



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:58 AM GMT

PDB ID : 1KMM  
Title : HISTIDYL-TRNA SYNTHETASE COMPLEXED WITH HISTIDYL-ADENYLATE  
Authors : Arnez, J.G.; Francklyn, C.S.; Moras, D.  
Deposited on : 1997-05-09  
Resolution : 2.60 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>

---

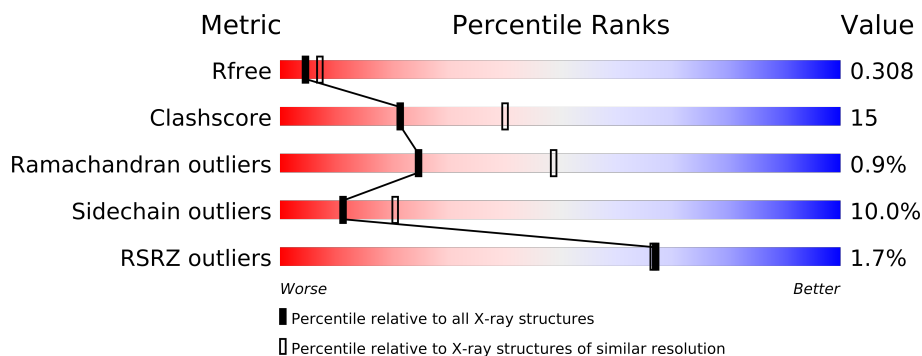
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	424	
1	B	424	
1	C	424	
1	D	424	

## 2 Entry composition i

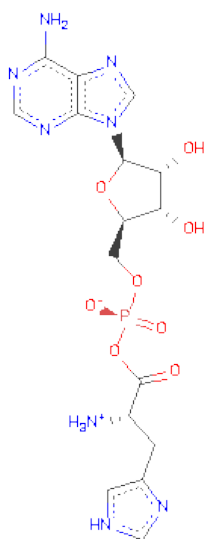
There are 3 unique types of molecules in this entry. The entry contains 14633 atoms, of which 2685 are hydrogens and 0 are deuterium.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	H	N	O	S	0	0	0
			3675	1884	682	535	563	11			
1	B	364	Total	C	H	N	O	S	0	0	0
			3472	1777	648	507	529	11			
1	C	387	Total	C	H	N	O	S	0	0	0
			3689	1892	684	538	564	11			
1	D	362	Total	C	H	N	O	S	0	0	0
			3453	1768	643	504	527	11			

- Molecule 2 is HISTIDYL-ADENOSINE MONOPHOSPHATE (three-letter code: HAM) (formula:  $C_{16}H_{21}N_8O_8P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			40	16	7	8	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			40	16	7	8	8	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	
			40	16	7	8	8	1	
2	D	1	Total	C	H	N	O	P	
			40	16	7	8	8	1	

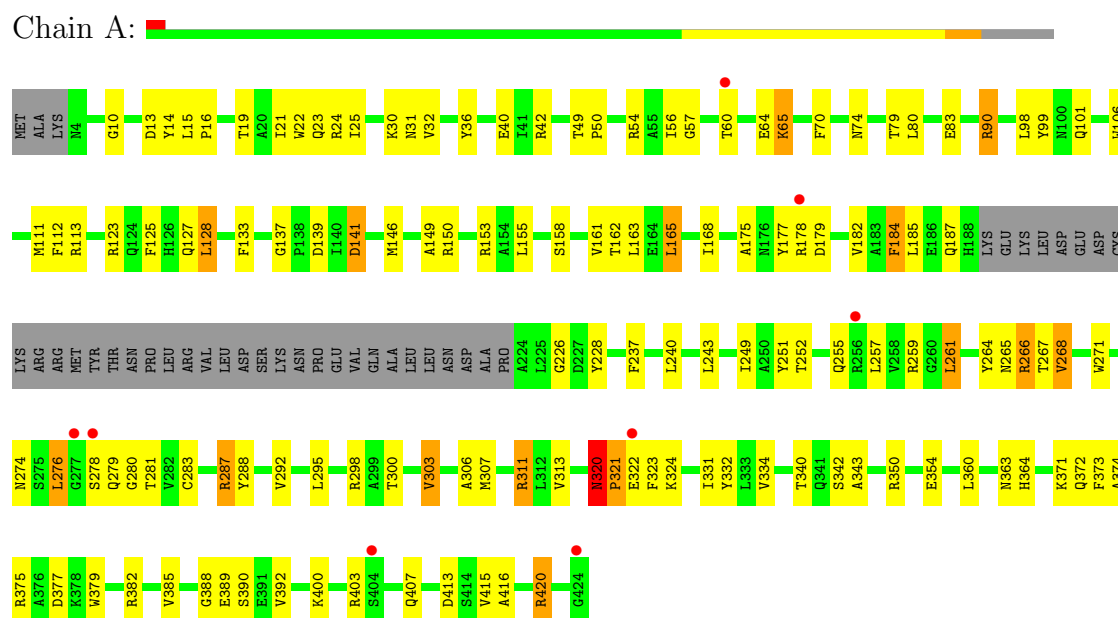
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O		
			45	45	0	0
3	B	50	Total	O		
			50	50	0	0
3	C	55	Total	O		
			55	55	0	0
3	D	34	Total	O		
			34	34	0	0

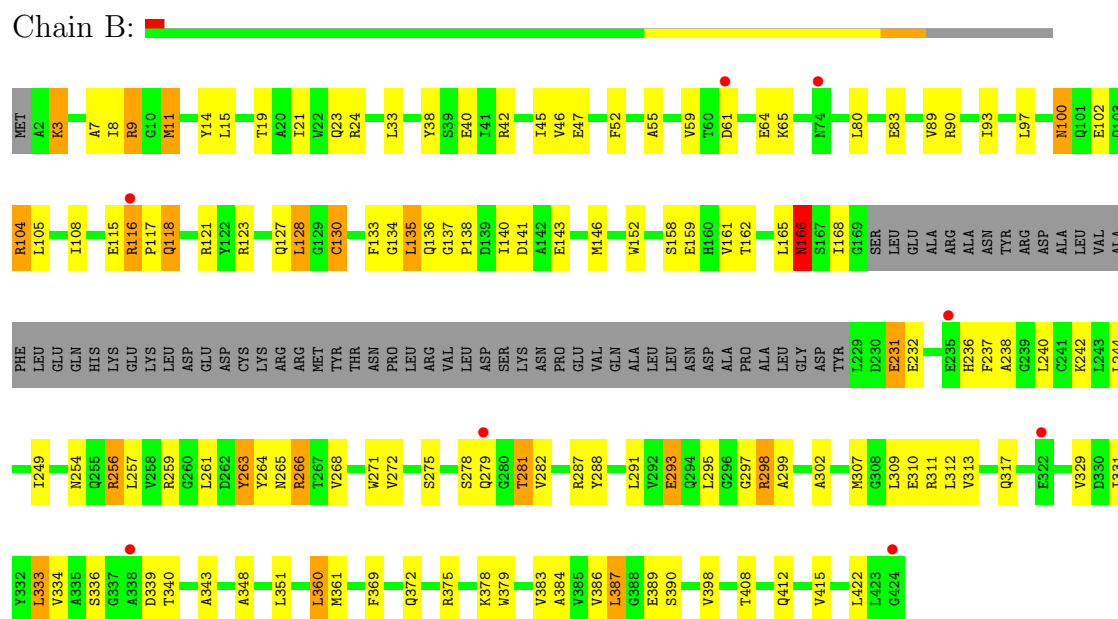
### 3 Residue-property plots

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

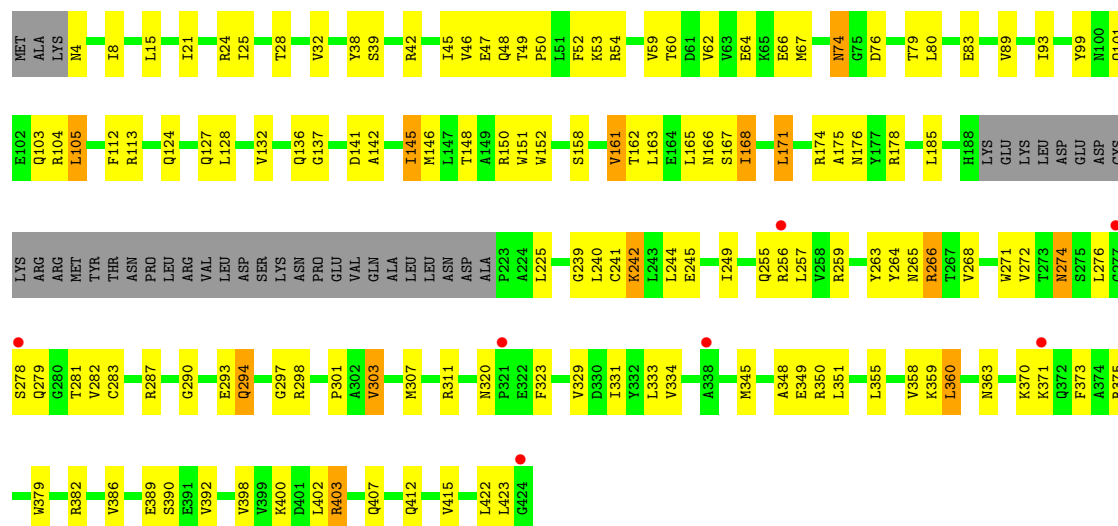


#### • Molecule 1: HISTIDYL-TRNA SYNTHETASE



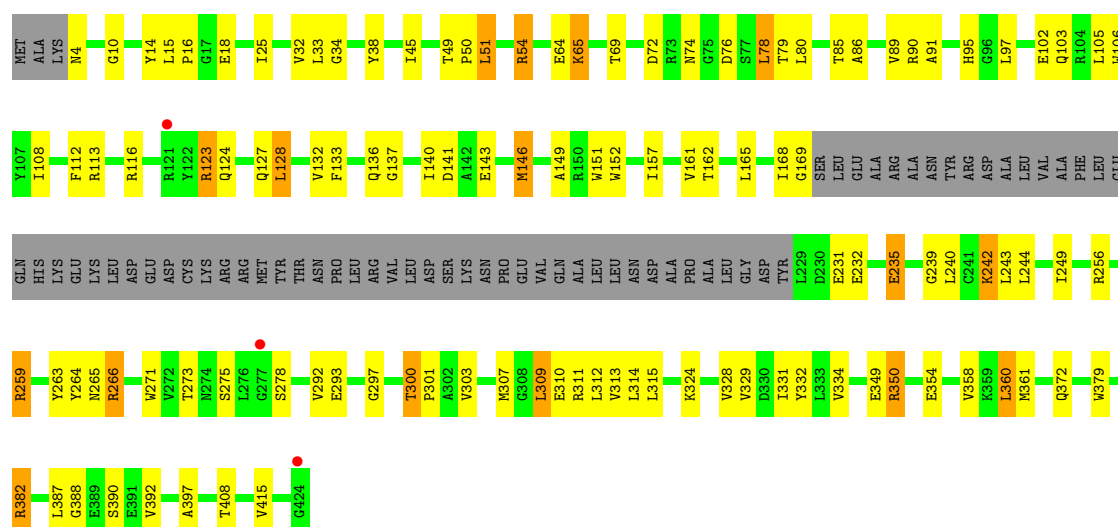
● Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain C: 



● Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.40Å 110.70Å 108.70Å 115.00° 97.40° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 12.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	68.0 (12.00-2.60) 84.9 (12.04-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.66 (at 2.59Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.221 , 0.297 0.252 , 0.308	Depositor DCC
$R_{free}$ test set	1679 reflections (2.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 66471 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% 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: HAM

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	0.59	0/3047	0.85	6/4123 (0.1%)
1	B	0.60	1/2875 (0.0%)	0.80	5/3888 (0.1%)
1	C	0.58	0/3061	0.80	4/4142 (0.1%)
1	D	0.57	0/2861	0.77	2/3870 (0.1%)
All	All	0.59	1/11844 (0.0%)	0.81	17/16023 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	CYS	CB-SG	-6.51	1.71	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASN	C-N-CD	-12.73	92.60	120.60
1	B	387	LEU	CA-CB-CG	7.16	131.76	115.30
1	A	323	PHE	N-CA-C	-6.18	94.31	111.00
1	C	323	PHE	N-CA-C	-5.88	95.12	111.00
1	D	360	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	128	LEU	N-CA-C	-5.54	96.03	111.00
1	A	303	VAL	CB-CA-C	-5.51	100.92	111.40
1	B	360	LEU	CA-CB-CG	5.47	127.87	115.30
1	B	257	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	128	LEU	CA-CB-CG	-5.36	102.98	115.30
1	C	128	LEU	N-CA-C	-5.33	96.60	111.00
1	C	360	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	128	LEU	N-CA-C	-5.28	96.75	111.00
1	A	261	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	105	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	311	ARG	NE-CZ-NH1	5.18	122.89	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	LEU	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2993	682	2269	88	0
1	B	2824	648	2152	110	0
1	C	3005	684	2279	94	0
1	D	2810	643	2139	86	0
2	A	33	7	14	2	0
2	B	33	7	14	1	0
2	C	33	7	14	2	0
2	D	33	7	14	5	0
3	A	45	0	0	1	0
3	B	50	0	0	1	0
3	C	55	0	0	1	0
3	D	34	0	0	0	0
All	All	11948	2685	8895	358	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 15.

All (358) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:382:ARG:HH11	1:D:382:ARG:HG2	1.36	0.89
1:B:3:LYS:NZ	1:B:3:LYS:HB3	1.87	0.89
1:B:89:VAL:HG21	1:B:291:LEU:HD22	1.55	0.89
1:D:311:ARG:NH1	2:D:450:HAM:H2'	1.88	0.89
1:A:161:VAL:HG12	1:A:271:TRP:HE3	1.38	0.88
1:D:311:ARG:HH12	2:D:450:HAM:H2'	1.42	0.85
1:B:8:ILE:HB	1:B:11:MET:HG3	1.55	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:PRO:O	1:A:19:THR:HG22	1.75	0.85
1:B:298:ARG:HG3	1:B:298:ARG:HH11	1.43	0.84
1:B:278:SER:HA	1:B:311:ARG:HD2	1.62	0.81
1:A:278:SER:CB	1:A:311:ARG:HD3	2.11	0.80
1:B:278:SER:CA	1:B:311:ARG:HD2	2.14	0.78
1:B:116:ARG:HD2	1:B:116:ARG:H	1.49	0.76
1:C:239:GLY:O	1:C:242:LYS:HG3	1.88	0.73
1:A:161:VAL:HG12	1:A:271:TRP:CE3	2.24	0.73
1:A:292:VAL:HG21	1:A:300:THR:HG22	1.69	0.72
1:B:115:GLU:HA	1:B:116:ARG:NH1	2.05	0.71
1:B:333:LEU:HD23	1:B:348:ALA:HB2	1.72	0.71
1:C:168:ILE:HG23	1:C:174:ARG:HE	1.56	0.71
1:A:334:VAL:HG21	1:A:373:PHE:CE1	2.26	0.71
1:B:240:LEU:O	1:B:244:LEU:HD23	1.89	0.70
1:C:355:LEU:O	1:C:358:VAL:HG22	1.91	0.69
1:B:9:ARG:H	1:B:9:ARG:HD3	1.56	0.69
1:C:278:SER:CB	1:C:311:ARG:HD3	2.23	0.69
1:D:328:VAL:HG23	1:D:329:VAL:HG23	1.75	0.69
1:A:165:LEU:HD22	1:A:237:PHE:HE1	1.57	0.69
1:A:146:MET:HG2	1:A:249:ILE:HD11	1.75	0.68
1:D:146:MET:HG3	1:D:249:ILE:HD11	1.74	0.68
1:A:19:THR:HG21	1:B:40:GLU:O	1.94	0.67
1:C:171:LEU:HA	1:C:174:ARG:NH1	2.09	0.67
1:D:273:THR:HG21	1:D:315:LEU:HD22	1.76	0.67
1:A:364:HIS:HD2	1:B:104:ARG:HH22	1.43	0.67
1:C:175:ALA:HA	1:C:178:ARG:HE	1.57	0.67
1:B:3:LYS:HZ1	1:B:3:LYS:HB3	1.59	0.67
1:A:364:HIS:HD2	1:B:104:ARG:NH2	1.92	0.67
1:D:157:ILE:HD12	1:D:315:LEU:HD23	1.76	0.67
1:B:375:ARG:HA	1:B:378:LYS:HD2	1.76	0.66
1:C:67:MET:HE2	1:C:79:THR:HG21	1.77	0.66
1:B:293:GLU:HA	1:B:297:GLY:O	1.96	0.66
1:D:382:ARG:NH1	1:D:382:ARG:HG2	2.07	0.66
1:C:168:ILE:HG22	1:C:265:ASN:O	1.95	0.65
1:D:256:ARG:NE	1:D:256:ARG:HA	2.12	0.65
1:A:165:LEU:HD22	1:A:237:PHE:CE1	2.32	0.65
1:A:382:ARG:HD2	1:A:403:ARG:HH21	1.61	0.65
1:A:14:TYR:HB2	1:B:42:ARG:HB2	1.80	0.64
1:D:310:GLU:O	1:D:314:LEU:HG	1.98	0.63
1:C:311:ARG:NH1	2:C:450:HAM:H2'	2.14	0.63
1:C:45:ILE:H	1:D:124:GLN:HE21	1.46	0.63
1:A:57:GLY:O	1:A:60:THR:HG22	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:171:LEU:HG	1:C:174:ARG:HH12	1.64	0.62
1:A:15:LEU:HD22	1:B:97:LEU:HD11	1.80	0.62
1:C:279:GLN:HB2	1:C:311:ARG:NH2	2.14	0.62
1:B:102:GLU:HA	1:B:133:PHE:O	2.00	0.61
1:D:311:ARG:NH1	2:D:450:HAM:C2'	2.62	0.61
1:A:388:GLY:O	1:A:392:VAL:HG23	2.01	0.60
1:B:412:GLN:O	1:B:415:VAL:HG22	2.01	0.60
1:A:49:THR:N	1:A:50:PRO:HD2	2.17	0.60
1:B:115:GLU:HA	1:B:116:ARG:HH11	1.67	0.60
1:D:331:ILE:HD12	1:D:358:VAL:HG11	1.83	0.60
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.37	0.60
1:D:239:GLY:O	1:D:242:LYS:HG3	2.02	0.59
1:B:168:ILE:HG13	1:B:265:ASN:O	2.02	0.59
1:C:136:GLN:HG3	1:C:301:PRO:HG2	1.83	0.59
1:B:298:ARG:HG3	1:B:298:ARG:NH1	2.17	0.59
1:B:116:ARG:N	1:B:116:ARG:HD2	2.17	0.59
1:B:3:LYS:HZ2	1:B:3:LYS:HB3	1.68	0.58
1:D:259:ARG:HB2	1:D:264:TYR:CD2	2.38	0.58
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.85	0.58
1:D:89:VAL:HG13	1:D:292:VAL:HG22	1.86	0.58
1:A:24:ARG:NH1	1:A:324:LYS:O	2.36	0.57
1:D:334:VAL:HG13	1:D:372:GLN:OE1	2.04	0.57
1:A:175:ALA:O	1:A:178:ARG:HG2	2.04	0.57
1:C:290:GLY:O	1:C:294:GLN:HB2	2.04	0.57
1:A:22:TRP:CE2	1:A:313:VAL:HG21	2.38	0.57
1:B:336:SER:HB3	1:B:369:PHE:CZ	2.39	0.57
1:A:30:LYS:HE2	1:A:106:TRP:HH2	1.70	0.57
1:D:168:ILE:HB	1:D:265:ASN:O	2.05	0.56
1:D:293:GLU:HA	1:D:297:GLY:O	2.06	0.56
1:C:412:GLN:HA	1:C:415:VAL:HG23	1.86	0.56
1:D:49:THR:N	1:D:50:PRO:HD2	2.20	0.56
1:B:89:VAL:O	1:B:93:ILE:HG13	2.05	0.56
1:A:30:LYS:HE2	1:A:106:TRP:CH2	2.41	0.56
1:A:400:LYS:HE2	1:A:407:GLN:HE22	1.71	0.56
1:D:85:THR:O	1:D:89:VAL:HG23	2.05	0.56
1:D:242:LYS:HE2	1:D:243:LEU:HG	1.88	0.56
1:A:10:GLY:HA3	1:A:123:ARG:HG3	1.87	0.56
1:B:166:ASN:ND2	1:B:268:VAL:HG23	2.21	0.55
1:B:15:LEU:H	1:B:15:LEU:HD22	1.70	0.55
1:B:89:VAL:HG21	1:B:291:LEU:CD2	2.32	0.55
1:A:320:ASN:O	1:A:322:GLU:N	2.39	0.55
1:B:165:LEU:O	1:B:166:ASN:HB3	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:259:ARG:NH1	1:C:264:TYR:OH	2.39	0.55
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.89	0.55
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.72	0.55
1:D:64:GLU:HB3	1:D:65:LYS:HD3	1.89	0.55
1:C:112:PHE:CE2	1:C:124:GLN:HG3	2.42	0.55
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.88	0.55
1:C:274:ASN:C	1:C:276:LEU:H	2.10	0.54
1:A:276:LEU:HD13	1:A:278:SER:O	2.07	0.54
1:C:350:ARG:HD2	1:C:351:LEU:HD12	1.87	0.54
1:D:128:LEU:HB2	1:D:309:LEU:HD11	1.89	0.54
1:A:49:THR:HG23	1:A:79:THR:OG1	2.07	0.54
1:A:36:TYR:HE1	1:A:150:ARG:HD2	1.71	0.54
1:C:375:ARG:O	1:C:379:TRP:CD1	2.61	0.54
1:A:364:HIS:CD2	1:B:104:ARG:NH2	2.75	0.54
1:C:163:LEU:HG	1:C:165:LEU:HD12	1.90	0.54
1:A:279:GLN:HG2	1:A:311:ARG:NH2	2.23	0.54
1:A:178:ARG:HG3	1:A:179:ASP:H	1.73	0.54
1:A:266:ARG:HB3	3:A:576:HOH:O	2.06	0.54
1:D:256:ARG:CZ	1:D:256:ARG:HA	2.38	0.54
1:B:254:ASN:OD1	1:B:256:ARG:HG3	2.08	0.54
1:C:8:ILE:HD11	1:D:78:LEU:HG	1.90	0.54
1:D:102:GLU:HA	1:D:133:PHE:O	2.07	0.54
1:A:112:PHE:HZ	1:B:45:ILE:HG13	1.73	0.54
1:A:182:VAL:HA	1:A:185:LEU:HD12	1.90	0.53
1:C:148:THR:O	1:C:151:TRP:HB2	2.08	0.53
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.91	0.53
1:C:271:TRP:HB2	1:C:283:CYS:HB3	1.90	0.53
1:A:21:ILE:O	1:A:25:ILE:HG13	2.07	0.53
1:D:329:VAL:CG2	1:D:379:TRP:HB3	2.38	0.53
1:B:115:GLU:OE1	1:B:121:ARG:HD2	2.08	0.53
1:D:259:ARG:NH1	1:D:264:TYR:OH	2.41	0.53
1:C:175:ALA:HA	1:C:178:ARG:NE	2.23	0.53
1:A:400:LYS:HG3	1:A:407:GLN:HB3	1.91	0.52
1:D:162:THR:O	1:D:271:TRP:HA	2.10	0.52
1:B:33:LEU:HD11	1:B:128:LEU:HD21	1.91	0.52
1:C:4:ASN:N	1:D:54:ARG:HH22	2.07	0.52
1:C:46:VAL:HG22	1:C:80:LEU:HD12	1.90	0.52
1:C:21:ILE:N	1:C:21:ILE:HD12	2.23	0.52
1:A:420:ARG:HH11	1:A:420:ARG:HG2	1.73	0.52
1:C:287:ARG:NH2	1:C:303:VAL:CG2	2.73	0.52
1:A:163:LEU:HD23	1:A:251:TYR:HB3	1.92	0.52
1:C:287:ARG:NH2	1:C:303:VAL:HG21	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:265:ASN:OD1	1:D:266:ARG:HG3	2.09	0.52
1:A:161:VAL:CG1	1:A:271:TRP:HE3	2.17	0.52
1:D:361:MET:HE2	1:D:379:TRP:NE1	2.24	0.52
1:C:241:CYS:O	1:C:245:GLU:HG3	2.09	0.52
1:A:264:TYR:HA	1:A:287:ARG:O	2.10	0.52
1:C:99:TYR:O	1:C:101:GLN:HG3	2.10	0.52
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.45	0.51
1:A:13:ASP:OD2	1:B:90:ARG:NH2	2.43	0.51
1:C:278:SER:CB	1:C:311:ARG:HB3	2.41	0.51
1:C:47:GLU:HB2	1:C:52:PHE:CE2	2.45	0.51
1:A:350:ARG:NH2	1:A:413:ASP:HA	2.26	0.51
1:B:291:LEU:O	1:B:291:LEU:HD23	2.11	0.51
1:C:171:LEU:HA	1:C:174:ARG:HH12	1.76	0.51
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.45	0.51
1:A:178:ARG:HG3	1:A:179:ASP:N	2.26	0.51
1:B:102:GLU:OE2	1:B:135:LEU:HD11	2.10	0.51
1:A:184:PHE:CD1	1:A:184:PHE:C	2.84	0.51
1:D:350:ARG:HD3	1:D:354:GLU:OE1	2.11	0.51
1:C:389:GLU:O	1:C:392:VAL:HG22	2.11	0.51
1:D:278:SER:CB	1:D:311:ARG:HG3	2.40	0.50
1:B:162:THR:O	1:B:271:TRP:HA	2.10	0.50
1:A:267:THR:H	1:A:287:ARG:HG3	1.77	0.50
1:C:333:LEU:CD1	1:C:348:ALA:HB2	2.42	0.50
1:D:49:THR:HG23	1:D:79:THR:OG1	2.12	0.50
1:C:171:LEU:HD23	1:C:178:ARG:HH22	1.75	0.50
1:B:281:THR:O	1:B:311:ARG:NH1	2.45	0.49
1:A:332:TYR:CE2	1:A:363:ASN:HB2	2.47	0.49
1:D:232:GLU:HG3	1:D:266:ARG:NH2	2.27	0.49
1:B:278:SER:CB	1:B:311:ARG:HB3	2.42	0.49
1:D:265:ASN:OD1	1:D:266:ARG:N	2.46	0.49
1:A:177:TYR:HD1	1:A:228:TYR:CD1	2.30	0.49
1:B:311:ARG:HG3	1:B:311:ARG:HH11	1.77	0.49
1:C:171:LEU:CD2	1:C:178:ARG:HH22	2.25	0.49
1:C:175:ALA:HB2	1:C:178:ARG:HH21	1.77	0.49
1:C:403:ARG:NH2	1:C:422:LEU:O	2.46	0.49
1:B:59:VAL:HG22	1:B:59:VAL:O	2.13	0.49
1:D:307:MET:SD	1:D:312:LEU:HD22	2.52	0.49
1:C:112:PHE:HZ	1:D:45:ILE:HD12	1.78	0.49
1:D:169:GLY:H	1:D:266:ARG:HA	1.78	0.48
1:B:264:TYR:HA	1:B:287:ARG:O	2.13	0.48
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	0.48
1:C:331:ILE:O	1:C:360:LEU:HA	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:TYR:O	1:A:101:GLN:HG3	2.12	0.48
1:A:259:ARG:HG2	1:A:268:VAL:HG22	1.95	0.48
1:B:136:GLN:HA	1:B:287:ARG:NH1	2.28	0.48
1:A:226:GLY:H	1:A:255:GLN:HE22	1.60	0.48
1:A:259:ARG:NH1	1:A:264:TYR:OH	2.46	0.48
1:A:259:ARG:HG2	1:A:268:VAL:CG2	2.44	0.48
1:C:49:THR:HG22	1:C:53:LYS:HE2	1.96	0.48
1:B:38:TYR:CD1	1:B:38:TYR:N	2.82	0.48
1:D:141:ASP:HB2	1:D:240:LEU:HD13	1.96	0.48
1:C:334:VAL:HG21	1:C:373:PHE:CE1	2.49	0.47
1:C:168:ILE:CG2	1:C:174:ARG:HE	2.27	0.47
1:C:8:ILE:CD1	1:D:78:LEU:HG	2.45	0.47
1:C:21:ILE:O	1:C:25:ILE:HG13	2.15	0.47
1:D:141:ASP:CB	1:D:240:LEU:HD13	2.45	0.47
1:B:238:ALA:O	1:B:242:LYS:HG2	2.15	0.47
1:A:271:TRP:HB2	1:A:283:CYS:HB3	1.96	0.47
1:B:311:ARG:HG3	1:B:311:ARG:NH1	2.29	0.47
1:D:140:ILE:HD12	1:D:143:GLU:HB3	1.97	0.47
1:D:103:GLN:O	1:D:132:VAL:HA	2.15	0.47
1:B:134:GLY:C	1:B:135:LEU:HD13	2.34	0.47
1:C:74:ASN:HD22	1:C:74:ASN:C	2.18	0.47
1:B:21:ILE:N	1:B:21:ILE:HD12	2.29	0.47
1:B:313:VAL:O	1:B:317:GLN:HG3	2.15	0.47
1:B:102:GLU:OE2	1:B:135:LEU:HD21	2.15	0.46
1:C:142:ALA:HB1	1:C:146:MET:HE3	1.97	0.46
1:D:15:LEU:HD22	1:D:15:LEU:H	1.79	0.46
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.64	0.46
1:D:74:ASN:HB3	1:D:76:ASP:OD2	2.14	0.46
1:C:166:ASN:HB3	1:C:268:VAL:HG23	1.96	0.46
1:C:168:ILE:HG23	1:C:174:ARG:NE	2.26	0.46
1:B:161:VAL:HA	1:B:272:VAL:O	2.16	0.46
1:C:163:LEU:HG	1:C:165:LEU:CD1	2.45	0.46
1:A:354:GLU:OE1	1:A:416:ALA:HB2	2.15	0.46
1:D:108:ILE:HA	1:D:127:GLN:O	2.16	0.46
1:C:67:MET:CE	1:C:79:THR:HG21	2.45	0.46
1:D:91:ALA:O	1:D:95:HIS:HD2	1.99	0.46
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.70	0.46
1:C:400:LYS:HD3	1:C:407:GLN:NE2	2.31	0.46
1:C:359:LYS:HG2	1:D:34:GLY:O	2.16	0.46
1:A:278:SER:C	1:A:280:GLY:N	2.67	0.46
1:B:329:VAL:CG2	1:B:379:TRP:HB3	2.45	0.46
1:D:334:VAL:HG22	1:D:372:GLN:HB3	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:72:ASP:C	1:D:74:ASN:H	2.19	0.46
1:C:163:LEU:HD21	1:C:165:LEU:HD11	1.98	0.46
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.98	0.46
1:D:32:VAL:HB	1:D:151:TRP:HE1	1.82	0.45
1:B:361:MET:HE2	1:B:379:TRP:NE1	2.32	0.45
1:B:61:ASP:HA	1:B:64:GLU:HB2	1.99	0.45
1:B:108:ILE:HA	1:B:127:GLN:O	2.15	0.45
1:C:127:GLN:HA	1:C:307:MET:O	2.16	0.45
1:B:38:TYR:HD1	1:B:38:TYR:N	2.15	0.45
1:B:115:GLU:O	1:B:117:PRO:HD3	2.16	0.45
1:B:291:LEU:C	1:B:291:LEU:HD23	2.37	0.45
1:C:375:ARG:O	1:C:379:TRP:HD1	1.98	0.45
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.99	0.45
1:B:278:SER:C	1:B:311:ARG:HD2	2.37	0.45
1:B:278:SER:HA	1:B:311:ARG:HB3	1.98	0.45
1:D:232:GLU:O	1:D:235:GLU:HG2	2.16	0.45
1:A:298:ARG:HG3	1:A:298:ARG:HH11	1.82	0.45
1:C:386:VAL:HB	1:C:398:VAL:HB	1.97	0.45
1:B:146:MET:HG3	1:B:249:ILE:HD11	1.98	0.45
1:D:278:SER:CB	1:D:311:ARG:CG	2.95	0.45
1:D:146:MET:O	1:D:149:ALA:HB3	2.16	0.45
1:A:127:GLN:HA	1:A:307:MET:O	2.15	0.45
1:C:333:LEU:HD13	1:C:348:ALA:HB2	1.98	0.45
1:C:89:VAL:O	1:C:93:ILE:HG13	2.16	0.45
1:D:382:ARG:HH11	1:D:382:ARG:CG	2.20	0.45
1:B:278:SER:CB	1:B:282:VAL:HG22	2.47	0.45
1:D:361:MET:CE	1:D:379:TRP:NE1	2.80	0.45
1:B:138:PRO:HD3	1:B:236:HIS:CD2	2.52	0.45
1:A:320:ASN:HA	1:A:321:PRO:HD2	1.64	0.44
1:B:261:LEU:HD12	1:B:263:TYR:OH	2.17	0.44
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.31	0.44
1:C:113:ARG:NH2	2:C:450:HAM:O2P	2.47	0.44
1:C:67:MET:HE2	1:C:67:MET:HB3	1.74	0.44
1:D:152:TRP:CD1	1:D:161:VAL:HG21	2.52	0.44
1:B:288:TYR:CD2	1:B:288:TYR:O	2.70	0.44
1:C:150:ARG:NH2	1:D:349:GLU:OE1	2.49	0.44
1:A:340:THR:O	1:A:343:ALA:HB3	2.18	0.44
1:D:331:ILE:O	1:D:360:LEU:HA	2.18	0.44
1:C:282:VAL:O	1:C:307:MET:HG3	2.17	0.44
1:C:145:ILE:HG22	1:C:249:ILE:HD13	1.98	0.44
1:B:386:VAL:HB	1:B:398:VAL:HB	2.00	0.44
1:B:55:ALA:HB2	1:B:295:LEU:HD11	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:62:VAL:HA	1:C:66:GLU:HB2	2.00	0.44
1:C:274:ASN:C	1:C:276:LEU:N	2.69	0.44
1:B:133:PHE:CD1	1:B:302:ALA:HB2	2.53	0.44
1:A:363:ASN:OD1	1:A:372:GLN:HG2	2.18	0.44
1:B:128:LEU:HB2	1:B:309:LEU:HD21	1.98	0.44
1:C:266:ARG:HB3	3:C:505:HOH:O	2.18	0.44
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.53	0.43
1:C:38:TYR:N	1:C:38:TYR:CD1	2.86	0.43
1:A:113:ARG:NH2	2:A:450:HAM:O2P	2.48	0.43
1:A:64:GLU:CB	1:A:65:LYS:HD3	2.47	0.43
1:B:166:ASN:HA	1:B:237:PHE:CZ	2.53	0.43
1:D:38:TYR:CD1	1:D:38:TYR:N	2.86	0.43
1:B:231:GLU:HG2	1:B:232:GLU:N	2.33	0.43
1:C:28:THR:O	1:C:32:VAL:HG23	2.19	0.43
1:D:146:MET:HG3	1:D:249:ILE:CD1	2.45	0.43
1:D:388:GLY:O	1:D:392:VAL:HG23	2.18	0.43
1:B:259:ARG:HB2	1:B:264:TYR:CD2	2.53	0.43
1:A:385:VAL:HG23	1:A:385:VAL:O	2.18	0.43
1:C:103:GLN:HB3	1:C:105:LEU:HD21	2.01	0.43
1:A:274:ASN:C	1:A:276:LEU:H	2.22	0.43
1:A:111:MET:HB2	1:A:125:PHE:CZ	2.54	0.43
1:B:152:TRP:HE3	1:B:152:TRP:HA	1.84	0.43
1:A:32:VAL:O	1:A:36:TYR:HD1	2.01	0.43
1:A:149:ALA:O	1:A:153:ARG:HG3	2.19	0.43
1:A:16:PRO:HG3	1:B:105:LEU:HD22	2.01	0.42
1:B:121:ARG:NH1	2:B:450:HAM:N7	2.66	0.42
1:A:371:LYS:O	1:A:374:ALA:HB3	2.20	0.42
1:A:375:ARG:O	1:A:379:TRP:CD1	2.72	0.42
1:A:98:LEU:HD22	1:A:133:PHE:CG	2.54	0.42
1:D:259:ARG:HB2	1:D:264:TYR:HD2	1.82	0.42
1:D:331:ILE:CD1	1:D:358:VAL:HG11	2.47	0.42
1:D:69:THR:HG23	1:D:79:THR:OG1	2.19	0.42
1:A:374:ALA:HA	1:A:377:ASP:OD2	2.19	0.42
1:C:293:GLU:HA	1:C:297:GLY:O	2.18	0.42
1:B:46:VAL:HG22	1:B:80:LEU:HD13	2.02	0.42
1:C:74:ASN:ND2	1:C:76:ASP:H	2.17	0.42
1:A:334:VAL:HG21	1:A:373:PHE:HE1	1.81	0.42
1:B:259:ARG:NH1	1:B:264:TYR:OH	2.50	0.42
1:B:331:ILE:O	1:B:360:LEU:HA	2.19	0.42
1:C:167:SER:HA	1:C:266:ARG:O	2.19	0.42
1:C:345:MET:O	1:C:349:GLU:HG2	2.20	0.42
1:B:141:ASP:HB2	1:B:240:LEU:HD13	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:300:THR:HA	1:D:301:PRO:HD3	1.90	0.42
1:C:276:LEU:C	1:C:278:SER:N	2.72	0.42
1:D:38:TYR:HD1	1:D:38:TYR:N	2.18	0.42
1:D:397:ALA:HB3	1:D:415:VAL:HG21	2.02	0.42
1:C:174:ARG:C	1:C:176:ASN:H	2.23	0.41
1:D:329:VAL:HG21	1:D:379:TRP:HB3	2.02	0.41
1:B:279:GLN:HA	1:B:279:GLN:NE2	2.35	0.41
1:C:60:THR:O	1:C:64:GLU:HG3	2.20	0.41
1:A:274:ASN:HA	1:A:274:ASN:HD22	1.70	0.41
1:A:306:ALA:HB3	2:A:450:HAM:HB2	2.01	0.41
1:C:259:ARG:CZ	1:C:259:ARG:HB3	2.50	0.41
1:C:32:VAL:HG13	1:C:150:ARG:HD2	2.01	0.41
1:D:113:ARG:NH1	2:D:450:HAM:O2P	2.52	0.41
1:A:161:VAL:CG1	1:A:271:TRP:CE3	2.97	0.41
1:D:33:LEU:HG	1:D:151:TRP:HZ2	1.85	0.41
1:A:56:ILE:HG22	1:A:60:THR:HG21	2.03	0.41
1:B:152:TRP:CE3	1:B:152:TRP:HA	2.55	0.41
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.85	0.41
1:C:48:GLN:HB3	1:C:50:PRO:HD2	2.02	0.41
1:B:307:MET:SD	1:B:312:LEU:HD22	2.60	0.41
1:B:152:TRP:CE3	1:B:152:TRP:CA	3.03	0.41
1:D:25:ILE:HD12	1:D:313:VAL:HG22	2.03	0.41
1:B:334:VAL:HG13	1:B:372:GLN:OE1	2.21	0.41
1:D:259:ARG:NH2	2:D:450:HAM:O1P	2.54	0.41
1:B:298:ARG:HD2	1:B:299:ALA:N	2.36	0.41
1:C:67:MET:HE2	1:C:79:THR:CG2	2.50	0.41
1:D:112:PHE:N	1:D:112:PHE:CD1	2.89	0.41
1:A:331:ILE:O	1:A:360:LEU:HA	2.21	0.41
1:C:382:ARG:O	1:C:402:LEU:HB2	2.20	0.41
1:D:165:LEU:HD11	1:D:244:LEU:CD1	2.50	0.41
1:B:140:ILE:HD12	1:B:143:GLU:HB3	2.03	0.41
1:B:298:ARG:NH1	1:B:299:ALA:O	2.54	0.41
1:B:278:SER:HA	1:B:311:ARG:CD	2.42	0.41
1:B:118:GLN:HG2	1:B:121:ARG:HB2	2.03	0.41
1:B:118:GLN:HE22	1:B:121:ARG:HG3	1.85	0.41
1:B:9:ARG:HE	1:B:123:ARG:NH2	2.19	0.41
1:B:42:ARG:HA	3:B:597:HOH:O	2.20	0.41
1:A:113:ARG:O	1:A:123:ARG:HA	2.21	0.41
1:C:331:ILE:HD11	1:C:423:LEU:HD11	2.03	0.41
1:A:70:PHE:HE1	1:A:80:LEU:CD1	2.34	0.41
1:D:332:TYR:HE1	1:D:361:MET:HE2	1.85	0.41
1:B:133:PHE:HD1	1:B:302:ALA:HB2	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:10:GLY:HA3	1:D:123:ARG:HG3	2.02	0.41
1:B:383:VAL:HG12	1:B:384:ALA:N	2.36	0.41
1:B:295:LEU:HD23	1:B:295:LEU:HA	1.85	0.40
1:A:141:ASP:HB2	1:A:240:LEU:HD13	2.03	0.40
1:A:168:ILE:HG12	1:A:265:ASN:O	2.21	0.40
1:B:298:ARG:HH11	1:B:298:ARG:CG	2.24	0.40
1:C:38:TYR:HD1	1:C:38:TYR:N	2.19	0.40
1:C:161:VAL:HA	1:C:272:VAL:O	2.20	0.40
1:B:422:LEU:HA	1:B:422:LEU:HD23	1.90	0.40
1:B:340:THR:O	1:B:343:ALA:HB3	2.21	0.40
1:B:19:THR:O	1:B:23:GLN:HG3	2.21	0.40
1:A:162:THR:HG22	1:A:163:LEU:N	2.36	0.40
1:B:351:LEU:HD21	1:B:415:VAL:HG23	2.03	0.40
1:C:152:TRP:HB3	1:C:158:SER:HA	2.03	0.40
1:B:100:ASN:ND2	1:B:100:ASN:O	2.54	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	382/424 (90%)	360 (94%)	16 (4%)	6 (2%)	14	28
1	B	360/424 (85%)	340 (94%)	17 (5%)	3 (1%)	27	53
1	C	383/424 (90%)	358 (94%)	23 (6%)	2 (0%)	38	67
1	D	358/424 (84%)	342 (96%)	14 (4%)	2 (1%)	33	63
All	All	1483/1696 (87%)	1400 (94%)	70 (5%)	13 (1%)	25	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	PRO
1	A	137	GLY
1	B	137	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	137	GLY
1	A	266	ARG
1	D	137	GLY
1	A	187	GLN
1	A	288	TYR
1	B	166	ASN
1	B	266	ARG
1	D	266	ARG
1	A	320	ASN
1	C	59	VAL

### 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	304/342 (89%)	275 (90%)	29 (10%)	12	23
1	B	289/342 (84%)	259 (90%)	30 (10%)	10	18
1	C	306/342 (90%)	274 (90%)	32 (10%)	10	18
1	D	288/342 (84%)	260 (90%)	28 (10%)	12	22
All	All	1187/1368 (87%)	1068 (90%)	119 (10%)	11	20

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	31	ASN
1	A	54	ARG
1	A	65	LYS
1	A	74	ASN
1	A	83	GLU
1	A	90	ARG
1	A	128	LEU
1	A	139	ASP
1	A	141	ASP
1	A	155	LEU
1	A	158	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	LEU
1	A	184	PHE
1	A	243	LEU
1	A	252	THR
1	A	257	LEU
1	A	261	LEU
1	A	268	VAL
1	A	276	LEU
1	A	281	THR
1	A	287	ARG
1	A	295	LEU
1	A	303	VAL
1	A	342	SER
1	A	389	GLU
1	A	390	SER
1	A	415	VAL
1	A	420	ARG
1	B	3	LYS
1	B	9	ARG
1	B	11	MET
1	B	24	ARG
1	B	65	LYS
1	B	83	GLU
1	B	100	ASN
1	B	104	ARG
1	B	116	ARG
1	B	118	GLN
1	B	130	CYS
1	B	135	LEU
1	B	158	SER
1	B	159	GLU
1	B	166	ASN
1	B	231	GLU
1	B	256	ARG
1	B	263	TYR
1	B	266	ARG
1	B	275	SER
1	B	281	THR
1	B	293	GLU
1	B	298	ARG
1	B	310	GLU
1	B	333	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	339	ASP
1	B	387	LEU
1	B	389	GLU
1	B	390	SER
1	B	408	THR
1	C	24	ARG
1	C	39	SER
1	C	54	ARG
1	C	74	ASN
1	C	83	GLU
1	C	141	ASP
1	C	145	ILE
1	C	161	VAL
1	C	162	THR
1	C	168	ILE
1	C	171	LEU
1	C	225	LEU
1	C	240	LEU
1	C	242	LYS
1	C	244	LEU
1	C	255	GLN
1	C	256	ARG
1	C	257	LEU
1	C	263	TYR
1	C	266	ARG
1	C	274	ASN
1	C	281	THR
1	C	294	GLN
1	C	298	ARG
1	C	303	VAL
1	C	320	ASN
1	C	329	VAL
1	C	363	ASN
1	C	370	LYS
1	C	371	LYS
1	C	390	SER
1	C	403	ARG
1	D	4	ASN
1	D	16	PRO
1	D	18	GLU
1	D	51	LEU
1	D	54	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	65	LYS
1	D	78	LEU
1	D	80	LEU
1	D	90	ARG
1	D	105	LEU
1	D	116	ARG
1	D	123	ARG
1	D	146	MET
1	D	231	GLU
1	D	235	GLU
1	D	242	LYS
1	D	259	ARG
1	D	263	TYR
1	D	275	SER
1	D	300	THR
1	D	303	VAL
1	D	309	LEU
1	D	324	LYS
1	D	350	ARG
1	D	382	ARG
1	D	387	LEU
1	D	390	SER
1	D	408	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	12	ASN
1	A	23	GLN
1	A	74	ASN
1	A	160	HIS
1	A	236	HIS
1	A	255	GLN
1	A	274	ASN
1	A	364	HIS
1	A	407	GLN
1	B	23	GLN
1	B	166	ASN
1	B	341	GLN
1	B	418	HIS
1	C	48	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	74	ASN
1	C	100	ASN
1	C	160	HIS
1	C	274	ASN
1	D	114	HIS
1	D	124	GLN
1	D	136	GLN
1	D	236	HIS
1	D	364	HIS

### 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	HAM	A	450	-	36,36,36	1.31	4 (11%)	53,53,53	1.79	6 (11%)
2	HAM	B	450	-	36,36,36	1.54	4 (11%)	53,53,53	1.36	5 (9%)
2	HAM	C	450	-	36,36,36	1.40	3 (8%)	53,53,53	1.68	5 (9%)
2	HAM	D	450	-	36,36,36	1.34	4 (11%)	53,53,53	1.25	3 (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	HAM	A	450	-	-	0/21/39/39	0/2/4/4
2	HAM	B	450	-	-	0/21/39/39	0/2/4/4
2	HAM	C	450	-	-	0/21/39/39	0/2/4/4
2	HAM	D	450	-	-	0/21/39/39	0/2/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	HAM	CA-C	5.67	1.59	1.52
2	C	450	HAM	P-O3P	5.15	1.70	1.61
2	B	450	HAM	P-O3P	4.88	1.69	1.61
2	A	450	HAM	P-O3P	4.45	1.68	1.61
2	C	450	HAM	CA-C	4.44	1.58	1.52
2	D	450	HAM	CA-C	4.35	1.58	1.52
2	A	450	HAM	CA-C	4.00	1.57	1.52
2	D	450	HAM	P-O3P	3.70	1.67	1.61
2	D	450	HAM	O3P-C	-3.66	1.32	1.37
2	B	450	HAM	O3P-C	-3.03	1.33	1.37
2	B	450	HAM	CD2-NE2	2.52	1.40	1.36
2	D	450	HAM	CD2-NE2	2.26	1.40	1.36
2	C	450	HAM	O3P-C	-2.24	1.34	1.37
2	A	450	HAM	O-C	2.20	1.26	1.21
2	A	450	HAM	O3P-C	-2.15	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	HAM	O3P-C-O	9.65	129.75	122.11
2	C	450	HAM	O3P-C-O	8.75	129.04	122.11
2	D	450	HAM	O3P-C-O	5.36	126.35	122.11
2	B	450	HAM	O3P-C-O	4.83	125.93	122.11
2	C	450	HAM	O-C-CA	-4.51	108.59	121.64
2	A	450	HAM	O-C-CA	-4.26	109.31	121.64
2	B	450	HAM	O-C-CA	-4.25	109.33	121.64
2	B	450	HAM	O3P-C-CA	4.22	124.57	113.90
2	D	450	HAM	O-C-CA	-3.86	110.46	121.64
2	D	450	HAM	O3P-C-CA	3.59	122.98	113.90
2	C	450	HAM	O3P-C-CA	3.27	122.18	113.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	HAM	C-CA-N	3.13	112.71	108.53
2	C	450	HAM	O3P-P-O5'	3.10	109.19	101.80
2	A	450	HAM	O3P-P-O5'	3.10	109.17	101.80
2	A	450	HAM	O3P-C-CA	2.78	120.92	113.90
2	B	450	HAM	O3P-P-O5'	2.49	107.73	101.80
2	C	450	HAM	C-CA-N	2.19	111.45	108.53
2	A	450	HAM	O2P-P-O3P	2.17	114.92	107.76
2	B	450	HAM	CB-CA-C	2.04	116.72	111.77

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	386/424 (91%)	-0.16	8 (2%) 60 58	19, 43, 78, 94	0
1	B	364/424 (85%)	-0.17	8 (2%) 59 56	20, 45, 81, 108	0
1	C	387/424 (91%)	-0.15	7 (1%) 65 64	19, 45, 77, 98	0
1	D	362/424 (85%)	-0.12	3 (0%) 83 85	20, 44, 81, 107	0
All	All	1499/1696 (88%)	-0.15	26 (1%) 67 66	19, 44, 80, 108	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	3.7
1	C	338	ALA	3.4
1	C	424	GLY	3.3
1	A	278	SER	3.0
1	D	277	GLY	2.9
1	B	235	GLU	2.9
1	D	424	GLY	2.8
1	B	74	ASN	2.8
1	A	424	GLY	2.7
1	C	278	SER	2.7
1	B	279	GLN	2.6
1	A	60	THR	2.6
1	C	321	PRO	2.5
1	A	322	GLU	2.5
1	B	424	GLY	2.4
1	C	277	GLY	2.4
1	A	277	GLY	2.3
1	C	371	LYS	2.3
1	D	121	ARG	2.3
1	B	338	ALA	2.2
1	A	404	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	256	ARG	2.2
1	C	256	ARG	2.1
1	B	116	ARG	2.1
1	B	322	GLU	2.1
1	B	61	ASP	2.0

## 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
2	HAM	C	450	33/33	0.15	0.70	0,31,35,37	0
2	HAM	A	450	33/33	0.16	0.66	0,28,35,37	0
2	HAM	D	450	33/33	0.18	0.34	0,49,54,54	0
2	HAM	B	450	33/33	0.17	0.27	0,42,49,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.