



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:40 PM GMT

PDB ID : 2VQI  
Title : STRUCTURE OF THE P PILUS USHER (PAPC) TRANSLOCATION PORE  
Authors : Remaut, H.; Tang, C.; Henderson, N.S.; Pinkner, J.S.; Wang, T.; Hultgren, S.J.; Thanassi, D.G.; Li, H.; Waksman, G.  
Deposited on : 2008-03-16  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

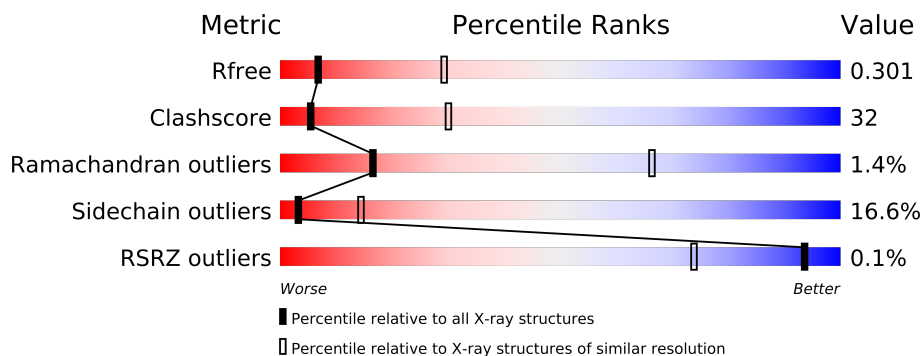
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	515	
1	B	515	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	LDA	B	1639	-	X
3	C8E	B	1638	-	X

## 2 Entry composition

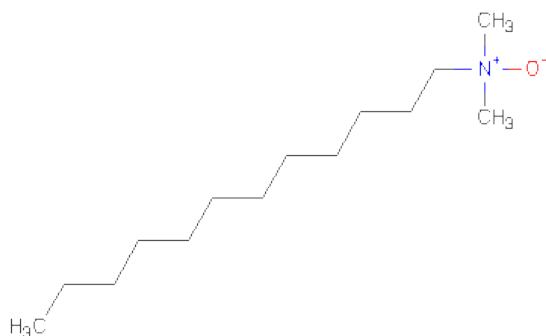
There are 4 unique types of molecules in this entry. The entry contains 7625 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called OUTER MEMBRANE USHER PROTEIN PAPC.

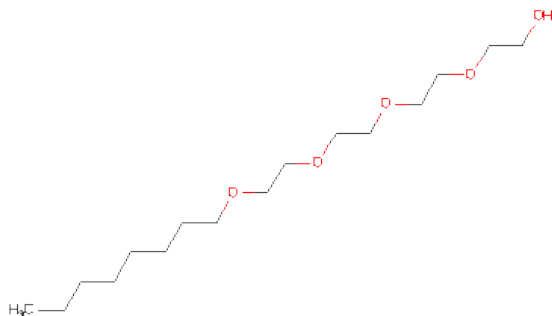
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	Se	0	0	0
			3767	2353	675	731	8			
1	B	477	Total	C	N	O	Se	0	0	0
			3750	2342	674	726	8			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

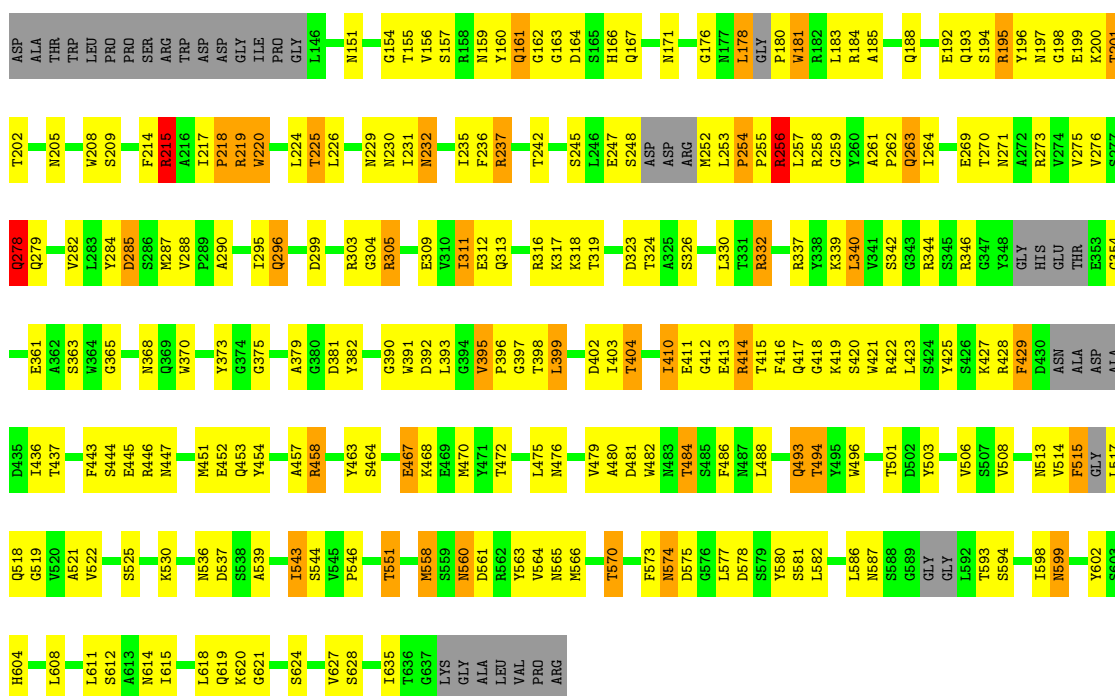
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	19	Total	O	0	0
			19	19		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

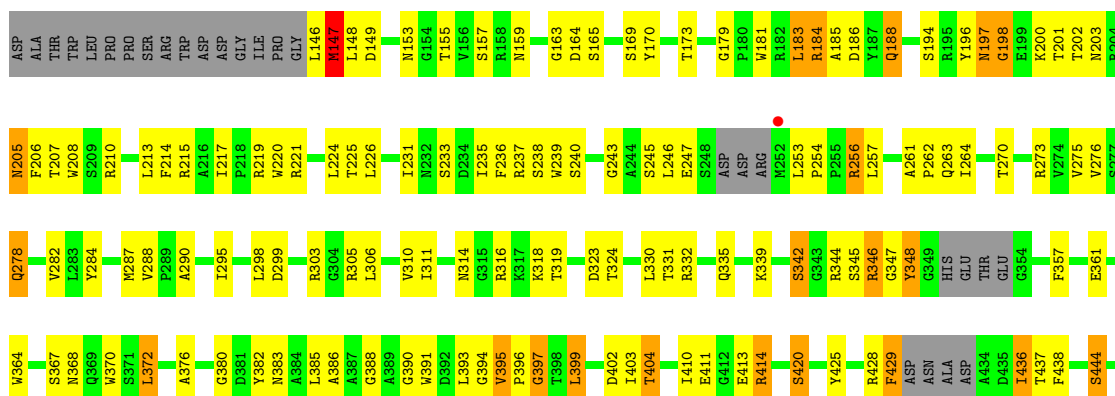
#### • Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC

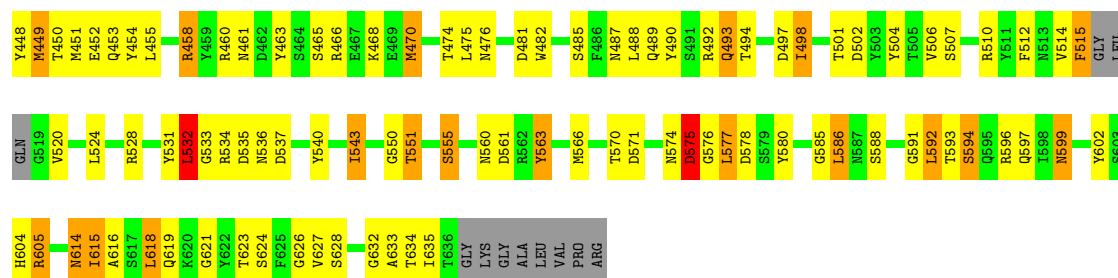
Chain A:



#### • Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.50Å 101.90Å 113.70Å 90.00° 128.20° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-3.20) 99.9 (15.00-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.259 , 0.296 0.264 , 0.301	Depositor DCC
$R_{free}$ test set	1228 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 11.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 47935 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, C8E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/3840	0.66	0/5184
1	B	0.52	2/3825 (0.1%)	0.71	1/5167 (0.0%)
All	All	0.47	2/7665 (0.0%)	0.68	1/10351 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	8
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	MSE	CG-SE	13.54	2.41	1.95
1	B	147	MSE	SE-CE	6.98	2.36	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	147	MSE	CG-SE-CE	-6.68	84.21	98.90

There are no chirality outliers.

All (13) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	162	GLY	Peptide
1	A	199	GLU	Peptide
1	A	215	ARG	Sidechain
1	A	218	PRO	Peptide
1	A	278	GLN	Peptide
1	B	179	GLY	Peptide
1	B	219	ARG	Peptide
1	B	345	SER	Peptide
1	B	346	ARG	Peptide
1	B	397	GLY	Peptide
1	B	575	ASP	Peptide
1	B	591	GLY	Peptide
1	B	592	LEU	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3767	0	3590	245	0
1	B	3750	0	3576	225	0
2	A	16	0	31	6	0
2	B	16	0	31	3	0
3	B	42	0	68	6	0
4	A	15	0	0	4	0
4	B	19	0	0	2	0
All	All	7625	0	7296	464	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (464) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:395:VAL:HB	1:B:429:PHE:CE1	1.67	1.28
1:B:181:TRP:CZ3	1:B:215:ARG:HB3	1.70	1.27
1:B:147:MSE:CE	1:B:147:MSE:SE	2.36	1.23
1:A:180:PRO:O	1:A:215:ARG:HB2	1.40	1.20

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:147:MSE:SE	1:B:147:MSE:CG	2.41	1.19
1:A:316:ARG:HH21	1:A:318:LYS:NZ	1.41	1.19
1:B:394:GLY:O	1:B:395:VAL:HG13	1.44	1.17
1:B:394:GLY:C	1:B:395:VAL:HG13	1.73	1.07
1:A:256:ARG:HB2	1:A:256:ARG:HH11	1.16	1.07
1:A:403:ILE:HD12	1:A:421:TRP:CD1	1.90	1.06
1:B:574:ASN:O	1:B:575:ASP:HB2	1.47	1.05
1:B:395:VAL:N	1:B:396:PRO:HD2	1.72	1.04
1:A:342:SER:HB2	2:A:1638:LDA:H12	1.33	1.03
1:B:436:ILE:HD13	1:B:436:ILE:H	1.20	1.03
1:A:365:GLY:HA3	4:A:2006:HOH:O	1.59	1.03
1:B:510:ARG:HH12	3:B:1637:C8E:H191	1.23	1.02
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.23	1.00
1:B:394:GLY:C	1:B:396:PRO:CD	2.30	1.00
1:A:522:VAL:HG22	1:A:543:ILE:HG22	1.39	1.00
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.24	0.98
1:A:403:ILE:HD12	1:A:421:TRP:HD1	1.28	0.97
1:A:551:THR:HG23	1:A:570:THR:HG23	1.47	0.96
1:B:577:LEU:HB3	1:B:605:ARG:O	1.64	0.96
1:B:395:VAL:N	1:B:396:PRO:CD	2.31	0.93
1:B:551:THR:HG23	1:B:570:THR:HG23	1.48	0.93
1:B:577:LEU:HD13	1:B:577:LEU:N	1.82	0.93
1:B:394:GLY:C	1:B:396:PRO:HD2	1.89	0.92
1:A:264:ILE:HD11	1:A:295:ILE:HD12	1.52	0.91
1:A:413:GLU:O	1:A:414:ARG:HB2	1.69	0.90
1:B:264:ILE:HD11	1:B:306:LEU:HD12	1.52	0.90
1:A:316:ARG:NH2	1:A:318:LYS:NZ	2.20	0.89
1:B:394:GLY:O	1:B:396:PRO:HD3	1.73	0.88
1:B:577:LEU:N	1:B:577:LEU:CD1	2.37	0.88
1:B:394:GLY:C	1:B:395:VAL:CG1	2.41	0.87
1:B:395:VAL:HB	1:B:429:PHE:HE1	1.06	0.87
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.36	0.87
1:B:181:TRP:CZ3	1:B:215:ARG:CB	2.58	0.87
1:B:181:TRP:CE3	1:B:215:ARG:CB	2.58	0.86
1:A:402:ASP:C	1:A:403:ILE:HD13	1.96	0.86
1:A:342:SER:CB	2:A:1638:LDA:H12	2.04	0.86
1:B:534:ARG:HG3	1:B:535:ASP:H	1.40	0.86
1:A:254:PRO:HG2	1:A:257:LEU:HD12	1.56	0.85
1:B:181:TRP:CE3	1:B:215:ARG:HB3	2.11	0.85
1:B:394:GLY:C	1:B:396:PRO:HD3	1.97	0.85
1:A:271:ASN:ND2	1:A:599:ASN:HD21	1.74	0.85
1:A:395:VAL:N	1:A:396:PRO:HD2	1.92	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:316:ARG:HH21	1:A:318:LYS:HZ2	1.24	0.83
1:B:253:LEU:HD12	1:B:257:LEU:HD23	1.60	0.83
1:A:217:ILE:CG2	1:A:218:PRO:HD2	2.08	0.83
1:A:342:SER:HB3	2:A:1638:LDA:H41	1.60	0.83
1:B:253:LEU:HB2	1:B:254:PRO:HD2	1.59	0.83
1:B:510:ARG:NH1	3:B:1637:C8E:H191	1.95	0.81
1:A:256:ARG:CB	1:A:256:ARG:HH11	1.93	0.81
1:A:217:ILE:HG23	1:A:218:PRO:HD2	1.61	0.81
1:A:196:TYR:HD2	1:A:197:ASN:H	1.26	0.81
1:B:395:VAL:CB	1:B:429:PHE:HE1	1.90	0.81
1:A:486:PHE:HD1	1:A:508:VAL:HG22	1.47	0.80
1:A:515:PHE:C	1:A:517:LEU:N	2.36	0.80
1:A:395:VAL:HG12	1:A:429:PHE:CE1	2.17	0.80
1:A:463:TYR:CG	1:B:592:LEU:HD11	2.17	0.79
1:A:482:TRP:O	1:A:484:THR:HG22	1.82	0.79
1:B:596:ARG:H	1:B:619:GLN:HB3	1.48	0.79
1:B:214:PHE:HB2	1:B:225:THR:HG22	1.62	0.78
1:A:316:ARG:HH21	1:A:318:LYS:HZ3	1.28	0.78
1:A:253:LEU:HB3	1:A:254:PRO:HD2	1.64	0.78
1:B:534:ARG:HG3	1:B:535:ASP:N	1.99	0.78
1:B:413:GLU:O	1:B:414:ARG:HB2	1.82	0.78
1:B:577:LEU:HD13	1:B:577:LEU:H	1.45	0.78
1:A:395:VAL:N	1:A:396:PRO:CD	2.47	0.77
1:A:219:ARG:HG3	1:A:219:ARG:NH1	1.98	0.77
1:B:618:LEU:HB3	1:B:621:GLY:HA3	1.65	0.77
1:B:181:TRP:CE3	1:B:215:ARG:HB2	2.20	0.76
1:B:436:ILE:H	1:B:436:ILE:CD1	1.95	0.76
1:A:256:ARG:NH1	1:A:256:ARG:HB2	1.99	0.76
1:B:184:ARG:CG	1:B:184:ARG:HH11	1.98	0.76
1:B:316:ARG:HD3	4:B:2004:HOH:O	1.85	0.76
1:B:436:ILE:HD13	1:B:436:ILE:N	2.00	0.75
1:B:181:TRP:HZ3	1:B:215:ARG:HB3	1.48	0.75
1:A:340:LEU:O	1:A:340:LEU:HG	1.85	0.75
3:B:1637:C8E:O9	3:B:1637:C8E:C13	2.35	0.75
1:A:332:ARG:HG3	1:A:332:ARG:NH1	1.91	0.74
1:B:510:ARG:HH12	3:B:1637:C8E:C19	2.00	0.74
1:B:183:LEU:HB2	1:B:213:LEU:HD23	1.69	0.74
1:A:254:PRO:HG2	1:A:257:LEU:CD1	2.18	0.74
1:B:394:GLY:O	1:B:395:VAL:CG1	2.30	0.73
1:A:271:ASN:ND2	1:A:599:ASN:ND2	2.36	0.73
1:B:465:SER:HA	1:B:498:ILE:HD11	1.70	0.73
1:B:576:GLY:H	1:B:577:LEU:HD13	1.53	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:217:ILE:HG22	1:B:220:TRP:H	1.54	0.73
1:A:235:ILE:HG12	1:A:361:GLU:OE2	1.89	0.73
1:B:149:ASP:HB2	1:B:173:THR:HG23	1.70	0.72
1:A:429:PHE:CD2	1:A:429:PHE:N	2.55	0.72
1:A:194:SER:O	1:A:200:LYS:HA	1.90	0.72
1:B:148:LEU:HB3	1:B:633:ALA:HB3	1.71	0.71
1:A:196:TYR:OH	1:B:460:ARG:NH1	2.21	0.71
1:A:403:ILE:CD1	1:A:421:TRP:HD1	2.04	0.70
1:A:275:VAL:HB	1:A:285:ASP:HB2	1.73	0.70
1:B:498:ILE:H	1:B:498:ILE:HD13	1.57	0.70
1:B:287:MSE:HE3	1:B:614:ASN:HD22	1.56	0.69
1:A:418:GLY:HA2	1:A:445:GLU:OE1	1.92	0.69
1:B:146:LEU:HD12	1:B:635:ILE:CD1	2.22	0.69
1:A:635:ILE:HG13	1:A:635:ILE:O	1.92	0.68
1:A:395:VAL:H	1:A:396:PRO:HD2	1.58	0.68
1:B:395:VAL:HB	1:B:429:PHE:CZ	2.27	0.68
1:A:427:LYS:HB3	1:A:437:THR:CG2	2.23	0.68
1:B:515:PHE:CD2	1:B:515:PHE:C	2.67	0.67
1:A:309:GLU:OE2	1:A:317:LYS:HD3	1.93	0.67
1:A:220:TRP:N	1:A:220:TRP:CD1	2.62	0.67
1:A:417:GLN:O	1:A:447:ASN:HB2	1.95	0.67
1:B:615:ILE:C	1:B:615:ILE:HD13	2.15	0.67
1:A:379:ALA:HB3	1:A:382:TYR:O	1.95	0.67
1:B:386:ALA:HB2	1:B:404:THR:HB	1.77	0.67
1:A:395:VAL:HG12	1:A:429:PHE:HE1	1.58	0.66
1:B:376:ALA:HB2	1:B:385:LEU:HD12	1.77	0.66
1:B:504:TYR:HB3	1:B:528:ARG:HG2	1.77	0.66
1:B:214:PHE:CB	1:B:225:THR:HG22	2.26	0.66
1:B:566:MSE:HE2	1:B:585:GLY:HA3	1.77	0.66
1:A:479:VAL:C	1:A:481:ASP:H	2.00	0.65
1:A:410:ILE:HD11	1:A:416:PHE:HE1	1.60	0.65
1:B:256:ARG:HA	1:B:428:ARG:NH2	2.12	0.64
1:A:514:VAL:C	1:A:515:PHE:HD1	2.00	0.64
1:A:395:VAL:H	1:A:396:PRO:CD	2.10	0.63
1:B:514:VAL:O	1:B:514:VAL:HG13	1.98	0.63
1:B:278:GLN:NE2	1:B:305:ARG:O	2.32	0.63
1:B:420:SER:OG	1:B:444:SER:HB3	1.98	0.63
1:A:271:ASN:HD21	1:A:599:ASN:HD21	1.47	0.63
1:A:580:TYR:CD1	1:A:602:TYR:HB2	2.34	0.63
1:B:264:ILE:HD11	1:B:306:LEU:CD1	2.25	0.62
1:B:146:LEU:HD12	1:B:635:ILE:HD11	1.81	0.62
1:A:332:ARG:CG	1:A:332:ARG:HH11	2.05	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ILE:HD11	1:A:361:GLU:HB2	1.81	0.62
1:A:232:ASN:H	1:A:232:ASN:HD22	1.47	0.62
1:B:393:LEU:HB2	1:B:396:PRO:HG2	1.82	0.61
1:A:342:SER:HB2	2:A:1638:LDA:C1	2.22	0.61
1:B:217:ILE:HG21	1:B:220:TRP:HB2	1.83	0.61
1:A:425:TYR:OH	1:A:427:LYS:HB2	2.01	0.61
1:B:449:MSE:HE2	1:B:466:ARG:NH1	2.16	0.61
1:A:503:TYR:OH	1:A:530:LYS:HE2	1.99	0.61
1:A:403:ILE:HD13	1:A:403:ILE:N	2.13	0.61
1:A:414:ARG:HH21	1:A:416:PHE:HE2	1.47	0.61
1:A:253:LEU:CB	1:A:254:PRO:HD2	2.30	0.61
1:A:159:ASN:HB3	1:A:161:GLN:HG2	1.83	0.61
1:B:498:ILE:HD13	1:B:498:ILE:N	2.16	0.60
1:A:458:ARG:C	1:A:458:ARG:HD3	2.22	0.60
1:B:184:ARG:CG	1:B:184:ARG:NH1	2.62	0.60
1:A:514:VAL:C	1:A:515:PHE:CD1	2.75	0.60
1:A:312:GLU:HG3	1:A:318:LYS:HE2	1.84	0.60
1:B:449:MSE:HE2	1:B:466:ARG:HH12	1.67	0.60
1:B:243:GLY:HA3	1:B:342:SER:O	2.02	0.59
1:B:270:THR:C	1:B:290:ALA:HB2	2.23	0.59
1:A:570:THR:HB	1:A:581:SER:HB3	1.84	0.59
1:A:580:TYR:HD1	1:A:602:TYR:HB2	1.65	0.59
1:A:235:ILE:HD13	1:A:361:GLU:HG3	1.85	0.59
1:B:402:ASP:OD1	1:B:402:ASP:N	2.35	0.59
1:A:416:PHE:HB3	1:A:447:ASN:HB3	1.85	0.59
1:A:468:LYS:HG3	1:A:496:TRP:CE2	2.37	0.59
1:B:256:ARG:HA	1:B:428:ARG:CZ	2.33	0.58
1:B:437:THR:HA	1:B:474:THR:O	2.03	0.58
1:A:468:LYS:HB3	1:A:494:THR:OG1	2.03	0.58
1:A:337:ARG:HB2	1:A:363:SER:HB3	1.84	0.58
1:A:419:LYS:HG3	1:A:421:TRP:CH2	2.39	0.58
1:B:246:LEU:HB2	2:B:1639:LDA:H91	1.86	0.58
1:A:414:ARG:HG2	1:A:415:THR:H	1.69	0.58
1:A:410:ILE:HD11	1:A:416:PHE:CE1	2.38	0.58
1:B:615:ILE:HD13	1:B:616:ALA:N	2.19	0.57
1:A:218:PRO:HB2	1:A:219:ARG:HG2	1.87	0.57
1:A:316:ARG:HH22	1:A:536:ASN:HD21	1.52	0.57
1:A:252:MSE:HA	1:A:258:ARG:NH2	2.18	0.57
1:A:256:ARG:NH1	1:A:256:ARG:CB	2.63	0.57
1:B:287:MSE:HE3	1:B:614:ASN:ND2	2.19	0.57
1:A:463:TYR:CD1	1:B:592:LEU:HD11	2.40	0.57
1:A:262:PRO:HB3	1:A:324:THR:HG22	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:550:GLY:HA2	1:B:571:ASP:HA	1.85	0.57
1:A:330:LEU:CD2	1:A:390:GLY:HA3	2.34	0.56
1:B:348:TYR:CE1	1:B:455:LEU:HD13	2.39	0.56
1:B:531:TYR:CD2	1:B:532:LEU:HD22	2.41	0.56
1:B:488:LEU:C	1:B:488:LEU:HD23	2.24	0.56
1:A:402:ASP:O	1:A:403:ILE:HD13	2.06	0.56
1:B:574:ASN:O	1:B:575:ASP:CB	2.34	0.56
1:A:392:ASP:OD1	1:A:393:LEU:N	2.38	0.56
1:B:254:PRO:HD3	1:B:332:ARG:NH1	2.20	0.56
1:A:413:GLU:O	1:A:414:ARG:CB	2.48	0.56
1:A:577:LEU:HD23	4:A:2014:HOH:O	2.05	0.56
1:B:391:TRP:HE3	1:B:399:LEU:HD23	1.71	0.55
1:B:368:ASN:CB	1:B:370:TRP:HE3	2.18	0.55
1:A:217:ILE:HG22	1:A:218:PRO:HD2	1.88	0.55
1:A:264:ILE:O	1:A:264:ILE:HG13	2.06	0.55
1:A:181:TRP:CE3	1:A:215:ARG:HB3	2.42	0.55
1:A:413:GLU:OE1	1:B:592:LEU:HD22	2.06	0.55
1:B:342:SER:HB3	2:B:1639:LDA:H61	1.88	0.55
1:B:476:ASN:ND2	1:B:487:ASN:ND2	2.56	0.54
1:A:470:MSE:HE3	1:A:472:THR:HG22	1.90	0.54
1:A:468:LYS:HG3	1:A:496:TRP:CZ2	2.42	0.54
1:B:287:MSE:CE	1:B:614:ASN:HD22	2.20	0.54
1:B:284:TYR:CD2	1:B:295:ILE:HD13	2.42	0.54
1:B:376:ALA:HB2	1:B:385:LEU:CD1	2.37	0.54
1:A:420:SER:HB3	1:A:444:SER:CB	2.37	0.54
1:B:159:ASN:HB2	1:B:163:GLY:H	1.73	0.54
1:B:386:ALA:CB	1:B:404:THR:HB	2.38	0.53
1:A:219:ARG:CG	1:A:219:ARG:NH1	2.66	0.53
1:B:231:ILE:HD11	1:B:238:SER:HA	1.90	0.53
1:B:451:MSE:O	1:B:455:LEU:HG	2.09	0.53
1:A:521:ALA:HB3	1:A:544:SER:OG	2.08	0.53
1:A:255:PRO:HA	1:A:258:ARG:HE	1.72	0.53
1:A:181:TRP:HA	1:A:181:TRP:CE3	2.43	0.53
1:B:184:ARG:NH1	1:B:186:ASP:OD1	2.42	0.53
1:A:479:VAL:C	1:A:481:ASP:N	2.62	0.53
1:A:515:PHE:CD1	1:A:515:PHE:N	2.77	0.52
1:A:519:GLY:O	1:A:546:PRO:HD3	2.08	0.52
1:A:391:TRP:CD1	1:A:392:ASP:N	2.78	0.52
4:A:2002:HOH:O	1:B:348:TYR:HA	2.09	0.52
1:A:427:LYS:HB3	1:A:437:THR:HG23	1.91	0.52
1:B:393:LEU:CB	1:B:396:PRO:HG2	2.38	0.52
1:B:146:LEU:CD1	1:B:635:ILE:HD11	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:ILE:HG13	1:A:311:ILE:O	2.10	0.52
1:A:419:LYS:HG2	1:A:445:GLU:CD	2.30	0.52
1:A:156:VAL:HG22	1:A:166:HIS:HD2	1.74	0.52
1:A:271:ASN:O	1:A:313:GLN:HG3	2.10	0.52
1:B:157:SER:HB3	1:B:624:SER:HB3	1.91	0.52
1:A:373:TYR:CE2	1:A:402:ASP:OD1	2.62	0.52
1:A:160:TYR:HE2	1:B:461:ASN:HB2	1.75	0.52
1:A:160:TYR:CE2	1:B:461:ASN:HB2	2.45	0.52
1:A:342:SER:CB	2:A:1638:LDA:H41	2.36	0.51
1:A:501:THR:HG23	1:A:501:THR:O	2.10	0.51
1:A:330:LEU:HD21	1:A:390:GLY:HA3	1.93	0.51
1:B:347:GLY:C	1:B:348:TYR:CG	2.84	0.51
1:A:573:PHE:CE1	1:A:578:ASP:HB2	2.46	0.51
1:A:264:ILE:HD13	1:A:276:VAL:HG22	1.92	0.51
1:A:395:VAL:C	1:A:397:GLY:H	2.13	0.51
1:B:146:LEU:HD12	1:B:635:ILE:HG13	1.91	0.51
1:A:156:VAL:HG22	1:A:166:HIS:CD2	2.46	0.51
1:B:157:SER:CB	1:B:624:SER:HB3	2.40	0.51
1:B:599:ASN:OD1	1:B:599:ASN:C	2.48	0.51
1:A:271:ASN:HD21	1:A:599:ASN:ND2	2.04	0.51
1:B:253:LEU:CD1	1:B:257:LEU:HD23	2.37	0.51
1:A:564:VAL:HG22	1:A:587:ASN:OD1	2.11	0.51
1:B:148:LEU:O	1:B:632:GLY:HA2	2.10	0.51
1:A:269:GLU:OE1	1:A:318:LYS:NZ	2.44	0.51
1:A:264:ILE:CG1	1:A:295:ILE:HB	2.40	0.51
1:A:443:PHE:HA	1:A:468:LYS:O	2.11	0.51
1:A:411:GLU:C	1:A:413:GLU:H	2.14	0.51
1:B:368:ASN:HB3	1:B:370:TRP:HE3	1.76	0.51
1:A:393:LEU:HB2	1:A:397:GLY:O	2.11	0.50
1:A:326:SER:HB2	1:A:422:ARG:HH21	1.74	0.50
1:B:206:PHE:CD1	1:B:207:THR:N	2.78	0.50
1:B:586:LEU:HD22	1:B:594:SER:HB2	1.92	0.50
1:A:463:TYR:CD1	1:B:592:LEU:CD1	2.94	0.50
1:B:403:ILE:HD12	1:B:403:ILE:N	2.27	0.50
1:A:192:GLU:O	1:A:202:THR:HA	2.11	0.50
1:A:419:LYS:HG2	1:A:445:GLU:OE1	2.12	0.50
1:A:403:ILE:CD1	1:A:421:TRP:CD1	2.79	0.50
1:A:515:PHE:N	1:A:515:PHE:HD1	2.10	0.50
1:B:465:SER:HA	1:B:498:ILE:CD1	2.41	0.49
1:B:235:ILE:HG23	1:B:236:PHE:CD1	2.47	0.49
1:A:188:GLN:OE1	1:A:282:VAL:HG23	2.11	0.49
1:A:215:ARG:HG3	1:A:215:ARG:O	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:411:GLU:O	1:A:413:GLU:N	2.45	0.49
1:B:466:ARG:HG2	1:B:497:ASP:OD1	2.12	0.49
1:A:176:GLY:N	1:A:183:LEU:HB3	2.27	0.49
1:B:580:TYR:CE1	1:B:602:TYR:HB2	2.47	0.49
1:A:368:ASN:C	1:A:370:TRP:H	2.15	0.49
1:B:263:GLN:HE22	1:B:487:ASN:HD21	1.59	0.49
1:A:344:ARG:HB3	1:A:354:GLY:O	2.12	0.49
1:A:521:ALA:O	1:A:543:ILE:HA	2.12	0.49
1:B:382:TYR:CE2	1:B:451:MSE:HG2	2.47	0.49
1:B:231:ILE:C	1:B:231:ILE:HD12	2.32	0.49
1:A:263:GLN:CG	1:A:296:GLN:HB3	2.42	0.49
1:A:264:ILE:HD13	1:A:276:VAL:CG2	2.42	0.49
1:A:232:ASN:N	1:A:232:ASN:HD22	2.09	0.49
1:A:514:VAL:HG12	1:A:515:PHE:CE1	2.47	0.49
1:A:570:THR:CB	1:A:581:SER:HB3	2.42	0.49
1:B:146:LEU:HD12	1:B:635:ILE:CG1	2.43	0.48
1:A:181:TRP:CZ3	1:A:215:ARG:HB3	2.48	0.48
1:B:493:GLN:HB3	1:B:501:THR:HG22	1.95	0.48
1:A:611:LEU:HD23	1:A:612:SER:N	2.28	0.48
1:A:458:ARG:HD3	1:A:458:ARG:O	2.14	0.48
1:A:413:GLU:HG2	1:A:463:TYR:OH	2.14	0.48
1:B:330:LEU:HD21	1:B:390:GLY:HA3	1.96	0.48
1:A:275:VAL:HA	1:A:284:TYR:O	2.13	0.48
1:A:180:PRO:O	1:A:215:ARG:CB	2.35	0.48
1:B:217:ILE:HG21	1:B:220:TRP:CB	2.42	0.48
1:A:573:PHE:CD1	1:A:578:ASP:HB2	2.48	0.48
1:A:411:GLU:C	1:A:413:GLU:N	2.66	0.48
1:B:388:GLY:HA3	1:B:402:ASP:HB3	1.96	0.48
1:B:531:TYR:CD2	1:B:532:LEU:CD2	2.97	0.48
1:B:264:ILE:HD12	1:B:276:VAL:HG11	1.96	0.48
1:A:198:GLY:HA3	1:B:205:ASN:HD22	1.79	0.48
1:B:395:VAL:HG23	1:B:395:VAL:O	2.13	0.48
1:A:427:LYS:HB3	1:A:437:THR:HG22	1.96	0.48
1:A:242:THR:OG1	1:A:346:ARG:HD2	2.14	0.48
1:A:237:ARG:HH22	1:A:467:GLU:CD	2.16	0.48
1:B:514:VAL:O	1:B:514:VAL:CG1	2.62	0.47
1:A:176:GLY:H	1:A:183:LEU:HB3	1.78	0.47
1:A:543:ILE:HD13	1:A:543:ILE:H	1.79	0.47
1:A:257:LEU:HD22	1:A:330:LEU:HB2	1.95	0.47
1:A:429:PHE:N	1:A:429:PHE:HD2	2.07	0.47
1:B:217:ILE:CG2	1:B:220:TRP:HB2	2.43	0.47
1:B:391:TRP:CE3	1:B:399:LEU:HD23	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:580:TYR:CD1	1:B:602:TYR:HB2	2.48	0.47
1:B:397:GLY:HA3	1:B:425:TYR:CE1	2.49	0.47
1:A:164:ASP:HB2	1:A:195:ARG:HH12	1.79	0.47
1:B:240:SER:HB2	1:B:346:ARG:NH1	2.29	0.47
1:B:231:ILE:CG1	1:B:238:SER:HA	2.45	0.47
1:B:170:TYR:OH	1:B:206:PHE:HD2	1.98	0.47
1:A:218:PRO:HG2	1:A:219:ARG:CG	2.45	0.47
1:A:479:VAL:O	1:A:481:ASP:N	2.47	0.47
1:A:193:GLN:HA	1:A:201:THR:O	2.14	0.47
1:A:365:GLY:CA	4:A:2006:HOH:O	2.37	0.47
1:A:235:ILE:HG12	1:A:361:GLU:CD	2.35	0.47
1:B:256:ARG:HA	1:B:428:ARG:NH1	2.30	0.47
1:A:159:ASN:HB2	1:A:163:GLY:H	1.79	0.47
1:B:437:THR:OG1	1:B:475:LEU:HD23	2.14	0.47
1:A:578:ASP:OD1	1:A:604:HIS:ND1	2.48	0.47
1:B:185:ALA:HB1	1:B:208:TRP:CZ3	2.50	0.47
1:B:153:ASN:HB2	1:B:169:SER:OG	2.15	0.47
1:A:373:TYR:OH	1:A:402:ASP:OD1	2.27	0.47
1:B:448:TYR:O	1:B:466:ARG:NH2	2.48	0.47
1:A:235:ILE:CD1	1:A:375:GLY:HA3	2.44	0.47
1:B:512:PHE:N	1:B:520:VAL:O	2.41	0.47
1:B:488:LEU:HD23	1:B:489:GLN:N	2.30	0.47
1:A:514:VAL:HB	1:A:515:PHE:HD1	1.80	0.46
1:A:468:LYS:HE3	1:A:496:TRP:CZ3	2.49	0.46
1:B:410:ILE:CD1	1:B:454:TYR:CE1	2.98	0.46
1:B:460:ARG:HG2	1:B:460:ARG:HH11	1.80	0.46
1:B:206:PHE:CD1	1:B:206:PHE:C	2.89	0.46
1:A:224:LEU:C	1:A:224:LEU:HD23	2.35	0.46
1:A:278:GLN:NE2	1:A:305:ARG:O	2.49	0.46
1:A:231:ILE:HD12	1:A:231:ILE:C	2.35	0.46
1:A:391:TRP:HD1	1:A:392:ASP:N	2.13	0.46
1:A:224:LEU:HD23	1:A:225:THR:N	2.31	0.46
1:A:420:SER:HB3	1:A:444:SER:HB3	1.96	0.46
1:A:486:PHE:CD1	1:A:508:VAL:HG22	2.38	0.46
1:B:566:MSE:CE	1:B:597:GLN:OE1	2.63	0.46
1:B:634:THR:O	1:B:634:THR:HG23	2.15	0.46
1:A:264:ILE:HG12	1:A:295:ILE:HB	1.97	0.46
1:A:436:ILE:HD11	1:A:476:ASN:HB2	1.97	0.46
1:A:410:ILE:CD1	1:A:416:PHE:HE1	2.27	0.46
1:B:514:VAL:HG12	1:B:520:VAL:HG21	1.98	0.46
1:B:224:LEU:C	1:B:224:LEU:HD23	2.36	0.46
1:B:481:ASP:O	1:B:482:TRP:CD1	2.69	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:LEU:O	1:A:254:PRO:C	2.54	0.45
1:B:257:LEU:HD11	1:B:330:LEU:HB2	1.98	0.45
1:B:364:TRP:HE3	1:B:372:LEU:O	1.98	0.45
1:B:458:ARG:HD3	1:B:458:ARG:C	2.37	0.45
1:A:279:GLN:HE22	1:A:452:GLU:CD	2.19	0.45
1:B:196:TYR:CG	1:B:197:ASN:N	2.84	0.45
1:B:311:ILE:HD12	1:B:311:ILE:N	2.31	0.45
1:B:188:GLN:OE1	1:B:282:VAL:HG23	2.16	0.45
1:B:543:ILE:HD13	1:B:543:ILE:N	2.31	0.45
1:B:262:PRO:HB3	1:B:324:THR:HB	1.99	0.45
1:A:419:LYS:N	1:A:445:GLU:OE1	2.50	0.45
1:B:536:ASN:HA	1:B:560:ASN:OD1	2.17	0.45
1:A:404:THR:O	1:A:419:LYS:HA	2.16	0.45
1:B:514:VAL:O	1:B:515:PHE:HB3	2.16	0.45
1:A:263:GLN:HG3	1:A:296:GLN:HB3	1.98	0.45
1:A:619:GLN:C	1:A:621:GLY:N	2.69	0.45
1:A:573:PHE:N	1:A:573:PHE:CD2	2.84	0.45
1:A:525:SER:O	1:A:539:ALA:HA	2.17	0.45
1:B:368:ASN:HB2	1:B:370:TRP:HE3	1.82	0.45
3:B:1637:C8E:O9	3:B:1637:C8E:H132	2.14	0.45
1:A:235:ILE:CD1	1:A:361:GLU:HG3	2.47	0.45
1:B:615:ILE:CD1	1:B:615:ILE:C	2.85	0.45
1:A:237:ARG:NH2	1:A:467:GLU:OE1	2.50	0.45
1:B:262:PRO:O	1:B:298:LEU:HD12	2.17	0.45
1:A:454:TYR:O	1:A:457:ALA:HB3	2.16	0.45
1:B:231:ILE:HG13	1:B:238:SER:HA	1.99	0.44
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.79	0.44
1:A:185:ALA:HB1	1:A:208:TRP:CZ3	2.51	0.44
1:B:577:LEU:O	1:B:605:ARG:N	2.50	0.44
1:A:488:LEU:HD13	1:A:488:LEU:C	2.38	0.44
1:A:373:TYR:CZ	1:A:402:ASP:OD1	2.71	0.44
1:A:551:THR:HG23	1:A:570:THR:CG2	2.33	0.44
1:B:155:THR:HA	1:B:626:GLY:HA2	1.99	0.44
1:A:225:THR:CG2	1:A:245:SER:OG	2.66	0.44
1:B:217:ILE:CG2	1:B:220:TRP:CB	2.96	0.44
1:A:202:THR:O	1:B:201:THR:HA	2.17	0.44
1:B:470:MSE:O	1:B:470:MSE:HE3	2.18	0.44
1:A:627:VAL:HG12	1:A:628:SER:N	2.32	0.44
1:B:197:ASN:HD22	1:B:198:GLY:N	2.15	0.44
1:A:235:ILE:HG13	1:A:236:PHE:CD1	2.53	0.44
1:A:159:ASN:HB2	1:A:163:GLY:N	2.32	0.44
1:B:231:ILE:CD1	1:B:238:SER:HA	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:380:GLY:O	1:B:383:ASN:ND2	2.51	0.44
1:A:316:ARG:NH2	1:A:318:LYS:HZ3	2.05	0.43
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.83	0.43
1:A:253:LEU:O	1:A:258:ARG:CZ	2.66	0.43
1:A:513:ASN:OD1	1:A:518:GLN:HA	2.18	0.43
1:A:470:MSE:O	1:A:470:MSE:HE2	2.18	0.43
1:A:259:GLY:HA3	1:A:303:ARG:NH2	2.33	0.43
1:B:413:GLU:HG3	1:B:463:TYR:OH	2.18	0.43
1:A:304:GLY:O	1:A:324:THR:HG23	2.19	0.43
1:A:225:THR:HG23	1:A:245:SER:OG	2.18	0.43
1:B:623:THR:HG23	1:B:623:THR:O	2.19	0.43
1:A:543:ILE:N	1:A:543:ILE:HD13	2.33	0.43
1:B:330:LEU:CD2	1:B:390:GLY:HA3	2.47	0.43
1:B:314:ASN:HD21	1:B:316:ARG:HD2	1.83	0.43
1:A:399:LEU:HD12	1:A:425:TYR:CD1	2.54	0.43
1:B:540:TYR:CE2	1:B:555:SER:HB3	2.54	0.43
1:B:194:SER:O	1:B:200:LYS:HA	2.18	0.43
1:A:157:SER:HB3	1:A:624:SER:HB2	2.01	0.43
1:B:237:ARG:HD2	1:B:450:THR:HG21	2.01	0.43
1:A:316:ARG:NH2	1:A:318:LYS:HZ2	1.98	0.43
1:B:368:ASN:CB	1:B:370:TRP:CE3	3.00	0.43
1:B:490:TYR:OH	1:B:492:ARG:HD2	2.19	0.43
1:B:224:LEU:CD1	2:B:1639:LDA:H123	2.49	0.42
1:B:586:LEU:CD2	1:B:594:SER:HB2	2.49	0.42
1:B:233:SER:HB3	1:B:236:PHE:O	2.19	0.42
1:A:382:TYR:CE2	1:A:451:MSE:HG2	2.55	0.42
1:B:532:LEU:H	1:B:532:LEU:HD22	1.83	0.42
1:A:270:THR:C	1:A:290:ALA:HB2	2.39	0.42
1:A:261:ALA:HA	1:A:262:PRO:HD3	1.79	0.42
1:B:438:PHE:CD2	1:B:438:PHE:C	2.92	0.42
1:B:231:ILE:HG12	1:B:239:TRP:CE3	2.54	0.42
1:B:240:SER:HB2	1:B:346:ARG:HH12	1.85	0.42
1:A:273:ARG:HA	1:A:287:MSE:HA	2.02	0.42
1:B:563:TYR:HD2	1:B:588:SER:HG	1.66	0.42
1:B:310:VAL:HB	1:B:318:LYS:HB2	2.00	0.42
1:A:463:TYR:CD2	1:B:592:LEU:HD11	2.54	0.42
1:B:507:SER:HA	1:B:524:LEU:O	2.19	0.42
1:B:627:VAL:HG12	1:B:628:SER:N	2.34	0.42
1:B:410:ILE:CD1	1:B:454:TYR:HE1	2.32	0.42
1:A:275:VAL:HG13	1:A:309:GLU:HB3	2.02	0.42
1:A:208:TRP:O	1:A:209:SER:C	2.58	0.42
1:A:574:ASN:N	1:A:574:ASN:HD22	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:348:TYR:OH	1:B:452:GLU:OE2	2.38	0.42
1:B:531:TYR:O	1:B:533:GLY:N	2.48	0.42
1:A:573:PHE:O	1:A:574:ASN:HB2	2.20	0.42
1:A:514:VAL:HG12	1:A:515:PHE:HE1	1.85	0.41
1:A:619:GLN:O	1:A:621:GLY:N	2.53	0.41
1:A:493:GLN:C	1:A:493:GLN:HE21	2.23	0.41
1:A:151:ASN:HB3	1:A:171:ASN:O	2.19	0.41
1:B:592:LEU:HA	1:B:592:LEU:HD23	1.77	0.41
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.57	0.41
1:B:253:LEU:CB	1:B:254:PRO:HD2	2.35	0.41
1:A:470:MSE:CE	1:A:472:THR:HG22	2.49	0.41
1:A:381:ASP:HB2	1:A:454:TYR:OH	2.19	0.41
1:B:395:VAL:C	1:B:397:GLY:H	2.24	0.41
1:B:256:ARG:HA	1:B:428:ARG:HH22	1.84	0.41
1:A:235:ILE:HG13	1:A:236:PHE:N	2.35	0.41
1:B:368:ASN:HB3	1:B:370:TRP:CE3	2.54	0.41
1:B:410:ILE:HD12	1:B:410:ILE:HG23	1.85	0.41
1:A:558:MSE:HE3	1:A:560:ASN:O	2.20	0.41
1:B:468:LYS:HB3	1:B:494:THR:HG23	2.01	0.41
1:B:575:ASP:HB3	1:B:576:GLY:H	1.65	0.41
1:B:316:ARG:CD	4:B:2004:HOH:O	2.55	0.41
2:A:1638:LDA:H41	2:A:1638:LDA:H12	1.85	0.41
1:A:262:PRO:CB	1:A:324:THR:HG22	2.50	0.41
1:B:261:ALA:HA	1:B:262:PRO:HD3	1.81	0.41
1:B:357:PHE:CD1	1:B:357:PHE:C	2.94	0.41
1:B:578:ASP:CG	1:B:604:HIS:HD1	2.24	0.41
1:A:154:GLY:HA2	1:A:167:GLN:O	2.19	0.41
1:B:575:ASP:HB3	1:B:577:LEU:HD13	2.03	0.41
1:B:619:GLN:C	1:B:621:GLY:N	2.73	0.40
1:A:403:ILE:CD1	1:A:403:ILE:N	2.83	0.40
1:A:463:TYR:CD1	1:A:463:TYR:N	2.89	0.40
1:B:273:ARG:HA	1:B:287:MSE:HA	2.03	0.40
3:B:1637:C8E:O9	3:B:1637:C8E:H131	2.16	0.40
1:B:402:ASP:C	1:B:403:ILE:HD12	2.41	0.40
1:A:229:ASN:OD1	1:A:230:ASN:N	2.51	0.40
1:A:247:GLU:HB3	1:A:339:LYS:HG2	2.03	0.40
1:B:247:GLU:CG	1:B:339:LYS:HG2	2.52	0.40
1:B:497:ASP:OD2	1:B:498:ILE:HD12	2.21	0.40
1:A:425:TYR:CZ	1:A:427:LYS:HB2	2.57	0.40
1:B:504:TYR:OH	1:B:506:VAL:HG21	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/515 (90%)	416 (90%)	40 (9%)	7 (2%)	15	64
1	B	467/515 (91%)	424 (91%)	37 (8%)	6 (1%)	18	68
All	All	930/1030 (90%)	840 (90%)	77 (8%)	13 (1%)	16	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	ARG
1	B	395	VAL
1	B	414	ARG
1	B	575	ASP
1	A	480	ALA
1	A	256	ARG
1	B	198	GLY
1	B	411	GLU
1	B	532	LEU
1	A	254	PRO
1	A	593	THR
1	A	412	GLY
1	A	620	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/414 (96%)	327 (83%)	69 (17%)	3	13
1	B	392/414 (95%)	330 (84%)	62 (16%)	4	16
All	All	788/828 (95%)	657 (83%)	131 (17%)	3	14

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	THR
1	A	161	GLN
1	A	178	LEU
1	A	181	TRP
1	A	195	ARG
1	A	201	THR
1	A	205	ASN
1	A	214	PHE
1	A	215	ARG
1	A	219	ARG
1	A	220	TRP
1	A	225	THR
1	A	226	LEU
1	A	232	ASN
1	A	237	ARG
1	A	248	SER
1	A	256	ARG
1	A	263	GLN
1	A	278	GLN
1	A	285	ASP
1	A	288	VAL
1	A	296	GLN
1	A	299	ASP
1	A	305	ARG
1	A	311	ILE
1	A	319	THR
1	A	323	ASP
1	A	332	ARG
1	A	340	LEU
1	A	395	VAL
1	A	398	THR
1	A	399	LEU
1	A	404	THR
1	A	410	ILE
1	A	423	LEU
1	A	428	ARG
1	A	429	PHE
1	A	446	ARG
1	A	453	GLN
1	A	458	ARG
1	A	464	SER
1	A	467	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	475	LEU
1	A	484	THR
1	A	493	GLN
1	A	494	THR
1	A	506	VAL
1	A	515	PHE
1	A	537	ASP
1	A	543	ILE
1	A	551	THR
1	A	558	MSE
1	A	560	ASN
1	A	561	ASP
1	A	563	TYR
1	A	565	ASN
1	A	566	MSE
1	A	570	THR
1	A	574	ASN
1	A	575	ASP
1	A	582	LEU
1	A	586	LEU
1	A	594	SER
1	A	598	ILE
1	A	599	ASN
1	A	608	LEU
1	A	614	ASN
1	A	615	ILE
1	A	618	LEU
1	B	147	MSE
1	B	164	ASP
1	B	165	SER
1	B	183	LEU
1	B	184	ARG
1	B	188	GLN
1	B	197	ASN
1	B	202	THR
1	B	203	ASN
1	B	205	ASN
1	B	210	ARG
1	B	221	ARG
1	B	226	LEU
1	B	245	SER
1	B	256	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	275	VAL
1	B	278	GLN
1	B	288	VAL
1	B	299	ASP
1	B	303	ARG
1	B	319	THR
1	B	323	ASP
1	B	331	THR
1	B	335	GLN
1	B	342	SER
1	B	344	ARG
1	B	348	TYR
1	B	361	GLU
1	B	367	SER
1	B	372	LEU
1	B	399	LEU
1	B	404	THR
1	B	420	SER
1	B	429	PHE
1	B	436	ILE
1	B	444	SER
1	B	449	MSE
1	B	453	GLN
1	B	458	ARG
1	B	470	MSE
1	B	485	SER
1	B	493	GLN
1	B	498	ILE
1	B	502	ASP
1	B	515	PHE
1	B	532	LEU
1	B	537	ASP
1	B	543	ILE
1	B	551	THR
1	B	555	SER
1	B	561	ASP
1	B	563	TYR
1	B	575	ASP
1	B	577	LEU
1	B	586	LEU
1	B	593	THR
1	B	594	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	599	ASN
1	B	605	ARG
1	B	614	ASN
1	B	615	ILE
1	B	618	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	166	HIS
1	A	167	GLN
1	A	232	ASN
1	A	278	GLN
1	A	279	GLN
1	A	493	GLN
1	A	536	ASN
1	A	565	ASN
1	A	597	GLN
1	A	599	ASN
1	B	151	ASN
1	B	197	ASN
1	B	205	ASN
1	B	278	GLN
1	B	314	ASN
1	B	335	GLN
1	B	369	GLN
1	B	476	ASN
1	B	487	ASN
1	B	493	GLN
1	B	595	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LDA	A	1638	-	15,15,15	3.96	2 (13%)	17,17,17	1.34	1 (5%)
3	C8E	B	1637	-	20,20,20	0.38	0	19,19,19	0.39	0
3	C8E	B	1638	-	20,20,20	0.38	0	19,19,19	0.39	0
2	LDA	B	1639	-	15,15,15	3.96	2 (13%)	17,17,17	1.34	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	A	1638	-	-	0/13/13/13	0/0/0/0
3	C8E	B	1637	-	-	0/18/18/18	0/0/0/0
3	C8E	B	1638	-	-	0/18/18/18	0/0/0/0
2	LDA	B	1639	-	-	0/13/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1638	LDA	O1-N1	-14.89	1.25	1.39
2	B	1639	LDA	O1-N1	-14.87	1.25	1.39
2	A	1638	LDA	C1-N1	-3.08	1.45	1.51
2	B	1639	LDA	C1-N1	-3.07	1.45	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1639	LDA	C2-C1-N1	-5.14	104.94	113.80
2	A	1638	LDA	C2-C1-N1	-5.11	104.99	113.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	477/515 (92%)	-0.25	0 100 100	18, 47, 75, 91	33 (6%)
1	B	477/515 (92%)	-0.24	1 (0%) 93 66	21, 47, 75, 91	33 (6%)
All	All	954/1030 (92%)	-0.25	1 (0%) 93 74	18, 47, 75, 91	66 (6%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	MSE	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	C8E	B	1638	21/21	0.29	3.41	81,90,93,94	0
2	LDA	B	1639	16/16	0.29	2.04	54,57,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C8E	B	1637	21/21	0.36	1.89	77,83,86,86	0
2	LDA	A	1638	16/16	0.27	1.58	78,83,89,90	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.