



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:08 pm BST

PDB ID : 1D6Y  
Title : CRYSTAL STRUCTURE OF E. COLI COPPER-CONTAINING AMINE  
OXIDASE ANAEROBICALLY REDUCED WITH BETA-PHENYLETH  
YLAMINE AND COMPLEXED WITH NITRIC OXIDE.  
Authors : Wilmot, C.M.; Hajdu, J.; McPherson, M.J.; Knowles, P.F.; Phillips, S.E.V.  
Deposited on : 1999-10-16  
Resolution : 2.40 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

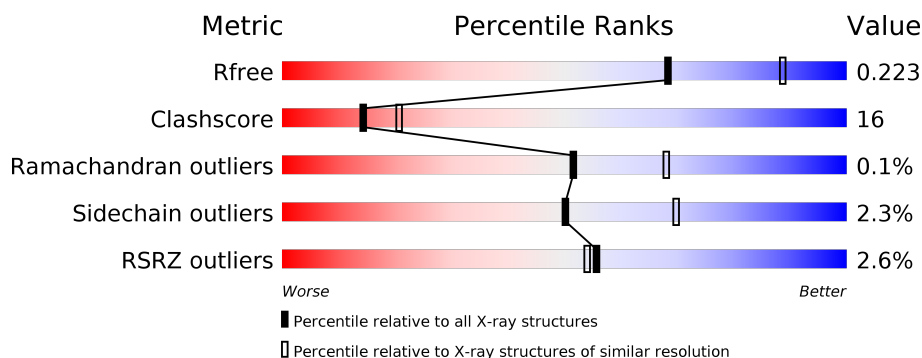
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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  $\leq 5\%$ . 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	727	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	727	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HY1	A	2001	-	-	X	-
4	HY1	B	3001	-	-	X	-
7	GOL	B	2004	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12823 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5664	3602	965	1075	22			
1	B	720	Total	C	N	O	S	0	0	0
			5683	3614	970	1077	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	TYQ	TYR	MODIFIED RESIDUE	UNP P46883
B	466	TYQ	TYR	MODIFIED RESIDUE	UNP P46883

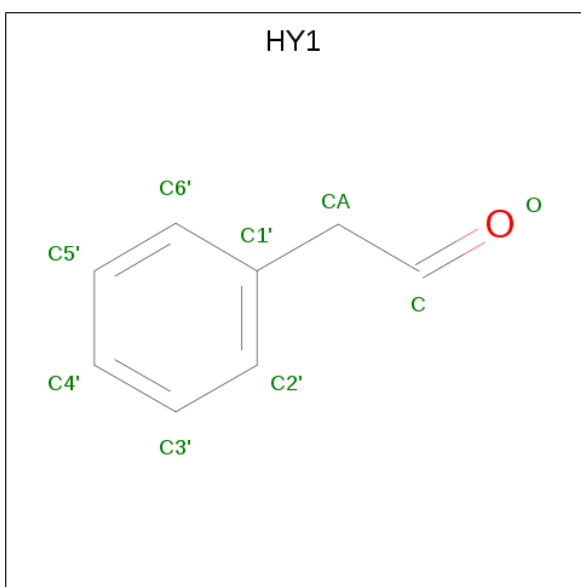
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

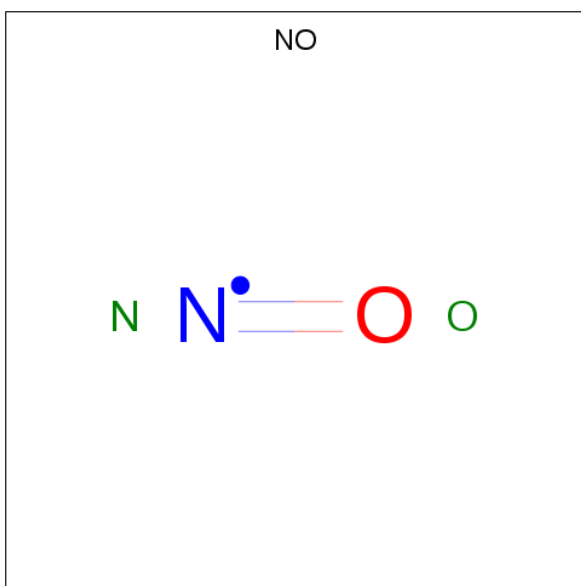
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PHENYLACETALDEHYDE (three-letter code: HY1) (formula: C<sub>8</sub>H<sub>8</sub>O).



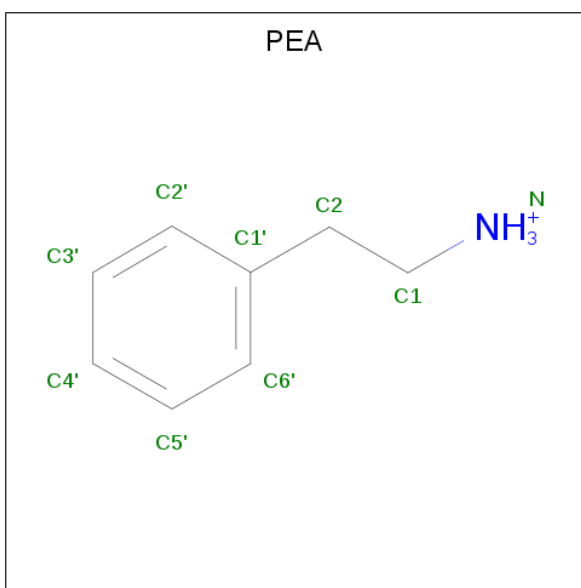
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	8	1		
4	B	1	Total	C	O	0	0
			9	8	1		

- Molecule 5 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



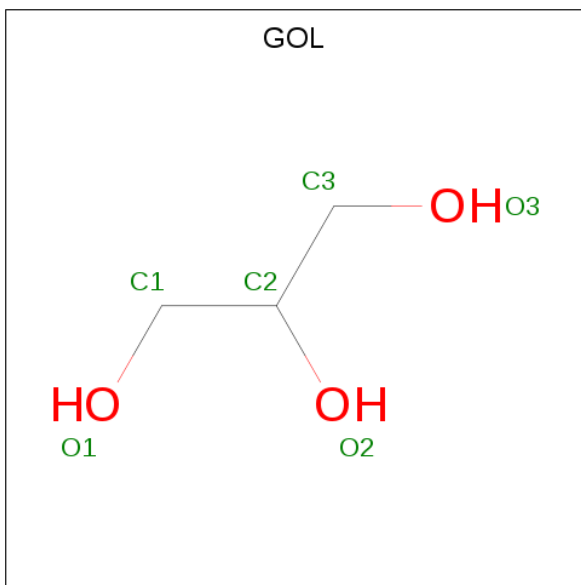
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			2	1	1		
5	B	1	Total	N	O	0	0
			2	1	1		

- Molecule 6 is 2-PHENYLETHYLAMINE (three-letter code: PEA) (formula:  $C_8H_{12}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			9	8	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

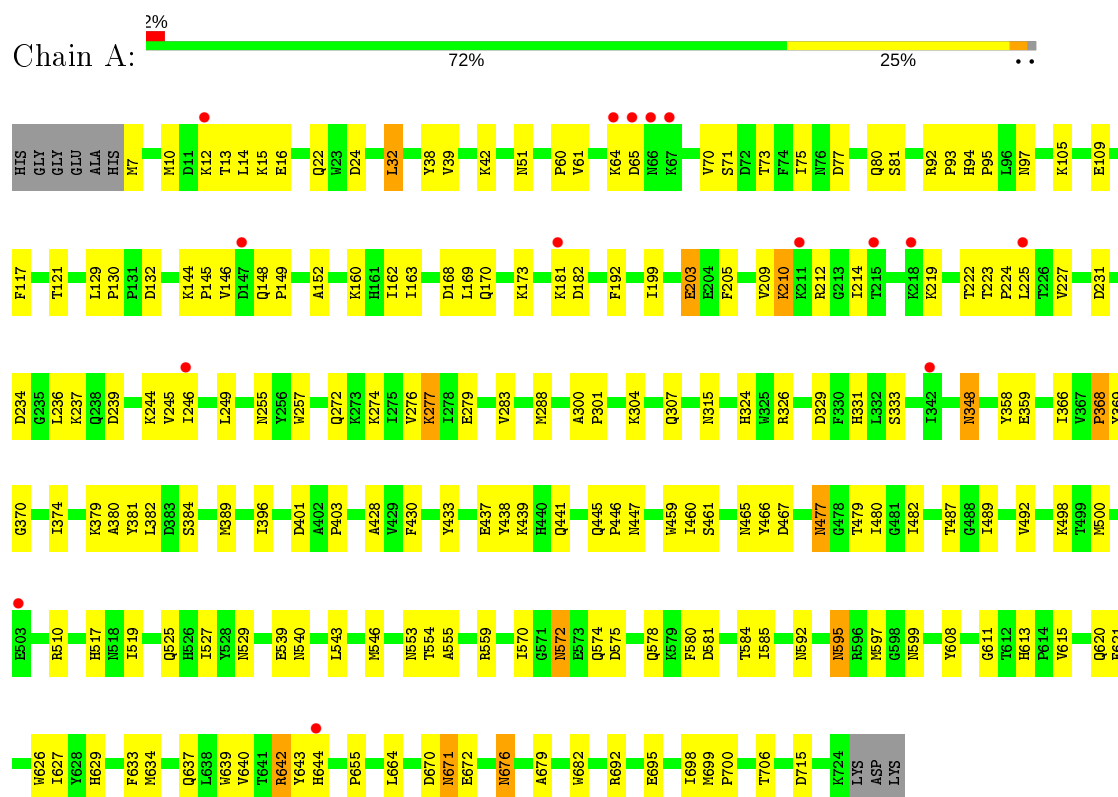
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	746	Total 746	O 746	0	0
8	B	681	Total 681	O 681	0	0

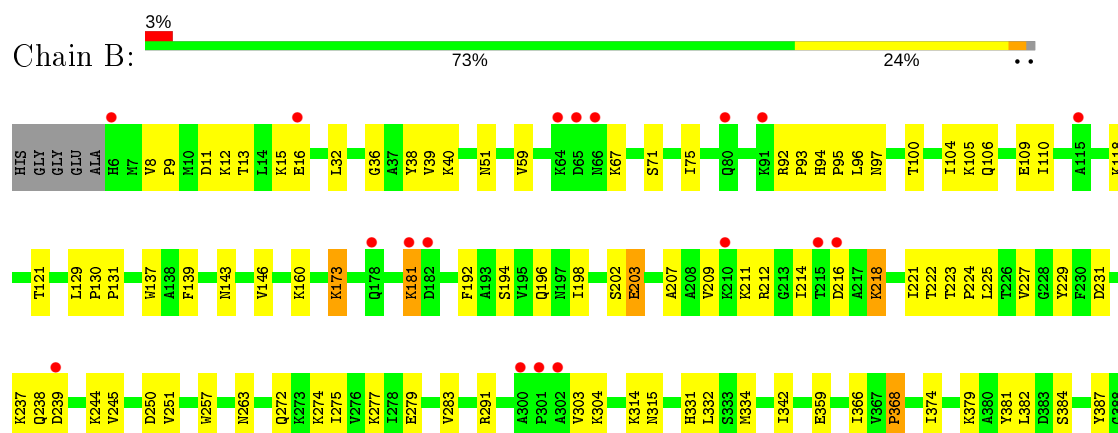
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

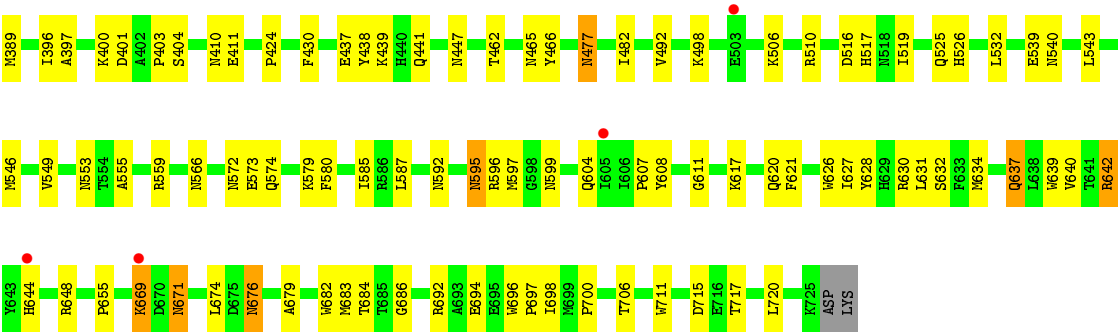
#### • Molecule 1: COPPER AMINE OXIDASE



#### • Molecule 1: COPPER AMINE OXIDASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.24Å 166.48Å 79.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 92.6 (29.37-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.181 , 0.231 0.178 , 0.223	Depositor DCC
$R_{free}$ test set	2274 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NO, CA, TYQ, HY1, PEA, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/5793	0.68	0/7886
1	B	0.33	0/5813	0.67	0/7912
All	All	0.33	0/11606	0.67	0/15798

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5664	0	5542	192	0
1	B	5683	0	5562	179	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	8	6	0
4	B	9	0	8	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	9	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	12	0	16	1	0
8	A	746	0	0	14	0
8	B	681	0	0	8	0
All	All	12823	0	11148	350	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 16.

All (350) 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:B:181:LYS:HE2	1:B:181:LYS:H	0.99	1.11
1:A:304:LYS:H	1:B:315:ASN:HD21	0.97	0.97
1:A:642:ARG:HH11	1:A:642:ARG:HB2	1.28	0.96
1:B:181:LYS:CE	1:B:181:LYS:H	1.81	0.91
1:B:181:LYS:HE2	1:B:181:LYS:N	1.84	0.91
1:B:572:ASN:HB2	1:B:671:ASN:HD21	1.38	0.87
1:B:642:ARG:HH11	1:B:642:ARG:HB2	1.41	0.86
1:B:572:ASN:HB2	1:B:671:ASN:ND2	1.92	0.82
1:B:669:LYS:NZ	1:B:669:LYS:HA	1.96	0.81
1:A:38:TYR:H	1:A:51:ASN:HD21	1.29	0.80
1:A:580:PHE:H	1:A:637:GLN:HE21	1.29	0.79
1:B:525:GLN:HE22	1:B:620:GLN:H	1.30	0.79
1:A:304:LYS:H	1:B:315:ASN:ND2	1.79	0.79
1:A:553:ASN:ND2	1:A:555:ALA:H	1.81	0.78
1:A:227:VAL:HG12	1:A:244:LYS:HG3	1.63	0.78
1:A:210:LYS:HA	1:A:210:LYS:HE2	1.66	0.77
1:A:642:ARG:HH11	1:A:642:ARG:CB	1.98	0.77
1:B:221:ILE:HD11	1:B:250:ASP:HB2	1.66	0.77
1:A:71:SER:OG	1:A:73:THR:HG22	1.86	0.76
8:A:2268:HOH:O	1:B:400:LYS:HD2	1.83	0.76
1:B:525:GLN:NE2	1:B:620:GLN:H	1.84	0.76
1:A:38:TYR:H	1:A:51:ASN:ND2	1.84	0.76
1:B:227:VAL:HG12	1:B:244:LYS:HG3	1.68	0.75
1:A:249:LEU:HD23	1:A:288:MET:HE1	1.67	0.75
1:A:22:GLN:NE2	1:A:307:GLN:HE22	1.86	0.73
1:B:237:LYS:HE2	1:B:239:ASP:HB3	1.70	0.73
1:B:644:HIS:HB3	8:B:3315:HOH:O	1.87	0.73
1:A:358:TYR:CD2	1:A:359:GLU:HG3	2.24	0.72
1:A:279:GLU:OE1	1:A:374:ILE:HD11	1.89	0.72
1:A:379:LYS:HG3	1:A:381:TYR:CZ	2.25	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:O	1:B:16:GLU:HG2	1.90	0.72
1:A:315:ASN:HD21	1:B:304:LYS:H	1.36	0.71
1:A:7:MET:HE2	1:A:7:MET:HA	1.72	0.71
1:B:221:ILE:CD1	1:B:250:ASP:HB2	2.21	0.70
1:B:580:PHE:H	1:B:637:GLN:NE2	1.89	0.69
1:B:8:VAL:HG23	1:B:9:PRO:HD2	1.73	0.69
1:B:94:HIS:HD2	1:B:96:LEU:H	1.39	0.69
1:A:203:GLU:CD	1:A:203:GLU:H	1.96	0.69
1:A:525:GLN:NE2	1:A:620:GLN:H	1.90	0.69
1:A:304:LYS:N	1:B:315:ASN:HD21	1.81	0.69
1:B:540:ASN:HB3	1:B:676:ASN:ND2	2.08	0.68
1:A:525:GLN:HE22	1:A:620:GLN:H	1.42	0.68
1:B:94:HIS:CD2	1:B:96:LEU:H	2.12	0.68
1:A:225:LEU:HD22	1:A:381:TYR:CE1	2.29	0.67
1:A:540:ASN:HB3	1:A:676:ASN:ND2	2.10	0.67
1:A:209:VAL:HG12	1:A:214:ILE:HB	1.77	0.67
1:A:272:GLN:HE21	1:A:274:LYS:HZ3	1.44	0.66
1:B:366:ILE:HD11	1:B:627:ILE:HD11	1.78	0.65
1:B:498:LYS:O	1:B:517:HIS:HD2	1.78	0.65
1:B:8:VAL:CG2	1:B:9:PRO:HD2	2.26	0.65
1:A:670:ASP:OD2	1:A:672:GLU:HG3	1.96	0.65
1:A:237:LYS:NZ	1:A:239:ASP:HB3	2.12	0.65
1:A:592:ASN:HD21	1:A:676:ASN:HD21	1.45	0.64
1:B:572:ASN:HD22	1:B:671:ASN:HD21	1.45	0.64
1:B:642:ARG:HH11	1:B:642:ARG:CB	2.11	0.64
1:B:231:ASP:HB2	1:B:626:TRP:CZ2	2.33	0.64
1:B:669:LYS:HA	1:B:669:LYS:HZ1	1.63	0.64
1:A:94:HIS:HB3	1:A:97:ASN:ND2	2.14	0.63
1:A:227:VAL:CG1	1:A:244:LYS:HG3	2.29	0.62
1:A:22:GLN:HE22	1:A:307:GLN:HE22	1.44	0.62
1:A:272:GLN:NE2	1:A:274:LYS:NZ	2.48	0.62
1:A:500:MET:HG3	1:B:599:ASN:ND2	2.15	0.61
1:B:381:TYR:CD2	1:B:466:TYQ:N5	2.66	0.61
1:B:574:GLN:H	1:B:671:ASN:ND2	1.98	0.61
1:A:441:GLN:OE1	1:A:447:ASN:HB2	2.00	0.61
1:B:13:THR:HG22	1:B:75:ILE:HD11	1.83	0.61
1:A:149:PRO:HA	1:A:170:GLN:HE21	1.65	0.60
1:B:387:TYR:CZ	4:B:3001:HY1:HA1	2.35	0.60
1:B:580:PHE:H	1:B:637:GLN:HE21	1.49	0.60
1:A:288:MET:CE	1:A:288:MET:HA	2.32	0.60
1:B:553:ASN:ND2	1:B:555:ALA:H	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HD12	1:A:214:ILE:N	2.17	0.59
1:B:382:LEU:N	1:B:382:LEU:HD12	2.18	0.59
1:A:570:ILE:HD13	1:A:578:GLN:HE22	1.67	0.59
1:B:257:TRP:HH2	4:B:3001:HY1:H3	1.67	0.59
1:B:441:GLN:OE1	1:B:447:ASN:HB2	2.02	0.59
1:B:692:ARG:NH1	1:B:694:GLU:HB2	2.16	0.59
1:A:580:PHE:H	1:A:637:GLN:NE2	1.97	0.59
1:B:717:THR:HB	1:B:720:LEU:HG	1.83	0.59
1:B:225:LEU:HD22	1:B:381:TYR:CE1	2.38	0.58
1:B:291:ARG:NH1	1:B:516:ASP:OD2	2.36	0.58
1:B:679:ALA:HB2	8:B:3366:HOH:O	2.03	0.58
1:A:439:LYS:HZ2	1:A:447:ASN:HD21	1.51	0.58
1:A:629:HIS:HB2	8:A:2378:HOH:O	2.02	0.58
1:A:326:ARG:HH12	1:B:303:VAL:HG22	1.68	0.58
1:A:381:TYR:HD2	1:A:466:TYQ:HN52	1.40	0.58
1:A:73:THR:HG23	1:A:77:ASP:OD2	2.03	0.58
1:A:77:ASP:O	1:A:81:SER:HB3	2.03	0.58
1:A:12:LYS:O	1:A:16:GLU:HG3	2.04	0.58
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.03	0.58
1:B:209:VAL:HG12	1:B:214:ILE:HB	1.86	0.58
1:B:173:LYS:HB3	1:B:173:LYS:NZ	2.20	0.57
1:A:219:LYS:HD3	8:A:2377:HOH:O	2.04	0.57
1:B:368:PRO:HB2	1:B:621:PHE:CZ	2.41	0.56
1:A:38:TYR:N	1:A:51:ASN:HD21	2.02	0.56
1:A:643:TYR:O	1:A:644:HIS:CD2	2.59	0.56
1:A:13:THR:HG22	1:A:75:ILE:HD11	1.88	0.56
1:A:276:VAL:O	1:A:277:LYS:HB2	2.05	0.56
1:A:381:TYR:CD2	1:A:466:TYQ:N5	2.67	0.56
1:B:366:ILE:HD12	1:B:631:LEU:CD1	2.36	0.56
1:A:572:ASN:HD21	1:A:575:ASP:CG	2.09	0.55
1:A:492:VAL:HB	1:A:519:ILE:HG23	1.88	0.55
1:B:639:TRP:HB2	1:B:682:TRP:HB2	1.87	0.55
1:A:129:LEU:HD12	1:A:130:PRO:HD2	1.87	0.55
1:B:251:VAL:O	1:B:251:VAL:HG12	2.07	0.55
1:B:379:LYS:HG3	1:B:381:TYR:CZ	2.41	0.54
1:A:692:ARG:HG3	1:A:695:GLU:HG3	1.90	0.54
1:B:404:SER:HB2	7:B:3003:GOL:H12	1.88	0.54
1:A:149:PRO:HA	1:A:170:GLN:NE2	2.22	0.54
1:A:664:LEU:HD21	1:A:682:TRP:CD2	2.43	0.54
1:B:579:LYS:HA	1:B:637:GLN:NE2	2.22	0.54
1:B:546:MET:HB2	1:B:585:ILE:HB	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:HB	1:B:71:SER:HB2	1.89	0.54
1:A:237:LYS:HZ3	1:A:239:ASP:HB3	1.71	0.53
1:B:221:ILE:N	1:B:221:ILE:HD12	2.22	0.53
1:A:160:LYS:HB2	8:A:2542:HOH:O	2.09	0.53
1:A:574:GLN:H	1:A:671:ASN:ND2	2.05	0.53
1:B:214:ILE:HD12	1:B:214:ILE:N	2.23	0.53
1:B:617:LYS:HA	8:B:3241:HOH:O	2.08	0.53
1:A:105:LYS:O	1:A:109:GLU:HG3	2.09	0.52
1:A:94:HIS:HB3	1:A:97:ASN:HD21	1.73	0.52
1:A:203:GLU:N	1:A:203:GLU:CD	2.63	0.52
1:A:498:LYS:HB3	1:A:498:LYS:NZ	2.25	0.52
1:A:382:LEU:HD13	1:A:655:PRO:HB2	1.91	0.52
1:A:477:ASN:HD22	1:A:477:ASN:C	2.12	0.52
1:A:572:ASN:C	1:A:572:ASN:HD22	2.11	0.52
1:A:482:ILE:HB	1:A:706:THR:OG1	2.09	0.52
1:A:10:MET:HG3	1:A:14:LEU:HD23	1.92	0.52
1:B:181:LYS:HE3	8:B:3672:HOH:O	2.09	0.52
1:A:326:ARG:HH12	1:B:303:VAL:CG2	2.23	0.52
1:B:543:LEU:HD22	1:B:640:VAL:HG21	1.91	0.52
1:A:163:ILE:HD12	1:A:163:ILE:N	2.25	0.51
1:A:633:PHE:HA	1:A:639:TRP:CZ2	2.45	0.51
1:B:595:ASN:HD22	1:B:595:ASN:C	2.12	0.51
1:A:117:PHE:CZ	1:A:121:THR:HB	2.45	0.51
1:A:368:PRO:HB2	1:A:621:PHE:CZ	2.45	0.51
1:B:384:SER:HA	1:B:389:MET:HG3	1.92	0.51
1:B:574:GLN:HB2	1:B:671:ASN:CG	2.31	0.51
1:B:94:HIS:HB3	1:B:97:ASN:ND2	2.26	0.51
1:A:396:ILE:CD1	1:A:428:ALA:HB2	2.40	0.51
1:A:543:LEU:HD22	1:A:640:VAL:HG21	1.92	0.51
1:B:94:HIS:CD2	1:B:96:LEU:HB2	2.46	0.51
1:A:595:ASN:ND2	1:A:599:ASN:H	2.09	0.51
1:A:24:ASP:OD2	1:B:40:LYS:NZ	2.33	0.50
1:B:129:LEU:HD12	1:B:130:PRO:HD2	1.92	0.50
8:A:2268:HOH:O	1:B:397:ALA:HB1	2.10	0.50
1:B:203:GLU:H	1:B:203:GLU:CD	2.14	0.50
1:A:366:ILE:HD11	1:A:627:ILE:HD11	1.93	0.50
1:A:595:ASN:HB2	1:A:715:ASP:OD1	2.12	0.50
1:A:597:MET:SD	1:B:516:ASP:HA	2.52	0.50
1:A:368:PRO:HB2	1:A:621:PHE:HZ	1.75	0.50
1:B:194:SER:O	1:B:198:ILE:HG13	2.11	0.50
1:A:366:ILE:HA	1:A:381:TYR:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASP:HB3	1:B:519:ILE:HB	1.94	0.50
1:A:639:TRP:HB2	1:A:682:TRP:HB2	1.93	0.50
1:A:231:ASP:HB2	1:A:626:TRP:CZ2	2.46	0.49
1:A:272:GLN:NE2	1:A:274:LYS:HZ1	2.10	0.49
1:A:288:MET:HA	1:A:288:MET:HE2	1.93	0.49
1:B:368:PRO:HB2	1:B:621:PHE:HZ	1.77	0.49
1:A:527:ILE:HD12	1:A:634:MET:CE	2.42	0.49
1:A:210:LYS:HE2	1:A:214:ILE:O	2.11	0.49
1:A:7:MET:HE2	1:A:71:SER:HA	1.94	0.49
1:B:100:THR:O	1:B:104:ILE:HG13	2.13	0.49
1:A:366:ILE:HG12	1:A:368:PRO:HD3	1.94	0.49
1:A:527:ILE:HD12	1:A:634:MET:HE3	1.94	0.49
1:A:326:ARG:NH1	1:B:303:VAL:HG22	2.26	0.49
1:A:403:PRO:HG3	1:A:430:PHE:CD2	2.47	0.49
1:A:439:LYS:NZ	1:A:447:ASN:HD21	2.11	0.49
1:B:334:MET:HE2	1:B:411:GLU:HG3	1.94	0.49
1:A:42:LYS:HD2	8:A:2468:HOH:O	2.12	0.49
1:B:595:ASN:ND2	1:B:595:ASN:C	2.66	0.49
1:A:381:TYR:CD2	4:A:2001:HY1:H	2.48	0.48
1:B:218:LYS:N	1:B:218:LYS:HD2	2.27	0.48
1:A:15:LYS:HE2	8:A:2448:HOH:O	2.12	0.48
1:A:60:PRO:HD2	8:A:2673:HOH:O	2.13	0.48
1:B:272:GLN:HE21	1:B:274:LYS:HD3	1.77	0.48
1:B:580:PHE:N	1:B:637:GLN:HE21	2.12	0.48
1:A:553:ASN:HD22	1:A:554:THR:N	2.12	0.48
1:A:517:HIS:CE1	1:B:596:ARG:HH11	2.31	0.48
1:A:64:LYS:O	1:A:65:ASP:HB3	2.14	0.48
1:A:553:ASN:HD21	1:A:555:ALA:H	1.57	0.48
1:B:36:GLY:HA2	1:B:314:LYS:HE2	1.95	0.48
1:B:492:VAL:HB	1:B:519:ILE:HG23	1.96	0.48
1:B:477:ASN:HD22	1:B:477:ASN:C	2.16	0.47
1:A:370:GLY:HA2	1:B:559:ARG:HH22	1.79	0.47
1:B:227:VAL:CG1	1:B:244:LYS:HG3	2.40	0.47
1:B:587:LEU:HD23	1:B:604:GLN:HA	1.96	0.47
1:B:209:VAL:CG1	1:B:214:ILE:HB	2.44	0.47
1:B:572:ASN:CB	1:B:671:ASN:HD21	2.19	0.47
1:B:105:LYS:O	1:B:109:GLU:HG3	2.14	0.47
1:B:118:LYS:HB2	1:B:121:THR:OG1	2.15	0.47
1:A:574:GLN:HG2	1:A:671:ASN:CG	2.34	0.47
1:B:466:TYQ:HN51	4:B:3001:HY1:C	2.27	0.47
1:A:32:LEU:HB2	1:A:39:VAL:HB	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLN:HE22	1:B:222:THR:H	1.61	0.47
1:A:467:ASP:HB2	1:A:487:THR:HG23	1.97	0.47
1:A:7:MET:CE	1:A:71:SER:HA	2.44	0.47
1:B:439:LYS:NZ	1:B:447:ASN:HD21	2.13	0.47
1:A:160:LYS:NZ	1:A:239:ASP:OD1	2.45	0.46
1:A:192:PHE:CE2	4:A:2001:HY1:H5	2.51	0.46
1:B:332:LEU:HD13	1:B:342:ILE:HD13	1.96	0.46
1:A:595:ASN:C	1:A:595:ASN:ND2	2.68	0.46
1:B:595:ASN:ND2	1:B:597:MET:H	2.14	0.46
1:A:438:TYR:CD1	1:B:698:ILE:HD13	2.50	0.46
1:B:439:LYS:HZ2	1:B:447:ASN:HD21	1.62	0.46
1:A:162:ILE:C	1:A:163:ILE:HD12	2.36	0.46
1:B:277:LYS:HE2	1:B:279:GLU:HG2	1.97	0.46
1:A:529:ASN:HD21	1:A:682:TRP:HE3	1.61	0.46
1:A:595:ASN:C	1:A:595:ASN:HD22	2.19	0.46
1:A:510:ARG:HH11	1:A:510:ARG:HG3	1.80	0.46
1:B:382:LEU:HD22	1:B:655:PRO:HB2	1.97	0.46
1:A:396:ILE:HG23	1:A:401:ASP:HB2	1.98	0.46
1:B:579:LYS:HA	1:B:637:GLN:HE22	1.82	0.46
1:B:572:ASN:ND2	1:B:671:ASN:HD21	2.13	0.46
1:A:439:LYS:NZ	1:A:447:ASN:ND2	2.64	0.45
1:B:160:LYS:HE3	1:B:239:ASP:OD1	2.16	0.45
1:A:581:ASP:HB3	1:A:584:THR:HG23	1.97	0.45
1:A:572:ASN:HB2	1:A:671:ASN:ND2	2.32	0.45
1:A:466:TYQ:N5	4:A:2001:HY1:H	2.32	0.45
1:B:291:ARG:HH11	1:B:291:ARG:HG3	1.82	0.45
1:A:382:LEU:CD1	1:A:655:PRO:HB2	2.47	0.45
1:B:549:VAL:HG11	1:B:566:ASN:ND2	2.32	0.45
1:B:580:PHE:CD2	1:B:607:PRO:HD2	2.52	0.45
1:A:433:TYR:CE2	1:B:403:PRO:HD3	2.52	0.45
1:B:573:GLU:HA	1:B:674:LEU:HD11	1.99	0.45
1:B:207:ALA:O	1:B:211:LYS:HG2	2.16	0.45
1:A:608:TYR:HE2	1:B:608:TYR:HE2	1.64	0.45
1:B:632:SER:HB3	8:B:3243:HOH:O	2.16	0.45
1:A:192:PHE:HE2	4:A:2001:HY1:H5	1.81	0.45
1:B:196:GLN:NE2	1:B:222:THR:H	2.15	0.45
1:A:222:THR:HB	1:A:245:VAL:CG1	2.46	0.44
1:A:331:HIS:HE1	1:A:333:SER:HB3	1.82	0.44
1:A:546:MET:HE3	8:A:2534:HOH:O	2.17	0.44
1:B:251:VAL:O	1:B:251:VAL:CG1	2.64	0.44
1:B:410:ASN:OD1	1:B:424:PRO:HA	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.31	0.44
1:A:459:TRP:CZ2	1:A:461:SER:HB2	2.52	0.44
1:B:203:GLU:N	1:B:203:GLU:CD	2.71	0.44
1:A:225:LEU:HD22	1:A:381:TYR:CZ	2.52	0.44
1:B:143:ASN:OD1	1:B:143:ASN:O	2.36	0.44
1:B:212:ARG:NH1	1:B:283:VAL:HA	2.33	0.44
1:B:549:VAL:HG11	1:B:566:ASN:HD22	1.82	0.44
1:B:592:ASN:HD21	1:B:676:ASN:HD21	1.65	0.44
1:A:437:GLU:OE2	1:B:700:PRO:HB3	2.17	0.44
1:B:173:LYS:HB3	1:B:173:LYS:HZ3	1.83	0.44
1:B:580:PHE:N	1:B:637:GLN:NE2	2.64	0.44
1:B:8:VAL:CG2	1:B:9:PRO:CD	2.96	0.44
1:A:209:VAL:CG1	1:A:214:ILE:HB	2.46	0.44
1:A:227:VAL:HG12	1:A:244:LYS:CG	2.42	0.44
1:B:595:ASN:HB2	1:B:715:ASP:OD1	2.18	0.44
1:A:181:LYS:HG3	1:A:182:ASP:OD2	2.18	0.43
1:A:611:GLY:HA3	8:A:2221:HOH:O	2.18	0.43
1:A:698:ILE:HD13	1:B:438:TYR:CD1	2.53	0.43
1:A:539:GLU:HB2	8:A:2438:HOH:O	2.18	0.43
1:A:132:ASP:OD2	1:A:148:GLN:OE1	2.37	0.43
1:A:255:ASN:HA	8:A:2358:HOH:O	2.18	0.43
1:B:506:LYS:HE2	1:B:510:ARG:HH12	1.83	0.43
1:A:324:HIS:HD2	1:A:329:ASP:OD1	2.01	0.43
1:A:396:ILE:HD12	1:A:428:ALA:HB2	2.01	0.43
1:B:139:PHE:O	1:B:143:ASN:HA	2.19	0.43
1:A:10:MET:HG3	1:A:14:LEU:CD2	2.49	0.43
1:A:559:ARG:NH2	1:B:621:PHE:HE1	2.16	0.43
1:B:238:GLN:HE21	1:B:238:GLN:HA	1.83	0.43
1:B:482:ILE:HB	1:B:706:THR:OG1	2.19	0.43
1:B:585:ILE:HD13	1:B:711:TRP:CH2	2.52	0.43
1:A:234:ASP:OD2	1:A:236:LEU:HD12	2.19	0.43
1:B:396:ILE:HG23	1:B:401:ASP:HB2	1.99	0.43
1:A:205:PHE:O	1:A:209:VAL:HG23	2.19	0.43
1:B:637:GLN:HA	1:B:684:THR:HB	2.01	0.43
1:A:225:LEU:HD12	1:A:246:ILE:HG12	2.01	0.43
1:A:695:GLU:HB3	1:A:699:MET:HG3	2.01	0.43
1:B:465:ASN:HD21	1:B:466:TYQ:CE1	2.32	0.43
1:B:229:TYR:HB3	1:B:630:ARG:HD2	2.00	0.43
1:A:368:PRO:HG3	1:A:634:MET:HE1	2.01	0.43
1:B:642:ARG:CG	1:B:642:ARG:HH11	2.32	0.43
1:A:445:GLN:HE21	1:A:446:PRO:HD3	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:HG2	1:A:671:ASN:CB	2.49	0.42
1:B:516:ASP:OD1	1:B:517:HIS:N	2.52	0.42
1:B:696:TRP:CD2	1:B:697:PRO:HA	2.55	0.42
1:B:366:ILE:HA	1:B:381:TYR:O	2.20	0.42
1:A:381:TYR:CG	4:A:2001:HY1:H	2.54	0.42
1:A:348:ASN:HD22	1:A:348:ASN:C	2.21	0.42
1:B:332:LEU:HD13	1:B:342:ILE:CD1	2.50	0.42
1:B:611:GLY:HA3	8:B:3246:HOH:O	2.20	0.42
1:A:130:PRO:HB3	8:A:2298:HOH:O	2.18	0.42
1:A:152:ALA:HB2	1:A:169:LEU:HD11	2.01	0.42
1:A:61:VAL:HG22	1:A:70:VAL:HG12	2.01	0.42
1:B:202:SER:OG	1:B:275:ILE:HD12	2.20	0.42
1:A:214:ILE:N	1:A:214:ILE:CD1	2.82	0.42
1:A:222:THR:HB	1:A:245:VAL:HG13	2.02	0.42
1:A:437:GLU:O	1:B:700:PRO:HA	2.20	0.42
1:A:92:ARG:HA	1:A:93:PRO:HD2	1.90	0.42
1:B:106:GLN:O	1:B:110:ILE:HG13	2.20	0.42
1:B:532:LEU:HD11	1:B:683:MET:HE2	2.01	0.42
1:B:669:LYS:HA	1:B:669:LYS:HZ2	1.79	0.42
1:A:144:LYS:HA	1:A:145:PRO:HD3	1.92	0.42
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.88	0.42
1:A:366:ILE:CD1	1:A:627:ILE:HD11	2.50	0.42
1:B:403:PRO:HG3	1:B:430:PHE:CD2	2.54	0.42
1:A:479:THR:HG22	1:A:480:ILE:N	2.35	0.41
1:B:381:TYR:CG	4:B:3001:HY1:H	2.55	0.41
1:A:212:ARG:NH1	1:A:283:VAL:HA	2.35	0.41
1:B:222:THR:HB	1:B:245:VAL:HG13	2.01	0.41
1:B:94:HIS:HD2	1:B:96:LEU:HB2	1.85	0.41
1:A:498:LYS:HB3	1:A:498:LYS:HZ3	1.84	0.41
1:B:130:PRO:HA	1:B:131:PRO:HD3	1.81	0.41
1:B:238:GLN:NE2	1:B:238:GLN:HA	2.35	0.41
1:B:462:THR:HG23	1:B:466:TYQ:O	2.20	0.41
1:A:237:LYS:HZ2	1:A:239:ASP:HB3	1.84	0.41
1:A:379:LYS:HE2	1:A:381:TYR:OH	2.21	0.41
1:A:384:SER:HA	1:A:389:MET:HG3	2.03	0.41
1:A:608:TYR:CZ	1:A:615:VAL:HG21	2.55	0.41
1:A:465:ASN:HB2	1:A:489:ILE:O	2.21	0.41
1:B:634:MET:HB3	1:B:634:MET:HE2	1.90	0.41
1:B:637:GLN:HB2	1:B:637:GLN:HE21	1.68	0.41
1:A:546:MET:HB2	1:A:585:ILE:HB	2.02	0.41
1:B:15:LYS:HE2	8:B:3496:HOH:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:MET:CE	1:B:411:GLU:HG3	2.50	0.41
1:A:700:PRO:HB3	1:B:437:GLU:OE2	2.21	0.41
1:A:51:ASN:N	1:A:51:ASN:HD22	2.17	0.41
1:A:257:TRP:HH2	4:A:2001:HY1:H3	1.86	0.41
1:A:366:ILE:HD11	1:A:380:ALA:HB1	2.02	0.41
1:A:664:LEU:HD21	1:A:682:TRP:CE2	2.55	0.41
1:B:223:THR:HA	1:B:224:PRO:HD3	1.83	0.41
1:A:460:ILE:HG21	1:B:439:LYS:HE2	2.03	0.41
1:B:627:ILE:HG23	1:B:628:TYR:N	2.36	0.41
1:A:595:ASN:HD21	1:A:599:ASN:H	1.69	0.41
1:A:396:ILE:HD13	1:A:428:ALA:HB2	2.02	0.41
1:A:477:ASN:HD22	1:A:479:THR:H	1.69	0.41
1:A:22:GLN:NE2	1:A:307:GLN:NE2	2.62	0.40
1:A:369:TYR:CD1	1:A:379:LYS:HG2	2.56	0.40
1:A:572:ASN:CG	1:A:671:ASN:HD21	2.24	0.40
1:A:679:ALA:HB2	8:A:2694:HOH:O	2.21	0.40
1:B:97:ASN:ND2	1:B:331:HIS:NE2	2.70	0.40
1:B:38:TYR:H	1:B:51:ASN:ND2	2.19	0.40
1:A:168:ASP:HB3	1:A:173:LYS:HG2	2.03	0.40
1:B:95:PRO:HB3	1:B:146:VAL:HG21	2.03	0.40
1:B:67:LYS:HE2	1:B:67:LYS:HB3	1.86	0.40
1:A:129:LEU:HD12	1:A:130:PRO:CD	2.51	0.40
1:B:359:GLU:CD	1:B:648:ARG:HH22	2.24	0.40
1:A:223:THR:HA	1:A:224:PRO:HD3	1.95	0.40
1:B:192:PHE:HE2	4:B:3001:HY1:H5	1.87	0.40
1:B:32:LEU:HB2	1:B:39:VAL:HB	2.04	0.40
1:B:263:ASN:HA	1:B:374:ILE:HD11	2.03	0.40
1:A:95:PRO:HB3	1:A:146:VAL:HG21	2.03	0.40
1:A:199:ILE:HG23	1:A:205:PHE:CD2	2.57	0.40
1:B:221:ILE:HD13	1:B:250:ASP:HB2	2.03	0.40
1:B:526:HIS:O	1:B:686:GLY:HA2	2.21	0.40
1:B:92:ARG:HA	1:B:93:PRO:HD2	1.85	0.40
1:B:9:PRO:HB2	8:B:3583:HOH:O	2.20	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	715/727 (98%)	689 (96%)	25 (4%)	1 (0%)	51	68
1	B	717/727 (99%)	692 (96%)	25 (4%)	0	100	100
All	All	1432/1454 (98%)	1381 (96%)	50 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	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	609/615 (99%)	596 (98%)	13 (2%)	53	72
1	B	611/615 (99%)	596 (98%)	15 (2%)	47	67
All	All	1220/1230 (99%)	1192 (98%)	28 (2%)	50	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	80	GLN
1	A	203	GLU
1	A	210	LYS
1	A	348	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	368	PRO
1	A	477	ASN
1	A	572	ASN
1	A	595	ASN
1	A	613	HIS
1	A	642	ARG
1	A	671	ASN
1	A	676	ASN
1	B	11	ASP
1	B	137	TRP
1	B	173	LYS
1	B	181	LYS
1	B	203	GLU
1	B	218	LYS
1	B	368	PRO
1	B	477	ASN
1	B	539	GLU
1	B	595	ASN
1	B	637	GLN
1	B	642	ARG
1	B	669	LYS
1	B	671	ASN
1	B	676	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	51	ASN
1	A	97	ASN
1	A	120	ASN
1	A	148	GLN
1	A	170	GLN
1	A	178	GLN
1	A	196	GLN
1	A	200	ASN
1	A	201	ASN
1	A	272	GLN
1	A	315	ASN
1	A	324	HIS
1	A	327	ASN
1	A	348	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	445	GLN
1	A	447	ASN
1	A	477	ASN
1	A	517	HIS
1	A	525	GLN
1	A	529	ASN
1	A	541	ASN
1	A	553	ASN
1	A	567	GLN
1	A	572	ASN
1	A	578	GLN
1	A	595	ASN
1	A	604	GLN
1	A	637	GLN
1	A	671	ASN
1	A	676	ASN
1	B	51	ASN
1	B	94	HIS
1	B	97	ASN
1	B	143	ASN
1	B	148	GLN
1	B	196	GLN
1	B	200	ASN
1	B	201	ASN
1	B	238	GLN
1	B	263	ASN
1	B	272	GLN
1	B	307	GLN
1	B	315	ASN
1	B	327	ASN
1	B	350	ASN
1	B	447	ASN
1	B	477	ASN
1	B	517	HIS
1	B	525	GLN
1	B	529	ASN
1	B	541	ASN
1	B	553	ASN
1	B	566	ASN
1	B	567	GLN
1	B	572	ASN
1	B	595	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	599	ASN
1	B	637	GLN
1	B	671	ASN
1	B	676	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	TYQ	A	466	1	13,14,15	1.16	2 (15%)	15,19,21	0.96	1 (6%)
1	TYQ	B	466	1	13,14,15	1.01	1 (7%)	15,19,21	1.19	1 (6%)

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
1	TYQ	A	466	1	-	0/5/6/8	0/1/1/1
1	TYQ	B	466	1	-	2/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TYQ	CE2-N5	2.55	1.46	1.37
1	B	466	TYQ	CE2-N5	2.39	1.45	1.37
1	A	466	TYQ	CE2-CZ	-2.13	1.38	1.40



All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TYQ	CB-CA-C	-3.59	104.74	111.47
1	A	466	TYQ	CB-CA-C	-2.59	106.62	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	466	TYQ	O-C-CA-CB
1	B	466	TYQ	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	466	TYQ	3	0
1	B	466	TYQ	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
5	NO	B	3002	2	0,1,1	0.00	-	-		
7	GOL	B	3003	-	5,5,5	0.39	0	5,5,5	0.41	0
5	NO	A	2002	-	0,1,1	0.00	-	-		
4	HY1	B	3001	-	9,9,9	1.23	1 (11%)	10,10,10	0.78	1 (10%)
7	GOL	B	2004	-	5,5,5	0.46	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HY1	A	2001	-	9,9,9	1.52	2 (22%)	10,10,10	0.68	0
6	PEA	A	2003	-	8,9,9	1.23	0	9,10,10	0.60	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
4	HY1	B	3001	-	-	0/3/3/3	0/1/1/1
4	HY1	A	2001	-	-	0/3/3/3	0/1/1/1
7	GOL	B	3003	-	-	0/4/4/4	-
7	GOL	B	2004	-	-	2/4/4/4	-
6	PEA	A	2003	-	-	1/3/3/3	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	HY1	C3'-C2'	2.73	1.44	1.38
4	A	2001	HY1	C5'-C6'	2.11	1.43	1.38
4	B	3001	HY1	C3'-C2'	2.03	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3001	HY1	C1'-CA-C	-2.16	109.24	114.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	PEA	N-C1-C2-C1'
7	B	2004	GOL	C1-C2-C3-O3
7	B	2004	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3003	GOL	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3001	HY1	5	0
4	A	2001	HY1	6	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	717/727 (98%)	-0.33	15 (2%) 63 61	22, 37, 59, 82	0
1	B	719/727 (98%)	-0.18	22 (3%) 49 47	26, 41, 63, 74	0
All	All	1436/1454 (98%)	-0.26	37 (2%) 56 54	22, 39, 62, 82	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	ALA	6.0
1	A	64	LYS	4.6
1	B	669	LYS	4.4
1	B	301	PRO	4.4
1	B	66	ASN	4.0
1	B	65	ASP	3.9
1	A	503	GLU	3.7
1	B	91	LYS	3.6
1	B	215	THR	3.6
1	B	6	HIS	3.5
1	B	644	HIS	3.4
1	B	216	ASP	3.3
1	B	239	ASP	3.1
1	A	12	LYS	3.0
1	A	218	LYS	2.9
1	B	178	GLN	2.9
1	B	605	ILE	2.8
1	B	182	ASP	2.8
1	B	64	LYS	2.8
1	B	115	ALA	2.8
1	B	80	GLN	2.8
1	A	211	LYS	2.8
1	A	65	ASP	2.8
1	B	210	LYS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	181	LYS	2.7
1	B	503	GLU	2.6
1	A	67	LYS	2.6
1	A	66	ASN	2.4
1	A	147	ASP	2.2
1	A	181	LYS	2.2
1	B	16	GLU	2.2
1	A	644	HIS	2.2
1	B	300	ALA	2.1
1	A	342	ILE	2.1
1	A	215	THR	2.1
1	A	225	LEU	2.0
1	A	246	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TYQ	A	466	14/15	0.88	0.20	39,53,58,61	0
1	TYQ	B	466	14/15	0.88	0.21	36,55,61,63	0

## 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
7	GOL	B	2004	6/6	0.80	0.46	58,60,61,61	0
4	HY1	B	3001	9/9	0.84	0.27	52,54,62,67	0
7	GOL	B	3003	6/6	0.86	0.29	56,57,57,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HY1	A	2001	9/9	0.88	0.18	54,55,57,60	0
3	CA	A	803	1/1	0.91	0.14	72,72,72,72	0
6	PEA	A	2003	9/9	0.91	0.16	35,37,38,39	0
5	NO	B	3002	2/2	0.92	0.29	48,48,48,49	0
3	CA	B	803	1/1	0.96	0.17	74,74,74,74	0
3	CA	A	802	1/1	0.99	0.11	33,33,33,33	0
3	CA	B	802	1/1	0.99	0.10	39,39,39,39	0
5	NO	A	2002	2/2	0.99	0.30	60,60,60,60	0
2	CU	A	801	1/1	0.99	0.08	43,43,43,43	0
2	CU	B	801	1/1	1.00	0.08	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.