



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:08 AM GMT

PDB ID : 3DJA  
Title : Crystal Structure of cpaf solved with MAD  
Authors : Chai, J.; Huang, Z.  
Deposited on : 2008-06-22  
Resolution : 2.90 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

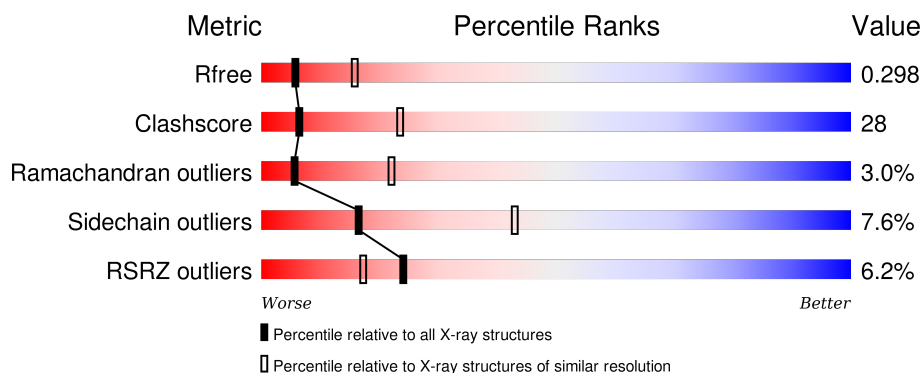
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	579	
1	B	579	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8290 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 Protein CT\_858.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	Se	0	0	0
			4145	2654	694	784	7	6			
1	B	527	Total	C	N	O	S	Se	0	0	0
			4145	2654	694	784	7	6			

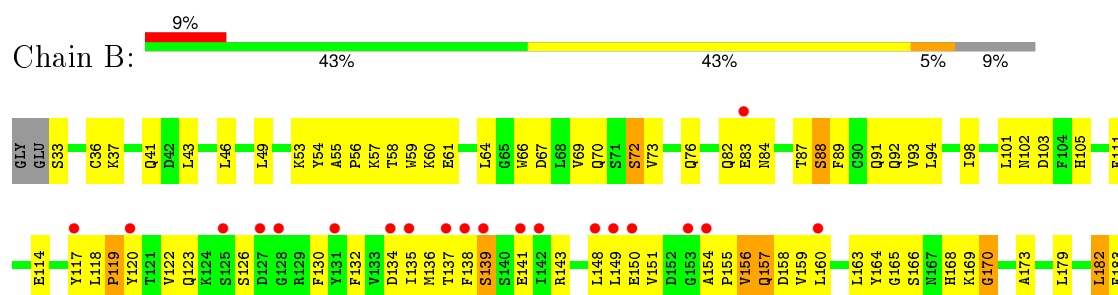
### 3 Residue-property plots

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: Protein CT\_858



#### • Molecule 1: Protein CT\_858





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.87Å 124.87Å 241.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 41.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.90) 100.0 (41.02-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.245 , 0.290 0.256 , 0.298	Depositor DCC
$R_{free}$ test set	2150 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43092 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.49	0/4237	0.72	0/5750
1	B	0.47	1/4237 (0.0%)	0.69	3/5750 (0.1%)
All	All	0.48	1/8474 (0.0%)	0.70	3/11500 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	MSE	CG-SE	-5.14	1.77	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	ASP	N-CA-C	-8.41	88.29	111.00
1	B	600	THR	N-CA-C	-8.27	88.67	111.00
1	B	328	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4145	0	4091	189	1
1	B	4145	0	4091	285	0
All	All	8290	0	8182	454	1

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 28.

All (454) 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:204:ARG:NH1	1:A:204:ARG:HB3	1.61	1.14
1:A:204:ARG:HH11	1:A:204:ARG:HB3	1.14	1.05
1:B:359:PHE:O	1:B:363:THR:HG22	1.64	0.97
1:B:516:ILE:H	1:B:565:HIS:HD2	1.08	0.95
1:B:297:ILE:HD11	1:B:313:SER:HB2	1.49	0.94
1:A:186:MSE:H	1:A:191:HIS:HD2	1.16	0.90
1:B:433:ASN:ND2	1:B:436:GLY:H	1.70	0.89
1:B:433:ASN:HD22	1:B:436:GLY:H	1.18	0.87
1:B:149:LEU:HD11	1:B:203:ARG:HB2	1.56	0.87
1:B:186:MSE:H	1:B:191:HIS:HD2	1.18	0.87
1:A:151:VAL:HB	1:A:159:VAL:HG21	1.56	0.86
1:A:502:ASP:O	1:A:506:VAL:HG23	1.76	0.85
1:A:33:SER:O	1:A:37:LYS:HG3	1.77	0.85
1:B:238:LEU:HD13	1:B:239:GLN:H	1.41	0.85
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.12	0.84
1:A:432:ASP:HA	1:A:439:VAL:HB	1.60	0.83
1:B:427:ARG:HG2	1:B:432:ASP:HA	1.60	0.83
1:B:302:TRP:HB3	1:B:312:ILE:HG12	1.59	0.83
1:A:404:GLN:HG3	1:B:538:GLY:HA2	1.60	0.82
1:A:197:ARG:NH1	1:A:213:ARG:HE	1.76	0.82
1:A:366:LEU:HD13	1:A:368:ILE:HD11	1.62	0.82
1:B:143:ARG:HH22	1:B:204:ARG:HD2	1.44	0.82
1:A:516:ILE:H	1:A:565:HIS:HD2	1.26	0.81
1:B:516:ILE:H	1:B:565:HIS:CD2	1.97	0.81
1:A:493:ILE:HD11	1:A:564:PRO:HB3	1.62	0.81
1:A:192:LYS:HB2	1:A:192:LYS:NZ	1.95	0.81
1:A:367:ILE:HD11	1:A:591:VAL:HG21	1.61	0.80
1:B:567:ASP:OD1	1:B:569:PRO:HD3	1.81	0.80
1:B:297:ILE:HD11	1:B:313:SER:CB	2.11	0.79
1:B:509:LYS:HB2	1:B:516:ILE:HD12	1.64	0.79
1:B:120:TYR:HB2	1:B:183:PHE:CD1	2.18	0.79
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.63	0.79
1:B:186:MSE:H	1:B:191:HIS:CD2	2.01	0.78
1:A:366:LEU:HD22	1:A:368:ILE:HD12	1.65	0.77
1:B:297:ILE:HD12	1:B:311:TYR:HE1	1.49	0.77
1:A:186:MSE:H	1:A:191:HIS:CD2	2.01	0.77
1:B:59:TRP:HE1	1:B:559:ASN:HD22	1.33	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD21	1:B:182:LEU:HG	1.68	0.76
1:B:517:VAL:HG13	1:B:566:ILE:HB	1.67	0.76
1:B:367:ILE:HD13	1:B:490:CYS:HB3	1.68	0.75
1:A:534:PRO:HG2	1:B:49:LEU:HD22	1.68	0.75
1:B:82:GLN:HG3	1:B:89:PHE:CZ	2.22	0.75
1:A:404:GLN:H	1:A:404:GLN:NE2	1.85	0.75
1:A:515:LEU:HG	1:A:601:ILE:HD11	1.69	0.75
1:A:538:GLY:HA2	1:B:404:GLN:HG3	1.68	0.74
1:A:594:LEU:HD21	1:A:601:ILE:HD11	1.68	0.74
1:B:182:LEU:HD13	1:B:183:PHE:CE2	2.22	0.73
1:B:321:LYS:HE2	1:B:323:HIS:HE1	1.54	0.73
1:B:54:TYR:CZ	1:B:56:PRO:HG2	2.24	0.72
1:B:122:VAL:HG12	1:B:123:GLN:N	2.04	0.72
1:A:395:LEU:HD21	1:A:477:ILE:HD13	1.71	0.71
1:B:197:ARG:HG2	1:B:215:LYS:HB2	1.72	0.71
1:A:594:LEU:HD22	1:A:599:GLY:HA2	1.72	0.71
1:A:368:ILE:HD13	1:A:489:ILE:HG23	1.73	0.71
1:B:302:TRP:HB3	1:B:312:ILE:CG1	2.20	0.70
1:B:297:ILE:HD12	1:B:311:TYR:CE1	2.26	0.70
1:A:602:ILE:HG22	1:A:603:LEU:H	1.55	0.70
1:B:332:THR:HA	1:B:373:ASN:OD1	1.92	0.69
1:A:515:LEU:HG	1:A:601:ILE:CD1	2.22	0.69
1:B:568:LEU:HD13	1:B:583:TYR:CD1	2.27	0.69
1:B:352:PHE:HD2	1:B:387:MSE:HE3	1.57	0.69
1:A:404:GLN:CG	1:B:538:GLY:HA2	2.23	0.69
1:B:536:ARG:HG3	1:B:536:ARG:HH11	1.55	0.69
1:B:160:LEU:CD2	1:B:182:LEU:HG	2.23	0.68
1:B:238:LEU:HD13	1:B:239:GLN:N	2.09	0.68
1:B:535:ASN:HD21	1:B:539:ILE:HB	1.58	0.68
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.29	0.68
1:B:334:SER:O	1:B:336:GLN:N	2.27	0.68
1:A:204:ARG:HH11	1:A:204:ARG:CB	1.99	0.68
1:A:395:LEU:HD11	1:A:477:ILE:HD12	1.74	0.68
1:B:509:LYS:HB2	1:B:516:ILE:CD1	2.25	0.67
1:B:316:THR:HG22	1:B:322:SER:OG	1.94	0.67
1:B:516:ILE:N	1:B:565:HIS:HD2	1.88	0.67
1:B:155:PRO:HG2	1:B:158:ASP:OD2	1.95	0.66
1:A:123:GLN:HE21	1:A:133:VAL:HG11	1.60	0.66
1:B:591:VAL:O	1:B:595:ILE:HD12	1.95	0.66
1:A:470:PRO:HG2	1:A:473:GLY:HA2	1.76	0.66
1:B:284:GLY:N	1:B:289:SER:HG	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:CD1	1:B:311:TYR:HE1	2.09	0.64
1:A:516:ILE:H	1:A:565:HIS:CD2	2.12	0.64
1:B:114:GLU:HG2	1:B:193:VAL:HG21	1.79	0.64
1:A:67:ASP:HB3	1:A:70:GLN:HB2	1.79	0.64
1:A:103:ASP:HB3	1:A:106:ALA:HB3	1.80	0.64
1:B:499:SER:O	1:B:502:ASP:HB2	1.99	0.63
1:A:432:ASP:CA	1:A:439:VAL:HB	2.28	0.63
1:A:404:GLN:HG3	1:B:538:GLY:CA	2.30	0.62
1:A:204:ARG:NH1	1:A:205:PRO:HD2	2.15	0.62
1:B:151:VAL:HG13	1:B:200:LEU:HD23	1.80	0.62
1:A:499:SER:O	1:A:502:ASP:HB2	1.99	0.62
1:A:602:ILE:HG22	1:A:603:LEU:N	2.14	0.62
1:A:413:TRP:CZ3	1:A:447:LEU:HD13	2.34	0.62
1:B:120:TYR:HB2	1:B:183:PHE:HD1	1.62	0.62
1:B:591:VAL:O	1:B:594:LEU:HB2	2.00	0.62
1:B:335:TRP:HB2	1:B:348:PRO:CG	2.31	0.61
1:B:123:GLN:HE22	1:B:285:TYR:HE2	1.48	0.61
1:B:503:PHE:HA	1:B:506:VAL:HG12	1.82	0.61
1:B:543:SER:O	1:B:544:LEU:HD23	2.00	0.61
1:A:335:TRP:HB2	1:A:348:PRO:HG3	1.83	0.60
1:A:538:GLY:HA2	1:B:404:GLN:CG	2.31	0.60
1:B:33:SER:O	1:B:37:LYS:HG3	2.00	0.60
1:B:64:LEU:HD23	1:B:169:LYS:HD2	1.83	0.60
1:A:399:ARG:HD2	1:A:466:SER:O	2.01	0.60
1:A:427:ARG:HD3	1:A:432:ASP:HB2	1.83	0.60
1:A:82:GLN:HG3	1:A:89:PHE:CE2	2.37	0.60
1:B:330:ILE:HD11	1:B:352:PHE:CE1	2.37	0.59
1:A:53:LYS:HB3	1:A:529:PHE:HZ	1.67	0.59
1:B:297:ILE:HD13	1:B:298:GLY:N	2.18	0.59
1:B:535:ASN:ND2	1:B:539:ILE:HB	2.18	0.59
1:A:321:LYS:HE3	1:A:323:HIS:HE1	1.66	0.59
1:B:586:LYS:O	1:B:590:LEU:HG	2.01	0.59
1:B:392:PRO:HA	1:B:477:ILE:O	2.03	0.59
1:A:538:GLY:CA	1:B:404:GLN:HG3	2.32	0.59
1:A:321:LYS:HE3	1:A:323:HIS:CE1	2.38	0.59
1:B:143:ARG:HH22	1:B:204:ARG:CD	2.11	0.58
1:A:494:ASN:HD22	1:A:496:GLN:HB2	1.67	0.58
1:B:157:GLN:N	1:B:157:GLN:OE1	2.35	0.58
1:B:499:SER:OG	1:B:500:CYS:N	2.36	0.58
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.34	0.58
1:B:198:THR:N	1:B:214:VAL:O	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ASN:OD1	1:B:441:LEU:HB2	2.03	0.58
1:A:534:PRO:HG2	1:B:49:LEU:CD2	2.34	0.58
1:B:503:PHE:O	1:B:506:VAL:HG12	2.03	0.58
1:B:150:GLU:OE1	1:B:201:LYS:HD3	2.04	0.58
1:A:520:ARG:HA	1:A:562:VAL:O	2.04	0.58
1:B:122:VAL:CG1	1:B:123:GLN:N	2.67	0.58
1:A:204:ARG:CZ	1:A:204:ARG:HB3	2.32	0.58
1:B:156:VAL:O	1:B:159:VAL:HB	2.03	0.58
1:A:597:ASN:O	1:A:598:ASP:HB2	2.04	0.58
1:B:587:VAL:O	1:B:591:VAL:HG23	2.04	0.57
1:B:111:PHE:CE1	1:B:540:LYS:HA	2.38	0.57
1:B:339:GLU:O	1:B:340:ASP:HB2	2.04	0.57
1:A:206:PHE:HE1	1:A:208:THR:HG1	1.52	0.57
1:A:192:LYS:HB2	1:A:192:LYS:HZ3	1.69	0.57
1:A:127:ASP:OD1	1:A:129:ARG:NH2	2.38	0.57
1:B:367:ILE:HD11	1:B:591:VAL:CG2	2.34	0.57
1:A:402:LEU:HB2	1:A:463:ILE:HB	1.87	0.57
1:B:536:ARG:HG3	1:B:536:ARG:NH1	2.20	0.57
1:B:143:ARG:NH2	1:B:204:ARG:HD2	2.18	0.57
1:B:122:VAL:HG12	1:B:123:GLN:H	1.69	0.57
1:B:367:ILE:HD11	1:B:591:VAL:HG22	1.86	0.57
1:A:427:ARG:CD	1:A:432:ASP:HB2	2.35	0.57
1:B:87:THR:O	1:B:91:GLN:HG3	2.04	0.57
1:B:201:LYS:HE3	1:B:209:THR:HG21	1.86	0.56
1:A:594:LEU:HD21	1:A:601:ILE:CD1	2.35	0.56
1:A:390:ASP:OD1	1:A:391:ARG:HG2	2.06	0.56
1:B:352:PHE:CD2	1:B:387:MSE:HE3	2.39	0.56
1:B:492:LEU:HD22	1:B:583:TYR:OH	2.06	0.56
1:A:509:LYS:HG3	1:A:516:ILE:HD13	1.88	0.56
1:A:192:LYS:HB2	1:A:192:LYS:HZ2	1.70	0.56
1:B:401:ILE:HG12	1:B:464:GLU:O	2.05	0.56
1:B:122:VAL:HB	1:B:179:LEU:HD21	1.86	0.56
1:B:209:THR:O	1:B:210:ARG:HD3	2.06	0.56
1:A:602:ILE:CG2	1:A:603:LEU:H	2.13	0.56
1:B:192:LYS:O	1:B:194:PRO:HD3	2.06	0.56
1:A:499:SER:OG	1:A:500:CYS:N	2.38	0.55
1:A:197:ARG:NH1	1:A:213:ARG:NE	2.51	0.55
1:B:122:VAL:CG1	1:B:123:GLN:H	2.20	0.55
1:A:498:PHE:N	1:A:498:PHE:CD1	2.73	0.55
1:A:70:GLN:HE21	1:A:70:GLN:N	2.05	0.55
1:B:316:THR:HA	1:B:321:LYS:O	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:HIS:CE1	1:A:170:GLY:HA2	2.42	0.55
1:B:119:PRO:HG3	1:B:217:ARG:HH22	1.70	0.55
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.88	0.55
1:A:54:TYR:CZ	1:A:56:PRO:HG2	2.41	0.55
1:B:182:LEU:O	1:B:183:PHE:HD2	1.90	0.54
1:A:105:HIS:CE1	1:A:528:VAL:HG22	2.41	0.54
1:B:450:PHE:O	1:B:454:VAL:HG23	2.07	0.54
1:B:53:LYS:HB3	1:B:529:PHE:CZ	2.42	0.54
1:B:204:ARG:HB2	1:B:208:THR:HG22	1.89	0.54
1:B:314:SER:O	1:B:315:VAL:HG23	2.08	0.54
1:B:375:GLY:HA3	1:B:499:SER:OG	2.08	0.54
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.72	0.54
1:B:600:THR:O	1:B:602:ILE:N	2.41	0.54
1:A:192:LYS:CB	1:A:192:LYS:NZ	2.70	0.54
1:B:159:VAL:HG11	1:B:182:LEU:HD21	1.91	0.53
1:B:197:ARG:HA	1:B:215:LYS:HA	1.89	0.53
1:A:336:GLN:CD	1:A:336:GLN:H	2.11	0.53
1:A:399:ARG:HD3	1:A:468:PRO:HD3	1.91	0.53
1:B:182:LEU:HD13	1:B:183:PHE:HE2	1.72	0.53
1:A:206:PHE:HE1	1:A:208:THR:OG1	1.92	0.53
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.44	0.53
1:B:330:ILE:HD11	1:B:352:PHE:HE1	1.72	0.53
1:A:415:THR:HA	1:A:418:GLU:HG3	1.90	0.53
1:B:149:LEU:O	1:B:155:PRO:HA	2.08	0.53
1:A:516:ILE:HD12	1:A:516:ILE:N	2.23	0.53
1:B:363:THR:HG23	1:B:485:TYR:OH	2.09	0.53
1:B:596:ASN:O	1:B:597:ASN:HB3	2.08	0.52
1:B:156:VAL:HB	1:B:157:GLN:OE1	2.09	0.52
1:B:143:ARG:NH2	1:B:204:ARG:CZ	2.72	0.52
1:B:329:ARG:HD2	1:B:369:ASP:OD1	2.08	0.52
1:B:57:LYS:O	1:B:61:GLU:HG3	2.09	0.52
1:A:515:LEU:HD23	1:A:565:HIS:CD2	2.45	0.52
1:A:57:LYS:O	1:A:61:GLU:HG3	2.10	0.52
1:B:105:HIS:CG	1:B:528:VAL:HG13	2.45	0.52
1:A:316:THR:HA	1:A:321:LYS:O	2.09	0.52
1:B:515:LEU:HD13	1:B:517:VAL:HG22	1.91	0.52
1:B:150:GLU:HB3	1:B:154:ALA:O	2.10	0.52
1:B:163:LEU:HD11	1:B:185:ARG:HH21	1.74	0.52
1:A:493:ILE:HD13	1:A:519:THR:O	2.10	0.52
1:B:566:ILE:HD12	1:B:590:LEU:CD1	2.40	0.52
1:B:64:LEU:CD2	1:B:169:LYS:HD2	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.92	0.52
1:B:155:PRO:CG	1:B:158:ASP:OD2	2.58	0.51
1:B:574:ASP:OD1	1:B:582:GLU:HB2	2.11	0.51
1:B:494:ASN:ND2	1:B:496:GLN:H	2.08	0.51
1:A:204:ARG:NH1	1:A:206:PHE:CE2	2.78	0.51
1:A:577:TYR:O	1:A:579:GLY:N	2.44	0.51
1:A:230:ALA:N	1:A:231:PRO:HD2	2.26	0.51
1:B:134:ASP:O	1:B:135:ILE:HD13	2.10	0.51
1:B:60:LYS:HZ3	1:B:558:GLU:HG3	1.76	0.51
1:A:536:ARG:HA	1:B:404:GLN:NE2	2.26	0.51
1:A:142:ILE:HD12	1:A:202:ILE:HG21	1.93	0.51
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.92	0.51
1:B:563:GLU:O	1:B:563:GLU:HG2	2.09	0.51
1:B:88:SER:O	1:B:92:GLN:HG3	2.11	0.51
1:A:551:ARG:HG3	1:A:557:ILE:HD11	1.92	0.51
1:A:600:THR:HG22	1:A:600:THR:O	2.11	0.51
1:B:197:ARG:HA	1:B:214:VAL:O	2.11	0.51
1:B:503:PHE:HA	1:B:506:VAL:CG1	2.41	0.51
1:B:117:TYR:CG	1:B:118:LEU:N	2.78	0.51
1:B:506:VAL:HB	1:B:562:VAL:HG21	1.91	0.51
1:A:155:PRO:O	1:A:158:ASP:HB2	2.12	0.50
1:B:480:HIS:ND1	1:B:481:PRO:HD2	2.27	0.50
1:A:382:TYR:CD1	1:A:477:ILE:HD11	2.46	0.50
1:A:427:ARG:HB3	1:A:432:ASP:HB3	1.93	0.50
1:A:393:LEU:HD21	1:A:513:ARG:HG3	1.93	0.50
1:A:593:GLN:OE1	1:A:603:LEU:O	2.29	0.50
1:B:297:ILE:HD13	1:B:297:ILE:N	2.27	0.50
1:A:366:LEU:HB2	1:A:485:TYR:CE2	2.47	0.50
1:B:66:TRP:CZ2	1:B:101:LEU:HD21	2.47	0.50
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.46	0.50
1:B:417:LEU:HB2	1:B:448:LYS:HD2	1.94	0.50
1:A:489:ILE:HG22	1:A:490:CYS:N	2.26	0.50
1:B:516:ILE:O	1:B:565:HIS:N	2.42	0.50
1:A:499:SER:H	1:A:524:ALA:HB3	1.77	0.50
1:A:325:VAL:CG1	1:A:367:ILE:HD13	2.40	0.50
1:A:537:THR:HG22	1:A:537:THR:O	2.12	0.50
1:B:517:VAL:CG1	1:B:566:ILE:HB	2.39	0.49
1:B:297:ILE:HD13	1:B:298:GLY:H	1.76	0.49
1:A:599:GLY:O	1:A:600:THR:C	2.49	0.49
1:A:548:LEU:HD22	1:A:556:PHE:HD2	1.77	0.49
1:B:329:ARG:HH11	1:B:369:ASP:CG	2.16	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:OD1	1:B:105:HIS:HB2	2.12	0.49
1:A:376:GLY:O	1:A:500:CYS:SG	2.64	0.49
1:A:404:GLN:H	1:A:404:GLN:CD	2.12	0.49
1:B:566:ILE:HD12	1:B:590:LEU:HD13	1.94	0.49
1:B:138:PHE:O	1:B:139:SER:C	2.50	0.49
1:A:105:HIS:HB3	1:A:528:VAL:HG13	1.95	0.49
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.77	0.49
1:A:49:LEU:CD2	1:B:534:PRO:HG2	2.42	0.49
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.95	0.49
1:B:545:THR:HG22	1:B:547:SER:H	1.77	0.49
1:A:302:TRP:CH2	1:A:304:SER:HB3	2.47	0.49
1:B:126:SER:OG	1:B:571:THR:HG22	2.12	0.49
1:B:89:PHE:O	1:B:93:VAL:HG23	2.13	0.49
1:B:504:PHE:HB3	1:B:505:PRO:HD3	1.95	0.49
1:B:118:LEU:HD22	1:B:120:TYR:CE1	2.48	0.48
1:B:157:GLN:CD	1:B:157:GLN:H	2.15	0.48
1:A:366:LEU:HD22	1:A:368:ILE:CD1	2.38	0.48
1:A:60:LYS:NZ	1:A:559:ASN:HD21	2.11	0.48
1:B:230:ALA:N	1:B:231:PRO:HD2	2.27	0.48
1:A:48:HIS:O	1:A:52:VAL:HG22	2.13	0.48
1:B:290:THR:O	1:B:329:ARG:HD3	2.12	0.48
1:B:370:GLN:HB3	1:B:370:GLN:HE21	1.49	0.48
1:A:353:ALA:O	1:A:357:GLN:HG3	2.14	0.48
1:A:105:HIS:CE1	1:A:499:SER:HB3	2.48	0.48
1:A:602:ILE:O	1:A:603:LEU:C	2.51	0.48
1:B:329:ARG:HB2	1:B:369:ASP:HB3	1.95	0.48
1:B:43:LEU:O	1:B:43:LEU:HD23	2.13	0.48
1:B:499:SER:H	1:B:524:ALA:HB3	1.78	0.48
1:B:53:LYS:HB3	1:B:529:PHE:HZ	1.75	0.48
1:B:132:PHE:CZ	1:B:148:LEU:HD13	2.49	0.48
1:B:143:ARG:NH2	1:B:204:ARG:NE	2.61	0.48
1:A:59:TRP:HE1	1:A:559:ASN:HD22	1.60	0.48
1:A:182:LEU:HD13	1:A:183:PHE:CZ	2.49	0.48
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.28	0.48
1:A:548:LEU:HD22	1:A:556:PHE:CD2	2.49	0.48
1:B:537:THR:HG22	1:B:537:THR:O	2.13	0.48
1:A:359:PHE:O	1:A:363:THR:HG22	2.14	0.48
1:A:192:LYS:HZ3	1:A:192:LYS:CB	2.27	0.48
1:B:355:ILE:HG22	1:B:359:PHE:CE1	2.49	0.47
1:B:114:GLU:HA	1:B:219:VAL:O	2.14	0.47
1:A:572:ALA:O	1:A:576:ARG:HB2	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HB2	1:B:485:TYR:CE2	2.50	0.47
1:A:197:ARG:CZ	1:A:213:ARG:HE	2.27	0.47
1:B:173:ALA:HA	1:B:495:GLU:HB2	1.96	0.47
1:B:98:ILE:N	1:B:98:ILE:HD12	2.29	0.47
1:B:201:LYS:HE3	1:B:209:THR:CG2	2.44	0.47
1:A:321:LYS:HG2	1:A:323:HIS:CE1	2.49	0.47
1:A:494:ASN:O	1:A:521:THR:HA	2.14	0.47
1:B:148:LEU:HG	1:B:156:VAL:CG2	2.45	0.47
1:A:70:GLN:HE21	1:A:70:GLN:CA	2.27	0.47
1:B:179:LEU:HD23	1:B:179:LEU:O	2.15	0.47
1:A:53:LYS:HB3	1:A:529:PHE:CZ	2.46	0.47
1:B:328:LEU:C	1:B:328:LEU:HD13	2.35	0.47
1:B:370:GLN:O	1:B:497:ASP:OD1	2.31	0.47
1:A:229:ILE:HD13	1:B:458:TRP:O	2.14	0.47
1:B:297:ILE:CD1	1:B:297:ILE:N	2.78	0.47
1:B:155:PRO:O	1:B:156:VAL:C	2.53	0.47
1:A:432:ASP:C	1:A:432:ASP:OD1	2.53	0.47
1:B:494:ASN:HD22	1:B:494:ASN:C	2.17	0.47
1:B:297:ILE:H	1:B:297:ILE:CD1	2.28	0.47
1:B:449:SER:O	1:B:453:GLN:HG3	2.15	0.46
1:B:94:LEU:O	1:B:98:ILE:HD13	2.15	0.46
1:B:118:LEU:O	1:B:120:TYR:N	2.48	0.46
1:A:371:THR:HA	1:A:494:ASN:HB2	1.98	0.46
1:A:407:VAL:O	1:A:410:ALA:HB3	2.15	0.46
1:A:601:ILE:HD12	1:A:601:ILE:H	1.81	0.46
1:B:55:ALA:N	1:B:56:PRO:HD2	2.30	0.46
1:A:304:SER:O	1:A:306:GLY:N	2.49	0.46
1:B:356:ILE:O	1:B:357:GLN:C	2.52	0.46
1:B:395:LEU:HD11	1:B:477:ILE:CD1	2.45	0.46
1:B:333:TYR:CE2	1:B:381:LEU:HD23	2.50	0.46
1:A:395:LEU:HD11	1:A:477:ILE:CD1	2.43	0.46
1:A:363:THR:CG2	1:A:485:TYR:OH	2.64	0.46
1:B:123:GLN:NE2	1:B:285:TYR:HE2	2.11	0.46
1:A:516:ILE:N	1:A:565:HIS:HD2	2.05	0.45
1:B:310:ALA:HA	1:B:327:PHE:O	2.16	0.45
1:B:325:VAL:HG12	1:B:326:GLY:N	2.30	0.45
1:A:404:GLN:NE2	1:B:536:ARG:HA	2.31	0.45
1:B:214:VAL:HG12	1:B:215:LYS:N	2.30	0.45
1:A:70:GLN:HE21	1:A:70:GLN:H	1.63	0.45
1:B:72:SER:O	1:B:76:GLN:HG3	2.16	0.45
1:A:380:TYR:CE1	1:A:384:LEU:HD21	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:C	1:B:183:PHE:HD2	2.19	0.45
1:A:370:GLN:HE21	1:A:370:GLN:HB3	1.51	0.45
1:B:149:LEU:C	1:B:150:GLU:HG3	2.37	0.45
1:B:471:LEU:O	1:B:472:PHE:HB2	2.17	0.45
1:B:294:LEU:HD13	1:B:584:LEU:HD21	1.99	0.45
1:A:56:PRO:O	1:A:60:LYS:HG2	2.16	0.45
1:B:132:PHE:CE1	1:B:148:LEU:HD13	2.52	0.45
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.81	0.45
1:B:366:LEU:HD23	1:B:367:ILE:N	2.32	0.45
1:B:55:ALA:HA	1:B:401:ILE:HD11	1.98	0.45
1:B:165:GLY:H	1:B:168:HIS:HB2	1.81	0.45
1:B:595:ILE:H	1:B:595:ILE:HD12	1.82	0.44
1:B:506:VAL:HB	1:B:562:VAL:CG2	2.48	0.44
1:A:558:GLU:O	1:A:559:ASN:HB2	2.17	0.44
1:B:69:VAL:O	1:B:73:VAL:HG23	2.17	0.44
1:B:579:GLY:O	1:B:581:SER:N	2.50	0.44
1:B:493:ILE:HG13	1:B:493:ILE:O	2.16	0.44
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.47	0.44
1:B:515:LEU:CD1	1:B:517:VAL:HG22	2.48	0.44
1:A:60:LYS:HZ2	1:A:559:ASN:HD21	1.65	0.44
1:B:568:LEU:HD23	1:B:568:LEU:HA	1.80	0.44
1:A:391:ARG:NH2	1:A:511:ASN:O	2.48	0.44
1:B:195:SER:HB3	1:B:218:TYR:CD1	2.53	0.44
1:B:117:TYR:O	1:B:118:LEU:HG	2.17	0.44
1:B:137:THR:HG23	1:B:138:PHE:N	2.33	0.44
1:B:59:TRP:HE1	1:B:559:ASN:ND2	2.09	0.44
1:B:126:SER:OG	1:B:571:THR:HA	2.18	0.44
1:B:579:GLY:C	1:B:581:SER:N	2.70	0.44
1:A:408:VAL:HG21	1:B:111:PHE:HB3	1.99	0.44
1:A:407:VAL:HG13	1:A:455:LEU:CD2	2.47	0.44
1:B:168:HIS:CE1	1:B:170:GLY:H	2.36	0.44
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.89	0.44
1:A:328:LEU:HD11	1:A:352:PHE:HE1	1.83	0.44
1:A:493:ILE:HD12	1:A:519:THR:H	1.83	0.43
1:B:352:PHE:HD2	1:B:387:MSE:CE	2.29	0.43
1:A:408:VAL:CG2	1:B:111:PHE:HB3	2.48	0.43
1:B:328:LEU:O	1:B:368:ILE:HA	2.18	0.43
1:A:451:GLY:O	1:A:455:LEU:HG	2.18	0.43
1:A:83:GLU:O	1:A:84:ASN:C	2.56	0.43
1:B:558:GLU:O	1:B:559:ASN:HB2	2.19	0.43
1:B:33:SER:HB3	1:B:36:CYS:HB3	2.01	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:THR:HG22	1:B:542:CYS:N	2.33	0.43
1:A:427:ARG:HB3	1:A:432:ASP:CB	2.49	0.43
1:A:368:ILE:HD13	1:A:489:ILE:CG2	2.46	0.43
1:A:368:ILE:HD12	1:A:368:ILE:N	2.33	0.43
1:B:433:ASN:ND2	1:B:436:GLY:N	2.53	0.43
1:B:579:GLY:C	1:B:581:SER:H	2.21	0.43
1:A:576:ARG:O	1:A:577:TYR:CD2	2.72	0.43
1:B:342:ASP:HA	1:B:343:PRO:HD2	1.77	0.43
1:A:534:PRO:CG	1:B:49:LEU:HD22	2.43	0.43
1:B:494:ASN:ND2	1:B:494:ASN:C	2.72	0.43
1:B:359:PHE:O	1:B:363:THR:CG2	2.52	0.43
1:B:55:ALA:HA	1:B:401:ILE:HG13	2.01	0.43
1:A:530:ASN:HB3	1:A:541:THR:CG2	2.49	0.43
1:B:516:ILE:HG22	1:B:564:PRO:HA	2.00	0.43
1:A:335:TRP:HB2	1:A:348:PRO:CG	2.46	0.43
1:B:393:LEU:HB2	1:B:477:ILE:HB	2.00	0.43
1:A:35:VAL:HG21	1:A:227:ALA:HB2	2.01	0.43
1:B:589:LYS:O	1:B:593:GLN:HG3	2.19	0.43
1:B:210:ARG:O	1:B:211:GLU:HG2	2.19	0.42
1:B:164:TYR:HB3	1:B:168:HIS:CG	2.54	0.42
1:A:111:PHE:CE1	1:B:405:ASP:HB2	2.54	0.42
1:B:150:GLU:OE1	1:B:201:LYS:CD	2.66	0.42
1:A:366:LEU:HB2	1:A:485:TYR:CZ	2.54	0.42
1:B:119:PRO:HG3	1:B:217:ARG:NH2	2.34	0.42
1:A:142:ILE:HD13	1:A:202:ILE:HD13	2.00	0.42
1:A:461:GLY:HA2	1:B:229:ILE:CG2	2.49	0.42
1:A:392:PRO:HA	1:A:477:ILE:O	2.19	0.42
1:A:382:TYR:CG	1:A:477:ILE:HD11	2.54	0.42
1:A:504:PHE:HB3	1:A:505:PRO:HD3	2.02	0.42
1:B:474:PHE:CD1	1:B:474:PHE:N	2.88	0.42
1:B:159:VAL:CG1	1:B:182:LEU:HD21	2.50	0.42
1:B:210:ARG:O	1:B:211:GLU:CG	2.67	0.42
1:A:105:HIS:ND1	1:A:528:VAL:HG22	2.35	0.42
1:B:363:THR:HG23	1:B:485:TYR:HH	1.85	0.42
1:B:149:LEU:HD11	1:B:203:ARG:CB	2.40	0.42
1:A:355:ILE:HG22	1:A:359:PHE:CE1	2.54	0.42
1:B:352:PHE:CD2	1:B:384:LEU:HD22	2.54	0.42
1:B:382:TYR:CD1	1:B:477:ILE:HD11	2.55	0.42
1:A:404:GLN:HE22	1:B:536:ARG:HA	1.85	0.42
1:A:449:SER:OG	1:A:453:GLN:NE2	2.50	0.42
1:B:317:ASP:OD2	1:B:321:LYS:HB3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:HB3	1:B:464:GLU:HB3	2.02	0.42
1:B:464:GLU:HA	1:B:464:GLU:OE2	2.19	0.42
1:B:498:PHE:HA	1:B:502:ASP:OD2	2.20	0.42
1:B:339:GLU:O	1:B:340:ASP:CB	2.68	0.42
1:B:186:MSE:N	1:B:191:HIS:HD2	2.00	0.41
1:A:602:ILE:O	1:A:603:LEU:O	2.38	0.41
1:B:520:ARG:HG3	1:B:520:ARG:HH11	1.84	0.41
1:B:67:ASP:HB3	1:B:70:GLN:HB3	2.02	0.41
1:B:111:PHE:CZ	1:B:540:LYS:HG3	2.55	0.41
1:B:130:PHE:N	1:B:130:PHE:CD1	2.88	0.41
1:B:342:ASP:O	1:B:344:SER:N	2.54	0.41
1:B:118:LEU:HD22	1:B:120:TYR:HE1	1.85	0.41
1:A:33:SER:HB3	1:A:36:CYS:HB3	2.01	0.41
1:A:82:GLN:HG3	1:A:89:PHE:CZ	2.56	0.41
1:B:325:VAL:CG1	1:B:326:GLY:N	2.84	0.41
1:B:433:ASN:HB2	1:B:437:TYR:O	2.21	0.41
1:B:148:LEU:HG	1:B:156:VAL:HG22	2.03	0.41
1:B:143:ARG:CB	1:B:143:ARG:HH11	2.34	0.41
1:B:143:ARG:NH2	1:B:204:ARG:CD	2.79	0.41
1:A:335:TRP:C	1:A:337:ASP:H	2.23	0.41
1:B:46:LEU:HD13	1:B:98:ILE:HD11	2.02	0.41
1:A:471:LEU:O	1:A:472:PHE:HB2	2.20	0.41
1:A:516:ILE:HD12	1:A:516:ILE:H	1.84	0.41
1:A:53:LYS:HD3	1:A:53:LYS:HA	1.89	0.41
1:B:135:ILE:CG2	1:B:137:THR:HG22	2.50	0.41
1:B:492:LEU:HA	1:B:517:VAL:O	2.21	0.41
1:A:381:LEU:HD13	1:A:381:LEU:C	2.41	0.41
1:B:503:PHE:O	1:B:504:PHE:C	2.59	0.41
1:B:571:THR:O	1:B:572:ALA:C	2.59	0.41
1:B:317:ASP:CG	1:B:321:LYS:HB3	2.41	0.41
1:B:503:PHE:CA	1:B:506:VAL:HG12	2.49	0.41
1:B:599:GLY:O	1:B:600:THR:OG1	2.36	0.41
1:B:370:GLN:OE1	1:B:501:ALA:HA	2.21	0.41
1:A:163:LEU:HD13	1:A:181:THR:HG22	2.03	0.41
1:B:532:GLN:HE21	1:B:532:GLN:HB2	1.59	0.41
1:A:476:LYS:HE2	1:A:476:LYS:HB3	1.91	0.41
1:A:519:THR:O	1:A:520:ARG:C	2.59	0.41
1:B:317:ASP:HB3	1:B:592:CYS:SG	2.61	0.41
1:A:133:VAL:O	1:A:578:LYS:HD3	2.21	0.41
1:B:494:ASN:HA	1:B:519:THR:OG1	2.21	0.41
1:A:407:VAL:HG11	1:B:223:VAL:HG13	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:O	1:A:93:VAL:HG23	2.21	0.40
1:A:43:LEU:HD23	1:A:94:LEU:CD2	2.52	0.40
1:B:351:GLU:O	1:B:355:ILE:HG13	2.20	0.40
1:B:114:GLU:O	1:B:193:VAL:HG21	2.20	0.40
1:B:363:THR:CG2	1:B:485:TYR:OH	2.69	0.40
1:B:586:LYS:O	1:B:586:LYS:HD3	2.22	0.40
1:B:135:ILE:HG22	1:B:137:THR:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:NH1	1:A:204:ARG:NH2[7_465]	2.19	0.01

## 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	523/579 (90%)	477 (91%)	32 (6%)	14 (3%)	6	25
1	B	523/579 (90%)	449 (86%)	57 (11%)	17 (3%)	5	20
All	All	1046/1158 (90%)	926 (88%)	89 (8%)	31 (3%)	5	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLU
1	A	466	SER
1	A	578	LYS
1	A	602	ILE
1	B	83	GLU
1	B	156	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	335	TRP
1	B	466	SER
1	B	600	THR
1	A	306	GLY
1	A	335	TRP
1	B	141	GLU
1	B	166	SER
1	B	170	GLY
1	B	601	ILE
1	A	315	VAL
1	B	139	SER
1	B	343	PRO
1	B	499	SER
1	B	576	ARG
1	A	600	THR
1	B	119	PRO
1	B	580	TYR
1	B	597	ASN
1	A	499	SER
1	A	597	ASN
1	B	299	PRO
1	A	56	PRO
1	A	465	LEU
1	A	156	VAL
1	A	479	PRO

### 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	456/495 (92%)	420 (92%)	36 (8%)	15	41
1	B	456/495 (92%)	423 (93%)	33 (7%)	18	46
All	All	912/990 (92%)	843 (92%)	69 (8%)	16	43

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	70	GLN
1	A	84	ASN
1	A	102	ASN
1	A	175	GLU
1	A	179	LEU
1	A	182	LEU
1	A	192	LYS
1	A	203	ARG
1	A	204	ARG
1	A	213	ARG
1	A	226	LEU
1	A	239	GLN
1	A	328	LEU
1	A	334	SER
1	A	363	THR
1	A	366	LEU
1	A	370	GLN
1	A	384	LEU
1	A	391	ARG
1	A	404	GLN
1	A	432	ASP
1	A	448	LYS
1	A	463	ILE
1	A	467	THR
1	A	477	ILE
1	A	483	VAL
1	A	484	GLN
1	A	495	GLU
1	A	498	PHE
1	A	513	ARG
1	A	515	LEU
1	A	528	VAL
1	A	548	LEU
1	A	553	HIS
1	A	568	LEU
1	B	41	GLN
1	B	58	THR
1	B	72	SER
1	B	84	ASN
1	B	88	SER
1	B	102	ASN
1	B	136	MSE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	157	GLN
1	B	182	LEU
1	B	238	LEU
1	B	297	ILE
1	B	301	ILE
1	B	312	ILE
1	B	328	LEU
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	386	SER
1	B	404	GLN
1	B	416	LEU
1	B	421	ASP
1	B	424	VAL
1	B	441	LEU
1	B	483	VAL
1	B	494	ASN
1	B	513	ARG
1	B	517	VAL
1	B	528	VAL
1	B	532	GLN
1	B	568	LEU
1	B	586	LYS
1	B	592	CYS
1	B	603	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	70	GLN
1	A	84	ASN
1	A	102	ASN
1	A	123	GLN
1	A	168	HIS
1	A	191	HIS
1	A	239	GLN
1	A	323	HIS
1	A	370	GLN
1	A	404	GLN
1	A	442	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	494	ASN
1	A	496	GLN
1	A	559	ASN
1	A	565	HIS
1	A	593	GLN
1	A	596	ASN
1	B	84	ASN
1	B	102	ASN
1	B	123	GLN
1	B	191	HIS
1	B	239	GLN
1	B	286	ASN
1	B	323	HIS
1	B	370	GLN
1	B	404	GLN
1	B	433	ASN
1	B	442	GLN
1	B	494	ASN
1	B	532	GLN
1	B	559	ASN
1	B	565	HIS
1	B	596	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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	521/579 (89%)	0.04	13 (2%) 61 55	18, 36, 68, 119	0
1	B	521/579 (89%)	0.51	52 (9%) 9 5	23, 54, 105, 159	0
All	All	1042/1158 (89%)	0.27	65 (6%) 24 17	18, 43, 94, 159	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	GLN	8.4
1	B	137	THR	5.2
1	B	142	ILE	5.1
1	B	204	ARG	4.8
1	B	196	GLY	4.8
1	B	120	TYR	4.7
1	A	239	GLN	4.6
1	A	305	GLU	4.2
1	B	206	PHE	4.2
1	A	140	SER	4.0
1	A	319	ASP	3.8
1	B	319	ASP	3.8
1	B	571	THR	3.8
1	B	141	GLU	3.7
1	B	317	ASP	3.7
1	B	149	LEU	3.7
1	B	320	GLY	3.7
1	B	208	THR	3.5
1	B	199	THR	3.5
1	A	318	GLY	3.5
1	B	139	SER	3.3
1	B	318	GLY	3.3
1	B	198	THR	3.2
1	A	577	TYR	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	3.2
1	B	214	VAL	3.1
1	A	139	SER	3.1
1	B	209	THR	3.1
1	B	316	THR	2.9
1	B	603	LEU	2.9
1	B	213	ARG	2.9
1	B	205	PRO	2.9
1	B	138	PHE	2.8
1	B	154	ALA	2.8
1	B	322	SER	2.8
1	B	210	ARG	2.8
1	B	599	GLY	2.8
1	B	600	THR	2.7
1	B	212	VAL	2.7
1	B	148	LEU	2.6
1	A	138	PHE	2.6
1	B	602	ILE	2.5
1	A	83	GLU	2.5
1	A	602	ILE	2.4
1	B	194	PRO	2.4
1	B	153	GLY	2.4
1	B	575	ILE	2.4
1	B	83	GLU	2.3
1	A	321	LYS	2.3
1	B	125	SER	2.3
1	B	135	ILE	2.3
1	B	128	GLY	2.3
1	B	200	LEU	2.3
1	B	297	ILE	2.2
1	B	127	ASP	2.2
1	B	131	TYR	2.2
1	B	323	HIS	2.1
1	B	134	ASP	2.1
1	A	141	GLU	2.1
1	B	160	LEU	2.0
1	B	150	GLU	2.0
1	B	598	ASP	2.0
1	B	117	TYR	2.0
1	B	193	VAL	2.0
1	B	215	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.