU:O	2.13	0.48
1:A:401:LEU:CD2	1:A:403:LEU:HG	2.42	0.48
1:B:211:VAL:HA	1:B:238:VAL:O	2.13	0.48
1:B:123:ILE:HD13	1:B:155:PHE:CD1	2.49	0.48
1:A:150:ILE:HD13	1:B:153:LEU:HB3	1.96	0.48
1:A:55:TYR:HE2	1:A:56:MET:CE	2.27	0.47
1:B:412:ASN:HD22	1:B:415:THR:HG23	1.79	0.47
1:B:49:ALA:HA	1:B:52:MET:HE2	1.95	0.47
1:A:224:ARG:O	1:A:227:ALA:HB3	2.14	0.47
1:B:360:PHE:CE1	1:B:386:CYS:SG	3.04	0.47
1:A:297:ALA:HB1	1:A:332:ILE:HD12	1.97	0.47
1:A:197:VAL:HG11	1:A:229:PHE:O	2.14	0.47
1:A:226:ILE:HD11	1:A:237:ILE:HD13	1.95	0.47
1:A:355:ILE:HA	1:A:383:LEU:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLY:O	1:B:12:VAL:N	2.47	0.47
1:B:470:VAL:HB	1:B:494:VAL:CG1	2.44	0.47
1:A:215:THR:O	1:A:241:TYR:HB2	2.14	0.47
1:B:249:VAL:HB	1:B:250:PRO:HD3	1.96	0.47
1:B:180:GLU:O	1:B:189:LYS:HG2	2.15	0.47
1:A:110:GLY:HA2	1:B:51:THR:O	2.15	0.47
1:B:303:THR:N	1:B:304:LYS:HZ2	2.13	0.47
1:A:223:ARG:HG3	1:A:224:ARG:H	1.79	0.47
1:A:265:ARG:NH1	1:A:265:ARG:HG3	2.30	0.46
1:B:401:LEU:HD12	1:B:481:ALA:CB	2.45	0.46
1:A:341:THR:O	1:A:342:LYS:C	2.52	0.46
1:B:488:ILE:H	1:B:488:ILE:HD13	1.79	0.46
1:B:422:LEU:HD21	1:B:467:ARG:NH2	2.31	0.46
1:A:63:THR:OG1	1:A:67:ALA:HB3	2.15	0.46
1:B:433:GLY:HA2	1:B:467:ARG:NH2	2.29	0.46
1:B:389:PHE:C	1:B:389:PHE:CD2	2.88	0.46
1:A:447:GLU:H	1:A:447:GLU:CD	2.17	0.46
1:A:393:ILE:HD12	1:A:497:ILE:CD1	2.39	0.46
1:A:400:VAL:HG23	1:A:401:LEU:N	2.30	0.46
1:A:427:LYS:N	1:A:428:ASN:HA	2.31	0.46
1:A:379:ASN:OD1	1:A:503:LYS:HG2	2.16	0.46
1:B:393:ILE:HD12	1:B:497:ILE:HD13	1.96	0.46
1:A:116:ILE:HA	1:A:117:PRO:HA	1.70	0.46
1:B:200:LEU:O	1:B:204:GLY:N	2.49	0.46
1:A:369:ILE:HD11	1:A:394:VAL:HG12	1.97	0.46
1:A:104:ARG:HD3	1:B:47:VAL:HG23	1.96	0.46
1:A:254:GLU:HG3	1:A:275:LEU:HD11	1.97	0.46
1:B:432:LEU:CG	1:B:433:GLY:H	2.28	0.46
1:B:12:VAL:HG22	1:B:146:THR:HA	1.98	0.46
1:A:369:ILE:HG22	1:A:370:LYS:N	2.30	0.45
1:B:266:LEU:HB2	1:B:268:LEU:HD12	1.98	0.45
1:B:326:ARG:HG3	2:B:603:HOH:O	2.16	0.45
1:A:264:SER:O	1:A:266:LEU:N	2.48	0.45
1:B:395:GLU:OE1	1:B:399:ASP:OD2	2.33	0.45
1:B:32:ARG:NH2	1:B:254:GLU:OE1	2.49	0.45
1:A:369:ILE:CG2	1:A:370:LYS:N	2.78	0.45
1:B:57:HIS:HB2	2:B:551:HOH:O	2.15	0.45
1:A:381:PRO:HA	1:A:504:PHE:O	2.17	0.45
1:A:4:LYS:NZ	1:A:268:LEU:HD21	2.32	0.45
1:A:408:SER:HA	1:A:420:ILE:O	2.16	0.45
1:A:270:ASP:O	1:A:271:ARG:HB2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:HA3	1:A:18:LYS:HG3	1.97	0.45
1:B:32:ARG:HG2	1:B:273:VAL:HG13	1.98	0.45
1:B:360:PHE:HZ	2:B:598:HOH:O	1.99	0.45
1:B:32:ARG:HH11	1:B:263:LEU:CD1	2.30	0.45
1:B:444:ILE:HB	1:B:488:ILE:CD1	2.46	0.45
1:A:17:GLY:O	1:A:18:LYS:C	2.55	0.45
1:B:116:ILE:N	1:B:116:ILE:HD12	2.32	0.45
1:B:305:LEU:CD2	1:B:307:ASP:H	2.30	0.45
1:B:32:ARG:C	1:B:34:TYR:H	2.20	0.45
1:B:291:LYS:HD2	1:B:324:GLY:O	2.17	0.45
1:A:360:PHE:HE1	1:A:386:CYS:HG	1.60	0.45
1:B:296:ILE:N	1:B:296:ILE:HD12	2.32	0.45
1:A:221:GLU:HG2	1:A:222:THR:HG23	1.99	0.45
1:B:11:GLY:C	1:B:13:LEU:H	2.21	0.45
1:A:469:GLU:CD	1:A:493:LEU:HD13	2.37	0.45
1:B:260:SER:CB	1:B:271:ARG:HH12	2.30	0.45
1:A:488:ILE:HD13	1:A:488:ILE:H	1.81	0.45
1:B:264:SER:O	1:B:266:LEU:N	2.50	0.44
1:A:264:SER:C	1:A:266:LEU:N	2.70	0.44
1:B:422:LEU:HD23	1:B:434:GLY:HA3	2.00	0.44
1:B:146:THR:HB	1:B:149:ASP:OD2	2.18	0.44
1:B:393:ILE:HD11	1:B:497:ILE:HD13	1.98	0.44
1:B:292:LYS:HD2	1:B:292:LYS:HA	1.82	0.44
1:A:55:TYR:CE2	1:A:56:MET:CE	3.01	0.44
1:A:180:GLU:HG2	1:A:189:LYS:HE3	1.98	0.44
1:A:269:GLU:O	1:A:269:GLU:HG3	2.17	0.44
1:B:257:LYS:O	1:B:260:SER:N	2.49	0.44
1:A:288:ILE:O	1:A:289:ASN:HB2	2.16	0.44
1:B:387:PHE:HZ	1:B:411:ILE:HD11	1.81	0.44
1:A:396:PHE:CE2	1:A:483:LEU:HB2	2.52	0.44
1:B:10:GLY:O	1:B:12:VAL:HG23	2.18	0.44
1:B:381:PRO:HB3	1:B:504:PHE:HB3	2.00	0.44
1:B:401:LEU:HD11	1:B:478:LEU:HA	2.00	0.44
1:B:193:LEU:HD21	1:B:226:ILE:HB	2.00	0.44
1:A:188:LEU:HD11	1:A:190:THR:HG22	2.00	0.43
1:B:345:ASN:ND2	1:B:378:HIS:CE1	2.69	0.43
1:A:227:ALA:HB2	1:A:237:ILE:HD12	1.99	0.43
1:B:201:ARG:NH2	1:B:206:GLN:OE1	2.52	0.43
1:A:469:GLU:OE2	1:A:493:LEU:HD13	2.19	0.43
1:B:301:LYS:HD2	1:B:302:TYR:CD1	2.54	0.43
1:B:8:VAL:HA	1:B:174:VAL:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HA	1:B:117:PRO:HA	1.76	0.43
1:B:358:PRO:HG3	1:B:385:ILE:CG2	2.48	0.43
1:B:303:THR:HB	1:B:331:TRP:HB3	1.99	0.43
1:B:42:ASP:HB3	1:B:44:TYR:CE2	2.53	0.43
1:A:389:PHE:CD2	1:A:389:PHE:C	2.91	0.43
1:B:74:GLY:HA3	2:B:541:HOH:O	2.17	0.43
1:A:147:VAL:HG11	1:A:200:LEU:CD2	2.49	0.43
1:B:21:LEU:O	1:B:25:ILE:HG13	2.19	0.43
1:B:313:LYS:NZ	2:B:550:HOH:O	2.47	0.43
1:A:189:LYS:O	1:A:189:LYS:HG3	2.18	0.43
1:B:489:SER:OG	1:B:493:LEU:HB2	2.17	0.43
1:B:209:PHE:HE2	1:B:261:LYS:HB3	1.83	0.43
1:B:198:GLN:NE2	1:B:199:GLU:HG2	2.34	0.43
1:A:376:ARG:HB2	1:A:505:PHE:CE1	2.53	0.43
1:B:360:PHE:CE1	1:B:387:PHE:HB2	2.54	0.43
1:B:292:LYS:HG3	1:B:293:THR:N	2.34	0.43
1:A:134:ASN:O	1:A:135:ASN:HB2	2.18	0.43
1:A:57:HIS:NE2	1:B:112:THR:HG23	2.34	0.43
1:B:188:LEU:O	1:B:188:LEU:HD12	2.19	0.43
1:B:275:LEU:O	1:B:276:THR:C	2.57	0.43
1:A:104:ARG:HA	1:A:104:ARG:HD2	1.61	0.43
1:B:225:LYS:HB3	1:B:225:LYS:HE3	1.70	0.43
1:A:383:LEU:HD12	1:A:506:VAL:O	2.19	0.42
1:B:383:LEU:HD12	1:B:384:GLY:N	2.34	0.42
1:A:55:TYR:O	1:A:56:MET:HB2	2.20	0.42
1:B:251:ILE:HD11	1:B:278:TRP:HD1	1.84	0.42
1:B:209:PHE:O	1:B:210:ILE:HD13	2.18	0.42
1:A:405:GLU:O	1:A:415:THR:OG1	2.34	0.42
1:B:197:VAL:HA	1:B:200:LEU:HD12	2.00	0.42
1:B:224:ARG:NH1	1:B:228:LEU:CD1	2.82	0.42
1:B:326:ARG:HA	1:B:327:PRO:HD3	1.88	0.42
1:B:208:ASP:N	1:B:208:ASP:OD1	2.52	0.42
1:A:95:VAL:HG13	1:A:122:GLN:CG	2.49	0.42
1:A:197:VAL:HG21	1:A:230:THR:CA	2.40	0.42
1:A:7:VAL:HG21	1:A:159:VAL:HG13	2.01	0.42
1:B:532:VAL:C	1:B:534:SER:H	2.23	0.42
1:B:223:ARG:HG3	1:B:224:ARG:N	2.31	0.42
1:B:432:LEU:HD12	1:B:434:GLY:N	2.35	0.42
1:B:360:PHE:HB3	1:B:410:GLU:OE2	2.19	0.42
1:B:213:ARG:HD2	1:B:240:SER:O	2.19	0.42
1:B:294:ILE:HA	1:B:352:ASN:ND2	2.35	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:SER:HA	1:B:420:ILE:HB	2.01	0.42
1:B:438:LEU:HA	1:B:464:HIS:O	2.20	0.42
1:B:226:ILE:HG13	1:B:227:ALA:N	2.34	0.42
1:B:221:GLU:O	1:B:222:THR:C	2.58	0.42
1:B:238:VAL:HG11	1:B:258:LEU:HD22	2.00	0.42
1:A:219:ASP:OD1	1:A:222:THR:HG23	2.19	0.42
1:A:211:VAL:HG22	1:A:238:VAL:HG12	2.02	0.42
1:A:201:ARG:H	1:A:201:ARG:HG2	1.68	0.41
1:B:147:VAL:HG11	1:B:200:LEU:CD2	2.50	0.41
1:A:265:ARG:O	1:A:265:ARG:HG3	2.19	0.41
1:A:153:LEU:HB2	1:A:154:PRO:HD3	2.02	0.41
1:A:342:LYS:HB3	1:A:342:LYS:HE2	1.74	0.41
1:B:356:VAL:HG21	1:B:372:ILE:HG13	2.02	0.41
1:B:437:ARG:HB3	1:B:441:GLN:HE21	1.85	0.41
1:B:41:ILE:HG21	1:B:155:PHE:CD1	2.55	0.41
1:A:112:THR:HB	1:B:52:MET:SD	2.61	0.41
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.79	0.41
1:A:421:THR:HG23	1:A:423:LEU:CD1	2.50	0.41
1:B:446:LYS:O	1:B:452:TYR:HB2	2.21	0.41
1:B:275:LEU:O	1:B:277:ASP:N	2.54	0.41
1:A:408:SER:HA	1:A:420:ILE:HB	2.02	0.41
1:A:344:LEU:HA	1:A:346:GLU:OE1	2.21	0.41
1:B:247:TYR:O	1:B:250:PRO:HD2	2.20	0.41
1:B:389:PHE:HA	1:B:507:ALA:HB1	2.01	0.41
1:B:381:PRO:HA	1:B:504:PHE:O	2.20	0.41
1:A:423:LEU:O	1:A:435:THR:HG23	2.19	0.41
1:B:433:GLY:CA	1:B:467:ARG:NH2	2.83	0.41
1:B:439:GLY:O	1:B:441:GLN:HG2	2.21	0.41
1:A:258:LEU:O	1:A:262:ILE:HG13	2.21	0.41
1:A:188:LEU:HD12	1:A:189:LYS:C	2.41	0.41
1:B:412:ASN:ND2	1:B:415:THR:HG23	2.35	0.41
1:A:150:ILE:HA	1:A:153:LEU:CD2	2.50	0.41
1:B:320:SER:CB	1:B:327:PRO:HG3	2.50	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.79	0.41
1:A:55:TYR:CE2	1:A:56:MET:HE2	2.53	0.41
1:B:337:LEU:HD23	1:B:371:ALA:HB2	2.03	0.41
1:A:450:ILE:O	1:A:454:LEU:HG	2.21	0.41
1:A:467:ARG:CG	1:A:467:ARG:NH1	2.63	0.40
1:A:328:LYS:HB3	1:A:328:LYS:HE2	1.80	0.40
1:A:95:VAL:HG13	1:A:122:GLN:HG2	2.03	0.40
1:B:445:LEU:O	1:B:458:LYS:HD2	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:SER:O	1:B:28:LEU:HG	2.22	0.40
1:B:271:ARG:HE	1:B:271:ARG:CA	2.29	0.40
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.86	0.40
1:A:11:GLY:O	1:A:18:LYS:HD2	2.22	0.40
1:A:425:GLU:O	1:A:426:GLN:CG	2.67	0.40
1:A:360:PHE:CE1	1:A:386:CYS:SG	3.14	0.40
1:A:104:ARG:CZ	1:B:47:VAL:HB	2.51	0.40
1:B:526:LEU:HD12	1:B:526:LEU:HA	1.74	0.40
1:A:445:LEU:HD12	1:A:457:LYS:O	2.22	0.40
1:B:397:ALA:HA	1:B:401:LEU:HB2	2.04	0.40
1:B:430:THR:CB	1:B:432:LEU:HD23	2.51	0.40
1:B:271:ARG:NE	1:B:271:ARG:CA	2.82	0.40
1:A:360:PHE:HE1	1:A:386:CYS:SG	2.43	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	531/535 (99%)	475 (90%)	42 (8%)	14 (3%)	7	10
1	B	531/535 (99%)	479 (90%)	35 (7%)	17 (3%)	5	6
All	All	1062/1070 (99%)	954 (90%)	77 (7%)	31 (3%)	6	8

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	A	426	GLN
1	A	427	LYS
1	A	432	LEU
1	B	12	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	341	THR
1	B	426	GLN
1	B	432	LEU
1	A	185	THR
1	A	271	ARG
1	A	345	ASN
1	B	11	GLY
1	B	342	LYS
1	A	272	GLN
1	A	362	SER
1	A	425	GLU
1	B	182	LEU
1	A	265	ARG
1	A	343	ASN
1	B	185	THR
1	B	221	GLU
1	B	265	ARG
1	B	267	LYS
1	B	276	THR
1	B	345	ASN
1	B	434	GLY
1	A	135	ASN
1	A	182	LEU
1	B	324	GLY
1	B	427	LYS
1	B	184	VAL

### 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	462/467 (99%)	411 (89%)	51 (11%)	8	14
1	B	462/467 (99%)	414 (90%)	48 (10%)	9	16
All	All	924/934 (99%)	825 (89%)	99 (11%)	8	15

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	36	VAL
1	A	44	TYR
1	A	59	GLU
1	A	73	LEU
1	A	104	ARG
1	A	135	ASN
1	A	153	LEU
1	A	157	GLU
1	A	168	GLU
1	A	185	THR
1	A	188	LEU
1	A	198	GLN
1	A	201	ARG
1	A	202	ARG
1	A	221	GLU
1	A	223	ARG
1	A	226	ILE
1	A	234	VAL
1	A	238	VAL
1	A	252	ILE
1	A	260	SER
1	A	263	LEU
1	A	272	GLN
1	A	277	ASP
1	A	304	LYS
1	A	305	LEU
1	A	337	LEU
1	A	346	GLU
1	A	352	ASN
1	A	360	PHE
1	A	362	SER
1	A	369	ILE
1	A	370	LYS
1	A	389	PHE
1	A	393	ILE
1	A	394	VAL
1	A	415	THR
1	A	423	LEU
1	A	425	GLU
1	A	431	GLN
1	A	457	LYS
1	A	465	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	467	ARG
1	A	473	LYS
1	A	476	ASP
1	A	488	ILE
1	A	494	VAL
1	A	503	LYS
1	A	519	THR
1	A	526	LEU
1	B	15	SER
1	B	20	THR
1	B	36	VAL
1	B	102	LYS
1	B	104	ARG
1	B	109	LEU
1	B	120	THR
1	B	153	LEU
1	B	170	ASN
1	B	172	ILE
1	B	185	THR
1	B	188	LEU
1	B	190	THR
1	B	198	GLN
1	B	202	ARG
1	B	203	ILE
1	B	208	ASP
1	B	223	ARG
1	B	228	LEU
1	B	234	VAL
1	B	238	VAL
1	B	239	SER
1	B	245	THR
1	B	268	LEU
1	B	271	ARG
1	B	273	VAL
1	B	277	ASP
1	B	279	ILE
1	B	301	LYS
1	B	304	LYS
1	B	329	LEU
1	B	334	SER
1	B	340	ASP
1	B	342	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	344	LEU
1	B	346	GLU
1	B	348	LEU
1	B	352	ASN
1	B	382	PHE
1	B	389	PHE
1	B	401	LEU
1	B	415	THR
1	B	422	LEU
1	B	437	ARG
1	B	465	ARG
1	B	488	ILE
1	B	494	VAL
1	B	503	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	57	HIS
1	A	295	ASN
1	A	379	ASN
1	B	378	HIS
1	B	441	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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	533/535 (99%)	0.40	43 (8%) <span>15</span> <span>16</span>	22, 51, 101, 185	2 (0%)
1	B	533/535 (99%)	0.58	68 (12%) <span>5</span> <span>5</span>	24, 57, 118, 187	2 (0%)
All	All	1066/1070 (99%)	0.49	111 (10%) <span>8</span> <span>8</span>	22, 54, 111, 187	4 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	THR	7.0
1	B	188	LEU	6.1
1	B	56	MET	5.7
1	A	182	LEU	5.7
1	A	186	GLY	5.5
1	B	184	VAL	5.4
1	B	13	LEU	5.4
1	B	182	LEU	5.4
1	B	340	ASP	5.4
1	A	425	GLU	5.2
1	A	427	LYS	5.1
1	B	183	SER	5.1
1	B	385	ILE	5.0
1	B	185	THR	5.0
1	B	426	GLN	4.8
1	A	184	VAL	4.8
1	B	187	GLU	4.8
1	A	340	ASP	4.4
1	B	273	VAL	4.3
1	B	275	LEU	4.3
1	A	432	LEU	4.3
1	B	197	VAL	4.2
1	B	274	ASP	4.1
1	B	6	ILE	4.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	269	GLU	4.0
1	B	201	ARG	4.0
1	A	385	ILE	3.9
1	A	174	VAL	3.9
1	B	383	LEU	3.9
1	A	183	SER	3.8
1	A	426	GLN	3.7
1	A	187	GLU	3.7
1	B	133	ILE	3.6
1	B	216	LEU	3.5
1	B	384	GLY	3.5
1	B	2	PRO	3.4
1	B	8	VAL	3.4
1	A	386	CYS	3.4
1	B	272	GLN	3.4
1	B	228	LEU	3.3
1	B	341	THR	3.3
1	B	181	TYR	3.2
1	A	428	ASN	3.2
1	A	221	GLU	3.1
1	B	434	GLY	3.1
1	A	508	THR	3.1
1	A	383	LEU	3.1
1	B	186	GLY	3.0
1	A	8	VAL	3.0
1	B	220	ASP	3.0
1	B	427	LYS	3.0
1	B	55	TYR	3.0
1	B	291	LYS	3.0
1	B	221	GLU	2.9
1	B	174	VAL	2.9
1	B	342	LYS	2.9
1	B	12	VAL	2.8
1	B	194	GLN	2.8
1	A	412	ASN	2.8
1	B	432	LEU	2.8
1	B	386	CYS	2.8
1	A	346	GLU	2.8
1	B	168	GLU	2.8
1	A	2	PRO	2.7
1	B	276	THR	2.6
1	B	15	SER	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	141	VAL	2.6
1	B	343	ASN	2.6
1	B	191	LYS	2.6
1	A	424	ASP	2.6
1	B	31	ARG	2.5
1	A	507	ALA	2.5
1	A	510	ALA	2.5
1	B	25	ILE	2.5
1	B	189	LYS	2.4
1	B	218	LEU	2.4
1	B	430	THR	2.4
1	B	508	THR	2.4
1	B	167	GLY	2.4
1	A	22	VAL	2.4
1	B	7	VAL	2.4
1	A	429	VAL	2.3
1	B	302	TYR	2.3
1	B	180	GLU	2.3
1	B	224	ARG	2.3
1	B	425	GLU	2.3
1	B	414	ASN	2.3
1	A	506	VAL	2.3
1	A	416	LYS	2.2
1	B	141	VAL	2.2
1	A	25	ILE	2.2
1	A	264	SER	2.2
1	A	344	LEU	2.2
1	B	22	VAL	2.2
1	A	6	ILE	2.2
1	B	195	HIS	2.2
1	B	363	ARG	2.2
1	B	271	ARG	2.2
1	A	384	GLY	2.1
1	B	431	GLN	2.1
1	A	203	ILE	2.1
1	A	497	ILE	2.1
1	B	198	GLN	2.1
1	A	389	PHE	2.1
1	A	423	LEU	2.0
1	A	176	ILE	2.0
1	B	21	LEU	2.0
1	A	201	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	2.0
1	A	140	LEU	2.0
1	A	185	THR	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.