



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2IOP  
Title : Crystal Structure of Full-length HtpG, the Escherichia coli Hsp90, Bound to ADP  
Authors : Shiau, A.K.; Harris, S.F.; Agard, D.A.  
Deposited on : 2006-10-10  
Resolution : 3.55 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

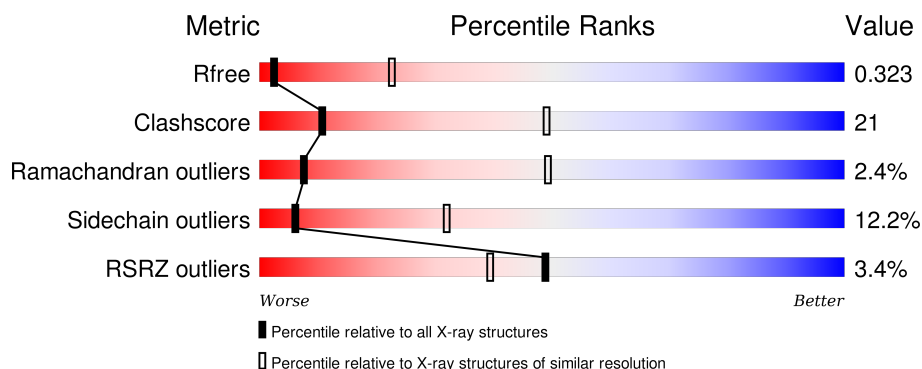
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	624	 3% 56% 37% 6%
1	B	624	 4% 54% 39% 6%
1	C	624	 5% 56% 34% 7%
1	D	624	 2% 54% 36% 6%

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
2	ADP	A	1001	X	-	-	-
2	ADP	B	1002	X	-	-	-
2	ADP	C	1003	X	-	-	-
2	ADP	D	1004	X	-	-	-

## 2 Entry composition [i](#)

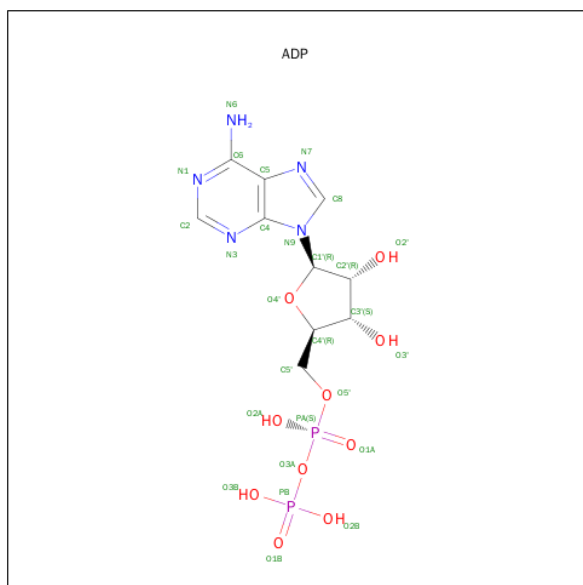
There are 2 unique types of molecules in this entry. The entry contains 19391 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4879	3079	840	947	13			
1	B	615	Total	C	N	O	S	0	0	0
			4878	3076	839	950	13			
1	C	606	Total	C	N	O	S	0	0	0
			4772	3016	821	922	13			
1	D	604	Total	C	N	O	S	0	0	0
			4754	3003	817	921	13			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

*Continued on next page...*

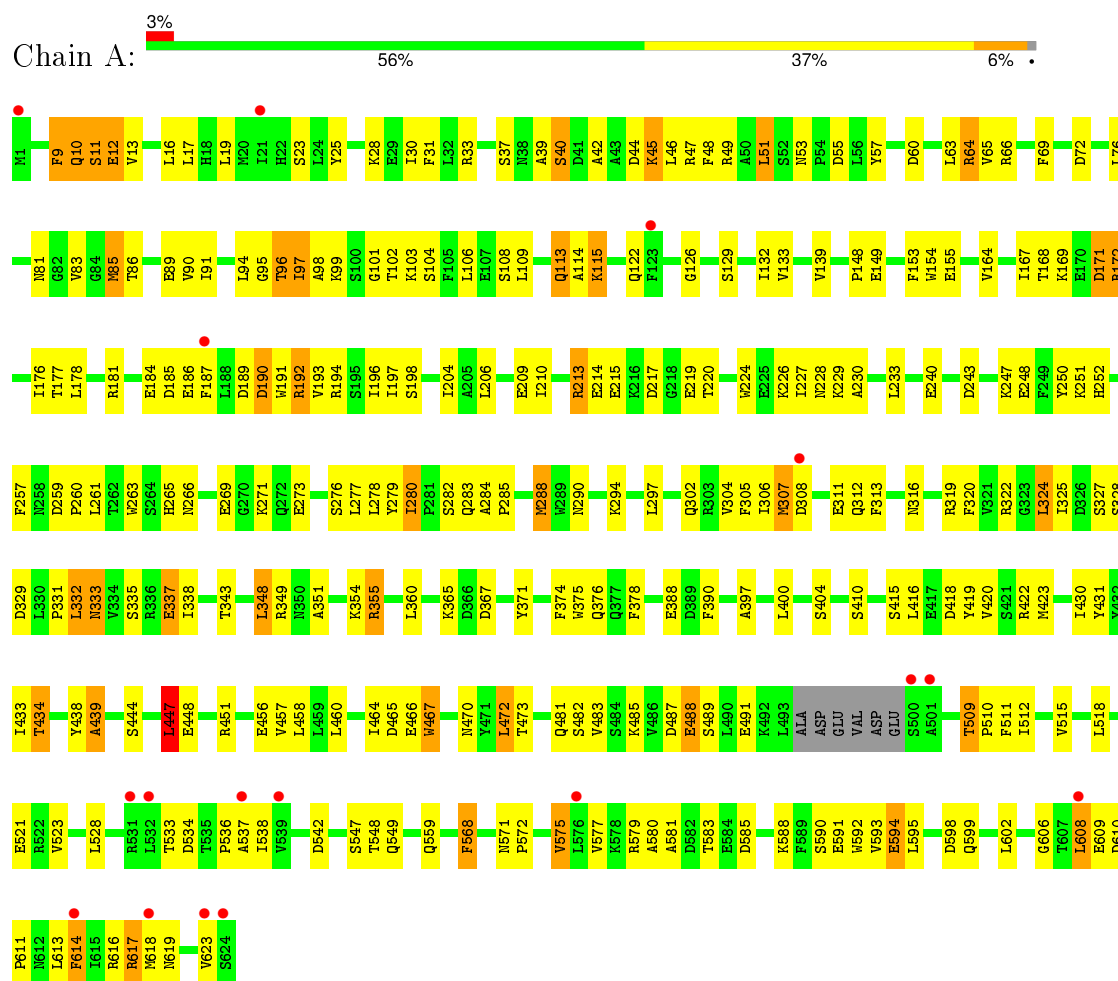
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

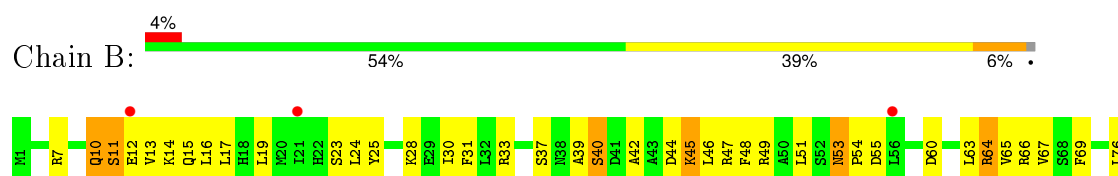
### 3 Residue-property plots

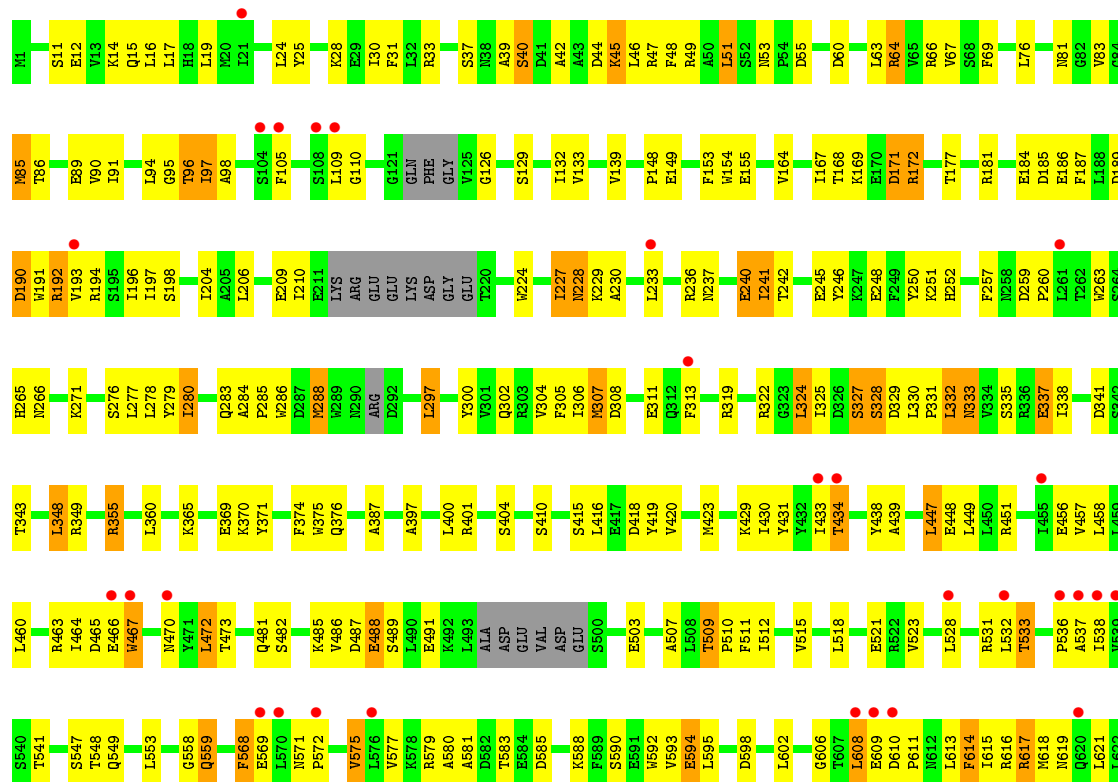
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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.

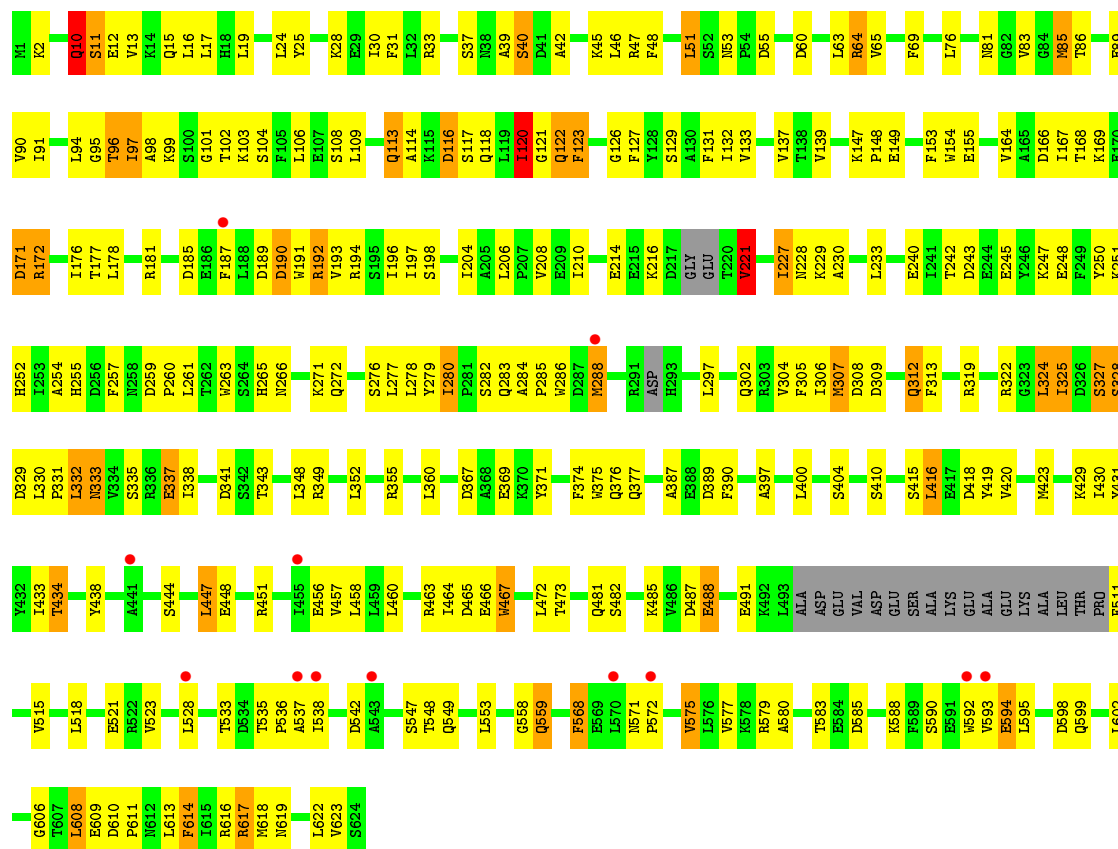
#### • Molecule 1: Chaperone protein htpG



#### • Molecule 1: Chaperone protein htpG









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.62Å 145.06Å 165.35Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	46.60 – 3.55 46.41 – 3.51	Depositor EDS
% Data completeness (in resolution range)	71.1 (46.60-3.55) 69.3 (46.41-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.317 , 0.357 0.286 , 0.323	Depositor DCC
$R_{free}$ test set	2599 reflections (8.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.3	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.9	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 36240 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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](#)

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

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	0.22	0/4969	0.42	0/6720
1	B	0.21	0/4967	0.43	1/6713 (0.0%)
1	C	0.21	0/4858	0.41	0/6568
1	D	0.22	0/4838	0.43	0/6540
All	All	0.22	0/19632	0.42	1/26541 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	4
1	D	0	7
All	All	0	21

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	291	ARG	CB-CA-C	5.65	121.71	110.40

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	307	MET	Peptide
1	A	327	SER	Peptide
1	A	447	LEU	Peptide
1	A	9	PHE	Peptide
1	B	10	GLN	Peptide
1	B	307	MET	Peptide
1	B	327	SER	Peptide
1	B	447	LEU	Peptide
1	B	7	ARG	Peptide
1	C	240	GLU	Peptide
1	C	307	MET	Peptide
1	C	311	GLU	Peptide
1	C	327	SER	Peptide
1	D	10	GLN	Peptide
1	D	120	ILE	Peptide
1	D	122	GLN	Peptide
1	D	221	VAL	Peptide
1	D	240	GLU	Peptide
1	D	307	MET	Peptide
1	D	327	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4879	0	4715	210	0
1	B	4878	0	4726	223	0
1	C	4772	0	4605	213	0
1	D	4754	0	4590	209	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
All	All	19391	0	18684	807	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 21.

All (807) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HA	1:C:286:TRP:HA	1.28	1.13
1:B:113:GLN:H	1:B:113:GLN:HE21	1.06	1.02
1:C:97:ILE:HG23	1:C:98:ALA:H	1.24	1.02
1:D:113:GLN:H	1:D:113:GLN:HE21	1.08	1.00
1:B:97:ILE:HG23	1:B:98:ALA:H	1.29	0.97
1:A:113:GLN:H	1:A:113:GLN:HE21	1.05	0.97
1:D:97:ILE:HG23	1:D:98:ALA:H	1.27	0.97
1:B:463:ARG:HH12	1:C:110:GLY:HA2	1.28	0.96
1:A:97:ILE:HG23	1:A:98:ALA:H	1.31	0.93
1:D:48:PHE:HA	1:D:331:PRO:HG3	1.51	0.89
1:A:284:ALA:HB1	1:A:288:MET:HG3	1.55	0.89
1:A:602:LEU:HD12	1:A:608:LEU:HD12	1.56	0.87
1:B:67:VAL:HB	1:B:210:ILE:HD13	1.56	0.87
1:B:284:ALA:HB1	1:B:288:MET:HG3	1.54	0.87
1:B:291:ARG:HG3	1:B:293:HIS:H	1.39	0.87
1:D:284:ALA:HB1	1:D:288:MET:HG3	1.57	0.85
1:A:48:PHE:CZ	1:D:338:ILE:HG23	2.11	0.85
1:C:602:LEU:HD12	1:C:608:LEU:HD12	1.59	0.84
1:A:575:VAL:HG21	1:B:623:VAL:HG13	1.61	0.82
1:C:284:ALA:HB1	1:C:288:MET:HG3	1.61	0.82
1:D:602:LEU:HD12	1:D:608:LEU:HD12	1.59	0.82
1:B:467:TRP:HE1	1:C:105:PHE:HE1	1.25	0.82
1:B:602:LEU:HD12	1:B:608:LEU:HD12	1.62	0.81
1:B:23:SER:HA	1:C:559:GLN:HE22	1.44	0.81
1:B:63:LEU:HA	1:B:81:ASN:HD21	1.48	0.79
1:C:528:LEU:HD22	1:C:572:PRO:HG3	1.65	0.78
1:B:528:LEU:HD22	1:B:572:PRO:HG3	1.65	0.78
1:D:10:GLN:HB2	1:D:11:SER:HA	1.63	0.78
1:A:10:GLN:O	1:A:13:VAL:HB	1.83	0.78
1:B:217:ASP:HB2	1:B:219:GLU:HG2	1.66	0.77
1:D:528:LEU:HD22	1:D:572:PRO:HG3	1.66	0.77
1:B:338:ILE:HD12	1:B:338:ILE:H	1.50	0.77
1:A:448:GLU:HB2	1:A:533:THR:HG21	1.67	0.77
1:A:338:ILE:H	1:A:338:ILE:HD12	1.50	0.76
1:C:63:LEU:HA	1:C:81:ASN:HD21	1.49	0.76
1:A:602:LEU:HD22	1:B:615:ILE:HD11	1.67	0.76
1:D:10:GLN:O	1:D:13:VAL:HB	1.85	0.76
1:B:463:ARG:NH1	1:C:110:GLY:HA2	2.01	0.75
1:D:63:LEU:HA	1:D:81:ASN:HD21	1.51	0.75
1:A:528:LEU:HD22	1:A:572:PRO:HG3	1.68	0.75
1:C:338:ILE:HD12	1:C:338:ILE:H	1.51	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HA	1:A:81:ASN:HD21	1.52	0.75
1:D:523:VAL:HG11	1:D:568:PHE:HB2	1.68	0.75
1:A:335:SER:H	1:A:338:ILE:HD13	1.52	0.74
1:A:294:LYS:HB2	1:A:311:GLU:HB3	1.69	0.74
1:C:335:SER:H	1:C:338:ILE:HD13	1.51	0.73
1:B:523:VAL:HG11	1:B:568:PHE:HB2	1.70	0.72
1:A:113:GLN:H	1:A:113:GLN:NE2	1.85	0.72
1:A:312:GLN:O	1:A:349:ARG:HD3	1.89	0.72
1:A:523:VAL:HG11	1:A:568:PHE:HB2	1.70	0.72
1:B:335:SER:H	1:B:338:ILE:HD13	1.53	0.72
1:C:523:VAL:HG11	1:C:568:PHE:HB2	1.70	0.71
1:B:28:LYS:HA	1:B:132:ILE:HD13	1.71	0.71
1:B:553:LEU:HG	1:C:109:LEU:HD21	1.73	0.70
1:D:113:GLN:H	1:D:113:GLN:NE2	1.88	0.70
1:C:623:VAL:HG22	1:D:575:VAL:HG11	1.72	0.70
1:B:105:PHE:HB2	1:B:123:PHE:CZ	2.26	0.70
1:A:28:LYS:HA	1:A:132:ILE:HD13	1.74	0.69
1:B:10:GLN:O	1:B:13:VAL:HB	1.92	0.69
1:D:335:SER:H	1:D:338:ILE:HD13	1.58	0.69
1:C:48:PHE:HA	1:C:331:PRO:HG3	1.75	0.69
1:A:97:ILE:HG23	1:A:98:ALA:N	2.06	0.68
1:B:12:GLU:O	1:B:16:LEU:HG	1.93	0.68
1:A:215:GLU:HA	1:A:220:THR:HA	1.76	0.68
1:D:28:LYS:HA	1:D:132:ILE:HD13	1.76	0.68
1:B:106:LEU:HD13	1:C:464:ILE:HG13	1.76	0.67
1:D:420:VAL:HA	1:D:423:MET:SD	2.34	0.67
1:D:338:ILE:HD12	1:D:338:ILE:H	1.59	0.67
1:B:16:LEU:O	1:B:19:LEU:HB3	1.95	0.67
1:A:397:ALA:HA	1:A:400:LEU:HD12	1.76	0.67
1:A:16:LEU:O	1:A:19:LEU:HB3	1.95	0.67
1:B:113:GLN:H	1:B:113:GLN:NE2	1.86	0.66
1:C:337:GLU:CD	1:C:337:GLU:H	1.96	0.66
1:D:85:MET:HE3	2:D:1004:ADP:H1'	1.77	0.66
1:B:371:TYR:O	1:B:374:PHE:HB3	1.96	0.66
1:B:397:ALA:HA	1:B:400:LEU:HD12	1.76	0.66
1:D:332:LEU:HD12	1:D:333:ASN:H	1.61	0.66
1:B:448:GLU:HB2	1:B:533:THR:HB	1.76	0.65
1:C:371:TYR:O	1:C:374:PHE:HB3	1.95	0.65
1:D:126:GLY:O	1:D:129:SER:HB3	1.97	0.65
1:A:371:TYR:O	1:A:374:PHE:HB3	1.96	0.65
1:A:115:LYS:O	1:D:558:GLY:HA3	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HG23	1:C:98:ALA:N	2.04	0.65
1:A:420:VAL:HA	1:A:423:MET:SD	2.37	0.65
1:A:337:GLU:H	1:A:337:GLU:CD	2.00	0.64
1:C:397:ALA:HA	1:C:400:LEU:HD12	1.79	0.64
1:D:12:GLU:O	1:D:16:LEU:HG	1.95	0.64
1:A:335:SER:N	1:A:338:ILE:HD13	2.13	0.64
1:C:28:LYS:HA	1:C:132:ILE:HD13	1.79	0.64
1:C:485:LYS:HG3	1:C:541:THR:O	1.97	0.64
1:C:16:LEU:O	1:C:19:LEU:HB3	1.97	0.64
1:D:193:VAL:O	1:D:197:ILE:HG13	1.98	0.64
1:D:397:ALA:HA	1:D:400:LEU:HD12	1.78	0.64
1:C:420:VAL:HA	1:C:423:MET:SD	2.38	0.64
1:B:335:SER:N	1:B:338:ILE:HD13	2.13	0.63
1:C:335:SER:N	1:C:338:ILE:HD13	2.12	0.63
1:B:85:MET:HE3	2:B:1002:ADP:H1'	1.81	0.63
1:B:420:VAL:HA	1:B:423:MET:SD	2.39	0.63
1:D:371:TYR:O	1:D:374:PHE:HB3	1.97	0.63
1:B:193:VAL:O	1:B:197:ILE:HG13	1.98	0.63
1:C:67:VAL:HB	1:C:210:ILE:HD12	1.80	0.63
1:D:16:LEU:O	1:D:19:LEU:HB3	1.99	0.62
1:D:97:ILE:HG23	1:D:98:ALA:N	2.07	0.62
1:D:337:GLU:CD	1:D:337:GLU:H	2.00	0.62
1:A:193:VAL:O	1:A:197:ILE:HG13	1.99	0.62
1:A:332:LEU:HD12	1:A:333:ASN:H	1.65	0.62
1:A:390:PHE:HE1	1:D:96:THR:HB	1.64	0.62
1:B:337:GLU:CD	1:B:337:GLU:H	2.02	0.62
1:B:332:LEU:HD12	1:B:333:ASN:H	1.65	0.61
1:B:25:TYR:O	1:B:28:LYS:HE3	2.00	0.61
1:C:193:VAL:O	1:C:197:ILE:HG13	2.00	0.61
1:B:203:HIS:HB2	1:D:255:HIS:CE1	2.36	0.61
1:A:302:GLN:NE2	1:A:328:SER:HB3	2.15	0.61
1:D:397:ALA:O	1:D:400:LEU:HB2	2.01	0.61
1:D:332:LEU:HD12	1:D:333:ASN:N	2.16	0.61
1:B:97:ILE:HG23	1:B:98:ALA:N	2.09	0.61
1:C:397:ALA:O	1:C:400:LEU:HB2	2.00	0.60
1:C:332:LEU:HD12	1:C:333:ASN:H	1.64	0.60
1:B:616:ARG:HA	1:B:619:ASN:ND2	2.16	0.60
1:A:11:SER:C	1:A:13:VAL:H	2.05	0.60
1:C:616:ARG:HA	1:C:619:ASN:ND2	2.17	0.60
1:A:616:ARG:HA	1:A:619:ASN:ND2	2.16	0.60
1:D:335:SER:N	1:D:338:ILE:HD13	2.16	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ALA:HB2	1:C:109:LEU:HD13	1.83	0.60
1:D:47:ARG:HH21	1:D:302:GLN:NE2	2.00	0.59
1:B:609:GLU:O	1:B:610:ASP:HB2	2.01	0.59
1:A:233:LEU:HD23	1:A:233:LEU:O	2.02	0.59
1:A:57:TYR:OH	1:A:329:ASP:HB3	2.01	0.59
1:C:613:LEU:HG	1:C:617:ARG:HH22	1.68	0.59
1:D:233:LEU:O	1:D:233:LEU:HD23	2.02	0.59
1:B:139:VAL:HB	1:B:154:TRP:HB3	1.84	0.59
1:B:397:ALA:O	1:B:400:LEU:HB2	2.01	0.59
1:A:294:LYS:NZ	1:A:311:GLU:HB2	2.17	0.59
1:B:233:LEU:HD23	1:B:233:LEU:O	2.01	0.59
1:D:227:ILE:HG13	1:D:228:ASN:N	2.17	0.58
1:C:265:HIS:HB2	1:C:277:LEU:HD13	1.85	0.58
1:A:470:ASN:HB3	1:D:13:VAL:HG23	1.85	0.58
1:D:25:TYR:O	1:D:28:LYS:HE3	2.02	0.58
1:A:332:LEU:O	1:A:333:ASN:HB3	2.02	0.58
1:C:139:VAL:HB	1:C:154:TRP:HB3	1.85	0.58
1:A:397:ALA:O	1:A:400:LEU:HB2	2.04	0.58
1:C:39:ALA:O	1:C:42:ALA:HB3	2.03	0.58
1:D:616:ARG:HA	1:D:619:ASN:ND2	2.18	0.58
1:A:588:LYS:HE2	1:A:592:TRP:HE1	1.67	0.58
1:C:96:THR:HG23	1:C:97:ILE:H	1.68	0.58
1:B:486:VAL:HG22	1:B:531:ARG:HH21	1.67	0.58
1:D:324:LEU:O	1:D:324:LEU:HD13	2.02	0.58
1:B:96:THR:HG23	1:B:97:ILE:H	1.68	0.58
1:A:98:ALA:O	1:A:102:THR:HG23	2.04	0.58
1:D:204:ILE:HG23	1:D:206:LEU:H	1.69	0.58
1:B:332:LEU:O	1:B:333:ASN:HB3	2.02	0.58
1:D:208:VAL:O	1:D:227:ILE:HG23	2.03	0.58
1:C:233:LEU:HD23	1:C:233:LEU:O	2.03	0.58
1:D:113:GLN:HG2	1:D:114:ALA:H	1.69	0.58
1:D:332:LEU:O	1:D:333:ASN:HB3	2.04	0.58
1:D:588:LYS:HE2	1:D:592:TRP:HE1	1.69	0.58
1:C:25:TYR:O	1:C:28:LYS:HE3	2.03	0.57
2:B:1002:ADP:O2B	2:B:1002:ADP:H4'	2.04	0.57
1:D:580:ALA:HB2	1:D:592:TRP:CE3	2.39	0.57
1:D:120:ILE:C	1:D:122:GLN:N	2.58	0.57
1:A:139:VAL:HB	1:A:154:TRP:HB3	1.86	0.57
1:C:404:SER:HB3	1:C:458:LEU:HD23	1.86	0.57
2:C:1003:ADP:H4'	2:C:1003:ADP:O2B	2.03	0.57
1:A:404:SER:HB3	1:A:458:LEU:HD23	1.85	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LEU:HD12	1:C:333:ASN:N	2.19	0.57
1:A:324:LEU:O	1:A:324:LEU:HD13	2.03	0.57
1:B:110:GLY:HA3	1:C:463:ARG:HH12	1.69	0.57
1:C:63:LEU:HD23	1:C:81:ASN:ND2	2.20	0.57
1:C:332:LEU:O	1:C:333:ASN:HB3	2.04	0.57
1:B:613:LEU:HG	1:B:617:ARG:HH22	1.70	0.57
1:B:115:LYS:O	1:C:558:GLY:HA3	2.04	0.57
1:D:404:SER:HB3	1:D:458:LEU:HD23	1.85	0.57
1:C:588:LYS:HE2	1:C:592:TRP:HE1	1.70	0.57
1:A:623:VAL:HG22	1:B:575:VAL:HG11	1.87	0.57
1:A:332:LEU:HD12	1:A:333:ASN:N	2.19	0.57
1:B:312:GLN:O	1:B:349:ARG:HD3	2.04	0.57
1:B:291:ARG:HG3	1:B:292:ASP:N	2.20	0.56
1:D:613:LEU:HG	1:D:617:ARG:HH22	1.68	0.56
1:A:25:TYR:O	1:A:28:LYS:HE3	2.04	0.56
1:C:328:SER:O	1:C:329:ASP:HB2	2.04	0.56
1:B:63:LEU:HD23	1:B:81:ASN:ND2	2.21	0.56
1:B:431:TYR:HA	1:B:481:GLN:O	2.06	0.56
1:C:609:GLU:O	1:C:610:ASP:HB2	2.05	0.56
2:A:1001:ADP:H4'	2:A:1001:ADP:O2B	2.05	0.56
1:A:580:ALA:HB2	1:A:592:TRP:CE3	2.41	0.56
1:C:280:ILE:HD12	1:C:360:LEU:HD21	1.87	0.56
1:C:204:ILE:HG23	1:C:206:LEU:H	1.71	0.56
1:A:447:LEU:HD13	1:A:451:ARG:HB2	1.87	0.56
1:A:280:ILE:HD12	1:A:360:LEU:HD21	1.87	0.56
1:B:332:LEU:HD12	1:B:333:ASN:N	2.20	0.56
1:D:609:GLU:O	1:D:610:ASP:HB2	2.05	0.56
1:B:39:ALA:O	1:B:42:ALA:HB3	2.05	0.56
1:A:126:GLY:O	1:A:129:SER:HB3	2.06	0.56
1:A:113:GLN:HG2	1:A:114:ALA:H	1.70	0.56
1:D:97:ILE:HG12	1:D:98:ALA:N	2.21	0.56
1:D:51:LEU:HD21	1:D:331:PRO:HD2	1.87	0.56
2:D:1004:ADP:O2B	2:D:1004:ADP:H4'	2.06	0.56
1:B:11:SER:O	1:B:14:LYS:HB3	2.05	0.56
1:B:588:LYS:HE2	1:B:592:TRP:HE1	1.70	0.56
1:A:602:LEU:HA	1:A:608:LEU:HG	1.88	0.56
1:D:25:TYR:HA	1:D:132:ILE:HD11	1.89	0.56
1:A:204:ILE:HG23	1:A:206:LEU:H	1.69	0.56
1:B:113:GLN:HG2	1:B:114:ALA:H	1.70	0.55
1:A:96:THR:HG23	1:A:97:ILE:H	1.71	0.55
1:A:48:PHE:HZ	1:D:338:ILE:HG23	1.68	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:TYR:HA	1:C:481:GLN:O	2.06	0.55
1:A:609:GLU:O	1:A:610:ASP:HB2	2.06	0.55
1:A:12:GLU:O	1:A:16:LEU:HG	2.07	0.55
1:C:47:ARG:HH21	1:C:302:GLN:NE2	2.04	0.55
1:B:265:HIS:HB2	1:B:277:LEU:HD13	1.89	0.55
1:C:585:ASP:HB3	1:C:588:LYS:HB3	1.88	0.55
1:C:313:PHE:O	1:C:349:ARG:HG3	2.07	0.55
1:D:2:LYS:O	1:D:166:ASP:HB2	2.07	0.55
1:A:599:GLN:HE21	1:B:618:MET:HE1	1.72	0.55
1:B:324:LEU:O	1:B:324:LEU:HD13	2.06	0.55
1:B:126:GLY:O	1:B:129:SER:HB3	2.05	0.55
1:A:613:LEU:HG	1:A:617:ARG:HH22	1.72	0.55
1:B:511:PHE:O	1:B:515:VAL:HG23	2.07	0.55
1:D:280:ILE:HD12	1:D:360:LEU:HD21	1.87	0.55
1:A:11:SER:C	1:A:13:VAL:N	2.60	0.55
1:B:204:ILE:HG23	1:B:206:LEU:H	1.71	0.55
1:D:96:THR:HG23	1:D:97:ILE:H	1.72	0.55
1:D:447:LEU:HD13	1:D:451:ARG:HB2	1.89	0.55
1:B:280:ILE:HD12	1:B:360:LEU:HD21	1.89	0.55
1:D:602:LEU:HA	1:D:608:LEU:HG	1.89	0.55
1:B:203:HIS:HB2	1:D:255:HIS:HE1	1.72	0.55
1:B:112:ASP:OD2	1:D:463:ARG:HB3	2.07	0.55
1:C:25:TYR:HA	1:C:132:ILE:HD11	1.88	0.55
1:A:485:LYS:HG3	1:A:542:ASP:HA	1.89	0.55
1:C:580:ALA:HB2	1:C:592:TRP:CE3	2.42	0.54
1:C:448:GLU:CB	1:C:533:THR:HG21	2.37	0.54
1:D:139:VAL:HB	1:D:154:TRP:HB3	1.89	0.54
1:A:25:TYR:HA	1:A:132:ILE:HD11	1.90	0.54
1:B:99:LYS:O	1:B:103:LYS:HB2	2.07	0.54
1:C:615:ILE:HG23	1:D:599:GLN:NE2	2.22	0.54
1:C:447:LEU:HD13	1:C:451:ARG:HB2	1.89	0.54
1:C:324:LEU:HD13	1:C:324:LEU:O	2.07	0.54
1:C:602:LEU:HA	1:C:608:LEU:HG	1.89	0.54
1:D:64:ARG:HD3	1:D:81:ASN:OD1	2.06	0.54
1:D:431:TYR:HA	1:D:481:GLN:O	2.06	0.54
1:C:241:ILE:HD12	1:C:246:TYR:CZ	2.42	0.54
1:D:39:ALA:O	1:D:42:ALA:HB3	2.08	0.54
1:A:63:LEU:HD23	1:A:81:ASN:ND2	2.23	0.54
1:A:47:ARG:HG2	1:A:329:ASP:HA	1.90	0.54
1:B:404:SER:HB3	1:B:458:LEU:HD23	1.89	0.54
1:A:585:ASP:HB3	1:A:588:LYS:HB3	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ASP:HB3	1:B:588:LYS:HB3	1.90	0.54
1:A:431:TYR:HA	1:A:481:GLN:O	2.07	0.54
1:C:575:VAL:HG11	1:D:623:VAL:HG13	1.88	0.54
1:A:90:VAL:HG13	1:A:94:LEU:HD12	1.89	0.54
1:B:580:ALA:HB2	1:B:592:TRP:CE3	2.43	0.54
1:D:277:LEU:HD12	1:D:278:LEU:N	2.23	0.54
1:D:585:ASP:HB3	1:D:588:LYS:HB3	1.89	0.53
1:D:375:TRP:HH2	1:D:400:LEU:HD23	1.74	0.53
1:B:602:LEU:HA	1:B:608:LEU:HG	1.90	0.53
1:B:447:LEU:HD13	1:B:451:ARG:HB2	1.89	0.53
1:A:598:ASP:HB3	1:A:614:PHE:HB2	1.89	0.53
1:C:375:TRP:HH2	1:C:400:LEU:HD23	1.74	0.53
1:B:46:LEU:HB2	1:B:83:VAL:HB	1.90	0.53
1:C:189:ASP:OD2	1:C:191:TRP:HB3	2.08	0.53
1:B:90:VAL:HG13	1:B:94:LEU:HD12	1.91	0.53
1:B:97:ILE:HG12	1:B:98:ALA:N	2.22	0.53
1:D:63:LEU:HD23	1:D:81:ASN:ND2	2.24	0.53
1:D:120:ILE:C	1:D:122:GLN:H	2.12	0.53
1:C:46:LEU:HB2	1:C:83:VAL:HB	1.91	0.53
1:D:99:LYS:O	1:D:103:LYS:HB2	2.08	0.53
1:D:148:PRO:O	1:D:168:THR:HG23	2.08	0.52
1:B:189:ASP:OD2	1:B:191:TRP:HB3	2.09	0.52
1:A:46:LEU:HB2	1:A:83:VAL:HB	1.90	0.52
1:B:48:PHE:CZ	1:C:338:ILE:HG23	2.44	0.52
1:D:10:GLN:HB2	1:D:11:SER:CA	2.31	0.52
1:D:133:VAL:HG11	1:D:187:PHE:HE1	1.74	0.52
1:A:39:ALA:O	1:A:42:ALA:HB3	2.09	0.52
1:B:466:GLU:OE1	1:B:549:GLN:HB3	2.09	0.52
1:C:619:ASN:O	1:C:623:VAL:HG23	2.09	0.52
1:D:132:ILE:HG23	1:D:133:VAL:HG13	1.91	0.52
1:B:332:LEU:O	1:B:333:ASN:CB	2.57	0.52
1:A:48:PHE:HA	1:A:331:PRO:HG3	1.89	0.52
1:A:375:TRP:HH2	1:A:400:LEU:HD23	1.75	0.52
1:A:410:SER:HA	1:A:438:TYR:CE1	2.45	0.52
1:B:25:TYR:HA	1:B:132:ILE:HD11	1.92	0.52
1:B:13:VAL:HG23	1:C:470:ASN:O	2.10	0.52
1:A:215:GLU:CB	1:A:220:THR:HG22	2.39	0.52
1:D:332:LEU:O	1:D:333:ASN:CB	2.58	0.52
1:C:278:LEU:N	1:C:278:LEU:HD12	2.25	0.52
1:A:45:LYS:HD2	1:D:341:ASP:HA	1.90	0.52
1:D:248:GLU:O	1:D:251:LYS:HB2	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:LEU:O	1:D:611:PRO:HD3	2.09	0.52
1:D:598:ASP:HB3	1:D:614:PHE:HB2	1.91	0.52
1:B:404:SER:HB2	1:B:457:VAL:O	2.10	0.52
1:B:598:ASP:HB3	1:B:614:PHE:HB2	1.91	0.52
1:B:608:LEU:O	1:B:611:PRO:HD3	2.10	0.51
1:A:332:LEU:O	1:A:333:ASN:CB	2.57	0.51
1:D:265:HIS:HB2	1:D:277:LEU:HD13	1.91	0.51
1:D:153:PHE:HE2	1:D:155:GLU:HB2	1.75	0.51
1:D:189:ASP:OD2	1:D:191:TRP:HB3	2.10	0.51
1:B:619:ASN:O	1:B:623:VAL:HG23	2.11	0.51
1:A:132:ILE:HG23	1:A:133:VAL:HG13	1.92	0.51
1:C:189:ASP:OD1	1:C:192:ARG:HB2	2.10	0.51
1:B:367:ASP:OD1	1:B:369:GLU:HB3	2.10	0.51
1:D:297:LEU:O	1:D:309:ASP:HA	2.10	0.51
1:C:332:LEU:O	1:C:333:ASN:CB	2.58	0.51
1:B:324:LEU:C	1:B:324:LEU:HD22	2.29	0.51
1:A:316:ASN:ND2	1:D:103:LYS:HD3	2.26	0.51
1:A:509:THR:H	1:A:510:PRO:HD2	1.75	0.51
1:C:228:ASN:N	1:C:228:ASN:ND2	2.58	0.51
1:C:598:ASP:HB3	1:C:614:PHE:HB2	1.91	0.51
1:C:410:SER:HA	1:C:438:TYR:CE1	2.46	0.51
1:A:460:LEU:HD13	1:A:465:ASP:HB3	1.93	0.51
1:A:189:ASP:OD2	1:A:191:TRP:HB3	2.11	0.51
1:B:375:TRP:HH2	1:B:400:LEU:HD23	1.75	0.51
1:B:410:SER:HA	1:B:438:TYR:CE1	2.45	0.51
1:D:367:ASP:OD1	1:D:369:GLU:HB3	2.10	0.51
1:D:404:SER:HB2	1:D:457:VAL:O	2.11	0.51
1:D:116:ASP:O	1:D:117:SER:HB2	2.10	0.51
1:C:248:GLU:O	1:C:251:LYS:HB2	2.10	0.51
1:A:99:LYS:O	1:A:103:LYS:HB2	2.10	0.51
1:B:217:ASP:HB2	1:B:219:GLU:CG	2.38	0.51
1:D:410:SER:HA	1:D:438:TYR:CE1	2.45	0.51
1:D:210:ILE:HG12	1:D:227:ILE:HG21	1.93	0.51
1:A:250:TYR:HD2	1:A:260:PRO:HD3	1.76	0.51
1:A:265:HIS:HB2	1:A:277:LEU:HD13	1.91	0.51
1:A:619:ASN:O	1:A:623:VAL:HG23	2.11	0.51
1:B:250:TYR:HD2	1:B:260:PRO:HD3	1.76	0.51
1:A:148:PRO:O	1:A:168:THR:HG23	2.10	0.51
1:B:278:LEU:N	1:B:278:LEU:HD12	2.25	0.51
1:A:210:ILE:CD1	1:A:227:ILE:HD11	2.41	0.51
1:A:608:LEU:O	1:A:611:PRO:HD3	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:O	1:B:251:LYS:HB2	2.11	0.50
1:A:277:LEU:HD12	1:A:278:LEU:N	2.26	0.50
1:B:419:TYR:CE2	1:B:430:ILE:HG23	2.46	0.50
1:A:213:ARG:HD3	1:A:213:ARG:H	1.76	0.50
1:D:313:PHE:HB3	1:D:352:LEU:HD12	1.92	0.50
1:D:63:LEU:HA	1:D:81:ASN:ND2	2.24	0.50
1:A:278:LEU:N	1:A:278:LEU:HD12	2.26	0.50
1:A:97:ILE:HG12	1:A:98:ALA:N	2.27	0.50
1:D:51:LEU:HD21	1:D:330:LEU:HD12	1.94	0.50
1:A:509:THR:H	1:A:510:PRO:CD	2.23	0.50
1:A:419:TYR:CE2	1:A:430:ILE:HG23	2.46	0.50
1:A:571:ASN:O	1:A:577:VAL:HG21	2.12	0.50
1:D:533:THR:HG23	1:D:535:THR:H	1.76	0.50
1:B:16:LEU:HD22	1:C:467:TRP:NE1	2.27	0.50
1:D:46:LEU:HB2	1:D:83:VAL:HB	1.94	0.50
1:A:488:GLU:HA	1:A:491:GLU:HB2	1.93	0.50
1:B:113:GLN:HE21	1:B:113:GLN:N	1.91	0.50
1:C:126:GLY:O	1:C:129:SER:HB3	2.12	0.50
1:B:559:GLN:OE1	1:C:19:LEU:HD11	2.11	0.50
1:B:63:LEU:HA	1:B:81:ASN:ND2	2.22	0.50
1:A:64:ARG:HD3	1:A:81:ASN:OD1	2.11	0.50
1:B:133:VAL:HG11	1:B:187:PHE:HE1	1.77	0.50
1:A:588:LYS:HE2	1:A:592:TRP:NE1	2.26	0.50
1:B:277:LEU:C	1:B:278:LEU:HD12	2.33	0.50
1:D:434:THR:OG1	1:D:466:GLU:HG2	2.12	0.50
1:B:583:THR:HG21	1:B:588:LYS:HG2	1.93	0.49
1:C:434:THR:OG1	1:C:466:GLU:HG2	2.12	0.49
1:D:250:TYR:HD2	1:D:260:PRO:HD3	1.77	0.49
1:C:571:ASN:O	1:C:577:VAL:HG21	2.12	0.49
1:B:467:TRP:HD1	1:B:553:LEU:HD21	1.77	0.49
1:B:13:VAL:N	1:C:470:ASN:HB3	2.28	0.49
1:C:532:LEU:O	1:C:533:THR:HB	2.11	0.49
1:B:197:ILE:HD12	1:B:210:ILE:HD11	1.93	0.49
1:C:63:LEU:HA	1:C:81:ASN:ND2	2.23	0.49
1:C:197:ILE:HB	1:C:227:ILE:HD13	1.93	0.49
1:C:448:GLU:HB2	1:C:533:THR:HG21	1.93	0.49
1:A:434:THR:OG1	1:A:466:GLU:HG2	2.12	0.49
1:D:131:PHE:CE2	1:D:137:VAL:HG23	2.48	0.49
1:B:122:GLN:HA	1:D:286:TRP:HA	1.94	0.49
1:C:153:PHE:HB2	1:C:167:ILE:HD13	1.93	0.49
1:A:172:ARG:HB3	1:A:172:ARG:HH11	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:C	1:D:19:LEU:H	2.14	0.49
1:C:90:VAL:HG13	1:C:94:LEU:HD12	1.94	0.49
1:C:583:THR:HG21	1:C:588:LYS:HG2	1.93	0.49
1:B:488:GLU:HA	1:B:491:GLU:HB2	1.94	0.49
1:C:189:ASP:CG	1:C:192:ARG:H	2.15	0.49
1:C:229:LYS:O	1:C:230:ALA:HB3	2.13	0.49
1:C:97:ILE:CG2	1:C:98:ALA:H	2.06	0.49
1:A:248:GLU:O	1:A:251:LYS:HB2	2.12	0.49
1:C:488:GLU:HA	1:C:491:GLU:HB2	1.95	0.49
1:D:448:GLU:HB2	1:D:533:THR:HG21	1.95	0.49
1:B:327:SER:OG	1:B:330:LEU:HB2	2.13	0.49
1:B:328:SER:C	1:B:330:LEU:H	2.16	0.49
1:B:460:LEU:HD13	1:B:465:ASP:HB3	1.94	0.49
1:D:485:LYS:HE3	1:D:542:ASP:HA	1.95	0.49
1:C:512:ILE:HD11	1:C:528:LEU:HG	1.95	0.49
1:B:571:ASN:O	1:B:577:VAL:HG21	2.13	0.49
1:B:217:ASP:OD2	1:B:217:ASP:N	2.45	0.49
1:A:133:VAL:HG11	1:A:187:PHE:HE1	1.78	0.49
1:D:511:PHE:O	1:D:515:VAL:HG23	2.13	0.49
1:D:390:PHE:CD2	1:D:390:PHE:N	2.81	0.49
1:B:86:THR:OG1	1:B:89:GLU:HG3	2.13	0.48
1:B:434:THR:OG1	1:B:466:GLU:HG2	2.12	0.48
1:C:169:LYS:HE2	1:C:171:ASP:OD1	2.12	0.48
1:C:460:LEU:HD13	1:C:465:ASP:HB3	1.95	0.48
1:D:619:ASN:O	1:D:623:VAL:HG23	2.13	0.48
1:D:278:LEU:HD12	1:D:278:LEU:N	2.28	0.48
1:D:488:GLU:HA	1:D:491:GLU:HB2	1.95	0.48
1:B:64:ARG:HD3	1:B:81:ASN:OD1	2.13	0.48
1:C:17:LEU:C	1:C:19:LEU:H	2.15	0.48
1:C:51:LEU:HG	1:C:331:PRO:HG3	1.95	0.48
1:C:192:ARG:O	1:C:196:ILE:HG13	2.14	0.48
1:C:66:ARG:HD3	1:C:224:TRP:CE3	2.48	0.48
1:D:169:LYS:HE2	1:D:171:ASP:OD1	2.13	0.48
1:C:67:VAL:HB	1:C:210:ILE:CD1	2.44	0.48
1:A:583:THR:HG21	1:A:588:LYS:HG2	1.95	0.48
1:D:419:TYR:CE2	1:D:430:ILE:HG23	2.48	0.48
1:B:85:MET:HE2	1:B:94:LEU:HG	1.94	0.48
1:A:306:ILE:HG22	1:A:307:MET:N	2.28	0.48
1:B:229:LYS:O	1:B:230:ALA:HB3	2.13	0.48
1:C:608:LEU:O	1:C:611:PRO:HD3	2.13	0.48
1:A:294:LYS:HD3	1:A:311:GLU:CD	2.34	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:TRP:CE2	1:D:106:LEU:HD21	2.48	0.48
1:C:64:ARG:HD3	1:C:81:ASN:OD1	2.13	0.48
1:B:537:ALA:HB1	1:B:568:PHE:HE1	1.79	0.48
1:D:192:ARG:O	1:D:196:ILE:HG13	2.13	0.48
1:B:123:PHE:O	1:D:286:TRP:HB3	2.14	0.48
1:A:31:PHE:HA	1:A:129:SER:OG	2.14	0.48
1:D:272:GLN:OE1	1:D:329:ASP:HB3	2.14	0.48
1:D:571:ASN:O	1:D:577:VAL:HG21	2.14	0.48
1:A:37:SER:O	1:A:40:SER:HB3	2.14	0.48
1:A:415:SER:HB3	1:A:418:ASP:CG	2.34	0.48
1:A:599:GLN:HE21	1:B:618:MET:CE	2.26	0.48
1:B:322:ARG:HA	1:B:322:ARG:HD2	1.64	0.48
1:B:415:SER:HB3	1:B:418:ASP:CG	2.34	0.48
1:C:97:ILE:HG12	1:C:98:ALA:N	2.29	0.47
1:A:523:VAL:HG11	1:A:568:PHE:H	1.78	0.47
1:B:17:LEU:C	1:B:19:LEU:H	2.17	0.47
1:D:583:THR:HG21	1:D:588:LYS:HG2	1.96	0.47
1:A:192:ARG:O	1:A:196:ILE:HG13	2.14	0.47
1:C:419:TYR:CE2	1:C:430:ILE:HG23	2.48	0.47
1:B:523:VAL:HG11	1:B:568:PHE:H	1.80	0.47
1:C:132:ILE:HG23	1:C:133:VAL:HG13	1.96	0.47
1:A:169:LYS:HE2	1:A:171:ASP:OD1	2.15	0.47
1:B:306:ILE:HG22	1:B:307:MET:N	2.29	0.47
1:C:404:SER:HB2	1:C:457:VAL:O	2.14	0.47
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.14	0.47
1:C:153:PHE:HE2	1:C:155:GLU:HB2	1.78	0.47
1:C:172:ARG:HB3	1:C:172:ARG:HH11	1.79	0.47
1:C:337:GLU:HG2	1:C:338:ILE:HD12	1.97	0.47
1:C:86:THR:OG1	1:C:89:GLU:HG3	2.14	0.47
1:A:17:LEU:C	1:A:19:LEU:H	2.16	0.47
1:B:133:VAL:HG11	1:B:187:PHE:CE1	2.50	0.47
1:B:122:GLN:O	1:B:123:PHE:HB2	2.14	0.47
1:D:133:VAL:HG11	1:D:187:PHE:CE1	2.50	0.47
1:C:12:GLU:O	1:C:16:LEU:HG	2.14	0.47
1:C:210:ILE:HD11	1:C:227:ILE:HD11	1.96	0.47
1:D:588:LYS:HE2	1:D:592:TRP:NE1	2.29	0.47
1:A:404:SER:HB2	1:A:457:VAL:O	2.15	0.47
1:B:277:LEU:HD12	1:B:278:LEU:N	2.29	0.47
1:D:153:PHE:CE2	1:D:155:GLU:HB2	2.50	0.47
1:D:90:VAL:HG13	1:D:94:LEU:HD12	1.95	0.47
1:B:45:LYS:HD2	1:C:341:ASP:HA	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:SER:O	1:D:40:SER:HB3	2.15	0.47
1:A:91:ILE:O	1:A:95:GLY:HA3	2.14	0.47
1:D:214:GLU:H	1:D:221:VAL:HA	1.80	0.47
1:B:148:PRO:O	1:B:168:THR:HG23	2.14	0.47
1:B:91:ILE:O	1:B:95:GLY:HA3	2.15	0.47
1:B:98:ALA:O	1:B:102:THR:HG23	2.15	0.47
1:D:537:ALA:HB1	1:D:568:PHE:HE1	1.80	0.47
1:A:537:ALA:HB1	1:A:568:PHE:HE1	1.80	0.47
1:D:229:LYS:O	1:D:230:ALA:HB3	2.15	0.47
1:A:217:ASP:C	1:A:219:GLU:H	2.18	0.47
1:C:250:TYR:HD2	1:C:260:PRO:HD3	1.79	0.47
1:A:153:PHE:HB2	1:A:167:ILE:HD13	1.97	0.47
1:B:105:PHE:HB2	1:B:123:PHE:HZ	1.72	0.46
1:B:554:PHE:HE2	1:C:19:LEU:HD13	1.80	0.46
1:B:588:LYS:HE2	1:B:592:TRP:NE1	2.30	0.46
1:D:618:MET:HB3	1:D:618:MET:HE3	1.53	0.46
1:D:460:LEU:HD13	1:D:465:ASP:HB3	1.96	0.46
1:C:69:PHE:CZ	1:C:190:ASP:HA	2.50	0.46
1:B:554:PHE:CE2	1:C:19:LEU:HD13	2.51	0.46
1:C:588:LYS:HE2	1:C:592:TRP:NE1	2.30	0.46
1:C:148:PRO:O	1:C:168:THR:HG23	2.14	0.46
1:C:486:VAL:HG21	1:C:569:GLU:OE2	2.16	0.46
1:C:523:VAL:HG11	1:C:568:PHE:H	1.80	0.46
1:C:419:TYR:HA	1:C:456:GLU:OE2	2.15	0.46
1:C:306:ILE:HG22	1:C:307:MET:N	2.30	0.46
1:C:602:LEU:HG	1:C:608:LEU:HB2	1.98	0.46
1:C:210:ILE:HG12	1:C:227:ILE:CG1	2.46	0.46
1:A:113:GLN:N	1:A:113:GLN:HE21	1.90	0.46
1:D:420:VAL:HA	1:D:423:MET:HG3	1.97	0.46
1:C:481:GLN:HG3	1:C:482:SER:N	2.31	0.46
1:B:433:ILE:HD12	1:B:434:THR:H	1.81	0.46
1:B:153:PHE:HE2	1:B:155:GLU:HB2	1.80	0.46
1:D:306:ILE:HG22	1:D:307:MET:N	2.30	0.46
1:D:523:VAL:HG11	1:D:568:PHE:H	1.81	0.46
1:C:420:VAL:HA	1:C:423:MET:HG3	1.97	0.46
1:D:243:ASP:O	1:D:247:LYS:HG3	2.16	0.46
1:A:191:TRP:O	1:A:194:ARG:HB3	2.15	0.46
1:B:153:PHE:HB2	1:B:167:ILE:HD13	1.98	0.46
1:B:31:PHE:HA	1:B:129:SER:OG	2.16	0.46
1:C:17:LEU:C	1:C:19:LEU:N	2.69	0.46
1:A:153:PHE:HE2	1:A:155:GLU:HB2	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HD13	1:A:30:ILE:HA	1.78	0.46
1:D:17:LEU:C	1:D:19:LEU:N	2.68	0.46
1:D:304:VAL:HG12	1:D:305:PHE:N	2.30	0.46
1:D:47:ARG:NH2	1:D:302:GLN:NE2	2.63	0.46
1:C:511:PHE:CE1	1:C:581:ALA:HA	2.50	0.46
1:B:408:ASP:N	1:B:408:ASP:OD1	2.49	0.46
1:B:30:ILE:HA	1:B:30:ILE:HD13	1.78	0.46
1:A:481:GLN:HG3	1:A:482:SER:N	2.31	0.46
1:B:192:ARG:O	1:B:196:ILE:HG13	2.16	0.46
1:D:86:THR:OG1	1:D:89:GLU:HG3	2.15	0.46
1:D:322:ARG:HA	1:D:322:ARG:HD2	1.63	0.46
1:D:12:GLU:CB	1:D:15:GLN:HB2	2.46	0.45
1:C:277:LEU:HD12	1:C:278:LEU:N	2.31	0.45
1:C:85:MET:HE2	1:C:94:LEU:HG	1.97	0.45
1:A:122:GLN:HA	1:C:286:TRP:CA	2.21	0.45
1:A:51:LEU:HD21	1:A:331:PRO:HD2	1.97	0.45
1:A:273:GLU:HB3	1:A:329:ASP:OD1	2.15	0.45
1:A:44:ASP:HA	1:A:47:ARG:HH11	1.81	0.45
1:C:86:THR:O	1:C:90:VAL:HG23	2.16	0.45
1:A:106:LEU:HD13	1:D:464:ILE:HG13	1.98	0.45
1:A:355:ARG:HA	1:A:355:ARG:HD3	1.78	0.45
1:B:191:TRP:O	1:B:194:ARG:HB3	2.16	0.45
1:D:153:PHE:HB2	1:D:167:ILE:HD13	1.98	0.45
1:D:419:TYR:HA	1:D:456:GLU:OE2	2.16	0.45
1:B:509:THR:N	1:B:510:PRO:CD	2.80	0.45
1:D:13:VAL:O	1:D:17:LEU:HD13	2.16	0.45
1:A:28:LYS:HE2	1:A:28:LYS:HB3	1.82	0.45
1:A:86:THR:O	1:A:90:VAL:HG23	2.17	0.45
1:C:509:THR:H	1:C:510:PRO:HD2	1.80	0.45
1:C:242:THR:HB	1:C:245:GLU:HG3	1.99	0.45
1:B:261:LEU:CD2	1:B:282:SER:HB3	2.46	0.45
1:A:229:LYS:O	1:A:230:ALA:HB3	2.15	0.45
1:D:420:VAL:HA	1:D:423:MET:CG	2.46	0.45
1:C:133:VAL:HG11	1:C:187:PHE:HE1	1.81	0.45
1:B:420:VAL:HA	1:B:423:MET:HG3	1.98	0.45
1:A:467:TRP:CD1	1:D:106:LEU:HD21	2.52	0.45
1:D:91:ILE:O	1:D:95:GLY:HA3	2.17	0.45
1:B:69:PHE:CZ	1:B:190:ASP:HA	2.51	0.45
1:B:51:LEU:HD21	1:B:331:PRO:HD2	1.98	0.45
1:C:277:LEU:C	1:C:278:LEU:HD12	2.37	0.45
1:D:191:TRP:O	1:D:194:ARG:HB3	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LYS:HE2	1:B:171:ASP:OD1	2.17	0.45
1:B:17:LEU:C	1:B:19:LEU:N	2.69	0.45
1:C:31:PHE:HA	1:C:129:SER:OG	2.17	0.45
1:A:616:ARG:O	1:A:619:ASN:HB2	2.17	0.45
1:C:91:ILE:O	1:C:95:GLY:HA3	2.15	0.45
1:A:63:LEU:HA	1:A:81:ASN:ND2	2.25	0.45
1:C:191:TRP:O	1:C:194:ARG:HB3	2.16	0.45
1:A:149:GLU:HA	1:A:168:THR:HG23	1.99	0.45
1:C:250:TYR:HB2	1:C:279:TYR:CE1	2.52	0.45
1:C:250:TYR:HB2	1:C:279:TYR:CD1	2.51	0.45
1:D:104:SER:O	1:D:108:SER:HB2	2.16	0.45
1:C:537:ALA:HB1	1:C:568:PHE:HE1	1.81	0.45
1:C:509:THR:H	1:C:510:PRO:CD	2.30	0.45
1:D:104:SER:HB3	1:D:123:PHE:CZ	2.52	0.45
1:B:518:LEU:HD23	1:B:593:VAL:HG11	1.99	0.45
1:A:17:LEU:C	1:A:19:LEU:N	2.70	0.45
1:D:24:LEU:HB2	1:D:132:ILE:HD12	1.99	0.45
1:B:189:ASP:OD1	1:B:192:ARG:HB2	2.17	0.45
1:B:153:PHE:O	1:B:164:VAL:HA	2.17	0.45
1:D:602:LEU:HG	1:D:608:LEU:HB2	1.98	0.44
1:A:133:VAL:HG11	1:A:187:PHE:CE1	2.52	0.44
1:A:190:ASP:CG	1:A:213:ARG:HH22	2.20	0.44
1:A:548:THR:HG23	1:A:549:GLN:N	2.32	0.44
1:D:312:GLN:O	1:D:349:ARG:HD3	2.18	0.44
1:B:132:ILE:HG23	1:B:133:VAL:HG13	1.99	0.44
1:C:616:ARG:O	1:C:619:ASN:HB2	2.18	0.44
1:B:12:GLU:HA	1:B:15:GLN:HB2	2.00	0.44
1:D:31:PHE:HA	1:D:129:SER:OG	2.17	0.44
1:C:24:LEU:HB2	1:C:132:ILE:HD12	1.98	0.44
1:D:481:GLN:HG3	1:D:482:SER:N	2.33	0.44
1:C:518:LEU:HD23	1:C:593:VAL:HG11	1.99	0.44
1:C:210:ILE:HG12	1:C:227:ILE:HG13	1.99	0.44
1:D:120:ILE:O	1:D:120:ILE:HG22	2.18	0.44
1:A:464:ILE:HG13	1:D:106:LEU:HD13	1.98	0.44
1:A:511:PHE:CE1	1:A:581:ALA:HA	2.52	0.44
1:B:129:SER:O	1:B:132:ILE:HG22	2.17	0.44
1:D:616:ARG:O	1:D:619:ASN:HB2	2.17	0.44
1:B:324:LEU:O	1:B:324:LEU:HD22	2.18	0.44
1:B:447:LEU:HD22	1:B:447:LEU:HA	1.82	0.44
1:B:419:TYR:HA	1:B:456:GLU:OE2	2.17	0.44
1:C:66:ARG:HG2	1:C:209:GLU:HB2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD21	1:D:467:TRP:CD1	2.52	0.44
1:B:13:VAL:O	1:B:17:LEU:HD13	2.17	0.44
1:A:420:VAL:HA	1:A:423:MET:HG3	1.98	0.44
1:C:313:PHE:HE1	1:C:348:LEU:HD13	1.82	0.44
1:A:169:LYS:HA	1:A:169:LYS:HD2	1.78	0.44
1:D:548:THR:HG23	1:D:549:GLN:N	2.33	0.44
1:D:172:ARG:HH11	1:D:172:ARG:HB3	1.81	0.44
1:B:104:SER:O	1:B:108:SER:HB2	2.18	0.44
1:C:85:MET:HE3	2:C:1003:ADP:H1'	1.99	0.44
1:B:481:GLN:HG3	1:B:482:SER:N	2.32	0.44
1:C:509:THR:N	1:C:510:PRO:CD	2.81	0.44
1:A:602:LEU:HG	1:A:608:LEU:HB2	1.99	0.44
1:B:602:LEU:HG	1:B:608:LEU:HB2	2.00	0.44
1:B:86:THR:O	1:B:90:VAL:HG23	2.18	0.44
1:C:449:LEU:HD23	1:C:531:ARG:HD3	1.98	0.44
1:D:30:ILE:HA	1:D:30:ILE:HD13	1.79	0.44
1:C:420:VAL:HA	1:C:423:MET:CG	2.48	0.44
1:D:250:TYR:HB2	1:D:279:TYR:CD1	2.53	0.44
1:B:616:ARG:O	1:B:619:ASN:HB2	2.18	0.44
1:D:10:GLN:HE21	1:D:10:GLN:H	1.66	0.44
1:A:13:VAL:O	1:A:17:LEU:HD13	2.17	0.44
1:A:57:TYR:CZ	1:A:329:ASP:HB3	2.53	0.44
1:D:120:ILE:HA	1:D:122:GLN:CB	2.47	0.44
1:D:153:PHE:O	1:D:164:VAL:HA	2.18	0.44
1:B:320:PHE:O	1:B:322:ARG:HD3	2.18	0.44
1:A:153:PHE:O	1:A:164:VAL:HA	2.18	0.44
1:B:153:PHE:CE2	1:B:155:GLU:HB2	2.53	0.44
1:B:243:ASP:O	1:B:247:LYS:HG3	2.18	0.44
1:D:518:LEU:HD23	1:D:593:VAL:HG11	1.99	0.44
1:A:104:SER:O	1:A:108:SER:HB2	2.17	0.44
1:A:322:ARG:HD2	1:A:322:ARG:HA	1.63	0.44
1:B:553:LEU:HA	1:B:553:LEU:HD12	1.90	0.43
1:B:553:LEU:CG	1:C:109:LEU:HD21	2.45	0.43
1:C:280:ILE:HD12	1:C:360:LEU:CD2	2.48	0.43
1:D:277:LEU:C	1:D:278:LEU:HD12	2.39	0.43
1:A:288:MET:CE	1:A:320:PHE:HB3	2.48	0.43
1:C:227:ILE:HG22	1:C:228:ASN:N	2.33	0.43
1:B:548:THR:HG23	1:B:549:GLN:N	2.33	0.43
1:A:214:GLU:N	1:A:214:GLU:OE1	2.52	0.43
1:A:277:LEU:C	1:A:278:LEU:HD12	2.38	0.43
1:A:467:TRP:CH2	1:D:102:THR:HB	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:HB1	1:C:467:TRP:HZ3	1.83	0.43
1:B:149:GLU:HA	1:B:168:THR:HG23	2.01	0.43
1:C:330:LEU:HD12	1:C:330:LEU:HA	1.86	0.43
1:B:37:SER:O	1:B:40:SER:HB3	2.18	0.43
1:D:69:PHE:CZ	1:D:190:ASP:HA	2.53	0.43
1:A:420:VAL:HA	1:A:423:MET:CG	2.49	0.43
1:C:133:VAL:HG11	1:C:187:PHE:CE1	2.54	0.43
1:D:302:GLN:NE2	1:D:328:SER:HB3	2.33	0.43
1:C:304:VAL:HG12	1:C:305:PHE:N	2.33	0.43
1:A:189:ASP:OD1	1:A:192:ARG:HB2	2.17	0.43
1:B:487:ASP:O	1:B:491:GLU:HB2	2.18	0.43
1:C:487:ASP:O	1:C:491:GLU:HB2	2.18	0.43
1:D:94:LEU:HD22	1:D:127:PHE:CZ	2.53	0.43
1:B:261:LEU:HD21	1:B:282:SER:HB3	2.00	0.43
1:C:548:THR:HG23	1:C:549:GLN:N	2.33	0.43
1:A:153:PHE:CE2	1:A:155:GLU:HB2	2.53	0.43
1:B:337:GLU:HG2	1:B:338:ILE:HD12	2.01	0.43
1:A:523:VAL:CG1	1:A:568:PHE:H	2.32	0.43
1:C:129:SER:O	1:C:132:ILE:HG22	2.19	0.43
1:C:241:ILE:HD12	1:C:246:TYR:OH	2.19	0.43
1:C:153:PHE:CE2	1:C:155:GLU:HB2	2.52	0.43
1:B:24:LEU:HD11	1:B:125:VAL:H	1.84	0.43
1:C:553:LEU:HA	1:C:553:LEU:HD12	1.87	0.43
1:A:243:ASP:O	1:A:247:LYS:HG3	2.19	0.43
1:D:149:GLU:HA	1:D:168:THR:HG23	1.99	0.43
1:B:618:MET:HE2	1:B:618:MET:HB3	1.66	0.43
1:C:447:LEU:HD22	1:C:447:LEU:HA	1.82	0.43
1:B:282:SER:O	1:B:377:GLN:HG3	2.19	0.43
1:B:44:ASP:HA	1:B:47:ARG:HH11	1.84	0.43
1:B:172:ARG:HB3	1:B:172:ARG:HH11	1.84	0.43
1:C:300:TYR:CD1	1:C:305:PHE:HA	2.54	0.43
1:D:189:ASP:OD1	1:D:192:ARG:HB2	2.18	0.43
1:C:153:PHE:O	1:C:164:VAL:HA	2.18	0.43
1:D:487:ASP:O	1:D:491:GLU:HB2	2.18	0.43
1:A:261:LEU:CD2	1:A:282:SER:HB3	2.49	0.43
1:A:518:LEU:HD23	1:A:593:VAL:HG11	2.00	0.43
1:A:269:GLU:HA	1:A:273:GLU:OE1	2.19	0.42
1:C:302:GLN:O	1:C:304:VAL:HG23	2.18	0.42
1:A:419:TYR:HA	1:A:456:GLU:OE2	2.18	0.42
1:A:313:PHE:HE1	1:A:348:LEU:HD13	1.83	0.42
1:A:45:LYS:O	1:A:49:ARG:HG2	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:CZ	1:A:190:ASP:HA	2.54	0.42
1:D:250:TYR:HB2	1:D:279:TYR:CE1	2.54	0.42
1:A:595:LEU:HD13	1:A:618:MET:HB2	2.01	0.42
1:C:602:LEU:CD2	1:D:611:PRO:HB3	2.49	0.42
1:C:415:SER:HB3	1:C:418:ASP:CG	2.38	0.42
1:A:263:TRP:HB3	1:A:279:TYR:CD2	2.54	0.42
1:C:464:ILE:O	1:C:464:ILE:HG12	2.19	0.42
1:D:28:LYS:HB3	1:D:28:LYS:HE2	1.85	0.42
1:D:47:ARG:HG2	1:D:329:ASP:HA	2.00	0.42
1:C:44:ASP:HA	1:C:47:ARG:HH11	1.84	0.42
1:C:327:SER:OG	1:C:330:LEU:HB2	2.20	0.42
1:B:184:GLU:C	1:B:186:GLU:H	2.22	0.42
1:D:242:THR:HB	1:D:245:GLU:HG3	2.00	0.42
1:C:355:ARG:HD3	1:C:355:ARG:HA	1.79	0.42
1:A:65:VAL:O	1:A:65:VAL:HG13	2.19	0.42
1:B:66:ARG:HG2	1:B:209:GLU:HB2	2.01	0.42
1:A:512:ILE:HD11	1:A:528:LEU:HG	2.01	0.42
1:B:280:ILE:HD12	1:B:360:LEU:CD2	2.50	0.42
1:A:433:ILE:HD12	1:A:434:THR:H	1.83	0.42
1:C:11:SER:O	1:C:15:GLN:HG2	2.20	0.42
1:B:16:LEU:HD11	1:C:470:ASN:HD22	1.83	0.42
1:B:533:THR:HG23	1:B:535:THR:HB	2.00	0.42
1:D:147:LYS:HA	1:D:148:PRO:HD3	1.92	0.42
1:C:263:TRP:HB3	1:C:279:TYR:CD2	2.54	0.42
1:D:595:LEU:HD13	1:D:618:MET:HB2	2.02	0.42
1:B:420:VAL:HA	1:B:423:MET:CG	2.49	0.42
1:D:433:ILE:HD12	1:D:434:THR:H	1.84	0.42
1:D:415:SER:HB3	1:D:418:ASP:CG	2.40	0.42
1:A:337:GLU:HG2	1:A:338:ILE:HD12	2.01	0.42
1:B:269:GLU:HA	1:B:273:GLU:OE1	2.20	0.42
1:A:85:MET:HE3	2:A:1001:ADP:H1'	2.01	0.42
1:B:466:GLU:CD	1:B:549:GLN:HB3	2.40	0.42
1:C:487:ASP:OD2	1:C:489:SER:HB2	2.19	0.42
1:C:66:ARG:HD3	1:C:224:TRP:CD2	2.55	0.42
1:B:313:PHE:HB3	1:B:352:LEU:HD12	2.02	0.42
1:B:263:TRP:HB3	1:B:279:TYR:CD2	2.54	0.42
1:D:261:LEU:CD2	1:D:282:SER:HB3	2.50	0.42
1:B:300:TYR:CD1	1:B:305:PHE:HA	2.55	0.42
1:B:400:LEU:O	1:B:401:ARG:HD3	2.20	0.42
1:A:487:ASP:O	1:A:491:GLU:HB2	2.20	0.42
1:D:106:LEU:O	1:D:109:LEU:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:O	1:C:40:SER:HB3	2.19	0.42
1:C:322:ARG:HA	1:C:322:ARG:HD2	1.65	0.42
1:D:416:LEU:HD23	1:D:416:LEU:HA	1.87	0.42
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.87	0.42
1:C:30:ILE:HA	1:C:30:ILE:HD13	1.78	0.42
1:C:227:ILE:O	1:C:228:ASN:C	2.59	0.41
1:D:302:GLN:O	1:D:304:VAL:HG23	2.20	0.41
1:B:45:LYS:O	1:B:49:ARG:HG2	2.21	0.41
1:D:464:ILE:O	1:D:464:ILE:HG12	2.19	0.41
1:C:184:GLU:C	1:C:186:GLU:H	2.22	0.41
1:A:66:ARG:HG2	1:A:209:GLU:HB2	2.01	0.41
1:B:387:ALA:HB1	1:B:467:TRP:HZ3	1.86	0.41
1:A:302:GLN:O	1:A:304:VAL:HG23	2.20	0.41
1:A:439:ALA:CB	1:B:609:GLU:O	2.68	0.41
1:D:280:ILE:HD12	1:D:360:LEU:CD2	2.50	0.41
1:D:590:SER:O	1:D:594:GLU:HB2	2.20	0.41
1:A:338:ILE:H	1:A:338:ILE:CD1	2.26	0.41
1:A:85:MET:HE2	1:A:94:LEU:HG	2.02	0.41
1:B:328:SER:O	1:B:329:ASP:HB2	2.20	0.41
1:A:23:SER:HA	1:D:559:GLN:HE22	1.85	0.41
1:C:369:GLU:HG3	1:C:370:LYS:N	2.35	0.41
1:B:595:LEU:HD13	1:B:618:MET:HB2	2.02	0.41
1:A:280:ILE:HD12	1:A:360:LEU:CD2	2.50	0.41
1:C:429:LYS:HD3	1:C:481:GLN:HB2	2.01	0.41
1:C:297:LEU:HA	1:C:297:LEU:HD22	1.83	0.41
1:D:65:VAL:O	1:D:65:VAL:HG13	2.19	0.41
1:A:575:VAL:CG2	1:B:623:VAL:HG13	2.43	0.41
1:C:458:LEU:HD23	1:C:458:LEU:HA	1.90	0.41
1:C:47:ARG:NH2	1:C:302:GLN:NE2	2.68	0.41
1:B:169:LYS:HD2	1:B:169:LYS:HA	1.79	0.41
1:C:590:SER:O	1:C:594:GLU:HB2	2.21	0.41
1:B:317:TYR:CE1	1:B:396:ILE:HD11	2.55	0.41
1:A:590:SER:O	1:A:594:GLU:HB2	2.21	0.41
1:C:338:ILE:CD1	1:C:338:ILE:H	2.26	0.41
1:A:302:GLN:HE22	1:A:328:SER:HB3	1.85	0.41
1:D:139:VAL:HG22	1:D:176:ILE:HD13	2.03	0.41
1:A:210:ILE:HD12	1:A:227:ILE:HD11	2.02	0.41
1:C:149:GLU:HA	1:C:168:THR:HG23	2.01	0.41
1:D:387:ALA:HB1	1:D:467:TRP:HZ3	1.85	0.41
1:B:53:ASN:HA	1:B:54:PRO:HD3	1.91	0.41
1:C:472:LEU:HD23	1:C:472:LEU:HA	1.88	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:LEU:HD12	1:D:553:LEU:HA	1.90	0.41
1:D:254:ALA:O	1:D:255:HIS:HB2	2.21	0.41
1:A:304:VAL:HG12	1:A:305:PHE:N	2.35	0.41
1:A:444:SER:O	1:A:447:LEU:HB2	2.21	0.41
1:D:447:LEU:HD22	1:D:447:LEU:HA	1.82	0.41
1:B:189:ASP:CG	1:B:192:ARG:H	2.24	0.41
1:B:433:ILE:HD13	1:B:483:VAL:HG23	2.03	0.41
1:A:464:ILE:HG12	1:A:464:ILE:O	2.19	0.41
1:A:324:LEU:CD1	1:A:324:LEU:N	2.84	0.41
1:C:592:TRP:CD2	1:C:621:LEU:HD11	2.56	0.41
1:C:47:ARG:HG2	1:C:329:ASP:HA	2.03	0.41
1:A:213:ARG:HD3	1:A:213:ARG:N	2.35	0.41
1:A:422:ARG:HD2	1:A:456:GLU:OE1	2.21	0.41
1:D:282:SER:O	1:D:377:GLN:HG3	2.21	0.41
1:D:622:LEU:HA	1:D:622:LEU:HD23	1.93	0.41
1:D:523:VAL:CG1	1:D:568:PHE:H	2.34	0.41
1:A:129:SER:O	1:A:132:ILE:HG22	2.21	0.41
1:B:106:LEU:HD21	1:C:467:TRP:CD1	2.55	0.41
1:C:465:ASP:C	1:C:467:TRP:N	2.74	0.41
1:C:210:ILE:CG1	1:C:227:ILE:HD11	2.51	0.41
1:A:189:ASP:CG	1:A:192:ARG:H	2.24	0.41
1:B:304:VAL:HG12	1:B:305:PHE:N	2.35	0.41
1:C:45:LYS:O	1:C:49:ARG:HG2	2.20	0.41
1:B:65:VAL:O	1:B:65:VAL:HG13	2.20	0.41
1:C:14:LYS:HE2	1:C:14:LYS:HB3	1.90	0.41
1:B:523:VAL:CG1	1:B:568:PHE:H	2.33	0.41
1:B:12:GLU:CA	1:B:15:GLN:HB2	2.51	0.41
1:D:444:SER:O	1:D:447:LEU:HB2	2.21	0.41
1:B:434:THR:OG1	1:B:549:GLN:HG3	2.20	0.41
1:A:487:ASP:OD2	1:A:489:SER:HB2	2.20	0.41
1:D:263:TRP:HB3	1:D:279:TYR:CD2	2.56	0.41
1:C:515:VAL:HG13	1:C:593:VAL:HG21	2.03	0.41
1:A:515:VAL:HG13	1:A:593:VAL:HG21	2.02	0.41
1:C:595:LEU:HD13	1:C:618:MET:HB2	2.03	0.41
1:B:590:SER:O	1:B:594:GLU:HB2	2.21	0.41
1:D:328:SER:O	1:D:329:ASP:HB2	2.20	0.40
1:B:429:LYS:HD3	1:B:481:GLN:CB	2.52	0.40
1:A:106:LEU:O	1:A:109:LEU:HB2	2.21	0.40
1:B:302:GLN:O	1:B:304:VAL:HG23	2.21	0.40
1:A:66:ARG:HD3	1:A:224:TRP:CD2	2.56	0.40
1:B:241:ILE:HD12	1:B:246:TYR:OH	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLU:C	1:A:186:GLU:H	2.24	0.40
1:C:51:LEU:HD21	1:C:331:PRO:HD2	2.03	0.40
1:C:400:LEU:O	1:C:401:ARG:HD3	2.21	0.40
1:C:237:ASN:O	1:C:240:GLU:HB3	2.21	0.40
1:D:46:LEU:O	1:D:46:LEU:HD12	2.21	0.40
1:A:433:ILE:HD13	1:A:483:VAL:HG23	2.03	0.40
1:B:488:GLU:HG3	1:B:488:GLU:H	1.60	0.40
1:C:169:LYS:HG3	1:C:171:ASP:CG	2.41	0.40
1:D:169:LYS:HD2	1:D:169:LYS:HA	1.79	0.40
1:A:176:ILE:HG22	1:A:178:LEU:HD12	2.02	0.40
1:D:325:ILE:HD13	1:D:325:ILE:C	2.42	0.40
1:B:464:ILE:HG12	1:B:464:ILE:O	2.20	0.40
1:A:96:THR:OG1	1:A:97:ILE:HG22	2.21	0.40
1:D:337:GLU:HG2	1:D:338:ILE:HD12	2.02	0.40
1:D:429:LYS:HD3	1:D:481:GLN:HB2	2.03	0.40
1:D:327:SER:OG	1:D:330:LEU:HB2	2.22	0.40
1:A:284:ALA:HB2	1:A:378:PHE:CE2	2.57	0.40
1:B:618:MET:HE3	1:B:619:ASN:OD1	2.22	0.40
1:D:375:TRP:CH2	1:D:400:LEU:HD23	2.55	0.40
1:B:94:LEU:HD22	1:B:127:PHE:CZ	2.57	0.40
1:C:236:ARG:HB3	1:C:240:GLU:HG3	2.04	0.40
1:C:236:ARG:O	1:C:241:ILE:HD11	2.22	0.40
1:B:485:LYS:HG3	1:B:542:ASP:OD2	2.21	0.40
1:A:588:LYS:O	1:A:591:GLU:HB2	2.22	0.40
1:D:176:ILE:HG22	1:D:178:LEU:HD12	2.03	0.40
1:C:433:ILE:HD12	1:C:434:THR:H	1.86	0.40
1:A:351:ALA:O	1:A:354:LYS:HB3	2.21	0.40
1:B:596:LEU:HA	1:B:596:LEU:HD23	1.90	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	614/624 (98%)	495 (81%)	102 (17%)	17 (3%)	6	45
1	B	609/624 (98%)	490 (80%)	105 (17%)	14 (2%)	8	50
1	C	596/624 (96%)	487 (82%)	97 (16%)	12 (2%)	9	53
1	D	596/624 (96%)	488 (82%)	92 (15%)	16 (3%)	6	46
All	All	2415/2496 (97%)	1960 (81%)	396 (16%)	59 (2%)	7	49

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	97	ILE
1	A	575	VAL
1	B	97	ILE
1	C	97	ILE
1	C	509	THR
1	D	11	SER
1	D	97	ILE
1	D	216	LYS
1	B	11	SER
1	B	293	HIS
1	B	312	GLN
1	B	575	VAL
1	C	575	VAL
1	D	121	GLY
1	D	575	VAL
1	A	12	GLU
1	A	115	LYS
1	A	271	LYS
1	A	509	THR
1	B	271	LYS
1	B	389	ASP
1	C	271	LYS
1	D	118	GLN
1	D	271	LYS
1	D	312	GLN
1	D	389	ASP
1	A	240	GLU
1	A	367	ASP
1	A	534	ASP
1	A	536	PRO
1	B	122	GLN
1	B	536	PRO

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	536	PRO
1	D	221	VAL
1	D	536	PRO
1	A	439	ALA
1	C	227	ILE
1	C	507	ALA
1	C	533	THR
1	D	101	GLY
1	D	120	ILE
1	A	72	ASP
1	C	439	ALA
1	A	53	ASN
1	B	53	ASN
1	C	53	ASN
1	D	53	ASN
1	A	606	GLY
1	B	610	ASP
1	C	606	GLY
1	A	285	PRO
1	B	101	GLY
1	B	285	PRO
1	B	606	GLY
1	C	285	PRO
1	D	285	PRO
1	D	606	GLY
1	A	101	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/547 (93%)	447 (88%)	63 (12%)	6	32
1	B	514/547 (94%)	451 (88%)	63 (12%)	6	32
1	C	496/547 (91%)	436 (88%)	60 (12%)	6	32
1	D	496/547 (91%)	436 (88%)	60 (12%)	6	32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2016/2188 (92%)	1770 (88%)	246 (12%)	6	32

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	33	ARG
1	A	40	SER
1	A	45	LYS
1	A	51	LEU
1	A	55	ASP
1	A	60	ASP
1	A	64	ARG
1	A	76	LEU
1	A	85	MET
1	A	96	THR
1	A	113	GLN
1	A	171	ASP
1	A	172	ARG
1	A	177	THR
1	A	181	ARG
1	A	185	ASP
1	A	190	ASP
1	A	192	ARG
1	A	198	SER
1	A	213	ARG
1	A	226	LYS
1	A	228	ASN
1	A	252	HIS
1	A	257	PHE
1	A	259	ASP
1	A	266	ASN
1	A	276	SER
1	A	280	ILE
1	A	283	GLN
1	A	288	MET
1	A	290	ASN
1	A	297	LEU
1	A	308	ASP
1	A	319	ARG
1	A	324	LEU
1	A	325	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	332	LEU
1	A	333	ASN
1	A	337	GLU
1	A	343	THR
1	A	348	LEU
1	A	355	ARG
1	A	365	LYS
1	A	376	GLN
1	A	388	GLU
1	A	416	LEU
1	A	434	THR
1	A	447	LEU
1	A	467	TRP
1	A	472	LEU
1	A	473	THR
1	A	488	GLU
1	A	521	GLU
1	A	538	ILE
1	A	547	SER
1	A	559	GLN
1	A	568	PHE
1	A	579	ARG
1	A	594	GLU
1	A	608	LEU
1	A	614	PHE
1	A	617	ARG
1	B	33	ARG
1	B	40	SER
1	B	45	LYS
1	B	55	ASP
1	B	60	ASP
1	B	64	ARG
1	B	76	LEU
1	B	85	MET
1	B	96	THR
1	B	113	GLN
1	B	116	ASP
1	B	142	ARG
1	B	171	ASP
1	B	172	ARG
1	B	177	THR
1	B	181	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	185	ASP
1	B	190	ASP
1	B	192	ARG
1	B	198	SER
1	B	217	ASP
1	B	228	ASN
1	B	239	SER
1	B	240	GLU
1	B	252	HIS
1	B	257	PHE
1	B	259	ASP
1	B	266	ASN
1	B	276	SER
1	B	280	ILE
1	B	283	GLN
1	B	288	MET
1	B	297	LEU
1	B	308	ASP
1	B	319	ARG
1	B	324	LEU
1	B	325	ILE
1	B	332	LEU
1	B	333	ASN
1	B	337	GLU
1	B	343	THR
1	B	348	LEU
1	B	355	ARG
1	B	376	GLN
1	B	408	ASP
1	B	416	LEU
1	B	434	THR
1	B	447	LEU
1	B	467	TRP
1	B	472	LEU
1	B	473	THR
1	B	488	GLU
1	B	521	GLU
1	B	534	ASP
1	B	538	ILE
1	B	547	SER
1	B	559	GLN
1	B	568	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	579	ARG
1	B	594	GLU
1	B	608	LEU
1	B	614	PHE
1	B	617	ARG
1	C	33	ARG
1	C	40	SER
1	C	45	LYS
1	C	51	LEU
1	C	55	ASP
1	C	60	ASP
1	C	64	ARG
1	C	76	LEU
1	C	85	MET
1	C	96	THR
1	C	171	ASP
1	C	172	ARG
1	C	177	THR
1	C	181	ARG
1	C	185	ASP
1	C	190	ASP
1	C	192	ARG
1	C	198	SER
1	C	228	ASN
1	C	241	ILE
1	C	252	HIS
1	C	257	PHE
1	C	259	ASP
1	C	266	ASN
1	C	276	SER
1	C	280	ILE
1	C	283	GLN
1	C	288	MET
1	C	297	LEU
1	C	308	ASP
1	C	319	ARG
1	C	324	LEU
1	C	325	ILE
1	C	328	SER
1	C	332	LEU
1	C	333	ASN
1	C	337	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	343	THR
1	C	348	LEU
1	C	355	ARG
1	C	365	LYS
1	C	376	GLN
1	C	416	LEU
1	C	434	THR
1	C	447	LEU
1	C	467	TRP
1	C	472	LEU
1	C	473	THR
1	C	488	GLU
1	C	503	GLU
1	C	521	GLU
1	C	538	ILE
1	C	547	SER
1	C	559	GLN
1	C	568	PHE
1	C	579	ARG
1	C	594	GLU
1	C	608	LEU
1	C	614	PHE
1	C	617	ARG
1	D	10	GLN
1	D	33	ARG
1	D	40	SER
1	D	45	LYS
1	D	51	LEU
1	D	55	ASP
1	D	60	ASP
1	D	64	ARG
1	D	76	LEU
1	D	85	MET
1	D	96	THR
1	D	113	GLN
1	D	116	ASP
1	D	123	PHE
1	D	171	ASP
1	D	172	ARG
1	D	177	THR
1	D	181	ARG
1	D	185	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	190	ASP
1	D	192	ARG
1	D	198	SER
1	D	227	ILE
1	D	252	HIS
1	D	257	PHE
1	D	259	ASP
1	D	266	ASN
1	D	276	SER
1	D	280	ILE
1	D	283	GLN
1	D	288	MET
1	D	308	ASP
1	D	319	ARG
1	D	324	LEU
1	D	325	ILE
1	D	328	SER
1	D	332	LEU
1	D	333	ASN
1	D	337	GLU
1	D	343	THR
1	D	348	LEU
1	D	355	ARG
1	D	376	GLN
1	D	416	LEU
1	D	434	THR
1	D	447	LEU
1	D	467	TRP
1	D	472	LEU
1	D	473	THR
1	D	488	GLU
1	D	521	GLU
1	D	538	ILE
1	D	547	SER
1	D	559	GLN
1	D	568	PHE
1	D	579	ARG
1	D	594	GLU
1	D	608	LEU
1	D	614	PHE
1	D	617	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	10	GLN
1	A	27	ASN
1	A	93	HIS
1	A	113	GLN
1	A	150	ASN
1	A	302	GLN
1	A	316	ASN
1	A	350	ASN
1	A	392	ASN
1	A	470	ASN
1	A	599	GLN
1	A	612	ASN
1	B	4	GLN
1	B	27	ASN
1	B	113	GLN
1	B	150	ASN
1	B	255	HIS
1	B	350	ASN
1	B	392	ASN
1	B	470	ASN
1	C	4	GLN
1	C	150	ASN
1	C	258	ASN
1	C	302	GLN
1	C	350	ASN
1	C	470	ASN
1	C	559	GLN
1	C	599	GLN
1	C	612	ASN
1	D	4	GLN
1	D	10	GLN
1	D	27	ASN
1	D	93	HIS
1	D	113	GLN
1	D	150	ASN
1	D	255	HIS
1	D	258	ASN
1	D	302	GLN
1	D	350	ASN
1	D	392	ASN
1	D	559	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	612	ASN

### 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](#)

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	$\# Z  > 2$
2	ADP	A	1001	-	22,29,29	3.50	7 (31%)	27,45,45	3.27	4 (14%)
2	ADP	B	1002	-	22,29,29	3.50	7 (31%)	27,45,45	3.30	4 (14%)
2	ADP	C	1003	-	22,29,29	3.50	7 (31%)	27,45,45	3.28	4 (14%)
2	ADP	D	1004	-	22,29,29	3.50	7 (31%)	27,45,45	3.31	4 (14%)

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
2	ADP	A	1001	-	1/1/6/6	0/12/32/32	0/3/3/3
2	ADP	B	1002	-	1/1/6/6	0/12/32/32	0/3/3/3
2	ADP	C	1003	-	1/1/6/6	0/12/32/32	0/3/3/3
2	ADP	D	1004	-	1/1/6/6	0/12/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	ADP	C5-C4	-6.31	1.26	1.40
2	A	1001	ADP	C5-C4	-6.30	1.26	1.40
2	D	1004	ADP	C5-C4	-6.27	1.26	1.40
2	C	1003	ADP	C5-C4	-6.23	1.26	1.40
2	B	1002	ADP	C6-N6	3.45	1.45	1.34
2	A	1001	ADP	C6-N6	3.45	1.45	1.34
2	C	1003	ADP	C6-N6	3.47	1.45	1.34
2	D	1004	ADP	C6-N6	3.48	1.45	1.34
2	D	1004	ADP	O4'-C1'	3.74	1.45	1.41
2	C	1003	ADP	O4'-C1'	3.75	1.45	1.41
2	B	1002	ADP	O4'-C1'	3.75	1.45	1.41
2	A	1001	ADP	O4'-C1'	3.75	1.45	1.41
2	A	1001	ADP	C8-N7	5.11	1.44	1.34
2	D	1004	ADP	C8-N7	5.12	1.44	1.34
2	C	1003	ADP	C8-N7	5.16	1.44	1.34
2	B	1002	ADP	C8-N7	5.17	1.44	1.34
2	C	1003	ADP	C2-N1	5.53	1.44	1.33
2	A	1001	ADP	C2-N1	5.53	1.44	1.33
2	D	1004	ADP	C2-N1	5.54	1.44	1.33
2	B	1002	ADP	C2-N1	5.58	1.44	1.33
2	B	1002	ADP	C4-N3	6.19	1.44	1.35
2	A	1001	ADP	C4-N3	6.28	1.44	1.35
2	C	1003	ADP	C4-N3	6.28	1.44	1.35
2	D	1004	ADP	C4-N3	6.32	1.45	1.35
2	B	1002	ADP	C2-N3	9.84	1.49	1.32
2	C	1003	ADP	C2-N3	9.86	1.49	1.32
2	A	1001	ADP	C2-N3	9.87	1.49	1.32
2	D	1004	ADP	C2-N3	9.88	1.49	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	ADP	N3-C2-N1	-15.16	117.29	128.89
2	B	1002	ADP	N3-C2-N1	-15.14	117.30	128.89
2	A	1001	ADP	N3-C2-N1	-15.10	117.33	128.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1003	ADP	N3-C2-N1	-15.10	117.34	128.89
2	D	1004	ADP	C2'-C1'-N9	-4.11	108.01	114.29
2	B	1002	ADP	C2'-C1'-N9	-4.05	108.11	114.29
2	D	1004	ADP	PA-O3A-PB	-3.90	119.59	132.67
2	B	1002	ADP	PA-O3A-PB	-3.89	119.63	132.67
2	C	1003	ADP	PA-O3A-PB	-3.89	119.64	132.67
2	A	1001	ADP	PA-O3A-PB	-3.88	119.65	132.67
2	C	1003	ADP	C4-C5-N7	-3.83	105.96	109.48
2	D	1004	ADP	C4-C5-N7	-3.82	105.96	109.48
2	A	1001	ADP	C4-C5-N7	-3.75	106.03	109.48
2	B	1002	ADP	C4-C5-N7	-3.71	106.07	109.48
2	C	1003	ADP	C2'-C1'-N9	-3.51	108.93	114.29
2	A	1001	ADP	C2'-C1'-N9	-3.36	109.16	114.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1004	ADP	C4'
2	B	1002	ADP	C4'
2	A	1001	ADP	C4'
2	C	1003	ADP	C4'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	2	0
2	B	1002	ADP	2	0
2	C	1003	ADP	2	0
2	D	1004	ADP	2	0

## 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	618/624 (99%)	0.11	17 (2%) 56 47	33, 101, 170, 231	0
1	B	615/624 (98%)	0.20	24 (3%) 43 35	34, 104, 171, 194	0
1	C	606/624 (97%)	0.21	31 (5%) 32 24	46, 114, 175, 239	0
1	D	604/624 (96%)	0.11	12 (1%) 68 59	28, 97, 167, 211	0
All	All	2443/2496 (97%)	0.16	84 (3%) 49 39	28, 104, 173, 239	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	624	SER	20.5
1	C	537	ALA	6.0
1	B	12	GLU	5.5
1	C	538	ILE	5.3
1	A	624	SER	5.2
1	C	569	GLU	4.2
1	C	466	GLU	4.0
1	C	623	VAL	3.9
1	C	572	PRO	3.8
1	A	1	MET	3.7
1	B	501	ALA	3.6
1	C	105	PHE	3.4
1	B	623	VAL	3.4
1	B	539	VAL	3.4
1	C	528	LEU	3.4
1	A	608	LEU	3.3
1	B	577	VAL	3.3
1	D	537	ALA	3.3
1	B	21	ILE	3.2
1	A	500	SER	3.2
1	A	532	LEU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	608	LEU	3.1
1	B	570	LEU	3.1
1	C	455	ILE	3.0
1	D	441	ALA	3.0
1	C	313	PHE	3.0
1	A	623	VAL	2.9
1	B	576	LEU	2.9
1	C	610	ASP	2.7
1	D	187	PHE	2.7
1	B	538	ILE	2.7
1	B	622	LEU	2.7
1	B	500	SER	2.6
1	C	21	ILE	2.6
1	D	572	PRO	2.6
1	C	532	LEU	2.6
1	C	109	LEU	2.6
1	C	609	GLU	2.6
1	A	501	ALA	2.5
1	D	528	LEU	2.5
1	C	108	SER	2.5
1	D	288	MET	2.5
1	C	261	LEU	2.5
1	C	467	TRP	2.4
1	B	568	PHE	2.4
1	C	576	LEU	2.4
1	C	536	PRO	2.4
1	C	104	SER	2.4
1	C	570	LEU	2.4
1	C	434	THR	2.3
1	A	308	ASP	2.3
1	B	569	GLU	2.3
1	B	234	TRP	2.3
1	A	123	PHE	2.3
1	D	593	VAL	2.3
1	A	21	ILE	2.2
1	B	537	ALA	2.2
1	B	526	VAL	2.2
1	C	470	ASN	2.2
1	C	620	GLN	2.2
1	D	570	LEU	2.2
1	B	146	GLU	2.2
1	A	531	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	164	VAL	2.2
1	A	576	LEU	2.2
1	A	539	VAL	2.2
1	A	614	PHE	2.1
1	B	56	LEU	2.1
1	C	539	VAL	2.1
1	D	538	ILE	2.1
1	B	431	TYR	2.1
1	C	193	VAL	2.1
1	B	531	ARG	2.1
1	D	543	ALA	2.1
1	B	467	TRP	2.1
1	A	537	ALA	2.1
1	C	233	LEU	2.1
1	D	592	TRP	2.1
1	C	433	ILE	2.1
1	B	490	LEU	2.0
1	A	187	PHE	2.0
1	A	618	MET	2.0
1	B	546	MET	2.0
1	D	455	ILE	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 ⓘ

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
2	ADP	B	1002	27/27	0.89	0.23	-0.44	78,84,91,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	D	1004	27/27	0.94	0.23	-0.59	38,41,51,55	0
2	ADP	C	1003	27/27	0.91	0.22	-0.63	53,64,80,80	0
2	ADP	A	1001	27/27	0.92	0.21	-0.77	74,86,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.