

Full wwPDB X-ray Structure Validation Report (i)

Nov 24, 2021 – 06:14 pm GMT

PDB ID	:	6Z9Y
Title	:	Copper transporter OprC
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Deposited on	:	2020-06-04
Resolution	:	2.95 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProhity		4 02b 467
Mon robity	·	4.020-407
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	3104 (3.00-2.92)		
Clashscore	141614	3462(3.00-2.92)		
Ramachandran outliers	138981	3340 (3.00-2.92)		
Sidechain outliers	138945	3343 (3.00-2.92)		
RSRZ outliers	127900	2986 (3.00-2.92)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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 o	f chain	
1	А	723	54%	33%	• 9%
1	В	723	3% 54%	37%	11%
1	C	723	4%	270	- 11/0
	0	123	46% 5%	37%	5% 11%
1	D	723	52%	35%	• 9%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20158 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	657	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	057	5092	3195	899	979	19	0		0
1	р	645	Total	С	Ν	0	S	0	0	0
	D	040	5004	3141	882	966	15	0		U
1	C	640	Total	С	Ν	0	S	0	0	0
			4970	3123	878	955	14	0		0
1	1 D	656	Total	С	Ν	0	S	0	1	0
			5088	3194	898	977	19	0		0

• Molecule 1 is a protein called Putative copper transport outer membrane porin OprC.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	323	ALA	HIS	engineered mutation	UNP G3XD89
В	323	ALA	HIS	engineered mutation	UNP G3XD89
С	323	ALA	HIS	engineered mutation	UNP G3XD89
D	323	ALA	HIS	engineered mutation	UNP G3XD89

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Cu 1 1	0	0
2	В	1	Total Cu 1 1	0	0
2	С	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Putative copper transport outer membrane porin OprC

• Molecule 1: Putative copper transport outer membrane porin OprC

Chain B: 54% 32% · 11%







PDB EIN DATA BANK

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# T671 N672 N673 N674 N673 N674 N675 S677 S677 N622 N622 N622 N622 N622 N622 N622 N623 N624 N625 N636 H231 N705 N706 N707 N708



### 4 Data and refinement statistics (i)

| Property                                           | Value                                           | Source    |
|----------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                        | P 1 21 1                                        | Depositor |
| Cell constants                                     | 67.34Å 197.67Å 171.75Å                          | Deperitor |
| a, b, c, $\alpha$ , $\beta$ , $\gamma$             | $90.00^{\circ}$ $88.75^{\circ}$ $90.00^{\circ}$ | Depositor |
| $\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$ | 85.85 - 2.95                                    | Depositor |
| Resolution (A)                                     | $171.71 \ - \ 2.95$                             | EDS       |
| % Data completeness                                | 98.0 (85.85-2.95)                               | Depositor |
| (in resolution range)                              | 93.7 (171.71-2.95)                              | EDS       |
| R <sub>merge</sub>                                 | (Not available)                                 | Depositor |
| $R_{sym}$                                          | (Not available)                                 | Depositor |
| $< I/\sigma(I) > 1$                                | $1.15 (at 2.96 \text{\AA})$                     | Xtriage   |
| Refinement program                                 | PHENIX 1.18_3855                                | Depositor |
| P. P.                                              | 0.242 , $0.302$                                 | Depositor |
| $n, n_{free}$                                      | 0.244 , $0.302$                                 | DCC       |
| $R_{free}$ test set                                | 4619 reflections $(4.91%)$                      | wwPDB-VP  |
| Wilson B-factor $(Å^2)$                            | 69.5                                            | Xtriage   |
| Anisotropy                                         | 0.404                                           | Xtriage   |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$        | (Not available), (Not available)                | EDS       |
| L-test for twinning <sup>2</sup>                   | $<  L  > = 0.47, < L^2 > = 0.30$                | Xtriage   |
| Estimated twinning fraction                        | 0.238 for h,-k,-l                               | Xtriage   |
| $F_o, F_c$ correlation                             | 0.88                                            | EDS       |
| Total number of atoms                              | 20158                                           | wwPDB-VP  |
| Average B, all atoms $(Å^2)$                       | 66.0                                            | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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: CU

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).

| Mal | Chain | Bo   | nd lengths     | Bond angles |                |  |
|-----|-------|------|----------------|-------------|----------------|--|
|     |       |      | # Z  > 5       | RMSZ        | # Z  > 5       |  |
| 1   | А     | 0.47 | 0/5218         | 0.69        | 2/7072~(0.0%)  |  |
| 1   | В     | 0.51 | 0/5127         | 0.70        | 0/6952         |  |
| 1   | С     | 0.49 | 1/5090~(0.0%)  | 0.70        | 1/6898~(0.0%)  |  |
| 1   | D     | 0.44 | 0/5217         | 0.67        | 2/7071~(0.0%)  |  |
| All | All   | 0.48 | 1/20652~(0.0%) | 0.69        | 5/27993~(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   | В     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Ζ    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | С     | 713 | ARG  | CG-CD | 5.56 | 1.65        | 1.51     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|----------|------|------------------|---------------|
| 1   | А     | 340 | PRO  | C-N-CA   | 8.15 | 142.09           | 121.70        |
| 1   | D     | 334 | ASP  | C-N-CD   | 6.40 | 141.84           | 128.40        |
| 1   | С     | 102 | LEU  | CA-CB-CG | 5.22 | 127.31           | 115.30        |
| 1   | D     | 222 | LEU  | CA-CB-CG | 5.21 | 127.29           | 115.30        |
| 1   | А     | 631 | LEU  | CA-CB-CG | 5.16 | 127.16           | 115.30        |

There are no chirality outliers.

All (1) planarity outliers are listed below:



| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | В     | 92  | PRO  | Peptide |

#### 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   | А     | 5092  | 0        | 4870     | 170     | 0            |
| 1   | В     | 5004  | 0        | 4779     | 171     | 0            |
| 1   | С     | 4970  | 0        | 4759     | 195     | 0            |
| 1   | D     | 5088  | 0        | 4870     | 164     | 0            |
| 2   | А     | 1     | 0        | 0        | 0       | 0            |
| 2   | В     | 1     | 0        | 0        | 0       | 0            |
| 2   | С     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 20158 | 0        | 19278    | 692     | 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 18.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom 1           | Atom 2           | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:B:171:VAL:HG22 | 1:B:414:GLU:HG3  | 1.51         | 0.93        |
| 1:B:504:ARG:HH12 | 1:B:555:ARG:HB3  | 1.37         | 0.90        |
| 1:A:630:SER:HB3  | 1:A:664:LEU:HD23 | 1.53         | 0.88        |
| 1:D:253:ASN:HD22 | 1:D:293:ARG:HH21 | 1.26         | 0.84        |
| 1:D:324:ILE:HG12 | 1:D:346:GLN:HG3  | 1.59         | 0.84        |
| 1:D:476:LEU:HD12 | 1:D:481:THR:HB   | 1.59         | 0.83        |
| 1:B:111:ILE:HG22 | 1:B:692:LEU:HB3  | 1.60         | 0.82        |
| 1:B:386:ASP:HB3  | 1:B:389:THR:HG22 | 1.61         | 0.82        |
| 1:B:374:MET:SD   | 1:B:376:ASN:ND2  | 2.53         | 0.82        |
| 1:C:466:PRO:HG2  | 1:D:466:PRO:HG2  | 1.62         | 0.82        |
| 1:A:445:SER:HB2  | 1:A:503:LYS:HE3  | 1.62         | 0.81        |
| 1:B:129:ARG:NH1  | 1:B:519:GLU:OE1  | 2.13         | 0.81        |
| 1:C:614:GLU:OE2  | 1:C:633:ARG:NE   | 2.12         | 0.81        |
| 1:C:695:ALA:HB2  | 1:C:708:VAL:HG23 | 1.60         | 0.81        |
| 1:A:72:THR:HB    | 1:A:631:LEU:HD22 | 1.63         | 0.81        |



|                  | io ao pagom      | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:B:671:THR:HG23 | 1:B:673:ASN:H    | 1.46         | 0.80        |
| 1:C:300:PHE:HZ   | 1:C:302:LYS:HD2  | 1.47         | 0.80        |
| 1:D:548:ASP:HB3  | 1:D:567:ASN:HD22 | 1.47         | 0.80        |
| 1:D:172:LEU:HD21 | 1:D:414:GLU:HB2  | 1.62         | 0.80        |
| 1:C:695:ALA:HB3  | 1:C:707:THR:HA   | 1.64         | 0.79        |
| 1:B:672:ARG:H    | 1:B:672:ARG:HD2  | 1.47         | 0.78        |
| 1:C:286:MET:HG2  | 1:C:327:ASN:HB3  | 1.64         | 0.78        |
| 1:C:147:MET:HB3  | 1:C:284:ARG:HE   | 1.48         | 0.77        |
| 1:A:664:LEU:HB2  | 1:A:680:VAL:HG22 | 1.65         | 0.77        |
| 1:C:82:ILE:HD11  | 1:C:166:LYS:HE3  | 1.64         | 0.77        |
| 1:C:164:VAL:HG22 | 1:C:182:ILE:HG13 | 1.66         | 0.77        |
| 1:D:260:TRP:HB3  | 1:D:268:ILE:HD11 | 1.66         | 0.77        |
| 1:B:521:THR:HG23 | 1:B:546:VAL:HG22 | 1.67         | 0.76        |
| 1:A:466:PRO:HG2  | 1:B:466:PRO:HG2  | 1.68         | 0.76        |
| 1:C:612:PRO:HG3  | 1:C:638:GLN:HB2  | 1.68         | 0.76        |
| 1:D:176:GLY:HA3  | 1:D:492:ARG:HG3  | 1.67         | 0.75        |
| 1:A:499:LEU:HD22 | 1:A:513:PHE:HA   | 1.69         | 0.75        |
| 1:C:203:LEU:HB3  | 1:C:211:ASP:HB3  | 1.68         | 0.74        |
| 1:A:91:GLN:NE2   | 1:A:665:ASN:HB3  | 2.02         | 0.74        |
| 1:A:616:ARG:HE   | 1:A:633:ARG:HD2  | 1.52         | 0.74        |
| 1:D:671:THR:HG22 | 1:D:674:VAL:HG12 | 1.68         | 0.73        |
| 1:B:133:LEU:HD11 | 1:B:173:TRP:HB3  | 1.71         | 0.73        |
| 1:C:492:ARG:NH2  | 1:C:519:GLU:OE2  | 2.21         | 0.73        |
| 1:B:495:ASP:HB2  | 1:B:498:GLU:HG3  | 1.70         | 0.73        |
| 1:A:671:THR:HG22 | 1:A:674:VAL:HG12 | 1.70         | 0.72        |
| 1:B:203:LEU:HD12 | 1:B:718:LYS:HB2  | 1.71         | 0.72        |
| 1:A:129:ARG:NH1  | 1:A:519:GLU:OE1  | 2.23         | 0.72        |
| 1:B:504:ARG:HB3  | 1:B:564:GLN:HG3  | 1.71         | 0.72        |
| 1:A:99:ALA:HA    | 1:A:102:LEU:HD12 | 1.70         | 0.71        |
| 1:B:230:ASN:ND2  | 1:B:253:ASN:OD1  | 2.22         | 0.71        |
| 1:A:698:ALA:H    | 1:A:702:PHE:HB2  | 1.55         | 0.70        |
| 1:C:467:SER:HB3  | 1:C:490:ALA:HA   | 1.73         | 0.70        |
| 1:A:91:GLN:HB3   | 1:A:92:PRO:HD3   | 1.74         | 0.70        |
| 1:C:653:PHE:HD1  | 1:C:654:ASP:H    | 1.38         | 0.69        |
| 1:B:465:LEU:HB3  | 1:B:491:GLU:HB2  | 1.74         | 0.69        |
| 1:C:441:GLN:O    | 1:C:454:ASN:N    | 2.25         | 0.69        |
| 1:D:584:THR:HG22 | 1:D:587:TRP:HB2  | 1.75         | 0.69        |
| 1:C:221:ARG:O    | 1:C:261:THR:OG1  | 2.09         | 0.69        |
| 1:C:379:ARG:HA   | 1:C:402:LYS:HA   | 1.75         | 0.69        |
| 1:D:643:ARG:HH21 | 1:D:653:PHE:HE1  | 1.41         | 0.69        |
| 1:C:87:LYS:NZ    | 1:C:157:GLU:O    | 2.26         | 0.68        |



|                  |                  | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:D:175:PRO:O    | 1:D:177:ALA:N    | 2.23         | 0.68        |
| 1:C:97:ASP:OD2   | 1:C:117:ASN:N    | 2.24         | 0.68        |
| 1:A:335:PRO:HA   | 1:A:340:PRO:HB3  | 1.76         | 0.68        |
| 1:D:163:THR:HB   | 1:D:183:LEU:HB2  | 1.75         | 0.68        |
| 1:D:455:PRO:HG3  | 1:D:510:VAL:HB   | 1.75         | 0.68        |
| 1:B:495:ASP:HB3  | 1:B:497:TRP:H    | 1.59         | 0.67        |
| 1:C:290:GLN:HB3  | 1:C:324:ILE:HG13 | 1.77         | 0.67        |
| 1:A:403:ASP:HB2  | 1:A:440:ARG:HG2  | 1.75         | 0.67        |
| 1:A:613:LEU:HD12 | 1:A:614:GLU:H    | 1.58         | 0.67        |
| 1:D:138:MET:HE3  | 1:D:140:LEU:HD21 | 1.77         | 0.67        |
| 1:C:214:LEU:HD12 | 1:C:215:ASP:H    | 1.60         | 0.67        |
| 1:C:465:LEU:HB3  | 1:C:491:GLU:HB2  | 1.77         | 0.67        |
| 1:B:84:THR:HG23  | 1:B:162:LEU:HB3  | 1.77         | 0.67        |
| 1:C:372:ASP:OD2  | 1:C:430:ARG:NH2  | 2.28         | 0.67        |
| 1:D:288:GLY:HA2  | 1:D:325:MET:HG2  | 1.77         | 0.67        |
| 1:C:274:LYS:HB2  | 1:C:292:LYS:HZ1  | 1.60         | 0.66        |
| 1:A:122:LEU:HG   | 1:A:123:ARG:HG3  | 1.78         | 0.66        |
| 1:A:583:LEU:HD12 | 1:A:587:TRP:HB3  | 1.78         | 0.66        |
| 1:A:497:TRP:O    | 1:A:501:SER:HB2  | 1.96         | 0.66        |
| 1:D:614:GLU:OE2  | 1:D:616:ARG:NH2  | 2.28         | 0.66        |
| 1:C:129:ARG:NH1  | 1:C:519:GLU:OE2  | 2.30         | 0.65        |
| 1:B:91:GLN:O     | 1:B:93:VAL:N     | 2.29         | 0.65        |
| 1:B:584:THR:HB   | 1:B:586:ASN:H    | 1.61         | 0.65        |
| 1:A:547:GLN:HG3  | 1:B:433:ARG:HH12 | 1.61         | 0.65        |
| 1:C:283:GLY:HA2  | 1:C:695:ALA:HA   | 1.77         | 0.65        |
| 1:D:441:GLN:NE2  | 1:D:458:ASN:OD1  | 2.29         | 0.65        |
| 1:B:672:ARG:HD2  | 1:B:672:ARG:N    | 2.12         | 0.65        |
| 1:C:274:LYS:HB2  | 1:C:292:LYS:NZ   | 2.11         | 0.65        |
| 1:D:467:SER:HB2  | 1:D:490:ALA:HA   | 1.78         | 0.65        |
| 1:C:584:THR:HB   | 1:C:586:ASN:H    | 1.62         | 0.65        |
| 1:C:682:ASN:HD22 | 1:C:712:GLY:HA2  | 1.61         | 0.65        |
| 1:D:616:ARG:HE   | 1:D:633:ARG:HD2  | 1.62         | 0.64        |
| 1:A:203:LEU:HD12 | 1:A:718:LYS:HB2  | 1.79         | 0.64        |
| 1:C:361:ARG:NH2  | 1:C:363:ASP:O    | 2.30         | 0.64        |
| 1:D:341:MET:HB3  | 1:D:385:TYR:HD1  | 1.62         | 0.64        |
| 1:D:503:LYS:HD3  | 1:D:562:SER:HB2  | 1.80         | 0.64        |
| 1:B:638:GLN:HG2  | 1:B:691:HIS:NE2  | 2.12         | 0.64        |
| 1:A:587:TRP:HZ3  | 1:A:619:LEU:HD21 | 1.63         | 0.64        |
| 1:B:635:VAL:HG11 | 1:B:659:PHE:CZ   | 2.32         | 0.64        |
| 1:B:83:VAL:HG22  | 1:B:163:THR:HG23 | 1.80         | 0.63        |
| 1:C:300:PHE:CZ   | 1:C:302:LYS:HD2  | 2.31         | 0.63        |



|                  | 1 · · · · ·      | Interatomic             | Clash       |
|------------------|------------------|-------------------------|-------------|
| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 1:D:428:GLY:N    | 1:D:469:PHE:O    | 2.30                    | 0.63        |
| 1:B:122:LEU:HG   | 1:B:123:ARG:HD3  | 1.80                    | 0.63        |
| 1:B:484:TYR:OH   | 1:B:540:SER:HB2  | 1.98                    | 0.63        |
| 1:C:116:SER:OG   | 1:C:117:ASN:N    | 2.31                    | 0.62        |
| 1:C:546:VAL:HG11 | 1:C:549:PHE:HD1  | 1.64                    | 0.62        |
| 1:C:264:GLU:CD   | 1:C:264:GLU:H    | 2.03                    | 0.62        |
| 1:B:586:ASN:ND2  | 1:B:622:GLU:O    | 2.30                    | 0.61        |
| 1:A:548:ASP:HB3  | 1:A:567:ASN:HD22 | 1.65                    | 0.61        |
| 1:B:456:THR:HG21 | 1:B:511:ASN:HD21 | 1.65                    | 0.61        |
| 1:C:206:SER:HG   | 1:C:715:PHE:H    | 1.48                    | 0.61        |
| 1:D:465:LEU:HB3  | 1:D:491:GLU:HB2  | 1.82                    | 0.61        |
| 1:A:437:LYS:HD3  | 1:A:439:TYR:CZ   | 2.36                    | 0.61        |
| 1:D:262:PRO:HD2  | 1:D:266:THR:HB   | 1.82                    | 0.61        |
| 1:A:141:GLY:O    | 1:A:349:ARG:HD3  | 2.00                    | 0.61        |
| 1:D:236:ASP:HB3  | 1:D:245:VAL:O    | 2.01                    | 0.61        |
| 1:B:693:ASN:OD1  | 1:B:693:ASN:N    | 2.25                    | 0.61        |
| 1:C:407:HIS:HB2  | 1:C:435:SER:HB3  | 1.83                    | 0.61        |
| 1:B:111:ILE:HD11 | 1:B:119:ASP:HB3  | 1.83                    | 0.60        |
| 1:B:128:SER:OG   | 1:B:495:ASP:OD1  | 2.19                    | 0.60        |
| 1:D:236:ASP:OD2  | 1:D:280:ARG:NH1  | 2.34                    | 0.60        |
| 1:C:289:SER:OG   | 1:C:326:ASP:OD2  | 2.13                    | 0.60        |
| 1:D:125:MET:HE3  | 1:D:572:ILE:HG21 | 1.82                    | 0.60        |
| 1:B:638:GLN:HG2  | 1:B:691:HIS:CD2  | 2.36                    | 0.60        |
| 1:C:682:ASN:ND2  | 1:C:712:GLY:HA2  | 2.16                    | 0.60        |
| 1:C:237:TYR:OH   | 1:C:709:PRO:O    | 2.10                    | 0.60        |
| 1:C:260:TRP:CE2  | 1:C:262:PRO:HG3  | 2.36                    | 0.60        |
| 1:C:555:ARG:O    | 1:C:562:SER:N    | 2.34                    | 0.60        |
| 1:D:129:ARG:NH2  | 1:D:519:GLU:OE2  | 2.35                    | 0.60        |
| 1:A:608:PRO:HG3  | 1:A:645:GLN:HB3  | 1.84                    | 0.60        |
| 1:B:311:LYS:HB3  | 1:B:359:THR:HG22 | 1.84                    | 0.60        |
| 1:A:203:LEU:HB3  | 1:A:211:ASP:HB2  | 1.84                    | 0.59        |
| 1:D:620:THR:HG22 | 1:D:629:GLY:HA3  | 1.84                    | 0.59        |
| 1:D:203:LEU:HB3  | 1:D:211:ASP:HB2  | 1.84                    | 0.59        |
| 1:C:417:TRP:CE2  | 1:C:419:ALA:HB2  | 2.37                    | 0.59        |
| 1:C:125:MET:HE3  | 1:C:572:ILE:HG21 | 1.84                    | 0.59        |
| 1:A:113:ASN:HB3  | 1:A:281:TYR:HD1  | 1.68                    | 0.59        |
| 1:C:614:GLU:OE2  | 1:C:616:ARG:NH2  | 2.35                    | 0.59        |
| 1:A:509:SER:OG   | 1:A:510:VAL:N    | 2.33                    | 0.59        |
| 1:A:551:LEU:HD11 | 1:A:608:PRO:HG2  | 1.85                    | 0.59        |
| 1:B:123:ARG:NH1  | 1:B:576:GLU:OE1  | 2.35                    | 0.59        |
| 1:D:91:GLN:HG2   | 1:D:665:ASN:HB3  | 1.85                    | 0.59        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:D:203:LEU:HD12 | 1:D:718:LYS:HB2  | 1.84         | 0.59        |
| 1:D:548:ASP:HB3  | 1:D:567:ASN:ND2  | 2.17         | 0.59        |
| 1:C:91:GLN:NE2   | 1:C:681:ASP:OD1  | 2.34         | 0.59        |
| 1:C:616:ARG:HE   | 1:C:633:ARG:HD2  | 1.67         | 0.59        |
| 1:A:416:THR:HG23 | 1:A:426:ILE:HG13 | 1.85         | 0.58        |
| 1:A:628:ALA:HA   | 1:A:666:GLY:HA2  | 1.85         | 0.58        |
| 1:B:555:ARG:HD2  | 1:B:556:GLU:H    | 1.68         | 0.58        |
| 1:D:493:PHE:CD1  | 1:D:494:PRO:HD2  | 2.38         | 0.58        |
| 1:D:294:GLU:HB2  | 1:D:320:TYR:HB3  | 1.85         | 0.58        |
| 1:B:209:ARG:HD2  | 1:B:234:SER:HB2  | 1.85         | 0.58        |
| 1:B:123:ARG:HG2  | 1:B:542:TYR:CE2  | 2.39         | 0.58        |
| 1:A:363:ASP:OD1  | 1:A:364:ASP:N    | 2.34         | 0.58        |
| 1:B:638:GLN:HE22 | 1:B:640:ARG:HB2  | 1.67         | 0.58        |
| 1:A:533:ASP:OD1  | 1:A:534:LYS:N    | 2.37         | 0.58        |
| 1:B:688:TYR:CE2  | 1:B:710:GLU:HG3  | 2.38         | 0.58        |
| 1:A:189:GLU:OE1  | 1:A:197:ARG:NH2  | 2.37         | 0.57        |
| 1:C:573:MET:HG3  | 1:C:597:TRP:HB3  | 1.85         | 0.57        |
| 1:B:339:MET:HG2  | 1:B:343:MET:SD   | 2.45         | 0.57        |
| 1:A:479:SER:OG   | 1:A:481:THR:OG1  | 2.21         | 0.57        |
| 1:C:441:GLN:HG3  | 1:C:457:ALA:HB1  | 1.86         | 0.57        |
| 1:D:705:ASN:OD1  | 1:D:705:ASN:N    | 2.33         | 0.57        |
| 1:C:394:ASP:O    | 1:C:396:ASP:N    | 2.30         | 0.57        |
| 1:A:209:ARG:NH1  | 1:A:211:ASP:OD2  | 2.32         | 0.57        |
| 1:A:622:GLU:HB3  | 1:A:627:SER:HB3  | 1.86         | 0.57        |
| 1:B:93:VAL:HG12  | 1:B:681:ASP:OD2  | 2.05         | 0.57        |
| 1:A:76:GLN:HE21  | 1:A:529:GLN:NE2  | 2.03         | 0.56        |
| 1:C:443:LEU:HD23 | 1:C:454:ASN:N    | 2.20         | 0.56        |
| 1:D:609:GLN:NE2  | 1:D:652:ASP:OD1  | 2.36         | 0.56        |
| 1:A:338:MET:HE3  | 1:A:339:MET:H    | 1.71         | 0.56        |
| 1:A:646:GLY:HA3  | 1:A:651:LYS:HA   | 1.86         | 0.56        |
| 1:B:583:LEU:HD12 | 1:B:587:TRP:HB3  | 1.87         | 0.56        |
| 1:D:201:SER:HB3  | 1:D:213:VAL:HB   | 1.86         | 0.56        |
| 1:D:260:TRP:NE1  | 1:D:262:PRO:HG3  | 2.21         | 0.56        |
| 1:B:364:ASP:HB3  | 1:B:418:PHE:HB2  | 1.87         | 0.56        |
| 1:A:213:VAL:HG23 | 1:A:230:ASN:HB3  | 1.87         | 0.56        |
| 1:A:78:SER:O     | 1:A:529:GLN:NE2  | 2.38         | 0.56        |
| 1:A:206:SER:HB2  | 1:A:714:THR:HG23 | 1.88         | 0.56        |
| 1:B:311:LYS:HB3  | 1:B:359:THR:CG2  | 2.35         | 0.56        |
| 1:C:441:GLN:NE2  | 1:C:458:ASN:OD1  | 2.39         | 0.56        |
| 1:A:260:TRP:NE1  | 1:A:262:PRO:HG3  | 2.21         | 0.56        |
| 1:C:581:TYR:HD2  | 1:C:582:GLN:H    | 1.53         | 0.56        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:C:497:TRP:O    | 1:C:502:PRO:HD3  | 2.05         | 0.56        |
| 1:D:494:PRO:HB2  | 1:D:499:LEU:HD22 | 1.88         | 0.56        |
| 1:B:238:GLU:HG3  | 1:B:244:THR:HG22 | 1.87         | 0.56        |
| 1:C:339:MET:HG3  | 1:C:340:PRO:HD3  | 1.87         | 0.55        |
| 1:C:653:PHE:CZ   | 1:C:707:THR:HG21 | 2.41         | 0.55        |
| 1:D:608:PRO:HG3  | 1:D:645:GLN:HB3  | 1.87         | 0.55        |
| 1:A:616:ARG:HA   | 1:A:632:TRP:O    | 2.06         | 0.55        |
| 1:C:85:ASN:O     | 1:C:87:LYS:N     | 2.40         | 0.55        |
| 1:C:189:GLU:OE1  | 1:C:197:ARG:NH2  | 2.35         | 0.55        |
| 1:A:667:ALA:HB2  | 1:A:677:SER:HB3  | 1.89         | 0.55        |
| 1:C:151:THR:HA   | 1:C:154:ILE:HG13 | 1.89         | 0.55        |
| 1:B:133:LEU:CD1  | 1:B:173:TRP:HB3  | 2.35         | 0.55        |
| 1:B:689:THR:HG22 | 1:B:709:PRO:HA   | 1.89         | 0.55        |
| 1:C:140:LEU:HB3  | 1:C:349:ARG:HD3  | 1.88         | 0.55        |
| 1:C:521:THR:HG23 | 1:C:546:VAL:HG22 | 1.88         | 0.55        |
| 1:D:682:ASN:HD22 | 1:D:712:GLY:HA2  | 1.71         | 0.55        |
| 1:B:112:ARG:HB3  | 1:B:693:ASN:HB3  | 1.87         | 0.55        |
| 1:C:141:GLY:O    | 1:C:349:ARG:HD2  | 2.07         | 0.55        |
| 1:C:498:GLU:HG2  | 1:C:550:ILE:HG21 | 1.87         | 0.55        |
| 1:A:698:ALA:HA   | 1:A:702:PHE:H    | 1.72         | 0.55        |
| 1:D:91:GLN:HB3   | 1:D:92:PRO:HD3   | 1.89         | 0.55        |
| 1:A:598:GLY:HA3  | 1:A:607:LEU:HD12 | 1.88         | 0.54        |
| 1:B:85:ASN:O     | 1:B:87:LYS:N     | 2.40         | 0.54        |
| 1:C:608:PRO:HB2  | 1:C:646:GLY:HA2  | 1.90         | 0.54        |
| 1:A:143:CYS:SG   | 1:A:147:MET:HG3  | 2.47         | 0.54        |
| 1:A:491:GLU:OE2  | 1:A:520:LYS:HE3  | 2.08         | 0.54        |
| 1:B:432:ASP:O    | 1:B:464:THR:HA   | 2.06         | 0.54        |
| 1:B:672:ARG:H    | 1:B:672:ARG:CD   | 2.18         | 0.54        |
| 1:C:616:ARG:HH21 | 1:C:633:ARG:NE   | 2.06         | 0.54        |
| 1:D:463:ASP:OD1  | 1:D:464:THR:N    | 2.40         | 0.54        |
| 1:D:690:GLU:HB2  | 1:D:693:ASN:OD1  | 2.07         | 0.54        |
| 1:A:198:VAL:HG23 | 1:A:216:ALA:HB2  | 1.88         | 0.54        |
| 1:C:301:VAL:HG22 | 1:C:313:GLU:HG2  | 1.89         | 0.54        |
| 1:A:260:TRP:CE2  | 1:A:262:PRO:HG3  | 2.43         | 0.54        |
| 1:A:603:ASP:HB3  | 1:A:605:ARG:HE   | 1.72         | 0.54        |
| 1:C:360:TRP:HE1  | 1:C:369:THR:CG2  | 2.21         | 0.54        |
| 1:D:169:GLN:OE1  | 1:D:471:ARG:NH1  | 2.40         | 0.54        |
| 1:C:143:CYS:SG   | 1:C:147:MET:HG2  | 2.47         | 0.54        |
| 1:C:364:ASP:N    | 1:C:364:ASP:OD1  | 2.41         | 0.54        |
| 1:A:301:VAL:HA   | 1:A:312:VAL:O    | 2.08         | 0.54        |
| 1:A:91:GLN:HE21  | 1:A:665:ASN:HB3  | 1.73         | 0.54        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:C:223:GLY:HA2  | 1:C:261:THR:HG23 | 1.90         | 0.54        |
| 1:A:442:THR:O    | 1:A:443:LEU:HD23 | 2.08         | 0.53        |
| 1:B:101:TYR:CD1  | 1:B:156:PRO:HG2  | 2.42         | 0.53        |
| 1:D:584:THR:OG1  | 1:D:585:GLY:N    | 2.40         | 0.53        |
| 1:D:143:CYS:SG   | 1:D:147:MET:HG3  | 2.48         | 0.53        |
| 1:D:359:THR:HG23 | 1:D:368:VAL:HG12 | 1.91         | 0.53        |
| 1:D:141:GLY:O    | 1:D:349:ARG:HD3  | 2.09         | 0.53        |
| 1:D:171:VAL:HG22 | 1:D:414:GLU:HG3  | 1.91         | 0.53        |
| 1:C:583:LEU:HD12 | 1:C:587:TRP:HB3  | 1.90         | 0.53        |
| 1:C:547:GLN:NE2  | 1:D:433:ARG:HE   | 2.05         | 0.53        |
| 1:C:190:ARG:HE   | 1:C:190:ARG:HA   | 1.74         | 0.53        |
| 1:D:628:ALA:HA   | 1:D:666:GLY:HA2  | 1.91         | 0.53        |
| 1:C:74:VAL:CG2   | 1:C:105:ILE:HG12 | 2.39         | 0.53        |
| 1:C:682:ASN:HD22 | 1:C:712:GLY:CA   | 2.22         | 0.53        |
| 1:D:261:THR:O    | 1:D:261:THR:OG1  | 2.24         | 0.52        |
| 1:B:265:ASP:OD1  | 1:B:304:ASN:ND2  | 2.42         | 0.52        |
| 1:D:96:SER:O     | 1:D:96:SER:OG    | 2.25         | 0.52        |
| 1:A:84:THR:HG22  | 1:A:162:LEU:HB3  | 1.92         | 0.52        |
| 1:B:171:VAL:HG23 | 1:B:412:PHE:HB2  | 1.90         | 0.52        |
| 1:C:385:TYR:CG   | 1:C:386:ASP:N    | 2.75         | 0.52        |
| 1:D:671:THR:CG2  | 1:D:674:VAL:HG12 | 2.37         | 0.52        |
| 1:A:506:PRO:HB2  | 1:A:515:LYS:HD3  | 1.91         | 0.52        |
| 1:B:157:GLU:OE1  | 1:B:718:LYS:NZ   | 2.27         | 0.52        |
| 1:C:586:ASN:HB3  | 1:C:621:TYR:CE2  | 2.45         | 0.52        |
| 1:C:613:LEU:HD23 | 1:C:614:GLU:H    | 1.75         | 0.52        |
| 1:A:108:PHE:HZ   | 1:A:182:ILE:HD11 | 1.74         | 0.52        |
| 1:B:326:ASP:HA   | 1:B:343:MET:O    | 2.10         | 0.52        |
| 1:B:471:ARG:HD2  | 1:B:473:GLU:OE2  | 2.10         | 0.52        |
| 1:C:123:ARG:HB3  | 1:C:542:TYR:OH   | 2.10         | 0.52        |
| 1:C:555:ARG:NH2  | 1:C:562:SER:OG   | 2.43         | 0.52        |
| 1:C:609:GLN:NE2  | 1:C:652:ASP:OD1  | 2.35         | 0.52        |
| 1:D:119:ASP:OD2  | 1:D:146:ARG:NH1  | 2.43         | 0.52        |
| 1:D:290:GLN:HB3  | 1:D:324:ILE:H    | 1.74         | 0.52        |
| 1:A:363:ASP:CG   | 1:A:364:ASP:H    | 2.12         | 0.52        |
| 1:C:475:ASP:N    | 1:C:475:ASP:OD1  | 2.42         | 0.52        |
| 1:D:479:SER:OG   | 1:D:481:THR:OG1  | 2.14         | 0.52        |
| 1:A:209:ARG:HD2  | 1:A:234:SER:HB2  | 1.92         | 0.52        |
| 1:B:189:GLU:HB2  | 1:B:224:TYR:CD2  | 2.45         | 0.52        |
| 1:B:403:ASP:HB2  | 1:B:440:ARG:HG2  | 1.92         | 0.52        |
| 1:D:76:GLN:HE21  | 1:D:166:LYS:HE3  | 1.74         | 0.52        |
| 1:D:341:MET:HB3  | 1:D:385:TYR:CD1  | 2.44         | 0.52        |



|                  | A la C           | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:A:613:LEU:HD12 | 1:A:614:GLU:N    | 2.25         | 0.51        |
| 1:B:682:ASN:HB3  | 1:B:712:GLY:O    | 2.10         | 0.51        |
| 1:C:343:MET:HB2  | 1:C:383:SER:OG   | 2.11         | 0.51        |
| 1:B:203:LEU:HB3  | 1:B:211:ASP:HB2  | 1.92         | 0.51        |
| 1:C:438:ASP:OD1  | 1:C:439:TYR:N    | 2.43         | 0.51        |
| 1:D:348:ASP:OD2  | 1:D:379:ARG:NH2  | 2.43         | 0.51        |
| 1:B:103:LYS:HG2  | 1:B:110:VAL:HG21 | 1.91         | 0.51        |
| 1:D:91:GLN:CG    | 1:D:665:ASN:HB3  | 2.40         | 0.51        |
| 1:C:203:LEU:HD12 | 1:C:718:LYS:HG3  | 1.92         | 0.51        |
| 1:C:613:LEU:HD23 | 1:C:614:GLU:N    | 2.25         | 0.51        |
| 1:A:202:LEU:HD13 | 1:C:225:LEU:HD12 | 1.93         | 0.51        |
| 1:A:115:GLY:N    | 1:A:247:SER:HB2  | 2.26         | 0.51        |
| 1:D:309:LEU:HD12 | 1:D:360:TRP:CH2  | 2.46         | 0.51        |
| 1:D:577:LEU:CD2  | 1:D:593:LEU:HB3  | 2.41         | 0.51        |
| 1:A:314:ALA:HB2  | 1:A:356:LEU:HD12 | 1.93         | 0.51        |
| 1:A:623:GLU:O    | 1:A:625:ASP:N    | 2.40         | 0.51        |
| 1:D:614:GLU:OE2  | 1:D:633:ARG:NE   | 2.31         | 0.51        |
| 1:A:671:THR:HG22 | 1:A:674:VAL:CG1  | 2.40         | 0.51        |
| 1:D:445:SER:OG   | 1:D:445:SER:O    | 2.26         | 0.50        |
| 1:A:74:VAL:HG23  | 1:A:104:THR:O    | 2.11         | 0.50        |
| 1:B:176:GLY:O    | 1:B:492:ARG:HD3  | 2.11         | 0.50        |
| 1:C:138:MET:O    | 1:C:319:ASN:ND2  | 2.40         | 0.50        |
| 1:A:126:PHE:CG   | 1:A:127:GLY:N    | 2.79         | 0.50        |
| 1:A:386:ASP:HB3  | 1:A:391:TYR:H    | 1.75         | 0.50        |
| 1:B:498:GLU:HB3  | 1:B:550:ILE:HG21 | 1.92         | 0.50        |
| 1:C:461:ARG:NH1  | 1:C:513:PHE:O    | 2.43         | 0.50        |
| 1:C:549:PHE:N    | 1:C:568:VAL:O    | 2.35         | 0.50        |
| 1:B:91:GLN:HE22  | 1:B:663:SER:HB3  | 1.76         | 0.50        |
| 1:B:172:LEU:HD21 | 1:B:414:GLU:HB2  | 1.93         | 0.50        |
| 1:B:260:TRP:CE2  | 1:B:262:PRO:HG3  | 2.47         | 0.50        |
| 1:B:586:ASN:ND2  | 1:B:623:GLU:HB2  | 2.26         | 0.50        |
| 1:C:463:ASP:OD1  | 1:C:464:THR:N    | 2.43         | 0.50        |
| 1:C:84:THR:HG21  | 1:C:90:ARG:HH12  | 1.76         | 0.50        |
| 1:D:512:ALA:O    | 1:D:514:ASP:N    | 2.45         | 0.50        |
| 1:A:549:PHE:HE2  | 1:A:551:LEU:HD13 | 1.75         | 0.50        |
| 1:C:202:LEU:O    | 1:C:718:LYS:HA   | 2.12         | 0.50        |
| 1:C:642:ALA:O    | 1:C:652:ASP:HB2  | 2.11         | 0.50        |
| 1:D:97:ASP:HA    | 1:D:154:ILE:O    | 2.11         | 0.50        |
| 1:A:671:THR:HG23 | 1:A:673:ASN:H    | 1.77         | 0.50        |
| 1:C:171:VAL:HG22 | 1:C:414:GLU:OE2  | 2.12         | 0.50        |
| 1:C:287:ASP:OD1  | 1:C:331:ARG:HD3  | 2.12         | 0.50        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:C:379:ARG:HD2  | 1:C:400:TRP:HB3  | 1.92         | 0.50        |
| 1:C:618:GLY:HA2  | 1:C:630:SER:O    | 2.12         | 0.50        |
| 1:A:379:ARG:HG2  | 1:A:402:LYS:HB2  | 1.94         | 0.49        |
| 1:A:544:GLY:O    | 1:A:572:ILE:HG13 | 2.11         | 0.49        |
| 1:C:661:VAL:HG21 | 1:C:688:TYR:CZ   | 2.47         | 0.49        |
| 1:D:72:THR:HG22  | 1:D:631:LEU:HD22 | 1.92         | 0.49        |
| 1:A:238:GLU:HA   | 1:A:243:ASN:O    | 2.11         | 0.49        |
| 1:C:148:ASP:HB3  | 1:C:291:PHE:CE1  | 2.47         | 0.49        |
| 1:A:248:ARG:HD3  | 1:A:280:ARG:NH2  | 2.27         | 0.49        |
| 1:B:113:ASN:HB3  | 1:B:281:TYR:CD1  | 2.47         | 0.49        |
| 1:D:454:ASN:OD1  | 1:D:456:THR:N    | 2.43         | 0.49        |
| 1:D:586:ASN:N    | 1:D:586:ASN:OD1  | 2.46         | 0.49        |
| 1:B:703:SER:O    | 1:B:703:SER:OG   | 2.23         | 0.49        |
| 1:A:633:ARG:NH2  | 1:A:690:GLU:OE1  | 2.41         | 0.49        |
| 1:A:236:ASP:N    | 1:A:236:ASP:OD1  | 2.43         | 0.49        |
| 1:A:339:MET:HE2  | 1:A:343:MET:HB3  | 1.94         | 0.49        |
| 1:D:84:THR:HG23  | 1:D:162:LEU:HB3  | 1.95         | 0.49        |
| 1:D:497:TRP:O    | 1:D:501:SER:HB2  | 2.13         | 0.49        |
| 1:D:554:TYR:CD2  | 1:D:651:LYS:HB3  | 2.48         | 0.49        |
| 1:A:113:ASN:HB3  | 1:A:281:TYR:CD1  | 2.47         | 0.49        |
| 1:B:494:PRO:HA   | 1:B:498:GLU:OE1  | 2.12         | 0.49        |
| 1:A:287:ASP:OD2  | 1:A:331:ARG:HG2  | 2.13         | 0.49        |
| 1:C:155:SER:HB3  | 1:C:158:THR:HG23 | 1.95         | 0.49        |
| 1:C:234:SER:HB3  | 1:C:249:TRP:CE2  | 2.48         | 0.49        |
| 1:A:91:GLN:O     | 1:A:93:VAL:N     | 2.45         | 0.48        |
| 1:C:70:VAL:HG22  | 1:C:89:PRO:HB2   | 1.94         | 0.48        |
| 1:D:513:PHE:HD1  | 1:D:513:PHE:O    | 1.96         | 0.48        |
| 1:D:584:THR:HG23 | 1:D:586:ASN:N    | 2.28         | 0.48        |
| 1:A:119:ASP:HB3  | 1:A:126:PHE:HE1  | 1.77         | 0.48        |
| 1:B:91:GLN:HG3   | 1:B:665:ASN:CG   | 2.33         | 0.48        |
| 1:B:91:GLN:HG2   | 1:B:716:TRP:HZ2  | 1.78         | 0.48        |
| 1:D:95:ALA:HB3   | 1:D:100:ASP:OD2  | 2.13         | 0.48        |
| 1:D:197:ARG:CZ   | 1:D:197:ARG:HB2  | 2.41         | 0.48        |
| 1:A:164:VAL:HG13 | 1:A:182:ILE:HD13 | 1.96         | 0.48        |
| 1:A:269:GLU:O    | 1:A:298:LEU:HD12 | 2.13         | 0.48        |
| 1:B:224:TYR:OH   | 1:B:269:GLU:OE1  | 2.19         | 0.48        |
| 1:A:82:ILE:HD11  | 1:A:166:LYS:HE2  | 1.96         | 0.48        |
| 1:B:306:SER:OG   | 1:B:307:ASP:N    | 2.46         | 0.48        |
| 1:C:203:LEU:HB3  | 1:C:211:ASP:CB   | 2.40         | 0.48        |
| 1:C:309:LEU:HD13 | 1:C:360:TRP:CE3  | 2.49         | 0.48        |
| 1:A:552:PHE:HB2  | 1:A:647:ASN:HA   | 1.95         | 0.48        |



|                  | is as pagem      | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 1:C:698:ALA:HB2  | 1:C:702:PHE:HB2  | 1.96         | 0.48        |
| 1:A:630:SER:HB2  | 1:A:662:PHE:CZ   | 2.49         | 0.48        |
| 1:B:264:GLU:CD   | 1:B:264:GLU:H    | 2.16         | 0.48        |
| 1:B:475:ASP:OD1  | 1:B:475:ASP:N    | 2.46         | 0.48        |
| 1:B:206:SER:HG   | 1:B:715:PHE:H    | 1.61         | 0.48        |
| 1:C:162:LEU:HD13 | 1:C:184:PHE:CE2  | 2.49         | 0.48        |
| 1:C:578:GLY:HA2  | 1:C:592:SER:HA   | 1.94         | 0.48        |
| 1:D:151:THR:HA   | 1:D:154:ILE:HD12 | 1.96         | 0.48        |
| 1:D:467:SER:HB2  | 1:D:489:HIS:O    | 2.14         | 0.48        |
| 1:A:428:GLY:O    | 1:A:429:LEU:HD23 | 2.14         | 0.48        |
| 1:A:668:TYR:HE2  | 1:A:670:VAL:HG22 | 1.78         | 0.48        |
| 1:B:280:ARG:HA   | 1:B:287:ASP:HB3  | 1.95         | 0.48        |
| 1:C:494:PRO:HB2  | 1:C:499:LEU:HG   | 1.95         | 0.48        |
| 1:C:497:TRP:O    | 1:C:501:SER:HB2  | 2.14         | 0.48        |
| 1:D:631:LEU:HD12 | 1:D:632:TRP:N    | 2.28         | 0.48        |
| 1:B:99:ALA:HB1   | 1:B:110:VAL:HG13 | 1.94         | 0.48        |
| 1:C:432:ASP:O    | 1:C:464:THR:HA   | 2.14         | 0.48        |
| 1:C:515:LYS:NZ   | 1:D:514:ASP:OD2  | 2.47         | 0.48        |
| 1:D:298:LEU:O    | 1:D:315:GLN:HA   | 2.14         | 0.48        |
| 1:D:423:ASP:OD2  | 1:D:472:TYR:OH   | 2.28         | 0.48        |
| 1:D:584:THR:HG23 | 1:D:586:ASN:H    | 1.78         | 0.48        |
| 1:A:445:SER:O    | 1:A:445:SER:OG   | 2.27         | 0.48        |
| 1:D:101:TYR:CD1  | 1:D:156:PRO:HG2  | 2.49         | 0.48        |
| 1:D:197:ARG:HH12 | 1:D:217:ALA:HB3  | 1.79         | 0.48        |
| 1:D:577:LEU:HD21 | 1:D:593:LEU:HB3  | 1.96         | 0.48        |
| 1:A:79:PRO:HB3   | 1:A:484:TYR:CD2  | 2.48         | 0.47        |
| 1:A:495:ASP:HB2  | 1:A:498:GLU:HG3  | 1.96         | 0.47        |
| 1:A:694:LYS:HB3  | 1:A:694:LYS:HE3  | 1.55         | 0.47        |
| 1:B:584:THR:HG22 | 1:B:585:GLY:H    | 1.78         | 0.47        |
| 1:B:635:VAL:HG22 | 1:B:636:ALA:O    | 2.14         | 0.47        |
| 1:C:520:LYS:NZ   | 1:D:464:THR:O    | 2.38         | 0.47        |
| 1:D:80:LEU:HD22  | 1:D:166:LYS:O    | 2.14         | 0.47        |
| 1:B:309:LEU:HD21 | 1:B:358:ALA:HB1  | 1.96         | 0.47        |
| 1:A:91:GLN:HB3   | 1:A:92:PRO:CD    | 2.42         | 0.47        |
| 1:A:128:SER:OG   | 1:A:495:ASP:OD1  | 2.24         | 0.47        |
| 1:B:84:THR:OG1   | 1:B:85:ASN:N     | 2.41         | 0.47        |
| 1:B:236:ASP:OD2  | 1:B:280:ARG:NH1  | 2.47         | 0.47        |
| 1:B:501:SER:N    | 1:B:502:PRO:HD2  | 2.30         | 0.47        |
| 1:C:82:ILE:HG21  | 1:C:105:ILE:HD13 | 1.96         | 0.47        |
| 1:D:325:MET:HE2  | 1:D:325:MET:HB2  | 1.73         | 0.47        |
| 1:C:74:VAL:HG23  | 1:C:105:ILE:HG12 | 1.97         | 0.47        |



| Interatomic Clash |                  |              |             |  |  |  |
|-------------------|------------------|--------------|-------------|--|--|--|
| Atom-1            | Atom-2           | distance (Å) | overlap (Å) |  |  |  |
| 1:C:176:GLY:HA3   | 1:C:492:ABG:HG3  | 1.96         | 0.47        |  |  |  |
| 1:C:314:ALA:HB2   | 1:C:356:LEU:HD12 | 1.94         | 0.47        |  |  |  |
| 1:C:588:LYS:HB3   | 1:C:620:THR:OG1  | 2.15         | 0.47        |  |  |  |
| 1:A:432:ASP:O     | 1:A:464:THR:HA   | 2.14         | 0.47        |  |  |  |
| 1:A:491:GLU:HA    | 1:A:519:GLU:O    | 2.14         | 0.47        |  |  |  |
| 1:D:438:ASP:OD1   | 1:D:439:TYR:N    | 2.48         | 0.47        |  |  |  |
| 1:B:334:ASP:O     | 1:B:337:SER:OG   | 2.33         | 0.47        |  |  |  |
| 1:D:334:ASP:N     | 1:D:334:ASP:OD1  | 2.47         | 0.47        |  |  |  |
| 1:A:431:LEU:HD13  | 1:A:466:PRO:HB3  | 1.97         | 0.47        |  |  |  |
| 1:B:635:VAL:HG11  | 1:B:659:PHE:CE2  | 2.50         | 0.47        |  |  |  |
| 1:B:661:VAL:HG21  | 1:B:688:TYR:CZ   | 2.50         | 0.47        |  |  |  |
| 1:C:385:TYR:O     | 1:C:386:ASP:HB2  | 2.14         | 0.47        |  |  |  |
| 1:B:143:CYS:SG    | 1:B:147:MET:HG3  | 2.55         | 0.47        |  |  |  |
| 1:B:305:VAL:HB    | 1:B:309:LEU:HB3  | 1.96         | 0.47        |  |  |  |
| 1:B:350:ARG:HH22  | 1:B:379:ARG:NH2  | 2.13         | 0.47        |  |  |  |
| 1:C:91:GLN:O      | 1:C:93:VAL:N     | 2.47         | 0.47        |  |  |  |
| 1:D:214:LEU:HD12  | 1:D:215:ASP:N    | 2.29         | 0.47        |  |  |  |
| 1:A:681:ASP:O     | 1:A:713:ARG:HA   | 2.15         | 0.47        |  |  |  |
| 1:B:213:VAL:HG22  | 1:B:230:ASN:HB2  | 1.97         | 0.47        |  |  |  |
| 1:B:221:ARG:NH1   | 1:B:264:GLU:OE2  | 2.48         | 0.47        |  |  |  |
| 1:B:517:LYS:HD3   | 1:B:548:ASP:OD2  | 2.14         | 0.47        |  |  |  |
| 1:D:108:PHE:HA    | 1:D:121:VAL:O    | 2.15         | 0.47        |  |  |  |
| 1:D:463:ASP:HB3   | 1:D:465:LEU:HD11 | 1.97         | 0.47        |  |  |  |
| 1:B:84:THR:CG2    | 1:B:162:LEU:HB3  | 2.43         | 0.46        |  |  |  |
| 1:B:638:GLN:NE2   | 1:B:640:ARG:HB2  | 2.29         | 0.46        |  |  |  |
| 1:C:204:ALA:HA    | 1:C:209:ARG:O    | 2.16         | 0.46        |  |  |  |
| 1:A:101:TYR:OH    | 1:A:157:GLU:HG3  | 2.14         | 0.46        |  |  |  |
| 1:B:91:GLN:HG3    | 1:B:665:ASN:OD1  | 2.16         | 0.46        |  |  |  |
| 1:B:491:GLU:HA    | 1:B:519:GLU:O    | 2.15         | 0.46        |  |  |  |
| 1:C:373:ALA:HA    | 1:C:408:ASN:O    | 2.15         | 0.46        |  |  |  |
| 1:C:672:ARG:HG2   | 1:C:672:ARG:HH21 | 1.80         | 0.46        |  |  |  |
| 1:D:108:PHE:CE1   | 1:D:122:LEU:HB2  | 2.49         | 0.46        |  |  |  |
| 1:A:257:ALA:HA    | 1:A:270:LEU:O    | 2.15         | 0.46        |  |  |  |
| 1:B:491:GLU:OE1   | 1:B:520:LYS:HG2  | 2.16         | 0.46        |  |  |  |
| 1:C:489:HIS:HA    | 1:C:521:THR:O    | 2.16         | 0.46        |  |  |  |
| 1:D:407:HIS:HB2   | 1:D:435:SER:OG   | 2.15         | 0.46        |  |  |  |
| 1:C:97:ASP:O      | 1:C:101:TYR:HD1  | 1.98         | 0.46        |  |  |  |
| 1:D:139:MET:O     | 1:D:140:LEU:HD23 | 2.16         | 0.46        |  |  |  |
| 1:A:556:GLU:OE1   | 1:A:561:SER:HB3  | 2.15         | 0.46        |  |  |  |
| 1:A:593:LEU:HD21  | 1:A:613:LEU:HD11 | 1.98         | 0.46        |  |  |  |
| 1:B:626:TRP:HB3   | 1:B:668:TYR:HD1  | 1.81         | 0.46        |  |  |  |



|                  | o uo puge        | Interatomic  | Clash       |  |  |
|------------------|------------------|--------------|-------------|--|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |  |
| 1:C:266:THR:OG1  | 1:C:302:LYS:HE3  | 2.16         | 0.46        |  |  |
| 1:C:436:VAL:HG22 | 1:C:513:PHE:HE2  | 1.81         | 0.46        |  |  |
| 1:C:691:HIS:O    | 1:C:691:HIS:ND1  | 2.49         | 0.46        |  |  |
| 1:B:91:GLN:NE2   | 1:B:664:LEU:O    | 2.49         | 0.46        |  |  |
| 1:B:111:ILE:HG12 | 1:B:119:ASP:O    | 2.15         | 0.46        |  |  |
| 1:B:638:GLN:NE2  | 1:B:640:ARG:H    | 2.13         | 0.46        |  |  |
| 1:D:204:ALA:HA   | 1:D:209:ARG:O    | 2.15         | 0.46        |  |  |
| 1:D:593:LEU:HD12 | 1:D:615:ALA:HB2  | 1.98         | 0.46        |  |  |
| 1:A:287:ASP:CG   | 1:A:331:ARG:HE   | 2.19         | 0.46        |  |  |
| 1:B:73:GLY:HA2   | 1:B:104:THR:O    | 2.14         | 0.46        |  |  |
| 1:C:555:ARG:HH12 | 1:C:564:GLN:HB2  | 1.81         | 0.46        |  |  |
| 1:A:240:GLY:HA3  | 1:A:687:ASP:HA   | 1.98         | 0.46        |  |  |
| 1:B:93:VAL:HG11  | 1:B:716:TRP:CD1  | 2.51         | 0.46        |  |  |
| 1:C:555:ARG:HB3  | 1:C:555:ARG:CZ   | 2.46         | 0.46        |  |  |
| 1:C:672:ARG:HG2  | 1:C:672:ARG:NH2  | 2.31         | 0.46        |  |  |
| 1:D:267:LEU:HD12 | 1:D:268:ILE:H    | 1.81         | 0.46        |  |  |
| 1:A:464:THR:C    | 1:A:465:LEU:HD23 | 2.36         | 0.46        |  |  |
| 1:D:248:ARG:HD3  | 1:D:280:ARG:NH2  | 2.31         | 0.46        |  |  |
| 1:D:689:THR:HG23 | 1:D:708:VAL:O    | 2.16         | 0.45        |  |  |
| 1:A:359:THR:HG23 | 1:A:368:VAL:HG22 | 1.97         | 0.45        |  |  |
| 1:A:623:GLU:HG2  | 1:A:626:TRP:NE1  | 2.30         | 0.45        |  |  |
| 1:A:667:ALA:CB   | 1:A:677:SER:HB3  | 2.45         | 0.45        |  |  |
| 1:A:710:GLU:HG3  | 1:A:711:PRO:HD2  | 1.97         | 0.45        |  |  |
| 1:B:690:GLU:HB2  | 1:B:693:ASN:OD1  | 2.17         | 0.45        |  |  |
| 1:D:267:LEU:HD12 | 1:D:268:ILE:N    | 2.31         | 0.45        |  |  |
| 1:B:81:THR:HG22  | 1:B:165:ILE:HD13 | 1.99         | 0.45        |  |  |
| 1:A:429:LEU:HD21 | 1:B:429:LEU:HD11 | 1.99         | 0.45        |  |  |
| 1:D:89:PRO:HG3   | 1:D:718:LYS:HD3  | 1.99         | 0.45        |  |  |
| 1:A:171:VAL:HB   | 1:A:430:ARG:HB3  | 1.99         | 0.45        |  |  |
| 1:A:612:PRO:HB3  | 1:A:638:GLN:HB2  | 1.99         | 0.45        |  |  |
| 1:B:367:LEU:HD12 | 1:B:414:GLU:O    | 2.16         | 0.45        |  |  |
| 1:D:504:ARG:HG3  | 1:D:564:GLN:HG3  | 1.98         | 0.45        |  |  |
| 1:D:673:ASN:OD1  | 1:D:673:ASN:N    | 2.48         | 0.45        |  |  |
| 1:B:202:LEU:O    | 1:B:718:LYS:HA   | 2.15         | 0.45        |  |  |
| 1:D:139:MET:SD   | 1:D:319:ASN:HB3  | 2.57         | 0.45        |  |  |
| 1:A:158:THR:CG2  | 1:A:230:ASN:HD22 | 2.29         | 0.45        |  |  |
| 1:B:103:LYS:HG2  | 1:B:110:VAL:CG2  | 2.45         | 0.45        |  |  |
| 1:B:327:ASN:OD1  | 1:B:342:PRO:HA   | 2.17         | 0.45        |  |  |
| 1:C:170:THR:HG21 | 1:C:173:TRP:HD1  | 1.81         | 0.45        |  |  |
| 1:C:694:LYS:HB3  | 1:C:695:ALA:H    | 1.69         | 0.45        |  |  |
| 1:D:437:LYS:HD3  | 1:D:439:TYR:CZ   | 2.52         | 0.45        |  |  |



|                  |                  | Interatomic             | Clash       |
|------------------|------------------|-------------------------|-------------|
| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 1:C:214:LEU:HD12 | 1:C:215:ASP:N    | 2.29                    | 0.45        |
| 1:C:276:ASP:OD1  | 1:C:277:GLY:N    | 2.44                    | 0.45        |
| 1:C:437:LYS:HG3  | 1:C:459:ASP:O    | 2.17                    | 0.45        |
| 1:B:651:LYS:HB3  | 1:B:651:LYS:HE2  | 1.55                    | 0.45        |
| 1:C:230:ASN:OD1  | 1:C:253:ASN:ND2  | 2.47                    | 0.45        |
| 1:C:638:GLN:N    | 1:C:656:SER:OG   | 2.36                    | 0.45        |
| 1:D:198:VAL:CG1  | 1:D:723:PHE:HB2  | 2.47                    | 0.45        |
| 1:D:472:TYR:CZ   | 1:D:474:HIS:HB2  | 2.51                    | 0.45        |
| 1:A:250:LYS:HB2  | 1:A:278:GLU:HG2  | 1.98                    | 0.44        |
| 1:A:661:VAL:HG21 | 1:A:688:TYR:CE1  | 2.52                    | 0.44        |
| 1:D:438:ASP:OD1  | 1:D:440:ARG:HG3  | 2.17                    | 0.44        |
| 1:D:515:LYS:O    | 1:D:516:ILE:HG12 | 2.17                    | 0.44        |
| 1:A:108:PHE:CE2  | 1:A:122:LEU:HD13 | 2.53                    | 0.44        |
| 1:B:120:PRO:HG3  | 1:B:151:THR:HG21 | 1.98                    | 0.44        |
| 1:D:158:THR:OG1  | 1:D:186:ARG:NH2  | 2.50                    | 0.44        |
| 1:A:313:GLU:O    | 1:A:356:LEU:HA   | 2.17                    | 0.44        |
| 1:A:697:ASP:C    | 1:A:699:GLY:H    | 2.21                    | 0.44        |
| 1:B:555:ARG:HD2  | 1:B:556:GLU:N    | 2.32                    | 0.44        |
| 1:B:359:THR:OG1  | 1:B:368:VAL:HG22 | 2.16                    | 0.44        |
| 1:C:371:VAL:HA   | 1:C:411:ALA:HA   | 1.99                    | 0.44        |
| 1:D:343:MET:HA   | 1:D:392:TYR:HE2  | 1.81                    | 0.44        |
| 1:A:698:ALA:N    | 1:A:702:PHE:HB2  | 2.28                    | 0.44        |
| 1:C:710:GLU:HB3  | 1:C:711:PRO:HD2  | 1.99                    | 0.44        |
| 1:A:443:LEU:HG   | 1:A:454:ASN:HB2  | 1.98                    | 0.44        |
| 1:C:367:LEU:HB2  | 1:C:415:LEU:HD23 | 2.00                    | 0.44        |
| 1:A:86:PRO:HG2   | 1:A:159:TYR:O    | 2.18                    | 0.44        |
| 1:B:476:LEU:HD23 | 1:B:476:LEU:HA   | 1.84                    | 0.44        |
| 1:C:113:ASN:HB2  | 1:C:281:TYR:HD2  | 1.82                    | 0.44        |
| 1:C:374:MET:SD   | 1:C:376:ASN:ND2  | 2.89                    | 0.44        |
| 1:D:374:MET:HE3  | 1:D:408:ASN:HB3  | 2.00                    | 0.44        |
| 1:A:494:PRO:HB2  | 1:A:499:LEU:HG   | 1.99                    | 0.44        |
| 1:B:481:THR:HA   | 1:B:529:GLN:O    | 2.17                    | 0.44        |
| 1:B:516:ILE:HA   | 1:B:516:ILE:HD13 | 1.80                    | 0.44        |
| 1:D:350:ARG:HH22 | 1:D:379:ARG:NH2  | 2.16                    | 0.44        |
| 1:A:189:GLU:HB2  | 1:A:224:TYR:CD1  | 2.52                    | 0.44        |
| 1:A:661:VAL:HG21 | 1:A:688:TYR:CZ   | 2.53                    | 0.44        |
| 1:B:304:ASN:OD1  | 1:B:304:ASN:N    | 2.50                    | 0.44        |
| 1:B:428:GLY:O    | 1:B:429:LEU:HD23 | 2.18                    | 0.44        |
| 1:D:84:THR:CG2   | 1:D:162:LEU:HB3  | 2.48                    | 0.44        |
| 1:D:85:ASN:ND2   | 1:D:88:GLU:HG2   | 2.33                    | 0.44        |
| 1:D:597:TRP:CH2  | 1:D:599:LYS:HB2  | 2.53                    | 0.44        |



|                  | • • • • • •      | Interatomic  | Clash       |  |  |
|------------------|------------------|--------------|-------------|--|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |  |
| 1:D:608:PRO:HB3  | 1:D:642:ALA:HB3  | 2.00         | 0.44        |  |  |
| 1:A:157:GLU:H    | 1:A:157:GLU:CD   | 2.21         | 0.43        |  |  |
| 1:B:125:MET:HB3  | 1:B:129:ARG:HD2  | 2.00         | 0.43        |  |  |
| 1:C:133:LEU:HD13 | 1:C:136:GLY:O    | 2.17         | 0.43        |  |  |
| 1:C:140:LEU:HB3  | 1:C:349:ARG:CD   | 2.48         | 0.43        |  |  |
| 1:D:76:GLN:HE21  | 1:D:166:LYS:CE   | 2.31         | 0.43        |  |  |
| 1:B:111:ILE:CG2  | 1:B:692:LEU:HB3  | 2.39         | 0.43        |  |  |
| 1:B:189:GLU:OE1  | 1:B:226:ARG:HD2  | 2.18         | 0.43        |  |  |
| 1:C:284:ARG:NH1  | 1:C:694:LYS:HG3  | 2.32         | 0.43        |  |  |
| 1:C:292:LYS:HB3  | 1:C:322:ASP:HB3  | 2.00         | 0.43        |  |  |
| 1:C:581:TYR:CD2  | 1:C:582:GLN:N    | 2.86         | 0.43        |  |  |
| 1:D:326:ASP:OD2  | 1:D:329:ARG:NE   | 2.51         | 0.43        |  |  |
| 1:B:149:ALA:O    | 1:B:152:SER:N    | 2.42         | 0.43        |  |  |
| 1:C:84:THR:CG2   | 1:C:90:ARG:HH12  | 2.31         | 0.43        |  |  |
| 1:D:334:ASP:HB2  | 1:D:335:PRO:HD3  | 2.00         | 0.43        |  |  |
| 1:A:78:SER:HB2   | 1:A:81:THR:HB    | 2.01         | 0.43        |  |  |
| 1:A:154:ILE:HG21 | 1:A:184:PHE:CD2  | 2.54         | 0.43        |  |  |
| 1:A:162:LEU:HD13 | 1:A:184:PHE:CE1  | 2.52         | 0.43        |  |  |
| 1:B:438:ASP:HB2  | 1:B:513:PHE:CE2  | 2.53         | 0.43        |  |  |
| 1:C:116:SER:HG   | 1:C:117:ASN:H    | 1.66         | 0.43        |  |  |
| 1:C:524:LEU:HD23 | 1:C:543:VAL:HG22 | 2.01         | 0.43        |  |  |
| 1:A:249:TRP:O    | 1:A:250:LYS:HG2  | 2.18         | 0.43        |  |  |
| 1:A:288:GLY:HA3  | 1:A:291:PHE:CZ   | 2.53         | 0.43        |  |  |
| 1:A:438:ASP:HB2  | 1:A:513:PHE:CE2  | 2.54         | 0.43        |  |  |
| 1:B:577:LEU:HD11 | 1:B:593:LEU:HD22 | 2.00         | 0.43        |  |  |
| 1:B:324:ILE:HG12 | 1:B:346:GLN:HG3  | 2.01         | 0.43        |  |  |
| 1:B:612:PRO:HG2  | 1:B:635:VAL:CG2  | 2.49         | 0.43        |  |  |
| 1:C:278:GLU:HA   | 1:C:288:GLY:O    | 2.18         | 0.43        |  |  |
| 1:D:234:SER:OG   | 1:D:235:ASP:N    | 2.51         | 0.43        |  |  |
| 1:D:584:THR:HG23 | 1:D:587:TRP:H    | 1.83         | 0.43        |  |  |
| 1:B:85:ASN:C     | 1:B:87:LYS:H     | 2.22         | 0.43        |  |  |
| 1:B:363:ASP:CG   | 1:B:364:ASP:H    | 2.20         | 0.43        |  |  |
| 1:C:261:THR:OG1  | 1:C:261:THR:O    | 2.36         | 0.43        |  |  |
| 1:C:346:GLN:NE2  | 1:C:381:ARG:HD2  | 2.33         | 0.43        |  |  |
| 1:C:581:TYR:HD2  | 1:C:582:GLN:N    | 2.16         | 0.43        |  |  |
| 1:A:635:VAL:HG21 | 1:A:659:PHE:CZ   | 2.54         | 0.43        |  |  |
| 1:B:91:GLN:NE2   | 1:B:680:VAL:O    | 2.52         | 0.43        |  |  |
| 1:B:248:ARG:HG2  | 1:B:249:TRP:N    | 2.34         | 0.43        |  |  |
| 1:B:255:ASP:HA   | 1:B:273:GLY:HA3  | 2.00         | 0.43        |  |  |
| 1:C:199:ASN:HB2  | 1:C:215:ASP:HB3  | 2.01         | 0.43        |  |  |
| 1:C:515:LYS:HB2  | 1:C:515:LYS:HE2  | 1.89         | 0.43        |  |  |



|                  | ti a             | Interatomic  | Clash       |  |  |
|------------------|------------------|--------------|-------------|--|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |  |
| 1:A:143:CYS:HB2  | 1:A:325:MET:SD   | 2.59         | 0.43        |  |  |
| 1:B:203:LEU:O    | 1:B:210:PHE:HA   | 2.19         | 0.43        |  |  |
| 1:C:371:VAL:HG12 | 1:C:411:ALA:HB2  | 2.01         | 0.43        |  |  |
| 1:C:405:VAL:O    | 1:C:436:VAL:HA   | 2.17         | 0.43        |  |  |
| 1:C:363:ASP:OD2  | 1:C:363:ASP:N    | 2.51         | 0.43        |  |  |
| 1:D:334:ASP:HB2  | 1:D:335:PRO:CD   | 2.48         | 0.43        |  |  |
| 1:A:587:TRP:CZ3  | 1:A:619:LEU:HD21 | 2.49         | 0.42        |  |  |
| 1:C:203:LEU:HB2  | 1:C:718:LYS:HG3  | 2.01         | 0.42        |  |  |
| 1:C:672:ARG:N    | 1:C:672:ARG:HD3  | 2.34         | 0.42        |  |  |
| 1:A:289:SER:HB3  | 1:A:330:LEU:CD1  | 2.49         | 0.42        |  |  |
| 1:D:189:GLU:HB2  | 1:D:224:TYR:CZ   | 2.53         | 0.42        |  |  |
| 1:A:341:MET:H    | 1:A:341:MET:HG2  | 1.66         | 0.42        |  |  |
| 1:A:631:LEU:HD12 | 1:A:632:TRP:N    | 2.33         | 0.42        |  |  |
| 1:D:443:LEU:O    | 1:D:452:MET:HB2  | 2.19         | 0.42        |  |  |
| 1:A:93:VAL:HG12  | 1:A:681:ASP:OD2  | 2.20         | 0.42        |  |  |
| 1:C:673:ASN:OD1  | 1:C:673:ASN:N    | 2.52         | 0.42        |  |  |
| 1:D:102:LEU:HD22 | 1:D:108:PHE:CE2  | 2.54         | 0.42        |  |  |
| 1:D:143:CYS:HA   | 1:D:144:PRO:HD3  | 1.83         | 0.42        |  |  |
| 1:D:489:HIS:HA   | 1:D:521:THR:O    | 2.19         | 0.42        |  |  |
| 1:A:101:TYR:CD1  | 1:A:156:PRO:HG2  | 2.54         | 0.42        |  |  |
| 1:A:501:SER:N    | 1:A:502:PRO:HD2  | 2.34         | 0.42        |  |  |
| 1:C:678:ALA:HA   | 1:C:716:TRP:O    | 2.20         | 0.42        |  |  |
| 1:D:469:PHE:HA   | 1:D:488:GLY:HA2  | 2.01         | 0.42        |  |  |
| 1:A:145:ASN:O    | 1:A:284:ARG:NH1  | 2.49         | 0.42        |  |  |
| 1:A:245:VAL:CG2  | 1:A:709:PRO:HG2  | 2.50         | 0.42        |  |  |
| 1:B:309:LEU:HG   | 1:B:360:TRP:CZ3  | 2.55         | 0.42        |  |  |
| 1:C:638:GLN:OE1  | 1:C:640:ARG:N    | 2.41         | 0.42        |  |  |
| 1:D:163:THR:O    | 1:D:183:LEU:N    | 2.51         | 0.42        |  |  |
| 1:A:608:PRO:HB3  | 1:A:645:GLN:O    | 2.20         | 0.42        |  |  |
| 1:C:271:THR:O    | 1:C:297:GLY:N    | 2.53         | 0.42        |  |  |
| 1:C:333:PRO:O    | 1:C:335:PRO:HD3  | 2.20         | 0.42        |  |  |
| 1:D:189:GLU:OE1  | 1:D:197:ARG:NH1  | 2.52         | 0.42        |  |  |
| 1:A:139:MET:HE1  | 1:A:293:ARG:HG3  | 2.01         | 0.42        |  |  |
| 1:B:91:GLN:HG3   | 1:B:665:ASN:HB3  | 2.01         | 0.42        |  |  |
| 1:B:202:LEU:HD23 | 1:B:721:PHE:HE2  | 1.85         | 0.42        |  |  |
| 1:C:375:ARG:HA   | 1:C:406:PHE:O    | 2.20         | 0.42        |  |  |
| 1:D:350:ARG:NH2  | 1:D:379:ARG:NH2  | 2.68         | 0.42        |  |  |
| 1:B:425:LEU:O    | 1:B:426:ILE:HG13 | 2.20         | 0.42        |  |  |
| 1:B:495:ASP:HB2  | 1:B:498:GLU:H    | 1.84         | 0.42        |  |  |
| 1:B:540:SER:O    | 1:B:540:SER:OG   | 2.38         | 0.42        |  |  |
| 1:B:586:ASN:HB3  | 1:B:621:TYR:CE1  | 2.55         | 0.42        |  |  |



|                  |                  | Interatomic  | Clash       |  |  |
|------------------|------------------|--------------|-------------|--|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |  |
| 1:D:130:LEU:HD23 | 1:D:179:ALA:HB3  | 2.01         | 0.42        |  |  |
| 1:D:467:SER:CB   | 1:D:490:ALA:HA   | 2.48         | 0.42        |  |  |
| 1:D:571:ARG:HG3  | 1:D:601:SER:OG   | 2.19         | 0.42        |  |  |
| 1:B:79:PRO:O     | 1:B:81:THR:HG23  | 2.19         | 0.42        |  |  |
| 1:B:499:LEU:HD23 | 1:B:516:ILE:HB   | 2.01         | 0.42        |  |  |
| 1:C:101:TYR:OH   | 1:C:157:GLU:HG2  | 2.20         | 0.42        |  |  |
| 1:C:381:ARG:NH1  | 1:C:396:ASP:OD1  | 2.52         | 0.42        |  |  |
| 1:A:98:GLY:HA2   | 1:A:156:PRO:CG   | 2.50         | 0.41        |  |  |
| 1:A:633:ARG:O    | 1:A:660:GLY:HA2  | 2.20         | 0.41        |  |  |
| 1:B:628:ALA:HA   | 1:B:666:GLY:HA2  | 2.02         | 0.41        |  |  |
| 1:C:253:ASN:HB3  | 1:C:293:ARG:HH12 | 1.85         | 0.41        |  |  |
| 1:C:379:ARG:HG2  | 1:C:402:LYS:HB3  | 2.01         | 0.41        |  |  |
| 1:D:111:ILE:HG23 | 1:D:692:LEU:O    | 2.20         | 0.41        |  |  |
| 1:A:225:LEU:HD23 | 1:A:226:ARG:N    | 2.34         | 0.41        |  |  |
| 1:C:125:MET:CE   | 1:C:572:ILE:HG21 | 2.48         | 0.41        |  |  |
| 1:D:339:MET:O    | 1:D:339:MET:HG3  | 2.19         | 0.41        |  |  |
| 1:A:155:SER:HB3  | 1:A:157:GLU:OE1  | 2.20         | 0.41        |  |  |
| 1:A:553:SER:O    | 1:A:563:THR:HA   | 2.19         | 0.41        |  |  |
| 1:B:571:ARG:NH2  | 1:B:599:LYS:HD3  | 2.35         | 0.41        |  |  |
| 1:C:598:GLY:O    | 1:C:607:LEU:HB2  | 2.21         | 0.41        |  |  |
| 1:A:101:TYR:CD2  | 1:A:156:PRO:HB2  | 2.55         | 0.41        |  |  |
| 1:C:479:SER:OG   | 1:C:481:THR:HG23 | 2.19         | 0.41        |  |  |
| 1:C:688:TYR:CE1  | 1:C:710:GLU:HB2  | 2.55         | 0.41        |  |  |
| 1:D:301:VAL:HA   | 1:D:312:VAL:O    | 2.21         | 0.41        |  |  |
| 1:A:132:ILE:HA   | 1:A:182:ILE:HB   | 2.03         | 0.41        |  |  |
| 1:A:447:HIS:CE1  | 1:A:448:MET:HG2  | 2.55         | 0.41        |  |  |
| 1:A:465:LEU:HB3  | 1:A:491:GLU:HB2  | 2.03         | 0.41        |  |  |
| 1:C:174:GLY:HA2  | 1:C:430:ARG:NH2  | 2.35         | 0.41        |  |  |
| 1:C:261:THR:HG22 | 1:C:267:LEU:HD23 | 2.03         | 0.41        |  |  |
| 1:C:290:GLN:OE1  | 1:C:292:LYS:HB2  | 2.21         | 0.41        |  |  |
| 1:D:286:MET:HG3  | 1:D:326:ASP:O    | 2.20         | 0.41        |  |  |
| 1:D:311:LYS:HE2  | 1:D:313:GLU:HB2  | 2.01         | 0.41        |  |  |
| 1:A:593:LEU:HD23 | 1:A:594:ALA:N    | 2.36         | 0.41        |  |  |
| 1:B:111:ILE:HD13 | 1:B:111:ILE:HG21 | 1.74         | 0.41        |  |  |
| 1:C:113:ASN:HB2  | 1:C:281:TYR:CD2  | 2.55         | 0.41        |  |  |
| 1:C:125:MET:HE3  | 1:C:572:ILE:HD13 | 2.03         | 0.41        |  |  |
| 1:D:174:GLY:O    | 1:D:430:ARG:NH1  | 2.53         | 0.41        |  |  |
| 1:A:155:SER:CB   | 1:A:230:ASN:HD21 | 2.34         | 0.41        |  |  |
| 1:A:524:LEU:O    | 1:A:542:TYR:HA   | 2.21         | 0.41        |  |  |
| 1:A:668:TYR:CE2  | 1:A:670:VAL:HG22 | 2.55         | 0.41        |  |  |
| 1:B:328:PHE:CD1  | 1:B:342:PRO:HB2  | 2.55         | 0.41        |  |  |



|                  |                  | Interatomic  | Clash       |  |
|------------------|------------------|--------------|-------------|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |
| 1:B:455:PRO:HB2  | 1:B:510:VAL:CG1  | 2.51         | 0.41        |  |
| 1:B:583:LEU:HB2  | 1:B:587:TRP:HB2  | 2.01         | 0.41        |  |
| 1:C:362:TRP:CD1  | 1:C:365:PHE:HB2  | 2.56         | 0.41        |  |
| 1:B:103:LYS:CG   | 1:B:110:VAL:HG21 | 2.51         | 0.41        |  |
| 1:B:417:TRP:CE2  | 1:B:419:ALA:HA   | 2.55         | 0.41        |  |
| 1:C:367:LEU:HB2  | 1:C:415:LEU:CD2  | 2.51         | 0.41        |  |
| 1:C:671:THR:OG1  | 1:C:672:ARG:N    | 2.53         | 0.41        |  |
| 1:A:455:PRO:HB2  | 1:A:510:VAL:CG1  | 2.50         | 0.41        |  |
| 1:A:696:GLY:HA3  | 1:A:702:PHE:CG   | 2.56         | 0.41        |  |
| 1:B:261:THR:HG22 | 1:B:267:LEU:HD13 | 2.03         | 0.41        |  |
| 1:B:318:TYR:OH   | 1:B:350:ARG:HD3  | 2.20         | 0.41        |  |
| 1:B:428:GLY:HA3  | 1:B:469:PHE:CE1  | 2.56         | 0.41        |  |
| 1:C:203:LEU:HA   | 1:C:717:THR:O    | 2.21         | 0.41        |  |
| 1:D:82:ILE:HD11  | 1:D:166:LYS:HE2  | 2.03         | 0.41        |  |
| 1:D:86:PRO:C     | 1:D:88:GLU:H     | 2.24         | 0.41        |  |
| 1:D:90:ARG:HB2   | 1:D:94:PRO:HD3   | 2.03         | 0.41        |  |
| 1:D:182:ILE:O    | 1:D:183:LEU:HD23 | 2.21         | 0.41        |  |
| 1:D:349:ARG:HH12 | 1:D:496:TYR:HB3  | 1.85         | 0.41        |  |
| 1:D:497:TRP:HB3  | 1:D:648:VAL:HG21 | 2.03         | 0.41        |  |
| 1:D:570:ALA:HB1  | 1:D:607:LEU:HD11 | 2.03         | 0.41        |  |
| 1:B:94:PRO:HG2   | 1:B:101:TYR:CZ   | 2.56         | 0.41        |  |
| 1:B:360:TRP:HB2  | 1:B:362:TRP:HZ3  | 1.86         | 0.41        |  |
| 1:B:692:LEU:HD23 | 1:B:692:LEU:HA   | 1.79         | 0.41        |  |
| 1:C:202:LEU:HA   | 1:C:202:LEU:HD23 | 1.84         | 0.41        |  |
| 1:D:126:PHE:CG   | 1:D:127:GLY:N    | 2.89         | 0.41        |  |
| 1:A:134:THR:HG23 | 1:A:134:THR:O    | 2.21         | 0.40        |  |
| 1:A:139:MET:O    | 1:A:150:PRO:HB3  | 2.22         | 0.40        |  |
| 1:A:304:ASN:N    | 1:A:310:GLU:O    | 2.50         | 0.40        |  |
| 1:A:348:ASP:OD2  | 1:A:379:ARG:NH2  | 2.46         | 0.40        |  |
| 1:B:138:MET:SD   | 1:B:140:LEU:HD11 | 2.61         | 0.40        |  |
| 1:B:188:PRO:HG3  | 1:B:299:ARG:HH22 | 1.85         | 0.40        |  |
| 1:B:629:GLY:N    | 1:B:665:ASN:O    | 2.49         | 0.40        |  |
| 1:C:554:TYR:HB2  | 1:C:644:ASP:O    | 2.21         | 0.40        |  |
| 1:C:635:VAL:HG12 | 1:C:636:ALA:O    | 2.21         | 0.40        |  |
| 1:D:79:PRO:O     | 1:D:81:THR:N     | 2.54         | 0.40        |  |
| 1:D:200:ALA:HB3  | 1:D:721:PHE:HB2  | 2.03         | 0.40        |  |
| 1:D:438:ASP:HB2  | 1:D:513:PHE:CE2  | 2.56         | 0.40        |  |
| 1:D:568:VAL:HB   | 1:D:602:SER:HB2  | 2.02         | 0.40        |  |
| 1:B:285:GLY:HA2  | 1:B:331:ARG:HH12 | 1.86         | 0.40        |  |
| 1:B:461:ARG:HE   | 1:B:461:ARG:HB2  | 1.65         | 0.40        |  |
| 1:C:111:ILE:HG23 | 1:C:692:LEU:O    | 2.21         | 0.40        |  |



| A 4 1            | A +              | Interatomic             | Clash       |  |
|------------------|------------------|-------------------------|-------------|--|
| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |  |
| 1:C:360:TRP:HE1  | 1:C:369:THR:HG21 | 1.84                    | 0.40        |  |
| 1:C:690:GLU:H    | 1:C:693:ASN:ND2  | 2.19                    | 0.40        |  |
| 1:D:513:PHE:O    | 1:D:513:PHE:CD1  | 2.75                    | 0.40        |  |
| 1:A:339:MET:N    | 1:A:340:PRO:HD3  | 2.36                    | 0.40        |  |
| 1:A:454:ASN:HA   | 1:A:455:PRO:HD3  | 1.96                    | 0.40        |  |
| 1:B:435:SER:HB3  | 1:B:462:ALA:HB2  | 2.03                    | 0.40        |  |
| 1:C:329:ARG:HE   | 1:C:329:ARG:HB2  | 1.57                    | 0.40        |  |
| 1:C:503:LYS:HB3  | 1:C:503:LYS:NZ   | 2.37                    | 0.40        |  |
| 1:C:535:LEU:HD23 | 1:C:535:LEU:C    | 2.42                    | 0.40        |  |
| 1:D:81:THR:HA    | 1:D:164:VAL:O    | 2.22                    | 0.40        |  |
| 1:D:625:ASP:HB3  | 1:D:626:TRP:HD1  | 1.85                    | 0.40        |  |
| 1:A:166:LYS:HB2  | 1:A:166:LYS:HE3  | 1.84                    | 0.40        |  |
| 1:B:98:GLY:HA3   | 1:B:151:THR:HB   | 2.03                    | 0.40        |  |
| 1:B:534:LYS:HB2  | 1:B:581:TYR:HE1  | 1.87                    | 0.40        |  |
| 1:A:157:GLU:OE1  | 1:A:157:GLU:N    | 2.50                    | 0.40        |  |
| 1:B:135:ASN:HD21 | 1:B:186:ARG:NH1  | 2.20                    | 0.40        |  |
| 1:B:515:LYS:HD2  | 1:B:515:LYS:O    | 2.22                    | 0.40        |  |
| 1:B:552:PHE:HB2  | 1:B:647:ASN:HA   | 2.03                    | 0.40        |  |
| 1:C:181:THR:C    | 1:C:182:ILE:HD12 | 2.41                    | 0.40        |  |
| 1:C:673:ASN:O    | 1:C:722:SER:N    | 2.51                    | 0.40        |  |
| 1:D:223:GLY:N    | 1:D:261:THR:HG23 | 2.35                    | 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 | Pe | erce | entiles |
|-----|-------|---------------|-----------|----------|----------|----|------|---------|
| 1   | А     | 653/723~(90%) | 577 (88%) | 68 (10%) | 8 (1%)   |    | 13   | 43      |
| 1   | В     | 639/723~(88%) | 582 (91%) | 50 (8%)  | 7 (1%)   |    | 14   | 46      |
| 1   | С     | 630/723~(87%) | 541 (86%) | 74 (12%) | 15 (2%)  |    | 6    | 26      |
| 1   | D     | 653/723~(90%) | 578 (88%) | 60 (9%)  | 15 (2%)  |    | 6    | 27      |



| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|----------|-------------|
| All | All   | 2575/2892~(89%) | 2278 (88%) | 252 (10%) | 45 (2%)  | 9 34        |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 624 | GLY  |
| 1   | В     | 583 | LEU  |
| 1   | С     | 386 | ASP  |
| 1   | С     | 395 | ALA  |
| 1   | D     | 175 | PRO  |
| 1   | D     | 246 | PRO  |
| 1   | D     | 334 | ASP  |
| 1   | D     | 513 | PHE  |
| 1   | А     | 148 | ASP  |
| 1   | А     | 206 | SER  |
| 1   | В     | 584 | THR  |
| 1   | С     | 382 | GLY  |
| 1   | С     | 624 | GLY  |
| 1   | С     | 697 | ASP  |
| 1   | D     | 80  | LEU  |
| 1   | D     | 447 | HIS  |
| 1   | D     | 514 | ASP  |
| 1   | А     | 262 | PRO  |
| 1   | А     | 419 | ALA  |
| 1   | А     | 445 | SER  |
| 1   | В     | 695 | ALA  |
| 1   | D     | 420 | ALA  |
| 1   | D     | 516 | ILE  |
| 1   | В     | 123 | ARG  |
| 1   | С     | 363 | ASP  |
| 1   | C     | 694 | LYS  |
| 1   | С     | 698 | ALA  |
| 1   | D     | 362 | TRP  |
| 1   | D     | 388 | MET  |
| 1   | D     | 704 | ALA  |
| 1   | В     | 92  | PRO  |
| 1   | С     | 331 | ARG  |
| 1   | C     | 333 | PRO  |
| 1   | C     | 399 | PRO  |
| 1   | C     | 511 | ASN  |
| 1   | D     | 262 | PRO  |
| 1   | А     | 91  | GLN  |



| Conti | Commuted from previous page |                |      |  |  |  |
|-------|-----------------------------|----------------|------|--|--|--|
| Mol   | Chain                       | $\mathbf{Res}$ | Type |  |  |  |
| 1     | В                           | 336            | SER  |  |  |  |
| 1     | С                           | 508            | GLY  |  |  |  |
| 1     | D                           | 176            | GLY  |  |  |  |
| 1     | А                           | 92             | PRO  |  |  |  |
| 1     | В                           | 246            | PRO  |  |  |  |
| 1     | С                           | 149            | ALA  |  |  |  |
| 1     | С                           | 92             | PRO  |  |  |  |
| 1     | D                           | 399            | PRO  |  |  |  |

#### 5.3.2Protein 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  | $\mathbf{P}$ | $\mathbf{erc}$ | entiles |
|-----|-------|-----------------|------------|-----------|--------------|----------------|---------|
| 1   | А     | 525/572~(92%)   | 477 (91%)  | 48 (9%)   |              | 9              | 31      |
| 1   | В     | 516/572~(90%)   | 455 (88%)  | 61 (12%)  |              | 5              | 20      |
| 1   | С     | 512/572~(90%)   | 439 (86%)  | 73 (14%)  |              | 3              | 13      |
| 1   | D     | 524/572~(92%)   | 460 (88%)  | 64 (12%)  |              | 5              | 19      |
| All | All   | 2077/2288~(91%) | 1831 (88%) | 246 (12%) |              | 5              | 20      |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 78  | SER  |
| 1   | А     | 90  | ARG  |
| 1   | А     | 116 | SER  |
| 1   | А     | 130 | LEU  |
| 1   | А     | 139 | MET  |
| 1   | А     | 147 | MET  |
| 1   | А     | 158 | THR  |
| 1   | А     | 199 | ASN  |
| 1   | А     | 201 | SER  |
| 1   | А     | 203 | LEU  |
| 1   | А     | 210 | PHE  |
| 1   | А     | 212 | LYS  |
| 1   | А     | 221 | ARG  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | А     | 228 | THR  |
| 1   | А     | 236 | ASP  |
| 1   | А     | 250 | LYS  |
| 1   | А     | 256 | VAL  |
| 1   | А     | 286 | MET  |
| 1   | А     | 287 | ASP  |
| 1   | А     | 306 | SER  |
| 1   | А     | 307 | ASP  |
| 1   | А     | 336 | SER  |
| 1   | А     | 337 | SER  |
| 1   | А     | 339 | MET  |
| 1   | А     | 343 | MET  |
| 1   | А     | 362 | TRP  |
| 1   | А     | 364 | ASP  |
| 1   | А     | 388 | MET  |
| 1   | А     | 389 | THR  |
| 1   | А     | 425 | LEU  |
| 1   | А     | 435 | SER  |
| 1   | А     | 445 | SER  |
| 1   | А     | 470 | VAL  |
| 1   | А     | 478 | ASP  |
| 1   | А     | 481 | THR  |
| 1   | А     | 487 | LEU  |
| 1   | А     | 516 | ILE  |
| 1   | А     | 528 | LEU  |
| 1   | А     | 558 | MET  |
| 1   | А     | 563 | THR  |
| 1   | А     | 601 | SER  |
| 1   | А     | 619 | LEU  |
| 1   | А     | 625 | ASP  |
| 1   | A     | 631 | LEU  |
| 1   | A     | 651 | LYS  |
| 1   | А     | 654 | ASP  |
| 1   | A     | 672 | ARG  |
| 1   | А     | 722 | SER  |
| 1   | В     | 74  | VAL  |
| 1   | В     | 78  | SER  |
| 1   | В     | 93  | VAL  |
| 1   | В     | 97  | ASP  |
| 1   | В     | 104 | THR  |
| 1   | В     | 112 | ARG  |
| 1   | В     | 123 | ARG  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | В     | 147 | MET  |
| 1   | В     | 152 | SER  |
| 1   | В     | 155 | SER  |
| 1   | В     | 170 | THR  |
| 1   | В     | 178 | SER  |
| 1   | В     | 187 | GLU  |
| 1   | В     | 193 | GLU  |
| 1   | В     | 206 | SER  |
| 1   | В     | 230 | ASN  |
| 1   | В     | 253 | ASN  |
| 1   | В     | 270 | LEU  |
| 1   | В     | 287 | ASP  |
| 1   | В     | 303 | SER  |
| 1   | В     | 304 | ASN  |
| 1   | В     | 306 | SER  |
| 1   | В     | 308 | VAL  |
| 1   | В     | 309 | LEU  |
| 1   | В     | 325 | MET  |
| 1   | В     | 326 | ASP  |
| 1   | В     | 330 | LEU  |
| 1   | В     | 332 | THR  |
| 1   | В     | 338 | MET  |
| 1   | В     | 387 | MET  |
| 1   | В     | 389 | THR  |
| 1   | В     | 401 | SER  |
| 1   | В     | 425 | LEU  |
| 1   | В     | 475 | ASP  |
| 1   | В     | 487 | LEU  |
| 1   | В     | 501 | SER  |
| 1   | В     | 509 | SER  |
| 1   | В     | 514 | ASP  |
| 1   | В     | 523 | GLN  |
| 1   | В     | 540 | SER  |
| 1   | В     | 556 | GLU  |
| 1   | В     | 562 | SER  |
| 1   | В     | 577 | LEU  |
| 1   | В     | 580 | SER  |
| 1   | В     | 584 | THR  |
| 1   | В     | 604 | ASP  |
| 1   | В     | 623 | GLU  |
| 1   | В     | 630 | SER  |
| 1   | В     | 651 | LYS  |



| 1         B         654         ASP           1         B         672         ARG           1         B         676         LEU           1         B         677         SER           1         B         680         VAL           1         B         683         LEU           1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         703         SER           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         78         SER           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         155         SER           1         C         190         ARG           1         C         203 <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th> | Mol | Chain | Res | Type |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-------|-----|------|
| 1         B         672         ARG           1         B         676         LEU           1         B         677         SER           1         B         680         VAL           1         B         693         ASN           1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         78         SER           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203                                                         | 1   | В     | 654 | ASP  |
| 1         B         676         LEU           1         B         677         SER           1         B         680         VAL           1         B         693         ASN           1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         78         SER           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         139         MET           1         C         139         MET           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203 <td>1</td> <td>В</td> <td>672</td> <td>ARG</td>        | 1   | В     | 672 | ARG  |
| 1         B         677         SER           1         B         680         VAL           1         B         683         LEU           1         B         693         ASN           1         B         703         SER           1         B         703         SER           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         78         SER           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203 <td>1</td> <td>B</td> <td>676</td> <td>LEU</td>        | 1   | B     | 676 | LEU  |
| 1         B         680         VAL           1         B         683         LEU           1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         74         VAL           1         C         74         VAL           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         155         SER           1         C         190         ARG           1         C         203                                                          | 1   | B     | 677 | SER  |
| 1         B         683         LEU           1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         74         VAL           1         C         97         ASP           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         235                                                          | 1   | B     | 680 | VAL  |
| 1         B         693         ASN           1         B         703         SER           1         B         705         ASN           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         78         SER           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         140         LEU           1         C         151         THR           1         C         190         ARG           1         C         203         LEU           1         C         203         LEU           1         C         235                                                         | 1   | В     | 683 | LEU  |
| 1         B         703         SER           1         B         705         ASN           1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         78         SER           1         C         97         ASP           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         140         LEU           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203         GLN           1         C         235         ASP           1         C         236                                                          | 1   | В     | 693 | ASN  |
| 1       B $705$ ASN         1       B $714$ THR         1       B $722$ SER         1       B $723$ PHE         1       C $74$ VAL         1       C $74$ VAL         1       C $78$ SER         1       C $80$ LEU         1       C $130$ LEU         1       C $130$ LEU         1       C $133$ LEU         1       C $133$ LEU         1       C $133$ LEU         1       C $133$ MET         1       C $139$ MET         1       C $155$ SER         1       C $190$ ARG         1       C $190$ ARG         1       C $203$ LEU         1       C $235$ ASP         1       C $236$ ASP         1       C $253$ ASN                                                                                                                                                                                                                                                                                                                                                                                                          | 1   | В     | 703 | SER  |
| 1         B         714         THR           1         B         722         SER           1         B         723         PHE           1         C         74         VAL           1         C         74         VAL           1         C         78         SER           1         C         97         ASP           1         C         130         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         140         LEU           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203         GLN           1         C         235                                                          | 1   | В     | 705 | ASN  |
| 1       B       722       SER         1       B       723       PHE         1       C       74       VAL         1       C       78       SER         1       C       97       ASP         1       C       133       LEU         1       C       134       THR         1       C       139       MET         1       C       151       THR         1       C       155       SER         1       C       190       ARG         1       C       203       LEU         1       C       203       GLN         1       C       235       ASP         1       C       236       ASP         1       C       236       ASP         1       C       258       VAL         1 <t< td=""><td>1</td><td>В</td><td>714</td><td>THR</td></t<>                                                                                                       | 1   | В     | 714 | THR  |
| 1         B         723         PHE           1         C         74         VAL           1         C         78         SER           1         C         97         ASP           1         C         133         LEU           1         C         134         THR           1         C         140         LEU           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203         GLN           1         C         235         ASP           1         C         236         ASP           1         C         264 <td>1</td> <td>В</td> <td>722</td> <td>SER</td>         | 1   | В     | 722 | SER  |
| 1         C         74         VAL           1         C         78         SER           1         C         80         LEU           1         C         97         ASP           1         C         133         ASN           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         151         THR           1         C         155         SER           1         C         190         ARG           1         C         203         LEU           1         C         203         LEU           1         C         203         GLN           1         C         233         GLN           1         C         235         ASP           1         C         258         VAL           1         C         264                                                          | 1   | В     | 723 | PHE  |
| 1         C         78         SER           1         C         80         LEU           1         C         97         ASP           1         C         113         ASN           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         140         LEU           1         C         155         SER           1         C         190         ARG           1         C         201         SER           1         C         203         LEU           1         C         233         GLN           1         C         235         ASP           1         C         236         ASN           1         C         258         VAL           1         C         303                                                         | 1   | С     | 74  | VAL  |
| 1         C         80         LEU           1         C         97         ASP           1         C         113         ASN           1         C         130         LEU           1         C         133         LEU           1         C         133         LEU           1         C         133         LEU           1         C         134         THR           1         C         139         MET           1         C         140         LEU           1         C         151         THR           1         C         155         SER           1         C         190         ARG           1         C         190         SER           1         C         203         LEU           1         C         203         GLN           1         C         233         GLN           1         C         235         ASP           1         C         236         ASP           1         C         258         VAL           1         C         303 <td>1</td> <td>C</td> <td>78</td> <td>SER</td>         | 1   | C     | 78  | SER  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | C     | 80  | LEU  |
| 1C113ASN1C130LEU1C133LEU1C134THR1C139MET1C140LEU1C151THR1C155SER1C190ARG1C201SER1C203LEU1C203LEU1C235ASP1C236ASP1C253ASN1C258VAL1C264GLU1C303SER1C303SER1C309LEU1C330LEU1C331ARG1C332THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 1   | С     | 97  | ASP  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 113 | ASN  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 130 | LEU  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 133 | LEU  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 134 | THR  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 139 | MET  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 140 | LEU  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 151 | THR  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 155 | SER  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 190 | ARG  |
| 1         C         201         SER           1         C         203         LEU           1         C         206         SER           1         C         233         GLN           1         C         235         ASP           1         C         236         ASP           1         C         253         ASN           1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         330         LEU           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                | 1   | С     | 196 | SER  |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 201 | SER  |
| 1         C         206         SER           1         C         233         GLN           1         C         235         ASP           1         C         236         ASP           1         C         253         ASP           1         C         253         ASP           1         C         253         ASN           1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         330         LEU           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                | 1   | С     | 203 | LEU  |
| 1       C       233       GLN         1       C       235       ASP         1       C       236       ASP         1       C       253       ASN         1       C       253       ASN         1       C       258       VAL         1       C       264       GLU         1       C       289       SER         1       C       303       SER         1       C       309       LEU         1       C       329       ARG         1       C       330       LEU         1       C       331       ARG         1       C       332       THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 1   | С     | 206 | SER  |
| 1         C         235         ASP           1         C         236         ASP           1         C         253         ASN           1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         330         LEU           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 1   | С     | 233 | GLN  |
| 1         C         236         ASP           1         C         253         ASN           1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1   | С     | 235 | ASP  |
| 1         C         253         ASN           1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 1   | С     | 236 | ASP  |
| 1         C         258         VAL           1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 1   | С     | 253 | ASN  |
| 1         C         264         GLU           1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1   | С     | 258 | VAL  |
| 1         C         289         SER           1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 1   | С     | 264 | GLU  |
| 1         C         303         SER           1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 1   | С     | 289 | SER  |
| 1         C         309         LEU           1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 1   | С     | 303 | SER  |
| 1         C         329         ARG           1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 1   | С     | 309 | LEU  |
| 1         C         330         LEU           1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1   | С     | 329 | ARG  |
| 1         C         331         ARG           1         C         332         THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 1   | С     | 330 | LEU  |
| 1 C 332 THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 1   | С     | 331 | ARG  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 1   | С     | 332 | THR  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | С     | 334 | ASP  |
| 1   | С     | 339 | MET  |
| 1   | С     | 341 | MET  |
| 1   | С     | 362 | TRP  |
| 1   | С     | 363 | ASP  |
| 1   | С     | 364 | ASP  |
| 1   | С     | 368 | VAL  |
| 1   | С     | 369 | THR  |
| 1   | С     | 392 | TYR  |
| 1   | С     | 429 | LEU  |
| 1   | С     | 440 | ARG  |
| 1   | С     | 442 | THR  |
| 1   | C     | 467 | SER  |
| 1   | С     | 475 | ASP  |
| 1   | С     | 478 | ASP  |
| 1   | С     | 487 | LEU  |
| 1   | С     | 501 | SER  |
| 1   | С     | 507 | ASN  |
| 1   | С     | 517 | LYS  |
| 1   | С     | 524 | LEU  |
| 1   | С     | 525 | ASP  |
| 1   | С     | 529 | GLN  |
| 1   | С     | 530 | TYR  |
| 1   | С     | 553 | SER  |
| 1   | С     | 556 | GLU  |
| 1   | С     | 563 | THR  |
| 1   | С     | 584 | THR  |
| 1   | С     | 589 | THR  |
| 1   | C     | 593 | LEU  |
| 1   | С     | 616 | ARG  |
| 1   | С     | 627 | SER  |
| 1   | С     | 630 | SER  |
| 1   | С     | 648 | VAL  |
| 1   | С     | 649 | VAL  |
| 1   | С     | 653 | PHE  |
| 1   | С     | 654 | ASP  |
| 1   | С     | 663 | SER  |
| 1   | С     | 664 | LEU  |
| 1   | С     | 672 | ARG  |
| 1   | C     | 673 | ASN  |
| 1   | С     | 675 | LYS  |
| 1   | С     | 700 | PHE  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | С     | 722 | SER  |
| 1   | D     | 66  | LEU  |
| 1   | D     | 78  | SER  |
| 1   | D     | 91  | GLN  |
| 1   | D     | 112 | ARG  |
| 1   | D     | 116 | SER  |
| 1   | D     | 119 | ASP  |
| 1   | D     | 134 | THR  |
| 1   | D     | 146 | ARG  |
| 1   | D     | 152 | SER  |
| 1   | D     | 170 | THR  |
| 1   | D     | 193 | GLU  |
| 1   | D     | 197 | ARG  |
| 1   | D     | 203 | LEU  |
| 1   | D     | 209 | ARG  |
| 1   | D     | 230 | ASN  |
| 1   | D     | 247 | SER  |
| 1   | D     | 260 | TRP  |
| 1   | D     | 261 | THR  |
| 1   | D     | 287 | ASP  |
| 1   | D     | 289 | SER  |
| 1   | D     | 296 | LEU  |
| 1   | D     | 302 | LYS  |
| 1   | D     | 303 | SER  |
| 1   | D     | 305 | VAL  |
| 1   | D     | 306 | SER  |
| 1   | D     | 308 | VAL  |
| 1   | D     | 332 | THR  |
| 1   | D     | 341 | MET  |
| 1   | D     | 355 | ARG  |
| 1   | D     | 388 | MET  |
| 1   | D     | 393 | THR  |
| 1   | D     | 396 | ASP  |
| 1   | D     | 403 | ASP  |
| 1   | D     | 409 | TYR  |
| 1   | D     | 425 | LEU  |
| 1   | D     | 433 | ARG  |
| 1   | D     | 442 | THR  |
| 1   | D     | 456 | THR  |
| 1   | D     | 470 | VAL  |
| 1   | D     | 479 | SER  |
| 1   | D     | 487 | LEU  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 510 | VAL  |
| 1   | D     | 525 | ASP  |
| 1   | D     | 545 | VAL  |
| 1   | D     | 556 | GLU  |
| 1   | D     | 558 | MET  |
| 1   | D     | 559 | MET  |
| 1   | D     | 561 | SER  |
| 1   | D     | 562 | SER  |
| 1   | D     | 563 | THR  |
| 1   | D     | 586 | ASN  |
| 1   | D     | 588 | LYS  |
| 1   | D     | 593 | LEU  |
| 1   | D     | 605 | ARG  |
| 1   | D     | 613 | LEU  |
| 1   | D     | 619 | LEU  |
| 1   | D     | 630 | SER  |
| 1   | D     | 653 | PHE  |
| 1   | D     | 672 | ARG  |
| 1   | D     | 673 | ASN  |
| 1   | D     | 677 | SER  |
| 1   | 1 D   |     | ASP  |
| 1   | D     | 693 | ASN  |
| 1   | D     | 714 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | $\mathbf{Res}$ | Type |
|-----|-------|----------------|------|
| 1   | А     | 91             | GLN  |
| 1   | А     | 230            | ASN  |
| 1   | А     | 523            | GLN  |
| 1   | А     | 529            | GLN  |
| 1   | В     | 76             | GLN  |
| 1   | В     | 507            | ASN  |
| 1   | В     | 638            | GLN  |
| 1   | С     | 135            | ASN  |
| 1   | С     | 230            | ASN  |
| 1   | С     | 253            | ASN  |
| 1   | С     | 346            | GLN  |
| 1   | С     | 547            | GLN  |
| 1   | D     | 76             | GLN  |
| 1   | D     | 253            | ASN  |
| 1   | D     | 441            | GLN  |



Continued from previous page...

| Mol | Chain | $\operatorname{Res}$ | Type |
|-----|-------|----------------------|------|
| 1   | D     | 458                  | 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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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> | #RSRZ>2        | $OWAB(Å^2)$      | Q<0.9 |
|-----|-------|-----------------|---------------|----------------|------------------|-------|
| 1   | А     | 657/723~(90%)   | 0.38          | 26 (3%) 38 25  | 42, 61, 91, 122  | 0     |
| 1   | В     | 645/723~(89%)   | 0.36          | 19 (2%) 51 35  | 40, 59, 85, 121  | 0     |
| 1   | С     | 640/723~(88%)   | 0.41          | 28 (4%) 34 21  | 44, 67, 102, 132 | 0     |
| 1   | D     | 656/723~(90%)   | 0.42          | 36 (5%) 25 15  | 45, 68, 101, 131 | 0     |
| All | All   | 2598/2892~(89%) | 0.39          | 109 (4%) 36 23 | 40, 64, 96, 132  | 0     |

All (109) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 362 | TRP  | 7.2  |
| 1   | С     | 385 | TYR  | 5.7  |
| 1   | А     | 558 | MET  | 5.6  |
| 1   | D     | 723 | PHE  | 5.2  |
| 1   | С     | 389 | THR  | 4.9  |
| 1   | А     | 362 | TRP  | 4.8  |
| 1   | D     | 382 | GLY  | 4.5  |
| 1   | В     | 69  | SER  | 4.4  |
| 1   | D     | 514 | ASP  | 4.4  |
| 1   | С     | 701 | GLY  | 4.4  |
| 1   | С     | 386 | ASP  | 4.3  |
| 1   | С     | 192 | GLY  | 4.2  |
| 1   | В     | 702 | PHE  | 4.2  |
| 1   | В     | 626 | TRP  | 4.2  |
| 1   | С     | 700 | PHE  | 4.2  |
| 1   | С     | 515 | LYS  | 3.9  |
| 1   | С     | 387 | MET  | 3.7  |
| 1   | С     | 392 | TYR  | 3.7  |
| 1   | С     | 119 | ASP  | 3.7  |
| 1   | D     | 119 | ASP  | 3.6  |
| 1   | D     | 102 | LEU  | 3.6  |



| 6Z9Y |
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|      |
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| Mol | Chain | Res | Type    | RSRZ |  |
|-----|-------|-----|---------|------|--|
| 1   | D     | 313 | GLU     | 3.5  |  |
| 1   | В     | 697 | ASP     | 3.5  |  |
| 1   | А     | 417 | TRP     | 3.4  |  |
| 1   | В     | 338 | 338 MET |      |  |
| 1   | С     | 383 | 383 SER |      |  |
| 1   | D     | 69  | SER     | 3.3  |  |
| 1   | С     | 514 | ASP     | 3.3  |  |
| 1   | D     | 453 | ALA     | 3.2  |  |
| 1   | С     | 102 | LEU     | 3.1  |  |
| 1   | С     | 697 | ASP     | 3.1  |  |
| 1   | В     | 341 | MET     | 3.1  |  |
| 1   | В     | 270 | LEU     | 3.0  |  |
| 1   | В     | 510 | VAL     | 3.0  |  |
| 1   | D     | 356 | LEU     | 3.0  |  |
| 1   | С     | 96  | SER     | 3.0  |  |
| 1   | А     | 448 | MET     | 2.9  |  |
| 1   | D     | 384 | LYS     | 2.8  |  |
| 1   | D     | 455 | PRO     | 2.8  |  |
| 1   | А     | 119 | ASP     | 2.8  |  |
| 1   | D     | 383 | SER     | 2.8  |  |
| 1   | D     | 641 | ILE     | 2.7  |  |
| 1   | В     | 391 | TYR     | 2.6  |  |
| 1   | С     | 704 | ALA     | 2.6  |  |
| 1   | D     | 512 | ALA     | 2.6  |  |
| 1   | D     | 704 | ALA     | 2.6  |  |
| 1   | В     | 67  | ALA     | 2.6  |  |
| 1   | В     | 524 | LEU     | 2.6  |  |
| 1   | D     | 122 | LEU     | 2.6  |  |
| 1   | С     | 69  | SER     | 2.6  |  |
| 1   | А     | 365 | PHE     | 2.6  |  |
| 1   | С     | 382 | GLY     | 2.5  |  |
| 1   | А     | 487 | LEU     | 2.5  |  |
| 1   | А     | 444 | LYS     | 2.5  |  |
| 1   | С     | 365 | PHE     | 2.5  |  |
| 1   | В     | 393 | THR     | 2.5  |  |
| 1   | С     | 722 | SER     | 2.5  |  |
| 1   | D     | 696 | GLY     | 2.5  |  |
| 1   | С     | 696 | GLY     | 2.4  |  |
| 1   | D     | 515 | LYS     | 2.4  |  |
| 1   | В     | 493 | PHE     | 2.4  |  |
| 1   | D     | 510 | VAL     | 2.4  |  |
| 1   | А     | 84  | THR     | 2.4  |  |



| 6Z9Y |
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|      |

| Mol | Chain | Res   Type |     | RSRZ |  |
|-----|-------|------------|-----|------|--|
| 1   | А     | 122        | LEU | 2.4  |  |
| 1   | D     | 83         | VAL | 2.4  |  |
| 1   | А     | 173        | TRP | 2.4  |  |
| 1   | А     | 415        | LEU | 2.4  |  |
| 1   | А     | 514        | ASP | 2.3  |  |
| 1   | D     | 452        | MET | 2.3  |  |
| 1   | D     | 131        | ASN | 2.3  |  |
| 1   | D     | 511        | ASN | 2.3  |  |
| 1   | А     | 387        | MET | 2.3  |  |
| 1   | С     | 260        | TRP | 2.3  |  |
| 1   | С     | 384        | LYS | 2.3  |  |
| 1   | В     | 356        | LEU | 2.3  |  |
| 1   | А     | 144        | PRO | 2.3  |  |
| 1   | А     | 528        | LEU | 2.3  |  |
| 1   | D     | 91         | GLN | 2.3  |  |
| 1   | А     | 73         | GLY | 2.2  |  |
| 1   | D     | 109        | ALA | 2.2  |  |
| 1   | D     | 417        | TRP | 2.2  |  |
| 1   | В     | 701        | GLY | 2.2  |  |
| 1   | С     | 150        | PRO | 2.2  |  |
| 1   | D     | 365        | PHE | 2.2  |  |
| 1   | D     | 516        | ILE | 2.2  |  |
| 1   | D     | 385        | TYR | 2.2  |  |
| 1   | С     | 121        | VAL | 2.2  |  |
| 1   | D     | 82         | ILE | 2.2  |  |
| 1   | А     | 388        | MET | 2.2  |  |
| 1   | А     | 700        | PHE | 2.1  |  |
| 1   | А     | 83         | VAL | 2.1  |  |
| 1   | А     | 442        | THR | 2.1  |  |
| 1   | В     | 312        | VAL | 2.1  |  |
| 1   | A     | 300        | PHE | 2.1  |  |
| 1   | A     | 268        | ILE | 2.1  |  |
| 1   | А     | 341        | MET | 2.1  |  |
| 1   | A     | 138        | MET | 2.1  |  |
| 1   | A     | 82         | ILE | 2.1  |  |
| 1   | С     | 356        | LEU | 2.1  |  |
| 1   | С     | 653        | PHE | 2.1  |  |
| 1   | D     | 164        | VAL | 2.0  |  |
| 1   | D     | 352        | LEU | 2.0  |  |
| 1   | В     | 385        | TYR | 2.0  |  |
| 1   | D     | 305        | VAL | 2.0  |  |
| 1   | D     | 338        | MET | 2.0  |  |



Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 543 | VAL  | 2.0  |
| 1   | В     | 126 | PHE  | 2.0  |
| 1   | В     | 684 | PHE  | 2.0  |
| 1   | С     | 507 | ASN  | 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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  | $\mathbf{B}	ext{-factors}(\mathbf{A}^2)$ | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------------------------------------------|-------|
| 2   | CU   | В     | 801 | 1/1   | 0.92 | 0.11 | 99,99,99,99                              | 0     |
| 2   | CU   | С     | 801 | 1/1   | 0.92 | 0.14 | 109,109,109,109                          | 0     |
| 2   | CU   | А     | 801 | 1/1   | 0.94 | 0.18 | 85,85,85,85                              | 0     |
| 2   | CU   | D     | 801 | 1/1   | 0.98 | 0.12 | 98,98,98,98                              | 0     |

#### 6.5 Other polymers (i)

There are no such residues in this entry.

