



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:27 AM UTC

PDB ID : 9HIP / pdb_00009hip
EMDB ID : EMD-52197
Title : MnmE-MnmG a2b2 complex
Authors : Maes, L.; Galicia, C.; Fislage, M.; Versees, W.
Deposited on : 2024-11-27
Resolution : 3.31 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

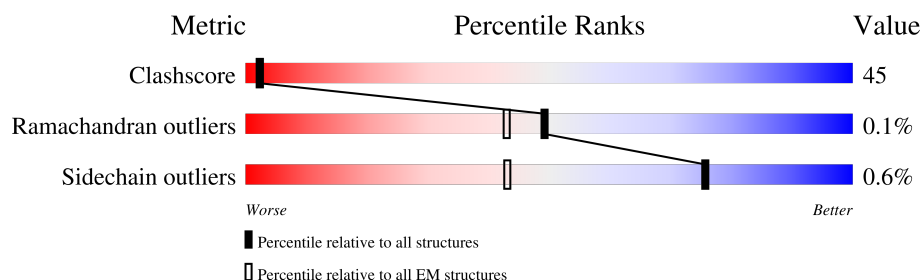
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	454	33% 67%
1	B	454	39% 60% .
2	C	649	46% 49% . .
2	D	649	33% 46% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNP	A	501	-	-	X	-
3	GNP	B	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15846 atoms, of which 26 are hydrogens and 0 are deuteriums.

In the tables below, 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 tRNA modification GTPase MnmE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3458	2164	618	668	8		
1	B	451	Total	C	N	O	S	0	0
			3418	2141	611	658	8		

- Molecule 2 is a protein called tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	624	Total	C	N	O	S	0	0
			4846	3035	872	917	22		
2	D	514	Total	C	N	O	S	0	0
			3981	2499	710	754	18		

There are 40 discrepancies between the modelled and reference sequences:

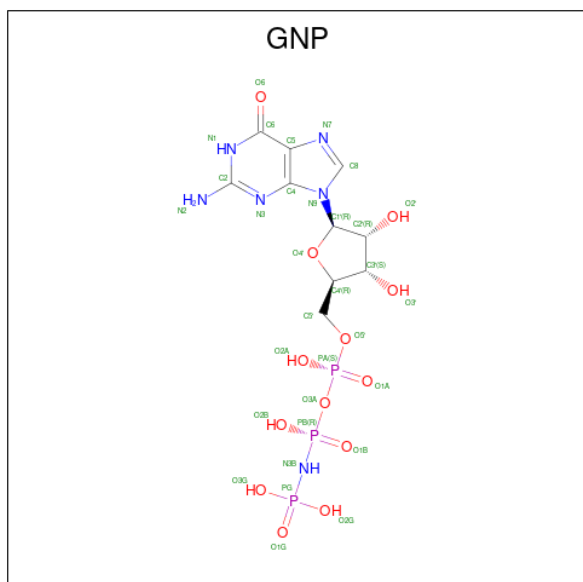
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P0A6U3
C	-18	GLY	-	expression tag	UNP P0A6U3
C	-17	SER	-	expression tag	UNP P0A6U3
C	-16	SER	-	expression tag	UNP P0A6U3
C	-15	HIS	-	expression tag	UNP P0A6U3
C	-14	HIS	-	expression tag	UNP P0A6U3
C	-13	HIS	-	expression tag	UNP P0A6U3
C	-12	HIS	-	expression tag	UNP P0A6U3
C	-11	HIS	-	expression tag	UNP P0A6U3
C	-10	HIS	-	expression tag	UNP P0A6U3
C	-9	SER	-	expression tag	UNP P0A6U3
C	-8	SER	-	expression tag	UNP P0A6U3
C	-7	GLY	-	expression tag	UNP P0A6U3
C	-6	GLU	-	expression tag	UNP P0A6U3
C	-5	ASN	-	expression tag	UNP P0A6U3
C	-4	LEU	-	expression tag	UNP P0A6U3

Continued on next page...

Continued from previous page...

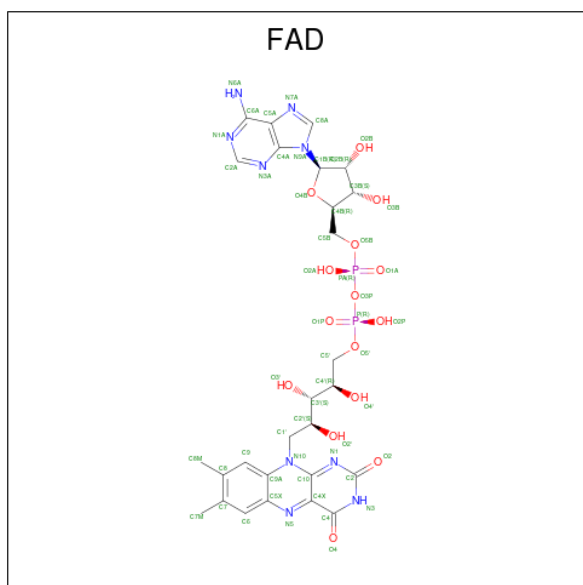
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP P0A6U3
C	-2	PHE	-	expression tag	UNP P0A6U3
C	-1	GLN	-	expression tag	UNP P0A6U3
C	0	GLY	-	expression tag	UNP P0A6U3
D	-19	MET	-	initiating methionine	UNP P0A6U3
D	-18	GLY	-	expression tag	UNP P0A6U3
D	-17	SER	-	expression tag	UNP P0A6U3
D	-16	SER	-	expression tag	UNP P0A6U3
D	-15	HIS	-	expression tag	UNP P0A6U3
D	-14	HIS	-	expression tag	UNP P0A6U3
D	-13	HIS	-	expression tag	UNP P0A6U3
D	-12	HIS	-	expression tag	UNP P0A6U3
D	-11	HIS	-	expression tag	UNP P0A6U3
D	-10	HIS	-	expression tag	UNP P0A6U3
D	-9	SER	-	expression tag	UNP P0A6U3
D	-8	SER	-	expression tag	UNP P0A6U3
D	-7	GLY	-	expression tag	UNP P0A6U3
D	-6	GLU	-	expression tag	UNP P0A6U3
D	-5	ASN	-	expression tag	UNP P0A6U3
D	-4	LEU	-	expression tag	UNP P0A6U3
D	-3	TYR	-	expression tag	UNP P0A6U3
D	-2	PHE	-	expression tag	UNP P0A6U3
D	-1	GLN	-	expression tag	UNP P0A6U3
D	0	GLY	-	expression tag	UNP P0A6U3

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 45	C 10	H 13	N 6	O 13	P 3	0
3	B	1	Total 45	C 10	H 13	N 6	O 13	P 3	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

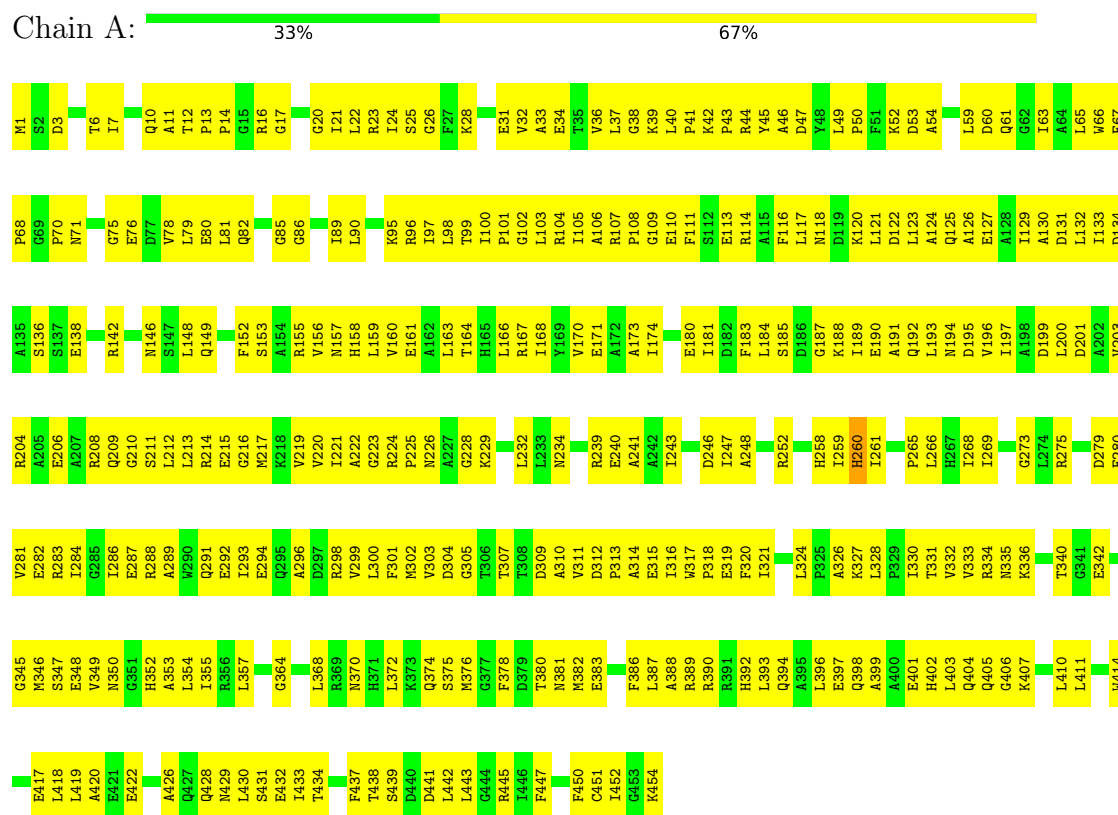


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			53	27	9	15	2	

3 Residue-property plots

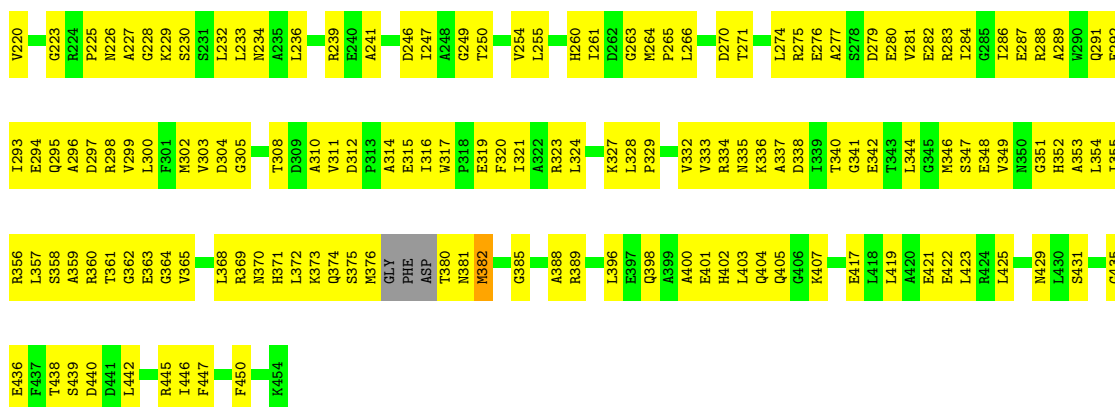
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: tRNA modification GTPase MnME



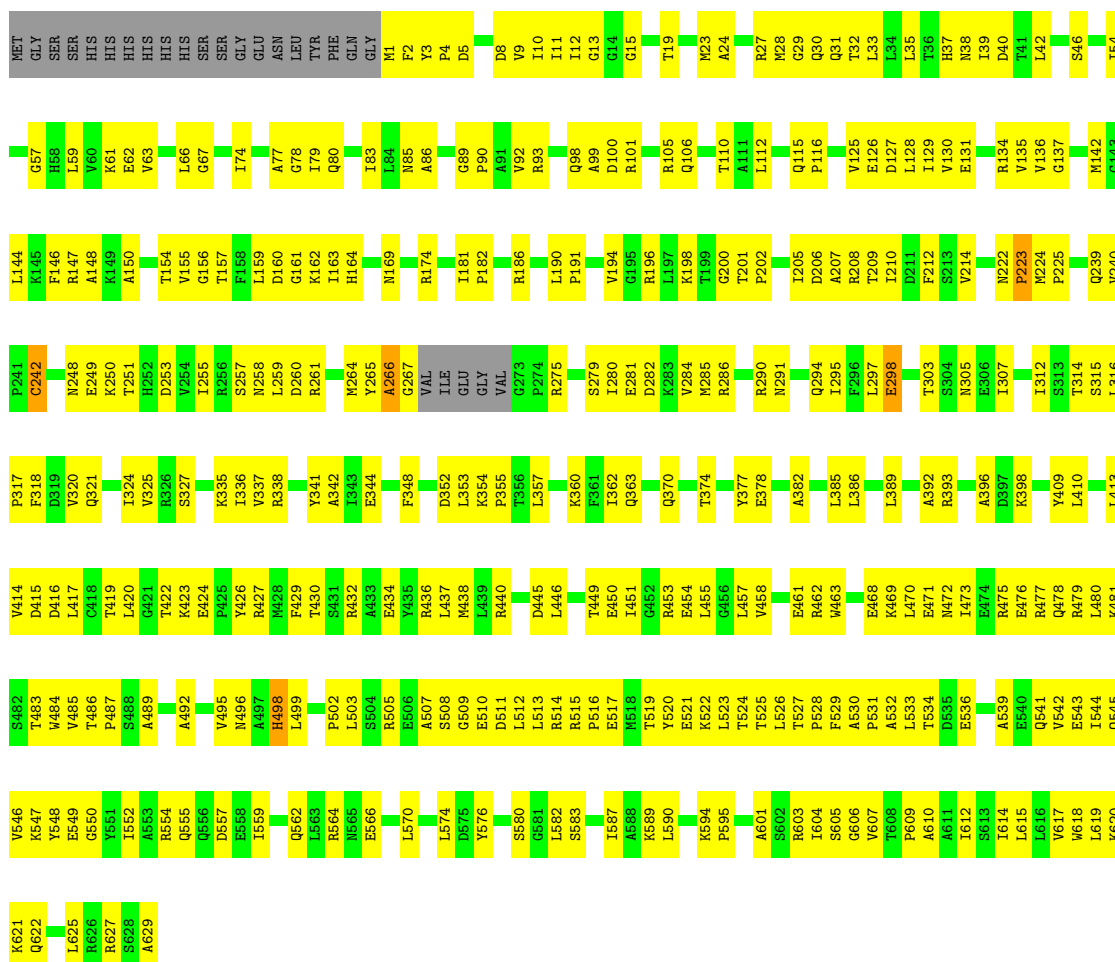
• Molecule 1: tRNA modification GTPase MnME





• Molecule 2: tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG

Chain C: 46% 49%



• Molecule 2: tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG

Chain D: 33% 46% 21%

GLN	GLY	MET	GLN	GLY	MET
ARG	LEU	GLY	LEU	GLY	GLY
ASN	ARG	SER	ASN	SER	SER
GLU	ASN	HIS	GLU	HIS	HIS
ASN	GLU	HIS	ASN	HIS	HIS
THR	THR	HIS	THR	HIS	HIS
LEU	LEU	HIS	LEU	HIS	HIS
PRO	PRO	HIS	PRO	HIS	HIS
ALA	ALA	SER	ALA	SER	SER
THR	THR	SER	THR	SER	SER
LEU	LEU	GLY	LEU	GLY	GLY
ASP	ASP	GLU	ASP	GLU	GLU
TYR	TYR	ASN	TYR	ASN	ASN
ARG	ARG	LEU	ARG	LEU	LEU
GLN	GLN	TYR	GLN	TYR	TYR
VAL	VAL	PHE	VAL	PHE	PHE
SER	SER	GLN	SER	GLN	GLN
GLY	GLY	GLY	GLY	GLY	GLY
LEU	LEU	M1	LEU	M1	M1
SER	SER	Y3	SER	Y3	Y3
ASN	ASN	P4	ASN	P4	P4
VAL	VAL	V9	VAL	V9	V9
GLU	GLU	I10	GLU	I10	I10
ASN	ASN	I11	ASN	I11	I11
ASP	ASP	G15	ASP	G15	G15
HIS	HIS	T19	HIS	T19	T19
LYS	LYS	M23	LYS	M23	M23
PRO	PRO	A24	PRO	A24	A24
ALA	ALA	A25	ALA	A25	A25
SER	SER	M28	SER	M28	M28
GLY	GLY	G29	GLY	G29	G29
LEU	LEU	Q31	LEU	Q31	Q31
THR	THR	T32	THR	T32	T32
PRO	PRO	L35	PRO	L35	L35
ALA	ALA	T36	ALA	T36	T36
ILE	ILE	H37	ILE	H37	H37
ARG	ARG	I39	ARG	I39	I39
GLN	GLN	Q44	GLN	Q44	Q44
LEU	LEU	M45	LEU	M45	M45
ASP	ASP	C47	ASP	C47	C47
VAL	VAL	N48	VAL	N48	N48
GLY	GLY	I51	GLY	I51	I51
LEU	LEU	G52	LEU	G52	G52
THR	THR	G53	THR	G53	G53
VAL	VAL	I54	VAL	I54	I54
LYS	LYS	G55	LYS	G55	G55
GLN	GLN	K56	GLN	K56	K56
GLY	GLY	L59	GLY	L59	L59
MET	MET	V60	MET	V60	V60
LEU	LEU	K61	LEU	K61	K61
ASN	ASN	E62	ASN	E62	E62
THR	THR	V63	THR	V63	V63
VAL	VAL	A71	VAL	A71	A71
SER	SER	I74	SER	I74	I74
GLY	GLY	A77	GLY	A77	A77
LEU	LEU	G78	LEU	G78	G78
ASP	ASP	I79	ASP	I79	I79
TYR	TYR	Q80	TYR	Q80	Q80
GLN	GLN	F81	GLN	F81	F81
LEU	LEU	R82	LEU	R82	R82
ASP	ASP	I83	ASP	I83	I83
VAL	VAL	S87	VAL	S87	S87
GLY	GLY	K88	GLY	K88	K88
LEU	LEU	G89	LEU	G89	G89
ASN	ASN	P90	ASN	P90	P90
THR	THR	A91	THR	A91	A91
VAL	VAL	V92	VAL	V92	V92
GLY	GLY	R93	GLY	R93	R93
LEU	LEU	T95	LEU	T95	T95
ASP	ASP	R96	ASP	R96	R96
THR	THR	H164	THR	H164	H164
VAL	VAL	I165	VAL	I165	I165
SER	SER	Q98	SER	Q98	Q98
GLY	GLY	A99	GLY	A99	A99
LEU	LEU	D100	LEU	D100	D100
ASN	ASN	R101	ASN	R101	R101
THR	THR	G172	THR	G172	G172
VAL	VAL	V102	VAL	V102	V102
GLY	GLY	L103	GLY	L103	L103
LEU	LEU	Y104	LEU	Y104	Y104
ASP	ASP	R105	ASP	R105	R105
THR	THR	Q106	THR	Q106	Q106
VAL	VAL	A107	VAL	A107	A107
GLY	GLY	V108	GLY	V108	V108
LEU	LEU	R109	LEU	R109	R109
ASN	ASN	L112	ASN	L112	L112
THR	THR	E113	THR	E113	E113
VAL	VAL	N114	VAL	N114	N114
GLY	GLY	Q115	GLY	Q115	Q115
LEU	LEU	P116	LEU	P116	P116
ASP	ASP	N117	ASP	N117	N117
THR	THR	I120	THR	I120	I120
VAL	VAL	Q123	VAL	Q123	Q123
GLY	GLY	A124	GLY	A124	A124
LEU	LEU	V125	LEU	V125	V125
ASP	ASP	E126	ASP	E126	E126
THR	THR	D127	THR	D127	D127
VAL	VAL	L128	VAL	L128	L128
GLY	GLY	I129	GLY	I129	I129
LEU	LEU	T209	LEU	T209	T209
ASN	ASN	I210	ASN	I210	I210
THR	THR	H219	THR	H219	H219
VAL	VAL	D221	VAL	D221	D221
GLY	GLY	N222	GLY	N222	N222
LEU	LEU	P223	LEU	P223	P223
ASP	ASP	M224	ASP	M224	M224
THR	THR	P225	THR	P225	P225
VAL	VAL	V226	VAL	V226	V226
GLY	GLY	F227	GLY	F227	F227
LEU	LEU	N232	LEU	N232	N232
ASN	ASN	A233	ASN	A233	A233
THR	THR	S234	THR	S234	S234
VAL	VAL	P237	VAL	P237	P237
GLY	GLY	Q238	GLY	Q238	Q238
LEU	LEU	V240	LEU	V240	V240
ASP	ASP	C242	ASP	C242	C242
THR	THR	Y243	THR	Y243	Y243
VAL	VAL	I244	VAL	I244	I244
GLY	GLY	T245	GLY	T245	T245
LEU	LEU	H246	LEU	H246	H246
ASN	ASN	T247	ASN	T247	T247
THR	THR	N248	THR	N248	N248
VAL	VAL	E249	VAL	E249	E249
GLY	GLY	K250	GLY	K250	K250
LEU	LEU	T251	LEU	T251	T251
ASP	ASP	V254	ASP	V254	V254
THR	THR	I255	THR	I255	I255
VAL	VAL	ARG	VAL	ARG	ARG
GLY	GLY	ASN	GLY	ASN	ASN
LEU	LEU	LEU	LEU	LEU	LEU
ASN	ASN	ASP	ASN	ASP	ASP
THR	THR	SER	THR	SER	SER
VAL	VAL	PRO	VAL	PRO	PRO
GLY	GLY	MET	GLY	MET	MET
LEU	LEU	TYR	LEU	TYR	TYR
ASP	ASP	ALA	ASP	ALA	ALA
THR	THR	GLY	THR	GLY	GLY
VAL	VAL	VAL	VAL	VAL	VAL
GLY	GLY	ILE	GLY	ILE	ILE
LEU	LEU	GLU	LEU	GLU	GLU
ASP	ASP	GLY	ASP	GLY	GLY
THR	THR	VAL	THR	VAL	VAL
VAL	VAL	GLY	VAL	GLY	GLY
GLY	GLY	Y341	GLY	Y341	Y341
LEU	LEU	A342	LEU	A342	A342
ASN	ASN	I343	ASN	I343	I343
THR	THR	E344	THR	E344	E344
VAL	VAL	Y345	VAL	Y345	Y345
GLY	GLY	D346	GLY	D346	D346
LEU	LEU	F347	LEU	F347	F347
ASP	ASP	F348	ASP	F348	F348
THR	THR	V320	THR	V320	V320
VAL	VAL	Q321	VAL	Q321	Q321
GLY	GLY	N322	GLY	N322	N322
LEU	LEU	Q323	LEU	Q323	Q323
ASN	ASN	I324	ASN	I324	I324
THR	THR	V325	THR	V325	V325
VAL	VAL	R326	VAL	R326	R326
GLY	GLY	S327	GLY	S327	S327
LEU	LEU	N328	LEU	N328	N328
ASP	ASP	Q329	ASP	Q329	Q329
THR	THR	R405	THR	R405	R405
VAL	VAL	M331	VAL	M331	M331
GLY	GLY	E332	GLY	E332	E332
LEU	LEU	N333	LEU	N333	N333
ASN	ASN	A334	ASN	A334	A334
THR	THR	F335	THR	F335	F335
VAL	VAL	I336	VAL	I336	I336
GLY	GLY	Y337	GLY	Y337	Y337
LEU	LEU	R338	LEU	R338	R338
ASP	ASP	A401	ASP	A401	A401
THR	THR	A402	THR	A402	A402
VAL	VAL	P403	VAL	P403	P403
GLY	GLY	A404	GLY	A404	A404
LEU	LEU	R405	LEU	R405	R405
ASN	ASN	S406	ASN	S406	S406
THR	THR	Q407	THR	Q407	Q407
VAL	VAL	A408	VAL	A408	A408
GLY	GLY	Y409	GLY	Y409	Y409
LEU	LEU	L410	LEU	L410	L410
ASP	ASP	G411	ASP	G411	G411
THR	THR	V412	THR	V412	V412
VAL	VAL	L413	VAL	L413	L413
GLY	GLY	V414	GLY	V414	V414
LEU	LEU	D415	LEU	D415	D415
ASP	ASP	T419	ASP	T419	T419
THR	THR	L420	THR	L420	L420
VAL	VAL	G421	VAL	G421	G421
GLY	GLY	T422	GLY	T422	T422
LEU	LEU	F423	LEU	F423	F423
ASN	ASN	N496	ASN	N496	N496

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

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: FAD, GNP

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	0.06	0/3511	0.20	0/4752
1	B	0.07	0/3469	0.21	0/4698
2	C	0.09	0/4934	0.25	0/6678
2	D	0.08	0/4055	0.25	1/5492 (0.0%)
All	All	0.08	0/15969	0.23	1/21620 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	312	ILE	N-CA-C	-5.47	107.95	113.20

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	3458	0	3452	436	0
1	B	3418	0	3409	346	0
2	C	4846	0	4847	340	0
2	D	3981	0	3966	334	0
3	A	32	13	13	14	0
3	B	32	13	13	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	53	0	31	2	0
All	All	15820	26	15731	1409	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 45.

All (1409) 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)
2:C:489:ALA:HB3	2:C:492:ALA:HB2	1.38	1.05
1:B:358:SER:HB3	1:B:363:GLU:HB2	1.33	1.04
2:D:156:GLY:HA2	2:D:370:GLN:HB2	1.38	1.03
2:D:472:ASN:HB3	2:D:533:LEU:HD11	1.41	1.02
2:D:28:MET:HE1	2:D:389:LEU:HA	1.40	0.99
2:C:389:LEU:HD13	2:C:457:LEU:HD11	1.45	0.98
1:B:357:LEU:HD22	1:B:368:LEU:HD11	1.47	0.96
1:A:3:ASP:HA	1:A:114:ARG:HH21	1.31	0.96
2:D:1:MET:HE3	2:D:145:LYS:HZ3	1.28	0.96
2:C:83:ILE:HD11	2:C:225:PRO:HG3	1.46	0.95
2:C:2:PHE:HE2	2:C:147:ARG:HG3	1.32	0.94
1:A:224:ARG:HG3	1:A:225:PRO:HD2	1.51	0.93
1:B:152:PHE:HA	1:B:206:GLU:HG2	1.49	0.92
2:C:285:MET:HA	2:C:285:MET:HE2	1.52	0.91
1:A:197:ILE:HD11	1:A:403:LEU:HB3	1.51	0.90
2:C:619:LEU:HB3	2:C:625:LEU:HD23	1.53	0.90
2:D:190:LEU:HD13	2:D:362:ILE:HD11	1.53	0.90
1:B:217:MET:HE3	1:B:380:THR:HA	1.54	0.90
1:B:264:MET:HE1	1:B:376:MET:HB2	1.53	0.89
2:C:496:ASN:HB3	2:C:502:PRO:HB3	1.54	0.89
1:A:442:LEU:HD12	1:A:445:ARG:HD2	1.55	0.88
2:D:420:LEU:HD22	2:D:422:THR:HB	1.53	0.87
1:B:225:PRO:HG2	1:B:275:ARG:HD3	1.56	0.87
2:D:487:PRO:HA	2:D:503:LEU:HD23	1.56	0.87
2:C:190:LEU:HG	2:C:191:PRO:HD2	1.56	0.86
1:A:336:LYS:HD3	3:A:501:GNP:N2	1.91	0.86
2:C:142:MET:HB3	2:D:165:ILE:HD12	1.58	0.86
1:A:336:LYS:HE2	3:A:501:GNP:N3	1.91	0.85
1:B:125:GLN:OE1	1:B:125:GLN:N	2.09	0.85
2:D:404:ALA:HB3	2:D:407:GLN:HG2	1.58	0.85
1:A:228:GLY:HA2	3:A:501:GNP:O2A	1.75	0.85
1:B:440:ASP:OD1	2:C:275:ARG:NH2	2.08	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:GLU:N	2:D:536:GLU:OE1	2.10	0.85
2:C:157:THR:HG22	2:C:370:GLN:HG2	1.59	0.84
2:D:513:LEU:HB2	2:D:523:LEU:HD11	1.59	0.84
1:A:100:ILE:HG23	1:A:103:LEU:HD23	1.59	0.84
2:C:564:ARG:NH2	2:C:627:ARG:O	2.10	0.83
1:A:240:GLU:OE2	1:B:288:ARG:NH1	2.11	0.83
2:C:281:GLU:N	2:C:281:GLU:OE1	2.12	0.83
2:C:526:LEU:HD23	2:C:528:PRO:HD2	1.59	0.83
2:D:210:ILE:HD12	2:D:331:MET:HG2	1.61	0.83
1:A:193:LEU:HD21	1:A:407:LYS:HB3	1.61	0.82
2:D:28:MET:CE	2:D:389:LEU:HA	2.08	0.82
2:C:78:GLY:HA2	2:C:99:ALA:HA	1.61	0.82
2:D:317:PRO:HG2	2:D:320:VAL:HG23	1.61	0.82
2:D:513:LEU:HA	2:D:518:MET:HG2	1.62	0.82
1:A:42:LYS:HD2	1:A:43:PRO:HD2	1.58	0.82
2:C:79:ILE:HD12	2:C:240:VAL:CG2	2.09	0.82
1:A:261:ILE:HG12	1:A:266:LEU:HD21	1.62	0.81
2:C:9:VAL:HG23	2:C:32:THR:HG23	1.60	0.81
2:C:618:TRP:HE3	2:C:619:LEU:HD22	1.46	0.81
2:D:190:LEU:CD1	2:D:362:ILE:HD11	2.11	0.81
1:B:344:LEU:HD11	1:B:363:GLU:HB3	1.62	0.81
1:A:17:GLY:HA2	1:B:382:MET:HE1	1.62	0.81
1:A:303:VAL:HG21	1:A:316:ILE:HG21	1.61	0.81
1:A:211:SER:HA	1:A:214:ARG:HG3	1.61	0.81
1:A:451:CYS:SG	1:B:16:ARG:NH1	2.53	0.81
2:C:24:ALA:HA	2:C:27:ARG:HH12	1.45	0.81
2:D:469:LYS:O	2:D:473:ILE:HG23	1.80	0.81
2:C:485:VAL:O	2:C:507:ALA:N	2.14	0.81
1:B:347:SER:O	1:B:354:LEU:N	2.13	0.80
2:D:433:ALA:O	2:D:436:ARG:NE	2.14	0.80
2:C:29:GLY:O	2:C:30:GLN:NE2	2.15	0.80
2:D:83:ILE:HD11	2:D:225:PRO:HG3	1.64	0.80
2:C:514:ARG:NH1	2:C:546:VAL:O	2.15	0.80
1:A:221:ILE:HG22	1:A:229:LYS:HD2	1.63	0.80
1:A:215:GLU:OE1	1:A:215:GLU:N	2.16	0.79
2:C:524:THR:HG21	2:C:532:ALA:HB2	1.63	0.79
1:A:203:VAL:O	1:A:206:GLU:HG2	1.81	0.79
2:C:224:MET:SD	2:C:239:GLN:NE2	2.56	0.79
2:C:198:LYS:HB2	2:C:344:GLU:HG3	1.66	0.78
2:C:527:THR:HB	2:C:528:PRO:HD3	1.64	0.78
1:B:42:LYS:HD2	1:B:45:TYR:HB2	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:326:ARG:HH12	2:D:333:ASN:HA	1.48	0.78
1:A:96:ARG:NH1	1:A:99:THR:OG1	2.17	0.78
2:C:125:VAL:HG22	4:C:701:FAD:H62A	1.48	0.78
1:A:347:SER:O	1:A:354:LEU:N	2.11	0.78
2:C:378:GLU:N	2:C:378:GLU:OE1	2.16	0.78
1:A:153:SER:O	1:A:157:ASN:ND2	2.15	0.77
1:A:319:GLU:N	1:A:319:GLU:OE1	2.18	0.77
2:D:196:ARG:NE	2:D:345:TYR:O	2.17	0.77
1:A:39:LYS:HE2	1:A:49:LEU:HD12	1.67	0.77
1:A:315:GLU:N	1:A:315:GLU:OE1	2.17	0.77
2:C:562:GLN:O	2:C:566:GLU:HG2	1.85	0.77
1:B:47:ASP:OD1	1:B:48:TYR:N	2.17	0.77
2:C:1:MET:O	2:C:144:LEU:HD12	1.84	0.77
1:A:214:ARG:HH12	1:A:389:ARG:HD3	1.50	0.77
1:B:155:ARG:HB2	1:B:203:VAL:HG22	1.65	0.77
2:C:3:TYR:HE2	2:C:5:ASP:HB2	1.49	0.77
2:C:27:ARG:NH2	2:C:67:GLY:O	2.18	0.77
2:C:316:LEU:HD13	2:C:320:VAL:HG11	1.66	0.76
2:D:164:HIS:HE1	2:D:344:GLU:HG2	1.50	0.76
2:C:468:GLU:O	2:C:472:ASN:ND2	2.18	0.76
2:D:102:VAL:O	2:D:106:GLN:HG2	1.86	0.76
2:D:487:PRO:HG3	2:D:503:LEU:HB3	1.68	0.76
1:A:228:GLY:HA2	3:A:501:GNP:PA	2.26	0.76
1:B:48:TYR:OH	1:B:61:GLN:OE1	2.03	0.76
1:A:155:ARG:HH22	1:A:159:LEU:HD21	1.48	0.76
2:D:306:GLU:OE2	2:D:338:ARG:NH1	2.16	0.76
2:C:434:GLU:N	2:C:434:GLU:OE1	2.17	0.76
1:A:393:LEU:O	1:A:397:GLU:HG2	1.86	0.75
1:B:400:ALA:O	1:B:404:GLN:HG2	1.85	0.75
1:A:6:THR:HG23	1:A:26:GLY:HA3	1.67	0.75
1:A:196:VAL:HA	1:A:199:ASP:OD2	1.85	0.75
1:A:301:PHE:O	1:A:333:VAL:N	2.15	0.75
1:B:344:LEU:CD1	1:B:363:GLU:HB3	2.17	0.75
2:C:3:TYR:CE2	2:C:5:ASP:HB2	2.21	0.75
1:A:213:LEU:O	1:A:265:PRO:HG3	1.85	0.75
2:C:415:ASP:OD2	2:C:603:ARG:NH1	2.18	0.75
2:C:542:VAL:O	2:C:546:VAL:HG22	1.87	0.75
1:A:402:HIS:HB3	1:A:426:ALA:HB2	1.67	0.75
2:C:77:ALA:O	2:C:100:ASP:N	2.20	0.75
1:B:98:LEU:HD11	1:B:105:ILE:HD11	1.68	0.75
1:B:174:ILE:HG23	2:C:92:VAL:HG21	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:ND2	1:A:239:ARG:O	2.19	0.74
1:A:314:ALA:HA	1:A:321:ILE:HD13	1.68	0.74
1:A:401:GLU:O	1:A:405:GLN:HG2	1.86	0.74
2:C:354:LYS:HB3	2:C:355:PRO:HD2	1.70	0.74
2:C:520:TYR:O	2:C:524:THR:HG23	1.87	0.74
1:A:110:GLU:HA	1:A:113:GLU:HB3	1.68	0.74
1:B:195:ASP:OD1	1:B:196:VAL:N	2.20	0.74
1:B:342:GLU:OE1	1:B:356:ARG:NE	2.18	0.74
1:B:303:VAL:HG21	1:B:332:VAL:HG13	1.69	0.74
2:C:415:ASP:O	2:C:419:THR:HG22	1.87	0.74
2:C:427:ARG:O	2:C:432:ARG:NH1	2.21	0.73
1:B:167:ARG:HA	1:B:170:VAL:HG12	1.70	0.73
1:B:336:LYS:HG2	3:B:501:GNP:C5	2.18	0.73
1:A:96:ARG:O	1:A:99:THR:OG1	2.06	0.73
1:B:184:LEU:O	1:B:189:ILE:HG13	1.88	0.73
2:D:309:PRO:HB2	2:D:312:ILE:HD12	1.69	0.73
1:B:53:ASP:OD1	1:B:57:SER:N	2.22	0.73
1:B:417:GLU:OE1	1:B:417:GLU:N	2.16	0.73
2:D:91:ALA:HB1	2:D:436:ARG:CG	2.19	0.73
1:A:301:PHE:N	1:A:331:THR:O	2.22	0.73
2:D:91:ALA:HB1	2:D:436:ARG:HG3	1.69	0.73
1:A:192:GLN:HA	1:A:195:ASP:OD2	1.88	0.72
2:D:83:ILE:HG12	2:D:221:ASP:OD2	1.88	0.72
1:A:97:ILE:O	1:A:100:ILE:HG22	1.89	0.72
1:B:308:THR:O	1:B:334:ARG:NH2	2.22	0.72
1:A:191:ALA:HA	1:A:194:ASN:ND2	2.03	0.72
2:C:28:MET:HE1	2:C:389:LEU:HD12	1.69	0.72
2:D:62:GLU:OE2	2:D:409:TYR:N	2.17	0.72
2:D:520:TYR:O	2:D:524:THR:HG23	1.89	0.72
1:B:230:SER:O	1:B:233:LEU:HG	1.88	0.72
2:C:483:THR:HG23	2:C:509:GLY:H	1.53	0.72
2:D:172:GLY:HA2	2:D:179:PRO:HG3	1.72	0.72
1:A:100:ILE:HD12	1:A:101:PRO:HD2	1.72	0.72
1:A:370:ASN:O	1:A:374:GLN:HG2	1.90	0.72
1:A:402:HIS:ND1	1:A:422:GLU:OE1	2.23	0.72
1:A:334:ARG:N	1:A:355:ILE:O	2.19	0.72
2:C:275:ARG:NE	2:C:424:GLU:OE2	2.18	0.72
1:B:31:GLU:N	1:B:31:GLU:OE1	2.21	0.71
2:D:92:VAL:HG13	2:D:430:THR:HG21	1.72	0.71
1:B:234:ASN:OD1	1:B:241:ALA:N	2.20	0.71
2:C:526:LEU:CD2	2:C:528:PRO:HD2	2.19	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:HA	1:B:321:ILE:HG13	1.72	0.71
2:C:79:ILE:HD12	2:C:240:VAL:HG22	1.71	0.71
1:A:167:ARG:O	1:A:171:GLU:HG2	1.90	0.71
2:C:495:VAL:HA	2:C:498:HIS:CE1	2.24	0.71
2:D:477:ARG:NH1	2:D:545:GLN:OE1	2.23	0.71
2:C:242:CYS:SG	2:C:298:GLU:HB3	2.30	0.71
2:C:524:THR:CG2	2:C:532:ALA:HB2	2.21	0.71
1:B:336:LYS:HE2	3:B:501:GNP:C8	2.20	0.71
2:D:506:GLU:OE1	2:D:506:GLU:HA	1.90	0.71
1:A:326:ALA:O	1:A:327:LYS:NZ	2.18	0.70
2:C:181:ILE:HB	2:C:182:PRO:HD3	1.72	0.70
2:C:539:ALA:O	2:C:542:VAL:HG22	1.91	0.70
2:D:520:TYR:OH	2:D:532:ALA:HB1	1.91	0.70
1:B:312:ASP:O	1:B:315:GLU:HG2	1.91	0.70
1:B:60:ASP:OD1	1:B:61:GLN:N	2.24	0.70
1:A:95:LYS:O	1:A:99:THR:HG23	1.90	0.70
1:B:320:PHE:CZ	1:B:324:LEU:HD11	2.26	0.70
2:C:618:TRP:CE3	2:C:619:LEU:HD22	2.27	0.70
2:D:389:LEU:HD12	2:D:457:LEU:HD11	1.73	0.70
1:A:54:ALA:HB2	1:A:96:ARG:NH2	2.07	0.70
1:B:127:GLU:OE1	1:B:127:GLU:N	2.20	0.70
1:B:227:ALA:HB1	1:B:302:MET:SD	2.32	0.70
1:B:277:ALA:HB2	1:B:286:ILE:HD12	1.72	0.70
2:D:224:MET:HE2	2:D:239:GLN:HG3	1.72	0.70
1:B:30:ARG:HG3	1:B:31:GLU:OE1	1.92	0.70
1:B:305:GLY:HA2	1:B:334:ARG:HH21	1.57	0.70
2:C:440:ARG:CZ	2:C:544:ILE:HG21	2.21	0.70
1:A:21:ILE:HG13	1:A:82:GLN:HG2	1.74	0.70
2:C:222:ASN:HB2	2:C:223:PRO:HD2	1.74	0.69
1:A:43:PRO:HB3	1:A:68:PRO:HD2	1.74	0.69
1:A:433:ILE:HD12	1:A:434:THR:HG23	1.73	0.69
1:B:16:ARG:HH21	1:B:260:HIS:HB3	1.55	0.69
1:B:29:ALA:HB3	1:B:77:ASP:HB3	1.74	0.69
1:A:42:LYS:HD2	1:A:43:PRO:CD	2.22	0.69
1:A:246:ASP:HA	3:A:501:GNP:O3'	1.92	0.69
2:C:160:ASP:OD1	2:C:162:LYS:NZ	2.24	0.69
2:C:562:GLN:N	2:C:562:GLN:OE1	2.26	0.69
1:A:311:VAL:HG23	1:A:349:VAL:HG21	1.71	0.69
1:B:371:HIS:HA	1:B:374:GLN:HG2	1.73	0.69
2:C:582:LEU:HB2	2:C:587:ILE:HD11	1.73	0.69
1:B:311:VAL:HB	1:B:354:LEU:HD22	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:513:LEU:HD22	2:C:546:VAL:HB	1.74	0.69
1:B:148:LEU:HD12	1:B:148:LEU:O	1.93	0.68
2:C:74:ILE:HD11	2:C:99:ALA:HB2	1.74	0.68
1:A:392:HIS:O	1:A:396:LEU:HG	1.93	0.68
1:B:9:ALA:HB3	1:B:111:PHE:HE2	1.58	0.68
1:B:344:LEU:HD22	1:B:357:LEU:HA	1.76	0.68
2:D:524:THR:HG22	2:D:532:ALA:HB2	1.75	0.68
2:C:530:ALA:HB1	2:C:531:PRO:HD2	1.76	0.68
2:D:401:TRP:CH2	2:D:403:PRO:HG3	2.29	0.68
1:A:44:ARG:NH2	1:A:71:ASN:O	2.27	0.68
1:A:44:ARG:HG2	1:A:67:PHE:CE1	2.29	0.68
2:D:519:THR:HG22	2:D:522:LYS:HE2	1.75	0.68
1:A:210:GLY:O	1:A:211:SER:OG	2.11	0.68
1:A:284:ILE:O	1:A:288:ARG:HG2	1.94	0.68
2:D:164:HIS:CE1	2:D:344:GLU:HG2	2.29	0.68
2:D:222:ASN:HB3	2:D:223:PRO:HD3	1.76	0.68
1:A:11:ALA:HB3	1:A:21:ILE:HG23	1.76	0.67
1:A:439:SER:OG	1:A:441:ASP:OD1	2.11	0.67
1:B:67:PHE:HB2	1:B:78:VAL:HG23	1.75	0.67
2:C:249:GLU:OE2	2:C:291:ASN:HB2	1.95	0.67
1:B:96:ARG:NH2	1:B:99:THR:OG1	2.27	0.67
2:C:471:GLU:HB3	2:C:475:ARG:HH21	1.57	0.67
2:D:98:GLN:NE2	2:D:298:GLU:OE1	2.28	0.67
2:D:480:LEU:O	2:D:483:THR:HG22	1.94	0.67
2:D:513:LEU:HB2	2:D:523:LEU:CD1	2.24	0.67
1:A:224:ARG:HG3	1:A:225:PRO:CD	2.24	0.67
1:A:442:LEU:O	1:A:445:ARG:HG2	1.95	0.67
1:B:368:LEU:O	1:B:372:LEU:HG	1.95	0.67
2:C:3:TYR:CD1	2:C:4:PRO:HD2	2.29	0.67
2:C:83:ILE:HD11	2:C:225:PRO:CG	2.24	0.67
2:D:367:PHE:HB3	2:D:372:ASN:HD21	1.60	0.67
1:A:53:ASP:OD1	1:A:54:ALA:N	2.27	0.67
2:C:13:GLY:O	2:C:154:THR:OG1	2.13	0.67
1:A:225:PRO:HG2	1:A:275:ARG:NE	2.09	0.67
1:A:124:ALA:HB3	1:A:152:PHE:HE2	1.58	0.67
1:B:96:ARG:NE	1:B:96:ARG:O	2.28	0.67
2:C:325:VAL:HG21	2:C:336:ILE:HD11	1.77	0.67
2:D:242:CYS:SG	2:D:243:TYR:N	2.68	0.67
2:D:354:LYS:HD2	2:D:358:GLU:HB3	1.76	0.67
1:A:320:PHE:O	1:A:324:LEU:HG	1.95	0.67
1:A:317:TRP:HD1	1:A:320:PHE:HB3	1.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:HB2	1:B:89:ILE:HD11	1.76	0.67
2:C:303:THR:HG23	2:D:109:ARG:HH22	1.59	0.66
2:D:127:ASP:OD1	2:D:128:LEU:N	2.28	0.66
2:C:190:LEU:CG	2:C:191:PRO:HD2	2.24	0.66
2:C:437:LEU:HB2	2:C:555:GLN:HE22	1.60	0.66
2:C:514:ARG:HB2	2:C:515:ARG:NH2	2.10	0.66
2:D:518:MET:SD	2:D:523:LEU:HG	2.35	0.66
1:A:184:LEU:HA	1:A:189:ILE:HD12	1.77	0.66
1:A:243:ILE:HG12	1:B:288:ARG:HH22	1.59	0.66
2:D:491:ALA:O	2:D:495:VAL:HG23	1.96	0.66
1:A:107:ARG:HA	1:A:107:ARG:CZ	2.26	0.66
2:D:326:ARG:NH1	2:D:333:ASN:HA	2.10	0.66
1:A:280:GLU:OE2	1:A:283:ARG:NH2	2.27	0.66
2:D:193:ARG:NH1	2:D:351:ARG:HD2	2.11	0.66
1:A:433:ILE:HD12	1:A:434:THR:N	2.09	0.66
2:D:131:GLU:N	2:D:131:GLU:OE1	2.28	0.66
1:B:360:ARG:HD2	3:B:501:GNP:N2	2.11	0.66
2:C:259:LEU:O	2:C:259:LEU:HD23	1.95	0.66
1:B:279:ASP:OD1	1:B:281:VAL:N	2.28	0.66
1:B:364:GLY:O	1:B:368:LEU:HD12	1.95	0.66
1:B:305:GLY:HA2	1:B:334:ARG:NH2	2.12	0.66
2:C:438:MET:HB3	2:C:552:ILE:CD1	2.26	0.66
2:D:496:ASN:OD1	2:D:503:LEU:N	2.17	0.66
2:D:513:LEU:HA	2:D:518:MET:CG	2.25	0.66
1:B:422:GLU:HA	1:B:422:GLU:OE1	1.96	0.65
2:C:186:ARG:CZ	2:C:186:ARG:HA	2.26	0.65
2:C:487:PRO:HD3	2:C:505:ARG:O	1.96	0.65
2:D:403:PRO:HG2	2:D:410:LEU:HD11	1.78	0.65
1:A:66:TRP:CD1	1:A:68:PRO:HD3	2.32	0.65
1:A:382:MET:SD	1:A:382:MET:N	2.70	0.65
2:C:135:VAL:HG12	2:C:363:GLN:O	1.97	0.65
2:D:135:VAL:HG21	2:D:365:LEU:HB2	1.78	0.65
1:B:277:ALA:HB3	1:B:283:ARG:HG2	1.79	0.65
2:D:1:MET:O	2:D:145:LYS:HG2	1.96	0.65
1:A:36:VAL:HG21	1:A:97:ILE:HD11	1.79	0.65
1:A:208:ARG:HH12	1:A:212:LEU:HD22	1.62	0.65
1:A:243:ILE:HD13	1:B:284:ILE:HG13	1.79	0.65
2:C:526:LEU:HD23	2:C:528:PRO:CD	2.27	0.65
1:A:53:ASP:HB2	1:A:59:LEU:HG	1.77	0.65
1:A:109:GLY:O	1:A:113:GLU:N	2.29	0.65
1:A:204:ARG:HH22	1:A:397:GLU:HA	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLY:O	1:B:274:LEU:N	2.21	0.65
2:C:536:GLU:OE1	2:C:536:GLU:N	2.23	0.65
2:D:410:LEU:HD12	2:D:411:GLY:N	2.11	0.65
2:D:251:THR:O	2:D:255:ILE:HG13	1.97	0.65
1:A:234:ASN:OD1	1:A:241:ALA:N	2.30	0.65
1:A:346:MET:HE1	1:A:353:ALA:CB	2.26	0.65
2:C:28:MET:CE	2:C:392:ALA:HB3	2.27	0.65
1:A:336:LYS:HE2	3:A:501:GNP:C2	2.27	0.64
1:B:167:ARG:NH2	1:B:442:LEU:HD22	2.12	0.64
2:C:131:GLU:OE1	2:C:131:GLU:N	2.31	0.64
1:B:168:ILE:HD11	1:B:445:ARG:HE	1.63	0.64
2:D:358:GLU:HB2	2:D:366:PHE:CE2	2.32	0.64
1:A:368:LEU:O	1:A:372:LEU:HD13	1.98	0.64
2:C:248:ASN:ND2	2:C:250:LYS:HG2	2.12	0.64
2:C:264:MET:SD	2:C:265:TYR:N	2.62	0.64
1:A:197:ILE:HD13	1:A:403:LEU:HD23	1.79	0.64
1:A:214:ARG:HD2	1:A:387:LEU:HD21	1.80	0.64
2:C:389:LEU:HD11	2:C:455:LEU:HD23	1.78	0.64
2:D:83:ILE:CD1	2:D:225:PRO:HG3	2.28	0.64
1:B:44:ARG:HA	1:B:67:PHE:HE1	1.63	0.64
1:B:156:VAL:O	1:B:160:VAL:HG13	1.98	0.64
2:C:24:ALA:HA	2:C:27:ARG:NH1	2.13	0.64
2:C:190:LEU:HD21	2:C:362:ILE:CD1	2.28	0.64
1:A:121:LEU:HD12	1:A:125:GLN:CD	2.23	0.64
1:B:353:ALA:HB1	1:B:355:ILE:HD11	1.80	0.64
2:C:583:SER:O	2:C:587:ILE:HG12	1.97	0.64
1:A:327:LYS:HG2	1:A:328:LEU:HD22	1.78	0.63
1:B:289:ALA:O	1:B:293:ILE:HG13	1.98	0.63
1:B:342:GLU:HB3	1:B:356:ARG:HD3	1.79	0.63
2:D:126:GLU:OE2	2:D:141:GLN:HG3	1.97	0.63
1:A:184:LEU:HB2	1:A:414:TRP:CZ3	2.34	0.63
1:A:317:TRP:NE1	1:A:319:GLU:HB2	2.13	0.63
1:A:429:ASN:HA	1:A:432:GLU:HG3	1.79	0.63
2:C:186:ARG:HA	2:C:186:ARG:NH1	2.13	0.63
2:D:484:TRP:HB3	2:D:506:GLU:OE2	1.98	0.63
1:A:232:LEU:HD11	1:A:368:LEU:CD2	2.28	0.63
2:C:130:VAL:HG22	2:C:135:VAL:HA	1.79	0.63
2:D:28:MET:CE	2:D:392:ALA:HB3	2.28	0.63
1:B:51:PHE:O	1:B:59:LEU:N	2.27	0.63
2:D:403:PRO:HG2	2:D:410:LEU:CD1	2.28	0.63
1:A:336:LYS:CD	3:A:501:GNP:N2	2.61	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:LEU:HD21	2:C:35:LEU:HD13	1.81	0.63
1:B:158:HIS:ND1	1:B:199:ASP:OD1	2.25	0.63
1:A:39:LYS:HE2	1:A:49:LEU:CD1	2.29	0.63
1:A:389:ARG:O	1:A:393:LEU:HD12	1.99	0.63
1:A:399:ALA:O	1:A:403:LEU:HD13	1.99	0.63
2:C:414:VAL:O	2:C:417:LEU:HG	1.98	0.63
1:A:70:PRO:HA	1:A:75:GLY:O	1.99	0.63
2:C:484:TRP:HD1	2:C:508:SER:HB3	1.62	0.63
2:D:445:ASP:O	2:D:449:THR:HG22	1.99	0.63
2:C:222:ASN:CB	2:C:223:PRO:HD2	2.29	0.63
2:C:495:VAL:HA	2:C:498:HIS:HE1	1.63	0.62
2:D:491:ALA:HB1	2:D:494:GLU:OE2	1.98	0.62
1:A:25:SER:CB	1:A:78:VAL:HG22	2.29	0.62
1:B:205:ALA:HA	1:B:208:ARG:NH1	2.14	0.62
2:C:127:ASP:OD1	2:C:128:LEU:N	2.31	0.62
2:C:414:VAL:HA	2:C:417:LEU:CD2	2.29	0.62
2:D:172:GLY:CA	2:D:179:PRO:HG3	2.29	0.62
1:A:390:ARG:HA	1:A:393:LEU:HD12	1.81	0.62
1:A:441:ASP:HB2	1:A:445:ARG:HH21	1.65	0.62
1:B:42:LYS:HD3	1:B:43:PRO:O	2.00	0.62
2:C:83:ILE:CD1	2:C:225:PRO:HG3	2.26	0.62
1:A:346:MET:HA	1:A:355:ILE:HD13	1.80	0.62
2:D:3:TYR:CD1	2:D:4:PRO:HD2	2.34	0.62
1:A:157:ASN:HA	1:A:160:VAL:HG12	1.82	0.62
1:A:200:LEU:O	1:A:204:ARG:HG2	1.99	0.62
1:A:252:ARG:NH2	1:B:250:THR:O	2.30	0.62
1:B:217:MET:HB2	1:B:266:LEU:HD23	1.79	0.62
2:C:527:THR:HB	2:C:528:PRO:CD	2.29	0.62
2:D:51:ILE:HD12	2:D:74:ILE:HD13	1.82	0.62
2:D:129:ILE:HB	2:D:136:VAL:O	2.00	0.62
2:C:453:ARG:HD3	2:C:463:TRP:CD2	2.35	0.62
2:D:408:ALA:O	2:D:412:VAL:HG23	1.99	0.62
2:D:472:ASN:HB3	2:D:533:LEU:CD1	2.25	0.62
1:A:155:ARG:HA	1:A:155:ARG:HH11	1.65	0.62
1:A:185:SER:HB3	1:A:414:TRP:HH2	1.64	0.62
1:A:201:ASP:HA	1:A:204:ARG:HG2	1.82	0.62
1:A:386:PHE:CE2	1:A:388:ALA:HB2	2.34	0.62
1:A:433:ILE:CD1	1:A:434:THR:HG23	2.30	0.62
1:B:217:MET:HE3	1:B:380:THR:CA	2.28	0.62
1:A:17:GLY:CA	1:B:382:MET:HE1	2.29	0.62
1:B:167:ARG:HA	1:B:170:VAL:CG1	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:N	1:B:215:GLU:OE1	2.33	0.62
2:D:353:LEU:HD12	2:D:357:LEU:HA	1.80	0.62
2:D:426:TYR:HE1	2:D:428:MET:HE2	1.64	0.62
2:D:155:VAL:HG11	2:D:159:LEU:CD2	2.30	0.61
2:D:499:LEU:HA	2:D:517:GLU:OE2	2.01	0.61
1:A:127:GLU:OE1	1:A:127:GLU:N	2.26	0.61
1:A:226:ASN:HA	3:A:501:GNP:PB	2.40	0.61
1:B:288:ARG:O	1:B:291:GLN:HG2	2.00	0.61
1:B:401:GLU:O	1:B:405:GLN:HG2	2.00	0.61
1:B:4:ASN:HB3	1:B:27:PHE:CD2	2.36	0.61
2:C:472:ASN:O	2:C:475:ARG:HG2	2.00	0.61
1:A:192:GLN:O	1:A:196:VAL:HG13	2.01	0.61
1:A:194:ASN:OD1	1:A:195:ASP:N	2.33	0.61
2:C:317:PRO:O	2:C:321:GLN:HG3	2.00	0.61
2:D:158:PHE:CD2	2:D:173:GLY:HA3	2.36	0.61
2:D:179:PRO:HG2	2:D:181:ILE:HD11	1.80	0.61
1:A:131:ASP:OD2	1:A:389:ARG:NH2	2.29	0.61
2:C:163:ILE:HG23	2:C:341:TYR:CD2	2.35	0.61
1:A:153:SER:HA	1:A:156:VAL:HG22	1.83	0.61
2:C:413:LEU:HD23	2:C:417:LEU:HD23	1.82	0.61
2:C:469:LYS:O	2:C:473:ILE:HG13	2.01	0.61
1:A:431:SER:O	1:A:434:THR:OG1	2.16	0.61
1:B:24:ILE:CD1	1:B:32:VAL:HG11	2.31	0.61
1:B:173:ALA:HB2	1:B:183:PHE:CG	2.36	0.61
1:B:197:ILE:CD1	1:B:403:LEU:HD23	2.31	0.61
1:B:226:ASN:HB3	3:B:501:GNP:H5'1	1.83	0.61
1:B:233:LEU:CD1	1:B:241:ALA:HB3	2.31	0.61
1:B:304:ASP:OD1	1:B:336:LYS:HD2	2.01	0.61
2:C:9:VAL:HG12	2:C:150:ALA:HB3	1.81	0.61
2:C:66:LEU:HD23	2:C:385:LEU:CD2	2.31	0.61
2:C:508:SER:O	2:C:512:LEU:N	2.33	0.61
1:A:349:VAL:HG11	1:A:354:LEU:HD12	1.83	0.61
1:B:49:LEU:HD12	1:B:50:PRO:HD2	1.82	0.61
1:B:303:VAL:O	1:B:334:ARG:HA	2.01	0.61
2:C:321:GLN:O	2:C:325:VAL:HG23	2.01	0.61
2:D:354:LYS:HG2	2:D:358:GLU:O	2.01	0.61
2:D:9:VAL:HB	2:D:32:THR:HG22	1.83	0.61
2:D:362:ILE:N	2:D:362:ILE:HD12	2.15	0.61
2:D:540:GLU:O	2:D:544:ILE:HG12	2.01	0.61
1:A:50:PRO:HG2	1:A:52:LYS:HE3	1.83	0.60
2:D:198:LYS:HZ2	2:D:344:GLU:HB3	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:O	1:A:32:VAL:HG23	2.01	0.60
1:A:199:ASP:O	1:A:203:VAL:HG13	2.01	0.60
1:B:280:GLU:HA	1:B:283:ARG:NH1	2.17	0.60
1:A:43:PRO:HB3	1:A:68:PRO:CD	2.31	0.60
1:B:312:ASP:O	1:B:316:ILE:HG13	2.01	0.60
2:C:80:GLN:HB3	2:C:98:GLN:HB2	1.84	0.60
2:D:427:ARG:O	2:D:432:ARG:NH1	2.35	0.60
1:A:50:PRO:HG2	1:A:52:LYS:NZ	2.17	0.60
1:B:299:VAL:C	1:B:300:LEU:HD12	2.27	0.60
1:A:310:ALA:HB1	1:A:315:GLU:HB2	1.84	0.60
1:B:49:LEU:CD1	1:B:50:PRO:HD2	2.32	0.60
2:C:251:THR:O	2:C:255:ILE:HG13	2.00	0.60
2:C:496:ASN:OD1	2:C:503:LEU:HD13	2.02	0.60
2:D:1:MET:O	2:D:145:LYS:NZ	2.30	0.60
1:A:317:TRP:CE2	1:A:319:GLU:HB2	2.37	0.60
1:A:220:VAL:HG23	1:A:296:ALA:HB2	1.83	0.60
1:B:166:LEU:O	1:B:170:VAL:HG12	2.01	0.60
1:B:357:LEU:HD22	1:B:368:LEU:CD1	2.25	0.60
2:D:346:ASP:OD1	2:D:347:PHE:N	2.34	0.60
2:D:519:THR:HG23	2:D:522:LYS:H	1.66	0.60
1:B:264:MET:HE1	1:B:376:MET:CB	2.30	0.60
2:C:615:LEU:O	2:C:619:LEU:HD23	2.02	0.60
1:A:402:HIS:CB	1:A:426:ALA:HB2	2.32	0.59
1:B:419:LEU:O	1:B:423:LEU:HD13	2.02	0.59
2:C:495:VAL:O	2:C:499:LEU:HB3	2.02	0.59
2:D:174:ARG:HG2	2:D:175:ALA:H	1.67	0.59
1:A:429:ASN:HA	1:A:432:GLU:CD	2.27	0.59
1:B:207:ALA:HB2	1:B:389:ARG:HH21	1.67	0.59
2:C:374:THR:HG22	2:C:426:TYR:HB3	1.82	0.59
1:A:225:PRO:HG3	1:A:273:GLY:HA3	1.83	0.59
1:A:332:VAL:O	1:A:354:LEU:HA	2.02	0.59
1:B:197:ILE:HD13	1:B:403:LEU:HD23	1.82	0.59
2:C:59:LEU:O	2:C:63:VAL:HG23	2.02	0.59
1:A:204:ARG:NH2	1:A:397:GLU:HA	2.17	0.59
1:A:287:GLU:O	1:A:291:GLN:HG3	2.02	0.59
1:B:51:PHE:N	1:B:60:ASP:O	2.28	0.59
2:D:30:GLN:O	2:D:117:ASN:HB3	2.01	0.59
1:A:159:LEU:O	1:A:163:LEU:HG	2.02	0.59
2:C:39:ILE:HG22	2:C:40:ASP:H	1.67	0.59
2:C:318:PHE:CD2	2:D:144:LEU:HD22	2.37	0.59
2:C:389:LEU:HD11	2:C:455:LEU:CD2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:VAL:HG11	2:D:159:LEU:HD21	1.84	0.59
1:B:217:MET:CE	1:B:380:THR:HA	2.29	0.59
2:C:249:GLU:CD	2:C:291:ASN:HB2	2.27	0.59
2:C:106:GLN:O	2:C:110:THR:HG23	2.02	0.59
2:D:10:ILE:HG12	2:D:148:ALA:CB	2.33	0.59
2:D:186:ARG:O	2:D:189:GLU:HG2	2.03	0.59
2:C:39:ILE:HB	2:D:338:ARG:NH2	2.18	0.59
2:C:190:LEU:HD21	2:C:362:ILE:HD11	1.83	0.59
2:C:520:TYR:CZ	2:C:539:ALA:HB1	2.38	0.59
2:D:2:PHE:CE1	2:D:145:LYS:HD2	2.38	0.59
1:A:247:ILE:HD11	1:B:280:GLU:HB3	1.84	0.59
1:A:294:GLU:OE1	1:A:294:GLU:N	2.27	0.59
2:C:79:ILE:HD12	2:C:240:VAL:HG21	1.84	0.59
2:C:550:GLY:O	2:C:554:ARG:HG3	2.03	0.58
2:D:28:MET:HE3	2:D:392:ALA:HB3	1.86	0.58
1:A:279:ASP:OD1	1:A:281:VAL:N	2.37	0.58
1:A:312:ASP:HB3	1:A:315:GLU:CD	2.28	0.58
2:D:450:GLU:HA	2:D:463:TRP:HZ3	1.68	0.58
1:B:5:ASP:O	1:B:114:ARG:NH2	2.33	0.58
2:D:127:ASP:O	2:D:138:ALA:HB1	2.03	0.58
1:A:3:ASP:HA	1:A:114:ARG:NH2	2.10	0.58
1:A:410:LEU:HB2	1:A:419:LEU:HD22	1.85	0.58
1:B:155:ARG:CB	1:B:203:VAL:HG22	2.33	0.58
1:B:187:GLY:O	1:B:190:GLU:HG3	2.03	0.58
1:B:225:PRO:HB3	1:B:249:GLY:H	1.67	0.58
1:B:254:VAL:O	1:B:255:LEU:HD23	2.03	0.58
1:B:4:ASN:HB3	1:B:27:PHE:CE2	2.37	0.58
1:B:6:THR:O	1:B:103:LEU:HD13	2.03	0.58
2:C:510:GLU:OE1	2:C:510:GLU:N	2.19	0.58
1:A:282:GLU:O	1:A:286:ILE:HG13	2.04	0.58
2:C:125:VAL:HG22	4:C:701:FAD:N6A	2.16	0.58
2:C:130:VAL:HA	2:C:134:ARG:O	2.04	0.58
2:C:513:LEU:CD1	2:C:546:VAL:HG21	2.33	0.58
2:D:251:THR:HG22	2:D:327:SER:HB2	1.85	0.58
1:B:64:ALA:C	1:B:65:LEU:HD12	2.28	0.58
2:C:511:ASP:O	2:C:515:ARG:NH2	2.37	0.58
2:C:564:ARG:HG2	2:C:629:ALA:C	2.28	0.58
2:D:55:GLY:CA	2:D:428:MET:HG3	2.33	0.58
1:B:1:MET:HA	1:B:5:ASP:OD2	2.04	0.58
2:D:306:GLU:OE2	2:D:338:ARG:HD2	2.04	0.58
2:D:475:ARG:HG3	2:D:476:GLU:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:O	1:A:203:VAL:HG22	2.04	0.58
1:B:369:ARG:NH1	1:B:373:LYS:HB3	2.19	0.58
2:C:416:ASP:O	2:C:420:LEU:HB2	2.03	0.58
2:D:61:LYS:HE3	2:D:227:PHE:O	2.04	0.58
2:D:250:LYS:O	2:D:254:VAL:HG23	2.04	0.58
1:A:25:SER:HB2	1:A:78:VAL:HG22	1.85	0.57
1:A:404:GLN:OE1	1:A:407:LYS:HD2	2.04	0.57
1:B:24:ILE:O	1:B:78:VAL:HA	2.04	0.57
2:D:494:GLU:O	2:D:498:HIS:ND1	2.21	0.57
1:A:34:GLU:O	1:A:38:GLY:N	2.37	0.57
1:A:174:ILE:HA	1:A:180:GLU:CD	2.29	0.57
1:A:331:THR:OG1	1:A:353:ALA:HB3	2.04	0.57
1:A:357:LEU:HB3	1:A:364:GLY:HA3	1.84	0.57
1:A:417:GLU:OE1	1:A:417:GLU:N	2.35	0.57
2:C:163:ILE:HG23	2:C:341:TYR:HD2	1.67	0.57
2:C:484:TRP:CD1	2:C:508:SER:HB3	2.38	0.57
1:A:153:SER:O	1:A:156:VAL:HG22	2.04	0.57
1:A:243:ILE:HG12	1:B:288:ARG:HH12	1.69	0.57
1:B:181:ILE:HB	1:B:183:PHE:CE1	2.39	0.57
2:C:86:ALA:O	2:C:93:ARG:NH1	2.38	0.57
1:A:118:ASN:HB2	1:A:120:LYS:HD3	1.86	0.57
2:D:533:LEU:HD22	2:D:535:ASP:H	1.69	0.57
1:A:16:ARG:HD2	1:B:381:ASN:HD22	1.69	0.57
2:D:77:ALA:O	2:D:99:ALA:HA	2.03	0.57
2:D:435:TYR:HB3	2:D:438:MET:SD	2.45	0.57
1:B:6:THR:HA	1:B:26:GLY:HA3	1.87	0.57
1:B:6:THR:HG1	1:B:28:LYS:H	1.49	0.57
2:D:513:LEU:CD2	2:D:546:VAL:HG11	2.34	0.57
2:C:12:ILE:HG21	2:C:125:VAL:HG21	1.87	0.57
2:C:290:ARG:NH1	2:C:290:ARG:HB2	2.18	0.57
2:D:162:LYS:HA	2:D:171:SER:HA	1.86	0.57
1:A:193:LEU:O	1:A:196:VAL:HG22	2.03	0.57
1:B:232:LEU:O	1:B:236:LEU:HD23	2.05	0.57
2:C:533:LEU:HD12	2:C:534:THR:H	1.70	0.57
2:D:144:LEU:HD12	2:D:145:LYS:H	1.70	0.57
2:D:533:LEU:HD22	2:D:535:ASP:HB2	1.86	0.57
2:C:312:ILE:HD11	2:C:324:ILE:HG22	1.87	0.57
1:B:28:LYS:HA	1:B:31:GLU:CD	2.30	0.56
2:D:530:ALA:HB1	2:D:531:PRO:HD2	1.87	0.56
1:A:166:LEU:O	1:A:170:VAL:HG23	2.05	0.56
1:B:436:GLU:OE1	1:B:436:GLU:N	2.33	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HB2	1:A:454:LYS:OXT	2.04	0.56
1:A:122:ASP:OD1	1:A:123:LEU:N	2.37	0.56
1:A:152:PHE:HB3	1:A:386:PHE:CD1	2.40	0.56
1:B:25:SER:O	1:B:114:ARG:NH1	2.38	0.56
1:B:230:SER:HA	1:B:233:LEU:CD2	2.35	0.56
1:B:275:ARG:NE	1:B:282:GLU:OE2	2.27	0.56
1:B:277:ALA:HB2	1:B:286:ILE:CD1	2.35	0.56
2:D:80:GLN:O	2:D:97:ALA:HA	2.04	0.56
2:D:317:PRO:O	2:D:321:GLN:HG3	2.05	0.56
1:A:6:THR:HB	1:A:103:LEU:HD13	1.86	0.56
1:A:7:ILE:HB	1:A:106:ALA:HB2	1.87	0.56
1:A:221:ILE:CG2	1:A:229:LYS:HB3	2.35	0.56
1:A:451:CYS:HB2	1:A:454:LYS:CD	2.35	0.56
1:B:66:TRP:NE1	1:B:68:PRO:HD3	2.21	0.56
2:C:382:ALA:HB1	2:C:410:LEU:HD13	1.87	0.56
2:C:475:ARG:O	2:C:479:ARG:HG2	2.05	0.56
2:C:477:ARG:O	2:C:480:LEU:HG	2.05	0.56
2:D:210:ILE:CD1	2:D:331:MET:HG2	2.34	0.56
2:D:435:TYR:HB3	2:D:438:MET:CG	2.35	0.56
2:D:511:ASP:HA	2:D:514:ARG:NH1	2.21	0.56
1:A:280:GLU:O	1:A:284:ILE:HG13	2.05	0.56
1:A:303:VAL:HG21	1:A:316:ILE:CG2	2.35	0.56
1:B:227:ALA:O	1:B:335:ASN:ND2	2.39	0.56
1:B:292:GLU:HA	1:B:295:GLN:OE1	2.05	0.56
1:B:337:ALA:O	1:B:341:GLY:N	2.26	0.56
2:C:207:ALA:HB2	2:C:307:ILE:HG12	1.86	0.56
1:A:6:THR:HG23	1:A:26:GLY:CA	2.35	0.56
1:A:331:THR:HG23	1:A:353:ALA:O	2.06	0.56
1:B:342:GLU:CB	1:B:356:ARG:HD3	2.36	0.56
1:B:354:LEU:C	1:B:355:ILE:HD12	2.30	0.56
1:B:431:SER:OG	1:B:435:GLY:O	2.05	0.56
2:C:142:MET:CB	2:D:165:ILE:HD12	2.33	0.56
2:C:316:LEU:HB3	2:C:317:PRO:HD2	1.87	0.56
2:C:574:LEU:O	2:C:594:LYS:NZ	2.38	0.56
1:A:21:ILE:HD11	1:A:80:GLU:HG2	1.87	0.56
1:A:225:PRO:CG	1:A:273:GLY:HA3	2.35	0.56
1:B:358:SER:HB3	1:B:363:GLU:CB	2.22	0.56
2:C:458:VAL:HG13	2:C:462:ARG:HB2	1.87	0.56
2:D:155:VAL:HG11	2:D:159:LEU:HG	1.87	0.56
2:D:513:LEU:HD21	2:D:543:GLU:OE1	2.05	0.56
1:B:310:ALA:O	1:B:334:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:HG3	1:A:66:TRP:CD1	2.41	0.56
1:A:96:ARG:HA	1:A:96:ARG:HH11	1.71	0.56
1:B:31:GLU:O	1:B:34:GLU:HG3	2.06	0.56
1:B:98:LEU:HD11	1:B:105:ILE:CD1	2.35	0.56
1:B:337:ALA:HA	1:B:340:THR:OG1	2.05	0.56
2:D:325:VAL:HG11	2:D:336:ILE:HD11	1.88	0.56
2:D:361:PHE:HB2	2:D:362:ILE:HD12	1.86	0.56
2:D:420:LEU:HD23	2:D:420:LEU:O	2.05	0.56
1:B:72:SER:HB2	1:B:78:VAL:HG21	1.87	0.56
2:C:589:LYS:NZ	2:C:606:GLY:HA3	2.20	0.56
1:B:349:VAL:N	1:B:352:HIS:O	2.22	0.55
2:C:11:ILE:N	2:C:11:ILE:HD12	2.21	0.55
2:C:357:LEU:CD1	2:C:386:LEU:HD23	2.37	0.55
2:D:53:GLY:CA	2:D:96:ARG:HG3	2.36	0.55
1:B:157:ASN:O	1:B:160:VAL:HG22	2.06	0.55
1:B:369:ARG:NH1	1:B:369:ARG:O	2.30	0.55
1:A:50:PRO:HG2	1:A:52:LYS:CE	2.36	0.55
1:B:220:VAL:HG21	1:B:296:ALA:HB2	1.88	0.55
2:C:42:LEU:HD13	2:C:112:LEU:HD23	1.87	0.55
2:D:123:GLN:HG3	2:D:140:THR:HB	1.88	0.55
2:D:520:TYR:HB2	2:D:543:GLU:OE2	2.07	0.55
1:A:110:GLU:OE2	1:A:114:ARG:HB2	2.06	0.55
1:A:121:LEU:HD12	1:A:125:GLN:CG	2.36	0.55
1:A:158:HIS:O	1:A:161:GLU:HG2	2.06	0.55
1:A:442:LEU:HA	1:A:445:ARG:HE	1.71	0.55
2:D:162:LYS:O	2:D:343:ILE:HG13	2.06	0.55
1:A:170:VAL:O	1:A:174:ILE:HG13	2.06	0.55
2:D:354:LYS:HB2	2:D:355:PRO:HD2	1.87	0.55
2:D:358:GLU:HA	2:D:366:PHE:HA	1.87	0.55
2:C:66:LEU:HD23	2:C:385:LEU:HD21	1.89	0.55
2:C:182:PRO:O	2:C:186:ARG:HG2	2.06	0.55
2:D:198:LYS:NZ	2:D:344:GLU:HB3	2.21	0.55
2:D:351:ARG:NH2	2:D:421:GLY:O	2.37	0.55
2:C:27:ARG:NH1	2:C:27:ARG:HB3	2.21	0.55
2:C:126:GLU:OE2	2:C:182:PRO:HG2	2.07	0.55
2:D:424:GLU:OE1	2:D:424:GLU:HA	2.06	0.55
1:A:212:LEU:O	1:A:216:GLY:HA2	2.07	0.55
2:C:210:ILE:HB	2:C:212:PHE:CZ	2.42	0.55
2:C:554:ARG:HA	2:C:557:ASP:OD1	2.07	0.55
2:C:595:PRO:HG2	2:C:601:ALA:HB2	1.89	0.55
2:D:181:ILE:HG22	2:D:185:ARG:NH1	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PHE:HE1	1:B:81:LEU:HD13	1.70	0.55
2:C:19:THR:O	2:C:23:MET:HG2	2.06	0.55
2:C:248:ASN:HD21	2:C:250:LYS:HG2	1.71	0.55
2:C:609:PRO:HA	2:C:612:ILE:HG12	1.88	0.55
2:D:314:THR:CG2	2:D:316:LEU:HG	2.36	0.55
1:A:228:GLY:C	1:A:302:MET:HE1	2.32	0.55
1:A:163:LEU:O	1:A:167:ARG:HG3	2.07	0.54
1:A:180:GLU:O	1:A:184:LEU:HG	2.07	0.54
2:D:83:ILE:HD11	2:D:225:PRO:CG	2.37	0.54
2:D:155:VAL:CG1	2:D:159:LEU:HG	2.37	0.54
2:D:499:LEU:HD11	2:D:515:ARG:CZ	2.36	0.54
1:B:226:ASN:ND2	1:B:246:ASP:O	2.40	0.54
1:A:10:GLN:HA	1:A:22:LEU:HD23	1.89	0.54
2:C:393:ARG:NH1	2:C:398:LYS:HD2	2.22	0.54
2:C:513:LEU:CD2	2:C:546:VAL:HB	2.36	0.54
2:D:15:GLY:O	2:D:19:THR:HG23	2.07	0.54
2:D:104:TYR:O	2:D:108:VAL:HG23	2.07	0.54
2:D:348:PHE:HE2	2:D:371:ILE:HD11	1.71	0.54
2:D:356:THR:O	2:D:390:ASN:ND2	2.35	0.54
2:D:499:LEU:HD11	2:D:515:ARG:NE	2.22	0.54
1:A:21:ILE:CG1	1:A:82:GLN:HG2	2.37	0.54
1:B:402:HIS:CE1	1:B:425:LEU:HB3	2.42	0.54
2:D:163:ILE:N	2:D:170:TYR:O	2.35	0.54
2:D:182:PRO:O	2:D:186:ARG:HG2	2.07	0.54
1:A:116:PHE:CZ	1:A:123:LEU:HD13	2.43	0.54
1:A:340:THR:OG1	1:A:342:GLU:HG3	2.08	0.54
1:B:334:ARG:HD3	1:B:356:ARG:CZ	2.38	0.54
2:C:453:ARG:NH1	2:C:458:VAL:O	2.40	0.54
2:C:609:PRO:O	2:C:612:ILE:HG12	2.07	0.54
2:D:28:MET:HE1	2:D:389:LEU:CA	2.27	0.54
1:A:146:ASN:O	1:A:149:GLN:HB2	2.07	0.54
2:C:555:GLN:O	2:C:559:ILE:HG13	2.08	0.54
2:D:496:ASN:HB3	2:D:502:PRO:HB3	1.90	0.54
1:A:12:THR:HG21	1:A:20:GLY:HA2	1.89	0.54
1:A:76:GLU:OE2	1:A:114:ARG:HD3	2.08	0.54
1:A:333:VAL:HA	1:A:355:ILE:O	2.08	0.54
1:A:438:THR:HG21	1:A:442:LEU:HD23	1.90	0.54
1:B:156:VAL:HG12	1:B:203:VAL:HG11	1.89	0.54
1:B:212:LEU:O	1:B:214:ARG:N	2.39	0.54
1:B:230:SER:HA	1:B:233:LEU:HD21	1.90	0.54
2:C:2:PHE:CE2	2:C:147:ARG:HG3	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASP:OD2	2:D:103:LEU:HG	2.07	0.54
2:D:379:GLU:N	2:D:379:GLU:OE1	2.41	0.54
2:D:492:ALA:HB1	2:D:503:LEU:HD22	1.89	0.54
1:A:346:MET:HA	1:A:355:ILE:CD1	2.37	0.54
1:B:6:THR:OG1	1:B:28:LYS:N	2.36	0.54
2:C:156:GLY:O	2:C:370:GLN:HB3	2.07	0.54
1:A:442:LEU:HA	1:A:445:ARG:NE	2.23	0.54
1:B:229:LYS:NZ	3:B:501:GNP:O1B	2.40	0.54
1:B:336:LYS:HA	3:B:501:GNP:O6	2.08	0.54
2:C:62:GLU:OE2	2:C:409:TYR:N	2.39	0.54
2:C:476:GLU:HA	2:C:479:ARG:HG2	1.89	0.54
1:A:383:GLU:N	1:A:383:GLU:OE1	2.41	0.53
2:C:46:SER:OG	2:C:174:ARG:NH1	2.41	0.53
1:A:191:ALA:HA	1:A:194:ASN:HD21	1.72	0.53
1:A:304:ASP:HB3	1:A:307:THR:HG23	1.89	0.53
1:B:282:GLU:O	1:B:286:ILE:HG13	2.08	0.53
2:C:437:LEU:HB2	2:C:555:GLN:NE2	2.22	0.53
2:D:181:ILE:HG22	2:D:185:ARG:HH11	1.74	0.53
1:A:63:ILE:N	1:A:82:GLN:O	2.38	0.53
1:A:121:LEU:HB2	1:A:125:GLN:OE1	2.08	0.53
2:C:514:ARG:HB2	2:C:515:ARG:HH21	1.73	0.53
1:A:160:VAL:O	1:A:164:THR:HG23	2.08	0.53
1:A:222:ALA:HA	1:A:229:LYS:HZ2	1.74	0.53
1:A:226:ASN:HA	3:A:501:GNP:O3A	2.08	0.53
1:A:311:VAL:HG23	1:A:349:VAL:CG2	2.39	0.53
1:A:381:ASN:HB3	1:A:382:MET:HE1	1.90	0.53
1:B:8:VAL:HG21	1:B:97:ILE:HG21	1.91	0.53
2:C:513:LEU:HD11	2:C:546:VAL:HG21	1.90	0.53
2:D:155:VAL:HG11	2:D:159:LEU:CG	2.39	0.53
2:D:404:ALA:N	2:D:407:GLN:OE1	2.41	0.53
2:D:420:LEU:HD22	2:D:422:THR:CB	2.33	0.53
1:A:226:ASN:ND2	1:A:248:ALA:HA	2.22	0.53
1:A:266:LEU:CD1	1:A:268:ILE:HG23	2.38	0.53
1:A:288:ARG:O	1:A:292:GLU:HG2	2.09	0.53
1:B:33:ALA:HB2	1:B:79:LEU:HD12	1.89	0.53
2:C:74:ILE:CD1	2:C:99:ALA:HB2	2.39	0.53
1:A:116:PHE:CE1	1:A:123:LEU:HD13	2.44	0.53
1:A:174:ILE:HG12	1:A:180:GLU:OE2	2.08	0.53
1:A:429:ASN:HA	1:A:432:GLU:CG	2.38	0.53
2:C:434:GLU:H	2:C:434:GLU:CD	2.16	0.53
2:D:51:ILE:HD12	2:D:74:ILE:CG1	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:513:LEU:HD23	2:D:546:VAL:HG11	1.91	0.53
2:D:25:ALA:CB	2:D:32:THR:HG21	2.39	0.53
2:D:249:GLU:OE1	2:D:249:GLU:N	2.35	0.53
1:A:326:ALA:O	1:A:327:LYS:HG2	2.08	0.53
1:B:50:PRO:HA	1:B:61:GLN:HA	1.91	0.53
1:B:193:LEU:HD21	1:B:407:LYS:HB2	1.90	0.53
1:B:327:LYS:O	1:B:329:PRO:HD3	2.09	0.53
1:B:358:SER:CB	1:B:363:GLU:HB2	2.24	0.53
2:C:625:LEU:O	2:C:625:LEU:HD12	2.08	0.53
2:D:28:MET:HE3	2:D:392:ALA:CB	2.39	0.53
2:D:254:VAL:HG21	2:D:323:GLN:OE1	2.09	0.53
1:A:47:ASP:CG	1:A:49:LEU:HD22	2.34	0.53
1:A:53:ASP:HB2	1:A:59:LEU:CD2	2.39	0.53
1:A:209:GLN:OE1	1:A:209:GLN:HA	2.09	0.53
1:A:228:GLY:CA	3:A:501:GNP:O2A	2.51	0.53
1:A:441:ASP:HB2	1:A:445:ARG:NH2	2.23	0.53
1:B:98:LEU:HD11	1:B:105:ILE:CG1	2.39	0.53
1:B:442:LEU:O	1:B:446:ILE:HG13	2.09	0.53
2:D:389:LEU:HD23	2:D:389:LEU:C	2.33	0.53
1:A:185:SER:HB3	1:A:414:TRP:CH2	2.44	0.53
1:A:220:VAL:HG23	1:A:296:ALA:CB	2.39	0.53
2:D:317:PRO:HG2	2:D:320:VAL:CG2	2.37	0.53
1:A:428:GLN:O	1:A:432:GLU:HG3	2.09	0.52
1:B:320:PHE:CE1	1:B:324:LEU:HD11	2.44	0.52
1:A:46:ALA:HB3	1:B:44:ARG:HG3	1.91	0.52
1:A:126:ALA:O	1:A:129:ILE:HB	2.09	0.52
1:A:260:HIS:O	1:A:260:HIS:ND1	2.42	0.52
1:B:49:LEU:HG	1:B:50:PRO:HD2	1.90	0.52
2:C:454:GLU:OE1	2:C:455:LEU:HD12	2.09	0.52
2:D:343:ILE:HG12	2:D:344:GLU:N	2.24	0.52
2:D:501:ALA:HB3	2:D:515:ARG:HH22	1.74	0.52
1:B:337:ALA:HA	1:B:340:THR:HG1	1.74	0.52
2:C:414:VAL:HA	2:C:417:LEU:HD21	1.92	0.52
1:A:53:ASP:HB2	1:A:59:LEU:CG	2.39	0.52
1:A:394:GLN:O	1:A:398:GLN:HG2	2.09	0.52
2:C:28:MET:CE	2:C:389:LEU:HD12	2.37	0.52
2:D:3:TYR:CG	2:D:4:PRO:HD2	2.44	0.52
2:D:321:GLN:O	2:D:325:VAL:HG12	2.09	0.52
1:A:201:ASP:HA	1:A:204:ARG:CG	2.38	0.52
1:A:390:ARG:HA	1:A:393:LEU:CD1	2.40	0.52
1:B:371:HIS:O	1:B:374:GLN:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:VAL:CG2	2:C:32:THR:HG23	2.37	0.52
2:C:472:ASN:HA	2:C:475:ARG:NE	2.25	0.52
2:C:513:LEU:C	2:C:513:LEU:HD23	2.34	0.52
2:D:183:LEU:O	2:D:187:LEU:HD13	2.09	0.52
2:D:426:TYR:CE2	2:D:432:ARG:HD2	2.45	0.52
1:A:247:ILE:CD1	1:B:280:GLU:HB3	2.40	0.52
1:A:336:LYS:HD3	3:A:501:GNP:HN22	1.74	0.52
2:D:413:LEU:C	2:D:413:LEU:HD23	2.34	0.52
1:A:107:ARG:HA	1:A:107:ARG:NE	2.25	0.52
1:B:9:ALA:HB3	1:B:111:PHE:CE2	2.41	0.52
1:B:25:SER:CB	1:B:78:VAL:HG12	2.40	0.52
2:C:521:GLU:CD	2:C:521:GLU:H	2.18	0.52
2:D:232:ASN:OD1	2:D:234:SER:N	2.23	0.52
2:D:473:ILE:HG13	2:D:474:GLU:N	2.24	0.52
2:D:499:LEU:HG	2:D:500:THR:O	2.09	0.52
1:A:136:SER:O	1:B:212:LEU:HD21	2.09	0.52
1:A:221:ILE:HG22	1:A:229:LYS:CD	2.37	0.52
1:A:226:ASN:HD21	1:A:248:ALA:HA	1.74	0.52
2:C:477:ARG:HA	2:C:480:LEU:HD21	1.91	0.52
1:A:13:PRO:HG3	1:B:17:GLY:HA3	1.91	0.52
1:A:16:ARG:HH22	1:B:376:MET:HE1	1.74	0.52
1:A:24:ILE:O	1:A:78:VAL:HG13	2.09	0.52
1:A:50:PRO:HG2	1:A:52:LYS:HZ1	1.75	0.52
2:D:358:GLU:HB2	2:D:366:PHE:CD2	2.44	0.52
1:A:188:LYS:HD3	1:A:192:GLN:NE2	2.25	0.51
1:A:317:TRP:HB3	1:A:320:PHE:HD2	1.75	0.51
2:C:127:ASP:C	2:C:128:LEU:HD12	2.36	0.51
2:D:47:CYS:SG	2:D:48:ASN:N	2.82	0.51
1:A:102:GLY:C	1:A:103:LEU:HD22	2.35	0.51
1:B:63:ILE:HD12	1:B:63:ILE:N	2.25	0.51
1:B:113:GLU:OE1	2:C:617:VAL:HG23	2.10	0.51
1:B:357:LEU:CD2	1:B:368:LEU:HD11	2.30	0.51
2:D:71:ALA:HA	2:D:74:ILE:HG22	1.91	0.51
2:C:445:ASP:OD1	2:C:446:LEU:N	2.43	0.51
2:C:458:VAL:CG1	2:C:462:ARG:HB2	2.41	0.51
2:D:137:GLY:HA3	2:D:146:PHE:O	2.11	0.51
1:A:1:MET:SD	1:A:107:ARG:HG2	2.50	0.51
1:A:336:LYS:HG2	3:A:501:GNP:C2	2.40	0.51
1:B:108:PRO:HG2	1:B:137:SER:HA	1.92	0.51
2:C:200:GLY:HA2	2:C:342:ALA:HA	1.92	0.51
2:D:353:LEU:HD13	2:D:367:PHE:HB2	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLN:NE2	1:A:437:PHE:HB2	2.25	0.51
1:B:139:GLN:OE1	1:B:381:ASN:HB3	2.10	0.51
1:B:298:ARG:HH21	1:B:375:SER:HB2	1.75	0.51
1:B:348:GLU:OE2	1:B:351:GLY:HA2	2.11	0.51
1:B:369:ARG:HH11	1:B:369:ARG:C	2.14	0.51
2:C:509:GLY:HA2	2:C:512:LEU:HB3	1.92	0.51
2:D:197:LEU:HB2	2:D:345:TYR:CZ	2.45	0.51
2:D:411:GLY:HA2	2:D:414:VAL:HG22	1.92	0.51
2:D:519:THR:HG23	2:D:522:LYS:HB2	1.92	0.51
1:A:213:LEU:C	1:A:265:PRO:HG3	2.35	0.51
1:A:312:ASP:HB3	1:A:315:GLU:OE1	2.10	0.51
1:A:380:THR:O	1:A:380:THR:HG22	2.10	0.51
2:D:404:ALA:HB3	2:D:407:GLN:CG	2.36	0.51
2:C:422:THR:O	2:C:423:LYS:HD2	2.11	0.51
2:C:450:GLU:OE2	2:C:451:ILE:HG13	2.11	0.51
2:D:140:THR:HG23	2:D:144:LEU:O	2.10	0.51
1:A:44:ARG:HH21	1:A:71:ASN:HB3	1.76	0.51
1:A:100:ILE:HD12	1:A:101:PRO:CD	2.38	0.51
1:B:45:TYR:HD1	1:B:46:ALA:N	2.09	0.51
1:B:396:LEU:C	1:B:396:LEU:HD23	2.36	0.51
2:C:297:LEU:HB3	2:C:307:ILE:HG21	1.93	0.51
2:C:337:VAL:HG12	2:D:120:ILE:O	2.11	0.51
1:A:133:ILE:CD1	1:B:84:HIS:HB3	2.41	0.51
1:B:122:ASP:OD1	1:B:123:LEU:N	2.39	0.51
2:C:312:ILE:HD11	2:C:324:ILE:CG2	2.41	0.51
2:C:353:LEU:O	2:C:353:LEU:HD23	2.11	0.51
2:D:87:SER:HB3	2:D:88:LYS:NZ	2.26	0.51
1:B:79:LEU:HD23	1:B:80:GLU:N	2.26	0.51
1:B:152:PHE:CD1	1:B:207:ALA:HB2	2.46	0.51
1:A:252:ARG:NH2	1:A:281:VAL:HG11	2.26	0.50
1:B:67:PHE:HB2	1:B:78:VAL:CG2	2.41	0.50
2:C:205:ILE:HG21	2:C:210:ILE:HD11	1.92	0.50
2:C:320:VAL:O	2:C:324:ILE:HG13	2.11	0.50
2:C:508:SER:HB2	2:C:510:GLU:CD	2.36	0.50
2:D:159:LEU:HD21	2:D:183:LEU:HD23	1.92	0.50
1:A:6:THR:HA	1:A:26:GLY:HA3	1.93	0.50
1:A:44:ARG:HG2	1:A:67:PHE:HE1	1.76	0.50
1:A:111:PHE:HB2	1:A:454:LYS:C	2.36	0.50
1:B:42:LYS:CD	1:B:45:TYR:HB2	2.39	0.50
2:C:115:GLN:OE1	2:C:116:PRO:HD2	2.11	0.50
2:C:130:VAL:HG13	2:C:134:ARG:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:444:ALA:HA	2:D:447:ARG:NH1	2.26	0.50
2:D:513:LEU:HD12	2:D:518:MET:HG3	1.92	0.50
2:D:519:THR:HG22	2:D:522:LYS:CE	2.40	0.50
1:A:226:ASN:HA	3:A:501:GNP:O2B	2.11	0.50
1:A:317:TRP:CD1	1:A:320:PHE:HB3	2.43	0.50
1:A:441:ASP:OD1	1:A:442:LEU:N	2.43	0.50
1:B:447:PHE:HB3	2:C:275:ARG:O	2.12	0.50
2:C:338:ARG:HH21	2:D:39:ILE:HB	1.76	0.50
1:A:21:ILE:HG21	1:B:19:VAL:HG11	1.93	0.50
1:A:309:ASP:HA	1:A:334:ARG:HH22	1.77	0.50
2:C:312:ILE:HG12	2:C:312:ILE:O	2.11	0.50
2:D:153:LEU:HG	2:D:155:VAL:HG23	1.93	0.50
1:A:311:VAL:C	1:A:349:VAL:HG21	2.36	0.50
1:A:429:ASN:HA	1:A:432:GLU:OE2	2.11	0.50
2:C:129:ILE:HB	2:C:136:VAL:O	2.12	0.50
2:C:413:LEU:CD2	2:C:417:LEU:HD23	2.41	0.50
2:C:450:GLU:N	2:C:450:GLU:OE1	2.43	0.50
2:D:136:VAL:O	2:D:136:VAL:HG23	2.12	0.50
2:D:481:LYS:HA	2:D:510:GLU:CD	2.35	0.50
1:A:219:VAL:CG1	1:A:268:ILE:HG22	2.41	0.50
1:B:319:GLU:O	1:B:323:ARG:HG3	2.11	0.50
1:B:369:ARG:O	1:B:369:ARG:HD2	2.12	0.50
2:D:420:LEU:CD2	2:D:422:THR:HB	2.36	0.50
1:A:335:ASN:HA	1:A:357:LEU:O	2.12	0.50
2:C:136:VAL:O	2:C:136:VAL:HG23	2.11	0.50
2:C:164:HIS:ND1	2:C:169:ASN:HB3	2.27	0.50
2:C:470:LEU:HD13	2:C:470:LEU:O	2.12	0.50
2:D:87:SER:HB3	2:D:88:LYS:HZ2	1.76	0.50
1:A:138:GLU:OE2	1:A:142:ARG:NH2	2.45	0.50
1:B:16:ARG:HE	1:B:260:HIS:CE1	2.30	0.50
1:B:125:GLN:O	1:B:129:ILE:HG12	2.12	0.50
2:C:28:MET:HE3	2:C:392:ALA:HB3	1.94	0.50
2:D:371:ILE:HG12	2:D:371:ILE:O	2.11	0.50
2:D:394:LEU:C	2:D:394:LEU:HD23	2.37	0.50
1:A:33:ALA:O	1:A:37:LEU:N	2.42	0.49
1:A:407:LYS:O	1:A:411:LEU:HG	2.12	0.49
2:C:352:ASP:OD1	2:C:352:ASP:N	2.44	0.49
2:D:314:THR:OG1	2:D:316:LEU:HG	2.11	0.49
2:D:453:ARG:NH2	2:D:460:ASP:OD1	2.45	0.49
2:D:525:THR:O	2:D:526:LEU:HD23	2.12	0.49
1:B:51:PHE:CE1	1:B:81:LEU:HD13	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HG2	3:B:501:GNP:C6	2.42	0.49
2:C:527:THR:CB	2:C:528:PRO:HD3	2.40	0.49
2:D:164:HIS:HA	2:D:169:ASN:CB	2.42	0.49
1:A:60:ASP:OD2	1:A:89:ILE:HD12	2.12	0.49
1:A:302:MET:HA	1:A:333:VAL:O	2.13	0.49
1:B:49:LEU:CG	1:B:50:PRO:HD2	2.42	0.49
2:C:39:ILE:HG22	2:C:40:ASP:N	2.27	0.49
2:C:57:GLY:O	2:C:61:LYS:HG2	2.11	0.49
2:C:516:PRO:HD2	2:C:517:GLU:OE1	2.13	0.49
2:C:589:LYS:HE3	2:C:606:GLY:C	2.37	0.49
1:A:211:SER:HA	1:A:214:ARG:CG	2.36	0.49
1:B:280:GLU:O	1:B:284:ILE:HG12	2.13	0.49
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.13	0.49
1:A:219:VAL:HG11	1:A:268:ILE:HG22	1.95	0.49
1:B:227:ALA:N	3:B:501:GNP:O1B	2.45	0.49
2:D:487:PRO:HA	2:D:503:LEU:CD2	2.34	0.49
1:A:95:LYS:HA	1:A:98:LEU:HG	1.93	0.49
1:A:126:ALA:HB1	1:A:447:PHE:HE1	1.76	0.49
1:B:186:ASP:OD1	1:B:186:ASP:N	2.45	0.49
1:B:276:GLU:HA	1:B:276:GLU:OE1	2.13	0.49
1:B:108:PRO:CG	1:B:137:SER:HA	2.43	0.49
1:B:353:ALA:HB1	1:B:355:ILE:CD1	2.42	0.49
2:D:245:THR:O	2:D:295:ILE:N	2.37	0.49
1:B:28:LYS:HA	1:B:31:GLU:OE1	2.13	0.49
2:C:396:ALA:HB1	2:C:398:LYS:HZ1	1.78	0.49
2:D:154:THR:HG22	2:D:368:ALA:O	2.13	0.49
2:D:378:GLU:CD	2:D:378:GLU:H	2.21	0.49
1:A:288:ARG:HA	1:A:291:GLN:CD	2.38	0.49
2:C:201:THR:OG1	2:C:202:PRO:HD2	2.13	0.49
2:D:25:ALA:HB1	2:D:32:THR:HG21	1.94	0.49
2:D:95:THR:HG23	2:D:227:PHE:CZ	2.47	0.49
2:D:316:LEU:HD13	2:D:320:VAL:CG1	2.42	0.49
2:D:518:MET:SD	2:D:519:THR:N	2.86	0.49
1:A:201:ASP:O	1:A:204:ARG:HG3	2.13	0.49
1:A:304:ASP:HB3	1:A:307:THR:CG2	2.43	0.49
1:A:381:ASN:HB3	1:A:382:MET:CE	2.42	0.49
1:A:442:LEU:CD1	1:A:445:ARG:HD2	2.36	0.49
2:C:10:ILE:HG13	2:C:148:ALA:HB2	1.95	0.49
2:D:415:ASP:O	2:D:419:THR:OG1	2.31	0.49
1:A:24:ILE:N	1:A:24:ILE:HD12	2.27	0.48
1:B:145:LEU:O	1:B:149:GLN:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:OE1	1:B:180:GLU:N	2.46	0.48
1:B:207:ALA:CB	1:B:389:ARG:HH21	2.25	0.48
2:C:194:VAL:HG12	2:C:348:PHE:CD1	2.48	0.48
2:C:478:GLN:HA	2:C:478:GLN:OE1	2.13	0.48
1:A:37:LEU:O	1:A:39:LYS:HG2	2.13	0.48
1:A:181:ILE:HA	1:A:414:TRP:HZ3	1.79	0.48
1:A:243:ILE:CG1	1:B:288:ARG:HH12	2.26	0.48
1:A:404:GLN:HA	1:A:407:LYS:HG2	1.95	0.48
1:B:159:LEU:HB2	1:B:199:ASP:OD2	2.12	0.48
1:B:346:MET:SD	1:B:355:ILE:HD11	2.53	0.48
2:C:209:THR:HG21	2:C:335:LYS:HG2	1.95	0.48
2:C:303:THR:HG23	2:D:109:ARG:NH2	2.26	0.48
2:C:360:LYS:NZ	2:C:594:LYS:O	2.44	0.48
2:D:56:LYS:O	2:D:378:GLU:HG2	2.13	0.48
2:D:219:HIS:ND1	2:D:241:PRO:HB3	2.28	0.48
2:D:487:PRO:CG	2:D:503:LEU:HB3	2.41	0.48
1:A:200:LEU:HA	1:A:203:VAL:HG22	1.95	0.48
1:A:225:PRO:CA	1:A:273:GLY:HA3	2.44	0.48
1:B:277:ALA:HB1	1:B:282:GLU:HB3	1.95	0.48
2:C:214:VAL:HG22	2:C:214:VAL:O	2.12	0.48
2:D:247:THR:HA	2:D:328:MET:HG3	1.96	0.48
2:D:496:ASN:OD1	2:D:503:LEU:HD13	2.14	0.48
2:D:533:LEU:CD2	2:D:535:ASP:H	2.26	0.48
1:A:45:TYR:CD2	1:A:47:ASP:HB2	2.47	0.48
1:A:346:MET:HE1	1:A:353:ALA:HB2	1.92	0.48
2:C:90:PRO:HG2	2:C:544:ILE:HD11	1.96	0.48
2:D:51:ILE:CD1	2:D:74:ILE:HD13	2.43	0.48
2:D:162:LYS:N	2:D:162:LYS:HD2	2.28	0.48
2:D:164:HIS:O	2:D:341:TYR:HB2	2.13	0.48
2:D:385:LEU:HD23	2:D:385:LEU:C	2.38	0.48
2:D:543:GLU:O	2:D:546:VAL:HG12	2.13	0.48
1:A:54:ALA:HB2	1:A:96:ARG:CZ	2.43	0.48
1:A:66:TRP:NE1	1:A:68:PRO:HD3	2.28	0.48
1:B:107:ARG:HB3	1:B:108:PRO:CD	2.43	0.48
1:B:181:ILE:HG23	1:B:450:PHE:CD1	2.49	0.48
2:C:28:MET:SD	2:C:389:LEU:HD12	2.53	0.48
2:C:196:ARG:HH21	2:C:344:GLU:HB3	1.78	0.48
2:C:520:TYR:OH	2:C:532:ALA:HB1	2.12	0.48
1:A:333:VAL:HG22	1:A:355:ILE:HB	1.96	0.48
2:C:127:ASP:O	2:C:128:LEU:HD12	2.13	0.48
1:A:49:LEU:N	1:A:49:LEU:HD23	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:OD1	1:A:200:LEU:N	2.46	0.48
1:A:313:PRO:HB2	1:A:321:ILE:HG21	1.96	0.48
1:A:438:THR:CG2	1:A:442:LEU:HD23	2.44	0.48
1:B:107:ARG:HB3	1:B:108:PRO:HD2	1.95	0.48
2:C:66:LEU:HD23	2:C:385:LEU:HD22	1.95	0.48
2:C:426:TYR:OH	2:C:432:ARG:HD3	2.14	0.48
2:D:53:GLY:O	2:D:94:ALA:HB1	2.13	0.48
2:D:53:GLY:HA2	2:D:96:ARG:HG3	1.95	0.48
2:D:312:ILE:HG22	2:D:312:ILE:O	2.13	0.48
1:B:205:ALA:HA	1:B:208:ARG:HH12	1.78	0.48
2:C:521:GLU:O	2:C:525:THR:HG23	2.14	0.48
2:C:38:ASN:OD1	2:C:39:ILE:N	2.47	0.48
2:C:222:ASN:O	2:C:223:PRO:C	2.56	0.48
1:A:130:ALA:O	1:A:131:ASP:HB2	2.13	0.48
1:A:432:GLU:O	1:A:438:THR:OG1	2.32	0.48
1:B:33:ALA:HB2	1:B:79:LEU:CD1	2.44	0.48
1:B:396:LEU:HD23	1:B:396:LEU:O	2.14	0.48
2:C:377:TYR:HB2	2:C:378:GLU:OE1	2.14	0.48
1:A:7:ILE:O	1:A:24:ILE:HG23	2.14	0.47
1:A:42:LYS:HE3	1:A:43:PRO:O	2.14	0.47
1:A:214:ARG:HH12	1:A:389:ARG:CD	2.24	0.47
1:B:132:LEU:O	1:B:132:LEU:HD23	2.13	0.47
1:B:261:ILE:HD12	1:B:369:ARG:HD3	1.96	0.47
2:D:222:ASN:CB	2:D:223:PRO:HD3	2.43	0.47
2:D:473:ILE:HG22	2:D:538:ALA:HB1	1.95	0.47
1:B:298:ARG:NH2	1:B:375:SER:HB2	2.29	0.47
1:B:417:GLU:OE2	2:C:89:GLY:HA3	2.15	0.47
2:C:589:LYS:NZ	2:C:605:SER:O	2.29	0.47
2:D:45:MET:HG2	2:D:377:TYR:CE2	2.49	0.47
2:D:312:ILE:O	2:D:312:ILE:CG2	2.61	0.47
1:A:134:ASP:OD2	1:B:16:ARG:HD3	2.14	0.47
1:A:331:THR:HG23	1:A:353:ALA:C	2.39	0.47
1:B:24:ILE:HD13	1:B:32:VAL:HG11	1.95	0.47
1:B:229:LYS:HE2	3:B:501:GNP:N3B	2.29	0.47
1:B:288:ARG:HD3	1:B:291:GLN:NE2	2.29	0.47
1:B:299:VAL:HG23	1:B:328:LEU:HD11	1.96	0.47
1:B:385:GLY:O	1:B:388:ALA:N	2.47	0.47
2:C:512:LEU:CD2	2:C:523:LEU:HD22	2.44	0.47
2:C:582:LEU:CB	2:C:587:ILE:HD11	2.42	0.47
2:D:80:GLN:HA	2:D:239:GLN:OE1	2.14	0.47
2:D:144:LEU:HD12	2:D:145:LYS:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLY:H	1:A:229:LYS:HZ3	1.62	0.47
2:D:51:ILE:HD12	2:D:74:ILE:CD1	2.43	0.47
2:C:519:THR:HG23	2:C:522:LYS:HE2	1.96	0.47
2:D:484:TRP:CD1	2:D:508:SER:HB3	2.49	0.47
1:A:157:ASN:HA	1:A:160:VAL:CG1	2.43	0.47
1:B:51:PHE:CE1	1:B:81:LEU:HD22	2.50	0.47
2:C:155:VAL:HG11	2:C:159:LEU:HG	1.96	0.47
2:D:83:ILE:N	2:D:221:ASP:OD2	2.46	0.47
2:D:316:LEU:HD13	2:D:320:VAL:HG11	1.97	0.47
1:A:1:MET:HE2	1:A:104:ARG:NH1	2.30	0.47
1:A:40:LEU:HD23	1:A:41:PRO:O	2.14	0.47
1:A:65:LEU:O	1:A:79:LEU:HD12	2.15	0.47
1:A:304:ASP:OD2	1:A:307:THR:HG23	2.14	0.47
1:A:317:TRP:HB3	1:A:320:PHE:CD2	2.49	0.47
1:B:260:HIS:CE1	1:B:265:PRO:HB3	2.49	0.47
1:B:438:THR:HG22	1:B:439:SER:H	1.79	0.47
2:C:10:ILE:HG13	2:C:148:ALA:CB	2.45	0.47
2:C:570:LEU:HD13	2:C:576:TYR:OH	2.14	0.47
2:C:589:LYS:HE3	2:C:606:GLY:HA3	1.97	0.47
2:D:181:ILE:HD12	2:D:181:ILE:N	2.30	0.47
2:D:322:MET:HA	2:D:325:VAL:HG12	1.97	0.47
1:A:50:PRO:HB3	1:A:61:GLN:NE2	2.29	0.47
1:A:299:VAL:O	1:A:330:ILE:HA	2.15	0.47
1:B:271:THR:HB	1:B:289:ALA:CB	2.45	0.47
1:B:303:VAL:HG21	1:B:332:VAL:CG1	2.41	0.47
1:B:336:LYS:HA	3:B:501:GNP:C6	2.44	0.47
1:B:319:GLU:OE1	1:B:319:GLU:N	2.32	0.47
1:B:357:LEU:HD12	1:B:359:ALA:N	2.30	0.47
2:C:512:LEU:HD23	2:C:523:LEU:HD22	1.97	0.47
2:D:125:VAL:HA	2:D:140:THR:HA	1.95	0.47
2:D:510:GLU:OE1	2:D:510:GLU:N	2.32	0.47
1:A:45:TYR:HD2	1:A:47:ASP:HB2	1.79	0.47
1:B:44:ARG:HA	1:B:67:PHE:CE1	2.45	0.47
1:B:291:GLN:HA	1:B:294:GLU:OE1	2.15	0.47
2:C:85:ASN:O	2:C:93:ARG:HG2	2.15	0.47
2:C:285:MET:HA	2:C:285:MET:CE	2.35	0.47
2:C:618:TRP:CZ2	2:C:622:GLN:HG3	2.50	0.47
2:D:130:VAL:HA	2:D:134:ARG:O	2.15	0.47
2:D:375:THR:OG1	2:D:376:GLY:N	2.47	0.47
1:A:138:GLU:HA	1:B:88:VAL:HG11	1.97	0.46
1:A:208:ARG:HD3	1:A:208:ARG:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HG3	1:A:273:GLY:CA	2.46	0.46
1:A:330:ILE:O	1:A:352:HIS:HB3	2.15	0.46
1:A:430:LEU:O	1:A:433:ILE:HG13	2.15	0.46
2:C:29:GLY:C	2:C:30:GLN:HE21	2.18	0.46
2:C:265:TYR:O	2:C:267:GLY:N	2.48	0.46
2:D:137:GLY:HA3	2:D:147:ARG:HA	1.96	0.46
2:D:350:PRO:HG3	2:D:372:ASN:HB3	1.97	0.46
1:A:113:GLU:O	1:A:117:LEU:HG	2.15	0.46
1:A:164:THR:O	1:A:168:ILE:HG13	2.15	0.46
1:A:336:LYS:HG2	3:A:501:GNP:N1	2.30	0.46
1:B:349:VAL:O	1:B:349:VAL:HG13	2.15	0.46
2:C:15:GLY:O	2:C:19:THR:HG23	2.14	0.46
2:C:294:GLN:O	2:C:295:ILE:HD13	2.15	0.46
1:A:451:CYS:HB2	1:A:454:LYS:HD3	1.96	0.46
1:B:279:ASP:OD1	1:B:280:GLU:N	2.47	0.46
2:C:161:GLY:HA2	2:C:344:GLU:O	2.16	0.46
2:C:483:THR:CG2	2:C:509:GLY:H	2.22	0.46
2:D:81:PHE:CD2	2:D:97:ALA:HB2	2.51	0.46
2:D:156:GLY:CA	2:D:370:GLN:HB2	2.26	0.46
1:A:129:ILE:HD13	1:A:148:LEU:HD11	1.97	0.46
2:C:625:LEU:HD12	2:C:625:LEU:C	2.40	0.46
2:D:188:ARG:HH11	2:D:194:VAL:HG11	1.80	0.46
2:D:449:THR:O	2:D:458:VAL:HG21	2.16	0.46
1:A:181:ILE:HG23	1:A:414:TRP:CZ3	2.51	0.46
1:A:347:SER:OG	1:A:354:LEU:HB3	2.16	0.46
1:B:319:GLU:H	1:B:319:GLU:CD	2.19	0.46
2:C:3:TYR:CG	2:C:4:PRO:HD2	2.51	0.46
2:C:159:LEU:HD23	2:C:159:LEU:HA	1.85	0.46
2:C:259:LEU:HD21	2:C:265:TYR:CB	2.45	0.46
1:A:313:PRO:CG	1:A:350:ASN:HD22	2.29	0.46
1:B:143:SER:O	1:B:144:ALA:HB3	2.16	0.46
1:B:239:ARG:CZ	1:B:239:ARG:HB2	2.45	0.46
1:B:271:THR:HB	1:B:289:ALA:HB2	1.98	0.46
1:B:438:THR:HG22	1:B:439:SER:N	2.31	0.46
2:C:461:GLU:N	2:C:461:GLU:OE1	2.49	0.46
2:D:356:THR:HB	2:D:390:ASN:ND2	2.31	0.46
1:A:225:PRO:HG2	1:A:275:ARG:HE	1.81	0.46
1:A:389:ARG:HG3	1:A:390:ARG:N	2.31	0.46
1:B:283:ARG:O	1:B:287:GLU:HG3	2.16	0.46
2:D:356:THR:O	2:D:357:LEU:HB2	2.16	0.46
1:A:171:GLU:OE2	1:A:420:ALA:HB1	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:OE1	1:A:402:HIS:N	2.49	0.46
1:B:132:LEU:HD23	1:B:132:LEU:C	2.41	0.46
1:B:228:GLY:N	3:B:501:GNP:O1B	2.40	0.46
1:B:338:ASP:HB3	1:B:358:SER:HB2	1.98	0.46
2:C:422:THR:C	2:C:423:LYS:HD2	2.40	0.46
2:D:90:PRO:HG3	2:D:544:ILE:HD12	1.98	0.46
1:B:62:GLY:HA3	1:B:82:GLN:O	2.16	0.46
2:D:92:VAL:HG12	2:D:92:VAL:O	2.15	0.46
1:A:96:ARG:NH1	1:A:96:ARG:HA	2.30	0.46
1:A:108:PRO:HG3	1:A:452:ILE:HG12	1.97	0.46
1:A:210:GLY:C	1:A:212:LEU:H	2.24	0.46
1:A:345:GLY:O	1:A:355:ILE:HD13	2.15	0.46
2:D:209:THR:HB	2:D:334:ALA:HA	1.97	0.46
2:D:224:MET:CE	2:D:239:GLN:HG3	2.44	0.46
2:D:533:LEU:HD22	2:D:535:ASP:CB	2.45	0.46
1:A:16:ARG:O	1:B:13:PRO:HG3	2.16	0.45
1:B:144:ALA:HA	1:B:147:SER:OG	2.16	0.45
1:B:362:GLY:O	1:B:365:VAL:HG13	2.16	0.45
2:C:258:ASN:OD1	2:C:261:ARG:HD3	2.15	0.45
2:C:281:GLU:O	2:C:284:VAL:HG12	2.16	0.45
2:C:282:ASP:O	2:C:286:ARG:HG2	2.16	0.45
2:D:78:GLY:HA2	2:D:98:GLN:O	2.15	0.45
2:D:112:LEU:CD2	2:D:120:ILE:HD11	2.46	0.45
2:D:357:LEU:O	2:D:366:PHE:HB3	2.16	0.45
1:A:349:VAL:HG12	1:A:354:LEU:HB2	1.99	0.45
1:B:13:PRO:HA	1:B:382:MET:HE3	1.99	0.45
2:C:513:LEU:O	2:C:547:LYS:NZ	2.49	0.45
2:D:329:GLN:HA	2:D:329:GLN:OE1	2.16	0.45
1:A:261:ILE:CG1	1:A:266:LEU:HD21	2.39	0.45
2:C:279:SER:HB2	2:C:281:GLU:OE1	2.15	0.45
2:D:513:LEU:HD13	2:D:523:LEU:HD12	1.99	0.45
1:A:37:LEU:O	1:A:39:LYS:NZ	2.42	0.45
1:A:305:GLY:HA2	1:A:334:ARG:NH1	2.31	0.45
2:D:191:PRO:O	2:D:192:LEU:HD12	2.16	0.45
1:A:116:PHE:CE1	1:A:123:LEU:HB2	2.50	0.45
1:B:47:ASP:O	1:B:63:ILE:HG23	2.17	0.45
1:B:317:TRP:O	1:B:321:ILE:HG12	2.17	0.45
1:B:334:ARG:HB2	1:B:356:ARG:HG2	1.98	0.45
2:C:305:ASN:ND2	2:D:113:GLU:HG2	2.31	0.45
2:D:354:LYS:CD	2:D:358:GLU:HB3	2.47	0.45
1:A:1:MET:SD	1:A:104:ARG:HD2	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HB	1:A:354:LEU:CD1	2.46	0.45
1:B:42:LYS:HD2	1:B:45:TYR:HD2	1.80	0.45
1:B:338:ASP:HB3	1:B:358:SER:OG	2.16	0.45
2:C:8:ASP:OD2	2:C:30:GLN:HB3	2.17	0.45
2:C:100:ASP:OD1	2:C:101:ARG:N	2.50	0.45
2:C:316:LEU:CD1	2:C:320:VAL:HG11	2.44	0.45
2:C:601:ALA:O	2:C:607:VAL:HG21	2.16	0.45
2:D:353:LEU:HD11	2:D:357:LEU:HD23	1.98	0.45
2:D:519:THR:CG2	2:D:522:LYS:HB2	2.46	0.45
1:A:219:VAL:CG1	1:A:268:ILE:HA	2.46	0.45
1:A:221:ILE:HG22	1:A:229:LYS:HB3	1.99	0.45
1:A:429:ASN:CA	1:A:432:GLU:HG3	2.47	0.45
2:C:487:PRO:HG3	2:C:503:LEU:C	2.42	0.45
2:D:320:VAL:O	2:D:324:ILE:HG13	2.16	0.45
1:A:81:LEU:C	1:A:81:LEU:HD23	2.42	0.45
1:A:243:ILE:HG12	1:B:288:ARG:NH2	2.30	0.45
2:C:485:VAL:HG12	2:C:486:THR:N	2.32	0.45
1:A:288:ARG:HA	1:A:291:GLN:OE1	2.17	0.45
2:C:514:ARG:NH1	2:C:549:GLU:OE2	2.50	0.45
2:C:574:LEU:HD23	2:C:576:TYR:CZ	2.52	0.45
2:D:35:LEU:HD13	2:D:125:VAL:CG1	2.47	0.45
2:D:112:LEU:C	2:D:112:LEU:HD23	2.41	0.45
2:D:112:LEU:HD21	2:D:120:ILE:HD11	1.99	0.45
1:A:44:ARG:HH21	1:A:71:ASN:CB	2.30	0.45
1:A:110:GLU:OE2	1:A:114:ARG:NH1	2.50	0.45
1:A:130:ALA:HB2	1:A:450:PHE:CE2	2.52	0.45
1:A:214:ARG:CD	1:A:387:LEU:HD21	2.46	0.45
1:B:180:GLU:HG2	1:B:180:GLU:O	2.16	0.45
2:C:206:ASP:OD1	2:C:208:ARG:HG2	2.17	0.45
2:C:610:ALA:O	2:C:614:ILE:HG13	2.18	0.45
2:D:115:GLN:OE1	2:D:116:PRO:HD2	2.16	0.45
1:A:157:ASN:O	1:A:160:VAL:HG12	2.17	0.44
1:A:327:LYS:HG2	1:A:328:LEU:CD2	2.46	0.44
1:A:442:LEU:HA	1:A:445:ARG:CD	2.46	0.44
1:B:369:ARG:NH1	1:B:370:ASN:HA	2.33	0.44
1:B:371:HIS:HA	1:B:374:GLN:CG	2.42	0.44
2:C:513:LEU:HD11	2:C:543:GLU:OE1	2.16	0.44
2:D:188:ARG:O	2:D:188:ARG:HG3	2.17	0.44
1:A:157:ASN:CA	1:A:160:VAL:HG12	2.47	0.44
2:D:476:GLU:OE1	2:D:476:GLU:HA	2.16	0.44
1:A:40:LEU:HD23	1:A:40:LEU:C	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HD3	1:A:209:GLN:N	2.33	0.44
1:A:386:PHE:HE2	1:A:388:ALA:HB2	1.81	0.44
1:A:447:PHE:HA	1:A:450:PHE:CD1	2.52	0.44
1:B:51:PHE:CZ	1:B:81:LEU:HB3	2.52	0.44
1:B:334:ARG:N	1:B:355:ILE:O	2.25	0.44
1:B:371:HIS:CA	1:B:374:GLN:HG2	2.42	0.44
2:C:66:LEU:HD12	2:C:66:LEU:HA	1.85	0.44
2:D:361:PHE:CB	2:D:362:ILE:HD12	2.47	0.44
2:D:499:LEU:HD11	2:D:515:ARG:CD	2.47	0.44
2:D:511:ASP:HA	2:D:514:ARG:HH12	1.82	0.44
1:A:221:ILE:HG21	1:A:229:LYS:HB3	1.99	0.44
1:A:266:LEU:C	1:A:266:LEU:HD12	2.42	0.44
1:A:289:ALA:O	1:A:293:ILE:HG13	2.17	0.44
1:A:350:ASN:HB3	1:A:352:HIS:CD2	2.52	0.44
1:A:376:MET:HE3	1:A:376:MET:HA	1.99	0.44
1:B:174:ILE:CG2	2:C:92:VAL:HG21	2.44	0.44
1:B:338:ASP:HB3	1:B:358:SER:CB	2.47	0.44
2:C:547:LYS:C	2:C:548:TYR:HD1	2.26	0.44
2:D:11:ILE:HD12	2:D:11:ILE:N	2.32	0.44
2:D:530:ALA:HB1	2:D:531:PRO:CD	2.47	0.44
1:A:116:PHE:HE1	1:A:123:LEU:HB2	1.83	0.44
1:A:213:LEU:H	1:A:213:LEU:CD2	2.31	0.44
1:A:300:LEU:HA	1:A:331:THR:O	2.18	0.44
1:A:318:PRO:O	1:A:321:ILE:HG12	2.17	0.44
1:A:332:VAL:O	1:A:355:ILE:N	2.45	0.44
2:D:81:PHE:CE2	2:D:97:ALA:HB2	2.53	0.44
2:D:411:GLY:O	2:D:414:VAL:HG22	2.18	0.44
1:A:124:ALA:CB	1:A:152:PHE:HE2	2.28	0.44
1:B:227:ALA:CB	1:B:302:MET:HE2	2.48	0.44
1:A:417:GLU:OE2	1:A:418:LEU:HG	2.18	0.44
2:C:79:ILE:O	2:C:239:GLN:HA	2.18	0.44
2:C:251:THR:HG22	2:C:327:SER:HB2	1.98	0.44
2:C:260:ASP:OD1	2:C:260:ASP:N	2.51	0.44
1:A:155:ARG:O	1:A:159:LEU:HG	2.18	0.44
2:D:163:ILE:N	2:D:163:ILE:HD12	2.32	0.44
2:D:473:ILE:HG22	2:D:538:ALA:CB	2.48	0.44
1:A:104:ARG:HG2	1:A:105:ILE:N	2.32	0.44
1:B:25:SER:HB2	1:B:78:VAL:HG12	1.99	0.44
1:B:164:THR:O	1:B:168:ILE:HG13	2.17	0.44
1:B:227:ALA:H	1:B:229:LYS:NZ	2.15	0.44
2:C:484:TRP:HA	2:C:507:ALA:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:541:GLN:O	2:C:545:GLN:HG3	2.17	0.44
2:D:62:GLU:OE2	2:D:409:TYR:HB2	2.17	0.44
2:D:128:LEU:HD23	2:D:138:ALA:CB	2.48	0.44
2:D:351:ARG:NE	2:D:421:GLY:O	2.49	0.44
1:A:258:HIS:CE1	1:B:212:LEU:HD22	2.53	0.43
1:A:300:LEU:C	1:A:300:LEU:HD12	2.42	0.43
2:D:10:ILE:CG1	2:D:148:ALA:CB	2.95	0.43
2:D:161:GLY:C	2:D:162:LYS:HD2	2.43	0.43
2:D:219:HIS:CE1	2:D:241:PRO:HB3	2.52	0.43
2:D:520:TYR:CZ	2:D:532:ALA:HB1	2.52	0.43
1:B:53:ASP:OD2	1:B:55:ASP:HB3	2.18	0.43
1:B:281:VAL:HA	1:B:284:ILE:HD11	2.01	0.43
2:C:589:LYS:CE	2:C:606:GLY:HA3	2.48	0.43
1:A:25:SER:OG	1:A:78:VAL:HG22	2.18	0.43
1:B:152:PHE:CE1	1:B:207:ALA:HB2	2.53	0.43
1:B:226:ASN:HA	3:B:501:GNP:O3A	2.19	0.43
1:B:361:THR:HG22	1:B:361:THR:O	2.18	0.43
2:C:27:ARG:HB3	2:C:27:ARG:HH11	1.83	0.43
2:C:40:ASP:O	2:C:105:ARG:HD3	2.18	0.43
2:C:290:ARG:HB2	2:C:290:ARG:CZ	2.48	0.43
2:D:495:VAL:CG1	2:D:503:LEU:HD11	2.48	0.43
1:A:7:ILE:CB	1:A:106:ALA:HB2	2.47	0.43
1:A:173:ALA:HA	1:A:183:PHE:HD2	1.81	0.43
1:A:184:LEU:HD23	1:A:189:ILE:CD1	2.48	0.43
1:A:193:LEU:CD2	1:A:407:LYS:HB3	2.37	0.43
1:B:28:LYS:O	1:B:32:VAL:HG23	2.19	0.43
1:B:312:ASP:HB3	1:B:315:GLU:CD	2.43	0.43
2:D:181:ILE:HB	2:D:182:PRO:HD3	1.99	0.43
2:D:246:HIS:NE2	2:D:294:GLN:HB3	2.33	0.43
2:D:350:PRO:HA	2:D:353:LEU:CD2	2.49	0.43
1:A:123:LEU:HD21	1:A:443:LEU:HD22	2.00	0.43
1:A:142:ARG:HH21	1:B:92:LEU:HD11	1.82	0.43
1:B:104:ARG:HH22	1:B:107:ARG:HD3	1.82	0.43
1:B:421:GLU:OE1	2:C:437:LEU:HD11	2.19	0.43
2:C:135:VAL:O	2:C:135:VAL:HG13	2.19	0.43
2:D:407:GLN:O	2:D:447:ARG:NE	2.50	0.43
2:D:486:THR:OG1	2:D:487:PRO:HD2	2.19	0.43
1:A:1:MET:HE2	1:A:104:ARG:HH11	1.83	0.43
1:A:95:LYS:O	1:A:98:LEU:HG	2.17	0.43
1:B:52:LYS:HA	1:B:57:SER:O	2.18	0.43
2:D:491:ALA:O	2:D:494:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HB3	1:B:45:TYR:CE1	2.54	0.43
1:A:193:LEU:HA	1:A:196:VAL:HG22	2.01	0.43
1:A:195:ASP:OD1	1:A:196:VAL:N	2.52	0.43
3:B:501:GNP:PA	3:B:501:GNP:H3'	2.58	0.43
2:C:280:ILE:HG22	2:C:314:THR:HB	2.01	0.43
2:D:348:PHE:CE2	2:D:371:ILE:HD11	2.52	0.43
2:D:353:LEU:HD23	2:D:353:LEU:H	1.84	0.43
2:D:446:LEU:HD21	2:D:469:LYS:HE2	2.01	0.43
1:A:42:LYS:HD2	1:A:43:PRO:N	2.34	0.43
1:A:406:GLY:O	1:A:419:LEU:HD13	2.18	0.43
1:B:195:ASP:OD1	1:B:196:VAL:HG23	2.19	0.43
2:D:524:THR:HG22	2:D:532:ALA:CB	2.45	0.43
2:D:530:ALA:O	2:D:531:PRO:C	2.61	0.43
1:A:20:GLY:HA3	1:A:90:LEU:HD11	2.00	0.43
1:A:130:ALA:C	1:A:132:LEU:H	2.27	0.43
1:A:155:ARG:HA	1:A:155:ARG:NH1	2.32	0.43
1:B:369:ARG:HH12	1:B:373:LYS:HB3	1.84	0.43
2:C:137:GLY:HA2	2:C:146:PHE:O	2.18	0.43
2:C:476:GLU:HA	2:C:479:ARG:CG	2.49	0.43
2:C:576:TYR:CE2	2:C:590:LEU:HD13	2.54	0.43
2:D:59:LEU:O	2:D:63:VAL:HG23	2.19	0.43
2:D:426:TYR:CE1	2:D:428:MET:HE2	2.48	0.43
1:A:86:GLY:O	1:A:89:ILE:HG12	2.19	0.43
1:A:95:LYS:HA	1:A:98:LEU:CG	2.49	0.43
1:B:148:LEU:HB2	1:B:153:SER:HB2	2.01	0.43
1:B:181:ILE:HG22	1:B:181:ILE:O	2.17	0.43
1:B:303:VAL:O	1:B:335:ASN:N	2.51	0.43
1:B:357:LEU:HB2	1:B:363:GLU:O	2.18	0.43
1:A:268:ILE:C	1:A:269:ILE:HD12	2.43	0.42
1:B:275:ARG:O	1:B:286:ILE:HD13	2.19	0.42
2:C:253:ASP:O	2:C:257:SER:OG	2.29	0.42
2:D:470:LEU:O	2:D:473:ILE:HG12	2.18	0.42
1:A:23:ARG:C	1:A:24:ILE:HD12	2.43	0.42
1:A:298:ARG:CZ	1:A:375:SER:HB2	2.50	0.42
1:B:16:ARG:NH2	1:B:260:HIS:HB3	2.27	0.42
1:B:229:LYS:HE2	1:B:229:LYS:HB2	1.89	0.42
1:B:332:VAL:HB	1:B:353:ALA:O	2.19	0.42
2:D:472:ASN:HA	2:D:475:ARG:HG2	2.01	0.42
1:A:17:GLY:O	1:A:85:GLY:HA3	2.19	0.42
1:A:43:PRO:HA	1:A:66:TRP:O	2.19	0.42
1:A:208:ARG:NH1	1:A:212:LEU:HD22	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:CD1	1:A:320:PHE:H	2.38	0.42
1:A:354:LEU:HD23	1:A:354:LEU:C	2.45	0.42
2:D:172:GLY:HA2	2:D:179:PRO:CG	2.47	0.42
1:B:167:ARG:CA	1:B:170:VAL:HG12	2.44	0.42
1:B:226:ASN:HD21	1:B:247:ILE:C	2.27	0.42
2:C:33:LEU:HD21	2:C:35:LEU:CD1	2.49	0.42
2:C:207:ALA:O	2:C:212:PHE:HE2	2.01	0.42
2:C:259:LEU:HD21	2:C:265:TYR:CG	2.54	0.42
2:C:508:SER:HB2	2:C:510:GLU:OE2	2.19	0.42
2:C:521:GLU:O	2:C:524:THR:OG1	2.23	0.42
2:D:53:GLY:N	2:D:96:ARG:HG3	2.34	0.42
2:D:71:ALA:HA	2:D:74:ILE:CG2	2.49	0.42
1:A:349:VAL:CG1	1:A:354:LEU:HD12	2.49	0.42
2:C:385:LEU:C	2:C:385:LEU:HD23	2.44	0.42
2:C:521:GLU:OE1	2:C:521:GLU:N	2.43	0.42
2:C:604:ILE:HG22	2:C:605:SER:N	2.35	0.42
2:D:44:GLN:OE1	2:D:105:ARG:HD3	2.19	0.42
2:D:78:GLY:O	2:D:237:PRO:HD2	2.19	0.42
1:A:23:ARG:HG2	1:A:111:PHE:HE2	1.85	0.42
2:C:54:ILE:HD11	2:C:85:ASN:OD1	2.20	0.42
2:C:486:THR:OG1	2:C:487:PRO:HD2	2.19	0.42
1:A:268:ILE:O	1:A:268:ILE:HG13	2.19	0.42
1:B:139:GLN:NE2	1:B:217:MET:HE1	2.35	0.42
2:C:430:THR:O	2:C:436:ARG:HD2	2.20	0.42
2:D:19:THR:O	2:D:23:MET:HG2	2.20	0.42
1:A:36:VAL:C	1:A:37:LEU:HD23	2.45	0.42
1:A:221:ILE:HG23	1:A:300:LEU:HD11	2.01	0.42
1:B:277:ALA:HA	1:B:282:GLU:OE1	2.20	0.42
2:C:478:GLN:HA	2:C:481:LYS:HE3	2.01	0.42
2:D:446:LEU:HA	2:D:466:PHE:HE1	1.84	0.42
2:D:449:THR:HG21	2:D:466:PHE:CD1	2.55	0.42
1:B:42:LYS:HD2	1:B:45:TYR:CD2	2.55	0.42
1:B:217:MET:HE3	1:B:380:THR:CB	2.49	0.42
1:B:349:VAL:HG12	1:B:352:HIS:O	2.20	0.42
1:B:372:LEU:O	1:B:375:SER:OG	2.35	0.42
2:C:489:ALA:HB3	2:C:492:ALA:CB	2.27	0.42
2:C:564:ARG:HD2	2:C:564:ARG:HA	1.69	0.42
2:D:405:ARG:HD2	2:D:415:ASP:OD2	2.20	0.42
2:D:487:PRO:CA	2:D:503:LEU:HD23	2.38	0.42
1:A:1:MET:CE	1:A:104:ARG:HD2	2.50	0.42
1:A:217:MET:HE1	1:A:219:VAL:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:HB2	1:B:270:ASP:HB3	2.01	0.42
1:B:431:SER:OG	1:B:436:GLU:HA	2.20	0.42
2:C:265:TYR:O	2:C:266:ALA:C	2.62	0.42
2:D:188:ARG:NH1	2:D:194:VAL:HG11	2.34	0.42
1:A:98:LEU:HD12	1:A:99:THR:N	2.35	0.41
1:B:230:SER:N	3:B:501:GNP:O2B	2.49	0.41
2:C:264:MET:O	2:C:265:TYR:C	2.63	0.41
2:D:55:GLY:HA2	2:D:428:MET:HG3	1.99	0.41
1:A:1:MET:HE1	1:A:104:ARG:HD2	2.02	0.41
1:A:14:PRO:HD2	1:B:263:GLY:O	2.19	0.41
1:A:121:LEU:CD1	1:A:125:GLN:HB3	2.50	0.41
1:B:74:THR:HG22	1:B:115:ALA:HB2	2.02	0.41
1:B:333:VAL:HG13	1:B:357:LEU:HD23	2.02	0.41
2:C:131:GLU:O	2:C:131:GLU:HG2	2.20	0.41
2:C:284:VAL:HG13	2:C:285:MET:N	2.35	0.41
2:C:519:THR:OG1	2:C:522:LYS:HG3	2.20	0.41
2:C:589:LYS:HD2	2:C:607:VAL:HG13	2.01	0.41
2:C:621:LYS:HD2	2:C:621:LYS:O	2.20	0.41
1:A:21:ILE:CD1	1:A:82:GLN:HG2	2.50	0.41
1:A:159:LEU:HB2	1:A:430:LEU:HD21	2.03	0.41
1:B:147:SER:O	1:B:389:ARG:NH1	2.49	0.41
2:C:314:THR:OG1	2:C:315:SER:N	2.53	0.41
2:D:160:ASP:OD2	2:D:162:LYS:NZ	2.53	0.41
1:B:130:ALA:HB1	2:C:580:SER:O	2.20	0.41
2:C:527:THR:CB	2:C:528:PRO:CD	2.97	0.41
1:A:187:GLY:HA2	1:A:190:GLU:OE1	2.20	0.41
1:A:225:PRO:N	1:A:273:GLY:HA3	2.35	0.41
1:A:269:ILE:HD12	1:A:269:ILE:N	2.36	0.41
1:A:404:GLN:O	1:A:407:LYS:HG2	2.21	0.41
1:B:125:GLN:O	1:B:125:GLN:HG2	2.21	0.41
1:B:229:LYS:O	1:B:233:LEU:HD23	2.20	0.41
1:B:261:ILE:HD13	1:B:261:ILE:HA	1.97	0.41
2:C:190:LEU:CD2	2:C:362:ILE:HD11	2.49	0.41
2:C:485:VAL:HB	2:C:507:ALA:HB3	2.02	0.41
2:D:410:LEU:HD12	2:D:410:LEU:C	2.45	0.41
1:B:346:MET:SD	1:B:353:ALA:HB1	2.61	0.41
2:D:82:ARG:HG2	2:D:220:GLY:HA2	2.02	0.41
2:D:304:SER:OG	2:D:305:ASN:N	2.54	0.41
1:A:259:ILE:HD11	1:A:266:LEU:HD11	2.02	0.41
1:B:28:LYS:HD2	1:B:31:GLU:HG2	2.03	0.41
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ALA:HB1	1:B:302:MET:HE2	2.03	0.41
1:B:284:ILE:HA	1:B:287:GLU:OE1	2.20	0.41
1:B:334:ARG:CB	1:B:356:ARG:HG2	2.51	0.41
1:B:371:HIS:C	1:B:374:GLN:HG2	2.46	0.41
2:D:450:GLU:OE1	2:D:451:ILE:N	2.53	0.41
2:D:539:ALA:O	2:D:542:VAL:HG12	2.20	0.41
1:A:44:ARG:HB3	1:B:45:TYR:HE1	1.85	0.41
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.90	0.41
1:B:175:ASP:OD2	2:C:429:PHE:HB3	2.21	0.41
1:B:229:LYS:NZ	3:B:501:GNP:N3B	2.68	0.41
1:B:277:ALA:HB3	1:B:283:ARG:CG	2.49	0.41
1:B:297:ASP:OD1	1:B:297:ASP:N	2.52	0.41
1:A:7:ILE:HD12	1:A:106:ALA:CB	2.51	0.41
1:A:16:ARG:HH22	1:B:376:MET:CE	2.34	0.41
1:A:110:GLU:HA	1:A:113:GLU:CB	2.43	0.41
1:A:212:LEU:HD23	1:A:378:PHE:HD1	1.86	0.41
1:A:214:ARG:HB2	1:A:215:GLU:OE1	2.20	0.41
1:A:387:LEU:HD23	1:A:388:ALA:N	2.35	0.41
1:B:14:PRO:HD3	1:B:382:MET:HG3	2.02	0.41
1:B:173:ALA:HB2	1:B:183:PHE:CD1	2.56	0.41
1:B:310:ALA:HB1	1:B:315:GLU:OE2	2.21	0.41
1:B:334:ARG:HB2	1:B:356:ARG:CG	2.50	0.41
2:C:410:LEU:O	2:C:414:VAL:HG23	2.20	0.41
2:C:449:THR:HG23	2:C:450:GLU:N	2.36	0.41
2:C:619:LEU:CB	2:C:625:LEU:HD23	2.37	0.41
2:D:181:ILE:HD12	2:D:181:ILE:H	1.85	0.41
1:A:53:ASP:HA	1:A:59:LEU:HD11	2.02	0.41
1:A:95:LYS:HA	1:A:98:LEU:CD2	2.51	0.41
2:C:362:ILE:HG22	2:C:363:GLN:N	2.36	0.41
2:D:153:LEU:HD12	2:D:153:LEU:HA	1.97	0.41
2:D:354:LYS:HG3	2:D:356:THR:OG1	2.21	0.41
1:A:197:ILE:CD1	1:A:403:LEU:HD23	2.48	0.40
1:A:225:PRO:HG3	1:A:273:GLY:C	2.47	0.40
1:B:117:LEU:CD2	2:C:620:LYS:HB2	2.51	0.40
1:B:220:VAL:CG2	1:B:296:ALA:HB2	2.51	0.40
1:B:355:ILE:HD12	1:B:355:ILE:N	2.35	0.40
2:C:205:ILE:HG22	2:C:206:ASP:N	2.35	0.40
2:C:517:GLU:OE1	2:C:517:GLU:N	2.39	0.40
1:A:124:ALA:HA	1:A:127:GLU:OE1	2.21	0.40
1:A:153:SER:CA	1:A:156:VAL:HG22	2.50	0.40
1:B:228:GLY:O	1:B:232:LEU:HG	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLN:O	1:B:429:ASN:ND2	2.54	0.40
2:C:8:ASP:HB2	2:C:31:GLN:O	2.21	0.40
2:D:472:ASN:O	2:D:475:ARG:HG2	2.21	0.40
1:A:220:VAL:CG2	1:A:296:ALA:HB2	2.51	0.40
1:A:223:GLY:N	1:A:229:LYS:HD3	2.36	0.40
1:A:317:TRP:O	1:A:320:PHE:CD2	2.74	0.40
1:B:3:ASP:OD1	1:B:3:ASP:N	2.54	0.40
2:C:513:LEU:HD23	2:C:513:LEU:O	2.21	0.40
2:D:445:ASP:OD2	2:D:469:LYS:NZ	2.49	0.40
2:D:537:GLN:O	2:D:541:GLN:HG2	2.21	0.40
1:A:13:PRO:HG3	1:B:16:ARG:C	2.46	0.40
1:B:44:ARG:HG2	1:B:44:ARG:O	2.21	0.40
1:B:123:LEU:HD23	1:B:123:LEU:C	2.46	0.40
2:C:297:LEU:HB3	2:C:307:ILE:CG2	2.51	0.40
2:D:322:MET:HA	2:D:325:VAL:CG1	2.51	0.40
1:A:98:LEU:HD12	1:A:98:LEU:C	2.46	0.40
1:A:348:GLU:HA	1:A:352:HIS:O	2.22	0.40
1:B:31:GLU:O	1:B:35:THR:OG1	2.37	0.40
1:B:320:PHE:O	1:B:324:LEU:HG	2.20	0.40
2:C:386:LEU:HB2	2:C:410:LEU:HD21	2.03	0.40
2:C:472:ASN:OD1	2:C:533:LEU:HD21	2.21	0.40
2:C:480:LEU:HD12	2:C:481:LYS:N	2.37	0.40
2:D:136:VAL:HA	2:D:148:ALA:O	2.21	0.40
2:D:377:TYR:CD1	2:D:377:TYR:N	2.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	452/454 (100%)	435 (96%)	17 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	447/454 (98%)	414 (93%)	33 (7%)	0	100	100
2	C	620/649 (96%)	579 (93%)	39 (6%)	2 (0%)	36	66
2	D	510/649 (79%)	478 (94%)	32 (6%)	0	100	100
All	All	2029/2206 (92%)	1906 (94%)	121 (6%)	2 (0%)	49	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	223	PRO
2	C	266	ALA

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 PDB entries followed by that with respect to all EM entries.

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	356/359 (99%)	355 (100%)	1 (0%)	86	85
1	B	350/359 (98%)	348 (99%)	2 (1%)	78	80
2	C	511/533 (96%)	506 (99%)	5 (1%)	68	75
2	D	417/533 (78%)	416 (100%)	1 (0%)	87	87
All	All	1634/1784 (92%)	1625 (99%)	9 (1%)	76	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	HIS
1	B	188	LYS
1	B	382	MET
2	C	37	HIS
2	C	242	CYS
2	C	298	GLU
2	C	498	HIS
2	C	529	PHE
2	D	37	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	350	ASN
1	B	84	HIS
1	B	226	ASN
1	B	402	HIS
2	C	16	HIS
2	C	106	GLN
2	C	218	GLN
2	C	238	GLN
2	C	248	ASN
2	C	323	GLN
2	C	390	ASN
2	C	472	ASN
2	C	555	GLN
2	D	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	GNP	B	501	-	34,34,34	1.67	6 (17%)	47,54,54	1.78	10 (21%)
4	FAD	C	701	-	58,58,58	1.29	3 (5%)	85,89,89	0.71	1 (1%)
3	GNP	A	501	-	34,34,34	1.53	6 (17%)	47,54,54	2.02	12 (25%)

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	GNP	B	501	-	-	9/18/38/38	0/3/3/3
4	FAD	C	701	-	-	12/34/50/50	0/6/6/6
3	GNP	A	501	-	-	11/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	FAD	P-O3P	6.55	1.66	1.59
3	B	501	GNP	PG-N3B	4.46	1.75	1.63
3	B	501	GNP	PB-N3B	4.21	1.74	1.63
3	A	501	GNP	PG-N3B	4.11	1.74	1.63
4	C	701	FAD	PA-O3P	3.98	1.63	1.59
3	B	501	GNP	C6-N1	-3.76	1.31	1.38
3	A	501	GNP	PB-N3B	3.72	1.73	1.63
3	A	501	GNP	C6-N1	-3.35	1.32	1.38
3	B	501	GNP	C5-C4	2.79	1.46	1.38
3	A	501	GNP	C4-N9	-2.54	1.31	1.38
3	A	501	GNP	C5-C4	2.53	1.45	1.38
3	A	501	GNP	C5-N7	-2.43	1.34	1.39
3	B	501	GNP	C5-N7	-2.38	1.34	1.39
4	C	701	FAD	C5X-N5	-2.19	1.35	1.39
3	B	501	GNP	C4-N9	-2.05	1.32	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GNP	C5-C4-N3	-5.96	118.91	128.39
3	B	501	GNP	C5-C4-N3	-5.92	118.97	128.39
3	B	501	GNP	N9-C4-N3	4.64	135.24	125.95
3	A	501	GNP	C2-N3-C4	4.50	120.05	112.30
3	B	501	GNP	C2-N3-C4	4.27	119.65	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GNP	O1B-PB-N3B	-4.17	105.64	111.77
3	A	501	GNP	C6-C5-N7	3.88	137.36	130.29
3	A	501	GNP	C4-C5-N7	-3.66	104.87	110.67
3	A	501	GNP	N9-C4-N3	3.65	133.24	125.95
3	A	501	GNP	O4'-C1'-N9	-3.17	101.17	108.36
3	B	501	GNP	C6-C5-N7	3.17	136.06	130.29
3	B	501	GNP	O2G-PG-O1G	-2.80	106.43	113.45
3	B	501	GNP	C4-C5-N7	-2.78	106.27	110.67
3	A	501	GNP	O3A-PB-N3B	2.74	114.19	106.59
3	A	501	GNP	C8-N7-C5	2.56	108.82	104.26
3	B	501	GNP	C8-N7-C5	2.32	108.39	104.26
3	A	501	GNP	O2B-PB-O3A	2.19	111.97	104.64
3	A	501	GNP	C3'-C2'-C1'	2.18	105.58	101.46
3	B	501	GNP	C8-N9-C4	2.14	110.03	106.03
3	B	501	GNP	N9-C8-N7	-2.10	109.51	113.40
4	C	701	FAD	O2P-P-O1P	2.08	122.14	112.44
3	B	501	GNP	O2B-PB-O3A	2.08	111.57	104.64
3	A	501	GNP	N9-C8-N7	-2.06	109.58	113.40

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GNP	PG-N3B-PB-O1B
3	A	501	GNP	PG-N3B-PB-O3A
3	A	501	GNP	PA-O3A-PB-O2B
3	A	501	GNP	C5'-O5'-PA-O1A
3	A	501	GNP	C5'-O5'-PA-O2A
3	B	501	GNP	PB-N3B-PG-O1G
3	B	501	GNP	PG-N3B-PB-O1B
3	B	501	GNP	PG-N3B-PB-O3A
3	B	501	GNP	C5'-O5'-PA-O3A
3	B	501	GNP	C5'-O5'-PA-O1A
4	C	701	FAD	C3'-C4'-C5'-O5'
4	C	701	FAD	O4'-C4'-C5'-O5'
3	A	501	GNP	O4'-C4'-C5'-O5'
3	A	501	GNP	C3'-C4'-C5'-O5'
3	B	501	GNP	O4'-C4'-C5'-O5'
4	C	701	FAD	O4B-C4B-C5B-O5B
4	C	701	FAD	C3B-C4B-C5B-O5B
4	C	701	FAD	O3'-C3'-C4'-C5'
4	C	701	FAD	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

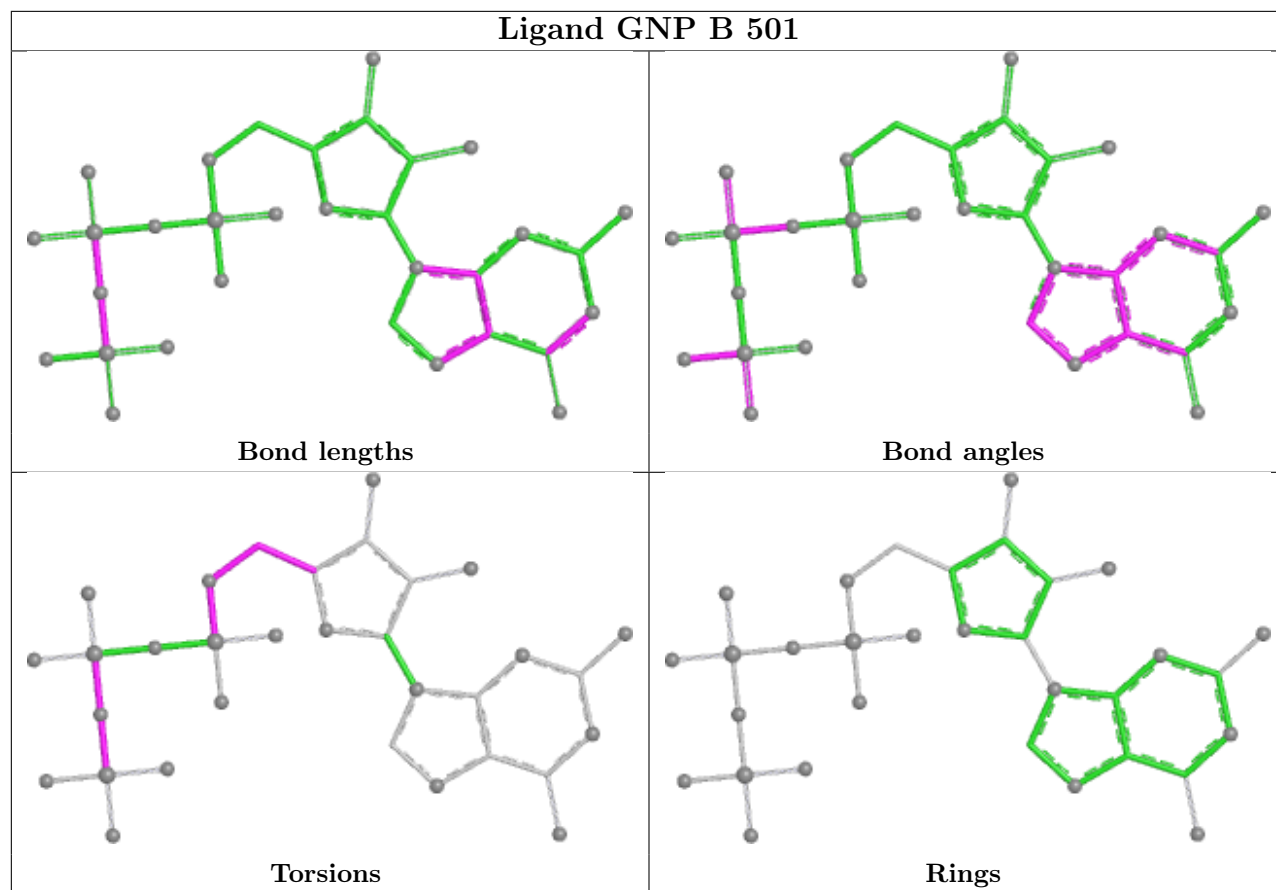
Mol	Chain	Res	Type	Atoms
4	C	701	FAD	C2'-C3'-C4'-O4'
4	C	701	FAD	O3'-C3'-C4'-O4'
3	B	501	GNP	C4'-C5'-O5'-PA
3	B	501	GNP	C3'-C4'-C5'-O5'
3	A	501	GNP	C4'-C5'-O5'-PA
4	C	701	FAD	C4'-C5'-O5'-P
3	A	501	GNP	C5'-O5'-PA-O3A
3	B	501	GNP	C5'-O5'-PA-O2A
4	C	701	FAD	C1'-C2'-C3'-O3'
4	C	701	FAD	O2'-C2'-C3'-C4'
4	C	701	FAD	O2'-C2'-C3'-O3'
3	A	501	GNP	PA-O3A-PB-O1B
3	A	501	GNP	C2'-C1'-N9-C8

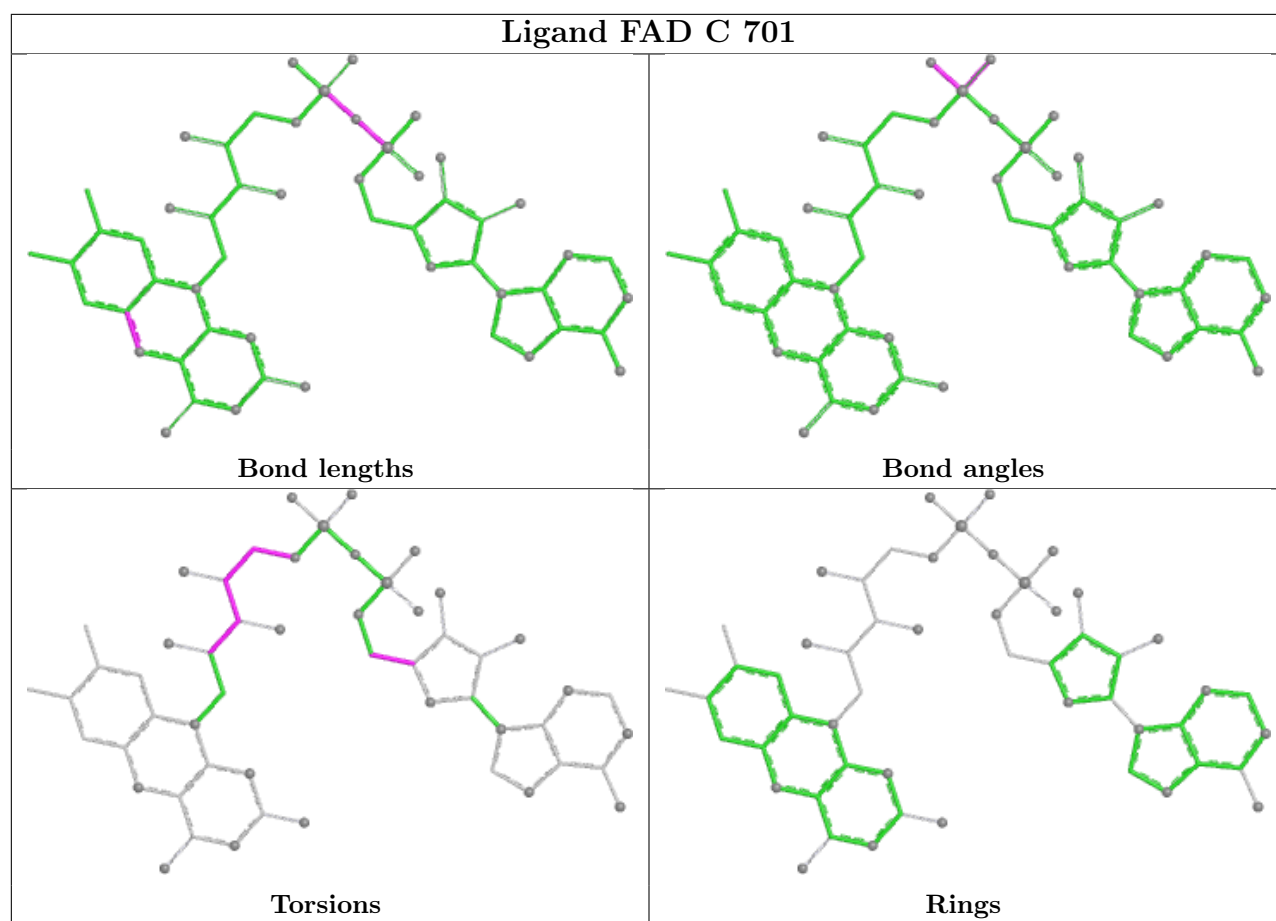
There are no ring outliers.

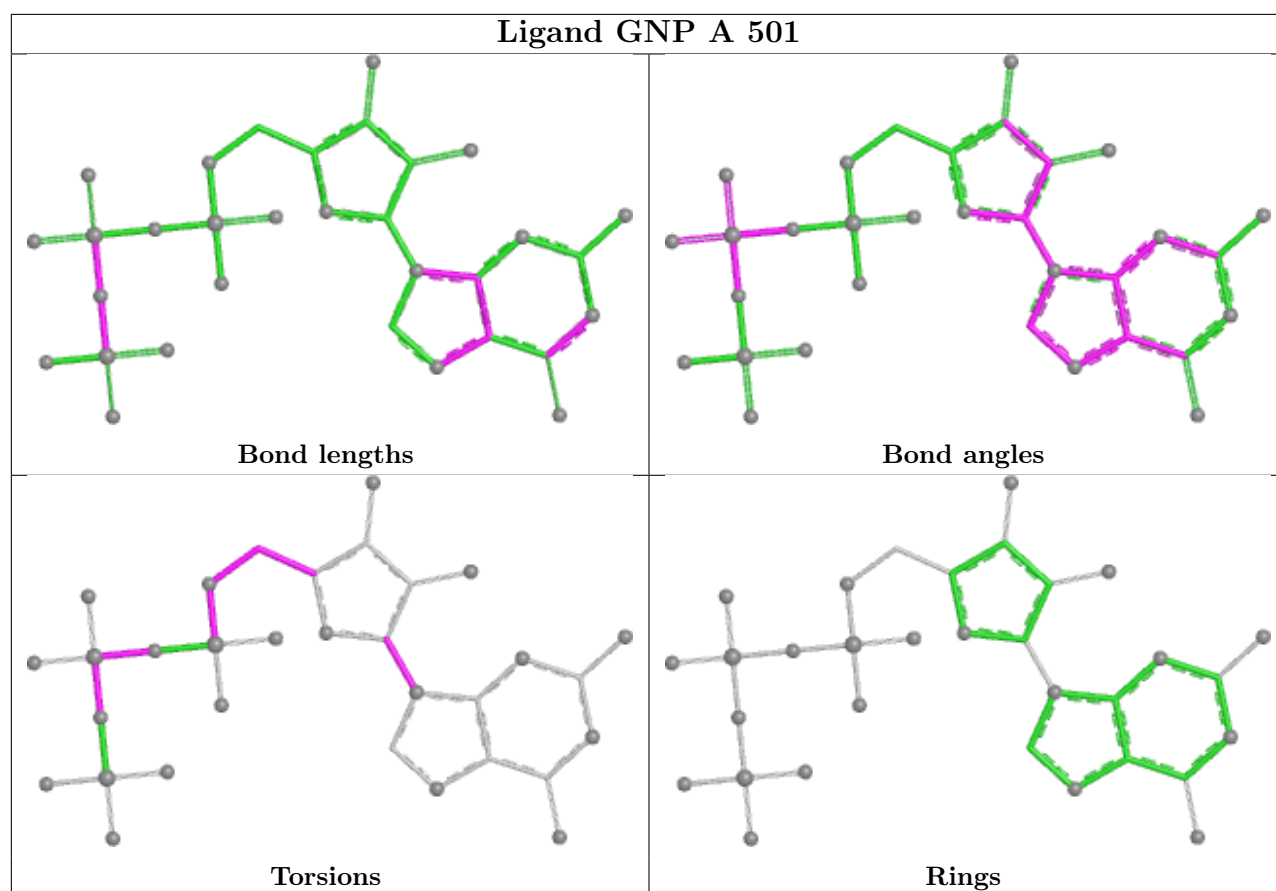
3 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	GNP	15	0
4	C	701	FAD	2	0
3	A	501	GNP	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 Map visualisation

This section contains visualisations of the EMDB entry EMD-52197. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.