



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:08 PM GMT

PDB ID : 1S9E  
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R129385  
Authors : Das, K.; Clark Jr., A.D.; Ludovici, D.W.; Kukla, M.J.; Decorte, B.; Lewi, P.J.; Hughes, S.H.; Janssen, P.A.; Arnold, E.  
Deposited on : 2004-02-04  
Resolution : 2.60 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

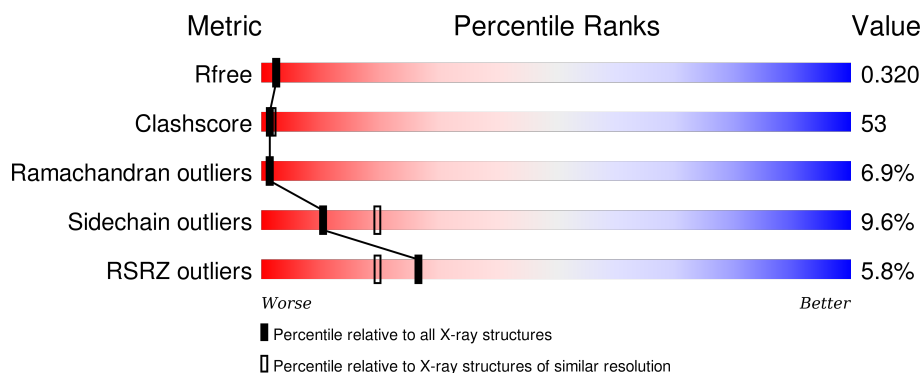
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	560	<div> <div>4%</div> <div>34%</div> <div>54%</div> <div>10%</div> <div>..</div> </div>
2	B	430	<div> <div>8%</div> <div>33%</div> <div>54%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8231 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 POL polyprotein [Contains:Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	122	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

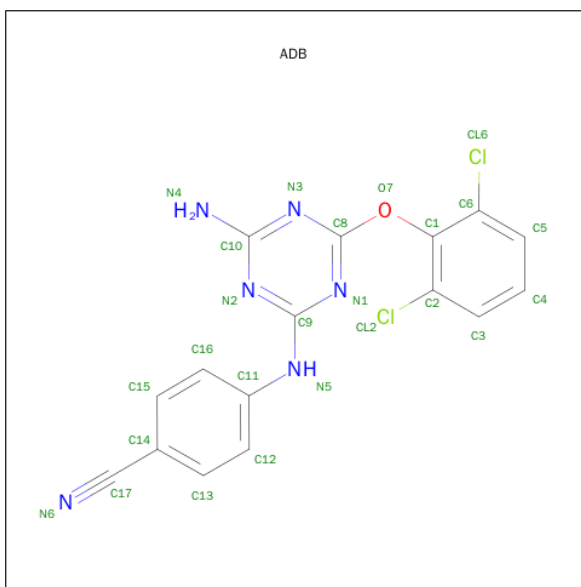
- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	56	0	0
			3529	2300	584	638	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is 4-[4-AMINO-6-(2,6-DICHLORO-PHENOXY)-[1,3,5]TRIAZIN-2-YLAMINO]-BENZONITRILE (three-letter code: ADB) (formula: C<sub>16</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			25	16	2	6	1		

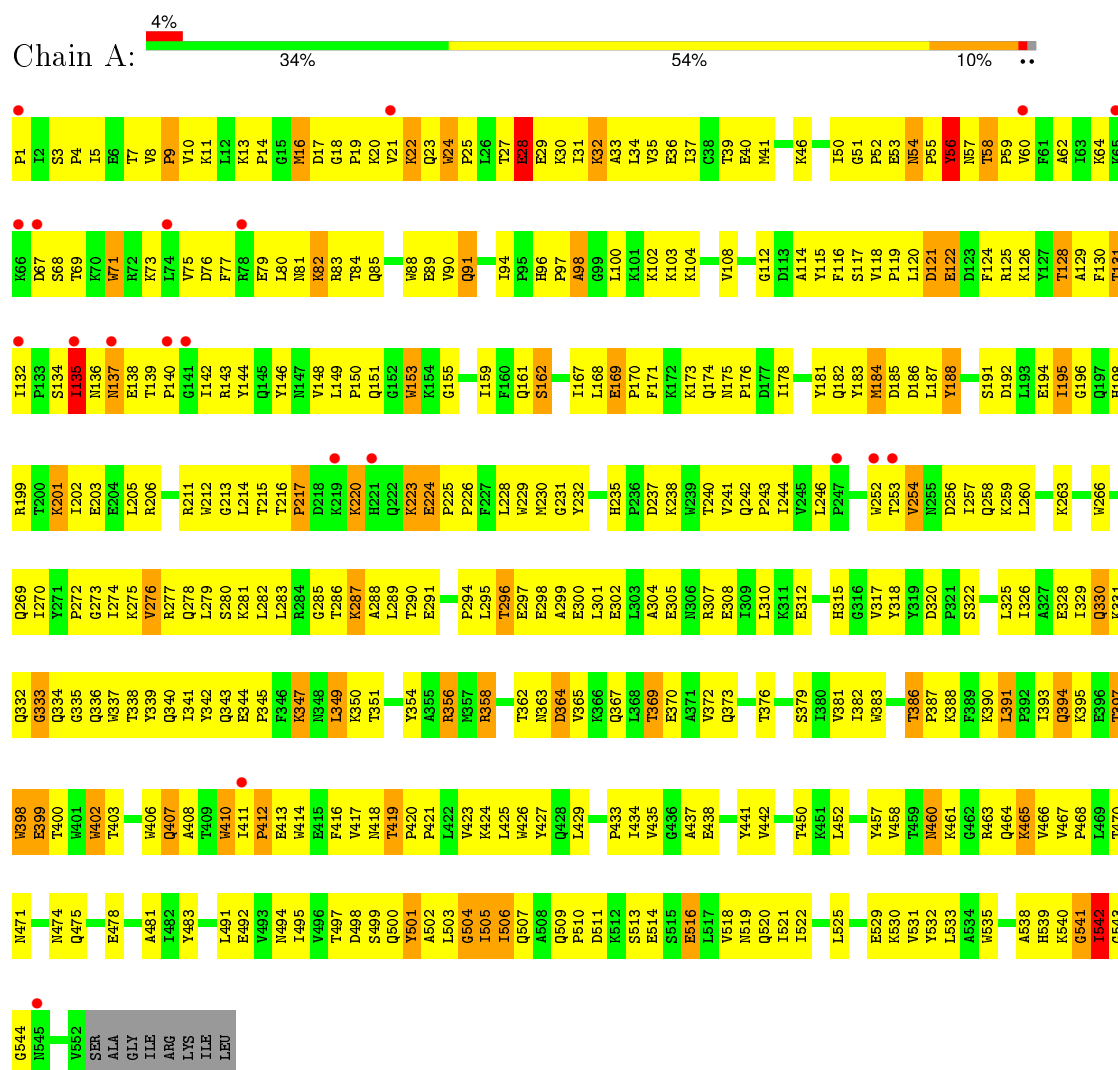
- Molecule 4 is water.

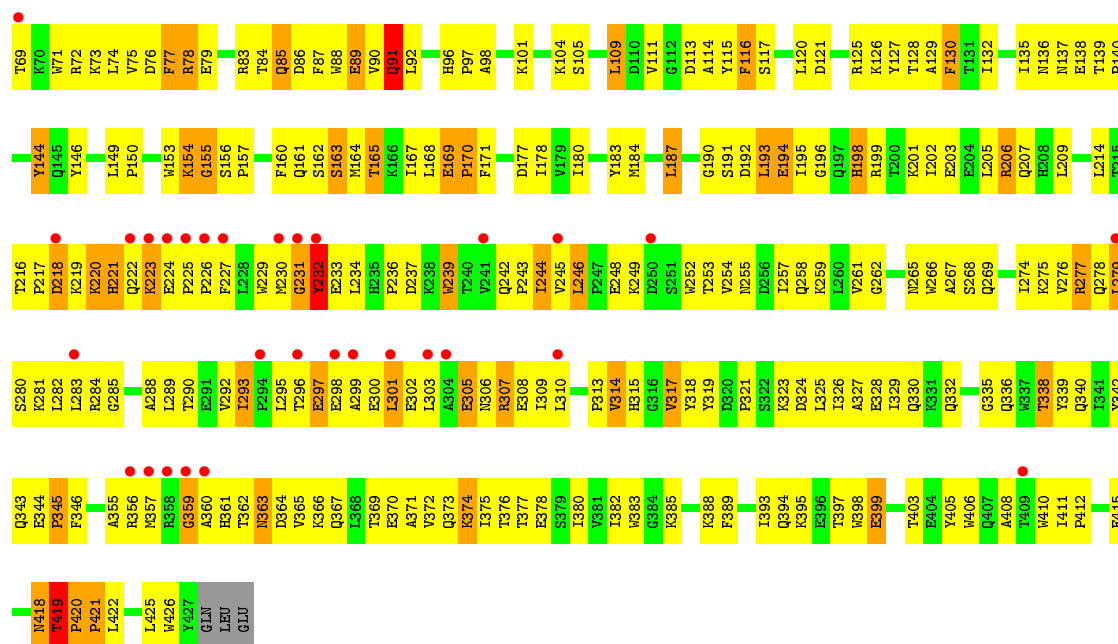
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	94	Total	O	0	0
			94	94		

### 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: POL polyprotein [Contains:Reverse transcriptase]





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.80Å 69.30Å 104.10Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 34.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-2.60) 95.8 (34.69-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.253 , 0.316 0.259 , 0.320	Depositor DCC
$R_{free}$ test set	2289 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45981 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

### 5.1 Standard geometry

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

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	0.67	0/4616	0.89	4/6271 (0.1%)
2	B	0.78	1/3634 (0.0%)	0.95	5/4940 (0.1%)
All	All	0.72	1/8250 (0.0%)	0.92	9/11211 (0.1%)

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
2	B	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	383	TRP	CB-CG	-5.55	1.40	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	THR	N-CA-C	8.01	132.63	111.00
1	A	381	VAL	CB-CA-C	-6.29	99.46	111.40
1	A	56	TYR	N-CA-C	-6.16	94.36	111.00
1	A	333	GLY	N-CA-C	5.61	127.12	113.10
2	B	78	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	B	89	GLU	N-CA-C	-5.56	95.98	111.00
1	A	135	ILE	N-CA-C	5.53	125.92	111.00
2	B	12	LEU	CA-CB-CG	5.39	127.71	115.30
2	B	155	GLY	N-CA-C	-5.11	100.33	113.10



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain
2	B	144	TYR	Sidechain
2	B	318	TYR	Sidechain

## 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	4498	0	4560	481	0
2	B	3529	0	3568	378	0
3	A	25	0	10	4	0
4	A	85	0	0	4	0
4	B	94	0	0	17	0
All	All	8231	0	8138	836	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 53.

All (836) 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:244:ILE:HD11	1:A:310:LEU:HD13	1.26	1.14
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.30	1.09
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.31	1.09
1:A:497:THR:HG22	1:A:499:SER:H	1.21	1.04
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.38	1.04
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.04
2:B:277:ARG:HD3	2:B:277:ARG:H	1.18	1.03
2:B:363:ASN:C	2:B:363:ASN:HD22	1.63	1.01
2:B:363:ASN:ND2	2:B:366:LYS:H	1.59	1.00
1:A:288:ALA:CB	1:A:291:GLU:HB2	1.91	0.98
2:B:5:ILE:HG22	2:B:6:GLU:H	1.29	0.98
2:B:65:LYS:HA	2:B:72:ARG:HG3	1.46	0.97
2:B:221:HIS:CE1	2:B:230:MET:HG2	2.01	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.45	0.95
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.05	0.94
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.50	0.94
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.03	0.94
2:B:363:ASN:HD21	2:B:366:LYS:H	1.02	0.93
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.47	0.92
1:A:503:LEU:HG	1:A:507:GLN:NE2	1.85	0.92
1:A:460:ASN:N	1:A:460:ASN:HD22	1.66	0.91
2:B:274:ILE:HG23	2:B:306:ASN:OD1	1.70	0.91
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.53	0.90
1:A:542:ILE:HD13	1:A:544:GLY:H	1.36	0.90
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.35	0.90
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.37	0.90
1:A:96:HIS:HD2	1:A:98:ALA:H	1.17	0.89
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.53	0.89
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.02	0.89
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.56	0.88
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.87	0.88
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.54	0.87
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.58	0.86
2:B:303:LEU:O	2:B:307:ARG:HB2	1.75	0.86
2:B:310:LEU:HD23	2:B:310:LEU:O	1.76	0.86
1:A:90:VAL:HG12	1:A:91:GLN:HG3	1.57	0.86
2:B:278:GLN:NE2	2:B:298:GLU:HB2	1.91	0.86
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.11	0.86
1:A:465:LYS:HG3	1:A:466:VAL:N	1.88	0.86
2:B:363:ASN:HD21	2:B:366:LYS:N	1.73	0.85
2:B:31:ILE:O	2:B:35:VAL:HG23	1.75	0.85
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.10	0.85
1:A:388:LYS:NZ	1:A:413:GLU:HG3	1.92	0.85
2:B:244:ILE:O	2:B:310:LEU:HD21	1.76	0.85
1:A:104:LYS:HE2	1:A:104:LYS:N	1.92	0.84
1:A:497:THR:HG22	1:A:498:ASP:N	1.89	0.84
1:A:460:ASN:H	1:A:460:ASN:HD22	1.25	0.84
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.59	0.84
1:A:148:VAL:O	1:A:150:PRO:HD3	1.77	0.84
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.77	0.84
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.07	0.84
1:A:254:VAL:O	1:A:257:ILE:HG22	1.78	0.84
1:A:542:ILE:HG12	1:A:543:GLY:H	1.43	0.83
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.61	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HG2	1:A:192:ASP:HA	1.61	0.82
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.07	0.82
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.59	0.81
1:A:96:HIS:CD2	1:A:98:ALA:H	1.99	0.81
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.15	0.81
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.62	0.81
1:A:64:LYS:HE3	1:A:68:SER:HB3	1.62	0.81
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.15	0.81
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.16	0.81
1:A:155:GLY:O	1:A:159:ILE:HG13	1.81	0.80
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.96	0.80
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.80	0.80
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.83	0.79
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.65	0.79
2:B:85:GLN:HG2	4:B:1089:HOH:O	1.81	0.79
1:A:206:ARG:HH22	1:A:217:PRO:C	1.86	0.78
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.11	0.78
1:A:298:GLU:CD	1:A:298:GLU:H	1.87	0.78
1:A:136:ASN:O	1:A:138:GLU:N	2.16	0.78
1:A:53:GLU:C	1:A:55:PRO:HD3	2.03	0.77
1:A:287:LYS:HG2	1:A:288:ALA:H	1.49	0.77
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.67	0.77
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.15	0.77
1:A:138:GLU:OE2	1:A:138:GLU:HA	1.85	0.77
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.00	0.77
1:A:220:LYS:HB2	4:A:1009:HOH:O	1.85	0.77
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.50	0.76
1:A:115:TYR:HD2	1:A:149:LEU:O	1.69	0.76
1:A:315:HIS:CE1	1:A:347:LYS:HD3	2.20	0.76
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.66	0.76
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.21	0.76
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.15	0.76
1:A:139:THR:HB	1:A:140:PRO:HD2	1.66	0.76
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.21	0.75
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.50	0.75
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.68	0.75
1:A:506:ILE:HG22	1:A:507:GLN:N	2.00	0.75
2:B:222:GLN:HG2	2:B:223:LYS:HG2	1.68	0.75
1:A:287:LYS:H	1:A:287:LYS:HD3	1.51	0.75
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.22	0.75
1:A:1:PRO:O	1:A:117:SER:HA	1.87	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG12	1:A:11:LYS:N	2.02	0.74
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.22	0.74
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.69	0.74
1:A:503:LEU:HG	1:A:507:GLN:HE22	1.51	0.74
1:A:509:GLN:N	1:A:510:PRO:HD3	2.02	0.74
1:A:183:TYR:CE2	1:A:230:MET:SD	2.81	0.74
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.23	0.74
1:A:497:THR:HG22	1:A:499:SER:N	2.01	0.74
1:A:96:HIS:HD2	1:A:98:ALA:N	1.85	0.74
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.68	0.74
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.68	0.74
1:A:388:LYS:HZ2	1:A:413:GLU:HG3	1.52	0.73
1:A:312:GLU:HG2	1:A:312:GLU:O	1.89	0.73
2:B:356:ARG:HG2	2:B:362:THR:HG21	1.69	0.73
1:A:540:LYS:HD2	2:B:265:ASN:HD21	1.52	0.73
2:B:356:ARG:HG3	2:B:357:MET:H	1.52	0.73
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.18	0.73
2:B:27:THR:CG2	2:B:29:GLU:HB3	2.19	0.73
1:A:542:ILE:HG12	1:A:543:GLY:N	2.04	0.73
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.22	0.73
1:A:28:GLU:HB3	1:A:135:ILE:HD13	1.71	0.73
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.04	0.73
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.54	0.72
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.70	0.72
2:B:278:GLN:HE22	2:B:298:GLU:HB2	1.53	0.72
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.55	0.72
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.71	0.72
1:A:435:VAL:HG13	2:B:290:THR:CG2	2.14	0.72
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.00	0.71
1:A:55:PRO:HD2	1:A:143:ARG:HH12	1.55	0.71
1:A:253:THR:OG1	1:A:290:THR:HA	1.90	0.71
1:A:64:LYS:HE3	1:A:68:SER:CB	2.21	0.71
1:A:424:LYS:HD3	1:A:425:LEU:N	2.05	0.71
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.31	0.71
2:B:278:GLN:OE1	2:B:297:GLU:HB2	1.90	0.71
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.20	0.71
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.54	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
1:A:301:LEU:O	1:A:305:GLU:HG3	1.90	0.70
2:B:221:HIS:HE1	2:B:230:MET:HG2	1.55	0.70
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.26	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HD13	1:A:544:GLY:N	2.06	0.70
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.74	0.70
1:A:30:LYS:O	1:A:33:ALA:N	2.25	0.70
2:B:278:GLN:HA	2:B:281:LYS:CE	2.18	0.70
1:A:507:GLN:O	1:A:509:GLN:HG3	1.91	0.70
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.74	0.70
1:A:373:GLN:OE1	2:B:397:THR:HA	1.91	0.70
2:B:298:GLU:HB3	2:B:301:LEU:CD1	2.22	0.69
2:B:418:ASN:O	2:B:419:THR:HG23	1.92	0.69
1:A:103:LYS:C	1:A:104:LYS:HE2	2.12	0.69
1:A:33:ALA:O	1:A:37:ILE:HG12	1.92	0.69
1:A:497:THR:CG2	1:A:499:SER:H	2.03	0.69
1:A:277:ARG:HD2	1:A:334:GLN:CB	2.23	0.69
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.75	0.68
1:A:27:THR:O	1:A:29:GLU:N	2.25	0.68
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.74	0.68
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.68
1:A:376:THR:HG23	1:A:386:THR:HG22	1.75	0.68
2:B:371:ALA:O	2:B:375:ILE:HG13	1.93	0.68
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.09	0.68
1:A:331:LYS:NZ	1:A:333:GLY:HA2	2.09	0.68
2:B:277:ARG:HD3	2:B:277:ARG:N	2.00	0.68
1:A:398:TRP:NE1	1:A:402:TRP:HD1	1.92	0.68
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.74	0.68
1:A:474:ASN:O	1:A:478:GLU:HG3	1.95	0.67
1:A:286:THR:O	1:A:286:THR:HG22	1.93	0.67
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.15	0.67
1:A:326:ILE:HD12	1:A:326:ILE:N	2.09	0.67
2:B:357:MET:HB2	2:B:361:HIS:HE2	1.59	0.67
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.20	0.67
1:A:354:TYR:OH	1:A:356:ARG:HD3	1.94	0.67
2:B:101:LYS:O	2:B:236:PRO:HB2	1.95	0.67
2:B:388:LYS:HE3	2:B:415:GLU:OE1	1.95	0.67
1:A:542:ILE:CD1	1:A:544:GLY:H	2.07	0.67
2:B:257:ILE:O	2:B:261:VAL:HG23	1.95	0.66
1:A:29:GLU:HA	1:A:29:GLU:OE1	1.94	0.66
2:B:357:MET:HB2	2:B:361:HIS:NE2	2.10	0.66
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.10	0.66
1:A:301:LEU:O	1:A:301:LEU:HD12	1.95	0.66
2:B:5:ILE:HG22	2:B:6:GLU:N	2.08	0.66
2:B:278:GLN:HE22	2:B:298:GLU:CB	2.07	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:O	1:A:417:VAL:HG12	1.96	0.66
2:B:86:ASP:O	2:B:89:GLU:HB3	1.95	0.66
1:A:460:ASN:N	1:A:460:ASN:ND2	2.40	0.66
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.65
1:A:27:THR:O	1:A:30:LYS:N	2.28	0.65
2:B:278:GLN:HE22	2:B:298:GLU:CG	2.09	0.65
1:A:290:THR:O	1:A:290:THR:HG22	1.96	0.65
2:B:422:LEU:O	2:B:425:LEU:HB2	1.96	0.65
2:B:23:GLN:HB2	4:B:1090:HOH:O	1.95	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.76	0.65
1:A:10:VAL:HG12	1:A:11:LYS:H	1.59	0.65
1:A:434:ILE:H	1:A:494:ASN:HD21	1.43	0.65
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.27	0.65
1:A:315:HIS:NE2	1:A:347:LYS:HD3	2.11	0.65
2:B:53:GLU:OE1	2:B:53:GLU:N	2.29	0.65
1:A:225:PRO:HA	1:A:226:PRO:C	2.17	0.65
1:A:298:GLU:CD	1:A:298:GLU:N	2.50	0.64
1:A:363:ASN:OD1	1:A:365:VAL:N	2.30	0.64
1:A:56:TYR:CD1	1:A:56:TYR:N	2.64	0.64
2:B:76:ASP:CG	2:B:78:ARG:HH21	2.00	0.64
2:B:411:ILE:HA	4:B:1088:HOH:O	1.97	0.64
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.62	0.64
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.25	0.64
2:B:339:TYR:C	2:B:340:GLN:OE1	2.36	0.64
2:B:46:LYS:CE	2:B:116:PHE:HD1	2.11	0.64
2:B:335:GLY:O	2:B:355:ALA:HA	1.97	0.64
2:B:85:GLN:HA	4:B:1089:HOH:O	1.98	0.63
1:A:270:ILE:O	1:A:272:PRO:HD3	1.98	0.63
2:B:156:SER:N	2:B:157:PRO:HD2	2.13	0.63
2:B:46:LYS:HD3	2:B:116:PHE:CD1	2.33	0.63
1:A:433:PRO:HG3	2:B:255:ASN:HD22	1.63	0.63
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.61	0.63
1:A:497:THR:CG2	1:A:498:ASP:N	2.59	0.63
1:A:373:GLN:HG2	2:B:394:GLN:HE22	1.64	0.63
2:B:363:ASN:C	2:B:363:ASN:ND2	2.39	0.63
2:B:359:GLY:O	2:B:361:HIS:N	2.32	0.63
1:A:50:ILE:HG13	1:A:51:GLY:N	2.13	0.63
2:B:195:ILE:HG23	2:B:196:GLY:N	2.13	0.62
1:A:420:PRO:HA	1:A:421:PRO:C	2.18	0.62
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.17	0.62
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:HG3	2:B:306:ASN:N	2.14	0.62
1:A:400:THR:O	1:A:403:THR:HB	1.99	0.62
2:B:217:PRO:O	2:B:219:LYS:N	2.32	0.62
1:A:287:LYS:CD	1:A:287:LYS:H	2.12	0.62
1:A:35:VAL:O	1:A:39:THR:HG23	1.98	0.62
2:B:357:MET:CB	2:B:361:HIS:HE2	2.13	0.62
2:B:282:LEU:CG	2:B:293:ILE:HD11	2.27	0.62
1:A:501:TYR:O	1:A:505:ILE:HD12	1.99	0.62
1:A:27:THR:O	1:A:27:THR:HG22	1.99	0.62
1:A:492:GLU:OE1	1:A:530:LYS:HD2	2.00	0.62
2:B:373:GLN:HG2	2:B:406:TRP:CH2	2.35	0.62
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.35	0.62
1:A:474:ASN:H	1:A:474:ASN:HD22	1.48	0.62
1:A:460:ASN:H	1:A:460:ASN:ND2	1.94	0.61
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.28	0.61
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.15	0.61
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.30	0.61
2:B:411:ILE:O	2:B:412:PRO:C	2.37	0.61
1:A:10:VAL:CG1	1:A:11:LYS:H	2.14	0.61
2:B:221:HIS:NE2	2:B:230:MET:HG2	2.16	0.61
2:B:224:GLU:O	2:B:226:PRO:HD3	2.00	0.61
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.65	0.61
1:A:398:TRP:CD1	1:A:402:TRP:HD1	2.18	0.61
2:B:87:PHE:O	2:B:91:GLN:HB2	2.00	0.60
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.87	0.60
2:B:255:ASN:O	2:B:258:GLN:HB2	2.01	0.60
1:A:90:VAL:HG12	1:A:91:GLN:CG	2.28	0.60
1:A:388:LYS:HZ3	1:A:413:GLU:HG3	1.66	0.60
2:B:369:THR:O	2:B:373:GLN:HG3	2.00	0.60
1:A:115:TYR:CD2	1:A:149:LEU:O	2.54	0.60
1:A:81:ASN:C	1:A:83:ARG:H	2.03	0.60
1:A:102:LYS:HG2	1:A:104:LYS:NZ	2.17	0.60
2:B:306:ASN:O	2:B:308:GLU:N	2.34	0.60
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.83	0.60
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.01	0.60
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.84	0.60
2:B:253:THR:HA	2:B:292:VAL:HA	1.84	0.60
2:B:27:THR:HG22	2:B:29:GLU:HB3	1.82	0.60
1:A:388:LYS:NZ	4:A:1155:HOH:O	2.28	0.60
2:B:376:THR:O	2:B:380:ILE:HG13	2.01	0.60
1:A:108:VAL:O	1:A:108:VAL:HG23	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:CG	1:A:507:GLN:HE22	2.13	0.60
1:A:57:ASN:OD1	1:A:131:THR:HB	2.01	0.60
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.17	0.60
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.67	0.60
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.64	0.60
2:B:61:PHE:HB3	4:B:1121:HOH:O	2.02	0.59
1:A:183:TYR:HE2	1:A:230:MET:SD	2.23	0.59
2:B:224:GLU:HG3	4:B:1151:HOH:O	2.01	0.59
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.83	0.59
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.38	0.59
1:A:134:SER:HB2	1:A:139:THR:OG1	2.02	0.59
1:A:10:VAL:CG1	1:A:11:LYS:N	2.65	0.59
1:A:195:ILE:HD11	1:A:199:ARG:CZ	2.32	0.59
2:B:105:SER:O	2:B:190:GLY:HA2	2.02	0.59
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.02	0.59
1:A:503:LEU:CG	1:A:507:GLN:NE2	2.64	0.59
1:A:125:ARG:O	1:A:128:THR:OG1	2.20	0.59
1:A:131:THR:OG1	1:A:143:ARG:HG3	2.01	0.59
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.38	0.59
2:B:84:THR:O	2:B:86:ASP:N	2.36	0.59
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.83	0.59
2:B:308:GLU:C	2:B:310:LEU:H	2.06	0.58
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.33	0.58
2:B:374:LYS:O	2:B:378:GLU:HG3	2.03	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
1:A:402:TRP:HE3	1:A:402:TRP:O	1.86	0.58
2:B:195:ILE:HD13	2:B:199:ARG:HH21	1.69	0.58
2:B:277:ARG:CD	2:B:277:ARG:H	1.96	0.58
1:A:501:TYR:CD1	1:A:505:ILE:HD11	2.38	0.58
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.68	0.58
2:B:27:THR:HG22	2:B:30:LYS:H	1.68	0.58
2:B:4:PRO:HG3	2:B:117:SER:HB2	1.85	0.58
1:A:173:LYS:O	1:A:176:PRO:HD3	2.04	0.58
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.69	0.58
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.23	0.57
1:A:253:THR:O	1:A:256:ASP:N	2.35	0.57
1:A:182:GLN:HB3	1:A:187:LEU:HD12	1.85	0.57
1:A:382:ILE:HG23	2:B:136:ASN:HD21	1.67	0.57
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.87	0.57
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.86	0.57
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.85	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.87	0.57
1:A:19:PRO:O	1:A:56:TYR:CB	2.53	0.57
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.70	0.57
2:B:342:TYR:CD1	2:B:342:TYR:C	2.78	0.57
1:A:100:LEU:HD21	3:A:701:ADB:CL2	2.41	0.57
1:A:81:ASN:O	1:A:83:ARG:N	2.38	0.57
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.40	0.56
1:A:100:LEU:HD22	3:A:701:ADB:C8	2.35	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.39	0.56
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.26	0.56
1:A:506:ILE:CG2	1:A:507:GLN:N	2.68	0.56
1:A:356:ARG:NH1	1:A:358:ARG:O	2.38	0.56
1:A:116:PHE:O	1:A:148:VAL:HG11	2.03	0.56
1:A:32:LYS:O	1:A:36:GLU:HG3	2.05	0.56
2:B:376:THR:HB	2:B:410:TRP:CH2	2.39	0.56
1:A:3:SER:HB3	1:A:212:TRP:C	2.26	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.56
1:A:121:ASP:O	1:A:122:GLU:C	2.43	0.56
2:B:222:GLN:HG2	2:B:223:LYS:N	2.21	0.56
2:B:5:ILE:CG2	2:B:6:GLU:H	2.11	0.56
1:A:22:LYS:CG	1:A:24:TRP:CZ2	2.83	0.56
2:B:13:LYS:O	2:B:16:MET:HB2	2.04	0.56
2:B:306:ASN:C	2:B:308:GLU:H	2.09	0.56
1:A:288:ALA:CB	1:A:291:GLU:CB	2.72	0.56
2:B:231:GLY:O	2:B:233:GLU:HG3	2.06	0.56
1:A:497:THR:HG22	1:A:498:ASP:H	1.66	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.38	0.56
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.37	0.56
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.18	0.56
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.40	0.56
1:A:362:THR:HG22	1:A:363:ASN:N	2.19	0.56
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.06	0.56
1:A:235:HIS:HB2	1:A:238:LYS:O	2.06	0.56
2:B:222:GLN:HG2	2:B:223:LYS:H	1.70	0.55
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.35	0.55
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.42	0.55
2:B:395:LYS:CG	2:B:399:GLU:OE1	2.55	0.55
2:B:98:ALA:O	2:B:101:LYS:HE2	2.07	0.55
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.40	0.55
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.21	0.55
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.70	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:HG12	2:B:246:LEU:O	2.06	0.55
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.22	0.55
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.37	0.55
1:A:277:ARG:CD	1:A:334:GLN:HB3	2.36	0.55
2:B:419:THR:O	2:B:420:PRO:C	2.42	0.55
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.41	0.55
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.41	0.55
1:A:434:ILE:N	1:A:494:ASN:HD21	2.04	0.55
2:B:246:LEU:N	2:B:246:LEU:HD23	2.22	0.55
2:B:301:LEU:O	2:B:305:GLU:HB3	2.07	0.55
2:B:308:GLU:C	2:B:310:LEU:N	2.59	0.55
1:A:19:PRO:O	1:A:57:ASN:N	2.40	0.55
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.06	0.55
1:A:369:THR:CG2	1:A:398:TRP:HH2	2.19	0.55
1:A:29:GLU:O	1:A:32:LYS:HE2	2.07	0.54
2:B:328:GLU:HB3	4:B:1149:HOH:O	2.06	0.54
2:B:78:ARG:HD3	2:B:411:ILE:O	2.07	0.54
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.37	0.54
1:A:242:GLN:O	1:A:243:PRO:C	2.46	0.54
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.08	0.54
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.42	0.54
2:B:2:ILE:O	2:B:2:ILE:HG23	2.06	0.54
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.36	0.54
1:A:82:LYS:HG2	1:A:82:LYS:O	2.08	0.54
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.40	0.54
2:B:296:THR:H	2:B:299:ALA:HB3	1.73	0.54
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.42	0.54
1:A:182:GLN:HA	1:A:187:LEU:HA	1.89	0.54
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.43	0.54
1:A:287:LYS:HG2	1:A:288:ALA:N	2.21	0.54
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.38	0.54
2:B:73:LYS:HE2	2:B:75:VAL:HG22	1.90	0.54
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.38	0.54
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.43	0.54
2:B:125:ARG:O	2:B:127:TYR:N	2.40	0.54
1:A:215:THR:HG22	1:A:216:THR:N	2.23	0.54
1:A:315:HIS:CE1	1:A:347:LYS:CD	2.90	0.53
1:A:139:THR:HB	1:A:140:PRO:CD	2.37	0.53
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.70	0.53
1:A:90:VAL:CG1	1:A:91:GLN:HG3	2.33	0.53
2:B:136:ASN:O	2:B:137:ASN:HB2	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:SER:H	2:B:157:PRO:HD2	1.72	0.53
1:A:257:ILE:CG2	1:A:283:LEU:HD13	2.38	0.53
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.09	0.53
2:B:276:VAL:O	2:B:279:LEU:N	2.40	0.53
2:B:330:GLN:NE2	2:B:330:GLN:H	2.06	0.53
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.53
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.08	0.53
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.23	0.53
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.39	0.53
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.53
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.39	0.53
2:B:340:GLN:CD	2:B:340:GLN:N	2.62	0.53
1:A:304:ALA:O	1:A:307:ARG:N	2.33	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.71	0.53
1:A:276:VAL:O	1:A:276:VAL:HG12	2.07	0.53
1:A:28:GLU:HB3	1:A:135:ILE:CD1	2.37	0.53
1:A:54:ASN:N	1:A:55:PRO:HD3	2.24	0.53
1:A:117:SER:CB	1:A:214:LEU:HD23	2.39	0.53
1:A:54:ASN:O	1:A:55:PRO:C	2.46	0.52
1:A:507:GLN:C	1:A:509:GLN:H	2.11	0.52
1:A:50:ILE:CG1	1:A:51:GLY:N	2.71	0.52
1:A:297:GLU:HB2	1:A:298:GLU:OE2	2.10	0.52
1:A:81:ASN:C	1:A:83:ARG:N	2.63	0.52
2:B:220:LYS:HD2	2:B:231:GLY:N	2.25	0.52
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.52
2:B:91:GLN:O	2:B:92:LEU:HD23	2.10	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
2:B:11:LYS:HG2	2:B:12:LEU:O	2.10	0.52
2:B:120:LEU:O	2:B:121:ASP:C	2.48	0.52
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.45	0.52
2:B:191:SER:OG	2:B:198:HIS:ND1	2.24	0.52
1:A:27:THR:O	1:A:28:GLU:C	2.48	0.52
1:A:50:ILE:HG13	1:A:51:GLY:H	1.75	0.52
2:B:406:TRP:NE1	2:B:408:ALA:HB3	2.25	0.52
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.52
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.52
1:A:19:PRO:O	1:A:56:TYR:HB3	2.10	0.52
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.74	0.52
1:A:240:THR:HG23	1:A:241:VAL:N	2.24	0.52
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.92	0.52
2:B:194:GLU:O	2:B:195:ILE:C	2.49	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:ND2	1:A:461:LYS:H	2.08	0.51
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.40	0.51
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.92	0.51
2:B:57:ASN:HA	2:B:129:ALA:O	2.11	0.51
1:A:356:ARG:HD2	1:A:358:ARG:HG3	1.91	0.51
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.45	0.51
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.92	0.51
2:B:184:MET:HE3	4:B:1037:HOH:O	2.08	0.51
1:A:509:GLN:N	1:A:510:PRO:CD	2.73	0.51
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.91	0.51
1:A:188:TYR:CD2	3:A:701:ADB:H5	2.45	0.51
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.45	0.51
1:A:407:GLN:OE1	2:B:394:GLN:N	2.44	0.51
1:A:420:PRO:HA	1:A:421:PRO:O	2.09	0.51
2:B:221:HIS:CD2	2:B:221:HIS:N	2.79	0.51
2:B:225:PRO:C	2:B:227:PHE:H	2.14	0.51
1:A:112:GLY:C	1:A:114:ALA:H	2.14	0.51
2:B:394:GLN:O	2:B:395:LYS:C	2.48	0.51
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.90	0.51
1:A:402:TRP:CE3	1:A:402:TRP:C	2.84	0.51
2:B:242:GLN:HB2	2:B:243:PRO:HD2	1.93	0.51
1:A:287:LYS:HE2	1:A:291:GLU:OE1	2.11	0.51
1:A:229:TRP:O	1:A:232:TYR:N	2.40	0.51
2:B:249:LYS:HD2	2:B:252:TRP:HZ3	1.73	0.51
2:B:296:THR:H	2:B:299:ALA:CB	2.24	0.51
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.45	0.51
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.92	0.51
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.31	0.51
2:B:330:GLN:HE21	2:B:338:THR:C	2.14	0.51
1:A:102:LYS:O	1:A:103:LYS:HD3	2.11	0.50
1:A:424:LYS:HD3	1:A:425:LEU:H	1.73	0.50
2:B:306:ASN:C	2:B:308:GLU:N	2.64	0.50
2:B:363:ASN:HD22	2:B:364:ASP:N	2.08	0.50
1:A:288:ALA:HB2	1:A:291:GLU:HB2	1.89	0.50
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.47	0.50
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.93	0.50
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.77	0.50
2:B:65:LYS:CA	2:B:72:ARG:HG3	2.31	0.50
1:A:3:SER:CB	1:A:4:PRO:HD2	2.41	0.50
1:A:168:LEU:O	1:A:169:GLU:C	2.48	0.50
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.40	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG22	1:A:76:ASP:O	2.12	0.50
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.94	0.50
2:B:193:LEU:HD12	2:B:198:HIS:N	2.27	0.50
1:A:501:TYR:C	1:A:505:ILE:HD12	2.32	0.50
2:B:171:PHE:CB	4:B:1153:HOH:O	2.60	0.50
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.42	0.50
2:B:276:VAL:O	2:B:280:SER:N	2.33	0.50
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.93	0.50
1:A:507:GLN:C	1:A:509:GLN:N	2.65	0.50
2:B:85:GLN:CG	2:B:154:LYS:HB2	2.41	0.50
2:B:195:ILE:HD13	2:B:199:ARG:NH2	2.27	0.50
1:A:17:ASP:O	1:A:83:ARG:CD	2.59	0.50
1:A:277:ARG:HH22	1:A:514:GLU:HG3	1.76	0.50
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.46	0.49
2:B:340:GLN:OE1	2:B:340:GLN:N	2.45	0.49
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.94	0.49
1:A:162:SER:HB2	2:B:52:PRO:CG	2.42	0.49
2:B:411:ILE:HG22	2:B:412:PRO:O	2.12	0.49
2:B:326:ILE:CG2	2:B:342:TYR:CE1	2.94	0.49
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.77	0.49
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.76	0.49
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.47	0.49
1:A:500:GLN:O	1:A:501:TYR:C	2.50	0.49
2:B:27:THR:O	2:B:31:ILE:HD12	2.13	0.49
2:B:345:PRO:C	2:B:346:PHE:CD1	2.86	0.49
2:B:221:HIS:NE2	2:B:230:MET:CE	2.75	0.49
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.48	0.49
2:B:85:GLN:C	2:B:85:GLN:OE1	2.51	0.49
1:A:203:GLU:O	1:A:206:ARG:HB3	2.13	0.49
1:A:173:LYS:C	1:A:175:ASN:H	2.16	0.49
2:B:22:LYS:HD2	2:B:22:LYS:N	2.28	0.49
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.61	0.49
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.12	0.49
1:A:30:LYS:O	1:A:33:ALA:HB3	2.13	0.49
1:A:20:LYS:HA	1:A:57:ASN:H	1.77	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.49
1:A:215:THR:HG22	1:A:216:THR:H	1.77	0.49
2:B:393:ILE:HG23	2:B:393:ILE:O	2.13	0.49
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.12	0.49
1:A:8:VAL:O	1:A:121:ASP:HB2	2.13	0.48
2:B:135:ILE:O	2:B:138:GLU:HG3	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HE3	1:A:192:ASP:OD1	2.13	0.48
1:A:57:ASN:ND2	1:A:58:THR:H	2.10	0.48
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.26	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD22	1.95	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48
1:A:376:THR:HG23	1:A:386:THR:CG2	2.41	0.48
1:A:499:SER:OG	1:A:502:ALA:HB3	2.13	0.48
2:B:88:TRP:CB	4:B:1089:HOH:O	2.61	0.48
1:A:182:GLN:NE2	1:A:182:GLN:H	2.10	0.48
2:B:42:GLU:OE1	2:B:49:LYS:HE3	2.13	0.48
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.44	0.48
2:B:314:VAL:CG2	2:B:315:HIS:N	2.77	0.48
2:B:246:LEU:HD12	2:B:303:LEU:HD11	1.96	0.48
1:A:22:LYS:HG2	1:A:24:TRP:HZ2	1.70	0.48
2:B:12:LEU:H	2:B:12:LEU:HD12	1.77	0.48
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.95	0.48
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.48
1:A:286:THR:O	1:A:286:THR:CG2	2.59	0.48
1:A:34:LEU:HB2	1:A:132:ILE:HD12	1.96	0.48
2:B:246:LEU:HD12	2:B:303:LEU:CD1	2.44	0.48
1:A:441:TYR:CD2	1:A:542:ILE:HD12	2.48	0.48
1:A:135:ILE:HG13	1:A:135:ILE:O	2.12	0.48
1:A:540:LYS:O	1:A:541:GLY:O	2.30	0.48
1:A:9:PRO:HG2	1:A:9:PRO:O	2.14	0.48
1:A:285:GLY:HA3	1:A:287:LYS:NZ	2.28	0.48
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.77	0.48
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.40	0.48
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.47	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.75	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.48
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.77	0.48
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.44	0.48
1:A:13:LYS:HD2	1:A:16:MET:CE	2.43	0.48
1:A:354:TYR:HA	4:A:1141:HOH:O	2.13	0.48
2:B:195:ILE:CG2	2:B:196:GLY:N	2.77	0.47
2:B:30:LYS:HD3	2:B:71:TRP:CH2	2.49	0.47
1:A:58:THR:HG22	1:A:59:PRO:CD	2.40	0.47
2:B:27:THR:HG23	4:B:1003:HOH:O	2.12	0.47
1:A:53:GLU:N	1:A:55:PRO:HD3	2.29	0.47
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.65	0.47
2:B:76:ASP:OD2	2:B:78:ARG:NH2	2.38	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.45	0.47
1:A:522:ILE:O	1:A:525:LEU:HB2	2.14	0.47
1:A:240:THR:HG23	1:A:241:VAL:O	2.14	0.47
1:A:20:LYS:HG2	1:A:56:TYR:HA	1.96	0.47
1:A:223:LYS:CD	1:A:223:LYS:H	2.27	0.47
2:B:198:HIS:O	2:B:199:ARG:C	2.52	0.47
2:B:161:GLN:O	2:B:162:SER:C	2.53	0.47
2:B:344:GLU:O	2:B:345:PRO:C	2.52	0.47
1:A:64:LYS:CE	1:A:68:SER:CB	2.91	0.47
1:A:56:TYR:HD1	1:A:56:TYR:H	1.58	0.47
2:B:298:GLU:O	2:B:301:LEU:CB	2.62	0.47
2:B:23:GLN:O	2:B:23:GLN:HG3	2.15	0.47
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.79	0.47
1:A:182:GLN:CD	1:A:182:GLN:H	2.18	0.47
2:B:232:TYR:HE1	2:B:234:LEU:HD21	1.80	0.47
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.44	0.47
2:B:419:THR:O	2:B:421:PRO:N	2.48	0.47
2:B:346:PHE:CD1	2:B:346:PHE:N	2.82	0.47
1:A:301:LEU:HD12	1:A:301:LEU:C	2.35	0.47
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.97	0.46
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.33	0.46
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.97	0.46
1:A:278:GLN:HG2	1:A:302:GLU:OE2	2.15	0.46
2:B:305:GLU:O	2:B:308:GLU:HB3	2.16	0.46
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.66	0.46
2:B:206:ARG:NH1	2:B:216:THR:HG1	2.12	0.46
1:A:279:LEU:HD23	1:A:299:ALA:CB	2.34	0.46
2:B:85:GLN:HB2	2:B:154:LYS:HB2	1.95	0.46
2:B:375:ILE:HB	2:B:389:PHE:HZ	1.80	0.46
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.46
1:A:173:LYS:O	1:A:175:ASN:N	2.48	0.46
2:B:11:LYS:NZ	2:B:14:PRO:HG3	2.31	0.46
1:A:24:TRP:N	1:A:25:PRO:CD	2.79	0.46
2:B:2:ILE:O	2:B:3:SER:C	2.54	0.46
1:A:53:GLU:C	1:A:55:PRO:CD	2.80	0.46
1:A:308:GLU:O	1:A:312:GLU:OE1	2.33	0.46
2:B:277:ARG:HA	2:B:280:SER:OG	2.16	0.46
1:A:402:TRP:HE3	1:A:402:TRP:C	2.19	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
2:B:411:ILE:O	2:B:412:PRO:O	2.34	0.46
3:A:701:ADB:N1	3:A:701:ADB:H16	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD21	2:B:310:LEU:HD13	1.98	0.46
1:A:540:LYS:HG3	1:A:541:GLY:N	2.31	0.46
1:A:329:ILE:HA	1:A:338:THR:O	2.16	0.46
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.97	0.46
2:B:222:GLN:CG	2:B:223:LYS:H	2.29	0.46
1:A:331:LYS:HZ3	1:A:333:GLY:HA2	1.80	0.46
1:A:3:SER:HB3	1:A:212:TRP:O	2.15	0.46
2:B:169:GLU:N	2:B:170:PRO:HD2	2.30	0.46
1:A:170:PRO:HG2	1:A:171:PHE:H	1.80	0.46
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.46
2:B:115:TYR:O	2:B:117:SER:N	2.49	0.46
1:A:13:LYS:HD2	1:A:16:MET:HE1	1.96	0.46
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.82	0.46
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.19	0.45
1:A:288:ALA:HB1	1:A:291:GLU:H	1.81	0.45
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.49	0.45
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.80	0.45
1:A:394:GLN:O	1:A:395:LYS:C	2.53	0.45
1:A:497:THR:CG2	1:A:498:ASP:H	2.27	0.45
1:A:429:LEU:HD11	1:A:506:ILE:HG23	1.98	0.45
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.81	0.45
2:B:319:TYR:O	2:B:321:PRO:HD3	2.17	0.45
1:A:426:TRP:O	1:A:427:TYR:HB3	2.16	0.45
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.29	0.45
1:A:120:LEU:O	1:A:122:GLU:N	2.49	0.45
1:A:356:ARG:HG2	1:A:367:GLN:HG3	1.98	0.45
1:A:104:LYS:CE	1:A:192:ASP:OD1	2.64	0.45
2:B:139:THR:HG23	2:B:140:PRO:CD	2.44	0.45
1:A:504:GLY:O	1:A:505:ILE:C	2.54	0.45
1:A:418:ASN:C	1:A:419:THR:HG22	2.37	0.45
1:A:53:GLU:H	1:A:55:PRO:HD3	1.80	0.45
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.99	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
1:A:398:TRP:O	1:A:400:THR:N	2.49	0.45
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.84	0.45
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.52	0.45
2:B:202:ILE:O	2:B:205:LEU:N	2.50	0.45
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.51	0.45
1:A:136:ASN:C	1:A:138:GLU:H	2.17	0.45
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.69	0.45
2:B:46:LYS:HD3	2:B:116:PHE:CE1	2.52	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:O	2:B:201:LYS:N	2.50	0.45
2:B:324:ASP:O	2:B:343:GLN:HG2	2.17	0.45
2:B:363:ASN:ND2	2:B:365:VAL:N	2.65	0.45
2:B:160:PHE:O	2:B:161:GLN:C	2.55	0.45
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.46	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.50	0.45
1:A:529:GLU:C	1:A:530:LYS:HG3	2.37	0.45
2:B:153:TRP:O	2:B:155:GLY:N	2.48	0.45
2:B:171:PHE:HB3	4:B:1153:HOH:O	2.15	0.44
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.16	0.44
2:B:274:ILE:HG22	2:B:275:LYS:N	2.32	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.47	0.44
2:B:205:LEU:O	2:B:206:ARG:C	2.54	0.44
1:A:102:LYS:HG2	1:A:104:LYS:HZ3	1.83	0.44
2:B:267:ALA:O	2:B:269:GLN:N	2.51	0.44
2:B:345:PRO:C	2:B:346:PHE:HD1	2.20	0.44
2:B:257:ILE:HD11	2:B:279:LEU:O	2.18	0.44
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.44
2:B:339:TYR:CG	2:B:375:ILE:HD13	2.52	0.44
1:A:369:THR:HG23	1:A:398:TRP:CH2	2.53	0.44
1:A:126:LYS:HB3	1:A:126:LYS:HE2	1.69	0.44
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.99	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:181:TYR:CD2	1:A:181:TYR:C	2.90	0.44
1:A:60:VAL:HG22	1:A:130:PHE:HB2	2.00	0.44
1:A:412:PRO:O	1:A:414:TRP:HD1	2.01	0.44
2:B:163:SER:O	2:B:167:ILE:HG13	2.17	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.66	0.44
1:A:253:THR:O	1:A:256:ASP:HB2	2.18	0.44
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.18	0.44
1:A:435:VAL:HA	2:B:290:THR:OG1	2.18	0.44
2:B:220:LYS:HD2	2:B:230:MET:C	2.38	0.44
1:A:504:GLY:O	1:A:507:GLN:N	2.50	0.44
1:A:37:ILE:O	1:A:41:MET:HB2	2.18	0.44
2:B:139:THR:HG22	2:B:140:PRO:O	2.17	0.44
1:A:411:ILE:HG13	1:A:412:PRO:HD2	2.00	0.44
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.99	0.44
1:A:80:LEU:O	1:A:84:THR:HG23	2.17	0.44
1:A:231:GLY:O	1:A:242:GLN:HG2	2.18	0.44
1:A:354:TYR:CZ	1:A:370:GLU:HB3	2.53	0.44
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.87	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:CE	1:A:104:LYS:N	2.75	0.44
2:B:104:LYS:O	2:B:105:SER:OG	2.34	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.44
2:B:40:GLU:O	2:B:41:MET:C	2.54	0.44
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.61	0.44
2:B:109:LEU:HA	2:B:218:ASP:OD2	2.18	0.44
1:A:320:ASP:OD2	1:A:322:SER:OG	2.36	0.44
2:B:259:LYS:O	2:B:262:GLY:N	2.50	0.44
1:A:235:HIS:HB2	1:A:238:LYS:HG2	2.00	0.43
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.95	0.43
1:A:51:GLY:O	1:A:53:GLU:N	2.51	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.80	0.43
1:A:397:THR:O	1:A:398:TRP:C	2.56	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.18	0.43
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.43
2:B:27:THR:HG21	2:B:29:GLU:HB3	1.99	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE2	2.18	0.43
1:A:30:LYS:O	1:A:31:ILE:C	2.56	0.43
2:B:411:ILE:C	2:B:412:PRO:O	2.56	0.43
1:A:241:VAL:HG12	1:A:242:GLN:N	2.33	0.43
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.00	0.43
2:B:30:LYS:HD2	2:B:62:ALA:HB3	2.01	0.43
1:A:57:ASN:ND2	1:A:58:THR:N	2.66	0.43
2:B:375:ILE:HD12	2:B:389:PHE:HE2	1.82	0.43
2:B:195:ILE:O	2:B:198:HIS:HB3	2.19	0.43
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.34	0.43
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.49	0.43
2:B:27:THR:HB	2:B:30:LYS:CG	2.49	0.43
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.99	0.43
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.53	0.43
1:A:342:TYR:HA	1:A:349:LEU:HB2	2.01	0.43
2:B:46:LYS:HZ3	2:B:116:PHE:HD1	1.66	0.43
2:B:13:LYS:O	2:B:16:MET:CB	2.64	0.43
1:A:331:LYS:HZ1	1:A:333:GLY:HA2	1.81	0.43
2:B:342:TYR:HD1	2:B:342:TYR:C	2.21	0.43
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.79	0.43
2:B:303:LEU:HD22	4:B:1143:HOH:O	2.19	0.43
2:B:308:GLU:O	2:B:310:LEU:N	2.51	0.43
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.30	0.43
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.33	0.43
2:B:366:LYS:HZ2	2:B:366:LYS:HB3	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:HG12	2:B:199:ARG:HG3	2.01	0.43
1:A:531:VAL:HG12	1:A:532:TYR:N	2.33	0.43
2:B:257:ILE:HG23	2:B:258:GLN:N	2.33	0.43
2:B:278:GLN:CA	2:B:281:LYS:HE3	2.22	0.43
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.01	0.43
2:B:283:LEU:O	2:B:285:GLY:N	2.51	0.43
2:B:283:LEU:C	2:B:285:GLY:N	2.72	0.43
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.36	0.43
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.49	0.43
1:A:30:LYS:HA	1:A:33:ALA:CB	2.49	0.43
1:A:128:THR:HB	1:A:146:TYR:HB2	2.01	0.42
1:A:257:ILE:HG21	1:A:283:LEU:HD13	2.01	0.42
1:A:137:ASN:O	1:A:138:GLU:HB3	2.18	0.42
1:A:491:LEU:HB3	1:A:529:GLU:HB2	2.00	0.42
2:B:329:ILE:N	4:B:1149:HOH:O	2.51	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.70	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.19	0.42
2:B:27:THR:O	2:B:28:GLU:C	2.56	0.42
2:B:30:LYS:O	2:B:31:ILE:C	2.57	0.42
1:A:64:LYS:HD3	1:A:71:TRP:CH2	2.54	0.42
1:A:424:LYS:CD	1:A:425:LEU:N	2.79	0.42
2:B:168:LEU:C	2:B:170:PRO:HD2	2.40	0.42
1:A:294:PRO:O	1:A:296:THR:N	2.53	0.42
2:B:90:VAL:O	2:B:91:GLN:C	2.57	0.42
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.54	0.42
2:B:236:PRO:HA	2:B:239:TRP:CG	2.53	0.42
1:A:195:ILE:O	1:A:199:ARG:HG3	2.19	0.42
1:A:427:TYR:CD1	1:A:427:TYR:C	2.93	0.42
1:A:457:TYR:CD2	1:A:457:TYR:C	2.93	0.42
1:A:183:TYR:C	1:A:184:MET:CG	2.82	0.42
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.54	0.42
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.54	0.42
2:B:13:LYS:HG2	2:B:14:PRO:O	2.20	0.42
2:B:314:VAL:HG22	2:B:315:HIS:N	2.34	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.55	0.42
2:B:40:GLU:O	2:B:43:LYS:N	2.52	0.42
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.49	0.42
1:A:470:THR:O	1:A:471:ASN:CB	2.67	0.42
2:B:195:ILE:HG23	2:B:196:GLY:H	1.81	0.42
1:A:19:PRO:HG2	1:A:80:LEU:HB2	2.01	0.42
2:B:222:GLN:CG	2:B:223:LYS:N	2.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:O	1:A:295:LEU:C	2.57	0.42
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.35	0.42
1:A:341:ILE:O	1:A:349:LEU:HB3	2.20	0.42
2:B:280:SER:O	2:B:281:LYS:C	2.58	0.42
2:B:302:GLU:O	2:B:306:ASN:HB2	2.19	0.42
1:A:542:ILE:HD13	1:A:544:GLY:CA	2.50	0.42
1:A:97:PRO:CG	1:A:232:TYR:CE2	2.99	0.42
1:A:59:PRO:O	1:A:75:VAL:HA	2.20	0.42
1:A:5:ILE:HD11	1:A:167:ILE:HD11	2.01	0.42
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.50	0.42
2:B:327:ALA:HA	4:B:1124:HOH:O	2.20	0.42
2:B:257:ILE:HD12	2:B:282:LEU:HD23	2.01	0.42
2:B:361:HIS:N	2:B:361:HIS:ND1	2.68	0.42
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.50	0.42
2:B:58:THR:N	4:B:1111:HOH:O	2.53	0.42
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.55	0.42
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.20	0.41
1:A:22:LYS:HB3	1:A:24:TRP:CE2	2.55	0.41
2:B:406:TRP:CE2	2:B:408:ALA:HB3	2.55	0.41
1:A:224:GLU:CB	1:A:225:PRO:CD	2.78	0.41
1:A:257:ILE:HD11	1:A:282:LEU:HB2	2.02	0.41
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.50	0.41
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.03	0.41
2:B:356:ARG:HB2	2:B:367:GLN:HG2	2.01	0.41
1:A:328:GLU:O	1:A:339:TYR:HA	2.20	0.41
1:A:434:ILE:O	1:A:437:ALA:HB3	2.21	0.41
2:B:46:LYS:CD	2:B:116:PHE:CD1	3.01	0.41
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.56	0.41
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.34	0.41
1:A:276:VAL:HG12	1:A:280:SER:OG	2.19	0.41
1:A:198:HIS:O	1:A:202:ILE:HG12	2.20	0.41
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.78	0.41
2:B:254:VAL:O	2:B:257:ILE:HG23	2.20	0.41
2:B:419:THR:H	2:B:420:PRO:CD	2.33	0.41
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.79	0.41
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.55	0.41
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.85	0.41
2:B:46:LYS:CD	2:B:116:PHE:HD1	2.33	0.41
1:A:211:ARG:NH1	1:A:211:ARG:HG3	2.35	0.41
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.85	0.41
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:O	2:B:196:GLY:C	2.59	0.41
2:B:84:THR:O	2:B:85:GLN:C	2.59	0.41
2:B:88:TRP:HB2	4:B:1089:HOH:O	2.20	0.41
1:A:59:PRO:HD2	1:A:76:ASP:O	2.21	0.41
1:A:11:LYS:HB2	1:A:85:GLN:OE1	2.21	0.41
1:A:369:THR:HG1	1:A:398:TRP:HH2	1.60	0.41
1:A:398:TRP:O	1:A:399:GLU:C	2.59	0.41
1:A:195:ILE:HG23	1:A:196:GLY:N	2.34	0.41
2:B:56:TYR:O	2:B:57:ASN:HB2	2.21	0.41
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.35	0.41
2:B:298:GLU:CA	2:B:301:LEU:HB2	2.51	0.41
1:A:542:ILE:CG1	1:A:543:GLY:N	2.79	0.41
1:A:104:LYS:CG	1:A:192:ASP:HA	2.42	0.41
1:A:275:LYS:NZ	1:A:332:GLN:HE21	2.18	0.41
1:A:470:THR:O	1:A:471:ASN:HB3	2.20	0.41
2:B:277:ARG:CD	2:B:277:ARG:N	2.70	0.41
1:A:410:TRP:HA	1:A:410:TRP:HE3	1.85	0.41
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.56	0.41
1:A:102:LYS:HG2	1:A:104:LYS:HZ1	1.84	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB2	2.03	0.41
1:A:108:VAL:CG2	1:A:108:VAL:O	2.68	0.41
1:A:215:THR:O	1:A:216:THR:HG22	2.21	0.41
1:A:3:SER:HB2	1:A:5:ILE:HG13	2.03	0.41
1:A:178:ILE:HG13	1:A:178:ILE:H	1.62	0.41
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.55	0.41
1:A:417:VAL:CG1	1:A:419:THR:CG2	3.00	0.40
1:A:298:GLU:O	1:A:299:ALA:C	2.59	0.40
2:B:224:GLU:HA	2:B:225:PRO:HD3	1.67	0.40
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.56	0.40
1:A:281:LYS:HE3	4:A:1074:HOH:O	2.19	0.40
2:B:220:LYS:HD3	2:B:229:TRP:O	2.21	0.40
1:A:382:ILE:HG22	1:A:383:TRP:CD1	2.57	0.40
2:B:164:MET:O	2:B:165:THR:C	2.58	0.40
1:A:131:THR:CG2	1:A:131:THR:O	2.70	0.40
1:A:474:ASN:C	1:A:478:GLU:HG3	2.40	0.40
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.40
2:B:382:ILE:O	2:B:382:ILE:CG2	2.67	0.40
2:B:249:LYS:HB2	2:B:252:TRP:CH2	2.56	0.40
1:A:411:ILE:HG23	1:A:411:ILE:O	2.22	0.40
1:A:132:ILE:CG2	1:A:142:ILE:O	2.69	0.40
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.51	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:O	1:A:263:LYS:HG3	2.22	0.40
1:A:235:HIS:CB	1:A:238:LYS:HG2	2.52	0.40
2:B:46:LYS:NZ	2:B:116:PHE:HD1	2.19	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	550/560 (98%)	429 (78%)	84 (15%)	37 (7%)	1	1
2	B	425/430 (99%)	327 (77%)	68 (16%)	30 (7%)	1	1
All	All	975/990 (98%)	756 (78%)	152 (16%)	67 (7%)	1	1

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	28	GLU
1	A	54	ASN
1	A	122	GLU
1	A	135	ILE
1	A	137	ASN
1	A	153	TRP
1	A	195	ILE
1	A	412	PRO
1	A	538	ALA
1	A	539	HIS
1	A	541	GLY
2	B	7	THR
2	B	77	PHE
2	B	85	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	116	PHE
2	B	218	ASP
2	B	295	LEU
2	B	360	ALA
2	B	419	THR
1	A	16	MET
1	A	82	LYS
1	A	89	GLU
1	A	121	ASP
1	A	174	GLN
1	A	224	GLU
1	A	276	VAL
1	A	398	TRP
1	A	505	ILE
1	A	516	GLU
2	B	126	LYS
2	B	154	LYS
2	B	220	LYS
2	B	288	ALA
2	B	297	GLU
2	B	307	ARG
2	B	421	PRO
1	A	52	PRO
1	A	213	GLY
1	A	254	VAL
2	B	68	SER
2	B	223	LYS
2	B	232	TYR
2	B	268	SER
1	A	23	GLN
1	A	98	ALA
1	A	162	SER
1	A	237	ASP
1	A	397	THR
1	A	501	TYR
1	A	542	ILE
2	B	18	GLY
2	B	231	GLY
2	B	284	ARG
2	B	345	PRO
1	A	399	GLU
2	B	65	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	91	GLN
2	B	198	HIS
2	B	359	GLY
1	A	69	THR
2	B	420	PRO
1	A	504	GLY
2	B	313	PRO
1	A	169	GLU
2	B	3	SER
1	A	24	TRP

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/500 (99%)	448 (91%)	46 (9%)	11	21
2	B	389/392 (99%)	350 (90%)	39 (10%)	9	18
All	All	883/892 (99%)	798 (90%)	85 (10%)	10	20

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	22	LYS
1	A	28	GLU
1	A	32	LYS
1	A	40	GLU
1	A	56	TYR
1	A	58	THR
1	A	67	ASP
1	A	71	TRP
1	A	91	GLN
1	A	128	THR
1	A	131	THR
1	A	135	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	161	GLN
1	A	184	MET
1	A	188	TYR
1	A	201	LYS
1	A	217	PRO
1	A	220	LYS
1	A	223	LYS
1	A	228	LEU
1	A	274	ILE
1	A	287	LYS
1	A	296	THR
1	A	300	GLU
1	A	317	VAL
1	A	330	GLN
1	A	347	LYS
1	A	349	LEU
1	A	356	ARG
1	A	358	ARG
1	A	364	ASP
1	A	369	THR
1	A	386	THR
1	A	391	LEU
1	A	394	GLN
1	A	402	TRP
1	A	407	GLN
1	A	410	TRP
1	A	419	THR
1	A	450	THR
1	A	460	ASN
1	A	465	LYS
1	A	506	ILE
1	A	511	ASP
1	A	542	ILE
2	B	1	PRO
2	B	7	THR
2	B	16	MET
2	B	22	LYS
2	B	36	GLU
2	B	67	ASP
2	B	69	THR
2	B	91	GLN
2	B	109	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	113	ASP
2	B	163	SER
2	B	165	THR
2	B	169	GLU
2	B	170	PRO
2	B	177	ASP
2	B	187	LEU
2	B	193	LEU
2	B	194	GLU
2	B	206	ARG
2	B	221	HIS
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	246	LEU
2	B	277	ARG
2	B	279	LEU
2	B	293	ILE
2	B	301	LEU
2	B	305	GLU
2	B	314	VAL
2	B	317	VAL
2	B	338	THR
2	B	363	ASN
2	B	372	VAL
2	B	374	LYS
2	B	399	GLU
2	B	403	THR
2	B	418	ASN
2	B	419	THR

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	235	HIS
1	A	269	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	332	GLN
1	A	361	HIS
1	A	367	GLN
1	A	460	ASN
1	A	474	ASN
1	A	475	GLN
1	A	494	ASN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
2	B	174	GLN
2	B	207	GLN
2	B	255	ASN
2	B	258	GLN
2	B	265	ASN
2	B	315	HIS
2	B	330	GLN
2	B	340	GLN
2	B	363	ASN
2	B	394	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADB	A	701	-	27,27,27	1.84	7 (25%)	37,37,37	2.65	11 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADB	A	701	-	-	0/10/10/10	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ADB	C4-C5	2.20	1.43	1.38
3	A	701	ADB	C1-C6	2.25	1.45	1.40
3	A	701	ADB	C1-C2	2.30	1.45	1.40
3	A	701	ADB	C13-C12	2.59	1.43	1.38
3	A	701	ADB	C16-C15	2.83	1.43	1.38
3	A	701	ADB	C10-N4	3.55	1.41	1.34
3	A	701	ADB	C16-C11	4.36	1.46	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	ADB	N2-C9-N1	-5.03	118.48	126.22
3	A	701	ADB	N3-C8-N1	-4.51	121.37	127.82
3	A	701	ADB	N3-C10-N2	-3.50	119.80	125.53
3	A	701	ADB	N4-C10-N2	2.03	120.57	117.20
3	A	701	ADB	N5-C9-N1	2.16	123.47	116.91
3	A	701	ADB	C1-C2-CL2	2.86	121.94	118.43
3	A	701	ADB	C1-C6-CL6	3.02	122.14	118.43
3	A	701	ADB	C8-N3-C10	3.41	118.61	113.08
3	A	701	ADB	C8-O7-C1	4.20	124.56	117.01
3	A	701	ADB	C10-N2-C9	5.19	121.14	113.57
3	A	701	ADB	C8-N1-C9	10.19	120.49	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ADB	4	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	545/560 (97%)	0.02	20 (3%) 45 37	25, 74, 99, 105	19 (3%)
2	B	427/430 (99%)	0.16	36 (8%) 14 9	17, 61, 101, 106	14 (3%)
All	All	972/990 (98%)	0.08	56 (5%) 26 20	17, 71, 100, 106	33 (3%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	6.6
2	B	1	PRO	5.8
2	B	225	PRO	5.6
2	B	2	ILE	5.3
2	B	4	PRO	5.2
2	B	230	MET	5.2
2	B	231	GLY	5.0
1	A	221	HIS	4.8
1	A	141	GLY	4.5
2	B	358	ARG	4.5
2	B	304	ALA	4.4
2	B	359	GLY	4.3
2	B	222	GLN	3.8
2	B	245	VAL	3.6
2	B	279	LEU	3.6
2	B	299	ALA	3.6
2	B	226	PRO	3.5
2	B	3	SER	3.5
1	A	74	LEU	3.4
2	B	218	ASP	3.4
1	A	132	ILE	3.2
2	B	5	ILE	3.2
2	B	301	LEU	3.1
1	A	140	PRO	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	223	LYS	3.0
1	A	135	ILE	3.0
1	A	1	PRO	3.0
1	A	21	VAL	2.9
2	B	296	THR	2.8
2	B	310	LEU	2.8
2	B	357	MET	2.7
1	A	78	ARG	2.7
1	A	219	LYS	2.7
2	B	250	ASP	2.5
1	A	65	LYS	2.5
1	A	253	THR	2.4
1	A	67	ASP	2.4
2	B	409	THR	2.3
2	B	227	PHE	2.3
1	A	545	ASN	2.3
2	B	224	GLU	2.2
2	B	298	GLU	2.2
2	B	241	VAL	2.2
2	B	232	TYR	2.2
1	A	252	TRP	2.2
2	B	303	LEU	2.2
2	B	356	ARG	2.2
1	A	137	ASN	2.1
1	A	247	PRO	2.1
2	B	294	PRO	2.1
2	B	69	THR	2.1
1	A	66	LYS	2.1
2	B	283	LEU	2.1
1	A	60	VAL	2.1
2	B	15	GLY	2.1
1	A	411	ILE	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](#)

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( $\text{\AA}^2$ )	Q<0.9
3	ADB	A	701	25/25	0.86	0.21	0.95	41,56,65,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.