



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GMX
Title : Selective Aminopyridine-Based C-Jun N-terminal Kinase inhibitors with cellular activity
Authors : Abad-Zapatero, C.
Deposited on : 2006-04-07
Resolution : 3.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

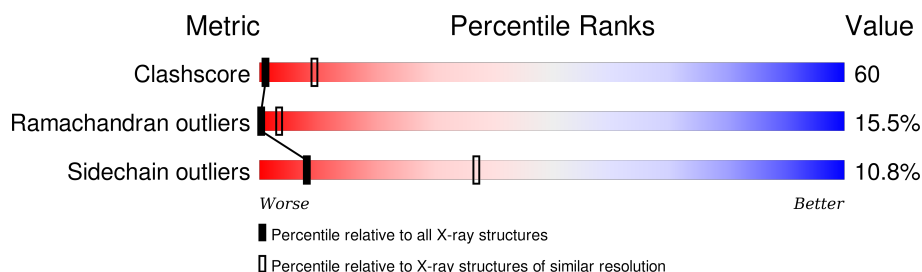
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	370	
1	B	370	
2	F	11	
2	G	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5966 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	1
			2868	1839	483	524	22			
1	B	358	Total	C	N	O	S	0	0	1
			2867	1838	483	524	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	ENGINEERED	UNP P45983
A	185	GLU	TYR	ENGINEERED	UNP P45983
A	365	HIS	-	EXPRESSION TAG	UNP P45983
A	366	HIS	-	EXPRESSION TAG	UNP P45983
A	367	HIS	-	EXPRESSION TAG	UNP P45983
A	368	HIS	-	EXPRESSION TAG	UNP P45983
A	369	HIS	-	EXPRESSION TAG	UNP P45983
A	370	HIS	-	EXPRESSION TAG	UNP P45983
B	183	GLU	THR	ENGINEERED	UNP P45983
B	185	GLU	TYR	ENGINEERED	UNP P45983
B	365	HIS	-	EXPRESSION TAG	UNP P45983
B	366	HIS	-	EXPRESSION TAG	UNP P45983
B	367	HIS	-	EXPRESSION TAG	UNP P45983
B	368	HIS	-	EXPRESSION TAG	UNP P45983
B	369	HIS	-	EXPRESSION TAG	UNP P45983
B	370	HIS	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is a protein called C-jun-amino-terminal kinase-interacting protein 1.

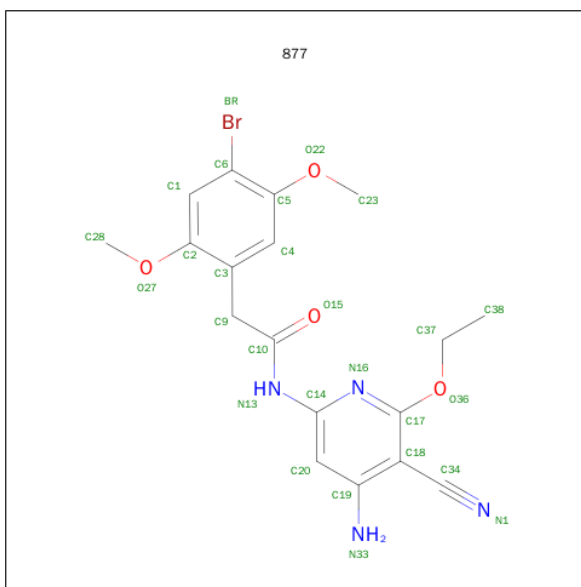
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			84	55	15	14			
2	G	10	Total	C	N	O	0	0	1
			73	46	15	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is N-(4-AMINO-5-CYANO-6-ETHOXYPYRIDIN-2-YL)-2-(4-BROMO-2,5-DIMETHOXYPHENYL)ACETAMIDE (three-letter code: 877) (formula: C₁₈H₁₉BrN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			27	1	18	4	4		
4	B	1	Total	Br	C	N	O	0	0
			27	1	18	4	4		

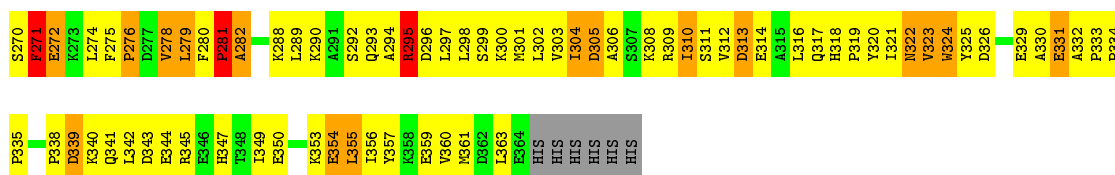
Note EDS was not executed.

- Chain A: 22% 54% 18%

MET	R69	L152	A193	Y259	A330
SER	A70	V133	P194	V260	E331
ARG	Y71	Q134	E195	E261	A332
SER	R72	M135	V196	N262	P333
LYS	E73	L136	I197	R263	P334
ARG	L74	C137	L198		P335
ASP	V75	G138	G199	F271	K336
N8	L76	I139	Y202	E272	I337
N9	M77	K140	K203	L273	P338
F10	V80	H141	K204	L274	K339
Y11	S81	L142	E204	F275	K340
S12	R82	H143	N205	F276	G341
V13	K83	A144	V206	D277	L342
E14	R84	G146	D207	F280	K345
I15	L85	I147	W208	P281	E346
G16	T86	I148	S210	A282	H347
L23	G87	H149	V211	D283	T348
K24	L88	R150	C212	S284	L349
R25	L89	D151	G213	E285	E350
Y26	N90	L152	I214	H286	E351
Q27	V91	K153	N215	N287	K352
N28	F92	P154	G216	K288	K353
L29	T93	S155	E217	L289	E354
I32	P94	M156	M218	K290	L355
G35	Q95	V157	V219	A291	E356
A36	X96	V158	C220	S292	Y357
Q37	S97	V159	H221	Q293	K358
G38	L98	K160	K222	A294	E359
I39	E99	S161	I223	K295	V360
V40	E100	D162	L224	L296	M361
Q41	F101	C163	F225	D297	K362
A42	Q102	T164	P226	L298	L363
A43	D103	L165	G227	S299	E364
Y44	V104	K166	K228	K300	H365
D45	Y105	I167	D229	H301	HIS
A46	I106	L168	Q232	L302	HIS
I47	V107	F170	Q233	K303	HIS
L48	L110	G171	W234	L304	HIS
E49	M111	L172	N235	T310	
R50	M114	A173	K236	S311	
A53	L115	T175	V237	V312	
I54	C116	T178	P244	E314	
K55	Q117	S179	C245	A315	
K56	V113	F180	P246	L316	
L57	L119	M181	E247	Q317	
S58	Q120	M182	F248	H318	
R59	E122	E183	M249	P319	
F61	L123	P184	K250	V320	
Q62	D124	E185	K251	N321	
M63	H125	V186	L252	N322	
Q64	E126	V187	Q253	W324	
T65	I127	T188	P254	K325	
H66	M128	R189	T255	D326	
S67	S129	V190	V256	P327	
K68	V130	Y191	R257	E328	
	L131	P192	T259	S329	

- Chain B:

Amino Acid	Count
Met	1
Ser	1
Arg	1
Ser	1
Lys	1
Arg	1
D7	1
N8	1
N9	1
F10	1
L11	1
S12	1
V13	1
K24	1
R25	1
Y26	1
Q27	1
R28	1
L29	1
K30	1
P31	1
I32	1
Q37	1
G38	1
I39	1
V40	1
C41	1
A42	1
A43	1
I47	1
L48	1
E49	1
I54	1
K55	1
K56	1
L57	1
S58	1
R59	1
P60	1
F61	1
Q62	1
T65	1
H66	1
A67	1
K68	1
R69	1
A70	1
Y71	1
R72	1
E73	1
L74	1
L75	1
V76	1
M77	1
V78	1
C79	1
V80	1
K83	1
N84	1
I85	1
I86	1
G87	1
L88	1
L89	1
N90	1
V91	1
F92	1
T93	1
P94	1
Q95	1
L98	1
F101	1
Q102	1
D103	1
V104	1
V105	1
I106	1
V107	1
M108	1
E109	1
L110	1
M111	1
D112	1
A113	1
N114	1
L115	1
C116	1
Q117	1
V118	1
F119	1
K120	1
M121	1
E122	1
L123	1
D124	1
H125	1
E126	1
R127	1
M128	1
S129	1
V130	1
L131	1
L132	1
V133	1
Q134	1
M135	1
L136	1
C137	1
G138	1
L139	1
K140	1
H141	1
L142	1
H143	1
S144	1
A145	1
I148	1
H149	1
L150	1
D151	1
L152	1
K153	1
P154	1
S155	1
V156	1
L157	1
V158	1
V159	1
K160	1
C163	1
T164	1
L165	1
K166	1
L167	1
L168	1
D169	1
F170	1
G171	1
L172	1
K173	1
T174	1
R175	1
A176	1
G177	1
L178	1
T179	1
S179	1
F180	1
M181	1
P184	1
E185	1
V186	1
V187	1
L188	1
R189	1
V190	1
V191	1
R192	1
A193	1
P194	1
E195	1
V196	1
L197	1
G201	1
Y202	1
K203	1
E204	1
N205	1
V206	1
D207	1
L208	1
W209	1
S210	1
V211	1
G212	1
C213	1
L214	1
M215	1
G216	1
E217	1
M218	1
V219	1
C220	1
E221	1
K222	1
L223	1
L224	1
F225	1
R226	1
G227	1
R228	1
D229	1
Y230	1
I231	1
D232	1
Q233	1
W234	1
N235	1
K236	1
V237	1
L238	1
E239	1
Q240	1
L241	1
G242	1
T243	1
P244	1
C245	1
P246	1
E247	1
F248	1
K249	



- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1



- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.79 Å 150.79 Å 118.66 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.91 – 3.50	Depositor
% Data completeness (in resolution range)	83.3 (19.91-3.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.266 , 0.351	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 877, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/2933	0.69	0/3971
1	B	0.40	0/2932	0.70	0/3970
2	F	0.38	0/86	0.69	0/114
2	G	0.58	0/74	0.81	0/100
All	All	0.40	0/6025	0.70	0/8155

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2868	0	2868	369	0
1	B	2867	0	2866	340	0
2	F	84	0	91	7	0
2	G	73	0	82	8	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	27	0	19	1	0
4	B	27	0	19	6	0
All	All	5966	0	5945	715	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 60.

All (715) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASN:HD21	1:B:309:ARG:HB3	1.20	1.03
1:B:172:LEU:HD21	1:B:186:VAL:HG21	1.40	0.99
1:B:186:VAL:HG13	1:B:187:VAL:H	1.28	0.97
1:B:13:VAL:HG21	1:B:29:LEU:HD13	1.45	0.97
1:A:304:ILE:HD12	1:A:304:ILE:H	1.30	0.97
1:A:132:LEU:O	1:A:136:LEU:HB2	1.67	0.95
1:A:88:LEU:HG	1:A:89:LEU:H	1.31	0.92
1:B:132:LEU:HD21	1:B:215:MET:HB2	1.53	0.91
1:A:190:TYR:H	1:A:190:TYR:HD2	1.00	0.91
1:A:318:HIS:ND1	1:A:319:PRO:HD2	1.86	0.89
1:A:84:ASN:O	1:A:166:LYS:HA	1.72	0.89
1:A:347:HIS:HB3	1:A:351:GLU:OE2	1.72	0.87
1:A:88:LEU:O	1:A:89:LEU:HB2	1.74	0.86
2:G:559:THR:HG22	2:G:560:LEU:H	1.37	0.86
1:A:167:ILE:HG22	1:A:168:LEU:H	1.41	0.86
1:A:244:PRO:HB3	1:A:248:PHE:HD2	1.41	0.85
1:A:208:LEU:HD12	1:A:301:MET:HE3	1.57	0.85
1:A:156:ASN:HD21	1:A:169:ASP:HB3	1.41	0.84
1:B:115:LEU:HD13	1:B:115:LEU:O	1.76	0.84
1:B:275:PHE:HB2	1:B:295:ARG:HD3	1.59	0.84
1:A:116:CYS:SG	1:A:154:PRO:HB2	2.19	0.83
1:A:134:GLN:HE22	1:A:164:THR:HA	1.43	0.82
1:A:190:TYR:CD2	1:A:190:TYR:N	2.46	0.82
1:A:60:PRO:HG2	1:A:61:PHE:H	1.44	0.82
1:A:148:ILE:HD13	1:A:148:ILE:H	1.45	0.82
1:B:39:ILE:HD12	1:B:39:ILE:H	1.43	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD21	1:B:186:VAL:CG2	2.10	0.81
1:A:164:THR:HG22	1:A:165:LEU:H	1.44	0.81
1:A:114:ASN:HD22	1:A:114:ASN:H	1.28	0.81
1:B:75:VAL:HG21	1:B:340:LYS:HG3	1.62	0.80
1:A:203:LYS:O	1:A:206:VAL:HG12	1.81	0.80
1:B:156:ASN:HD21	1:B:169:ASP:HB2	1.46	0.80
1:B:98:LEU:HD11	1:B:353:LYS:HG2	1.63	0.80
1:B:271:PHE:HZ	1:B:302:LEU:HB2	1.45	0.79
1:A:150:ARG:HH21	1:A:172:LEU:HB3	1.47	0.79
1:B:95:GLN:HG2	1:B:102:GLN:H	1.45	0.79
1:A:74:LEU:HD23	1:A:359:GLU:HG3	1.64	0.78
1:A:210:SER:O	1:A:214:ILE:HG12	1.83	0.78
1:B:208:LEU:HD12	1:B:310:ILE:CG2	2.14	0.78
1:B:208:LEU:HD12	1:B:310:ILE:HG23	1.66	0.78
1:B:154:PRO:HD3	1:B:191:TYR:CE2	2.18	0.78
1:A:290:LYS:HE2	1:A:292:SER:HB3	1.66	0.78
1:A:48:LEU:HD22	1:A:50:ARG:HE	1.47	0.78
1:B:32:ILE:HG12	1:B:42:ALA:HB2	1.65	0.78
1:A:253:GLN:HB3	1:A:254:PRO:HD2	1.67	0.77
1:A:45:ASP:OD2	1:A:48:LEU:HB2	1.84	0.77
1:A:80:VAL:HG11	1:A:85:ILE:HG21	1.66	0.76
1:A:300:LYS:O	1:A:310:ILE:HG22	1.86	0.75
1:A:61:PHE:HE2	1:A:353:LYS:HG3	1.49	0.75
1:A:215:MET:O	1:A:219:VAL:HG23	1.86	0.75
1:B:145:ALA:HB2	1:B:335:PRO:HD2	1.68	0.75
2:G:559:THR:O	2:G:560:LEU:HB2	1.85	0.74
1:A:337:ILE:HG23	1:A:338:PRO:HD2	1.67	0.74
1:B:259:TYR:CZ	1:B:263:ARG:HD3	2.22	0.74
1:B:271:PHE:CE1	1:B:299:SER:HA	2.23	0.74
1:B:275:PHE:HB3	1:B:280:PHE:HE2	1.52	0.74
1:A:53:ALA:HB2	1:A:110:LEU:HD12	1.69	0.73
1:B:305:ASP:CB	1:B:308:LYS:HE2	2.18	0.73
1:B:294:ALA:C	1:B:296:ASP:H	1.93	0.72
1:B:150:ARG:HD3	1:B:202:TYR:HE1	1.53	0.72
1:A:26:TYR:HB3	1:A:54:ILE:HD11	1.71	0.72
1:B:111:MET:HB2	4:B:1001:877:H91	1.71	0.72
1:A:316:LEU:HA	1:A:321:ILE:HG21	1.72	0.71
1:B:177:GLY:HA2	1:B:202:TYR:CE2	2.25	0.71
1:A:163:CYS:HA	2:F:560:LEU:HD12	1.71	0.71
1:B:87:GLY:HA3	1:B:109:GLU:OE2	1.90	0.71
1:A:208:LEU:HD12	1:A:301:MET:CE	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASP:O	1:B:170:PHE:HB2	1.91	0.71
1:B:189:ARG:NH1	1:B:229:ASP:HA	2.06	0.70
1:A:134:GLN:HE22	1:A:164:THR:CA	2.03	0.70
1:A:148:ILE:HG22	1:A:204:GLU:HA	1.73	0.70
1:A:90:ASN:HD22	1:A:91:VAL:H	1.40	0.70
1:B:326:ASP:HB2	2:G:556:ARG:HH22	1.55	0.70
1:A:189:ARG:HB2	1:A:192:ARG:HH21	1.57	0.69
1:A:310:ILE:HD11	1:A:315:ALA:HA	1.75	0.69
1:A:11:TYR:OH	1:A:27:GLN:HA	1.92	0.69
1:A:181:MET:O	1:A:184:PRO:HD3	1.92	0.69
1:A:150:ARG:NH1	1:A:174:ARG:HG2	2.07	0.69
1:B:275:PHE:HB3	1:B:280:PHE:CE2	2.27	0.69
1:B:102:GLN:HG2	1:B:103:ASP:OD1	1.93	0.69
1:B:10:PHE:CE1	1:B:94:PRO:HA	2.28	0.69
1:A:237:VAL:HG13	1:A:238:ILE:HG23	1.75	0.69
1:B:357:TYR:O	1:B:361:MET:HG2	1.92	0.68
1:B:187:VAL:HG22	1:B:192:ARG:HG2	1.74	0.68
1:A:271:PHE:HA	1:A:274:LEU:HB2	1.75	0.68
1:B:360:VAL:HA	1:B:363:LEU:HD11	1.75	0.68
1:B:153:LYS:HE2	1:B:155:SER:OG	1.93	0.68
1:B:275:PHE:CD2	1:B:298:LEU:HD13	2.29	0.68
1:B:114:ASN:ND2	1:B:116:CYS:HB2	2.09	0.68
1:B:115:LEU:HB2	1:B:157:ILE:HB	1.76	0.68
1:A:285:GLU:HB2	1:A:286:HIS:ND1	2.08	0.67
1:A:259:TYR:CZ	1:A:263:ARG:HD3	2.29	0.67
1:B:148:ILE:O	1:B:173:ALA:HA	1.94	0.67
1:B:187:VAL:O	1:B:192:ARG:HD3	1.94	0.67
1:B:61:PHE:HA	1:B:67:ALA:HB2	1.77	0.67
1:B:186:VAL:HG13	1:B:187:VAL:N	2.06	0.67
1:A:32:ILE:HG21	1:A:42:ALA:HB2	1.76	0.67
1:A:288:LYS:HD2	1:A:323:VAL:HG12	1.76	0.67
1:B:30:LYS:HB3	1:B:42:ALA:HB3	1.76	0.66
1:B:230:TYR:CE2	1:B:231:ILE:HG13	2.30	0.66
1:A:117:GLN:HE21	1:A:117:GLN:HA	1.60	0.66
1:A:158:VAL:O	1:A:165:LEU:HA	1.95	0.66
1:A:287:ASN:O	1:A:289:LEU:N	2.28	0.66
1:B:359:GLU:O	1:B:363:LEU:HG	1.95	0.66
1:B:318:HIS:ND1	1:B:319:PRO:HD2	2.10	0.66
1:B:288:LYS:O	1:B:293:GLN:HG2	1.96	0.66
1:A:189:ARG:HA	1:A:192:ARG:HE	1.59	0.66
1:A:257:ARG:O	1:A:261:GLU:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:CE2	1:A:238:ILE:HG21	2.31	0.66
1:A:128:MET:O	1:A:132:LEU:HD22	1.96	0.66
2:F:559:THR:HG22	2:F:560:LEU:H	1.61	0.66
1:A:115:LEU:HB2	1:A:157:ILE:HG22	1.78	0.65
1:B:78:LYS:HD3	1:B:363:LEU:HD22	1.79	0.65
1:A:165:LEU:HD23	1:A:165:LEU:C	2.17	0.65
1:A:356:ILE:O	1:A:360:VAL:HG23	1.96	0.65
1:A:220:CYS:O	1:A:221:HIS:HB2	1.97	0.65
1:B:133:TYR:HB2	1:B:321:ILE:HG23	1.77	0.65
1:A:149:HIS:C	1:A:150:ARG:HG3	2.17	0.65
1:A:101:PHE:HD2	1:A:357:TYR:HB2	1.61	0.65
1:B:303:VAL:HG21	1:B:309:ARG:HA	1.79	0.65
1:B:321:ILE:O	1:B:323:VAL:N	2.29	0.64
1:A:315:ALA:O	1:A:318:HIS:HB3	1.98	0.64
1:A:213:CYS:HA	1:A:224:LEU:HD22	1.79	0.64
1:B:95:GLN:HG2	1:B:102:GLN:N	2.12	0.64
1:B:60:PRO:HG2	1:B:61:PHE:CD2	2.33	0.64
1:A:289:LEU:O	1:A:293:GLN:HB2	1.98	0.64
1:A:244:PRO:HB3	1:A:248:PHE:CD2	2.28	0.64
1:A:234:TRP:CZ2	1:A:238:ILE:HG21	2.33	0.64
1:A:160:LYS:HB3	1:A:162:ASP:OD1	1.98	0.64
1:B:342:LEU:HB2	1:B:345:ARG:HD3	1.80	0.64
1:A:174:ARG:HD3	1:A:175:THR:O	1.98	0.63
1:A:142:LEU:HD11	1:A:147:ILE:HG21	1.81	0.63
1:A:64:GLN:HB3	1:A:346:GLU:CD	2.19	0.63
1:A:114:ASN:HD22	1:A:114:ASN:N	1.94	0.63
1:B:342:LEU:H	1:B:342:LEU:HD23	1.63	0.63
1:B:110:LEU:HD21	4:B:1001:877:H232	1.81	0.63
1:B:128:MET:HG3	1:B:218:MET:HE2	1.80	0.63
1:A:115:LEU:CD1	1:A:119:ILE:HG13	2.29	0.63
1:A:164:THR:O	1:A:165:LEU:HB2	1.99	0.63
1:B:259:TYR:CE1	1:B:263:ARG:HD3	2.34	0.62
1:A:101:PHE:CD2	1:A:357:TYR:HB2	2.34	0.62
1:A:115:LEU:C	1:A:117:GLN:H	2.01	0.62
1:A:235:ASN:HD21	1:A:263:ARG:NE	1.97	0.62
1:B:98:LEU:O	1:B:101:PHE:HB2	1.99	0.62
1:B:290:LYS:HB2	1:B:293:GLN:HB2	1.81	0.62
1:B:148:ILE:HG22	1:B:150:ARG:HG3	1.81	0.61
1:B:205:ASN:ND2	1:B:309:ARG:HB3	2.04	0.61
1:B:152:LEU:O	1:B:214:ILE:HD11	2.00	0.61
1:B:98:LEU:CD1	1:B:353:LYS:HG2	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CZ	1:B:299:SER:HA	2.36	0.61
1:B:215:MET:HE3	1:B:298:LEU:HG	1.81	0.61
1:A:90:ASN:HD22	1:A:91:VAL:N	1.97	0.61
1:B:275:PHE:CE2	1:B:298:LEU:HD13	2.36	0.61
1:B:13:VAL:HG21	1:B:29:LEU:CD1	2.28	0.61
1:B:113:ALA:HB1	1:B:117:GLN:OE1	2.00	0.61
1:B:342:LEU:CB	1:B:345:ARG:HD3	2.30	0.61
1:A:314:GLU:CD	1:A:314:GLU:H	2.04	0.61
1:A:143:HIS:C	1:A:145:ALA:H	2.04	0.61
1:B:84:ASN:O	1:B:85:ILE:HD13	2.01	0.61
1:B:77:MET:HB3	1:B:88:LEU:HD22	1.82	0.61
1:A:156:ASN:O	1:A:157:ILE:HD13	2.01	0.61
1:B:163:CYS:HA	2:G:560:LEU:HD22	1.81	0.61
1:B:225:PHE:HE1	1:B:240:GLN:HB2	1.66	0.61
1:A:115:LEU:HD13	1:A:119:ILE:HG13	1.83	0.60
1:B:125:HIS:ND1	1:B:289:LEU:O	2.34	0.60
1:A:88:LEU:HG	1:A:89:LEU:N	2.11	0.60
1:B:65:THR:C	1:B:67:ALA:H	2.04	0.60
1:A:143:HIS:O	1:A:145:ALA:N	2.34	0.60
1:B:78:LYS:NZ	1:B:363:LEU:HB2	2.17	0.60
1:B:128:MET:HG3	1:B:218:MET:CE	2.31	0.60
1:A:94:PRO:HG2	1:A:95:GLN:NE2	2.17	0.60
1:A:86:ILE:HA	1:A:166:LYS:HD3	1.83	0.60
1:B:28:ASN:HD22	1:B:29:LEU:N	1.99	0.60
1:B:215:MET:CE	1:B:298:LEU:HG	2.31	0.60
1:A:64:GLN:HB3	1:A:346:GLU:OE2	2.00	0.60
1:B:165:LEU:HD23	1:B:166:LYS:N	2.17	0.60
1:B:230:TYR:CD2	1:B:231:ILE:HG13	2.37	0.60
1:A:63:ASN:OD1	1:A:65:THR:HB	2.01	0.60
1:A:118:VAL:O	1:A:119:ILE:C	2.40	0.59
1:A:136:LEU:HA	1:A:139:ILE:HD12	1.84	0.59
1:A:148:ILE:CG2	1:A:204:GLU:HA	2.32	0.59
1:A:25:ARG:HG2	1:A:47:ILE:HB	1.85	0.59
1:B:194:PRO:HA	1:B:197:ILE:HD12	1.84	0.59
1:A:117:GLN:NE2	1:A:117:GLN:HA	2.17	0.59
1:B:193:ALA:HB2	1:B:209:TRP:CG	2.37	0.59
1:A:254:PRO:O	1:A:257:ARG:HB3	2.02	0.59
1:A:61:PHE:CE2	1:A:353:LYS:HG3	2.35	0.59
1:A:149:HIS:HA	1:A:173:ALA:CB	2.33	0.59
1:B:59:ARG:CB	1:B:62:GLN:HB2	2.33	0.59
1:B:305:ASP:HB2	1:B:308:LYS:HE2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:CE2	1:A:94:PRO:HA	2.38	0.59
1:A:167:ILE:HG22	1:A:168:LEU:N	2.14	0.59
1:A:74:LEU:HD23	1:A:359:GLU:CG	2.33	0.59
1:B:354:GLU:O	1:B:355:LEU:C	2.41	0.59
1:B:305:ASP:HB3	1:B:308:LYS:HE2	1.84	0.58
1:A:164:THR:HG22	1:A:165:LEU:N	2.17	0.58
1:B:39:ILE:HD12	1:B:39:ILE:N	2.15	0.58
1:A:189:ARG:CA	1:A:192:ARG:HH21	2.15	0.58
1:A:165:LEU:HD23	1:A:166:LYS:N	2.19	0.58
1:A:150:ARG:O	1:A:151:ASP:HB2	2.03	0.58
1:B:272:GLU:HA	1:B:295:ARG:HD2	1.85	0.58
1:B:11:TYR:CE1	1:B:24:LYS:HA	2.38	0.58
1:B:250:LYS:HD2	1:B:257:ARG:HH12	1.68	0.58
1:A:48:LEU:HD22	1:A:50:ARG:NE	2.17	0.58
1:A:125:HIS:ND1	1:A:320:TYR:OH	2.31	0.58
1:A:13:VAL:HG11	1:A:29:LEU:HB2	1.86	0.58
1:A:300:LYS:C	1:A:310:ILE:HG22	2.24	0.57
1:B:169:ASP:O	1:B:170:PHE:CB	2.52	0.57
1:B:220:CYS:O	1:B:221:HIS:HB2	2.03	0.57
1:A:189:ARG:CB	1:A:192:ARG:HH21	2.17	0.57
1:A:77:MET:CE	1:A:77:MET:HA	2.34	0.57
1:B:216:GLY:HA3	1:B:224:LEU:HD22	1.86	0.57
1:B:130:TYR:O	1:B:134:GLN:HB2	2.04	0.57
1:A:244:PRO:HB2	1:A:249:MET:CE	2.35	0.57
1:A:133:TYR:CE1	1:A:137:CYS:SG	2.97	0.57
1:B:119:ILE:HB	1:B:120:GLN:NE2	2.20	0.57
1:B:349:ILE:HG13	1:B:350:GLU:N	2.20	0.57
1:A:234:TRP:HA	1:A:237:VAL:HG12	1.86	0.56
1:B:193:ALA:HB2	1:B:209:TRP:CD1	2.39	0.56
1:B:270:SER:O	1:B:272:GLU:N	2.38	0.56
1:B:86:ILE:HG13	1:B:168:LEU:HD23	1.87	0.56
1:A:60:PRO:CG	1:A:61:PHE:H	2.17	0.56
1:A:148:ILE:N	1:A:148:ILE:HD13	2.17	0.56
1:A:133:TYR:HB2	1:A:324:TRP:HD1	1.70	0.56
1:A:342:LEU:HB2	1:A:345:ARG:HB3	1.87	0.56
1:B:140:LYS:HA	1:B:312:VAL:HG11	1.88	0.56
1:B:131:LEU:O	1:B:132:LEU:C	2.44	0.55
1:A:297:LEU:HD13	1:A:318:HIS:CD2	2.42	0.55
1:A:190:TYR:HB3	1:A:223:ILE:HG21	1.89	0.55
1:B:39:ILE:O	1:B:55:LYS:HA	2.06	0.55
1:A:234:TRP:NE1	1:A:238:ILE:HD13	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD12	1:A:128:MET:CA	2.37	0.55
1:B:127:ARG:O	1:B:131:LEU:HG	2.06	0.55
1:A:361:MET:O	1:A:363:LEU:N	2.39	0.55
1:A:325:TYR:O	1:A:326:ASP:HB2	2.06	0.55
1:B:89:LEU:O	1:B:90:ASN:HB2	2.05	0.55
1:B:192:ARG:HH22	1:B:230:TYR:HB2	1.72	0.55
2:F:560:LEU:HD22	2:F:562:LEU:HD21	1.88	0.55
1:B:30:LYS:O	1:B:42:ALA:N	2.35	0.55
1:A:111:MET:HG3	1:A:158:VAL:HB	1.88	0.55
1:A:129:SER:HB3	1:A:320:TYR:CE2	2.41	0.55
1:A:94:PRO:HG3	1:A:105:TYR:HE1	1.71	0.55
1:A:228:ARG:NH2	1:B:262:ASN:OD1	2.40	0.55
1:A:235:ASN:HD21	1:A:263:ARG:HE	1.55	0.55
1:B:115:LEU:CD1	1:B:119:ILE:HD11	2.37	0.55
1:A:25:ARG:HD3	1:A:45:ASP:OD1	2.07	0.55
1:A:192:ARG:HG2	1:A:196:VAL:HG11	1.89	0.55
1:A:197:ILE:HG22	1:A:198:LEU:N	2.20	0.55
1:A:93:THR:O	1:A:93:THR:HG23	2.07	0.55
1:B:321:ILE:O	1:B:322:ASN:C	2.44	0.54
1:A:234:TRP:O	1:A:236:LYS:N	2.40	0.54
1:B:325:TYR:HE1	1:B:330:ALA:HB3	1.72	0.54
1:B:11:TYR:HE1	1:B:24:LYS:HA	1.72	0.54
1:B:65:THR:O	1:B:68:LYS:HG2	2.08	0.54
1:B:137:CYS:SG	1:B:330:ALA:HB2	2.48	0.54
1:A:216:GLY:O	1:A:220:CYS:HB2	2.08	0.54
1:B:86:ILE:HG13	1:B:168:LEU:CD2	2.38	0.54
1:A:105:TYR:O	1:A:106:ILE:HD13	2.07	0.54
1:B:257:ARG:O	1:B:259:TYR:N	2.40	0.53
1:A:180:PHE:CG	1:A:181:MET:N	2.75	0.53
1:B:294:ALA:C	1:B:296:ASP:N	2.62	0.53
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.22	0.53
1:B:259:TYR:O	1:B:262:ASN:HB2	2.08	0.53
1:A:39:ILE:HG22	1:A:40:VAL:N	2.23	0.53
1:B:310:ILE:HG13	1:B:311:SER:H	1.73	0.53
1:A:233:GLN:HA	1:A:233:GLN:NE2	2.23	0.53
1:A:296:ASP:OD2	1:A:300:LYS:HE2	2.09	0.53
1:A:310:ILE:O	1:A:310:ILE:HG23	2.08	0.53
1:A:183:GLU:N	1:A:184:PRO:HD3	2.23	0.53
1:B:239:GLU:HA	1:B:266:TYR:CD1	2.44	0.53
1:B:211:VAL:HB	1:B:301:MET:HE1	1.91	0.53
1:A:10:PHE:N	1:A:10:PHE:CD1	2.75	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:CE1	1:A:104:VAL:HG22	2.44	0.53
1:A:194:PRO:HD3	1:A:209:TRP:CE2	2.44	0.53
1:B:172:LEU:CD2	1:B:186:VAL:HG21	2.25	0.53
1:B:149:HIS:O	1:B:150:ARG:HB2	2.09	0.53
1:B:175:THR:O	1:B:176:ALA:O	2.27	0.53
1:B:28:ASN:HD22	1:B:28:ASN:C	2.12	0.53
1:A:118:VAL:O	1:A:121:MET:HG2	2.09	0.53
1:B:271:PHE:HA	1:B:274:LEU:HD12	1.91	0.53
1:A:149:HIS:O	1:A:150:ARG:HG3	2.08	0.53
1:A:252:LEU:CD1	1:A:260:VAL:HG11	2.39	0.53
1:A:205:ASN:O	1:A:208:LEU:N	2.40	0.52
1:A:25:ARG:HE	1:A:47:ILE:HG21	1.74	0.52
1:B:139:ILE:HD11	1:B:152:LEU:CD1	2.39	0.52
1:A:197:ILE:HD11	1:A:233:GLN:HG3	1.89	0.52
1:A:154:PRO:C	1:A:156:ASN:H	2.13	0.52
1:A:325:TYR:OH	1:A:331:GLU:HG3	2.10	0.52
1:B:177:GLY:HA2	1:B:202:TYR:HE2	1.72	0.52
1:B:256:VAL:O	1:B:259:TYR:HB3	2.10	0.52
1:B:300:LYS:O	1:B:310:ILE:HB	2.09	0.52
1:A:53:ALA:CB	1:A:110:LEU:HD12	2.37	0.52
1:A:178:THR:HG22	1:A:179:SER:N	2.25	0.52
1:A:137:CYS:O	1:A:138:GLY:C	2.48	0.52
1:A:149:HIS:HA	1:A:173:ALA:HB2	1.92	0.52
1:B:9:ASN:O	1:B:24:LYS:HG3	2.10	0.52
1:B:297:LEU:HG	1:B:301:MET:SD	2.50	0.51
1:A:312:VAL:O	1:A:315:ALA:HB3	2.11	0.51
1:A:53:ALA:CA	1:A:110:LEU:HD12	2.40	0.51
1:A:234:TRP:C	1:A:236:LYS:H	2.14	0.51
1:B:201:GLY:O	1:B:202:TYR:HB3	2.10	0.51
1:B:270:SER:C	1:B:272:GLU:H	2.13	0.51
1:B:293:GLN:NE2	1:B:319:PRO:HG2	2.26	0.51
1:A:164:THR:O	1:A:165:LEU:CB	2.58	0.51
1:B:304:ILE:HD12	1:B:304:ILE:H	1.76	0.51
1:B:150:ARG:HH21	1:B:172:LEU:HB3	1.74	0.51
1:B:189:ARG:O	1:B:191:TYR:N	2.43	0.51
1:B:280:PHE:O	1:B:282:ALA:N	2.44	0.51
1:A:131:LEU:HA	1:A:134:GLN:HB2	1.92	0.51
1:B:356:ILE:O	1:B:360:VAL:HG23	2.10	0.51
1:A:314:GLU:HA	1:A:317:GLN:HB2	1.92	0.51
1:B:211:VAL:HB	1:B:301:MET:CE	2.41	0.51
1:A:293:GLN:HA	1:A:293:GLN:HE21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CD1	1:B:299:SER:HA	2.45	0.51
1:A:123:LEU:HD12	1:A:128:MET:HA	1.92	0.51
1:A:135:MET:O	1:A:139:ILE:HG13	2.10	0.51
1:A:10:PHE:HD1	1:A:10:PHE:N	2.09	0.51
1:B:294:ALA:HB2	1:B:320:TYR:CE1	2.45	0.50
1:A:115:LEU:C	1:A:117:GLN:N	2.65	0.50
1:A:84:ASN:O	1:A:166:LYS:CA	2.52	0.50
1:A:163:CYS:HB2	2:F:559:THR:O	2.11	0.50
1:B:40:VAL:HA	1:B:54:ILE:O	2.10	0.50
1:A:90:ASN:HB3	1:A:107:VAL:HB	1.93	0.50
1:B:107:VAL:O	1:B:108:MET:HB3	2.11	0.50
1:A:120:GLN:O	1:A:120:GLN:HG3	2.10	0.50
1:A:152:LEU:N	1:A:152:LEU:HD23	2.26	0.50
1:B:232:ASP:HA	1:B:235:ASN:ND2	2.26	0.50
1:B:153:LYS:HE2	1:B:155:SER:CB	2.41	0.50
1:A:88:LEU:CG	1:A:89:LEU:N	2.71	0.50
1:A:94:PRO:HG2	1:A:95:GLN:HE22	1.73	0.50
1:A:212:GLY:C	1:A:214:ILE:H	2.14	0.50
1:A:48:LEU:HD21	1:A:50:ARG:HH21	1.77	0.50
1:B:140:LYS:O	1:B:143:HIS:N	2.44	0.50
1:A:133:TYR:CB	1:A:324:TRP:HD1	2.24	0.50
1:A:255:THR:O	1:A:256:VAL:C	2.50	0.50
1:B:342:LEU:O	1:B:345:ARG:HB2	2.12	0.50
1:A:111:MET:HE3	1:A:160:LYS:N	2.26	0.50
1:B:217:GLU:CD	1:B:223:ILE:HD13	2.32	0.50
1:B:224:LEU:O	1:B:226:PRO:HD3	2.12	0.50
1:B:297:LEU:CD2	1:B:321:ILE:HD11	2.42	0.50
1:B:32:ILE:HD11	1:B:42:ALA:HA	1.93	0.50
1:B:122:GLU:O	1:B:123:LEU:HD23	2.11	0.50
1:A:125:HIS:CE1	1:A:320:TYR:HH	2.22	0.50
1:B:10:PHE:CZ	1:B:94:PRO:HA	2.47	0.50
1:B:207:ASP:O	1:B:211:VAL:HG23	2.12	0.50
1:B:281:PRO:O	1:B:282:ALA:O	2.30	0.50
1:A:101:PHE:CD1	1:A:102:GLN:N	2.79	0.50
1:B:205:ASN:HD21	1:B:309:ARG:CB	2.08	0.49
1:A:288:LYS:CD	1:A:323:VAL:HG12	2.42	0.49
1:A:61:PHE:HA	1:A:67:ALA:HB2	1.93	0.49
1:A:48:LEU:O	1:A:49:GLU:HB2	2.12	0.49
1:A:128:MET:CE	1:A:132:LEU:HD21	2.41	0.49
1:A:348:THR:HG22	1:A:349:ILE:H	1.77	0.49
1:B:174:ARG:HG3	1:B:175:THR:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:HD3	1:B:191:TYR:CZ	2.47	0.49
1:B:215:MET:CE	1:B:297:LEU:HB3	2.42	0.49
1:A:183:GLU:N	1:A:184:PRO:CD	2.75	0.49
1:B:114:ASN:C	1:B:114:ASN:HD22	2.14	0.49
1:B:67:ALA:O	1:B:70:ALA:HB3	2.10	0.49
1:A:38:GLY:HA3	1:A:56:LYS:O	2.12	0.49
1:B:118:VAL:HA	1:B:121:MET:CG	2.41	0.49
1:A:146:GLY:HA2	1:A:204:GLU:OE2	2.12	0.49
1:B:338:PRO:HG3	1:B:340:LYS:HE2	1.95	0.49
1:A:198:LEU:HD11	1:A:234:TRP:CH2	2.48	0.49
1:A:180:PHE:CD1	1:A:181:MET:N	2.81	0.49
1:A:9:ASN:O	1:A:24:LYS:HG3	2.12	0.49
1:B:125:HIS:CE1	1:B:289:LEU:O	2.66	0.49
1:B:172:LEU:O	1:B:173:ALA:C	2.49	0.49
1:A:334:PRO:HB2	1:A:336:LYS:HE2	1.93	0.49
1:B:303:VAL:HG11	1:B:308:LYS:HB2	1.94	0.49
1:A:248:PHE:O	1:A:251:LYS:HG3	2.12	0.49
1:B:313:ASP:O	1:B:317:GLN:HG2	2.13	0.49
1:B:209:TRP:C	1:B:209:TRP:CD1	2.86	0.49
1:A:294:ALA:O	1:A:297:LEU:HB3	2.12	0.49
1:B:111:MET:HE3	1:B:160:LYS:HB2	1.94	0.49
1:B:151:ASP:O	1:B:152:LEU:HD23	2.13	0.49
1:B:124:ASP:O	1:B:125:HIS:C	2.51	0.49
1:B:189:ARG:NH1	1:B:229:ASP:CA	2.76	0.49
1:B:27:GLN:HE21	1:B:28:ASN:H	1.59	0.49
2:G:559:THR:HG22	2:G:560:LEU:N	2.18	0.49
1:A:189:ARG:HG2	1:A:233:GLN:NE2	2.27	0.48
1:A:234:TRP:HA	1:A:237:VAL:CG1	2.43	0.48
2:F:559:THR:O	2:F:560:LEU:HB2	2.13	0.48
1:A:130:TYR:CZ	2:F:556:ARG:HD3	2.48	0.48
1:A:262:ASN:O	1:A:263:ARG:C	2.49	0.48
1:A:91:VAL:HG21	1:A:363:LEU:CD1	2.44	0.48
1:B:269:TYR:HB2	1:B:274:LEU:CD2	2.43	0.48
1:B:111:MET:CE	1:B:160:LYS:HB2	2.44	0.48
1:A:296:ASP:O	1:A:299:SER:HB2	2.13	0.48
1:B:32:ILE:HD11	1:B:41:CYS:O	2.14	0.48
1:B:189:ARG:HH12	1:B:229:ASP:HA	1.76	0.48
1:A:90:ASN:ND2	1:A:91:VAL:N	2.60	0.48
1:B:118:VAL:HA	1:B:121:MET:SD	2.54	0.48
1:A:229:ASP:OD1	1:A:232:ASP:CB	2.61	0.48
1:B:65:THR:O	1:B:67:ALA:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:O	1:B:188:THR:N	2.47	0.48
1:A:234:TRP:C	1:A:236:LYS:N	2.67	0.48
1:B:208:LEU:CD1	1:B:310:ILE:HG23	2.42	0.48
1:B:28:ASN:O	1:B:43:ALA:HA	2.13	0.48
1:A:134:GLN:HE22	1:A:164:THR:C	2.16	0.48
1:A:351:GLU:O	1:A:355:LEU:HD13	2.13	0.48
1:B:117:GLN:O	1:B:120:GLN:N	2.37	0.48
1:A:149:HIS:CG	1:A:152:LEU:HD21	2.49	0.48
1:A:283:ASP:HB2	1:A:291:ALA:HB2	1.95	0.48
1:B:257:ARG:O	1:B:258:THR:C	2.49	0.48
1:B:110:LEU:HD21	4:B:1001:877:C23	2.43	0.48
1:A:224:LEU:HD23	1:A:225:PHE:CZ	2.49	0.48
1:B:303:VAL:HG12	1:B:305:ASP:H	1.79	0.48
1:A:233:GLN:HA	1:A:233:GLN:HE21	1.79	0.48
1:B:140:LYS:O	1:B:142:LEU:N	2.47	0.48
1:B:89:LEU:H	1:B:108:MET:HA	1.79	0.48
1:B:27:GLN:NE2	1:B:28:ASN:H	2.12	0.47
1:B:29:LEU:HD12	1:B:29:LEU:N	2.29	0.47
1:B:257:ARG:C	1:B:259:TYR:N	2.64	0.47
1:A:32:ILE:CG1	1:A:40:VAL:HG13	2.44	0.47
1:A:189:ARG:HB2	1:A:192:ARG:NH2	2.27	0.47
1:A:29:LEU:HD12	1:A:43:ALA:CB	2.44	0.47
1:B:215:MET:HG2	1:B:215:MET:O	2.13	0.47
1:B:110:LEU:HD23	1:B:111:MET:O	2.14	0.47
1:B:355:LEU:O	1:B:359:GLU:N	2.43	0.47
1:B:27:GLN:O	1:B:28:ASN:HB3	2.15	0.47
1:A:360:VAL:O	1:A:361:MET:C	2.53	0.47
1:A:244:PRO:HB2	1:A:249:MET:HE1	1.94	0.47
1:A:72:ARG:NH1	1:A:174:ARG:HB3	2.29	0.47
1:B:169:ASP:HB3	1:B:170:PHE:H	1.37	0.47
1:B:290:LYS:O	1:B:293:GLN:HB3	2.14	0.47
1:A:259:TYR:HB2	1:B:229:ASP:HB2	1.96	0.47
1:A:110:LEU:HD21	4:A:901:877:H232	1.95	0.47
1:B:165:LEU:HD23	1:B:165:LEU:C	2.35	0.47
1:B:105:TYR:CD1	1:B:105:TYR:N	2.83	0.47
1:B:278:VAL:O	1:B:280:PHE:N	2.47	0.47
1:B:338:PRO:O	1:B:339:ASP:HB3	2.14	0.47
1:B:338:PRO:HG2	1:B:339:ASP:H	1.80	0.47
1:B:148:ILE:CD1	1:B:204:GLU:HA	2.44	0.47
1:B:186:VAL:CG1	1:B:187:VAL:H	2.12	0.47
1:A:153:LYS:NZ	1:A:188:THR:HG23	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:364:GLU:HB2	2.15	0.47
1:A:326:ASP:O	1:A:328:SER:N	2.47	0.47
1:B:244:PRO:HB3	1:B:248:PHE:CD2	2.50	0.47
1:A:285:GLU:HB2	1:A:286:HIS:CE1	2.50	0.47
1:B:293:GLN:HE21	1:B:319:PRO:HG2	1.80	0.47
1:A:69:ARG:HG3	1:A:171:GLY:O	2.15	0.47
1:B:189:ARG:NH2	1:B:227:GLY:O	2.48	0.47
1:A:332:ALA:HB1	1:A:333:PRO:HD2	1.97	0.47
1:B:189:ARG:HH11	1:B:230:TYR:N	2.12	0.46
1:A:207:ASP:O	1:A:210:SER:HB2	2.15	0.46
1:A:25:ARG:HG2	1:A:45:ASP:OD1	2.15	0.46
1:B:150:ARG:NH1	1:B:181:MET:SD	2.88	0.46
1:A:82:HIS:CD2	1:A:84:ASN:H	2.32	0.46
1:A:94:PRO:HD3	1:A:105:TYR:CD1	2.50	0.46
1:A:39:ILE:HG22	1:A:40:VAL:H	1.80	0.46
1:A:29:LEU:HD12	1:A:43:ALA:HB2	1.96	0.46
1:B:133:TYR:HB2	1:B:321:ILE:CG2	2.43	0.46
1:B:132:LEU:O	1:B:135:MET:HB3	2.15	0.46
1:B:133:TYR:CZ	1:B:137:CYS:SG	3.08	0.46
1:A:118:VAL:O	1:A:121:MET:N	2.47	0.46
1:A:190:TYR:HD1	1:A:223:ILE:HG21	1.80	0.46
1:A:257:ARG:HA	1:A:260:VAL:HG12	1.98	0.46
1:B:237:VAL:O	1:B:241:LEU:N	2.47	0.46
1:A:154:PRO:O	1:A:156:ASN:N	2.48	0.46
1:B:190:TYR:HA	1:B:233:GLN:OE1	2.15	0.46
1:B:123:LEU:CD1	1:B:128:MET:HB2	2.44	0.46
2:G:559:THR:O	2:G:560:LEU:CB	2.58	0.46
1:A:60:PRO:HG2	1:A:61:PHE:N	2.22	0.46
1:B:72:ARG:NH1	1:B:174:ARG:HB2	2.30	0.46
1:A:245:CYS:O	1:A:248:PHE:N	2.48	0.46
1:B:95:GLN:HG2	1:B:101:PHE:HA	1.98	0.46
1:B:192:ARG:O	1:B:197:ILE:HD11	2.16	0.46
1:A:194:PRO:HD3	1:A:209:TRP:CZ2	2.51	0.46
1:A:294:ALA:HB2	1:A:320:TYR:CE1	2.51	0.46
1:A:88:LEU:CG	1:A:89:LEU:H	2.03	0.46
1:B:117:GLN:O	1:B:118:VAL:C	2.54	0.46
1:A:220:CYS:O	1:A:221:HIS:CB	2.61	0.46
1:B:193:ALA:O	1:B:195:GLU:N	2.49	0.46
1:B:215:MET:HE1	1:B:297:LEU:HB3	1.98	0.46
1:A:205:ASN:O	1:A:206:VAL:C	2.53	0.46
1:B:293:GLN:NE2	1:B:319:PRO:CG	2.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD12	1:B:347:HIS:NE2	2.30	0.46
1:A:14:GLU:HG2	1:A:14:GLU:H	1.46	0.46
1:A:115:LEU:HB2	1:A:157:ILE:CG2	2.45	0.45
1:A:136:LEU:O	1:A:139:ILE:HB	2.16	0.45
1:A:287:ASN:O	1:A:288:LYS:C	2.55	0.45
1:A:211:VAL:O	1:A:214:ILE:HB	2.16	0.45
1:B:233:GLN:HA	1:B:233:GLN:HE21	1.81	0.45
1:B:131:LEU:O	1:B:134:GLN:N	2.49	0.45
1:A:252:LEU:HD13	1:A:260:VAL:HG11	1.98	0.45
1:B:111:MET:HE3	1:B:159:VAL:C	2.37	0.45
1:A:125:HIS:O	1:A:126:GLU:C	2.53	0.45
1:A:85:ILE:HD11	1:A:138:GLY:O	2.15	0.45
1:A:187:VAL:O	1:A:187:VAL:HG13	2.16	0.45
1:A:323:VAL:HG23	1:A:324:TRP:CD2	2.51	0.45
1:A:190:TYR:CD1	1:A:223:ILE:HG21	2.51	0.45
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.84	0.45
1:B:110:LEU:HD11	4:B:1001:877:H232	1.98	0.45
1:A:198:LEU:O	1:A:199:GLY:C	2.53	0.45
1:B:354:GLU:HB3	1:B:355:LEU:H	1.56	0.45
1:B:140:LYS:C	1:B:142:LEU:N	2.70	0.45
1:B:294:ALA:O	1:B:296:ASP:N	2.49	0.45
1:B:80:VAL:HG11	1:B:170:PHE:CE1	2.50	0.45
1:A:298:LEU:HD22	1:A:302:LEU:CD1	2.47	0.45
1:B:295:ARG:HG2	1:B:295:ARG:HH11	1.82	0.45
1:A:157:ILE:CD1	1:A:167:ILE:HA	2.46	0.45
1:B:338:PRO:O	1:B:339:ASP:CB	2.65	0.45
1:A:184:PRO:O	1:A:187:VAL:HG12	2.16	0.45
1:B:360:VAL:HA	1:B:363:LEU:CD1	2.44	0.45
1:B:234:TRP:O	1:B:235:ASN:C	2.54	0.45
1:B:296:ASP:O	1:B:300:LYS:N	2.46	0.45
1:B:11:TYR:OH	1:B:29:LEU:HD11	2.17	0.45
1:A:63:ASN:C	1:A:65:THR:H	2.20	0.45
1:A:127:ARG:O	1:A:130:TYR:N	2.49	0.45
1:A:57:LEU:HD12	1:A:57:LEU:N	2.31	0.45
1:B:354:GLU:O	1:B:357:TYR:N	2.50	0.45
1:B:104:VAL:HG21	1:B:360:VAL:HG21	1.98	0.45
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.79	0.45
1:B:139:ILE:O	1:B:142:LEU:HB2	2.17	0.45
1:B:214:ILE:O	1:B:217:GLU:N	2.39	0.45
1:B:90:ASN:O	1:B:107:VAL:N	2.50	0.45
1:B:72:ARG:HD2	1:B:173:ALA:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HE1	1:B:240:GLN:CB	2.30	0.44
1:A:134:GLN:NE2	1:A:163:CYS:O	2.50	0.44
1:A:149:HIS:CE1	1:A:151:ASP:HB3	2.52	0.44
1:B:84:ASN:O	1:B:166:LYS:HA	2.17	0.44
1:A:154:PRO:C	1:A:156:ASN:N	2.70	0.44
1:A:134:GLN:NE2	1:A:164:THR:C	2.71	0.44
1:A:257:ARG:O	1:A:260:VAL:HG12	2.17	0.44
1:A:118:VAL:HA	1:A:121:MET:HG2	2.00	0.44
1:A:143:HIS:O	1:A:146:GLY:N	2.41	0.44
1:A:45:ASP:O	1:A:46:ALA:C	2.55	0.44
1:B:233:GLN:NE2	1:B:233:GLN:HA	2.32	0.44
1:B:25:ARG:NH2	1:B:48:LEU:HD23	2.33	0.44
1:A:123:LEU:HD11	1:A:131:LEU:CD1	2.48	0.44
1:B:312:VAL:O	1:B:316:LEU:HD12	2.17	0.44
1:A:352:TRP:O	1:A:356:ILE:N	2.32	0.44
1:A:212:GLY:C	1:A:214:ILE:N	2.71	0.44
2:G:556:ARG:HA	2:G:557:PRO:HD3	1.56	0.44
1:A:232:ASP:O	1:A:233:GLN:C	2.56	0.44
1:B:318:HIS:CG	1:B:319:PRO:HD2	2.53	0.44
1:B:203:LYS:O	1:B:206:VAL:HG12	2.17	0.44
1:A:115:LEU:HD22	1:A:118:VAL:HB	1.99	0.44
1:A:295:ARG:O	1:A:296:ASP:C	2.56	0.44
1:A:125:HIS:HB3	1:A:289:LEU:HD23	1.98	0.44
1:B:259:TYR:O	1:B:262:ASN:N	2.36	0.44
1:A:27:GLN:O	1:A:28:ASN:HB3	2.17	0.44
1:A:274:LEU:HB3	1:A:275:PHE:CE2	2.52	0.44
1:B:11:TYR:CE2	1:B:13:VAL:HG23	2.52	0.44
1:A:140:LYS:HD2	1:A:140:LYS:O	2.18	0.44
1:A:286:HIS:O	1:A:287:ASN:C	2.56	0.44
1:A:208:LEU:HA	1:A:208:LEU:HD13	1.79	0.44
1:A:149:HIS:C	1:A:150:ARG:CG	2.86	0.44
1:B:123:LEU:HD12	1:B:128:MET:HB2	2.00	0.43
1:B:187:VAL:HG13	1:B:187:VAL:O	2.17	0.43
1:A:140:LYS:HA	1:A:312:VAL:HG11	2.00	0.43
1:B:360:VAL:O	1:B:363:LEU:HD12	2.18	0.43
1:B:65:THR:C	1:B:67:ALA:N	2.71	0.43
1:B:89:LEU:HB2	1:B:108:MET:HA	2.00	0.43
1:A:322:ASN:O	1:A:324:TRP:N	2.51	0.43
1:A:86:ILE:HD13	1:A:168:LEU:CD1	2.48	0.43
1:B:324:TRP:CD1	1:B:324:TRP:N	2.84	0.43
1:A:298:LEU:HD22	1:A:302:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG12	1:A:106:ILE:HD12	2.00	0.43
1:A:184:PRO:C	1:A:186:VAL:H	2.21	0.43
1:B:132:LEU:CD2	1:B:215:MET:HB2	2.36	0.43
1:A:92:PHE:CE1	1:A:105:TYR:HB2	2.53	0.43
1:A:283:ASP:OD1	1:A:290:LYS:HA	2.19	0.43
1:B:256:VAL:O	1:B:260:VAL:HG23	2.19	0.43
1:B:61:PHE:HA	1:B:67:ALA:CB	2.47	0.43
1:B:167:ILE:HG22	1:B:168:LEU:N	2.33	0.43
1:A:29:LEU:CD1	1:A:43:ALA:HB2	2.49	0.43
1:B:92:PHE:C	1:B:92:PHE:CD1	2.91	0.43
1:A:293:GLN:HE21	1:A:293:GLN:CA	2.32	0.43
1:A:226:PRO:O	1:A:233:GLN:NE2	2.43	0.43
1:B:106:ILE:HG22	1:B:108:MET:HE2	1.99	0.43
1:A:36:ALA:HB3	1:A:37:GLN:HE22	1.83	0.43
1:A:310:ILE:HD11	1:A:315:ALA:CA	2.48	0.43
1:A:256:VAL:O	1:A:260:VAL:HG12	2.19	0.43
1:A:244:PRO:HB2	1:A:249:MET:HE2	2.00	0.43
1:A:337:ILE:HG23	1:A:338:PRO:CD	2.42	0.43
1:A:42:ALA:CB	1:A:110:LEU:HD11	2.48	0.43
1:B:78:LYS:CE	1:B:363:LEU:HB2	2.49	0.43
1:A:143:HIS:C	1:A:145:ALA:N	2.71	0.43
1:B:111:MET:HE3	1:B:160:LYS:N	2.34	0.43
1:B:104:VAL:CG2	1:B:360:VAL:HG21	2.48	0.43
1:B:78:LYS:HE2	1:B:363:LEU:HB2	2.00	0.43
1:A:77:MET:HE3	1:A:77:MET:HA	2.00	0.43
1:B:47:ILE:HG22	1:B:47:ILE:O	2.18	0.43
1:B:332:ALA:HB1	1:B:333:PRO:HD2	2.00	0.43
1:B:278:VAL:O	1:B:279:LEU:C	2.58	0.43
1:B:26:TYR:O	1:B:27:GLN:C	2.55	0.43
1:A:190:TYR:HB3	1:A:223:ILE:CG2	2.48	0.43
1:A:244:PRO:CB	1:A:248:PHE:HD2	2.20	0.43
1:B:115:LEU:CB	1:B:157:ILE:HB	2.48	0.43
1:B:111:MET:HG3	1:B:158:VAL:HG23	2.01	0.43
1:B:193:ALA:O	1:B:196:VAL:N	2.48	0.42
1:B:148:ILE:HG23	1:B:207:ASP:OD2	2.19	0.42
1:A:163:CYS:SG	2:F:560:LEU:HD12	2.59	0.42
1:B:110:LEU:HA	4:B:1001:877:O15	2.19	0.42
1:B:213:CYS:HA	1:B:224:LEU:HD23	2.00	0.42
1:B:107:VAL:HG12	1:B:108:MET:N	2.32	0.42
1:B:233:GLN:CA	1:B:233:GLN:HE21	2.32	0.42
1:A:153:LYS:O	1:A:154:PRO:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG21	1:A:363:LEU:HD13	2.01	0.42
1:B:89:LEU:HD12	1:B:108:MET:C	2.39	0.42
1:B:249:MET:CE	1:B:261:GLU:HG2	2.49	0.42
1:B:204:GLU:O	1:B:206:VAL:N	2.52	0.42
1:B:28:ASN:C	1:B:28:ASN:ND2	2.71	0.42
1:A:126:GLU:HG3	1:A:285:GLU:OE2	2.20	0.42
1:A:131:LEU:O	1:A:135:MET:N	2.50	0.42
1:A:255:THR:O	1:A:258:THR:N	2.53	0.42
1:A:259:TYR:CD1	1:B:231:ILE:HD12	2.54	0.42
1:A:301:MET:O	1:A:303:VAL:N	2.51	0.42
1:B:271:PHE:CZ	1:B:302:LEU:HB2	2.37	0.42
1:A:42:ALA:HA	1:A:110:LEU:HD11	2.01	0.42
1:A:342:LEU:HD12	1:A:342:LEU:O	2.19	0.42
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.55	0.42
1:B:178:THR:O	1:B:179:SER:HB2	2.18	0.42
1:B:128:MET:O	1:B:131:LEU:HB2	2.20	0.42
1:B:280:PHE:CE1	1:B:294:ALA:HB3	2.55	0.42
1:B:244:PRO:CB	1:B:248:PHE:HD2	2.33	0.42
1:A:297:LEU:HD13	1:A:318:HIS:HD2	1.83	0.42
1:B:193:ALA:HA	1:B:209:TRP:CE2	2.54	0.42
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.76	0.42
1:A:128:MET:HE3	1:A:132:LEU:HD21	2.01	0.42
1:A:229:ASP:OD1	1:A:232:ASP:N	2.50	0.42
1:B:57:LEU:HD13	1:B:57:LEU:HA	1.67	0.42
1:A:348:THR:HB	1:A:351:GLU:HG3	2.01	0.42
1:A:214:ILE:O	1:A:217:GLU:N	2.50	0.42
1:A:25:ARG:CG	1:A:47:ILE:HB	2.49	0.42
1:A:61:PHE:N	1:A:61:PHE:CD1	2.86	0.42
1:A:148:ILE:O	1:A:173:ALA:HA	2.20	0.42
1:B:326:ASP:HB3	1:B:329:GLU:HB2	2.02	0.42
1:A:192:ARG:HG2	1:A:196:VAL:CG1	2.50	0.42
1:B:214:ILE:C	1:B:216:GLY:N	2.72	0.42
1:B:343:ASP:OD1	1:B:344:GLU:N	2.52	0.42
1:A:111:MET:CE	1:A:160:LYS:HB2	2.50	0.42
1:A:88:LEU:O	1:A:89:LEU:CB	2.56	0.42
1:A:89:LEU:O	1:A:90:ASN:HB2	2.20	0.42
2:G:559:THR:CG2	2:G:560:LEU:H	2.16	0.42
1:A:53:ALA:N	1:A:110:LEU:HD12	2.34	0.42
1:A:98:LEU:HA	1:A:357:TYR:CE2	2.55	0.42
1:B:275:PHE:N	1:B:276:PRO:HD3	2.35	0.41
1:B:118:VAL:HA	1:B:121:MET:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PRO:O	1:A:283:ASP:N	2.53	0.41
1:A:45:ASP:O	1:A:45:ASP:CG	2.59	0.41
1:B:361:MET:C	1:B:363:LEU:H	2.22	0.41
1:B:238:ILE:HG23	1:B:238:ILE:H	1.65	0.41
1:B:25:ARG:HB2	1:B:47:ILE:HG12	2.02	0.41
1:B:153:LYS:O	1:B:154:PRO:C	2.58	0.41
1:B:189:ARG:NH1	1:B:230:TYR:N	2.68	0.41
1:B:330:ALA:O	1:B:331:GLU:HG3	2.20	0.41
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.77	0.41
1:A:114:ASN:N	1:A:114:ASN:ND2	2.65	0.41
1:B:269:TYR:HB2	1:B:274:LEU:HD21	2.02	0.41
1:A:257:ARG:HD2	1:A:257:ARG:HH11	1.64	0.41
1:A:98:LEU:HA	1:A:357:TYR:CZ	2.55	0.41
1:A:124:ASP:OD2	1:A:127:ARG:HB2	2.19	0.41
1:A:115:LEU:O	1:A:117:GLN:N	2.53	0.41
1:A:142:LEU:O	1:A:147:ILE:HB	2.21	0.41
1:B:233:GLN:O	1:B:237:VAL:HG23	2.19	0.41
1:B:71:TYR:O	1:B:74:LEU:N	2.53	0.41
1:A:97:SER:HB3	1:A:100:GLU:HB2	2.01	0.41
1:B:111:MET:HG3	1:B:158:VAL:CG2	2.51	0.41
1:A:184:PRO:O	1:A:186:VAL:N	2.53	0.41
1:B:48:LEU:O	1:B:49:GLU:HB2	2.21	0.41
1:A:123:LEU:HD12	1:A:128:MET:CB	2.51	0.41
1:A:123:LEU:HD12	1:A:128:MET:HB2	2.02	0.41
1:A:211:VAL:CG1	1:A:301:MET:HE1	2.51	0.41
1:A:172:LEU:O	1:A:174:ARG:N	2.54	0.41
1:B:83:LYS:O	1:B:83:LYS:HG2	2.20	0.41
1:B:186:VAL:HG22	1:B:187:VAL:N	2.36	0.41
1:A:71:TYR:CE1	1:A:355:LEU:HB3	2.55	0.41
1:A:338:PRO:HG3	1:A:340:LYS:NZ	2.35	0.41
1:A:23:LEU:HD12	1:A:26:TYR:HE2	1.85	0.41
1:A:11:TYR:HH	1:A:27:GLN:HA	1.83	0.41
1:A:64:GLN:NE2	1:A:346:GLU:OE1	2.54	0.41
1:B:85:ILE:HD12	1:B:167:ILE:HB	2.02	0.41
1:B:309:ARG:C	1:B:310:ILE:O	2.58	0.41
1:A:288:LYS:CE	1:A:323:VAL:HG12	2.51	0.41
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.89	0.41
1:B:334:PRO:HA	1:B:335:PRO:HD3	1.79	0.41
1:B:234:TRP:O	1:B:236:LYS:N	2.54	0.41
1:A:262:ASN:O	1:A:263:ARG:O	2.39	0.41
1:B:9:ASN:HA	1:B:24:LYS:CE	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:CD2	1:A:165:LEU:C	2.88	0.41
1:A:353:LYS:O	1:A:354:GLU:C	2.59	0.41
1:A:254:PRO:HG2	1:A:255:THR:H	1.86	0.41
1:A:198:LEU:HD11	1:A:234:TRP:CZ3	2.56	0.41
1:A:333:PRO:HA	1:A:334:PRO:HD3	1.86	0.41
1:B:132:LEU:HD21	1:B:215:MET:CB	2.36	0.41
1:A:133:TYR:O	1:A:134:GLN:C	2.59	0.41
1:A:72:ARG:O	1:A:76:LEU:HG	2.21	0.41
1:B:76:LEU:O	1:B:80:VAL:HG12	2.20	0.41
1:A:329:GLU:HG3	1:A:329:GLU:O	2.21	0.41
1:B:172:LEU:N	1:B:172:LEU:HD12	2.36	0.40
1:B:193:ALA:HB3	1:B:206:VAL:HG23	2.03	0.40
1:B:275:PHE:CB	1:B:280:PHE:HE2	2.28	0.40
1:A:215:MET:SD	1:A:297:LEU:HD23	2.61	0.40
1:B:111:MET:O	4:B:1001:877:H4	2.22	0.40
1:B:214:ILE:C	1:B:216:GLY:H	2.24	0.40
1:B:206:VAL:HG13	1:B:207:ASP:N	2.36	0.40
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.83	0.40
1:B:238:ILE:HG13	1:B:266:TYR:CD2	2.56	0.40
1:A:295:ARG:O	1:A:298:LEU:N	2.55	0.40
1:A:181:MET:C	1:A:183:GLU:H	2.23	0.40
1:B:214:ILE:O	1:B:216:GLY:N	2.54	0.40
1:B:124:ASP:OD2	1:B:127:ARG:HG3	2.22	0.40
1:B:311:SER:H	1:B:314:GLU:HB2	1.87	0.40
1:A:245:CYS:HA	1:A:246:PRO:HD3	1.96	0.40
1:A:65:THR:C	1:A:67:ALA:H	2.24	0.40
1:A:337:ILE:HA	1:A:337:ILE:HD13	1.95	0.40
1:A:189:ARG:O	1:A:191:TYR:N	2.55	0.40
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.90	0.40
1:B:184:PRO:C	1:B:186:VAL:N	2.72	0.40
1:B:39:ILE:CD1	1:B:39:ILE:H	2.22	0.40
1:A:25:ARG:CD	1:A:45:ASP:OD1	2.70	0.40
1:A:330:ALA:C	1:A:332:ALA:H	2.25	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	356/370 (96%)	219 (62%)	74 (21%)	63 (18%)	0	2
1	B	356/370 (96%)	230 (65%)	80 (22%)	46 (13%)	0	5
2	F	8/11 (73%)	4 (50%)	1 (12%)	3 (38%)	0	0
2	G	8/11 (73%)	3 (38%)	4 (50%)	1 (12%)	0	6
All	All	728/762 (96%)	456 (63%)	159 (22%)	113 (16%)	0	3

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	111	MET
1	A	144	SER
1	A	151	ASP
1	A	165	LEU
1	A	169	ASP
1	A	173	ALA
1	A	226	PRO
1	A	282	ALA
1	A	287	ASN
1	A	288	LYS
1	A	289	LEU
1	A	322	ASN
1	A	327	PRO
1	A	338	PRO
1	A	361	MET
1	A	362	ASP
1	A	364	GLU
2	F	555	LYS
2	F	560	LEU
1	B	176	ALA
1	B	189	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	271	PHE
1	B	278	VAL
1	B	281	PRO
1	B	282	ALA
1	B	322	ASN
1	B	323	VAL
1	B	331	GLU
1	B	339	ASP
1	B	354	GLU
2	G	560	LEU
1	A	14	GLU
1	A	50	ARG
1	A	60	PRO
1	A	61	PHE
1	A	64	GLN
1	A	86	ILE
1	A	88	LEU
1	A	134	GLN
1	A	164	THR
1	A	181	MET
1	A	206	VAL
1	A	283	ASP
1	A	290	LYS
1	A	323	VAL
1	A	330	ALA
1	A	339	ASP
1	B	37	GLN
1	B	66	HIS
1	B	126	GLU
1	B	141	HIS
1	B	155	SER
1	B	170	PHE
1	B	187	VAL
1	B	190	TYR
1	B	205	ASN
1	B	279	LEU
1	B	305	ASP
1	B	306	ALA
1	A	180	PHE
1	A	185	GLU
1	A	188	THR
1	A	235	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	THR
1	A	284	SER
1	A	310	ILE
1	A	326	ASP
2	F	561	ASN
1	B	27	GLN
1	B	267	ALA
1	B	310	ILE
1	A	74	LEU
1	A	116	CYS
1	A	155	SER
1	A	246	PRO
1	A	302	LEU
1	B	28	ASN
1	B	71	TYR
1	B	117	GLN
1	B	125	HIS
1	B	194	PRO
1	B	292	SER
1	B	295	ARG
1	B	355	LEU
1	A	47	ILE
1	A	97	SER
1	A	119	ILE
1	A	123	LEU
1	A	167	ILE
1	A	190	TYR
1	A	250	LYS
1	A	299	SER
1	B	72	ARG
1	B	109	GLU
1	B	173	ALA
1	B	260	VAL
1	B	263	ARG
1	A	197	ILE
1	A	254	PRO
1	A	319	PRO
1	B	86	ILE
1	B	179	SER
1	B	186	VAL
1	A	16	GLY
1	A	35	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	PRO
1	B	118	VAL
1	B	276	PRO
1	A	59	ARG
1	A	256	VAL
1	A	321	ILE
1	B	59	ARG

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	316/334 (95%)	279 (88%)	37 (12%)	7	32
1	B	316/334 (95%)	284 (90%)	32 (10%)	9	40
2	F	10/11 (91%)	9 (90%)	1 (10%)	9	41
2	G	9/11 (82%)	9 (100%)	0	100	100
All	All	651/690 (94%)	581 (89%)	70 (11%)	8	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	11	TYR
1	A	14	GLU
1	A	28	ASN
1	A	48	LEU
1	A	61	PHE
1	A	73	GLU
1	A	74	LEU
1	A	90	ASN
1	A	114	ASN
1	A	123	LEU
1	A	124	ASP
1	A	132	LEU
1	A	136	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	ILE
1	A	156	ASN
1	A	163	CYS
1	A	184	PRO
1	A	188	THR
1	A	190	TYR
1	A	192	ARG
1	A	202	TYR
1	A	208	LEU
1	A	229	ASP
1	A	236	LYS
1	A	237	VAL
1	A	244	PRO
1	A	246	PRO
1	A	272	GLU
1	A	277	ASP
1	A	304	ILE
1	A	312	VAL
1	A	313	ASP
1	A	319	PRO
1	A	327	PRO
1	A	342	LEU
1	A	349	ILE
2	F	560	LEU
1	B	10	PHE
1	B	28	ASN
1	B	39	ILE
1	B	57	LEU
1	B	65	THR
1	B	90	ASN
1	B	91	VAL
1	B	114	ASN
1	B	122	GLU
1	B	124	ASP
1	B	156	ASN
1	B	169	ASP
1	B	184	PRO
1	B	188	THR
1	B	191	TYR
1	B	194	PRO
1	B	195	GLU
1	B	202	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	205	ASN
1	B	208	LEU
1	B	229	ASP
1	B	230	TYR
1	B	243	THR
1	B	246	PRO
1	B	271	PHE
1	B	272	GLU
1	B	281	PRO
1	B	295	ARG
1	B	304	ILE
1	B	313	ASP
1	B	324	TRP
1	B	341	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	27	GLN
1	A	28	ASN
1	A	37	GLN
1	A	64	GLN
1	A	66	HIS
1	A	84	ASN
1	A	90	ASN
1	A	102	GLN
1	A	114	ASN
1	A	117	GLN
1	A	134	GLN
1	A	141	HIS
1	A	156	ASN
1	A	233	GLN
1	A	235	ASN
1	A	293	GLN
1	B	27	GLN
1	B	28	ASN
1	B	82	HIS
1	B	114	ASN
1	B	120	GLN
1	B	141	HIS
1	B	156	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	205	ASN
1	B	233	GLN
1	B	235	ASN
1	B	293	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	SO4	A	501	-	4,4,4	1.72	0	6,6,6	0.06	0
3	SO4	A	601	-	4,4,4	1.19	0	6,6,6	0.09	0
4	877	A	901	-	28,28,28	2.09	12 (42%)	34,38,38	1.48	7 (20%)
4	877	B	1001	-	28,28,28	1.81	6 (21%)	34,38,38	1.42	3 (8%)
3	SO4	B	701	-	4,4,4	1.58	0	6,6,6	0.12	0
3	SO4	B	801	-	4,4,4	1.11	0	6,6,6	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	877	A	901	-	-	1/16/17/17	0/2/2/2
4	877	B	1001	-	-	1/16/17/17	0/2/2/2
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	877	C4-C5	2.06	1.42	1.38
4	A	901	877	BR-C6	2.14	1.95	1.89
4	A	901	877	C4-C3	2.15	1.43	1.39
4	A	901	877	O22-C5	2.15	1.40	1.37
4	B	1001	877	O27-C2	2.17	1.40	1.37
4	A	901	877	C19-C18	2.48	1.43	1.41
4	A	901	877	C1-C6	2.50	1.44	1.38
4	A	901	877	C2-C3	2.52	1.44	1.40
4	B	1001	877	C2-C3	2.96	1.45	1.40
4	B	1001	877	O22-C5	3.10	1.42	1.37
4	A	901	877	C1-C2	3.13	1.44	1.38
4	B	1001	877	C5-C6	3.26	1.46	1.39
4	A	901	877	O27-C2	3.26	1.42	1.37
4	A	901	877	C5-C6	3.49	1.46	1.39
4	B	1001	877	C17-N16	3.58	1.37	1.32
4	B	1001	877	O36-C17	3.83	1.40	1.34
4	A	901	877	O36-C17	4.32	1.41	1.34
4	A	901	877	C17-N16	4.44	1.38	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	877	C18-C17-N16	-4.18	121.17	124.11
4	B	1001	877	C18-C17-N16	-3.97	121.32	124.11
4	A	901	877	C23-O22-C5	-2.58	113.62	117.54
4	A	901	877	O22-C5-C4	-2.53	119.90	124.21
4	B	1001	877	O22-C5-C4	-2.21	120.44	124.21
4	A	901	877	BR-C6-C5	2.04	122.42	119.73
4	A	901	877	O15-C10-N13	2.04	127.37	123.72
4	A	901	877	C14-N13-C10	2.22	131.74	128.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	877	O22-C5-C6	3.40	121.41	116.87
4	B	1001	877	O22-C5-C6	3.61	121.69	116.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	877	C23-O22-C5-C6
4	B	1001	877	C23-O22-C5-C6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	877	1	0
4	B	1001	877	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.