



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:43 am GMT

PDB ID : 3VQX  
Title : Crystal structure of the catalytic domain of pyrrolysyl-tRNA synthetase in triclinic crystal form  
Authors : Yanagisawa, T.; Sumida, T.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2012-04-02  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

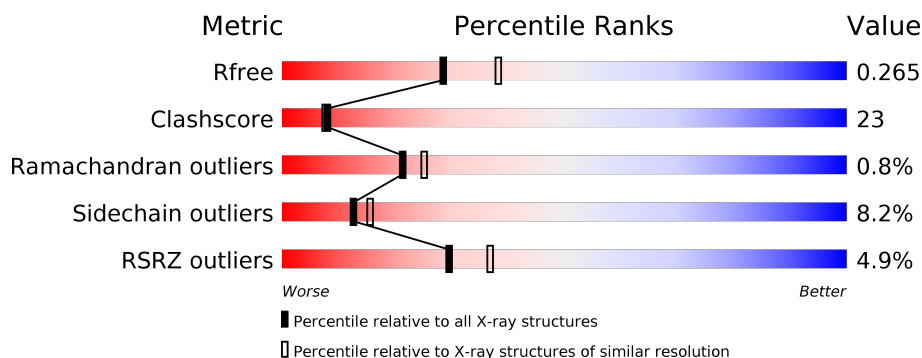
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>30%</div> <div>5%</div> <div>13%</div> </div> </div>
1	B	291	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>27%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	291	<div> <div>7%</div> <div> <div></div> <div>52%</div> <div>31%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	291	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>29%</div> <div>5%</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

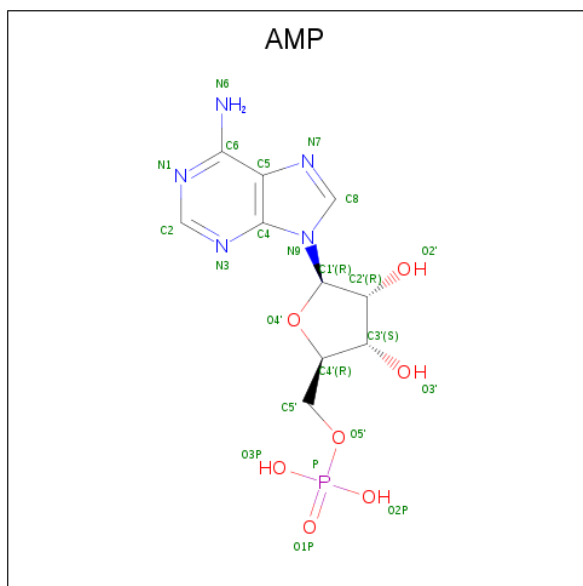
There are 5 unique types of molecules in this entry. The entry contains 8544 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyrrolysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			2062	1316	355	380	11			
1	B	246	Total	C	N	O	S	0	0	0
			2012	1288	347	368	9			
1	C	254	Total	C	N	O	S	0	0	0
			2069	1321	357	380	11			
1	D	257	Total	C	N	O	S	0	0	0
			2093	1334	360	388	11			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



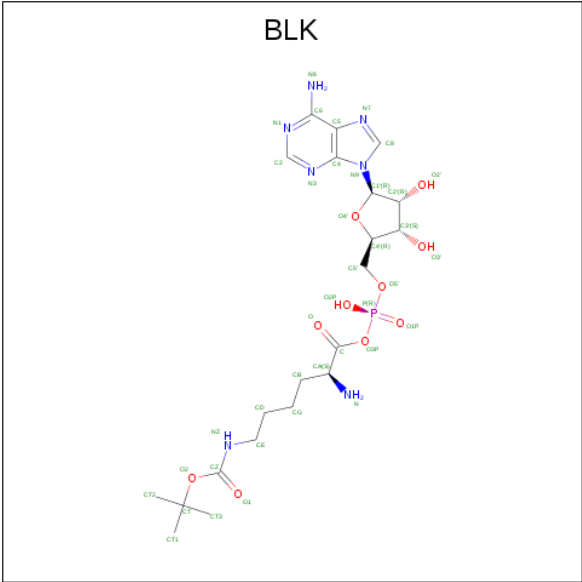
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] (2S)-2-azanyl-6-[(2-methylpropan-2-yl)oxycarbonylamino]hexanoate (three-letter code: BLK) (formula: C<sub>21</sub>H<sub>34</sub>N<sub>7</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			39	21	7	10	1		
4	D	1	Total	C	N	O	P	0	0
			39	21	7	10	1		

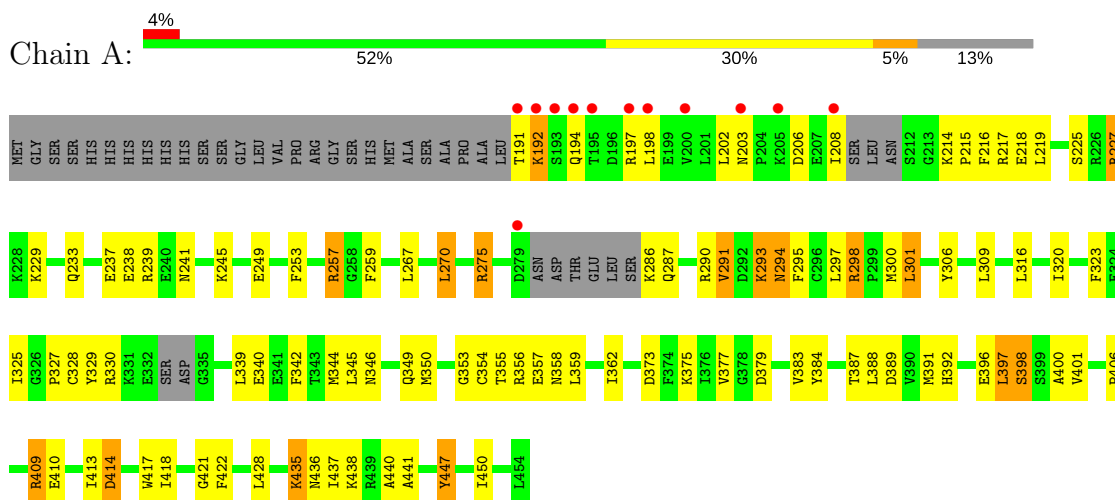
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	49	Total	O	0	0
			49	49		
5	C	39	Total	O	0	0
			39	39		
5	D	30	Total	O	0	0
			30	30		

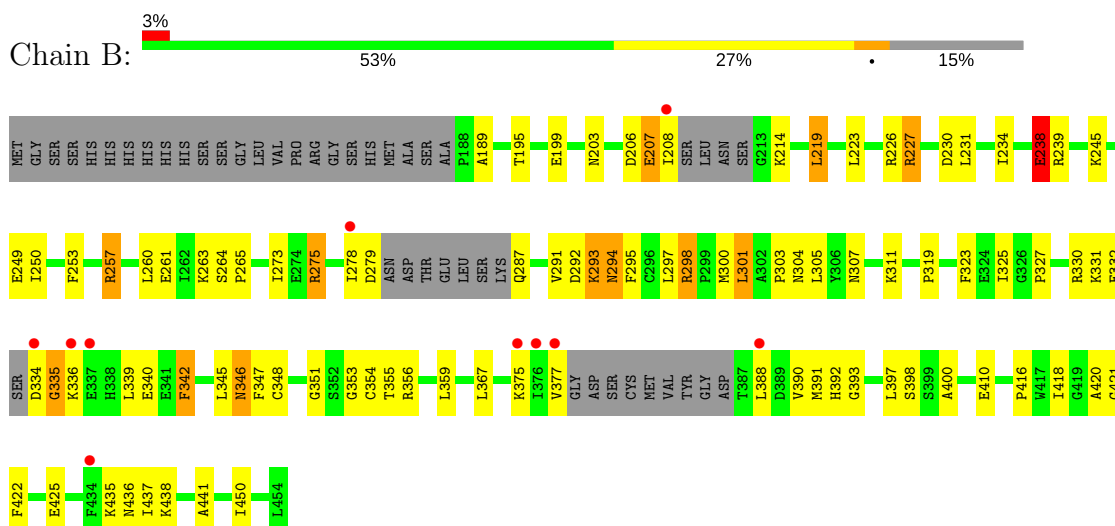
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Pyrrollysine-tRNA ligase

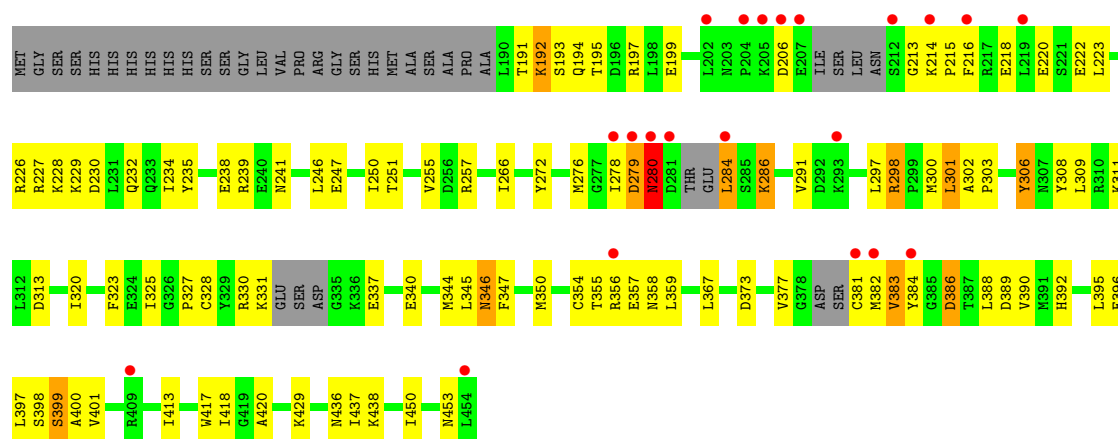


- Molecule 1: Pyrrollysine-tRNA ligase

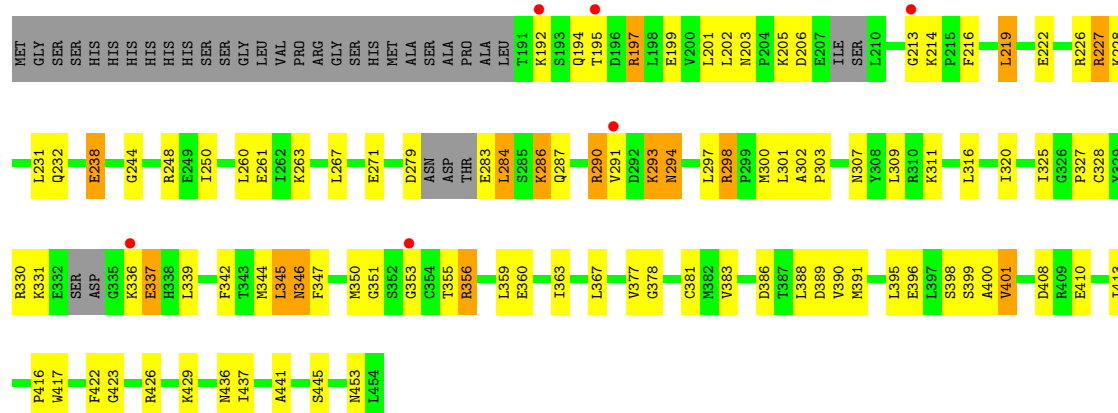


- Molecule 1: Pyrrollysine-tRNA ligase





### • Molecule 1: Pyrrolysine-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.80Å 69.42Å 83.33Å 106.92° 91.41° 113.83°	Depositor
Resolution (Å)	48.15 – 2.30 48.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.8 (48.15-2.30) 83.9 (48.15-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.270 0.210 , 0.265	Depositor DCC
$R_{free}$ test set	4573 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, PO4, BLK

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	0.40	0/2100	0.66	0/2817
1	B	0.39	0/2049	0.64	1/2749 (0.0%)
1	C	0.38	0/2106	0.62	0/2824
1	D	0.38	0/2131	0.64	0/2859
All	All	0.39	0/8386	0.64	1/11249 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	393	GLY	N-CA-C	-5.59	99.12	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2062	0	2077	103	0
1	B	2012	0	2035	77	0
1	C	2069	0	2087	109	0
1	D	2093	0	2105	99	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	C	39	0	33	12	0
4	D	39	0	33	9	0
5	A	46	0	0	3	0
5	B	49	0	0	4	0
5	C	39	0	0	1	0
5	D	30	0	0	0	0
All	All	8544	0	8394	383	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 23.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ARG:HD3	1:D:290:ARG:H	1.22	1.05
1:D:350:MET:HE1	1:D:413:ILE:HD12	1.41	1.03
1:A:350:MET:HE1	1:A:413:ILE:HD12	1.42	1.01
1:A:203:ASN:HB2	1:A:227:ARG:HH21	1.26	0.99
1:C:191:THR:HG22	1:C:193:SER:H	1.28	0.98
1:C:383:VAL:HG13	1:C:384:TYR:H	1.25	0.97
1:B:436:ASN:HD21	1:B:438:LYS:HB2	1.25	0.97
1:A:227:ARG:HH11	1:A:227:ARG:HA	1.28	0.96
1:A:214:LYS:NZ	1:A:218:GLU:HG2	1.82	0.93
1:D:356:ARG:HH21	1:D:378:GLY:HA3	1.31	0.93
1:C:399:SER:HB2	4:C:601:BLK:CB	1.99	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:LEU:HD13	1:D:350:MET:HE3	1.49	0.92
1:D:356:ARG:HE	1:D:388:LEU:HD21	1.35	0.91
1:A:309:LEU:HD13	1:A:350:MET:HE3	1.53	0.91
1:D:290:ARG:H	1:D:290:ARG:CD	1.79	0.90
1:D:286:LYS:NZ	1:D:286:LYS:HA	1.86	0.90
1:B:436:ASN:ND2	1:B:438:LYS:HB2	1.87	0.89
1:D:293:LYS:HD3	1:D:294:ASN:H	1.36	0.88
1:C:399:SER:HB2	4:C:601:BLK:H18	1.59	0.84
1:D:356:ARG:NE	1:D:388:LEU:HD21	1.92	0.84
1:A:203:ASN:HB2	1:A:227:ARG:NH2	1.90	0.84
1:C:436:ASN:HD21	1:C:438:LYS:HB2	1.41	0.84
1:A:217:ARG:HG3	5:A:613:HOH:O	1.77	0.84
1:B:351:GLY:O	1:B:416:PRO:HG2	1.78	0.83
1:A:202:LEU:HD21	1:A:208:ILE:HD12	1.60	0.83
1:C:247:GLU:HG3	1:C:325:ILE:HG21	1.61	0.82
1:C:337:GLU:OE2	1:C:429:LYS:HE3	1.82	0.80
1:A:286:LYS:NZ	1:A:287:GLN:HE21	1.78	0.80
1:A:192:LYS:HE2	1:A:192:LYS:HA	1.64	0.80
1:C:298:ARG:HD2	1:C:327:PRO:O	1.80	0.80
1:B:257:ARG:HG2	1:B:257:ARG:HH11	1.48	0.79
1:C:356:ARG:HE	1:C:388:LEU:HD11	1.45	0.79
1:C:313:ASP:HA	1:C:320:ILE:CD1	2.13	0.78
1:A:398:SER:HB2	1:A:421:GLY:O	1.83	0.78
1:B:275:ARG:HG3	1:B:410:GLU:HG3	1.64	0.78
1:D:356:ARG:O	1:D:360:GLU:HG3	1.84	0.77
1:A:409:ARG:O	1:A:409:ARG:HD3	1.82	0.77
1:C:191:THR:HB	1:C:194:GLN:HG3	1.67	0.77
1:A:227:ARG:CA	1:A:227:ARG:HH11	1.97	0.77
1:C:191:THR:HG22	1:C:193:SER:N	2.00	0.77
1:D:197:ARG:NH2	1:D:201:LEU:HD21	2.00	0.76
1:C:313:ASP:HA	1:C:320:ILE:HD11	1.67	0.76
1:D:337:GLU:OE1	1:D:429:LYS:HE3	1.85	0.76
1:C:215:PRO:HG2	1:C:218:GLU:HG2	1.68	0.76
1:A:286:LYS:HZ1	1:A:287:GLN:HE21	1.31	0.75
1:A:214:LYS:HZ1	1:A:218:GLU:HG2	1.49	0.75
1:A:214:LYS:HZ3	1:A:218:GLU:HG2	1.50	0.75
1:C:359:LEU:HD21	1:C:400:ALA:HB1	1.69	0.75
1:C:309:LEU:HD13	1:C:350:MET:HE3	1.69	0.74
1:D:283:GLU:CG	1:D:284:LEU:HD22	2.18	0.74
1:D:359:LEU:HD21	1:D:400:ALA:HB1	1.69	0.74
1:D:351:GLY:O	1:D:416:PRO:HG2	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:501:BLK:O1	4:D:501:BLK:H7	1.87	0.73
1:A:353:GLY:O	1:A:355:THR:HG23	1.88	0.72
1:D:283:GLU:HG3	1:D:284:LEU:HD22	1.70	0.72
1:A:293:LYS:HZ1	1:A:295:PHE:HE1	1.37	0.72
4:D:501:BLK:O1	4:D:501:BLK:H4	1.89	0.71
1:C:417:TRP:CH2	4:C:601:BLK:H9	2.25	0.71
1:C:278:ILE:HD13	1:C:284:LEU:HD13	1.71	0.71
1:D:286:LYS:HZ2	1:D:286:LYS:HA	1.56	0.70
1:D:353:GLY:O	1:D:355:THR:HG23	1.91	0.70
4:C:601:BLK:H7	4:C:601:BLK:O1	1.92	0.70
1:C:229:LYS:HG3	5:C:728:HOH:O	1.91	0.69
1:D:298:ARG:HD2	1:D:327:PRO:O	1.92	0.69
1:A:383:VAL:HG23	1:A:384:TYR:CD1	2.29	0.68
1:C:286:LYS:CE	1:C:286:LYS:HA	2.23	0.68
1:B:435:LYS:HB3	5:B:623:HOH:O	1.94	0.68
1:C:383:VAL:HG13	1:C:384:TYR:N	2.05	0.68
1:C:436:ASN:ND2	1:C:438:LYS:HB2	2.09	0.67
1:D:293:LYS:CD	1:D:294:ASN:H	2.07	0.67
1:B:293:LYS:NZ	1:B:293:LYS:HB3	2.11	0.66
1:C:356:ARG:NE	1:C:388:LEU:HD11	2.10	0.66
1:B:303:PRO:HG2	5:B:640:HOH:O	1.95	0.66
1:D:202:LEU:HD13	1:D:203:ASN:N	2.10	0.66
4:D:501:BLK:O1P	4:D:501:BLK:O	2.10	0.66
1:B:257:ARG:HG2	1:B:257:ARG:NH1	2.11	0.66
1:D:339:LEU:HD21	1:D:437:ILE:HG23	1.77	0.66
1:B:206:ASP:HB3	1:B:208:ILE:HG22	1.78	0.65
1:C:228:LYS:O	1:C:232:GLN:HG3	1.97	0.65
1:C:350:MET:HE1	1:C:413:ILE:HD12	1.77	0.65
1:C:301:LEU:HD13	1:C:328:CYS:SG	2.37	0.64
1:A:358:ASN:O	1:A:362:ILE:HG13	1.95	0.64
1:C:286:LYS:HE3	1:C:286:LYS:HA	1.80	0.64
1:B:353:GLY:O	1:B:355:THR:HG23	1.98	0.64
1:B:227:ARG:NH1	1:B:230:ASP:OD2	2.31	0.64
1:D:238:GLU:CD	1:D:238:GLU:H	2.00	0.64
1:D:293:LYS:H	1:D:293:LYS:HD2	1.63	0.64
1:A:293:LYS:HG3	1:A:294:ASN:H	1.63	0.63
1:A:350:MET:HE1	1:A:413:ILE:CD1	2.25	0.63
1:A:392:HIS:HB2	1:A:397:LEU:HD21	1.80	0.63
1:B:214:LYS:HB2	1:B:219:LEU:HD13	1.80	0.63
1:B:227:ARG:HH11	1:B:227:ARG:HA	1.64	0.63
1:C:453:ASN:HD21	1:D:311:LYS:NZ	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HB2	1:A:400:ALA:HB3	1.81	0.62
1:A:387:THR:CG2	1:A:388:LEU:N	2.61	0.62
1:A:197:ARG:HD2	1:A:216:PHE:HZ	1.65	0.62
1:B:238:GLU:O	1:B:239:ARG:HB2	1.98	0.62
1:B:307:ASN:O	1:B:311:LYS:HG3	2.00	0.61
1:A:202:LEU:HD11	1:A:208:ILE:HD13	1.82	0.61
1:A:359:LEU:HD21	1:A:400:ALA:HB1	1.81	0.61
1:B:245:LYS:O	1:B:249:GLU:HG3	2.01	0.61
1:C:417:TRP:CZ3	4:C:601:BLK:H9	2.35	0.61
1:A:298:ARG:HD2	1:A:327:PRO:O	2.01	0.61
1:C:381:CYS:HB3	1:C:384:TYR:O	2.01	0.61
1:C:226:ARG:HB3	1:C:227:ARG:HH12	1.65	0.60
1:D:367:LEU:HD11	1:D:390:VAL:HG11	1.83	0.60
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.67	0.60
1:B:275:ARG:HG3	1:B:410:GLU:CG	2.32	0.60
1:C:223:LEU:O	1:C:227:ARG:HG2	2.02	0.60
1:C:311:LYS:HE2	3:C:602:PO4:O2	2.00	0.60
1:B:287:GLN:HA	1:B:331:LYS:HB2	1.83	0.59
1:C:194:GLN:HB3	1:C:216:PHE:CD2	2.37	0.59
1:D:286:LYS:HZ1	1:D:290:ARG:NH2	2.00	0.59
1:A:238:GLU:O	1:A:239:ARG:HB2	2.02	0.59
1:B:332:GLU:HA	1:B:332:GLU:OE2	2.02	0.59
1:B:293:LYS:HG3	1:B:294:ASN:OD1	2.02	0.59
1:D:356:ARG:NH2	1:D:378:GLY:HA3	2.11	0.58
1:C:195:THR:O	1:C:199:GLU:HG3	2.03	0.57
1:C:383:VAL:O	1:C:386:ASP:HB2	2.04	0.57
1:B:293:LYS:HB3	1:B:293:LYS:HZ3	1.69	0.57
1:A:198:LEU:HD11	1:A:219:LEU:HD23	1.87	0.57
1:D:350:MET:HE1	1:D:413:ILE:CD1	2.24	0.57
1:C:191:THR:CG2	1:C:193:SER:H	2.10	0.57
1:D:377:VAL:HG23	1:D:377:VAL:O	2.03	0.57
1:A:435:LYS:HB2	1:A:435:LYS:NZ	2.19	0.57
1:D:307:ASN:O	1:D:311:LYS:HG3	2.04	0.57
1:C:367:LEU:HD11	1:C:390:VAL:HG11	1.86	0.56
4:C:601:BLK:H4	4:C:601:BLK:O1	2.05	0.56
1:D:426:ARG:NH1	4:D:501:BLK:H29	2.20	0.56
1:A:239:ARG:HA	1:B:260:LEU:HD12	1.86	0.56
1:C:309:LEU:HB3	1:C:350:MET:CE	2.34	0.56
1:A:192:LYS:CE	1:A:192:LYS:HA	2.35	0.56
1:C:309:LEU:HB3	1:C:350:MET:HE1	1.87	0.56
1:D:286:LYS:HZ3	1:D:286:LYS:HA	1.65	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:O	1:A:229:LYS:HG3	2.06	0.56
1:B:375:LYS:N	1:B:391:MET:O	2.39	0.56
1:A:267:LEU:HD11	1:A:291:VAL:HG11	1.88	0.56
1:C:227:ARG:HH11	1:C:227:ARG:HA	1.71	0.56
1:C:331:LYS:NZ	1:C:331:LYS:HB2	2.21	0.56
1:D:284:LEU:HB3	1:D:287:GLN:HE21	1.69	0.56
1:B:250:ILE:HG22	1:B:325:ILE:HD11	1.88	0.55
1:B:334:ASP:O	1:B:336:LYS:N	2.39	0.55
1:D:408:ASP:HB3	1:D:413:ILE:O	2.06	0.55
4:D:501:BLK:O1	4:D:501:BLK:CT3	2.51	0.55
1:A:436:ASN:HD22	1:A:438:LYS:HB2	1.69	0.55
1:D:301:LEU:HD21	1:D:344:MET:HB2	1.87	0.55
1:C:286:LYS:HZ2	1:C:286:LYS:HA	1.72	0.55
1:A:436:ASN:HD22	1:A:438:LYS:H	1.55	0.55
1:B:275:ARG:NH1	1:B:275:ARG:HG2	2.21	0.54
1:D:344:MET:SD	4:D:501:BLK:O4'	2.65	0.54
1:D:283:GLU:HG2	1:D:284:LEU:HD22	1.87	0.54
1:C:291:VAL:HG22	1:D:291:VAL:HG22	1.89	0.54
1:C:437:ILE:O	1:C:437:ILE:HG12	2.07	0.54
1:A:215:PRO:HG2	1:A:218:GLU:HB2	1.89	0.54
1:A:350:MET:CE	1:A:413:ILE:HD12	2.26	0.54
1:A:197:ARG:HD2	1:A:216:PHE:CZ	2.42	0.54
1:B:356:ARG:HE	1:B:388:LEU:HD21	1.73	0.54
1:D:287:GLN:O	1:D:330:ARG:HA	2.08	0.54
1:C:399:SER:HB2	4:C:601:BLK:H17	1.86	0.54
1:A:428:LEU:HD12	1:A:440:ALA:HB1	1.90	0.54
1:C:266:ILE:O	1:C:298:ARG:HG2	2.08	0.54
1:C:227:ARG:HH11	1:C:227:ARG:CA	2.22	0.53
1:D:346:ASN:HD22	1:D:347:PHE:N	2.06	0.53
1:B:367:LEU:HD11	1:B:390:VAL:HG11	1.90	0.53
1:C:239:ARG:HA	1:D:260:LEU:HD12	1.91	0.53
1:C:247:GLU:HG3	1:C:325:ILE:CG2	2.37	0.53
1:A:350:MET:HE2	1:A:413:ILE:HG23	1.91	0.52
1:D:194:GLN:HB3	1:D:216:PHE:CD2	2.45	0.52
1:B:195:THR:O	1:B:199:GLU:HG2	2.09	0.52
1:C:337:GLU:HG2	1:C:395:LEU:HD13	1.90	0.52
1:D:399:SER:HB3	4:D:501:BLK:H19	1.91	0.52
1:A:233:GLN:HG3	1:A:237:GLU:OE2	2.08	0.52
1:C:192:LYS:HD3	1:C:192:LYS:O	2.10	0.52
1:A:208:ILE:HG21	5:A:603:HOH:O	2.09	0.52
1:A:344:MET:HG2	5:A:636:HOH:O	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:CD1	1:B:346:ASN:HB3	2.40	0.52
1:C:350:MET:HE1	1:C:413:ILE:CD1	2.40	0.51
1:C:251:THR:HG23	1:C:323:PHE:HZ	1.76	0.51
1:C:388:LEU:HD22	1:C:388:LEU:N	2.25	0.51
1:D:279:ASP:O	1:D:283:GLU:N	2.44	0.51
1:C:251:THR:O	1:C:255:VAL:HG23	2.09	0.51
1:B:250:ILE:CG2	1:B:325:ILE:HD11	2.40	0.51
1:C:355:THR:OG1	1:C:357:GLU:HG2	2.10	0.51
1:A:350:MET:HE2	1:A:413:ILE:CG2	2.41	0.51
1:B:203:ASN:O	1:B:206:ASP:HB2	2.10	0.51
1:B:305:LEU:HD11	1:B:346:ASN:HB3	1.91	0.51
1:B:339:LEU:HD21	1:B:437:ILE:HG23	1.94	0.50
1:C:359:LEU:HD21	1:C:400:ALA:CB	2.40	0.50
1:A:373:ASP:O	1:A:392:HIS:HD2	1.93	0.50
1:D:222:GLU:O	1:D:226:ARG:HG3	2.11	0.50
1:A:275:ARG:HG3	1:A:410:GLU:CG	2.41	0.50
1:C:311:LYS:NZ	1:D:453:ASN:HD21	2.10	0.50
1:B:342:PHE:CD1	1:B:342:PHE:N	2.79	0.50
1:B:436:ASN:HD21	1:B:438:LYS:CB	2.11	0.50
1:A:267:LEU:CD1	1:A:291:VAL:HG11	2.41	0.50
1:C:278:ILE:CD1	1:C:284:LEU:HD13	2.40	0.50
1:D:302:ALA:N	1:D:303:PRO:HD2	2.27	0.50
1:C:227:ARG:N	1:C:227:ARG:HH11	2.09	0.50
1:B:207:GLU:HG3	1:B:226:ARG:HH12	1.77	0.49
4:C:601:BLK:CT3	4:C:601:BLK:O1	2.56	0.49
1:A:191:THR:HG22	1:A:194:GLN:CG	2.42	0.49
1:A:227:ARG:HD3	1:A:450:ILE:HG23	1.95	0.49
1:C:286:LYS:CA	1:C:286:LYS:HE3	2.41	0.49
1:C:234:ILE:HG23	1:C:238:GLU:HB2	1.94	0.49
1:C:306:TYR:CE1	4:C:601:BLK:H2	2.46	0.49
1:D:214:LYS:HD3	1:D:219:LEU:CD1	2.42	0.49
1:A:387:THR:HG22	1:A:388:LEU:N	2.28	0.49
1:B:345:LEU:O	1:B:421:GLY:HA2	2.13	0.49
1:B:273:ILE:HG23	1:B:278:ILE:HD12	1.95	0.49
1:C:306:TYR:CE1	4:C:601:BLK:CT1	2.96	0.49
1:A:191:THR:CG2	1:A:194:GLN:HG3	2.43	0.49
1:B:291:VAL:HG21	1:B:297:LEU:CD1	2.43	0.49
1:A:339:LEU:HD21	1:A:437:ILE:HG23	1.95	0.48
1:D:195:THR:O	1:D:199:GLU:HG2	2.13	0.48
1:A:325:ILE:HA	1:A:344:MET:O	2.12	0.48
1:C:214:LYS:HB3	1:C:215:PRO:HD2	1.93	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:HG2	1:B:294:ASN:H	1.79	0.48
1:D:228:LYS:O	1:D:232:GLN:HG3	2.13	0.48
1:D:316:LEU:HB2	1:D:320:ILE:HD12	1.94	0.48
1:A:275:ARG:HG3	1:A:410:GLU:HG3	1.96	0.48
1:B:339:LEU:HD13	1:B:441:ALA:HB2	1.95	0.48
1:A:316:LEU:HB2	1:A:320:ILE:CD1	2.44	0.48
1:A:377:VAL:HG23	1:A:389:ASP:HB2	1.96	0.48
1:B:377:VAL:HG23	1:B:377:VAL:O	2.14	0.48
1:C:377:VAL:O	1:C:377:VAL:HG23	2.14	0.48
1:A:387:THR:HG23	1:A:388:LEU:H	1.79	0.48
1:C:286:LYS:NZ	1:C:286:LYS:HA	2.29	0.48
1:C:230:ASP:HB3	1:C:450:ILE:HD13	1.94	0.48
1:D:290:ARG:N	1:D:290:ARG:CD	2.60	0.48
1:D:286:LYS:HE2	1:D:290:ARG:NH1	2.28	0.48
1:D:359:LEU:O	1:D:363:ILE:HG13	2.13	0.48
1:B:298:ARG:HD2	1:B:327:PRO:O	2.14	0.47
1:C:453:ASN:HD21	1:D:311:LYS:HZ1	1.61	0.47
1:D:301:LEU:HD22	1:D:328:CYS:SG	2.54	0.47
1:B:346:ASN:HD22	1:B:346:ASN:HA	1.50	0.47
1:C:213:GLY:O	1:C:214:LYS:HD2	2.13	0.47
1:D:377:VAL:CG2	1:D:377:VAL:O	2.62	0.47
1:A:355:THR:OG1	1:A:357:GLU:HB3	2.14	0.47
1:A:301:LEU:HD13	1:A:328:CYS:SG	2.54	0.47
1:C:325:ILE:HA	1:C:344:MET:O	2.15	0.47
1:B:264:SER:O	1:B:298:ARG:NH2	2.48	0.46
1:C:191:THR:HB	1:C:194:GLN:CG	2.42	0.46
1:C:279:ASP:O	1:C:280:ASN:C	2.53	0.46
1:B:335:GLY:C	1:B:336:LYS:HG3	2.35	0.46
1:A:245:LYS:HE2	1:A:249:GLU:OE1	2.16	0.46
1:B:301:LEU:HD23	1:B:346:ASN:HB2	1.98	0.46
1:A:241:ASN:ND2	1:B:263:LYS:HB2	2.31	0.46
1:A:286:LYS:NZ	1:A:287:GLN:NE2	2.55	0.46
1:B:398:SER:HB2	1:B:422:PHE:CD2	2.51	0.46
1:D:293:LYS:HD2	1:D:293:LYS:N	2.31	0.46
1:D:325:ILE:HA	1:D:344:MET:O	2.15	0.46
1:B:230:ASP:HB3	1:B:450:ILE:HD13	1.98	0.46
1:D:197:ARG:HH22	1:D:201:LEU:HD21	1.79	0.46
1:D:284:LEU:HG	1:D:287:GLN:HE21	1.81	0.46
1:B:356:ARG:NE	1:B:388:LEU:HD21	2.30	0.46
1:D:331:LYS:HB2	1:D:331:LYS:HE3	1.73	0.46
1:B:227:ARG:HD3	1:B:227:ARG:HA	1.78	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HG23	1:A:194:GLN:H	1.80	0.45
1:C:215:PRO:HG2	1:C:218:GLU:CG	2.43	0.45
1:C:302:ALA:HA	4:C:601:BLK:H5	1.98	0.45
1:B:298:ARG:HG3	1:B:298:ARG:O	2.16	0.45
1:C:222:GLU:O	1:C:226:ARG:HG3	2.16	0.45
1:C:347:PHE:CE1	1:C:420:ALA:HB3	2.51	0.45
1:D:213:GLY:O	1:D:214:LYS:HB2	2.17	0.45
1:A:414:ASP:OD2	1:A:414:ASP:N	2.49	0.45
1:B:264:SER:HB2	1:B:265:PRO:CD	2.47	0.45
1:C:230:ASP:HB3	1:C:450:ILE:CD1	2.45	0.45
1:C:347:PHE:CZ	1:C:420:ALA:HB3	2.52	0.45
1:C:197:ARG:NH1	1:C:220:GLU:OE2	2.50	0.45
1:D:346:ASN:HD22	1:D:346:ASN:C	2.20	0.45
1:D:401:VAL:HG22	1:D:417:TRP:CH2	2.52	0.45
1:A:323:PHE:HA	1:A:346:ASN:O	2.17	0.45
1:A:436:ASN:ND2	1:A:438:LYS:HB2	2.31	0.45
1:B:207:GLU:O	1:B:208:ILE:C	2.55	0.45
1:D:316:LEU:HB2	1:D:320:ILE:CD1	2.47	0.45
1:A:197:ARG:HB2	1:A:197:ARG:NH2	2.31	0.45
1:A:329:TYR:CD1	1:A:329:TYR:N	2.85	0.45
1:D:284:LEU:HG	1:D:287:GLN:NE2	2.32	0.45
1:C:272:TYR:O	1:C:276:MET:HG2	2.17	0.45
1:A:396:GLU:HG2	2:A:501:AMP:O3'	2.17	0.44
1:C:235:TYR:CG	1:D:316:LEU:HD13	2.53	0.44
1:C:239:ARG:HA	1:D:260:LEU:CD1	2.46	0.44
1:D:417:TRP:CH2	4:D:501:BLK:H1	2.53	0.44
1:C:357:GLU:H	1:C:357:GLU:CD	2.18	0.44
1:D:214:LYS:HD3	1:D:219:LEU:HD11	1.99	0.44
1:A:339:LEU:HD13	1:A:441:ALA:HB2	1.99	0.44
1:B:347:PHE:CZ	1:B:420:ALA:HB3	2.52	0.44
1:C:453:ASN:HD21	1:D:311:LYS:HZ3	1.66	0.44
1:D:339:LEU:HD13	1:D:441:ALA:HB2	2.00	0.44
1:A:245:LYS:O	1:A:249:GLU:HG3	2.17	0.44
1:A:286:LYS:HZ1	1:A:287:GLN:NE2	2.08	0.44
1:B:234:ILE:HD12	1:B:450:ILE:HD12	1.98	0.44
1:B:293:LYS:CB	1:B:293:LYS:NZ	2.78	0.44
1:B:275:ARG:CG	1:B:410:GLU:HG3	2.43	0.44
1:C:213:GLY:C	1:C:214:LYS:HD2	2.38	0.44
1:C:398:SER:OG	1:C:399:SER:N	2.51	0.44
1:D:206:ASP:OD2	1:D:227:ARG:NH2	2.50	0.44
1:A:191:THR:HG22	1:A:194:GLN:HG3	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:O	1:A:421:GLY:HA2	2.18	0.43
1:A:398:SER:HB3	1:A:422:PHE:CD2	2.53	0.43
1:B:253:PHE:O	1:B:257:ARG:HG3	2.18	0.43
1:C:331:LYS:NZ	1:C:331:LYS:CB	2.80	0.43
1:C:241:ASN:N	1:D:261:GLU:OE1	2.41	0.43
1:A:197:ARG:HB2	1:A:197:ARG:HH21	1.83	0.43
1:C:330:ARG:O	1:C:340:GLU:HA	2.19	0.43
1:D:250:ILE:HG21	1:D:345:LEU:HD22	2.00	0.43
1:A:291:VAL:HG22	1:A:291:VAL:O	2.17	0.43
1:D:291:VAL:HG21	1:D:297:LEU:HD13	2.01	0.43
1:D:286:LYS:HE2	1:D:290:ARG:HH12	1.83	0.43
1:D:423:GLY:HA3	4:D:501:BLK:H31	1.99	0.43
1:A:401:VAL:HG13	1:A:417:TRP:CZ3	2.54	0.43
1:A:359:LEU:HD23	1:A:388:LEU:HD12	2.01	0.43
1:B:348:CYS:HA	1:B:418:ILE:O	2.18	0.43
1:A:330:ARG:O	1:A:340:GLU:HA	2.19	0.43
1:A:379:ASP:O	1:A:387:THR:N	2.50	0.43
1:A:447:TYR:CZ	1:B:260:LEU:HD11	2.54	0.43
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.91	0.42
1:A:253:PHE:CE1	1:A:257:ARG:NH1	2.88	0.42
1:A:356:ARG:HE	1:A:388:LEU:HD21	1.84	0.42
1:C:238:GLU:O	1:C:239:ARG:HB2	2.20	0.42
1:D:377:VAL:HG22	1:D:389:ASP:HB2	2.01	0.42
1:B:319:PRO:HD2	5:B:617:HOH:O	2.18	0.42
1:C:206:ASP:OD2	1:C:227:ARG:NH2	2.52	0.42
1:D:391:MET:SD	1:D:396:GLU:HA	2.58	0.42
1:C:358:ASN:HD22	1:C:358:ASN:HA	1.63	0.42
1:D:309:LEU:HD13	1:D:350:MET:CE	2.36	0.42
1:B:425:GLU:HB2	5:B:637:HOH:O	2.19	0.42
1:C:323:PHE:HA	1:C:346:ASN:O	2.20	0.42
1:D:205:LYS:HA	1:D:205:LYS:HD3	1.93	0.42
1:A:202:LEU:HD11	1:A:208:ILE:CD1	2.50	0.42
1:A:270:LEU:HD11	1:A:290:ARG:HD2	2.02	0.42
1:A:301:LEU:HD22	1:A:344:MET:HB3	2.02	0.42
1:A:320:ILE:O	1:A:349:GLN:HA	2.20	0.42
1:B:392:HIS:HB2	1:B:397:LEU:HD22	2.02	0.42
1:C:302:ALA:N	1:C:303:PRO:HD2	2.34	0.42
1:A:409:ARG:C	1:A:409:ARG:HD3	2.39	0.42
1:B:292:ASP:HB3	1:B:293:LYS:H	1.45	0.41
1:D:356:ARG:NH1	1:D:386:ASP:OD1	2.53	0.41
1:A:259:PHE:CZ	1:A:349:GLN:NE2	2.87	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LYS:HA	1:D:263:LYS:HD3	1.92	0.41
1:A:214:LYS:HB3	1:A:219:LEU:HD13	2.02	0.41
1:C:291:VAL:HG21	1:C:297:LEU:CD1	2.49	0.41
1:C:298:ARG:HG3	1:C:298:ARG:O	2.20	0.41
1:C:350:MET:CE	1:C:413:ILE:HD12	2.49	0.41
1:D:286:LYS:CE	1:D:286:LYS:HA	2.50	0.41
1:A:375:LYS:N	1:A:391:MET:O	2.47	0.41
1:A:436:ASN:ND2	1:A:438:LYS:H	2.18	0.41
1:B:245:LYS:HE2	1:B:249:GLU:OE1	2.20	0.41
1:B:261:GLU:HA	1:B:323:PHE:CE1	2.55	0.41
1:D:244:GLY:O	1:D:248:ARG:HG3	2.21	0.41
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.94	0.41
1:C:192:LYS:HD3	1:C:192:LYS:C	2.40	0.41
1:B:223:LEU:HA	1:B:223:LEU:HD23	1.84	0.41
1:B:354:CYS:HB3	1:B:418:ILE:HG23	2.03	0.41
1:C:331:LYS:HZ1	1:C:331:LYS:HB2	1.85	0.41
1:C:354:CYS:SG	1:C:417:TRP:HA	2.60	0.41
1:C:373:ASP:O	1:C:392:HIS:HD2	2.03	0.41
1:D:388:LEU:HB2	1:D:400:ALA:HB3	2.02	0.41
1:A:198:LEU:CD1	1:A:219:LEU:HD23	2.50	0.41
1:B:295:PHE:N	1:B:295:PHE:CD1	2.88	0.41
1:A:359:LEU:HD13	1:A:418:ILE:HB	2.03	0.41
1:C:246:LEU:O	1:C:250:ILE:HG13	2.20	0.41
1:C:388:LEU:CD2	1:C:388:LEU:N	2.84	0.41
1:D:337:GLU:HG3	1:D:395:LEU:HD11	2.03	0.41
1:D:398:SER:HB2	1:D:422:PHE:CD2	2.55	0.41
1:A:301:LEU:HD23	1:A:346:ASN:HB2	2.03	0.41
1:B:359:LEU:HD21	1:B:400:ALA:HB1	2.02	0.41
1:D:342:PHE:CE2	1:D:344:MET:HG2	2.56	0.41
1:D:401:VAL:CG2	1:D:417:TRP:CH2	3.04	0.41
1:A:342:PHE:N	1:A:342:PHE:CD1	2.89	0.40
1:B:304:ASN:HD22	1:B:304:ASN:HA	1.68	0.40
1:C:395:LEU:HD12	1:C:396:GLU:N	2.36	0.40
1:D:336:LYS:HE2	1:D:336:LYS:HB2	1.88	0.40
1:C:399:SER:HB2	4:C:601:BLK:CA	2.51	0.40
1:A:206:ASP:OD2	1:A:227:ARG:NH2	2.55	0.40
1:C:286:LYS:CA	1:C:286:LYS:CE	2.96	0.40
1:D:311:LYS:HE2	3:D:502:PO4:O3	2.21	0.40
1:B:330:ARG:O	1:B:340:GLU:HA	2.21	0.40
1:C:354:CYS:HB3	1:C:418:ILE:HG23	2.03	0.40
1:D:377:VAL:CG2	1:D:389:ASP:HB2	2.51	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:CD1	1:D:297:LEU:HD12	2.52	0.40
1:D:271:GLU:CD	1:D:271:GLU:H	2.24	0.40
1:D:290:ARG:HD3	1:D:290:ARG:N	2.07	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/291 (84%)	235 (96%)	8 (3%)	2 (1%)	21	25
1	B	236/291 (81%)	221 (94%)	12 (5%)	3 (1%)	13	13
1	C	244/291 (84%)	233 (96%)	8 (3%)	3 (1%)	14	15
1	D	249/291 (86%)	233 (94%)	16 (6%)	0	100	100
All	All	974/1164 (84%)	922 (95%)	44 (4%)	8 (1%)	21	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	335	GLY
1	C	383	VAL
1	A	354	CYS
1	B	238	GLU
1	C	280	ASN
1	B	189	ALA
1	A	293	LYS
1	C	382	MET

### 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	227/259 (88%)	209 (92%)	18 (8%)	13	17
1	B	221/259 (85%)	206 (93%)	15 (7%)	17	22
1	C	228/259 (88%)	210 (92%)	18 (8%)	13	17
1	D	231/259 (89%)	208 (90%)	23 (10%)	8	10
All	All	907/1036 (88%)	833 (92%)	74 (8%)	12	15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	227	ARG
1	A	257	ARG
1	A	270	LEU
1	A	275	ARG
1	A	291	VAL
1	A	294	ASN
1	A	297	LEU
1	A	298	ARG
1	A	300	MET
1	A	301	LEU
1	A	306	TYR
1	A	397	LEU
1	A	398	SER
1	A	406	PRO
1	A	409	ARG
1	A	414	ASP
1	A	435	LYS
1	B	207	GLU
1	B	219	LEU
1	B	227	ARG
1	B	231	LEU
1	B	238	GLU
1	B	257	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	275	ARG
1	B	279	ASP
1	B	293	LYS
1	B	294	ASN
1	B	298	ARG
1	B	300	MET
1	B	301	LEU
1	B	342	PHE
1	B	346	ASN
1	C	192	LYS
1	C	257	ARG
1	C	279	ASP
1	C	280	ASN
1	C	284	LEU
1	C	286	LYS
1	C	298	ARG
1	C	300	MET
1	C	301	LEU
1	C	306	TYR
1	C	308	TYR
1	C	345	LEU
1	C	346	ASN
1	C	386	ASP
1	C	389	ASP
1	C	397	LEU
1	C	399	SER
1	C	401	VAL
1	D	192	LYS
1	D	197	ARG
1	D	219	LEU
1	D	227	ARG
1	D	231	LEU
1	D	238	GLU
1	D	284	LEU
1	D	286	LYS
1	D	290	ARG
1	D	293	LYS
1	D	294	ASN
1	D	298	ARG
1	D	300	MET
1	D	337	GLU
1	D	345	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	346	ASN
1	D	356	ARG
1	D	381	CYS
1	D	383	VAL
1	D	401	VAL
1	D	410	GLU
1	D	436	ASN
1	D	445	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	304	ASN
1	A	358	ASN
1	A	368	ASN
1	A	392	HIS
1	A	436	ASN
1	A	453	ASN
1	B	304	ASN
1	B	346	ASN
1	B	349	GLN
1	B	368	ASN
1	C	304	ASN
1	C	346	ASN
1	C	349	GLN
1	C	358	ASN
1	C	368	ASN
1	C	436	ASN
1	C	453	ASN
1	D	287	GLN
1	D	304	ASN
1	D	349	GLN
1	D	368	ASN
1	D	392	HIS
1	D	436	ASN
1	D	453	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	AMP	A	501	-	22,25,25	1.27	3 (13%)	23,38,38	2.12	5 (21%)
3	PO4	A	502	-	4,4,4	1.44	0	6,6,6	0.37	0
2	AMP	B	501	-	22,25,25	1.26	3 (13%)	23,38,38	2.12	4 (17%)
3	PO4	B	502	-	4,4,4	1.41	0	6,6,6	0.39	0
4	BLK	C	601	-	37,41,41	1.06	4 (10%)	40,60,60	2.09	8 (20%)
3	PO4	C	602	-	4,4,4	1.53	0	6,6,6	0.38	0
4	BLK	D	501	-	37,41,41	1.06	4 (10%)	40,60,60	2.19	9 (22%)
3	PO4	D	502	-	4,4,4	1.47	0	6,6,6	0.38	0

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	AMP	A	501	-	-	0/6/26/26	0/3/3/3
3	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	AMP	B	501	-	-	0/6/26/26	0/3/3/3
3	PO4	B	502	-	-	0/0/0/0	0/0/0/0
4	BLK	C	601	-	-	0/26/48/48	0/3/3/3
3	PO4	C	602	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BLK	D	501	-	-	0/26/48/48	0/3/3/3
3	PO4	D	502	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AMP	C8-N9	-2.82	1.33	1.36
2	B	501	AMP	C8-N9	-2.76	1.33	1.36
4	D	501	BLK	C8-N9	-2.67	1.33	1.36
4	D	501	BLK	O2-CT	-2.66	1.43	1.48
4	C	601	BLK	C8-N9	-2.64	1.33	1.36
4	C	601	BLK	O2-CT	-2.60	1.43	1.48
4	C	601	BLK	O4'-C1'	2.19	1.44	1.41
2	B	501	AMP	O4'-C1'	2.29	1.44	1.41
2	A	501	AMP	O4'-C1'	2.31	1.44	1.41
4	D	501	BLK	O4'-C1'	2.35	1.44	1.41
4	D	501	BLK	P-O1P	2.97	1.61	1.50
4	C	601	BLK	P-O1P	3.01	1.61	1.50
2	B	501	AMP	P-O1P	3.21	1.61	1.50
2	A	501	AMP	P-O1P	3.21	1.61	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	N3-C2-N1	-8.43	121.64	128.86
4	C	601	BLK	N3-C2-N1	-8.43	121.65	128.86
2	A	501	AMP	N3-C2-N1	-8.38	121.69	128.86
4	D	501	BLK	N3-C2-N1	-8.27	121.79	128.86
4	D	501	BLK	CT-O2-CZ	-6.50	110.61	121.01
4	C	601	BLK	CT-O2-CZ	-5.12	112.81	121.01
4	D	501	BLK	O2-CZ-O1	-3.45	119.05	125.58
4	C	601	BLK	O2-CZ-O1	-3.35	119.23	125.58
2	A	501	AMP	C2'-C3'-C4'	-2.93	96.99	102.62
4	C	601	BLK	C2'-C3'-C4'	-2.85	97.16	102.62
2	B	501	AMP	C2'-C3'-C4'	-2.80	97.25	102.62
4	C	601	BLK	C4'-O4'-C1'	-2.48	107.24	109.83
4	D	501	BLK	C2'-C3'-C4'	-2.31	98.18	102.62
4	C	601	BLK	C4-C5-N7	-2.29	107.20	109.41
4	D	501	BLK	C4-C5-N7	-2.28	107.20	109.41
4	D	501	BLK	CD-CG-CB	-2.22	105.82	113.59
4	D	501	BLK	CD-CE-NZ	-2.12	106.01	112.19
2	A	501	AMP	C4-C5-N7	-2.08	107.40	109.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AMP	C4'-O4'-C1'	-2.05	107.69	109.83
2	B	501	AMP	C4-C5-N7	-2.03	107.45	109.41
4	D	501	BLK	O3P-P-O5'	2.13	109.13	103.08
2	A	501	AMP	O2P-P-O5'	2.15	112.45	106.73
2	B	501	AMP	O2P-P-O5'	2.25	112.73	106.73
4	C	601	BLK	O2P-P-O3P	2.30	111.43	103.72
4	C	601	BLK	O2-CZ-NZ	4.78	117.46	109.98
4	D	501	BLK	O2-CZ-NZ	5.23	118.15	109.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	1	0
4	C	601	BLK	12	0
3	C	602	PO4	1	0
4	D	501	BLK	9	0
3	D	502	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	253/291 (86%)	0.20	12 (4%) 31 39	20, 42, 69, 86	0
1	B	246/291 (84%)	0.23	10 (4%) 37 44	26, 43, 69, 88	0
1	C	254/291 (87%)	0.50	21 (8%) 11 15	24, 47, 76, 99	0
1	D	257/291 (88%)	0.22	6 (2%) 60 67	23, 45, 73, 83	0
All	All	1010/1164 (86%)	0.29	49 (4%) 29 37	20, 44, 72, 99	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	281	ASP	6.0
1	A	208	ILE	5.4
1	C	214	LYS	5.3
1	B	208	ILE	5.2
1	C	382	MET	5.2
1	C	207	GLU	4.2
1	A	205	LYS	4.1
1	C	212	SER	4.0
1	C	381	CYS	4.0
1	C	278	ILE	4.0
1	A	197	ARG	3.9
1	B	376	ILE	3.7
1	D	353	GLY	3.7
1	C	219	LEU	3.6
1	B	336	LYS	3.6
1	B	278	ILE	3.6
1	D	213	GLY	3.5
1	A	192	LYS	3.5
1	C	409	ARG	3.4
1	C	216	PHE	3.4
1	C	280	ASN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	336	LYS	3.1
1	D	195	THR	2.9
1	C	205	LYS	2.9
1	A	198	LEU	2.9
1	C	384	TYR	2.7
1	A	193	SER	2.7
1	C	279	ASP	2.7
1	A	191	THR	2.7
1	D	291	VAL	2.6
1	B	377	VAL	2.5
1	B	375	LYS	2.5
1	C	454	LEU	2.4
1	C	293	LYS	2.4
1	A	195	THR	2.4
1	C	204	PRO	2.4
1	C	356	ARG	2.4
1	A	203	ASN	2.3
1	A	200	VAL	2.3
1	C	202	LEU	2.3
1	B	388	LEU	2.2
1	B	337	GLU	2.2
1	A	194	GLN	2.2
1	C	206	ASP	2.1
1	B	334	ASP	2.1
1	B	434	PHE	2.1
1	A	279	ASP	2.1
1	C	284	LEU	2.1
1	D	192	LYS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AMP	B	501	23/23	0.88	0.13	60,69,81,82	0
4	BLK	C	601	39/39	0.88	0.15	61,66,76,76	0
4	BLK	D	501	39/39	0.90	0.15	52,58,68,68	0
2	AMP	A	501	23/23	0.93	0.11	64,67,75,75	0
3	PO4	B	502	5/5	0.97	0.11	53,55,57,58	0
3	PO4	C	602	5/5	0.98	0.11	58,59,59,62	0
3	PO4	D	502	5/5	0.99	0.14	46,46,47,48	0
3	PO4	A	502	5/5	0.99	0.12	47,49,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.