



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 09:09 am GMT

PDB ID : 1EFK  
Title : STRUCTURE OF HUMAN MALIC ENZYME IN COMPLEX WITH KETOMALONATE  
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.  
Deposited on : 2000-02-09  
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

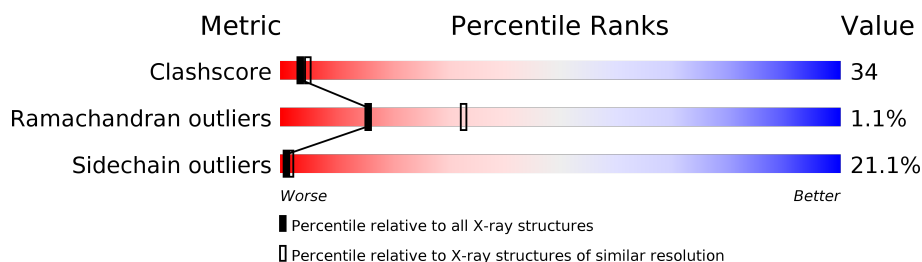
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	122078	3109 (2.60-2.60)
Ramachandran outliers	120005	3061 (2.60-2.60)
Sidechain outliers	119972	3061 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	
1	C	584	
1	D	584	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17931 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	177	MSE	MET	MODIFIED RESIDUE	UNP P23368

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

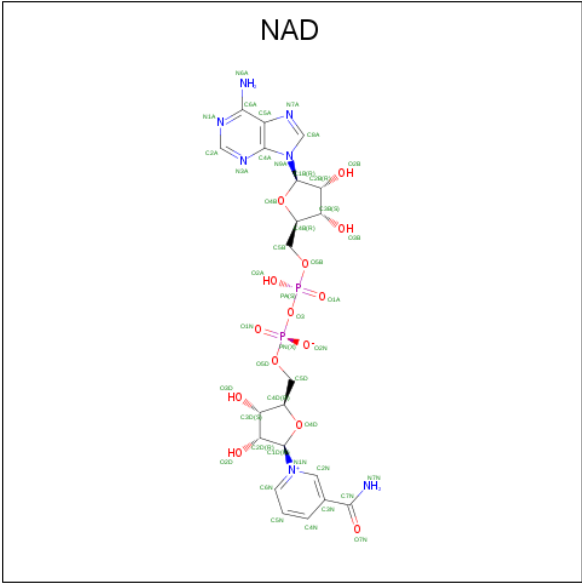
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

*Continued on next page...*

Continued from previous page...

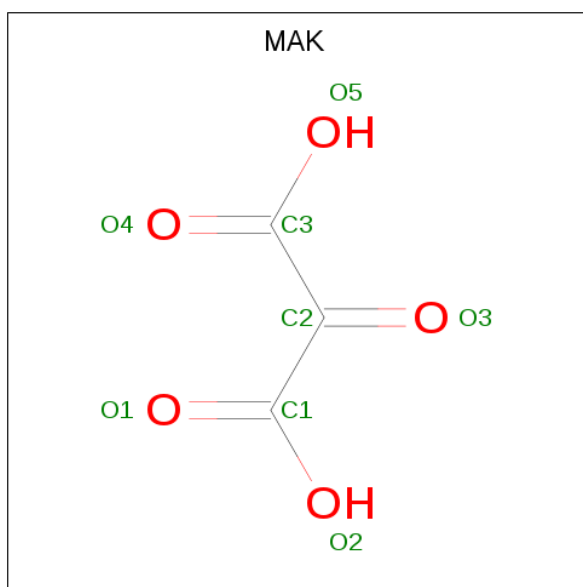
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	D	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
3	A	1	44	21	7	14	2	9	0
3	B	1	44	21	7	14	2	0	0
3	B	1	44	21	7	14	2	9	0
3	C	1	44	21	7	14	2	0	0
3	C	1	44	21	7	14	2	9	0
3	D	1	44	21	7	14	2	0	0
3	D	1	44	21	7	14	2	9	0

- Molecule 4 is ALPHA-KETOMALONIC ACID (three-letter code: MAK) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	3	5		
4	B	1	Total	C	O	0	0
			8	3	5		
4	C	1	Total	C	O	0	0
			8	3	5		
4	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 5 is water.

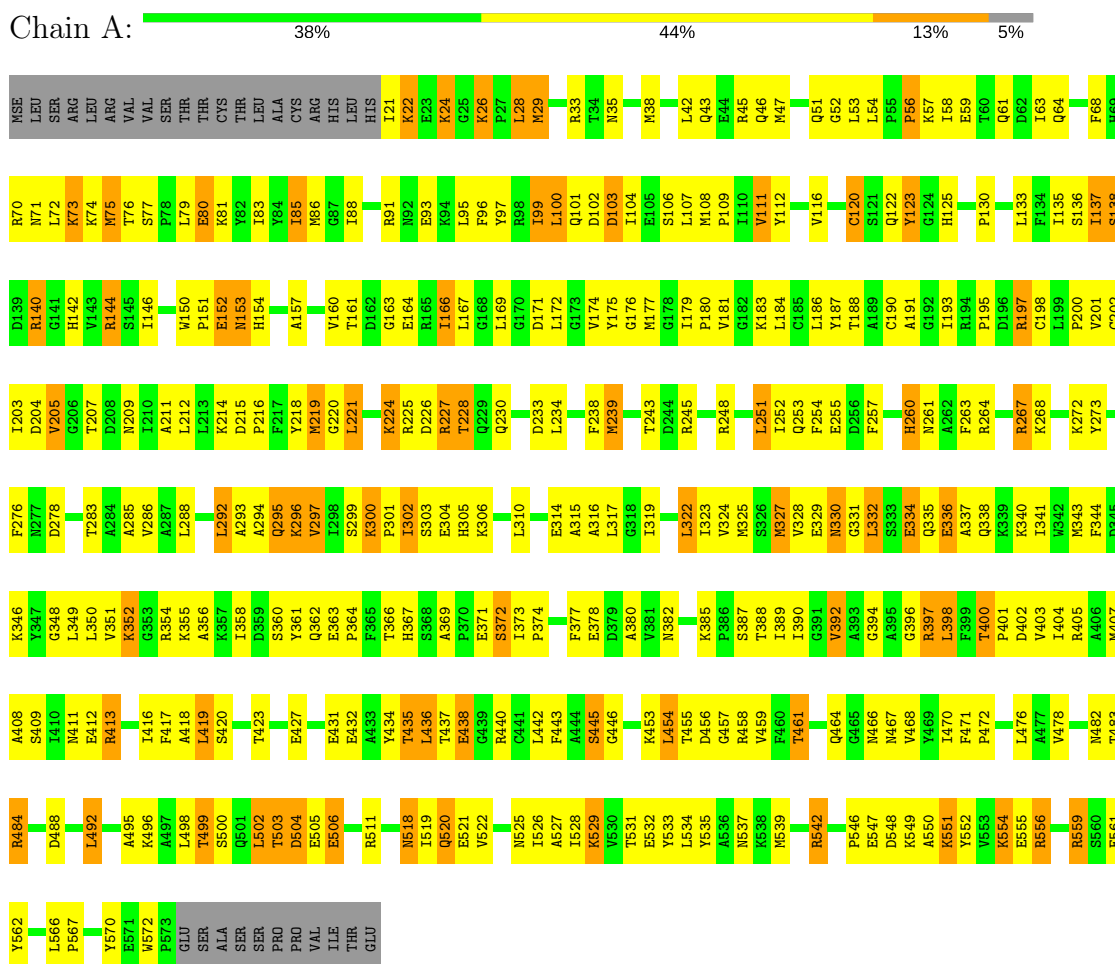
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	18	Total	O	0	0
			18	18		
5	C	16	Total	O	0	0
			16	16		
5	D	16	Total	O	0	0
			16	16		

### 3 Residue-property plots

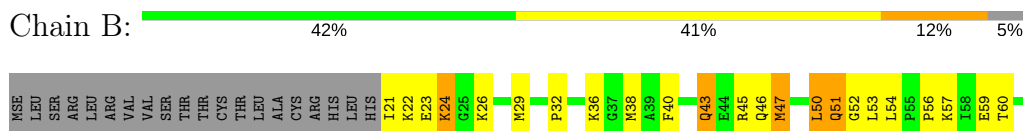
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

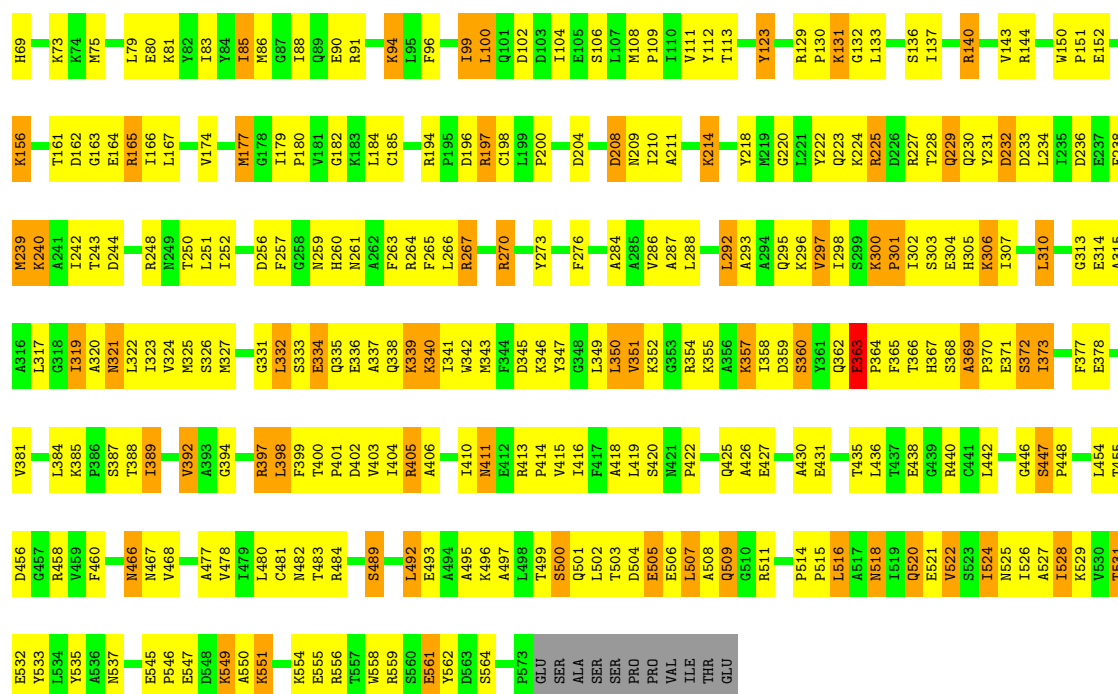
Note EDS was not executed.

#### • Molecule 1: MALIC ENZYME



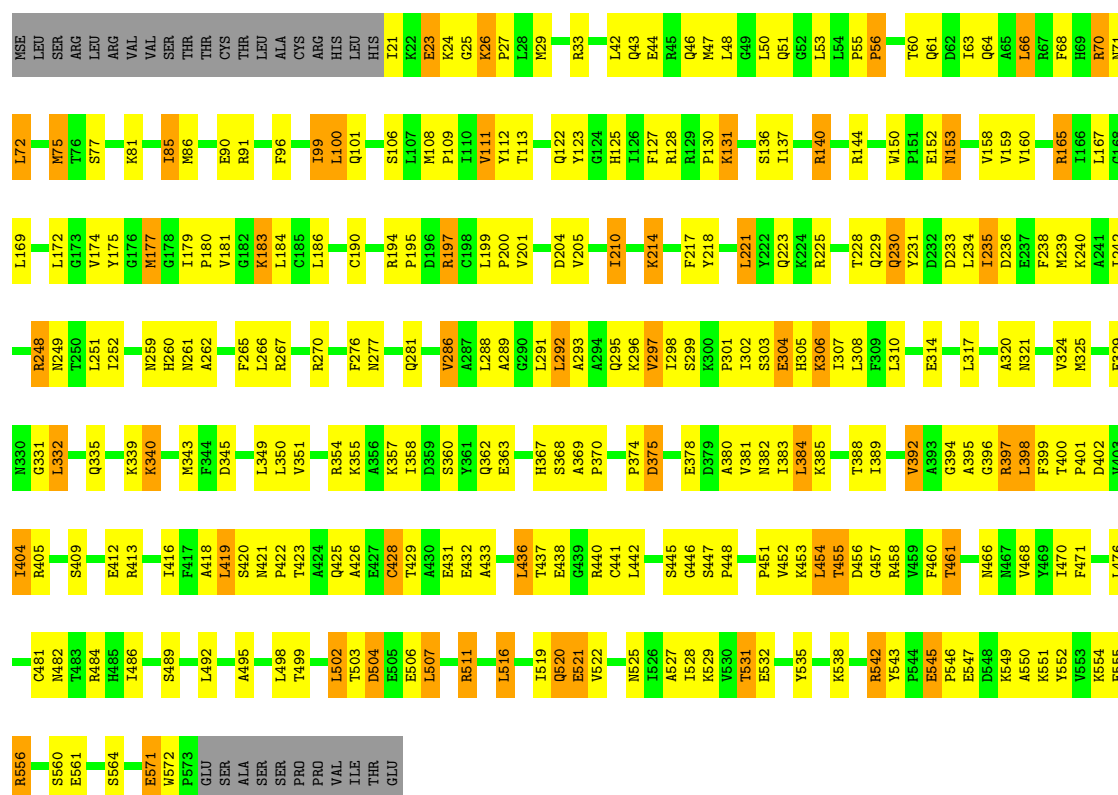
#### • Molecule 1: MALIC ENZYME





### • Molecule 1: MALIC ENZYME

Chain C: 47% 38% 9% 5%



### • Molecule 1: MALIC ENZYME

Chain D: 41% 39% 14% 5%





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.60Å 118.60Å 113.10Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (20.00-2.60)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.218 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 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: MG, MAK, NAD

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	0.44	0/4447	0.64	0/5998
1	B	0.45	0/4447	0.64	0/5998
1	C	0.46	0/4447	0.65	0/5998
1	D	0.45	1/4447 (0.0%)	0.64	0/5998
All	All	0.45	1/17788 (0.0%)	0.64	0/23992

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	CYS	CB-SG	-5.57	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4407	359	0
1	B	4367	0	4407	313	0
1	C	4367	0	4407	217	0
1	D	4367	0	4407	334	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	52	4	0
3	B	88	0	52	5	0
3	C	88	0	52	3	0
3	D	88	0	52	3	0
4	A	8	0	0	1	0
4	B	8	0	0	1	0
4	C	8	0	0	1	0
4	D	8	0	0	2	0
5	A	25	0	0	4	0
5	B	18	0	0	4	0
5	C	16	0	0	3	0
5	D	16	0	0	1	0
All	All	17931	0	17836	1198	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 34.

All (1198) 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:C:210:ILE:H	1:C:210:ILE:HD13	1.00	1.10
1:D:140:ARG:HH22	1:D:233:ASP:HB3	1.15	1.09
1:D:177:MSE:HE1	1:D:181:VAL:HG23	1.34	1.06
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.38	1.06
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.21	1.06
1:D:300:LYS:HE3	1:D:304:GLU:HB2	1.37	1.03
1:D:302:ILE:HG12	1:D:332:LEU:HD11	1.41	1.00
1:C:210:ILE:CD1	1:C:210:ILE:H	1.73	0.96
1:C:378:GLU:O	1:C:381:VAL:HG12	1.65	0.96
1:B:354:ARG:NE	1:B:358:ILE:HD11	1.81	0.96
1:A:86:MSE:HE1	1:A:111:VAL:HG23	1.48	0.95
1:A:492:LEU:HD22	1:A:496:LYS:HE3	1.49	0.94
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.32	0.94
1:B:339:LYS:HA	1:B:367:HIS:CE1	2.03	0.94
1:D:123:TYR:HD2	1:D:219:MSE:HE1	1.32	0.93
1:B:351:VAL:HG11	1:B:369:ALA:HA	1.50	0.93
1:D:374:PRO:HG3	1:D:383:ILE:HG13	1.49	0.92
1:C:454:LEU:HD11	1:C:460:PHE:HE2	1.32	0.91
1:D:137:ILE:HD12	1:D:205:VAL:HG12	1.51	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HD13	1:C:210:ILE:N	1.86	0.91
1:D:327:MSE:HG2	1:D:332:LEU:HD22	1.49	0.91
1:A:137:ILE:HB	1:A:205:VAL:HG12	1.53	0.90
1:D:261:ASN:HD22	1:D:264:ARG:NH2	1.68	0.90
1:D:527:ALA:O	1:D:531:THR:HG22	1.72	0.90
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.38	0.89
1:D:371:GLU:CD	1:D:371:GLU:H	1.73	0.89
1:B:29:MSE:HE2	1:B:50:LEU:HD22	1.56	0.88
1:B:266:LEU:O	1:B:270:ARG:HG2	1.74	0.87
1:C:527:ALA:O	1:C:531:THR:HG22	1.72	0.87
1:A:389:ILE:HB	1:A:407:MSE:HE2	1.57	0.87
1:C:81:LYS:O	1:C:85:ILE:HG23	1.74	0.87
1:A:261:ASN:ND2	1:A:264:ARG:HH21	1.72	0.86
1:B:339:LYS:HA	1:B:367:HIS:HE1	1.42	0.85
1:D:379:ASP:O	1:D:383:ILE:HG12	1.75	0.85
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.56	0.85
1:D:85:ILE:HD11	1:D:111:VAL:HG12	1.58	0.85
1:C:453:LYS:HE3	1:C:457:GLY:HA2	1.58	0.85
1:D:332:LEU:HD23	1:D:340:LYS:HE3	1.58	0.85
1:A:220:GLY:HA2	1:B:56:PRO:HG2	1.59	0.84
1:A:211:ALA:O	1:A:214:LYS:HG2	1.76	0.84
1:A:377:PHE:HE2	1:A:389:ILE:HD11	1.42	0.84
1:D:140:ARG:NH2	1:D:233:ASP:HB3	1.92	0.84
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.57	0.84
1:C:520:GLN:H	1:C:520:GLN:HE21	1.24	0.84
1:B:520:GLN:HE21	1:B:520:GLN:H	1.23	0.84
1:D:72:LEU:HD12	1:D:75:MSE:HE2	1.60	0.83
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.61	0.83
1:B:506:GLU:OE2	1:B:515:PRO:HD3	1.78	0.82
1:D:261:ASN:HD22	1:D:264:ARG:HH22	1.25	0.82
1:B:527:ALA:O	1:B:531:THR:HG23	1.80	0.82
1:C:23:GLU:OE1	1:C:23:GLU:HA	1.80	0.82
1:C:239:MSE:HE1	1:C:252:ILE:HD13	1.62	0.82
1:B:478:VAL:HG13	1:B:483:THR:HB	1.61	0.81
1:B:546:PRO:HG2	1:B:549:LYS:HD2	1.60	0.81
1:D:75:MSE:CE	1:D:81:LYS:HA	2.10	0.81
1:D:392:VAL:O	1:D:392:VAL:HG13	1.80	0.81
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.63	0.81
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.61	0.81
1:D:468:VAL:HA	1:D:471:PHE:CE2	2.15	0.80
1:C:397:ARG:HH21	1:C:426:ALA:HB3	1.46	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH2	1:A:233:ASP:HB3	1.95	0.80
1:B:371:GLU:H	1:B:371:GLU:CD	1.84	0.80
1:B:81:LYS:O	1:B:85:ILE:HG23	1.80	0.80
1:C:349:LEU:HD22	1:C:374:PRO:HG2	1.63	0.80
1:B:466:ASN:HB3	1:B:468:VAL:HG12	1.62	0.80
1:D:123:TYR:CD2	1:D:219:MSE:HE1	2.17	0.80
1:A:38:MSE:HE3	1:A:59:GLU:CD	2.02	0.80
1:D:437:THR:O	1:D:440:ARG:HG3	1.82	0.79
1:B:505:GLU:CD	1:B:505:GLU:H	1.85	0.79
1:D:324:VAL:O	1:D:328:VAL:HG23	1.83	0.79
1:B:528:ILE:O	1:B:532:GLU:HG3	1.81	0.79
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.45	0.79
1:B:51:GLN:HA	1:B:51:GLN:HE21	1.48	0.79
1:D:556:ARG:CG	1:D:556:ARG:HH11	1.96	0.78
1:D:177:MSE:CE	1:D:181:VAL:HG23	2.13	0.78
1:A:518:ASN:HA	1:A:520:GLN:OE1	1.84	0.78
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.48	0.78
1:B:208:ASP:O	1:B:210:ILE:HD12	1.83	0.77
1:B:377:PHE:O	1:B:381:VAL:HG23	1.84	0.77
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.46	0.77
1:B:342:TRP:CE3	1:B:349:LEU:HD21	2.19	0.77
1:C:140:ARG:HB2	1:C:140:ARG:NH1	2.00	0.77
1:D:261:ASN:ND2	1:D:264:ARG:NH2	2.33	0.77
1:B:229:GLN:NE2	1:B:232:ASP:HB2	1.99	0.77
1:C:422:PRO:HD2	1:C:425:GLN:NE2	2.00	0.77
1:B:79:LEU:O	1:B:83:ILE:HG13	1.84	0.77
1:D:377:PHE:HZ	1:D:389:ILE:HD11	1.49	0.77
1:A:43:GLN:HG2	1:A:566:LEU:HD11	1.67	0.76
1:D:548:ASP:OD2	1:D:551:LYS:HB2	1.85	0.76
1:A:260:HIS:O	1:A:264:ARG:HB2	1.85	0.76
1:D:301:PRO:HB2	1:D:304:GLU:HG3	1.65	0.76
1:D:177:MSE:HG2	1:D:202:CYS:HB2	1.67	0.76
1:D:302:ILE:CG1	1:D:332:LEU:HD11	2.14	0.76
1:C:454:LEU:HD11	1:C:460:PHE:CE2	2.18	0.76
1:B:239:MSE:HE1	1:B:252:ILE:HD13	1.68	0.75
1:A:85:ILE:HG12	1:A:86:MSE:HE2	1.68	0.75
1:A:552:TYR:HE1	1:A:556:ARG:NH2	1.85	0.74
1:C:433:ALA:O	1:C:437:THR:HG23	1.87	0.74
1:D:60:THR:O	1:D:63:ILE:HG22	1.87	0.74
1:A:535:TYR:OH	1:A:542:ARG:HB3	1.87	0.74
1:D:43:GLN:OE1	1:D:47:MSE:HE1	1.87	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:PRO:HD2	1:B:425:GLN:HE21	1.53	0.74
1:D:175:TYR:CE2	1:D:218:TYR:HA	2.21	0.74
1:D:397:ARG:NH2	1:D:426:ALA:HB3	2.03	0.74
1:D:294:ALA:O	1:D:297:VAL:HG22	1.88	0.74
1:B:229:GLN:HE21	1:B:229:GLN:HA	1.53	0.73
1:C:395:ALA:HB3	1:C:398:LEU:HD21	1.71	0.73
1:D:538:LYS:HZ3	1:D:538:LYS:H	1.34	0.73
1:B:305:HIS:O	1:B:340:LYS:HD3	1.89	0.73
1:B:505:GLU:N	1:B:505:GLU:CD	2.40	0.73
1:D:400:THR:OG1	1:D:403:VAL:HG23	1.89	0.73
1:D:75:MSE:HE3	1:D:81:LYS:HA	1.70	0.73
1:A:56:PRO:HG2	1:B:220:GLY:HA2	1.69	0.73
1:C:60:THR:OG1	1:C:63:ILE:HG13	1.88	0.73
1:D:377:PHE:CZ	1:D:389:ILE:HD11	2.23	0.73
1:A:392:VAL:O	1:A:392:VAL:HG13	1.88	0.72
1:B:334:GLU:O	1:B:338:GLN:HG3	1.89	0.72
1:A:525:ASN:O	1:A:529:LYS:HG2	1.89	0.72
1:B:177:MSE:O	1:B:180:PRO:HD2	1.89	0.72
1:A:520:GLN:NE2	1:A:521:GLU:N	2.37	0.72
1:B:351:VAL:CG1	1:B:369:ALA:HA	2.19	0.72
1:B:349:LEU:HD11	1:B:384:LEU:HD11	1.71	0.72
1:A:495:ALA:O	1:A:499:THR:HG22	1.89	0.72
1:D:556:ARG:HG2	1:D:556:ARG:HH11	1.52	0.72
1:B:29:MSE:HE2	1:B:50:LEU:CD2	2.19	0.72
1:C:248:ARG:HG3	1:C:248:ARG:HH11	1.54	0.72
1:A:52:GLY:O	1:B:133:LEU:HD23	1.89	0.72
1:B:334:GLU:HG3	1:B:338:GLN:NE2	2.04	0.72
1:B:446:GLY:O	1:B:466:ASN:ND2	2.23	0.72
1:D:249:ASN:C	1:D:249:ASN:HD22	1.92	0.72
1:C:378:GLU:OE1	1:C:402:ASP:HB3	1.90	0.72
1:A:225:ARG:HB2	5:A:4041:HOH:O	1.90	0.71
1:A:227:ARG:NH1	1:A:227:ARG:HG2	2.03	0.71
1:B:287:ALA:HB3	1:B:319:ILE:HG21	1.72	0.71
1:B:298:ILE:CG2	1:B:300:LYS:HB2	2.21	0.71
1:A:164:GLU:HG3	1:A:225:ARG:CZ	2.20	0.71
1:B:358:ILE:HG12	1:B:366:THR:HG21	1.72	0.71
1:D:94:LYS:HE3	1:D:558:TRP:CZ2	2.25	0.71
1:A:164:GLU:HG3	1:A:225:ARG:NE	2.05	0.71
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.73	0.71
1:C:382:ASN:O	1:C:385:LYS:HD2	1.91	0.71
1:C:542:ARG:HD2	1:C:552:TYR:OH	1.91	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASN:ND2	1:D:153:ASN:H	1.87	0.71
1:A:369:ALA:HB1	1:A:373:ILE:HD11	1.72	0.71
1:A:319:ILE:O	1:A:323:ILE:HG13	1.90	0.70
1:A:343:MSE:HB2	1:A:350:LEU:HD12	1.71	0.70
1:A:33:ARG:HD3	1:A:93:GLU:OE2	1.92	0.70
1:B:307:ILE:HD13	1:B:323:ILE:HD13	1.73	0.70
1:B:406:ALA:O	1:B:410:ILE:HD12	1.92	0.70
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.21	0.70
1:A:431:GLU:O	1:A:435:THR:OG1	2.09	0.70
1:B:137:ILE:O	1:B:140:ARG:HG2	1.91	0.70
1:B:401:PRO:HB2	1:B:405:ARG:HH21	1.56	0.70
1:C:47:MSE:O	1:C:48:LEU:HD23	1.91	0.70
1:D:137:ILE:HB	1:D:205:VAL:HG12	1.73	0.70
1:C:451:PRO:HG3	1:C:461:THR:HG23	1.73	0.70
1:A:138:SER:OG	1:A:221:LEU:HD21	1.92	0.70
1:A:86:MSE:CE	1:A:111:VAL:HG23	2.21	0.70
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.38	0.69
1:A:315:ALA:O	1:A:319:ILE:HD12	1.93	0.69
1:D:288:LEU:HG	1:D:292:LEU:HD22	1.73	0.69
1:B:397:ARG:HH21	1:B:426:ALA:HB3	1.58	0.69
1:B:489:SER:HB2	1:B:533:TYR:OH	1.91	0.69
1:A:144:ARG:NH2	1:A:245:ARG:HB2	2.08	0.69
1:A:295:GLN:HE22	1:A:300:LYS:N	1.91	0.69
1:B:315:ALA:O	1:B:319:ILE:HG13	1.91	0.69
1:C:235:ILE:HD13	1:C:265:PHE:CZ	2.28	0.69
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.73	0.69
1:B:267:ARG:HB2	5:B:4022:HOH:O	1.91	0.69
1:B:295:GLN:HA	1:B:295:GLN:OE1	1.93	0.69
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.21	0.68
1:B:518:ASN:O	1:B:522:VAL:HG23	1.93	0.68
1:A:81:LYS:O	1:A:85:ILE:HG23	1.94	0.68
1:B:397:ARG:NH2	1:B:426:ALA:HB3	2.08	0.68
1:D:68:PHE:CD2	1:D:99:ILE:HG13	2.28	0.68
1:D:401:PRO:HB3	1:D:436:LEU:HD21	1.74	0.68
1:D:381:VAL:HG21	1:D:403:VAL:HG13	1.75	0.68
1:A:334:GLU:O	1:A:338:GLN:HG3	1.94	0.68
1:C:454:LEU:HD12	1:C:458:ARG:HB2	1.75	0.68
1:B:108:MSE:CE	1:B:516:LEU:HD11	2.24	0.68
1:B:522:VAL:O	1:B:526:ILE:HG13	1.92	0.68
1:C:429:THR:OG1	1:C:432:GLU:HG3	1.93	0.68
1:B:422:PRO:HD2	1:B:425:GLN:NE2	2.09	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:TYR:CE2	1:C:545:GLU:HB2	2.29	0.68
1:D:194:ARG:HE	1:D:197:ARG:NH1	1.92	0.67
1:D:85:ILE:HD11	1:D:111:VAL:CG1	2.24	0.67
1:B:96:PHE:O	1:B:100:LEU:HD13	1.94	0.67
1:B:392:VAL:HG22	1:B:392:VAL:O	1.95	0.67
1:B:342:TRP:HE3	1:B:349:LEU:HD21	1.56	0.67
1:D:327:MSE:HE3	1:D:337:ALA:CB	2.24	0.67
1:A:267:ARG:NH1	1:A:361:TYR:OH	2.27	0.67
1:A:300:LYS:HZ3	1:A:304:GLU:HB2	1.59	0.67
1:A:350:LEU:HD22	1:A:358:ILE:HD11	1.77	0.67
1:C:528:ILE:HD13	1:C:550:ALA:HA	1.75	0.67
1:A:186:LEU:O	1:A:190:CYS:HB2	1.94	0.67
1:D:397:ARG:NH2	1:D:423:THR:O	2.27	0.67
1:A:492:LEU:O	1:A:496:LYS:HG3	1.95	0.67
1:D:556:ARG:HG2	1:D:556:ARG:NH1	2.09	0.67
1:A:389:ILE:HG22	1:A:416:ILE:HA	1.77	0.67
1:B:492:LEU:O	1:B:496:LYS:HG3	1.94	0.67
1:B:527:ALA:O	1:B:531:THR:CG2	2.43	0.67
1:C:325:MSE:O	1:C:329:GLU:HG3	1.95	0.67
1:A:140:ARG:NH2	1:A:230:GLN:HA	2.10	0.67
1:B:349:LEU:HD23	1:B:350:LEU:N	2.10	0.67
1:B:400:THR:OG1	1:B:403:VAL:HG23	1.95	0.67
1:D:535:TYR:O	1:D:538:LYS:NZ	2.28	0.66
1:A:432:GLU:O	1:A:436:LEU:HB2	1.94	0.66
1:A:226:ASP:OD1	1:A:228:THR:HG23	1.95	0.66
1:A:64:GLN:NE2	1:A:562:TYR:OH	2.25	0.66
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.77	0.66
1:B:239:MSE:HE1	1:B:252:ILE:CD1	2.25	0.66
1:A:520:GLN:NE2	1:A:521:GLU:H	1.91	0.66
1:C:546:PRO:HG2	1:C:549:LYS:HD3	1.77	0.66
1:A:288:LEU:HD23	1:A:322:LEU:HD23	1.78	0.66
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.59	0.66
1:D:22:LYS:O	1:D:22:LYS:HD3	1.96	0.66
1:D:75:MSE:HE1	1:D:81:LYS:HA	1.78	0.66
1:A:123:TYR:CD2	1:A:219:MSE:HE1	2.29	0.66
1:B:297:VAL:HG22	1:B:298:ILE:HD12	1.78	0.66
1:D:298:ILE:CG2	1:D:300:LYS:HB2	2.25	0.66
1:B:414:PRO:O	1:B:442:LEU:HD12	1.96	0.66
1:B:298:ILE:HG22	1:B:300:LYS:N	2.11	0.65
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.31	0.65
1:D:177:MSE:O	1:D:177:MSE:HE3	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:ARG:HG3	1:D:561:GLU:OE1	1.97	0.65
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.11	0.65
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.09	0.65
1:A:144:ARG:NH2	1:A:245:ARG:HG3	2.11	0.65
1:C:131:LYS:O	1:C:177:MSE:HE3	1.96	0.65
1:B:331:GLY:O	1:B:332:LEU:O	2.15	0.65
1:B:346:LYS:HG2	3:B:1601:NAD:O2B	1.97	0.64
1:B:301:PRO:HG2	1:B:304:GLU:HG3	1.79	0.64
1:D:266:LEU:HD12	1:D:280:ILE:HD12	1.78	0.64
1:A:467:ASN:O	1:A:471:PHE:HD2	1.81	0.64
1:D:363:GLU:HB3	1:D:364:PRO:HD3	1.79	0.64
1:C:317:LEU:HD23	1:C:343:MSE:HE1	1.79	0.64
1:B:261:ASN:ND2	1:B:264:ARG:NH2	2.46	0.64
1:C:331:GLY:O	1:C:332:LEU:O	2.15	0.64
1:A:550:ALA:O	1:A:554:LYS:HG2	1.98	0.64
1:B:29:MSE:HE1	1:B:53:LEU:CD1	2.28	0.64
1:C:546:PRO:O	1:C:549:LYS:NZ	2.31	0.64
1:A:552:TYR:CE1	1:A:556:ARG:NH2	2.65	0.64
1:B:505:GLU:N	1:B:505:GLU:OE2	2.31	0.64
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.81	0.63
1:D:342:TRP:CZ3	1:D:367:HIS:HB2	2.33	0.63
1:A:160:VAL:HG21	1:A:203:ILE:HD11	1.80	0.63
1:C:140:ARG:HH22	1:C:233:ASP:HB2	1.63	0.63
1:D:33:ARG:NH1	1:D:93:GLU:OE2	2.31	0.63
1:B:240:LYS:HE3	1:B:244:ASP:OD2	1.98	0.63
1:A:300:LYS:HZ1	1:A:304:GLU:C	2.02	0.63
1:B:112:TYR:CD2	1:B:113:THR:HG22	2.34	0.63
1:C:160:VAL:HG12	1:C:201:VAL:HB	1.80	0.63
1:A:21:ILE:HG22	1:A:21:ILE:O	1.98	0.63
1:A:404:ILE:HG22	1:A:437:THR:HG23	1.81	0.63
1:D:316:ALA:HB2	1:D:392:VAL:HG11	1.80	0.63
1:C:56:PRO:HB2	1:D:221:LEU:HD13	1.81	0.62
1:D:298:ILE:HG23	1:D:300:LYS:HB2	1.81	0.62
1:C:85:ILE:HD12	1:C:96:PHE:HE1	1.63	0.62
1:C:297:VAL:HG21	1:C:442:LEU:HD11	1.80	0.62
1:D:343:MSE:O	1:D:350:LEU:HD23	2.00	0.62
1:A:43:GLN:HG3	1:A:566:LEU:HD21	1.82	0.62
1:A:219:MSE:HG2	1:B:38:MSE:HE1	1.81	0.62
1:D:298:ILE:HD12	1:D:442:LEU:HD11	1.81	0.62
1:D:329:GLU:HG2	1:D:330:ASN:ND2	2.14	0.62
1:D:332:LEU:N	1:D:332:LEU:HD12	2.14	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:LEU:HD22	1:D:354:ARG:HH12	1.63	0.62
1:D:538:LYS:N	1:D:538:LYS:HZ3	1.97	0.62
1:D:537:ASN:C	1:D:538:LYS:HG2	2.20	0.61
1:A:177:MSE:HE3	1:A:180:PRO:HD2	1.82	0.61
1:B:238:PHE:CE1	1:B:242:ILE:HG13	2.36	0.61
1:B:288:LEU:HG	1:B:292:LEU:HD22	1.81	0.61
1:C:466:ASN:HB3	1:C:468:VAL:HG12	1.82	0.61
1:D:327:MSE:CE	1:D:337:ALA:HB1	2.28	0.61
1:D:81:LYS:O	1:D:85:ILE:HG23	1.99	0.61
1:D:432:GLU:O	1:D:436:LEU:HB2	2.00	0.61
1:D:555:GLU:HB3	1:D:556:ARG:NH1	2.15	0.61
1:A:324:VAL:HA	1:A:327:MSE:HE2	1.81	0.61
1:B:352:LYS:HE3	1:B:366:THR:O	2.00	0.61
1:D:538:LYS:N	1:D:538:LYS:NZ	2.48	0.61
1:B:370:PRO:HD2	1:B:373:ILE:HD12	1.81	0.61
1:B:496:LYS:O	1:B:500:SER:HB3	1.99	0.61
1:B:75:MSE:HG2	1:B:80:GLU:OE1	1.99	0.61
1:C:194:ARG:HB2	1:C:197:ARG:HG3	1.81	0.61
1:A:108:MSE:N	1:A:109:PRO:HD2	2.16	0.61
1:A:504:ASP:OD2	1:A:504:ASP:N	2.33	0.61
1:B:301:PRO:HG2	1:B:304:GLU:CD	2.21	0.61
1:B:64:GLN:NE2	1:B:562:TYR:OH	2.34	0.61
1:A:150:TRP:HE1	1:A:152:GLU:CD	2.03	0.61
1:D:137:ILE:CD1	1:D:205:VAL:HG12	2.29	0.61
1:D:538:LYS:NZ	1:D:538:LYS:H	1.99	0.61
1:B:301:PRO:HG2	1:B:304:GLU:CG	2.31	0.61
1:C:432:GLU:O	1:C:436:LEU:HB2	2.00	0.61
1:C:389:ILE:HG22	1:C:416:ILE:HA	1.82	0.61
1:D:23:GLU:O	1:D:28:LEU:HD21	2.01	0.61
1:A:332:LEU:H	1:A:332:LEU:HD12	1.66	0.60
1:A:548:ASP:OD2	1:A:551:LYS:HB2	2.00	0.60
1:B:239:MSE:HE3	1:B:239:MSE:HA	1.83	0.60
1:D:332:LEU:H	1:D:332:LEU:HD12	1.66	0.60
1:A:324:VAL:HA	1:A:327:MSE:CE	2.30	0.60
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.82	0.60
1:A:570:TYR:HE1	1:A:572:TRP:HE1	1.49	0.60
1:C:140:ARG:NH2	1:C:233:ASP:HB2	2.16	0.60
1:A:525:ASN:HA	1:A:528:ILE:HD12	1.82	0.60
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.15	0.60
1:D:137:ILE:HD12	1:D:205:VAL:CG1	2.29	0.60
1:D:174:VAL:HG12	1:D:219:MSE:HE2	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ARG:HD3	1:D:93:GLU:OE2	2.02	0.60
1:B:36:LYS:NZ	1:B:562:TYR:HB3	2.17	0.60
1:D:506:GLU:HG2	1:D:511:ARG:HD2	1.83	0.60
1:D:297:VAL:HG21	1:D:442:LEU:HD21	1.82	0.60
1:D:506:GLU:CB	1:D:511:ARG:HD2	2.32	0.60
1:B:108:MSE:HE2	1:B:516:LEU:HD11	1.84	0.59
1:C:551:LYS:O	1:C:555:GLU:HB2	2.01	0.59
1:D:153:ASN:H	1:D:153:ASN:HD22	1.48	0.59
1:D:36:LYS:HE3	1:D:562:TYR:HB3	1.84	0.59
1:D:89:GLN:HG2	1:D:131:LYS:HZ3	1.67	0.59
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.37	0.59
1:B:346:LYS:HB2	1:B:346:LYS:HZ3	1.66	0.59
1:B:480:LEU:HD22	1:B:556:ARG:HD3	1.85	0.59
1:D:59:GLU:HB3	1:D:63:ILE:HG21	1.83	0.59
1:B:315:ALA:HB3	1:B:392:VAL:HG21	1.82	0.59
1:A:472:PRO:HG2	5:A:4021:HOH:O	2.03	0.59
1:A:401:PRO:HA	1:A:404:ILE:HD12	1.83	0.59
1:B:310:LEU:HD21	1:B:398:LEU:HD23	1.84	0.59
1:B:29:MSE:HE1	1:B:53:LEU:HD12	1.85	0.59
1:D:261:ASN:ND2	1:D:264:ARG:HH21	2.01	0.59
1:A:144:ARG:NH2	1:A:245:ARG:CB	2.65	0.59
1:A:79:LEU:O	1:A:83:ILE:HG13	2.02	0.59
1:C:546:PRO:HG2	1:C:549:LYS:CD	2.32	0.59
1:B:400:THR:HB	1:B:401:PRO:HD2	1.83	0.59
1:C:140:ARG:NH2	1:C:230:GLN:O	2.34	0.59
1:C:286:VAL:HG11	1:C:466:ASN:O	2.03	0.59
1:A:47:MSE:SE	1:C:47:MSE:HE2	2.53	0.59
1:A:466:ASN:HB3	1:A:468:VAL:HG12	1.84	0.59
1:B:287:ALA:HB3	1:B:319:ILE:CG2	2.31	0.59
1:B:503:THR:HA	5:B:4040:HOH:O	2.01	0.59
1:B:60:THR:OG1	1:B:63:ILE:HG13	2.03	0.59
1:C:289:ALA:CB	1:C:498:LEU:HD23	2.33	0.59
1:C:85:ILE:HG13	1:C:86:MSE:N	2.17	0.59
1:D:186:LEU:HD13	1:D:468:VAL:HG23	1.85	0.59
1:C:43:GLN:O	1:C:47:MSE:HB2	2.02	0.58
1:D:412:GLU:HG3	1:D:413:ARG:HG2	1.85	0.58
1:D:286:VAL:HG11	1:D:466:ASN:O	2.03	0.58
1:A:316:ALA:HB2	1:A:392:VAL:HG11	1.85	0.58
1:B:307:ILE:HG23	1:B:388:THR:HB	1.85	0.58
1:C:305:HIS:O	1:C:340:LYS:HB3	2.03	0.58
1:D:374:PRO:HB3	1:D:379:ASP:HB2	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ILE:HG22	1:D:416:ILE:HA	1.84	0.58
1:B:136:SER:HA	1:B:204:ASP:O	2.04	0.58
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.85	0.58
1:D:331:GLY:O	1:D:332:LEU:O	2.21	0.58
1:C:42:LEU:O	1:C:46:GLN:HG3	2.03	0.58
1:D:175:TYR:HE2	1:D:218:TYR:HA	1.67	0.58
1:A:38:MSE:HE3	1:A:59:GLU:OE1	2.03	0.58
1:C:481:CYS:O	1:C:482:ASN:HB2	2.02	0.58
1:C:66:LEU:HD22	1:C:70:ARG:NH1	2.18	0.58
1:D:506:GLU:HB3	1:D:511:ARG:HD2	1.85	0.58
1:B:131:LYS:O	1:B:177:MSE:HE3	2.03	0.58
1:B:323:ILE:HG22	1:B:324:VAL:N	2.18	0.58
1:B:351:VAL:HG11	1:B:370:PRO:HD3	1.85	0.58
1:C:301:PRO:O	1:C:304:GLU:HG2	2.04	0.58
1:D:324:VAL:HA	1:D:327:MSE:HE2	1.86	0.58
1:D:392:VAL:O	1:D:392:VAL:CG1	2.52	0.58
1:A:154:HIS:O	1:A:197:ARG:HG3	2.04	0.58
1:A:239:MSE:HE1	1:A:254:PHE:HE1	1.68	0.58
1:C:33:ARG:HH21	1:C:152:GLU:HG3	1.69	0.58
1:D:502:LEU:CD1	1:D:507:LEU:HG	2.34	0.58
1:A:85:ILE:HA	1:A:88:ILE:HD12	1.86	0.58
1:B:363:GLU:HG2	1:B:364:PRO:N	2.19	0.58
1:B:418:ALA:HB1	1:B:427:GLU:HB2	1.85	0.58
1:D:551:LYS:O	1:D:555:GLU:HB2	2.04	0.58
1:A:332:LEU:HD23	1:A:340:LYS:NZ	2.19	0.58
1:D:41:THR:O	1:D:45:ARG:HG3	2.04	0.58
1:A:295:GLN:HE22	1:A:299:SER:CA	2.17	0.58
1:A:300:LYS:HZ2	1:A:300:LYS:HB3	1.68	0.58
1:B:260:HIS:CE1	1:B:264:ARG:NE	2.72	0.58
1:C:392:VAL:HG13	1:C:392:VAL:O	2.03	0.58
1:D:329:GLU:HG2	1:D:330:ASN:HD22	1.69	0.58
1:D:456:ASP:OD1	1:D:458:ARG:HG3	2.04	0.58
1:D:550:ALA:O	1:D:554:LYS:HG2	2.04	0.57
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.84	0.57
1:B:152:GLU:HG2	1:B:196:ASP:HB2	1.85	0.57
1:B:210:ILE:O	1:B:214:LYS:HG2	2.04	0.57
1:B:504:ASP:HB2	1:B:505:GLU:OE2	2.03	0.57
1:C:401:PRO:HB2	1:C:405:ARG:NH2	2.20	0.57
1:D:269:TYR:O	1:D:271:GLU:N	2.37	0.57
1:A:343:MSE:HE3	1:A:350:LEU:CD1	2.34	0.57
1:A:343:MSE:HE3	1:A:350:LEU:HD11	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HG	1:B:492:LEU:HD23	1.86	0.57
1:D:300:LYS:HE3	1:D:304:GLU:CB	2.24	0.57
1:A:325:MSE:HE1	1:A:488:ASP:HB2	1.85	0.57
1:D:316:ALA:HB2	1:D:392:VAL:CG1	2.35	0.57
1:A:166:ILE:HG13	1:A:172:LEU:HB2	1.86	0.57
1:A:503:THR:OG1	1:A:506:GLU:HG2	2.03	0.57
1:B:229:GLN:CA	1:B:229:GLN:HE21	2.18	0.57
1:D:191:ALA:HB3	1:D:193:ILE:HD12	1.87	0.57
1:A:295:GLN:NE2	1:A:299:SER:HA	2.19	0.57
1:B:358:ILE:HG23	1:B:362:GLN:HB2	1.86	0.57
1:C:504:ASP:HA	1:C:507:LEU:HB2	1.85	0.57
1:D:388:THR:HG23	1:D:415:VAL:HB	1.86	0.57
1:A:413:ARG:HH21	1:A:440:ARG:C	2.08	0.57
1:A:293:ALA:O	1:A:296:LYS:HB2	2.05	0.56
1:B:431:GLU:O	1:B:435:THR:HG23	2.04	0.56
1:D:165:ARG:NH2	4:D:3603:MAK:O1	2.38	0.56
1:A:157:ALA:HB1	1:A:187:TYR:HE2	1.71	0.56
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.87	0.56
1:A:392:VAL:CG1	1:A:392:VAL:O	2.52	0.56
1:B:456:ASP:OD2	1:B:458:ARG:NH1	2.38	0.56
1:D:431:GLU:HA	1:D:452:VAL:HG11	1.86	0.56
1:A:140:ARG:O	1:A:140:ARG:HG3	2.05	0.56
1:B:24:LYS:O	1:D:22:LYS:NZ	2.36	0.56
1:D:352:LYS:HG3	1:D:366:THR:HG22	1.86	0.56
1:B:229:GLN:HE21	1:B:232:ASP:HB2	1.69	0.56
1:D:153:ASN:ND2	1:D:153:ASN:N	2.50	0.56
1:D:471:PHE:CG	1:D:472:PRO:HD3	2.40	0.56
1:C:277:ASN:N	1:C:281:GLN:OE1	2.25	0.56
1:D:229:GLN:HG2	1:D:229:GLN:O	2.05	0.56
1:D:333:SER:HB3	1:D:336:GLU:HG3	1.87	0.56
1:D:363:GLU:C	1:D:363:GLU:OE1	2.43	0.56
1:B:430:ALA:HB3	5:B:4069:HOH:O	2.04	0.56
1:A:160:VAL:CG2	1:A:203:ILE:HD11	2.35	0.56
1:A:26:LYS:HG3	1:B:151:PRO:HG2	1.87	0.56
1:C:422:PRO:HD2	1:C:425:GLN:HE21	1.69	0.56
1:A:468:VAL:HA	1:A:471:PHE:HE2	1.71	0.56
1:B:306:LYS:NZ	1:B:384:LEU:O	2.38	0.56
1:B:86:MSE:CE	1:B:111:VAL:HG23	2.36	0.56
1:C:167:LEU:HD22	1:C:421:ASN:HB2	1.86	0.56
1:D:150:TRP:NE1	1:D:152:GLU:HG2	2.21	0.56
1:D:293:ALA:HA	1:D:296:LYS:HE2	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MSE:HG2	1:B:38:MSE:CE	2.35	0.56
1:A:344:PHE:CE2	1:A:348:GLY:HA2	2.40	0.56
1:B:293:ALA:O	1:B:296:LYS:HB2	2.05	0.56
1:B:298:ILE:HG21	1:B:300:LYS:HB2	1.87	0.56
1:D:184:LEU:HD12	1:D:200:PRO:HG3	1.88	0.56
1:C:295:GLN:HA	1:C:295:GLN:OE1	2.06	0.56
1:D:186:LEU:HD12	1:D:471:PHE:HZ	1.71	0.56
1:A:183:LYS:HA	1:A:186:LEU:HD12	1.89	0.56
1:A:552:TYR:CE1	1:A:556:ARG:CZ	2.89	0.56
1:B:332:LEU:HD12	1:B:332:LEU:H	1.70	0.56
1:D:334:GLU:O	1:D:338:GLN:HG3	2.06	0.56
1:A:527:ALA:O	1:A:531:THR:HG23	2.05	0.55
1:A:106:SER:OG	1:A:107:LEU:HD12	2.06	0.55
1:A:528:ILE:O	1:A:532:GLU:HG3	2.05	0.55
1:D:298:ILE:HD11	1:D:413:ARG:HB2	1.88	0.55
1:B:284:ALA:HA	1:B:319:ILE:HG23	1.87	0.55
1:C:455:THR:HG22	5:C:4002:HOH:O	2.06	0.55
1:A:227:ARG:CG	1:A:227:ARG:HH11	2.11	0.55
1:A:22:LYS:HD2	1:A:22:LYS:O	2.06	0.55
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.89	0.55
1:D:143:VAL:HG21	1:D:237:GLU:HG2	1.88	0.55
1:A:120:CYS:O	1:A:175:TYR:HB3	2.06	0.55
1:A:300:LYS:NZ	1:A:305:HIS:HD2	2.04	0.55
1:A:542:ARG:HD2	1:A:552:TYR:OH	2.06	0.55
1:B:551:LYS:O	1:B:555:GLU:HB2	2.06	0.55
1:D:530:VAL:O	1:D:534:LEU:HG	2.07	0.55
1:A:140:ARG:HH22	1:A:230:GLN:HA	1.70	0.55
1:C:140:ARG:HB2	1:C:140:ARG:HH11	1.72	0.55
1:B:335:GLN:O	1:B:339:LYS:HD2	2.07	0.55
1:B:36:LYS:HZ3	1:B:562:TYR:HB3	1.72	0.55
1:B:75:MSE:HG2	1:B:80:GLU:CD	2.26	0.55
1:D:332:LEU:HA	1:D:336:GLU:OE2	2.06	0.55
1:C:358:ILE:HG23	1:C:362:GLN:HB2	1.89	0.55
1:D:528:ILE:O	1:D:531:THR:HG23	2.07	0.55
1:A:104:ILE:HD13	1:A:519:ILE:HG21	1.89	0.55
1:A:215:ASP:OD1	1:A:216:PRO:HD2	2.06	0.55
1:A:261:ASN:ND2	1:A:264:ARG:NH2	2.50	0.55
1:A:332:LEU:HG	1:A:336:GLU:CD	2.28	0.55
1:A:401:PRO:CB	1:A:436:LEU:HD21	2.37	0.55
1:D:370:PRO:HB2	1:D:371:GLU:OE1	2.07	0.55
1:D:530:VAL:HG12	1:D:534:LEU:HD21	1.90	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MSE:HB2	1:A:350:LEU:CD1	2.35	0.54
1:B:69:HIS:HE1	1:B:102:ASP:OD2	1.90	0.54
1:B:45:ARG:HA	1:B:50:LEU:HD12	1.89	0.54
1:C:535:TYR:HE2	1:C:545:GLU:HB2	1.70	0.54
1:A:496:LYS:O	1:A:500:SER:HB3	2.07	0.54
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.90	0.54
1:D:207:THR:O	1:D:224:LYS:HA	2.07	0.54
1:D:371:GLU:CD	1:D:371:GLU:N	2.51	0.54
1:D:401:PRO:HA	1:D:436:LEU:HD23	1.89	0.54
1:A:350:LEU:HD23	1:A:354:ARG:NH1	2.23	0.54
1:D:166:ILE:HG13	1:D:172:LEU:HB2	1.89	0.54
1:B:518:ASN:HB3	1:B:521:GLU:OE2	2.07	0.54
1:A:419:LEU:O	3:A:601:NAD:H2N	2.08	0.54
1:B:130:PRO:O	1:B:131:LYS:HG3	2.07	0.54
1:B:21:ILE:HG13	1:B:23:GLU:H	1.73	0.54
1:A:358:ILE:HD12	1:A:366:THR:OG1	2.08	0.54
1:B:467:ASN:ND2	4:B:1603:MAK:O5	2.41	0.54
1:C:33:ARG:HH21	1:C:152:GLU:CG	2.21	0.54
1:C:276:PHE:HB3	1:C:486:ILE:HD12	1.90	0.54
1:C:91:ARG:NE	5:C:4011:HOH:O	2.39	0.54
1:C:388:THR:HG22	1:C:389:ILE:N	2.23	0.54
1:C:571:GLU:OE2	1:C:572:TRP:O	2.26	0.54
1:D:461:THR:HB	1:D:509:GLN:HB3	1.90	0.54
1:A:187:TYR:HE1	1:A:471:PHE:HD1	1.54	0.54
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.90	0.54
1:D:64:GLN:NE2	1:D:562:TYR:OH	2.24	0.54
1:A:534:LEU:CD2	1:A:539:MSE:HE2	2.38	0.54
1:A:546:PRO:HG3	1:A:552:TYR:CD2	2.43	0.54
1:C:127:PHE:CD2	1:D:38:MSE:HE2	2.43	0.54
1:B:516:LEU:O	1:B:516:LEU:HD12	2.08	0.54
1:C:153:ASN:C	1:C:153:ASN:HD22	2.11	0.54
1:D:51:GLN:HA	1:D:51:GLN:HE21	1.72	0.54
1:D:59:GLU:HB3	1:D:63:ILE:CG2	2.37	0.54
1:A:456:ASP:CG	1:A:458:ARG:HH11	2.10	0.53
1:B:373:ILE:O	1:B:373:ILE:HG22	2.08	0.53
1:A:175:TYR:CE2	1:A:218:TYR:HA	2.42	0.53
1:A:177:MSE:O	1:A:177:MSE:HG3	2.08	0.53
1:C:140:ARG:HE	1:C:230:GLN:HG2	1.73	0.53
1:C:61:GLN:HA	1:C:64:GLN:NE2	2.15	0.53
1:D:453:LYS:HG3	1:D:459:VAL:HG22	1.89	0.53
1:A:387:SER:HA	1:A:411:ASN:OD1	2.08	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HG3	1:A:471:PHE:CZ	2.43	0.53
1:C:248:ARG:CG	1:C:248:ARG:HH11	2.20	0.53
1:C:546:PRO:HG2	1:C:549:LYS:HE3	1.91	0.53
1:D:75:MSE:HE3	1:D:81:LYS:HG2	1.91	0.53
1:D:248:ARG:NH1	1:D:272:LYS:O	2.41	0.53
1:A:302:ILE:HG21	1:A:332:LEU:HD13	1.91	0.53
1:C:140:ARG:HB2	1:C:140:ARG:CZ	2.36	0.53
1:C:350:LEU:HD23	1:C:354:ARG:NH1	2.23	0.53
1:A:297:VAL:CG2	1:A:442:LEU:HD11	2.39	0.53
1:A:300:LYS:HZ2	1:A:305:HIS:HD2	1.57	0.53
1:B:324:VAL:HG13	1:B:337:ALA:HB3	1.91	0.53
1:B:354:ARG:HE	1:B:358:ILE:CD1	2.09	0.53
1:C:174:VAL:HG12	1:C:174:VAL:O	2.09	0.53
1:D:177:MSE:SE	5:D:4017:HOH:O	2.76	0.53
1:C:56:PRO:HG2	1:D:220:GLY:HA2	1.89	0.53
1:D:531:THR:HA	1:D:534:LEU:HG	1.90	0.53
1:A:153:ASN:HB3	1:A:245:ARG:HH21	1.74	0.53
1:A:518:ASN:N	1:A:518:ASN:OD1	2.42	0.53
1:C:503:THR:OG1	1:C:506:GLU:HG3	2.09	0.53
1:D:399:PHE:HB2	1:D:428:CYS:HB3	1.90	0.53
1:D:466:ASN:HB3	1:D:468:VAL:HG12	1.91	0.53
1:D:38:MSE:HE3	1:D:59:GLU:CD	2.28	0.53
1:B:525:ASN:HA	1:B:528:ILE:HG13	1.91	0.53
1:B:86:MSE:HE2	1:B:111:VAL:HG23	1.90	0.53
1:D:120:CYS:O	1:D:175:TYR:HB3	2.09	0.53
1:D:295:GLN:HE21	1:D:305:HIS:HE1	1.57	0.53
1:A:153:ASN:ND2	1:A:153:ASN:H	2.07	0.53
1:D:83:ILE:HD11	1:D:126:ILE:CG2	2.38	0.53
1:B:324:VAL:HG13	1:B:337:ALA:CB	2.39	0.52
1:B:43:GLN:HG2	1:B:47:MSE:HE1	1.89	0.52
1:C:351:VAL:CG1	1:C:369:ALA:HA	2.39	0.52
1:A:97:TYR:HA	1:A:100:LEU:HD22	1.91	0.52
1:B:112:TYR:CE2	1:B:113:THR:HG22	2.43	0.52
1:B:389:ILE:HG23	1:B:399:PHE:CE1	2.45	0.52
1:D:26:LYS:HB3	1:D:27:PRO:HD3	1.91	0.52
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.39	0.52
1:C:418:ALA:O	1:C:445:SER:HA	2.10	0.52
1:A:288:LEU:CD2	1:A:322:LEU:HD23	2.40	0.52
1:B:349:LEU:CD1	1:B:384:LEU:HD11	2.38	0.52
1:B:310:LEU:HD12	1:B:377:PHE:CD1	2.44	0.52
1:B:75:MSE:HG2	1:B:80:GLU:HG2	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HA	1:B:256:ASP:OD2	2.09	0.52
1:C:288:LEU:O	1:C:292:LEU:HD22	2.09	0.52
1:D:150:TRP:O	1:D:245:ARG:NH2	2.41	0.52
1:D:374:PRO:HB3	1:D:380:ALA:N	2.24	0.52
1:D:61:GLN:OE1	1:D:98:ARG:NH1	2.42	0.52
1:A:456:ASP:OD2	1:A:458:ARG:NH1	2.41	0.52
1:B:194:ARG:HB2	1:B:197:ARG:HG3	1.92	0.52
1:B:26:LYS:HA	1:B:29:MSE:HE3	1.91	0.52
1:D:363:GLU:O	1:D:363:GLU:OE1	2.28	0.52
1:C:90:GLU:OE1	1:C:131:LYS:HD2	2.09	0.52
1:D:161:THR:HA	1:D:257:PHE:CE1	2.45	0.52
1:D:327:MSE:HE3	1:D:337:ALA:CA	2.40	0.52
1:D:94:LYS:HG3	1:D:560:SER:O	2.09	0.52
1:B:298:ILE:HG22	1:B:300:LYS:H	1.73	0.52
1:C:137:ILE:O	1:C:140:ARG:HG2	2.10	0.52
1:C:504:ASP:OD2	1:C:504:ASP:N	2.42	0.52
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.33	0.52
1:A:46:GLN:HG3	1:A:51:GLN:HG3	1.92	0.52
1:A:552:TYR:HE1	1:A:556:ARG:CZ	2.23	0.52
1:D:307:ILE:HD13	1:D:388:THR:OG1	2.10	0.52
1:D:518:ASN:ND2	1:D:518:ASN:N	2.57	0.52
1:C:144:ARG:HD2	1:C:144:ARG:O	2.10	0.52
1:A:374:PRO:HB3	1:A:380:ALA:N	2.25	0.51
1:A:518:ASN:O	1:A:522:VAL:HG23	2.10	0.51
1:B:177:MSE:C	1:B:180:PRO:HD2	2.28	0.51
1:C:297:VAL:CG2	1:C:442:LEU:HD11	2.39	0.51
1:D:140:ARG:NH2	1:D:230:GLN:O	2.43	0.51
1:A:251:LEU:HD22	1:A:252:ILE:N	2.25	0.51
1:A:183:LYS:HG3	1:A:471:PHE:CE1	2.45	0.51
1:C:218:TYR:O	1:D:57:LYS:HE2	2.11	0.51
1:B:196:ASP:OD1	1:B:197:ARG:HG2	2.11	0.51
1:B:533:TYR:CZ	1:B:537:ASN:ND2	2.78	0.51
1:C:374:PRO:HG3	1:C:383:ILE:HD12	1.92	0.51
1:D:551:LYS:HD2	1:D:555:GLU:OE1	2.11	0.51
1:A:389:ILE:O	1:A:390:ILE:HD13	2.10	0.51
1:A:533:TYR:O	1:A:537:ASN:ND2	2.43	0.51
1:B:493:GLU:HG3	1:B:533:TYR:CD1	2.45	0.51
1:A:297:VAL:HG21	1:A:442:LEU:HD11	1.93	0.51
1:C:528:ILE:HA	1:C:531:THR:CG2	2.40	0.51
1:D:501:GLN:HE22	1:D:525:ASN:HB2	1.74	0.51
1:B:228:THR:OG1	1:B:230:GLN:HG3	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:NZ	1:A:457:GLY:HA2	2.24	0.51
1:B:354:ARG:CD	1:B:358:ILE:HD11	2.40	0.51
1:B:43:GLN:O	1:B:47:MSE:HE3	2.11	0.51
1:D:163:GLY:HA2	1:D:166:ILE:HD11	1.93	0.51
1:A:144:ARG:HH21	1:A:245:ARG:HG3	1.75	0.51
1:B:137:ILE:HA	1:B:234:LEU:HD22	1.93	0.51
1:B:401:PRO:HB3	1:B:436:LEU:HD21	1.92	0.51
1:C:167:LEU:HD23	4:C:2603:MAK:C1	2.41	0.51
1:C:288:LEU:HG	1:C:292:LEU:HD22	1.93	0.51
1:A:263:PHE:CZ	1:A:314:GLU:HA	2.46	0.51
1:B:296:LYS:NZ	1:B:507:LEU:HD11	2.25	0.51
1:D:226:ASP:OD1	1:D:226:ASP:C	2.49	0.51
1:B:505:GLU:O	1:B:509:GLN:HG2	2.11	0.51
1:D:283:THR:HA	1:D:286:VAL:HG23	1.92	0.51
1:A:239:MSE:O	1:A:243:THR:HG23	2.12	0.50
1:A:61:GLN:HG3	1:A:562:TYR:CE1	2.46	0.50
1:B:182:GLY:O	1:B:185:CYS:HB2	2.11	0.50
1:B:431:GLU:N	5:B:4069:HOH:O	2.44	0.50
1:A:350:LEU:HD22	1:A:358:ILE:CD1	2.40	0.50
1:C:441:CYS:O	1:C:442:LEU:HD23	2.11	0.50
1:D:108:MSE:HA	1:D:111:VAL:HG22	1.93	0.50
1:D:140:ARG:HG3	1:D:140:ARG:O	2.11	0.50
1:A:305:HIS:O	1:A:340:LYS:HD2	2.12	0.50
1:A:412:GLU:O	1:A:440:ARG:NH1	2.44	0.50
1:A:418:ALA:O	1:A:445:SER:HA	2.11	0.50
1:A:68:PHE:CD2	1:A:99:ILE:HD11	2.47	0.50
1:B:447:SER:HB3	1:B:448:PRO:HD2	1.93	0.50
1:C:160:VAL:HG11	1:C:238:PHE:CZ	2.46	0.50
1:D:191:ALA:O	1:D:476:LEU:HD22	2.10	0.50
1:B:251:LEU:HD23	1:B:252:ILE:N	2.27	0.50
1:B:418:ALA:CB	1:B:427:GLU:HB2	2.41	0.50
1:C:446:GLY:O	1:C:466:ASN:ND2	2.42	0.50
1:A:319:ILE:HG22	1:A:323:ILE:HD11	1.93	0.50
1:C:286:VAL:HG13	1:C:470:ILE:HG12	1.93	0.50
1:C:127:PHE:CE2	1:D:38:MSE:HE2	2.47	0.50
1:A:354:ARG:NE	1:A:356:ALA:O	2.44	0.50
1:A:413:ARG:HA	1:A:440:ARG:O	2.12	0.50
1:B:144:ARG:HH12	1:B:244:ASP:HB3	1.75	0.50
1:D:300:LYS:HE2	1:D:301:PRO:N	2.26	0.50
1:D:351:VAL:HB	1:D:369:ALA:HB2	1.94	0.50
1:A:26:LYS:HG3	1:B:151:PRO:CG	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:HH21	1:B:167:LEU:CA	2.24	0.50
1:C:358:ILE:HG23	1:C:362:GLN:HE21	1.76	0.50
1:C:396:GLY:HA2	1:C:425:GLN:HA	1.93	0.50
1:D:314:GLU:HB2	3:D:3601:NAD:O1N	2.12	0.50
1:D:437:THR:O	1:D:438:GLU:HB2	2.12	0.50
1:B:287:ALA:CB	1:B:319:ILE:HG21	2.39	0.50
1:B:94:LYS:HE2	1:B:558:TRP:CZ2	2.46	0.50
1:A:404:ILE:HD13	1:A:436:LEU:HD23	1.94	0.49
1:C:456:ASP:OD1	1:C:456:ASP:C	2.50	0.49
1:D:194:ARG:HE	1:D:197:ARG:HH11	1.59	0.49
1:D:404:ILE:CG2	1:D:436:LEU:HB3	2.42	0.49
1:A:226:ASP:OD1	1:A:226:ASP:C	2.48	0.49
1:A:295:GLN:HE22	1:A:299:SER:HA	1.77	0.49
1:C:210:ILE:O	1:C:214:LYS:HG2	2.12	0.49
1:D:394:GLY:HA2	1:D:420:SER:HB3	1.94	0.49
1:D:557:THR:O	1:D:559:ARG:NH2	2.45	0.49
1:A:243:THR:HG21	1:A:273:TYR:CE2	2.46	0.49
1:A:551:LYS:HZ2	1:A:551:LYS:HB3	1.76	0.49
1:D:186:LEU:HD13	1:D:468:VAL:CG2	2.42	0.49
1:A:294:ALA:O	1:A:297:VAL:HG13	2.12	0.49
1:B:174:VAL:HG12	1:B:174:VAL:O	2.10	0.49
1:B:370:PRO:HD2	1:B:373:ILE:CD1	2.42	0.49
1:D:177:MSE:HE1	1:D:181:VAL:CG2	2.24	0.49
1:A:332:LEU:CD2	1:A:340:LYS:NZ	2.75	0.49
1:A:529:LYS:NZ	1:A:532:GLU:OE1	2.46	0.49
1:A:61:GLN:HA	1:A:64:GLN:NE2	2.26	0.49
1:D:321:ASN:O	1:D:325:MSE:HG3	2.13	0.49
1:D:447:SER:HB3	1:D:448:PRO:HD2	1.95	0.49
1:A:482:ASN:HD21	3:A:602:NAD:H4B	1.78	0.49
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.23	0.49
1:A:174:VAL:HG12	1:A:219:MSE:HE2	1.95	0.49
1:A:461:THR:O	1:A:511:ARG:HG2	2.12	0.49
1:B:334:GLU:HG3	1:B:338:GLN:HE21	1.74	0.49
1:B:370:PRO:HG2	1:B:372:SER:O	2.12	0.49
1:D:132:GLY:HA2	1:D:200:PRO:HD2	1.93	0.49
1:D:329:GLU:C	1:D:330:ASN:HD22	2.16	0.49
1:A:478:VAL:HG13	1:A:483:THR:HB	1.95	0.49
1:C:47:MSE:C	1:C:48:LEU:HD23	2.33	0.49
1:B:320:ALA:O	1:B:324:VAL:HG23	2.13	0.49
1:B:75:MSE:HG2	1:B:80:GLU:CG	2.43	0.49
1:C:238:PHE:CE1	1:C:242:ILE:HG13	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LYS:HB2	1:C:306:LYS:HZ3	1.77	0.49
1:C:476:LEU:HD23	1:C:527:ALA:CB	2.43	0.49
1:C:495:ALA:O	1:C:499:THR:HG22	2.13	0.49
1:C:552:TYR:CD1	1:C:556:ARG:NH1	2.81	0.49
1:C:128:ARG:HG2	1:D:91:ARG:HD3	1.95	0.49
1:D:287:ALA:HB3	1:D:319:ILE:HG23	1.95	0.48
1:D:506:GLU:O	1:D:511:ARG:HG2	2.13	0.48
1:C:529:LYS:O	1:C:532:GLU:HB2	2.14	0.48
1:D:239:MSE:O	1:D:243:THR:HG23	2.12	0.48
1:A:227:ARG:CG	1:A:227:ARG:NH1	2.71	0.48
1:A:64:GLN:HB3	1:A:95:LEU:HD22	1.94	0.48
1:B:144:ARG:HH12	1:B:244:ASP:CB	2.26	0.48
1:B:481:CYS:SG	1:B:531:THR:HB	2.53	0.48
1:C:351:VAL:HG11	1:C:369:ALA:HA	1.96	0.48
1:D:104:ILE:O	1:D:108:MSE:HB2	2.13	0.48
1:D:115:THR:HG22	1:D:115:THR:O	2.13	0.48
1:D:174:VAL:C	1:D:176:GLY:H	2.17	0.48
1:A:174:VAL:C	1:A:176:GLY:H	2.16	0.48
1:A:261:ASN:HD22	1:A:264:ARG:NE	2.09	0.48
1:A:261:ASN:HD21	1:A:264:ARG:HH21	1.59	0.48
1:A:300:LYS:NZ	1:A:304:GLU:HB2	2.28	0.48
1:A:300:LYS:NZ	1:A:304:GLU:O	2.44	0.48
1:B:323:ILE:HG21	1:B:341:ILE:HD11	1.95	0.48
1:C:184:LEU:HD12	1:C:200:PRO:HG3	1.95	0.48
1:C:33:ARG:NH2	1:C:152:GLU:HG3	2.27	0.48
1:C:441:CYS:C	1:C:442:LEU:HD23	2.34	0.48
1:D:208:ASP:OD1	1:D:225:ARG:HG3	2.14	0.48
1:D:287:ALA:CB	1:D:319:ILE:HD13	2.43	0.48
1:D:397:ARG:HA	1:D:427:GLU:O	2.12	0.48
1:A:166:ILE:HG23	1:A:179:ILE:HG13	1.96	0.48
1:A:369:ALA:HB1	1:A:373:ILE:CD1	2.41	0.48
1:C:351:VAL:HA	1:C:367:HIS:O	2.14	0.48
1:C:400:THR:O	1:C:404:ILE:HG12	2.13	0.48
1:C:46:GLN:HG2	1:C:51:GLN:HG3	1.95	0.48
1:D:502:LEU:HD11	1:D:507:LEU:HG	1.95	0.48
1:A:332:LEU:CD2	1:A:340:LYS:HZ3	2.26	0.48
1:A:285:ALA:HB1	1:A:470:ILE:HD12	1.94	0.48
1:B:276:PHE:CD1	1:B:276:PHE:C	2.87	0.48
1:D:197:ARG:HG2	1:D:197:ARG:HH11	1.78	0.48
1:D:211:ALA:HA	1:D:214:LYS:HE3	1.95	0.48
1:D:404:ILE:HG21	1:D:436:LEU:HB3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:VAL:O	1:D:478:VAL:HG23	2.14	0.48
1:D:506:GLU:CG	1:D:511:ARG:HD2	2.43	0.48
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.96	0.48
1:B:297:VAL:HG21	1:B:442:LEU:HD21	1.95	0.48
1:D:91:ARG:NH1	1:D:91:ARG:HG3	2.23	0.48
1:A:144:ARG:NH2	1:A:245:ARG:CG	2.77	0.48
1:A:331:GLY:O	1:A:332:LEU:O	2.31	0.48
1:D:157:ALA:HB2	1:D:479:ILE:HD11	1.96	0.48
1:D:506:GLU:O	1:D:511:ARG:CG	2.62	0.48
1:B:533:TYR:CE1	1:B:537:ASN:ND2	2.80	0.48
1:C:447:SER:HB3	1:C:448:PRO:HD2	1.96	0.48
1:A:204:ASP:OD2	1:A:221:LEU:HB2	2.14	0.48
1:B:389:ILE:HG22	1:B:416:ILE:HA	1.96	0.48
1:D:555:GLU:HB3	1:D:556:ARG:HH11	1.79	0.48
1:A:253:GLN:HB2	1:A:276:PHE:CE2	2.49	0.47
1:A:396:GLY:O	1:A:398:LEU:HD23	2.14	0.47
1:B:69:HIS:CE1	1:B:102:ASP:OD2	2.67	0.47
1:B:401:PRO:HA	1:B:436:LEU:CD2	2.44	0.47
1:D:344:PHE:CZ	1:D:348:GLY:HA2	2.49	0.47
1:A:295:GLN:HE22	1:A:299:SER:C	2.17	0.47
1:B:415:VAL:C	1:B:416:ILE:HD12	2.34	0.47
1:B:549:LYS:N	1:B:549:LYS:HD3	2.28	0.47
1:C:177:MSE:O	1:C:181:VAL:HG23	2.14	0.47
1:D:144:ARG:HH12	1:D:244:ASP:HB2	1.79	0.47
1:D:329:GLU:CG	1:D:330:ASN:ND2	2.78	0.47
1:B:416:ILE:N	1:B:416:ILE:HD12	2.29	0.47
1:B:51:GLN:HA	1:B:51:GLN:NE2	2.24	0.47
1:C:521:GLU:HG3	1:C:522:VAL:N	2.28	0.47
1:D:204:ASP:OD2	1:D:221:LEU:HD22	2.13	0.47
1:D:249:ASN:C	1:D:249:ASN:ND2	2.65	0.47
1:D:557:THR:OG1	1:D:559:ARG:NH1	2.47	0.47
1:A:108:MSE:HG3	1:A:112:TYR:HB3	1.96	0.47
1:A:549:LYS:HD3	1:A:549:LYS:H	1.79	0.47
1:B:497:ALA:O	1:B:501:GLN:HG3	2.14	0.47
1:C:228:THR:OG1	1:C:230:GLN:HB2	2.14	0.47
1:C:546:PRO:O	1:C:549:LYS:CE	2.63	0.47
1:D:438:GLU:O	1:D:458:ARG:NH2	2.47	0.47
1:D:530:VAL:CG1	1:D:534:LEU:HD21	2.45	0.47
1:B:301:PRO:HB2	1:B:304:GLU:HG3	1.97	0.47
1:D:104:ILE:HG13	1:D:108:MSE:HE2	1.96	0.47
1:D:186:LEU:O	1:D:190:CYS:HB2	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLY:HA2	1:B:166:ILE:HD11	1.96	0.47
1:B:231:TYR:HE2	1:B:265:PHE:CZ	2.33	0.47
1:B:504:ASP:O	1:B:508:ALA:N	2.47	0.47
1:B:506:GLU:HA	1:B:509:GLN:HG3	1.97	0.47
1:C:525:ASN:O	1:C:529:LYS:HG2	2.15	0.47
1:D:43:GLN:O	1:D:47:MSE:HE3	2.14	0.47
1:A:404:ILE:HG23	1:A:416:ILE:HD13	1.97	0.47
1:C:400:THR:HB	1:C:401:PRO:HD2	1.96	0.47
1:D:136:SER:HB2	1:D:221:LEU:HD22	1.96	0.47
1:A:209:ASN:OD1	1:A:211:ALA:HB3	2.15	0.47
1:A:57:LYS:HD3	1:B:218:TYR:O	2.15	0.47
1:D:288:LEU:HG	1:D:292:LEU:CD2	2.42	0.47
1:A:392:VAL:CG1	5:A:4006:HOH:O	2.63	0.47
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.71	0.47
1:A:93:GLU:O	1:A:96:PHE:HB3	2.15	0.47
1:C:165:ARG:NH1	3:C:2601:NAD:O1N	2.45	0.47
1:D:107:LEU:O	1:D:111:VAL:HG13	2.15	0.47
1:D:68:PHE:CG	1:D:99:ILE:HG13	2.49	0.47
1:B:550:ALA:O	1:B:554:LYS:HG3	2.14	0.47
1:C:394:GLY:HA2	1:C:420:SER:HB3	1.97	0.47
1:B:302:ILE:HG13	1:B:332:LEU:HD11	1.97	0.46
1:B:419:LEU:O	3:B:1601:NAD:H2N	2.15	0.46
1:B:559:ARG:HB3	1:B:561:GLU:OE1	2.15	0.46
1:C:150:TRP:CE2	1:C:199:LEU:HD13	2.50	0.46
1:C:259:ASN:O	1:C:262:ALA:HB3	2.15	0.46
1:D:339:LYS:HA	1:D:367:HIS:NE2	2.31	0.46
1:A:96:PHE:O	1:A:100:LEU:HD22	2.15	0.46
1:B:165:ARG:HH21	1:B:167:LEU:HA	1.80	0.46
1:B:23:GLU:HG3	1:B:24:LYS:N	2.30	0.46
1:D:184:LEU:HD12	1:D:200:PRO:CG	2.44	0.46
1:A:175:TYR:CZ	1:A:218:TYR:HA	2.50	0.46
1:A:255:GLU:OE2	1:A:278:ASP:HB3	2.15	0.46
1:A:349:LEU:HD23	1:A:351:VAL:CG1	2.45	0.46
1:C:396:GLY:O	1:C:398:LEU:HD22	2.14	0.46
1:D:267:ARG:HB2	1:D:267:ARG:CZ	2.46	0.46
1:D:330:ASN:HD22	1:D:330:ASN:N	2.13	0.46
1:B:211:ALA:O	1:B:214:LYS:HG3	2.16	0.46
1:C:302:ILE:HG23	1:C:303:SER:N	2.31	0.46
1:C:516:LEU:O	1:C:516:LEU:HD12	2.16	0.46
1:C:68:PHE:CD2	1:C:99:ILE:CG1	2.99	0.46
1:A:142:HIS:HB3	1:D:568:ASP:OD1	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:C	1:A:330:ASN:H	2.19	0.46
1:A:372:SER:O	1:A:374:PRO:HD3	2.16	0.46
1:B:43:GLN:O	1:B:47:MSE:HB2	2.16	0.46
1:A:108:MSE:N	1:A:109:PRO:CD	2.78	0.46
1:A:42:LEU:HD11	1:A:46:GLN:NE2	2.30	0.46
1:B:333:SER:H	1:B:336:GLU:CG	2.28	0.46
1:B:57:LYS:HZ3	1:B:59:GLU:HG2	1.81	0.46
1:C:293:ALA:O	1:C:296:LYS:HB2	2.16	0.46
1:A:183:LYS:HE2	1:A:255:GLU:OE1	2.15	0.46
1:B:401:PRO:HA	1:B:436:LEU:HD23	1.97	0.46
1:C:298:ILE:HD11	1:C:413:ARG:O	2.16	0.46
1:D:535:TYR:OH	1:D:542:ARG:HB3	2.15	0.46
1:A:207:THR:O	1:A:224:LYS:HA	2.16	0.46
1:A:251:LEU:HD22	1:A:252:ILE:H	1.81	0.46
1:C:106:SER:O	1:C:109:PRO:HD2	2.16	0.46
1:C:308:LEU:HD13	1:C:384:LEU:HD23	1.97	0.46
1:C:72:LEU:HA	1:C:75:MSE:HG3	1.97	0.46
1:D:520:GLN:HE21	1:D:520:GLN:H	1.64	0.46
1:D:55:PRO:HA	1:D:56:PRO:HD3	1.86	0.46
1:A:171:ASP:OD1	1:A:207:THR:OG1	2.30	0.46
1:A:177:MSE:HE3	1:A:177:MSE:O	2.15	0.46
1:A:177:MSE:HE3	1:A:180:PRO:CG	2.45	0.46
1:B:32:PRO:HG3	1:B:90:GLU:O	2.15	0.46
1:B:404:ILE:HD12	1:B:436:LEU:HD22	1.98	0.46
1:A:420:SER:HA	3:A:601:NAD:H1D	1.98	0.46
1:A:72:LEU:HA	1:A:75:MSE:HG3	1.97	0.46
1:C:158:VAL:HG12	1:C:160:VAL:HG13	1.98	0.46
1:C:320:ALA:O	1:C:324:VAL:HG23	2.15	0.45
1:C:431:GLU:HA	1:C:452:VAL:HG11	1.98	0.45
1:D:502:LEU:HD13	1:D:507:LEU:HG	1.99	0.45
1:A:188:THR:HG21	1:A:195:PRO:HG3	1.99	0.45
1:A:161:THR:HA	1:A:257:PHE:CE1	2.52	0.45
1:A:295:GLN:NE2	1:A:299:SER:CA	2.79	0.45
1:B:156:LYS:HG3	1:B:197:ARG:CD	2.46	0.45
1:B:36:LYS:HB2	1:B:40:PHE:CE1	2.51	0.45
1:B:504:ASP:HA	1:B:507:LEU:HB2	1.98	0.45
1:D:338:GLN:HB2	1:D:339:LYS:NZ	2.31	0.45
1:D:397:ARG:HG2	1:D:397:ARG:H	1.63	0.45
1:A:295:GLN:HE22	1:A:300:LYS:H	1.63	0.45
1:A:332:LEU:CD1	1:A:332:LEU:H	2.28	0.45
1:A:522:VAL:O	1:A:526:ILE:HG12	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ILE:HG23	1:B:327:MSE:HE3	1.99	0.45
1:D:358:ILE:HG12	1:D:366:THR:OG1	2.16	0.45
1:D:552:TYR:CE1	1:D:556:ARG:CZ	2.99	0.45
1:A:382:ASN:O	1:A:385:LYS:NZ	2.42	0.45
1:A:404:ILE:CD1	1:A:436:LEU:HD23	2.46	0.45
1:A:167:LEU:HD23	4:A:603:MAK:O1	2.17	0.45
1:B:194:ARG:HG3	3:B:1602:NAD:C6A	2.45	0.45
1:D:77:SER:O	1:D:81:LYS:HG3	2.16	0.45
1:A:140:ARG:HB3	1:A:234:LEU:HD13	1.98	0.45
1:A:43:GLN:OE1	1:A:43:GLN:HA	2.17	0.45
1:A:95:LEU:O	1:A:95:LEU:HD12	2.17	0.45
1:C:310:LEU:HD21	1:C:398:LEU:HD23	1.99	0.45
1:D:191:ALA:HB1	1:D:476:LEU:HD22	1.97	0.45
1:D:534:LEU:HD23	1:D:534:LEU:N	2.31	0.45
1:A:467:ASN:O	1:A:471:PHE:CD2	2.67	0.45
1:A:392:VAL:O	3:A:601:NAD:H51N	2.17	0.45
1:B:229:GLN:NE2	1:B:232:ASP:CB	2.74	0.45
1:B:387:SER:HA	1:B:411:ASN:OD1	2.16	0.45
1:B:397:ARG:HA	1:B:427:GLU:O	2.15	0.45
1:B:210:ILE:H	1:B:210:ILE:HD12	1.81	0.45
1:B:359:ASP:O	1:B:360:SER:C	2.54	0.45
1:B:524:ILE:O	1:B:528:ILE:CG1	2.64	0.45
1:A:438:GLU:O	1:A:458:ARG:NH2	2.50	0.45
1:C:375:ASP:N	1:C:375:ASP:OD1	2.49	0.45
1:D:171:ASP:OD2	1:D:225:ARG:NE	2.43	0.45
1:D:471:PHE:N	1:D:472:PRO:CD	2.80	0.45
1:D:89:GLN:HG2	1:D:131:LYS:NZ	2.31	0.45
1:A:551:LYS:O	1:A:555:GLU:HG3	2.16	0.45
1:B:298:ILE:HG22	1:B:300:LYS:HB2	1.97	0.45
1:B:302:ILE:HD12	1:B:305:HIS:ND1	2.32	0.45
1:B:456:ASP:OD1	1:B:458:ARG:HD3	2.17	0.45
1:B:524:ILE:O	1:B:528:ILE:HG12	2.17	0.45
1:C:325:MSE:HE1	1:C:489:SER:HA	1.99	0.45
1:D:108:MSE:N	1:D:109:PRO:CD	2.80	0.45
1:D:22:LYS:CD	1:D:22:LYS:O	2.65	0.45
1:A:160:VAL:CG2	1:A:203:ILE:CD1	2.95	0.44
1:A:400:THR:O	1:A:403:VAL:HB	2.17	0.44
1:B:373:ILE:O	1:B:373:ILE:CG2	2.65	0.44
1:D:313:GLY:HA3	3:D:3601:NAD:O5B	2.17	0.44
1:D:374:PRO:HB3	1:D:379:ASP:CB	2.47	0.44
1:A:177:MSE:HE3	1:A:180:PRO:CD	2.45	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:HIS:O	1:A:340:LYS:CD	2.65	0.44
1:B:259:ASN:OD1	1:B:263:PHE:HE1	2.00	0.44
1:B:342:TRP:CZ3	1:B:349:LEU:HD21	2.50	0.44
1:B:349:LEU:HD22	1:B:351:VAL:HG13	2.00	0.44
1:B:298:ILE:HD11	1:B:442:LEU:CD1	2.47	0.44
1:B:65:ALA:HA	1:B:99:ILE:HD11	1.98	0.44
1:C:546:PRO:O	1:C:549:LYS:HE3	2.18	0.44
1:C:85:ILE:HD12	1:C:85:ILE:C	2.38	0.44
1:D:554:LYS:HG2	1:D:554:LYS:H	1.59	0.44
1:A:97:TYR:HA	1:A:100:LEU:CD2	2.47	0.44
1:A:177:MSE:CE	1:A:177:MSE:O	2.66	0.44
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.10	0.44
1:A:554:LYS:HE2	1:A:554:LYS:HB3	1.61	0.44
1:B:36:LYS:HB2	1:B:40:PHE:CD1	2.53	0.44
1:C:388:THR:CG2	1:C:389:ILE:N	2.80	0.44
1:D:266:LEU:O	1:D:270:ARG:HG2	2.18	0.44
1:A:96:PHE:O	1:A:99:ILE:HG22	2.17	0.44
1:B:321:ASN:O	1:B:325:MSE:HG3	2.17	0.44
1:B:358:ILE:HA	1:B:362:GLN:HE21	1.81	0.44
1:C:295:GLN:O	1:C:299:SER:N	2.45	0.44
1:C:412:GLU:O	1:C:440:ARG:HD2	2.17	0.44
1:D:83:ILE:HD11	1:D:126:ILE:HG21	1.99	0.44
1:D:346:LYS:HG2	3:D:3601:NAD:O2B	2.16	0.44
1:A:108:MSE:HE2	1:A:108:MSE:HB2	1.94	0.44
1:A:150:TRP:CD2	1:A:151:PRO:HD2	2.53	0.44
1:A:29:MSE:HE2	1:A:29:MSE:HB3	1.83	0.44
1:A:398:LEU:CD2	1:A:398:LEU:N	2.80	0.44
1:B:132:GLY:HA3	1:B:200:PRO:HG2	2.00	0.44
1:B:29:MSE:HE1	1:B:53:LEU:HD13	2.00	0.44
1:C:186:LEU:HD13	1:C:468:VAL:CG2	2.48	0.44
1:D:150:TRP:CE2	1:D:199:LEU:HD13	2.53	0.44
1:D:23:GLU:OE1	1:D:24:LYS:N	2.44	0.44
1:A:174:VAL:HG23	1:A:204:ASP:OD1	2.18	0.44
1:B:108:MSE:N	1:B:109:PRO:HD2	2.33	0.44
1:B:447:SER:HB3	1:B:448:PRO:CD	2.48	0.44
1:C:502:LEU:HD13	1:C:507:LEU:HG	2.00	0.44
1:D:293:ALA:O	1:D:296:LYS:HB2	2.18	0.44
1:D:559:ARG:HD3	1:D:559:ARG:HA	1.82	0.44
1:A:219:MSE:HB2	1:A:219:MSE:HE2	1.84	0.44
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.82	0.44
1:C:248:ARG:CG	1:C:248:ARG:NH1	2.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MSE:HE1	1:A:254:PHE:CE1	2.52	0.44
1:A:46:GLN:HG3	1:A:51:GLN:CG	2.47	0.44
1:C:130:PRO:C	1:C:131:LYS:HG2	2.38	0.44
1:C:172:LEU:O	1:C:175:TYR:HB2	2.17	0.44
1:C:186:LEU:O	1:C:190:CYS:HB2	2.18	0.44
1:C:455:THR:CG2	5:C:4002:HOH:O	2.66	0.44
1:D:75:MSE:HE1	1:D:84:TYR:CB	2.48	0.44
1:A:174:VAL:C	1:A:176:GLY:N	2.71	0.44
1:B:229:GLN:CA	1:B:229:GLN:NE2	2.79	0.44
1:B:401:PRO:O	1:B:405:ARG:HB2	2.18	0.44
1:B:477:ALA:CB	1:B:531:THR:HG22	2.47	0.44
1:C:136:SER:HB2	1:C:221:LEU:HD22	2.00	0.44
1:A:498:LEU:HB2	1:A:526:ILE:HD11	2.00	0.43
1:B:288:LEU:O	1:B:292:LEU:HD22	2.17	0.43
1:B:319:ILE:HG13	1:B:319:ILE:H	1.55	0.43
1:D:467:ASN:OD1	4:D:3603:MAK:O5	2.36	0.43
1:A:188:THR:HG23	1:A:193:ILE:O	2.18	0.43
1:A:85:ILE:HG12	1:A:86:MSE:N	2.33	0.43
1:C:261:ASN:HB3	1:C:265:PHE:CE1	2.54	0.43
1:C:286:VAL:HG11	1:C:466:ASN:C	2.38	0.43
1:D:197:ARG:NH1	1:D:197:ARG:HG2	2.33	0.43
1:A:332:LEU:HD23	1:A:340:LYS:HZ3	1.84	0.43
1:A:341:ILE:O	1:A:367:HIS:NE2	2.50	0.43
1:A:549:LYS:O	1:A:552:TYR:HB3	2.18	0.43
1:B:350:LEU:N	1:B:350:LEU:HD23	2.33	0.43
1:B:357:LYS:HG2	1:B:357:LYS:H	1.36	0.43
1:D:328:VAL:HA	1:D:332:LEU:O	2.18	0.43
1:D:359:ASP:O	1:D:360:SER:C	2.56	0.43
1:A:388:THR:CG2	1:A:390:ILE:HD11	2.48	0.43
1:C:68:PHE:CG	1:C:99:ILE:HG12	2.53	0.43
1:D:413:ARG:HA	1:D:440:ARG:O	2.18	0.43
1:A:453:LYS:HE2	1:A:459:VAL:HG22	2.01	0.43
1:A:46:GLN:CG	1:A:51:GLN:HG3	2.49	0.43
1:B:350:LEU:HD22	1:B:354:ARG:NH2	2.33	0.43
1:C:266:LEU:O	1:C:270:ARG:HG2	2.19	0.43
1:D:177:MSE:O	1:D:180:PRO:HD2	2.19	0.43
1:D:350:LEU:HD22	1:D:354:ARG:NH1	2.29	0.43
1:A:103:ASP:O	1:A:107:LEU:HD13	2.18	0.43
1:C:229:GLN:HG3	1:C:229:GLN:O	2.18	0.43
1:C:260:HIS:C	1:C:260:HIS:CD2	2.92	0.43
1:C:288:LEU:HG	1:C:292:LEU:CD2	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:VAL:CG1	1:C:382:ASN:N	2.81	0.43
1:C:453:LYS:HE3	1:C:457:GLY:CA	2.38	0.43
1:C:506:GLU:HB3	1:C:511:ARG:CD	2.49	0.43
1:D:286:VAL:HG21	1:D:467:ASN:HA	1.99	0.43
1:D:323:ILE:HG22	1:D:324:VAL:N	2.33	0.43
1:A:343:MSE:HE1	1:A:362:GLN:HG2	2.01	0.43
1:A:503:THR:HG23	1:A:506:GLU:CD	2.39	0.43
1:B:482:ASN:HD22	1:B:482:ASN:HA	1.61	0.43
1:B:524:ILE:N	1:B:524:ILE:CD1	2.80	0.43
1:C:26:LYS:HD3	1:D:151:PRO:CG	2.49	0.43
1:D:137:ILE:HB	1:D:205:VAL:CG1	2.46	0.43
1:D:298:ILE:O	1:D:299:SER:C	2.57	0.43
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.79	0.43
1:A:316:ALA:HB2	1:A:392:VAL:CG1	2.48	0.43
1:B:250:THR:O	1:B:252:ILE:HD12	2.19	0.43
1:B:288:LEU:HG	1:B:292:LEU:CD2	2.46	0.43
1:B:345:ASP:HB2	3:B:1601:NAD:O2B	2.19	0.43
1:C:304:GLU:H	1:C:304:GLU:HG2	1.55	0.43
1:D:75:MSE:HE3	1:D:81:LYS:CA	2.45	0.43
1:A:352:LYS:N	1:A:367:HIS:O	2.42	0.43
1:B:343:MSE:HB2	1:B:350:LEU:HG	2.01	0.43
1:B:410:ILE:HG22	1:B:411:ASN:CG	2.39	0.43
1:C:159:VAL:HG23	1:C:184:LEU:HD21	2.00	0.43
1:C:401:PRO:HA	1:C:404:ILE:HG13	2.01	0.43
1:D:308:LEU:O	1:D:389:ILE:HD13	2.18	0.43
1:D:389:ILE:HD13	1:D:389:ILE:HA	1.82	0.43
1:A:412:GLU:HG3	1:A:413:ARG:HG2	2.00	0.43
1:A:71:ASN:ND2	1:A:74:LYS:NZ	2.66	0.43
1:B:184:LEU:HD12	1:B:200:PRO:HB3	2.01	0.43
1:B:43:GLN:HG2	1:B:47:MSE:CE	2.49	0.43
1:D:301:PRO:O	1:D:302:ILE:C	2.57	0.43
1:D:546:PRO:HG2	1:D:552:TYR:CD2	2.54	0.43
1:A:177:MSE:O	1:A:180:PRO:HD2	2.19	0.42
1:A:29:MSE:O	1:A:35:ASN:ND2	2.51	0.42
1:A:389:ILE:CG2	1:A:416:ILE:HA	2.48	0.42
1:B:161:THR:HA	1:B:257:PHE:CE1	2.54	0.42
1:B:286:VAL:HG11	1:B:466:ASN:O	2.19	0.42
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.32	0.42
1:C:136:SER:HA	1:C:204:ASP:O	2.19	0.42
1:C:68:PHE:CD2	1:C:99:ILE:HG13	2.54	0.42
1:D:174:VAL:C	1:D:176:GLY:N	2.71	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ALA:O	1:D:319:ILE:HG13	2.19	0.42
1:D:552:TYR:O	1:D:556:ARG:NH1	2.52	0.42
1:A:137:ILE:HG13	1:A:137:ILE:O	2.18	0.42
1:A:310:LEU:HD21	1:A:398:LEU:CB	2.49	0.42
1:A:503:THR:HG23	1:A:506:GLU:CG	2.49	0.42
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.79	0.42
1:A:77:SER:OG	1:A:80:GLU:HB3	2.19	0.42
1:B:301:PRO:CG	1:B:304:GLU:HG3	2.47	0.42
1:B:46:GLN:HG2	1:B:51:GLN:HG3	2.01	0.42
1:B:535:TYR:HE2	1:B:545:GLU:HB2	1.84	0.42
1:C:29:MSE:SE	1:C:50:LEU:HD22	2.70	0.42
1:C:546:PRO:HG2	1:C:549:LYS:CE	2.49	0.42
1:D:85:ILE:HG13	1:D:86:MSE:N	2.31	0.42
1:A:295:GLN:OE1	1:A:295:GLN:HA	2.20	0.42
1:A:559:ARG:HD3	1:A:559:ARG:HA	1.84	0.42
1:B:260:HIS:CE1	1:B:264:ARG:HE	2.37	0.42
1:B:483:THR:CG2	1:B:484:ARG:N	2.82	0.42
1:B:524:ILE:HG22	1:B:528:ILE:HD11	2.01	0.42
1:C:194:ARG:HA	1:C:195:PRO:HD3	1.91	0.42
1:D:430:ALA:HA	1:D:443:PHE:CE2	2.55	0.42
1:D:456:ASP:OD1	1:D:458:ARG:NH1	2.53	0.42
1:B:143:VAL:HG11	1:B:238:PHE:HA	2.02	0.42
1:B:243:THR:HG21	1:B:273:TYR:CE2	2.55	0.42
1:B:300:LYS:HA	1:B:301:PRO:HD2	1.91	0.42
1:B:325:MSE:HB3	1:B:325:MSE:HE2	1.91	0.42
1:B:528:ILE:HG23	1:B:550:ALA:HA	2.01	0.42
1:C:23:GLU:CD	1:C:24:LYS:H	2.22	0.42
1:C:25:GLY:C	1:C:27:PRO:HD2	2.40	0.42
1:D:431:GLU:O	1:D:435:THR:HB	2.20	0.42
1:D:566:LEU:HA	1:D:567:PRO:HD3	1.86	0.42
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.89	0.42
1:A:22:LYS:HE3	1:C:24:LYS:O	2.19	0.42
1:A:390:ILE:CD1	1:A:417:PHE:HB2	2.50	0.42
1:A:43:GLN:HG3	1:A:47:MSE:CE	2.50	0.42
1:A:484:ARG:CZ	1:D:543:TYR:CD2	3.02	0.42
1:B:166:ILE:O	1:B:167:LEU:HB2	2.20	0.42
1:B:260:HIS:ND1	1:B:264:ARG:NE	2.67	0.42
1:C:128:ARG:HB2	1:C:128:ARG:HE	1.64	0.42
1:D:412:GLU:HG3	1:D:413:ARG:CG	2.48	0.42
1:D:66:LEU:HD22	1:D:70:ARG:CD	2.50	0.42
1:A:253:GLN:NE2	1:A:278:ASP:OD2	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TRP:HA	1:B:151:PRO:HD3	1.82	0.42
1:B:400:THR:O	1:B:403:VAL:HB	2.19	0.42
1:B:520:GLN:O	1:B:524:ILE:HD13	2.18	0.42
1:B:94:LYS:HE2	1:B:558:TRP:HZ2	1.84	0.42
1:D:104:ILE:HG13	1:D:104:ILE:O	2.19	0.42
1:D:136:SER:HB2	1:D:221:LEU:CD2	2.49	0.42
1:D:344:PHE:CD2	1:D:344:PHE:C	2.92	0.42
1:A:201:VAL:HG12	1:A:202:CYS:N	2.35	0.42
1:A:53:LEU:HD23	1:A:53:LEU:N	2.34	0.42
1:B:345:ASP:OD2	1:B:347:TYR:N	2.49	0.42
1:B:397:ARG:H	1:B:397:ARG:HG2	1.40	0.42
1:C:128:ARG:CG	1:D:91:ARG:NE	2.81	0.42
1:D:63:ILE:CG2	1:D:64:GLN:N	2.83	0.42
1:A:209:ASN:C	1:A:209:ASN:OD1	2.58	0.42
1:A:24:LYS:HA	1:A:28:LEU:CD1	2.50	0.42
1:A:434:TYR:CZ	1:A:443:PHE:HB3	2.55	0.42
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.91	0.42
1:B:314:GLU:HB2	3:B:1601:NAD:O1N	2.19	0.42
1:B:313:GLY:O	1:B:317:LEU:HD12	2.20	0.42
1:B:518:ASN:N	1:B:518:ASN:ND2	2.67	0.42
1:B:520:GLN:NE2	1:B:520:GLN:H	2.04	0.42
1:C:420:SER:HA	3:C:2601:NAD:H1D	2.02	0.42
1:D:407:MSE:HG3	1:D:414:PRO:HB3	2.01	0.42
1:B:252:ILE:O	1:B:252:ILE:HG22	2.20	0.42
1:B:358:ILE:CG2	1:B:359:ASP:N	2.82	0.42
1:B:288:LEU:HD23	1:B:495:ALA:CB	2.49	0.42
1:C:60:THR:O	1:C:64:GLN:HG3	2.20	0.42
1:D:239:MSE:HE1	1:D:254:PHE:HE1	1.85	0.42
1:C:307:ILE:HG22	1:C:308:LEU:N	2.34	0.42
1:C:419:LEU:O	3:C:2601:NAD:H2N	2.19	0.42
1:D:239:MSE:HE1	1:D:254:PHE:CE1	2.55	0.42
1:D:530:VAL:O	1:D:533:TYR:HB3	2.20	0.42
1:D:72:LEU:HD12	1:D:75:MSE:CE	2.42	0.42
1:D:68:PHE:CZ	1:D:72:LEU:HD13	2.55	0.42
1:D:75:MSE:HE1	1:D:84:TYR:HB3	2.02	0.42
1:C:165:ARG:O	1:C:165:ARG:NE	2.53	0.41
1:C:44:GLU:O	1:C:48:LEU:HG	2.20	0.41
1:D:115:THR:O	1:D:115:THR:CG2	2.68	0.41
1:D:217:PHE:O	1:D:218:TYR:C	2.59	0.41
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.28	0.41
1:A:43:GLN:HG3	1:A:47:MSE:HE3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:MSE:HE3	1:A:47:MSE:HB2	1.82	0.41
1:A:518:ASN:HB3	1:A:521:GLU:OE2	2.20	0.41
1:B:162:ASP:OD2	1:B:257:PHE:CD2	2.73	0.41
1:D:22:LYS:C	1:D:22:LYS:HD3	2.40	0.41
1:A:394:GLY:HA2	1:A:420:SER:CB	2.50	0.41
1:A:398:LEU:N	1:A:398:LEU:HD22	2.34	0.41
1:A:57:LYS:HE3	1:B:222:TYR:OH	2.20	0.41
1:C:108:MSE:N	1:C:109:PRO:HD2	2.35	0.41
1:C:549:LYS:HD3	1:C:549:LYS:HA	1.76	0.41
1:D:36:LYS:NZ	1:D:44:GLU:OE2	2.53	0.41
1:A:135:ILE:O	1:A:203:ILE:HA	2.20	0.41
1:A:136:SER:HA	1:A:204:ASP:O	2.19	0.41
1:A:292:LEU:HA	1:A:292:LEU:HD12	1.93	0.41
1:A:454:LEU:HD22	1:A:454:LEU:HA	1.72	0.41
1:B:345:ASP:OD1	1:B:350:LEU:HD21	2.20	0.41
1:B:365:PHE:O	1:B:367:HIS:CD2	2.73	0.41
1:C:85:ILE:HD11	1:C:111:VAL:CG1	2.50	0.41
1:C:369:ALA:HA	1:C:370:PRO:HD3	1.82	0.41
1:D:133:LEU:HA	1:D:133:LEU:HD23	1.82	0.41
1:A:268:LYS:HG2	1:A:268:LYS:O	2.20	0.41
1:B:501:GLN:NE2	1:B:522:VAL:HG12	2.36	0.41
1:C:109:PRO:HA	1:C:113:THR:O	2.20	0.41
1:C:205:VAL:HG11	1:C:231:TYR:HD1	1.86	0.41
1:D:85:ILE:HG13	1:D:86:MSE:HE2	2.01	0.41
1:A:122:GLN:O	1:A:125:HIS:HB2	2.21	0.41
1:A:130:PRO:HG3	1:B:54:LEU:HD23	2.02	0.41
1:A:150:TRP:NE1	1:A:152:GLU:CD	2.74	0.41
1:A:301:PRO:O	1:A:302:ILE:C	2.56	0.41
1:A:492:LEU:CD2	1:A:496:LYS:HE3	2.35	0.41
1:A:45:ARG:CZ	1:A:58:ILE:HD13	2.50	0.41
1:B:144:ARG:NH1	1:B:244:ASP:HB2	2.36	0.41
1:B:315:ALA:HB3	1:B:392:VAL:CG2	2.49	0.41
1:B:456:ASP:C	1:B:456:ASP:OD1	2.59	0.41
1:B:503:THR:OG1	1:B:506:GLU:OE1	2.38	0.41
1:D:105:GLU:HG3	1:D:516:LEU:HD23	2.02	0.41
1:D:177:MSE:HG2	1:D:202:CYS:CB	2.43	0.41
1:D:43:GLN:O	1:D:47:MSE:HB2	2.21	0.41
1:A:29:MSE:HE1	1:A:54:LEU:CD2	2.51	0.41
1:A:392:VAL:HG13	5:A:4006:HOH:O	2.20	0.41
1:A:191:ALA:O	1:A:476:LEU:HD22	2.21	0.41
1:B:152:GLU:CG	1:B:196:ASP:HB2	2.50	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HA	1:B:362:GLN:NE2	2.36	0.41
1:D:504:ASP:OD1	1:D:504:ASP:N	2.51	0.41
1:A:26:LYS:HA	1:A:29:MSE:HG3	2.02	0.41
1:A:300:LYS:HZ2	1:A:305:HIS:CD2	2.36	0.41
1:A:332:LEU:HD23	1:A:340:LYS:HZ1	1.86	0.41
1:A:371:GLU:OE2	1:A:371:GLU:N	2.36	0.41
1:B:164:GLU:OE1	1:B:225:ARG:HD3	2.21	0.41
1:B:394:GLY:HA2	1:B:420:SER:HB3	2.02	0.41
1:C:112:TYR:CG	1:C:113:THR:N	2.89	0.41
1:C:374:PRO:HB3	1:C:380:ALA:N	2.35	0.41
1:C:397:ARG:NH2	1:C:423:THR:O	2.54	0.41
1:C:50:LEU:HA	1:C:53:LEU:HD12	2.02	0.41
1:C:90:GLU:OE1	1:C:131:LYS:CD	2.68	0.41
1:C:99:ILE:HG22	1:C:100:LEU:HD13	2.03	0.41
1:D:407:MSE:HE2	1:D:407:MSE:HB2	1.92	0.41
1:D:493:GLU:HG2	1:D:533:TYR:CD1	2.55	0.41
1:A:446:GLY:O	1:A:466:ASN:ND2	2.46	0.41
1:A:79:LEU:O	1:A:79:LEU:HG	2.19	0.41
1:D:302:ILE:HD11	1:D:332:LEU:CD2	2.50	0.41
1:D:518:ASN:O	1:D:522:VAL:HG23	2.21	0.41
1:D:93:GLU:O	1:D:96:PHE:HB3	2.20	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.92	0.41
1:A:401:PRO:O	1:A:405:ARG:HG3	2.21	0.41
1:A:502:LEU:HD21	1:A:506:GLU:HB2	2.03	0.41
1:B:478:VAL:CG1	1:B:483:THR:HB	2.40	0.41
1:B:528:ILE:CG2	1:B:550:ALA:HA	2.51	0.41
1:C:358:ILE:CG2	1:C:362:GLN:HB2	2.51	0.41
1:A:343:MSE:CE	1:A:362:GLN:HG2	2.51	0.41
1:A:317:LEU:HD13	1:A:361:TYR:HB2	2.03	0.41
1:B:535:TYR:CE2	1:B:545:GLU:HB2	2.56	0.41
1:C:183:LYS:HG3	1:C:471:PHE:CZ	2.55	0.41
1:D:376:THR:HG23	1:D:379:ASP:OD2	2.21	0.41
1:D:458:ARG:HB2	1:D:460:PHE:HE2	1.86	0.41
1:A:29:MSE:HE1	1:A:54:LEU:HD21	2.03	0.40
1:A:85:ILE:HG12	1:A:86:MSE:CE	2.45	0.40
1:C:546:PRO:CD	1:C:549:LYS:HE3	2.51	0.40
1:C:55:PRO:HG3	1:D:134:PHE:CZ	2.56	0.40
1:D:522:VAL:HG12	1:D:526:ILE:HD12	2.03	0.40
1:A:112:TYR:O	1:A:116:VAL:HG12	2.21	0.40
1:A:303:SER:OG	1:A:304:GLU:HG3	2.22	0.40
1:A:503:THR:HG23	1:A:506:GLU:OE1	2.21	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ARG:HE	1:B:270:ARG:HB2	1.65	0.40
1:B:454:LEU:HD11	1:B:460:PHE:HE2	1.86	0.40
1:B:85:ILE:HA	1:B:88:ILE:HG13	2.03	0.40
1:C:137:ILE:HD12	1:C:234:LEU:HD22	2.02	0.40
1:A:329:GLU:HG3	1:A:329:GLU:O	2.20	0.40
1:A:71:ASN:ND2	1:A:74:LYS:HZ1	2.20	0.40
1:A:68:PHE:CG	1:A:99:ILE:HG13	2.55	0.40
1:B:112:TYR:CG	1:B:113:THR:N	2.90	0.40
1:B:298:ILE:HD11	1:B:442:LEU:HD13	2.03	0.40
1:B:346:LYS:HB2	1:B:346:LYS:NZ	2.32	0.40
1:D:366:THR:HG22	1:D:366:THR:O	2.21	0.40
1:D:533:TYR:C	1:D:533:TYR:CD2	2.95	0.40
1:D:91:ARG:NH1	1:D:91:ARG:CG	2.82	0.40
1:A:153:ASN:ND2	1:A:153:ASN:N	2.70	0.40
1:A:534:LEU:HD23	1:A:539:MSE:HE2	2.04	0.40
1:C:186:LEU:HD13	1:C:468:VAL:HG23	2.03	0.40
1:C:399:PHE:HB2	1:C:428:CYS:HB3	2.04	0.40
1:D:144:ARG:O	1:D:144:ARG:HD2	2.20	0.40
1:D:134:PHE:CE2	1:D:177:MSE:HG3	2.56	0.40
1:D:219:MSE:HB2	1:D:219:MSE:HE2	1.88	0.40
1:D:329:GLU:CG	1:D:330:ASN:HD22	2.32	0.40
1:D:339:LYS:HD3	1:D:339:LYS:HA	1.79	0.40
1:D:552:TYR:CD1	1:D:556:ARG:CZ	3.04	0.40
1:A:397:ARG:HG3	1:A:427:GLU:O	2.20	0.40
1:A:38:MSE:CB	1:A:59:GLU:HG3	2.51	0.40
1:B:520:GLN:HE21	1:B:520:GLN:N	2.03	0.40
1:C:217:PHE:O	1:C:218:TYR:C	2.59	0.40
1:C:301:PRO:HD2	1:C:304:GLU:OE1	2.21	0.40
1:C:511:ARG:HB3	1:C:511:ARG:HH11	1.86	0.40
1:D:194:ARG:HH21	1:D:197:ARG:NE	2.20	0.40
1:D:359:ASP:OD2	1:D:362:GLN:HG3	2.22	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	551/584 (94%)	512 (93%)	34 (6%)	5 (1%)	19	38
1	B	551/584 (94%)	512 (93%)	32 (6%)	7 (1%)	13	27
1	C	551/584 (94%)	513 (93%)	34 (6%)	4 (1%)	24	46
1	D	551/584 (94%)	499 (91%)	43 (8%)	9 (2%)	11	21
All	All	2204/2336 (94%)	2036 (92%)	143 (6%)	25 (1%)	16	33

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	LEU
1	B	332	LEU
1	C	332	LEU
1	D	270	ARG
1	D	332	LEU
1	B	360	SER
1	D	397	ARG
1	A	103	ASP
1	B	123	TYR
1	B	209	ASN
1	C	392	VAL
1	D	56	PRO
1	D	103	ASP
1	A	56	PRO
1	B	369	ALA
1	D	218	TYR
1	D	335	GLN
1	C	56	PRO
1	C	360	SER
1	A	302	ILE
1	B	392	VAL
1	D	302	ILE
1	A	166	ILE
1	B	363	GLU
1	D	392	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	469/483 (97%)	371 (79%)	98 (21%)	1	2
1	B	469/483 (97%)	374 (80%)	95 (20%)	1	2
1	C	469/483 (97%)	380 (81%)	89 (19%)	1	2
1	D	469/483 (97%)	356 (76%)	113 (24%)	1	1
All	All	1876/1932 (97%)	1481 (79%)	395 (21%)	1	2

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	24	LYS
1	A	26	LYS
1	A	28	LEU
1	A	29	MSE
1	A	63	ILE
1	A	70	ARG
1	A	73	LYS
1	A	75	MSE
1	A	76	THR
1	A	80	GLU
1	A	85	ILE
1	A	91	ARG
1	A	99	ILE
1	A	100	LEU
1	A	101	GLN
1	A	102	ASP
1	A	111	VAL
1	A	120	CYS
1	A	123	TYR
1	A	133	LEU
1	A	137	ILE
1	A	138	SER
1	A	140	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	144	ARG
1	A	152	GLU
1	A	153	ASN
1	A	169	LEU
1	A	197	ARG
1	A	205	VAL
1	A	212	LEU
1	A	219	MSE
1	A	221	LEU
1	A	224	LYS
1	A	227	ARG
1	A	228	THR
1	A	238	PHE
1	A	239	MSE
1	A	248	ARG
1	A	251	LEU
1	A	260	HIS
1	A	267	ARG
1	A	272	LYS
1	A	283	THR
1	A	286	VAL
1	A	292	LEU
1	A	295	GLN
1	A	296	LYS
1	A	297	VAL
1	A	300	LYS
1	A	306	LYS
1	A	322	LEU
1	A	327	MSE
1	A	330	ASN
1	A	334	GLU
1	A	335	GLN
1	A	336	GLU
1	A	346	LYS
1	A	352	LYS
1	A	355	LYS
1	A	360	SER
1	A	372	SER
1	A	378	GLU
1	A	392	VAL
1	A	397	ARG
1	A	398	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	400	THR
1	A	402	ASP
1	A	409	SER
1	A	413	ARG
1	A	419	LEU
1	A	423	THR
1	A	435	THR
1	A	436	LEU
1	A	438	GLU
1	A	445	SER
1	A	454	LEU
1	A	455	THR
1	A	461	THR
1	A	464	GLN
1	A	484	ARG
1	A	492	LEU
1	A	499	THR
1	A	502	LEU
1	A	503	THR
1	A	504	ASP
1	A	505	GLU
1	A	506	GLU
1	A	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	542	ARG
1	A	547	GLU
1	A	551	LYS
1	A	554	LYS
1	A	556	ARG
1	A	559	ARG
1	A	561	GLU
1	B	22	LYS
1	B	24	LYS
1	B	43	GLN
1	B	47	MSE
1	B	50	LEU
1	B	51	GLN
1	B	66	LEU
1	B	73	LYS
1	B	85	ILE
1	B	94	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	99	ILE
1	B	100	LEU
1	B	104	ILE
1	B	106	SER
1	B	123	TYR
1	B	129	ARG
1	B	131	LYS
1	B	140	ARG
1	B	156	LYS
1	B	165	ARG
1	B	177	MSE
1	B	197	ARG
1	B	208	ASP
1	B	214	LYS
1	B	223	GLN
1	B	224	LYS
1	B	225	ARG
1	B	227	ARG
1	B	229	GLN
1	B	232	ASP
1	B	233	ASP
1	B	236	ASP
1	B	239	MSE
1	B	240	LYS
1	B	248	ARG
1	B	267	ARG
1	B	270	ARG
1	B	292	LEU
1	B	297	VAL
1	B	300	LYS
1	B	301	PRO
1	B	303	SER
1	B	306	LYS
1	B	310	LEU
1	B	319	ILE
1	B	321	ASN
1	B	326	SER
1	B	334	GLU
1	B	339	LYS
1	B	340	LYS
1	B	350	LEU
1	B	351	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	355	LYS
1	B	357	LYS
1	B	363	GLU
1	B	368	SER
1	B	372	SER
1	B	373	ILE
1	B	378	GLU
1	B	385	LYS
1	B	389	ILE
1	B	397	ARG
1	B	398	LEU
1	B	402	ASP
1	B	405	ARG
1	B	411	ASN
1	B	413	ARG
1	B	438	GLU
1	B	440	ARG
1	B	447	SER
1	B	455	THR
1	B	466	ASN
1	B	489	SER
1	B	492	LEU
1	B	499	THR
1	B	500	SER
1	B	502	LEU
1	B	505	GLU
1	B	507	LEU
1	B	509	GLN
1	B	511	ARG
1	B	514	PRO
1	B	516	LEU
1	B	518	ASN
1	B	520	GLN
1	B	522	VAL
1	B	524	ILE
1	B	528	ILE
1	B	529	LYS
1	B	531	THR
1	B	547	GLU
1	B	549	LYS
1	B	551	LYS
1	B	561	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	564	SER
1	C	21	ILE
1	C	23	GLU
1	C	26	LYS
1	C	66	LEU
1	C	70	ARG
1	C	71	ASN
1	C	72	LEU
1	C	75	MSE
1	C	77	SER
1	C	85	ILE
1	C	99	ILE
1	C	100	LEU
1	C	101	GLN
1	C	111	VAL
1	C	122	GLN
1	C	123	TYR
1	C	125	HIS
1	C	131	LYS
1	C	140	ARG
1	C	153	ASN
1	C	165	ARG
1	C	169	LEU
1	C	177	MSE
1	C	183	LYS
1	C	197	ARG
1	C	210	ILE
1	C	214	LYS
1	C	221	LEU
1	C	223	GLN
1	C	225	ARG
1	C	230	GLN
1	C	235	ILE
1	C	236	ASP
1	C	240	LYS
1	C	248	ARG
1	C	249	ASN
1	C	251	LEU
1	C	267	ARG
1	C	286	VAL
1	C	291	LEU
1	C	292	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	297	VAL
1	C	304	GLU
1	C	306	LYS
1	C	314	GLU
1	C	321	ASN
1	C	335	GLN
1	C	339	LYS
1	C	340	LYS
1	C	345	ASP
1	C	355	LYS
1	C	357	LYS
1	C	363	GLU
1	C	368	SER
1	C	375	ASP
1	C	384	LEU
1	C	397	ARG
1	C	398	LEU
1	C	404	ILE
1	C	409	SER
1	C	419	LEU
1	C	428	CYS
1	C	436	LEU
1	C	438	GLU
1	C	454	LEU
1	C	455	THR
1	C	461	THR
1	C	484	ARG
1	C	492	LEU
1	C	502	LEU
1	C	504	ASP
1	C	507	LEU
1	C	511	ARG
1	C	516	LEU
1	C	519	ILE
1	C	520	GLN
1	C	521	GLU
1	C	531	THR
1	C	538	LYS
1	C	542	ARG
1	C	543	TYR
1	C	545	GLU
1	C	547	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	554	LYS
1	C	556	ARG
1	C	560	SER
1	C	561	GLU
1	C	564	SER
1	C	571	GLU
1	D	22	LYS
1	D	23	GLU
1	D	24	LYS
1	D	29	MSE
1	D	36	LYS
1	D	51	GLN
1	D	60	THR
1	D	62	ASP
1	D	66	LEU
1	D	70	ARG
1	D	74	LYS
1	D	75	MSE
1	D	85	ILE
1	D	89	GLN
1	D	91	ARG
1	D	94	LYS
1	D	99	ILE
1	D	100	LEU
1	D	120	CYS
1	D	123	TYR
1	D	125	HIS
1	D	133	LEU
1	D	140	ARG
1	D	144	ARG
1	D	152	GLU
1	D	153	ASN
1	D	156	LYS
1	D	165	ARG
1	D	169	LEU
1	D	177	MSE
1	D	183	LYS
1	D	197	ARG
1	D	205	VAL
1	D	210	ILE
1	D	214	LYS
1	D	221	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	227	ARG
1	D	229	GLN
1	D	236	ASP
1	D	237	GLU
1	D	245	ARG
1	D	249	ASN
1	D	251	LEU
1	D	261	ASN
1	D	266	LEU
1	D	267	ARG
1	D	270	ARG
1	D	283	THR
1	D	286	VAL
1	D	291	LEU
1	D	292	LEU
1	D	298	ILE
1	D	299	SER
1	D	300	LYS
1	D	303	SER
1	D	305	HIS
1	D	322	LEU
1	D	327	MSE
1	D	329	GLU
1	D	333	SER
1	D	335	GLN
1	D	336	GLU
1	D	339	LYS
1	D	350	LEU
1	D	355	LYS
1	D	358	ILE
1	D	360	SER
1	D	363	GLU
1	D	371	GLU
1	D	376	THR
1	D	384	LEU
1	D	387	SER
1	D	388	THR
1	D	389	ILE
1	D	392	VAL
1	D	397	ARG
1	D	405	ARG
1	D	409	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	412	GLU
1	D	428	CYS
1	D	431	GLU
1	D	436	LEU
1	D	440	ARG
1	D	445	SER
1	D	452	VAL
1	D	455	THR
1	D	456	ASP
1	D	464	GLN
1	D	489	SER
1	D	492	LEU
1	D	500	SER
1	D	502	LEU
1	D	504	ASP
1	D	507	LEU
1	D	509	GLN
1	D	512	LEU
1	D	518	ASN
1	D	520	GLN
1	D	529	LYS
1	D	531	THR
1	D	534	LEU
1	D	535	TYR
1	D	538	LYS
1	D	547	GLU
1	D	549	LYS
1	D	551	LYS
1	D	554	LYS
1	D	555	GLU
1	D	556	ARG
1	D	557	THR
1	D	559	ARG
1	D	561	GLU
1	D	571	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	71	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	122	GLN
1	A	153	ASN
1	A	261	ASN
1	A	295	GLN
1	A	305	HIS
1	A	330	ASN
1	A	482	ASN
1	A	520	GLN
1	B	43	GLN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	154	HIS
1	B	229	GLN
1	B	338	GLN
1	B	362	GLN
1	B	367	HIS
1	B	425	GLN
1	B	482	ASN
1	B	501	GLN
1	B	518	ASN
1	B	520	GLN
1	C	64	GLN
1	C	69	HIS
1	C	71	ASN
1	C	153	ASN
1	C	229	GLN
1	C	261	ASN
1	C	321	ASN
1	C	335	GLN
1	C	362	GLN
1	C	425	GLN
1	C	482	ASN
1	C	520	GLN
1	D	51	GLN
1	D	64	GLN
1	D	69	HIS
1	D	122	GLN
1	D	153	ASN
1	D	154	HIS
1	D	230	GLN
1	D	249	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	261	ASN
1	D	305	HIS
1	D	330	ASN
1	D	425	GLN
1	D	482	ASN
1	D	518	ASN
1	D	520	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
3	NAD	A	601	-	40,48,48	1.75	9 (22%)	44,73,73	1.75	3 (6%)
3	NAD	A	602	-	40,48,48	1.79	8 (20%)	44,73,73	1.77	3 (6%)
4	MAK	A	603	2	1,7,7	3.27	1 (100%)	0,9,9	0.00	-
3	NAD	B	1601	-	40,48,48	1.64	7 (17%)	44,73,73	1.91	4 (9%)
3	NAD	B	1602	-	40,48,48	1.86	10 (25%)	44,73,73	1.74	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAK	B	1603	2	1,7,7	3.13	1 (100%)	0,9,9	0.00	-
3	NAD	C	2601	-	40,48,48	1.65	8 (20%)	44,73,73	1.82	6 (13%)
3	NAD	C	2602	-	40,48,48	1.94	10 (25%)	44,73,73	1.74	3 (6%)
4	MAK	C	2603	2	1,7,7	3.15	1 (100%)	0,9,9	0.00	-
3	NAD	D	3601	-	40,48,48	1.86	8 (20%)	44,73,73	1.82	3 (6%)
3	NAD	D	3602	-	40,48,48	1.73	8 (20%)	44,73,73	1.81	4 (9%)
4	MAK	D	3603	2	1,7,7	3.09	1 (100%)	0,9,9	0.00	-

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
3	NAD	A	601	-	-	0/22/62/62	0/5/5/5
3	NAD	A	602	-	-	0/22/62/62	0/5/5/5
4	MAK	A	603	2	-	0/0/8/8	0/0/0/0
3	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
3	NAD	B	1602	-	-	0/22/62/62	0/5/5/5
4	MAK	B	1603	2	-	0/0/8/8	0/0/0/0
3	NAD	C	2601	-	-	0/22/62/62	0/5/5/5
3	NAD	C	2602	-	-	0/22/62/62	0/5/5/5
4	MAK	C	2603	2	-	0/0/8/8	0/0/0/0
3	NAD	D	3601	-	-	0/22/62/62	0/5/5/5
3	NAD	D	3602	-	-	0/22/62/62	0/5/5/5
4	MAK	D	3603	2	-	0/0/8/8	0/0/0/0

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3601	NAD	C5A-C4A	-3.33	1.33	1.40
3	B	1601	NAD	C5A-C4A	-3.18	1.33	1.40
3	C	2601	NAD	C5A-C4A	-3.18	1.33	1.40
3	A	601	NAD	C5A-C4A	-2.98	1.33	1.40
3	D	3602	NAD	C5A-C4A	-2.88	1.34	1.40
3	A	602	NAD	C5A-C4A	-2.72	1.34	1.40
3	D	3601	NAD	C5A-N7A	-2.61	1.30	1.39
3	A	602	NAD	C5A-N7A	-2.61	1.30	1.39
3	C	2601	NAD	C5A-N7A	-2.48	1.31	1.39
3	B	1602	NAD	C5A-C4A	-2.42	1.35	1.40
3	D	3602	NAD	C5A-N7A	-2.40	1.31	1.39

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2602	NAD	C5A-C4A	-2.36	1.35	1.40
3	B	1601	NAD	C5A-N7A	-2.30	1.31	1.39
3	C	2602	NAD	C5A-N7A	-2.25	1.31	1.39
3	A	601	NAD	C5A-N7A	-2.20	1.31	1.39
3	D	3602	NAD	C4N-C3N	2.04	1.42	1.39
3	C	2602	NAD	C4N-C3N	2.12	1.43	1.39
3	B	1602	NAD	C4N-C3N	2.13	1.43	1.39
3	B	1602	NAD	C2A-N1A	2.13	1.37	1.33
3	C	2602	NAD	C2A-N1A	2.16	1.38	1.33
3	A	601	NAD	C2A-N1A	2.16	1.38	1.33
3	C	2601	NAD	C5N-C4N	2.22	1.43	1.38
3	A	602	NAD	C4N-C3N	2.23	1.43	1.39
3	B	1602	NAD	O4D-C4D	2.24	1.50	1.45
3	C	2602	NAD	C8A-N9A	2.31	1.39	1.36
3	C	2601	NAD	O4D-C1D	2.36	1.44	1.41
3	A	601	NAD	C4N-C3N	2.47	1.43	1.39
3	C	2601	NAD	O4B-C1B	2.61	1.44	1.41
3	B	1602	NAD	C8A-N9A	2.67	1.40	1.36
3	B	1601	NAD	O4D-C1D	3.00	1.45	1.41
4	D	3603	MAK	O3-C2	3.09	1.28	1.22
3	C	2601	NAD	C6N-N1N	3.10	1.43	1.35
3	C	2602	NAD	C3N-C7N	3.12	1.55	1.50
3	D	3601	NAD	C4N-C3N	3.13	1.44	1.39
4	B	1603	MAK	O3-C2	3.13	1.28	1.22
3	B	1601	NAD	C2A-N3A	3.14	1.37	1.32
3	A	602	NAD	C3N-C7N	3.15	1.55	1.50
4	C	2603	MAK	O3-C2	3.15	1.28	1.22
3	D	3602	NAD	C3N-C7N	3.17	1.55	1.50
3	B	1602	NAD	C3N-C7N	3.19	1.55	1.50
3	B	1601	NAD	C6N-N1N	3.19	1.43	1.35
4	A	603	MAK	O3-C2	3.27	1.28	1.22
3	D	3601	NAD	C2A-N3A	3.30	1.37	1.32
3	D	3602	NAD	C2A-N3A	3.33	1.37	1.32
3	B	1602	NAD	C2A-N3A	3.45	1.37	1.32
3	A	601	NAD	C6N-N1N	3.48	1.44	1.35
3	A	601	NAD	C3N-C7N	3.48	1.56	1.50
3	B	1601	NAD	O4B-C1B	3.49	1.46	1.41
3	C	2601	NAD	C2A-N3A	3.50	1.37	1.32
3	D	3602	NAD	C6N-N1N	3.54	1.44	1.35
3	B	1602	NAD	C6N-N1N	3.58	1.44	1.35
3	C	2602	NAD	C6N-N1N	3.62	1.44	1.35
3	A	602	NAD	C6N-N1N	3.63	1.44	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3601	NAD	C6N-N1N	3.74	1.45	1.35
3	B	1601	NAD	C3N-C7N	3.82	1.56	1.50
3	A	602	NAD	O4D-C1D	3.83	1.46	1.41
3	A	601	NAD	O4B-C1B	3.87	1.46	1.41
3	C	2602	NAD	C2A-N3A	3.90	1.38	1.32
3	A	602	NAD	C2A-N3A	3.91	1.38	1.32
3	D	3602	NAD	O4D-C1D	3.95	1.46	1.41
3	A	601	NAD	C2A-N3A	3.97	1.38	1.32
3	A	601	NAD	O4D-C1D	4.08	1.46	1.41
3	D	3602	NAD	O4B-C1B	4.26	1.47	1.41
3	A	602	NAD	O4B-C1B	4.33	1.47	1.41
3	D	3601	NAD	O4B-C1B	4.33	1.47	1.41
3	B	1602	NAD	O4B-C1B	4.34	1.47	1.41
3	D	3601	NAD	C3N-C7N	4.60	1.57	1.50
3	D	3601	NAD	O4D-C1D	4.75	1.47	1.41
3	C	2601	NAD	C3N-C7N	4.84	1.58	1.50
3	C	2602	NAD	O4D-C1D	5.02	1.48	1.41
3	B	1602	NAD	O4D-C1D	5.20	1.48	1.41
3	C	2602	NAD	O4B-C1B	5.50	1.48	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1601	NAD	N3A-C2A-N1A	-9.96	120.34	128.86
3	D	3602	NAD	N3A-C2A-N1A	-9.53	120.71	128.86
3	D	3601	NAD	N3A-C2A-N1A	-9.47	120.76	128.86
3	C	2601	NAD	N3A-C2A-N1A	-9.26	120.94	128.86
3	A	602	NAD	N3A-C2A-N1A	-9.23	120.96	128.86
3	A	601	NAD	N3A-C2A-N1A	-9.08	121.09	128.86
3	C	2602	NAD	N3A-C2A-N1A	-9.06	121.11	128.86
3	B	1602	NAD	N3A-C2A-N1A	-8.94	121.21	128.86
3	D	3601	NAD	C4D-O4D-C1D	-2.70	107.01	109.83
3	B	1601	NAD	C3N-C7N-N7N	-2.62	114.71	117.76
3	C	2601	NAD	C3N-C7N-N7N	-2.49	114.87	117.76
3	C	2601	NAD	C4B-O4B-C1B	-2.48	107.24	109.83
3	A	601	NAD	C4D-O4D-C1D	-2.33	107.40	109.83
3	C	2601	NAD	C4D-O4D-C1D	-2.32	107.41	109.83
3	B	1601	NAD	C4D-O4D-C1D	-2.04	107.70	109.83
3	D	3602	NAD	C3N-C7N-N7N	-2.03	115.40	117.76
3	D	3602	NAD	C2D-C3D-C4D	2.07	106.60	102.62
3	C	2601	NAD	O7N-C7N-C3N	2.08	122.24	119.62
3	C	2602	NAD	C2D-C3D-C4D	2.17	106.78	102.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAD	C2D-C3D-C4D	2.17	106.79	102.62
3	B	1602	NAD	C2D-C3D-C4D	2.27	106.98	102.62
3	C	2602	NAD	C4A-C5A-N7A	4.26	113.53	109.41
3	B	1602	NAD	C4A-C5A-N7A	4.42	113.68	109.41
3	C	2601	NAD	C4A-C5A-N7A	4.43	113.69	109.41
3	D	3602	NAD	C4A-C5A-N7A	4.43	113.69	109.41
3	A	601	NAD	C4A-C5A-N7A	4.54	113.80	109.41
3	A	602	NAD	C4A-C5A-N7A	4.58	113.83	109.41
3	D	3601	NAD	C4A-C5A-N7A	4.64	113.89	109.41
3	B	1601	NAD	C4A-C5A-N7A	4.68	113.93	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAD	3	0
3	A	602	NAD	1	0
4	A	603	MAK	1	0
3	B	1601	NAD	4	0
3	B	1602	NAD	1	0
4	B	1603	MAK	1	0
3	C	2601	NAD	3	0
4	C	2603	MAK	1	0
3	D	3601	NAD	3	0
4	D	3603	MAK	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.