



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:52 am BST

PDB ID : 1KKQ
Title : Crystal structure of the human PPAR-alpha ligand-binding domain in complex with an antagonist GW6471 and a SMRT corepressor motif
Authors : Xu, H.E.; Stanley, T.B.; Montana, V.G.; Lambert, M.H.; Shearer, B.G.; Cobb, J.E.; McKee, D.D.; Galardi, C.M.; Nolte, R.T.; Parks, D.J.
Deposited on : 2001-12-10
Resolution : 3.00 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

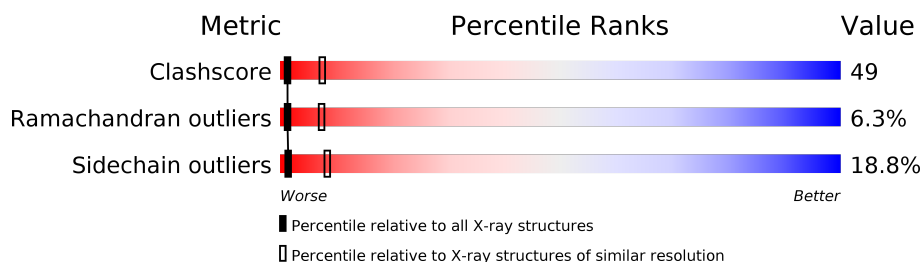
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	38% 48% 14%
1	B	269	43% 43% 12% .
1	C	269	39% 44% 13% .
1	D	269	44% 39% 15% .
2	E	19	16% 37% 37% 11%
2	F	19	32% 32% 32% 5%
2	G	19	37% 42% 21%
2	H	19	47% 26% 21% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9606 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.

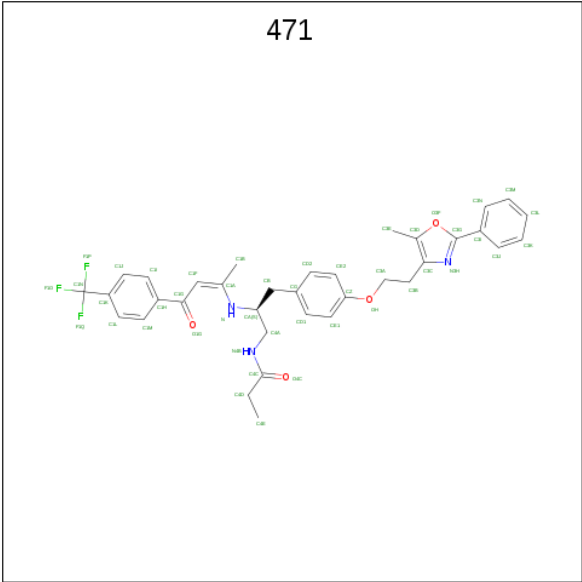
- Molecule 1 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	B	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	C	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	D	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			

- Molecule 2 is a protein called NUCLEAR RECEPTOR CO-REPRESSOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			
2	F	19	Total	C	N	O	S	0	0	0
			149	97	25	25	2			
2	G	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			
2	H	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			

- Molecule 3 is N-((2S)-2-((1Z)-1-METHYL-3-OXO-3-[4-(TRIFLUOROMETHYL) PHENYL]PROP-1-ENYL} AMINO)-3-{4-[2-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)ETHOXY]PHENYL}PROPYL)PROPANAMIDE (three-letter code: 471) (formula: C₃₅H₃₆F₃N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	B	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	C	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	D	1	Total	C	F	N	O	0	0
			45	35	3	3	4		

- Molecule 4 is water.

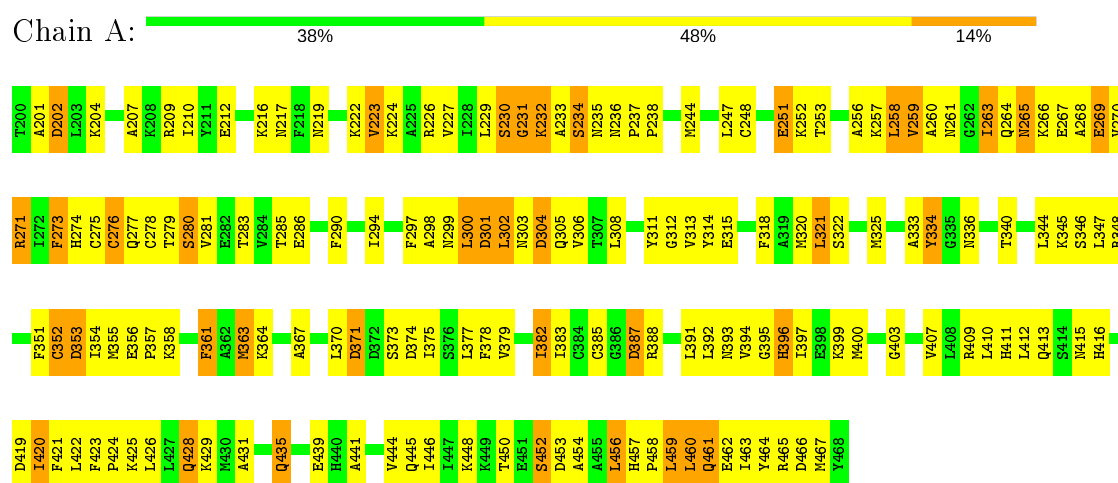
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	108	Total	O	0	0
			108	108		
4	C	55	Total	O	0	0
			55	55		
4	D	87	Total	O	0	0
			87	87		
4	E	4	Total	O	0	0
			4	4		
4	F	10	Total	O	0	0
			10	10		
4	G	1	Total	O	0	0
			1	1		
4	H	4	Total	O	0	0
			4	4		

3 Residue-property plots

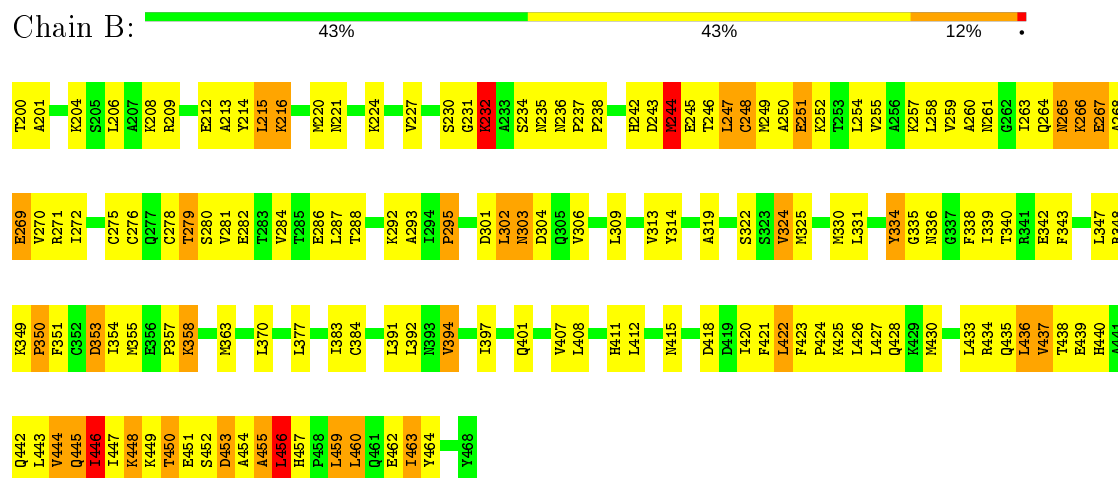
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR

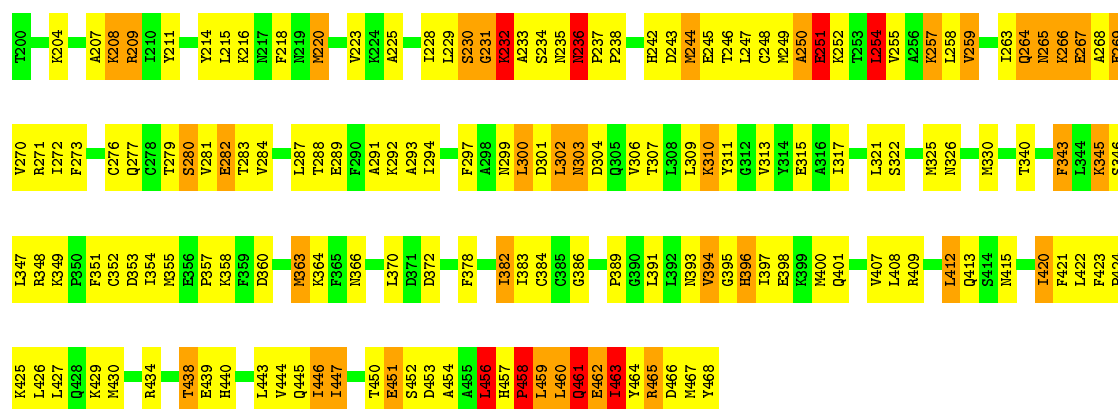


• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR



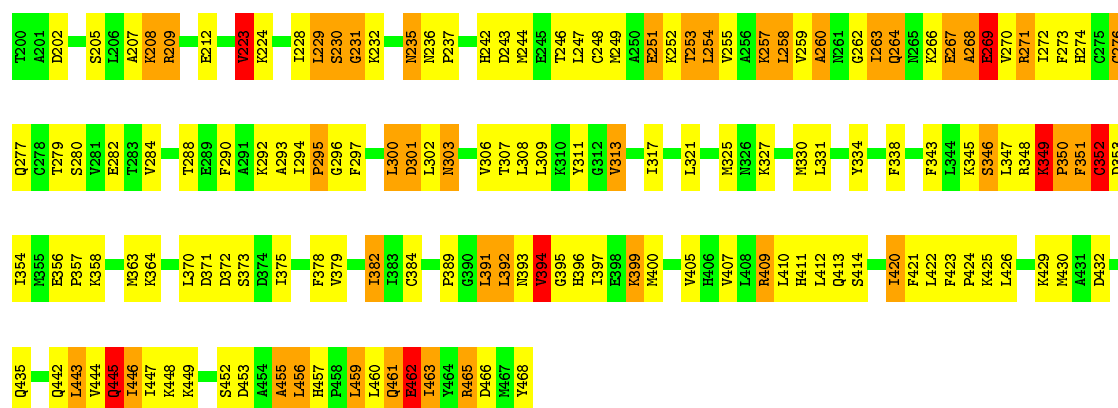
• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR





• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR

Chain D: 44% 39% 15%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain E: 16% 37% 37% 11%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain F: 32% 32% 32% 5%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain G: 37% 42% 21%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.41Å 112.77Å 123.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.99 – 3.00	Depositor
% Data completeness (in resolution range)	98.8 (20.99-3.00)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.258 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9606	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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:
471

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	0/2166	0.79	2/2920 (0.1%)
1	B	0.42	0/2166	0.82	2/2920 (0.1%)
1	C	0.39	0/2166	0.79	6/2920 (0.2%)
1	D	0.44	0/2166	0.78	3/2920 (0.1%)
2	E	0.63	0/147	0.99	1/195 (0.5%)
2	F	0.43	0/151	1.01	1/199 (0.5%)
2	G	0.55	0/147	1.17	2/195 (1.0%)
2	H	0.45	0/147	0.91	0/195
All	All	0.42	0/9256	0.81	17/12464 (0.1%)

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	D	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	GLU	N-CA-C	-7.76	90.04	111.00
2	F	695	GLY	N-CA-C	7.60	132.10	113.10
1	C	461	GLN	N-CA-C	-7.52	90.69	111.00
1	B	267	GLU	N-CA-C	-7.34	91.18	111.00
1	D	236	ASN	N-CA-C	-7.16	91.66	111.00
2	G	695	GLY	N-CA-C	6.84	130.20	113.10
1	D	462	GLU	N-CA-C	6.44	128.38	111.00
1	C	266	LYS	N-CA-C	-6.43	93.62	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	ASN	N-CA-C	-6.39	93.76	111.00
2	G	696	LYS	N-CA-C	6.24	127.84	111.00
1	C	456	LEU	N-CA-C	-6.18	94.32	111.00
1	A	236	ASN	N-CA-C	-5.92	95.02	111.00
1	B	265	ASN	CB-CA-C	-5.68	99.04	110.40
1	D	351	PHE	N-CA-C	5.58	126.06	111.00
1	C	458	PRO	N-CA-C	-5.40	98.06	112.10
2	E	685	LEU	CA-CB-CG	-5.34	103.01	115.30
1	A	231	GLY	N-CA-C	5.28	126.31	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	349	LYS	Mainchain

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	2128	0	2168	199	0
1	B	2128	0	2168	206	0
1	C	2128	0	2168	222	0
1	D	2128	0	2168	206	0
2	E	145	0	138	36	0
2	F	149	0	149	39	0
2	G	145	0	138	29	0
2	H	145	0	138	18	0
3	A	45	0	36	1	0
3	B	45	0	35	8	0
3	C	45	0	36	2	0
3	D	45	0	35	3	0
4	A	61	0	0	3	0
4	B	108	0	0	5	0
4	C	55	0	0	7	0
4	D	87	0	0	8	0
4	E	4	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	10	0	0	3	0
4	G	1	0	0	1	0
4	H	4	0	0	1	0
All	All	9606	0	9377	916	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 49.

All (916) 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:G:688:ILE:HD13	2:G:689:ILE:N	1.32	1.43
1:D:348:ARG:O	1:D:349:LYS:CG	1.74	1.35
2:G:685:LEU:O	2:G:688:ILE:CD1	1.92	1.16
1:A:269:GLU:HG3	1:A:348:ARG:HH11	1.09	1.16
1:D:348:ARG:O	1:D:349:LYS:HG2	1.33	1.14
2:E:685:LEU:HD23	2:E:685:LEU:H	1.12	1.14
1:A:207:ALA:HB2	1:A:407:VAL:HG11	1.29	1.14
1:A:258:LEU:HD22	1:A:263:ILE:HG13	1.30	1.13
1:A:269:GLU:HG3	1:A:348:ARG:NH1	1.64	1.12
2:G:688:ILE:CD1	2:G:689:ILE:H	1.64	1.10
1:B:200:THR:O	1:B:204:LYS:HD3	1.48	1.10
1:C:258:LEU:HD22	1:C:263:ILE:HD12	1.31	1.09
1:A:227:VAL:O	1:A:231:GLY:HA3	1.53	1.09
1:D:348:ARG:O	1:D:349:LYS:CB	1.99	1.08
2:E:685:LEU:HD23	2:E:685:LEU:N	1.67	1.08
1:D:457:HIS:HD2	1:D:459:LEU:HB2	1.15	1.05
1:D:457:HIS:CD2	1:D:459:LEU:HB2	1.91	1.05
1:C:231:GLY:O	1:C:233:ALA:N	1.90	1.05
1:A:456:LEU:HD22	1:A:456:LEU:H	1.21	1.03
1:B:456:LEU:H	1:B:456:LEU:HD23	1.23	1.02
1:B:456:LEU:N	1:B:456:LEU:HD23	1.74	1.02
1:B:459:LEU:O	1:B:459:LEU:HD12	1.58	1.02
1:C:300:LEU:HD12	1:C:300:LEU:H	1.22	1.01
1:D:209:ARG:HD2	2:H:700:TRP:HZ3	1.23	1.01
2:G:685:LEU:O	2:G:688:ILE:HD12	1.58	1.00
1:D:268:ALA:HB2	1:D:271:ARG:HH21	1.27	0.99
2:G:685:LEU:O	2:G:688:ILE:HD11	1.63	0.97
2:G:688:ILE:CD1	2:G:689:ILE:N	2.23	0.96
1:A:461:GLN:HG3	1:A:464:TYR:CD2	2.01	0.95
1:A:420:ILE:HD13	1:A:421:PHE:H	1.31	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:688:ILE:HD13	2:G:689:ILE:H	0.88	0.95
1:B:445:GLN:HA	1:B:445:GLN:HE21	1.31	0.94
1:C:230:SER:HB2	4:C:783:HOH:O	1.66	0.94
1:D:272:ILE:O	1:D:276:CYS:HB2	1.68	0.92
1:C:420:ILE:HD13	1:C:421:PHE:N	1.84	0.92
2:G:688:ILE:HD12	2:G:688:ILE:H	1.32	0.91
1:C:237:PRO:HB2	1:C:238:PRO:HD2	1.53	0.91
1:D:268:ALA:CB	1:D:271:ARG:HH21	1.83	0.91
1:D:268:ALA:HB2	1:D:271:ARG:NH2	1.87	0.90
1:D:391:LEU:HD12	1:D:397:ILE:HD12	1.53	0.90
1:C:209:ARG:HH22	1:C:293:ALA:HB1	1.35	0.90
1:B:460:LEU:HD23	1:B:460:LEU:N	1.85	0.90
1:C:317:ILE:O	1:C:321:LEU:HB2	1.73	0.89
2:G:688:ILE:HD12	2:G:688:ILE:N	1.87	0.89
1:B:450:THR:HG22	1:B:451:GLU:HG3	1.53	0.89
1:D:460:LEU:H	1:D:460:LEU:HD12	1.38	0.89
1:A:273:PHE:HD2	1:A:273:PHE:O	1.55	0.88
1:A:257:LYS:C	1:A:258:LEU:HD23	1.92	0.88
1:A:273:PHE:O	1:A:273:PHE:CD2	2.27	0.88
1:C:456:LEU:N	1:C:456:LEU:HD13	1.88	0.88
2:E:685:LEU:HA	4:E:169:HOH:O	1.70	0.88
1:C:230:SER:O	1:C:232:LYS:N	2.07	0.88
1:B:449:LYS:HA	1:B:452:SER:OG	1.73	0.88
1:B:451:GLU:O	1:B:453:ASP:OD1	1.92	0.88
1:A:244:MET:HE1	1:A:268:ALA:HB2	1.55	0.88
1:B:230:SER:O	1:B:232:LYS:HG3	1.73	0.88
1:C:461:GLN:O	1:C:465:ARG:HD2	1.72	0.87
1:D:230:SER:O	1:D:232:LYS:HD2	1.75	0.87
1:C:386:GLY:HA3	1:C:398:GLU:HG3	1.57	0.87
1:B:201:ALA:HA	1:B:204:LYS:HE2	1.56	0.86
1:D:459:LEU:O	1:D:459:LEU:HD12	1.75	0.85
1:A:207:ALA:HB2	1:A:407:VAL:CG1	2.06	0.85
1:A:223:VAL:O	1:A:227:VAL:HG23	1.76	0.85
1:A:258:LEU:HD22	1:A:263:ILE:CG1	2.06	0.85
1:C:457:HIS:CD2	1:C:458:PRO:HD3	2.12	0.84
1:A:456:LEU:HD22	1:A:456:LEU:N	1.93	0.84
1:D:457:HIS:HD2	1:D:459:LEU:CB	1.90	0.84
1:A:219:ASN:O	1:A:224:LYS:NZ	2.10	0.84
1:B:384:CYS:O	1:B:401:GLN:HB2	1.77	0.84
1:A:457:HIS:CG	1:A:458:PRO:HD2	2.12	0.84
1:A:461:GLN:HA	1:A:464:TYR:HB3	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD12	1:C:300:LEU:N	1.91	0.83
2:E:685:LEU:CD2	2:E:685:LEU:N	2.39	0.83
1:A:412:LEU:HD11	1:A:426:LEU:HD12	1.59	0.83
1:D:255:VAL:H	1:D:258:LEU:HD11	1.43	0.83
1:A:420:ILE:HD13	1:A:421:PHE:N	1.92	0.83
1:C:409:ARG:O	1:C:413:GLN:HB2	1.78	0.83
1:D:255:VAL:HB	1:D:258:LEU:HG	1.61	0.82
1:B:272:ILE:O	1:B:276:CYS:HB2	1.79	0.82
2:G:688:ILE:CD1	2:G:689:ILE:HG23	2.10	0.82
1:A:257:LYS:HE2	1:A:261:ASN:ND2	1.95	0.82
1:D:378:PHE:O	1:D:382:ILE:HG23	1.80	0.82
1:C:360:ASP:OD2	1:C:364:LYS:HE3	1.80	0.81
1:A:456:LEU:CD2	1:A:456:LEU:H	1.92	0.81
1:A:285:THR:HG23	2:E:692:ALA:HB1	1.63	0.81
1:B:457:HIS:ND1	1:B:459:LEU:HB2	1.95	0.81
2:E:697:TYR:O	2:E:698:ASP:HB2	1.80	0.81
1:D:209:ARG:CD	2:H:700:TRP:HZ3	1.94	0.80
1:C:236:ASN:OD1	1:C:236:ASN:O	1.99	0.80
1:C:315:GLU:HB2	1:C:382:ILE:HD13	1.64	0.80
1:D:244:MET:CE	1:D:268:ALA:HB3	2.10	0.80
2:H:697:TYR:O	2:H:698:ASP:HB2	1.81	0.80
1:A:396:HIS:O	1:A:399:LYS:HG2	1.82	0.80
1:C:209:ARG:NH2	1:C:293:ALA:HB1	1.96	0.80
2:F:696:LYS:O	2:F:696:LYS:HD2	1.82	0.79
1:A:374:ASP:OD2	1:A:416:HIS:HE1	1.65	0.79
1:A:273:PHE:CZ	1:A:454:ALA:O	2.36	0.79
1:B:459:LEU:O	1:B:459:LEU:CD1	2.31	0.78
2:E:697:TYR:O	2:E:697:TYR:HD1	1.66	0.78
2:G:688:ILE:HD11	2:G:689:ILE:HG23	1.65	0.78
1:C:235:ASN:OD1	1:C:236:ASN:N	2.16	0.78
1:B:444:VAL:HA	1:B:447:ILE:HD12	1.66	0.78
1:B:457:HIS:C	1:B:459:LEU:H	1.87	0.78
1:C:232:LYS:O	1:C:232:LYS:HG2	1.84	0.77
1:C:459:LEU:HG	1:C:459:LEU:O	1.82	0.77
1:C:248:CYS:SG	1:C:271:ARG:NH2	2.58	0.77
1:B:412:LEU:HD21	1:B:426:LEU:HD12	1.67	0.77
1:C:258:LEU:CD2	1:C:263:ILE:HD12	2.12	0.77
1:B:201:ALA:O	1:B:204:LYS:HE2	1.85	0.76
1:D:244:MET:HE1	1:D:268:ALA:HB3	1.65	0.76
1:D:230:SER:O	1:D:232:LYS:CD	2.33	0.76
2:E:683:MET:HG3	2:E:684:GLY:H	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HA	1:A:266:LYS:HZ3	1.50	0.76
1:B:454:ALA:O	1:B:455:ALA:HB2	1.84	0.76
1:A:321:LEU:O	1:A:325:MET:HG3	1.86	0.76
1:D:391:LEU:CD1	1:D:397:ILE:HD12	2.15	0.76
1:A:269:GLU:CG	1:A:348:ARG:HH11	1.95	0.75
1:D:345:LYS:O	1:D:352:CYS:HB3	1.85	0.75
1:D:394:VAL:O	1:D:394:VAL:HG13	1.86	0.75
1:D:255:VAL:HB	1:D:258:LEU:CG	2.15	0.75
1:A:248:CYS:SG	1:A:271:ARG:NH2	2.59	0.75
1:A:277:GLN:C	1:A:279:THR:H	1.89	0.75
1:A:396:HIS:HB3	1:A:399:LYS:NZ	2.01	0.75
1:C:297:PHE:HA	1:C:300:LEU:HD11	1.67	0.75
1:A:251:GLU:OE1	1:A:271:ARG:HG2	1.87	0.75
2:H:689:ILE:O	2:H:693:LEU:HD22	1.86	0.75
1:D:251:GLU:HA	1:D:254:LEU:HB2	1.66	0.75
1:D:274:HIS:O	1:D:277:GLN:HB2	1.87	0.75
1:D:302:LEU:HD13	1:D:302:LEU:O	1.87	0.74
1:A:311:TYR:HB2	1:A:388:ARG:HD2	1.69	0.74
1:B:355:MET:CE	3:B:776:471:HCE1	2.18	0.74
1:B:348:ARG:NH2	1:B:351:PHE:HE2	1.85	0.73
1:B:201:ALA:HA	1:B:204:LYS:CE	2.18	0.73
1:D:209:ARG:HD2	2:H:700:TRP:CZ3	2.16	0.73
1:A:257:LYS:HG2	1:A:257:LYS:O	1.87	0.73
1:A:409:ARG:HG2	1:A:413:GLN:HE21	1.52	0.73
1:C:292:LYS:HD3	2:G:693:LEU:HD12	1.71	0.73
2:F:685:LEU:HA	4:F:240:HOH:O	1.87	0.73
1:C:420:ILE:HD13	1:C:421:PHE:H	1.53	0.73
1:C:223:VAL:HG23	1:C:372:ASP:OD2	1.89	0.72
1:C:251:GLU:HA	1:C:254:LEU:HB2	1.70	0.72
1:D:232:LYS:HE2	4:D:828:HOH:O	1.88	0.72
1:D:249:MET:O	1:D:253:THR:HG23	1.89	0.72
1:A:456:LEU:HD11	3:A:775:471:H4E1	1.71	0.72
2:F:696:LYS:C	2:F:696:LYS:HD2	2.08	0.72
1:D:348:ARG:O	1:D:349:LYS:HB2	1.89	0.72
2:G:688:ILE:CD1	2:G:689:ILE:CG2	2.68	0.72
1:B:270:VAL:HG13	1:B:454:ALA:CB	2.20	0.72
1:B:314:TYR:HE1	3:B:776:471:H4A2	1.53	0.72
1:B:334:TYR:CD1	1:B:334:TYR:N	2.57	0.72
1:C:279:THR:HG21	4:C:816:HOH:O	1.90	0.72
1:A:306:VAL:HG13	2:E:689:ILE:HD11	1.71	0.72
1:B:227:VAL:HA	1:B:231:GLY:HA3	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:N	1:A:334:TYR:CD2	2.56	0.72
1:C:313:VAL:O	1:C:317:ILE:HG13	1.89	0.72
1:D:457:HIS:O	1:D:460:LEU:HD12	1.89	0.72
1:D:349:LYS:HD3	1:D:352:CYS:SG	2.30	0.71
1:B:230:SER:O	1:B:232:LYS:HE2	1.89	0.71
1:B:391:LEU:HD13	1:B:397:ILE:HD12	1.71	0.71
1:B:292:LYS:HZ1	2:F:696:LYS:CE	2.03	0.71
1:A:248:CYS:O	1:A:252:LYS:HB2	1.90	0.71
1:D:420:ILE:HD11	1:D:421:PHE:CE1	2.25	0.71
1:B:258:LEU:HD21	1:B:263:ILE:HD12	1.71	0.71
1:D:448:LYS:O	1:D:452:SER:HA	1.90	0.71
1:C:465:ARG:HD3	1:C:465:ARG:O	1.91	0.71
1:B:306:VAL:HA	2:F:689:ILE:HD11	1.72	0.71
1:B:270:VAL:CG1	1:B:454:ALA:CB	2.68	0.71
1:C:257:LYS:HG2	1:C:257:LYS:O	1.90	0.71
2:E:682:ASN:O	2:E:683:MET:HB2	1.90	0.71
1:D:396:HIS:HB3	4:D:838:HOH:O	1.91	0.71
1:D:449:LYS:HA	1:D:452:SER:OG	1.91	0.71
1:D:348:ARG:HG3	1:D:349:LYS:N	2.03	0.70
1:C:446:ILE:HG22	1:C:446:ILE:O	1.89	0.70
1:C:461:GLN:C	1:C:461:GLN:NE2	2.45	0.70
1:D:412:LEU:HD11	1:D:426:LEU:HD12	1.71	0.70
2:E:683:MET:HA	2:E:683:MET:CE	2.21	0.70
1:A:263:ILE:HA	1:A:266:LYS:NZ	2.06	0.70
1:B:247:LEU:HD12	1:B:247:LEU:O	1.89	0.70
1:D:409:ARG:HG2	1:D:410:LEU:HD23	1.73	0.70
1:A:333:ALA:C	1:A:334:TYR:HD2	1.94	0.70
1:B:235:ASN:O	1:B:236:ASN:HB3	1.91	0.70
1:C:378:PHE:O	1:C:382:ILE:HG23	1.91	0.70
1:C:460:LEU:HD23	1:C:464:TYR:CE2	2.27	0.70
1:B:292:LYS:HE3	2:F:696:LYS:HE2	1.73	0.69
1:D:297:PHE:HA	1:D:300:LEU:HD11	1.74	0.69
2:G:688:ILE:N	2:G:688:ILE:CD1	2.54	0.69
1:D:348:ARG:C	1:D:349:LYS:HG2	2.11	0.69
2:H:683:MET:HG3	2:H:684:GLY:H	1.58	0.69
1:A:274:HIS:HA	1:A:277:GLN:HE21	1.58	0.69
1:B:265:ASN:CG	1:B:265:ASN:O	2.27	0.69
1:C:453:ASP:CG	1:C:454:ALA:H	1.95	0.69
1:A:457:HIS:HB3	1:A:459:LEU:HD22	1.74	0.69
2:G:686:GLU:OE2	2:G:690:ARG:NH1	2.26	0.69
1:B:334:TYR:HD1	1:B:334:TYR:N	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ILE:HG23	1:B:446:ILE:O	1.92	0.68
1:C:309:LEU:O	1:C:313:VAL:HB	1.92	0.68
1:C:461:GLN:C	1:C:461:GLN:HE21	1.96	0.68
1:D:351:PHE:O	1:D:353:ASP:N	2.26	0.68
2:G:685:LEU:HA	4:G:260:HOH:O	1.93	0.68
1:A:258:LEU:CD2	1:A:263:ILE:HG13	2.17	0.68
1:A:363:MET:HE3	1:A:363:MET:HA	1.74	0.68
1:C:273:PHE:O	1:C:277:GLN:HG3	1.94	0.68
1:D:242:HIS:CE1	1:D:243:ASP:OD2	2.46	0.68
1:C:450:THR:O	1:C:451:GLU:HG2	1.94	0.68
1:B:201:ALA:CA	1:B:204:LYS:HE2	2.24	0.68
1:A:393:ASN:HB3	1:A:396:HIS:CE1	2.28	0.68
1:D:300:LEU:HD12	1:D:300:LEU:H	1.59	0.68
1:A:315:GLU:HB2	1:A:382:ILE:HD13	1.75	0.67
1:D:423:PHE:HB3	1:D:424:PRO:HD3	1.75	0.67
1:A:227:VAL:O	1:A:231:GLY:CA	2.39	0.67
1:D:447:ILE:N	1:D:447:ILE:HD12	2.09	0.67
2:G:688:ILE:HD11	2:G:689:ILE:CG2	2.24	0.67
1:B:450:THR:CG2	1:B:451:GLU:HG3	2.24	0.67
1:A:258:LEU:HB3	1:A:263:ILE:HG12	1.76	0.67
1:C:272:ILE:HG22	1:C:272:ILE:O	1.94	0.67
1:D:300:LEU:N	1:D:300:LEU:HD12	2.10	0.67
1:D:465:ARG:HG2	1:D:466:ASP:OD1	1.94	0.67
1:D:465:ARG:HH11	1:D:465:ARG:HG3	1.60	0.67
1:A:387:ASP:OD2	1:A:387:ASP:N	2.27	0.67
1:C:461:GLN:O	1:C:461:GLN:NE2	2.28	0.67
1:B:319:ALA:HB2	1:B:433:LEU:HD11	1.77	0.67
1:B:348:ARG:HH22	1:B:351:PHE:HE2	1.43	0.67
1:A:263:ILE:H	1:A:263:ILE:HD13	1.58	0.66
1:C:456:LEU:CD1	1:C:456:LEU:N	2.58	0.66
1:B:325:MET:HG2	1:B:330:MET:HB3	1.76	0.66
1:B:267:GLU:OE1	1:B:348:ARG:NH2	2.28	0.66
1:B:275:CYS:HA	1:B:278:CYS:SG	2.34	0.66
1:D:382:ILE:O	1:D:382:ILE:HD12	1.95	0.66
1:D:345:LYS:HA	1:D:352:CYS:HA	1.77	0.66
1:B:270:VAL:HG13	1:B:454:ALA:HB3	1.78	0.66
2:G:697:TYR:O	2:G:698:ASP:HB2	1.95	0.66
1:A:244:MET:HE1	1:A:271:ARG:HH21	1.59	0.66
1:B:453:ASP:OD1	1:B:453:ASP:N	2.27	0.66
1:A:461:GLN:HG3	1:A:464:TYR:HD2	1.61	0.65
1:A:259:VAL:O	1:A:259:VAL:CG1	2.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:HB3	1:A:422:LEU:HB2	1.78	0.65
1:C:232:LYS:O	1:C:232:LYS:CG	2.43	0.65
1:A:411:HIS:O	1:A:415:ASN:HB2	1.97	0.65
1:A:457:HIS:CD2	1:A:458:PRO:HD2	2.31	0.65
1:B:309:LEU:O	1:B:313:VAL:HB	1.97	0.65
1:D:235:ASN:C	1:D:235:ASN:ND2	2.48	0.65
1:D:422:LEU:HB3	4:D:795:HOH:O	1.96	0.65
1:D:263:ILE:HA	1:D:266:LYS:HE3	1.78	0.65
1:A:399:LYS:HG3	1:A:400:MET:N	2.11	0.65
1:A:428:GLN:O	1:A:431:ALA:HB3	1.95	0.65
1:C:393:ASN:O	1:C:395:GLY:N	2.29	0.65
1:A:285:THR:HG23	2:E:692:ALA:CB	2.26	0.65
2:F:694:MET:N	2:F:694:MET:HE2	2.11	0.65
1:B:243:ASP:OD1	1:B:245:GLU:HB3	1.96	0.65
1:D:348:ARG:CG	1:D:349:LYS:N	2.59	0.65
1:B:354:ILE:O	1:B:357:PRO:HD2	1.98	0.64
1:C:438:THR:HG22	1:C:439:GLU:N	2.11	0.64
1:A:391:LEU:HD13	1:A:397:ILE:HD12	1.79	0.64
2:E:683:MET:HE3	2:E:683:MET:HA	1.78	0.64
1:A:363:MET:CE	1:A:363:MET:HA	2.27	0.64
1:A:300:LEU:HD21	1:A:400:MET:CE	2.28	0.64
1:A:403:GLY:O	1:A:407:VAL:HG23	1.98	0.64
1:B:440:HIS:O	1:B:444:VAL:HB	1.98	0.64
1:D:409:ARG:HG2	1:D:410:LEU:N	2.11	0.64
1:C:266:LYS:O	1:C:267:GLU:C	2.35	0.64
1:B:331:LEU:HD22	1:B:335:GLY:HA2	1.80	0.64
1:A:420:ILE:HD11	1:A:421:PHE:CD1	2.33	0.64
1:B:455:ALA:O	1:B:457:HIS:N	2.31	0.64
1:C:456:LEU:HD13	1:C:456:LEU:H	1.61	0.64
1:C:461:GLN:HE22	1:C:465:ARG:NH1	1.96	0.64
1:A:396:HIS:HB3	1:A:399:LYS:HZ2	1.60	0.64
1:B:456:LEU:CD2	1:B:456:LEU:N	2.48	0.64
1:D:457:HIS:C	1:D:459:LEU:H	2.01	0.64
2:G:688:ILE:HD13	2:G:688:ILE:C	2.08	0.64
1:C:463:ILE:O	1:C:464:TYR:CD2	2.52	0.63
2:G:688:ILE:HD13	2:G:689:ILE:CG2	2.28	0.63
1:A:266:LYS:O	1:A:267:GLU:C	2.37	0.63
1:C:450:THR:O	1:C:450:THR:HG22	1.97	0.63
1:D:445:GLN:HE21	1:D:445:GLN:HA	1.63	0.63
1:B:358:LYS:HE3	1:B:436:LEU:HD21	1.80	0.63
1:B:279:THR:HG21	4:B:794:HOH:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:LEU:HB3	2:H:689:ILE:HD12	1.81	0.63
1:C:396:HIS:N	1:C:396:HIS:ND1	2.47	0.62
1:B:237:PRO:HB2	1:B:238:PRO:HD2	1.81	0.62
1:A:435:GLN:O	1:A:435:GLN:HG3	1.97	0.62
1:D:273:PHE:O	1:D:277:GLN:HG2	1.98	0.62
2:F:697:TYR:O	2:F:697:TYR:CG	2.51	0.62
1:A:361:PHE:C	1:A:361:PHE:CD1	2.72	0.62
1:C:268:ALA:HA	1:C:271:ARG:HD3	1.80	0.62
1:A:345:LYS:HG3	1:A:345:LYS:O	1.99	0.62
1:A:216:LYS:HD3	1:A:216:LYS:O	1.99	0.62
1:A:423:PHE:HB3	1:A:424:PRO:HD3	1.82	0.62
1:D:297:PHE:O	1:D:300:LEU:CD1	2.47	0.62
1:D:348:ARG:O	1:D:349:LYS:HG3	1.93	0.62
1:A:263:ILE:CG2	1:A:266:LYS:HZ3	2.13	0.62
1:A:298:ALA:HA	1:A:305:GLN:HE22	1.64	0.62
1:C:251:GLU:HA	1:C:254:LEU:HD22	1.81	0.62
1:C:457:HIS:CG	1:C:458:PRO:CD	2.83	0.62
1:B:248:CYS:O	1:B:252:LYS:HB2	1.99	0.62
1:B:270:VAL:HG21	1:B:453:ASP:OD2	1.99	0.62
1:A:233:ALA:O	1:A:234:SER:HB2	1.97	0.62
1:C:297:PHE:O	1:C:300:LEU:HD13	1.98	0.62
1:D:399:LYS:O	1:D:399:LYS:HG3	1.97	0.62
1:D:270:VAL:CG2	1:D:348:ARG:NH2	2.64	0.61
1:D:373:SER:OG	1:D:411:HIS:CE1	2.53	0.61
1:C:235:ASN:CG	1:C:236:ASN:H	2.03	0.61
1:A:378:PHE:O	1:A:382:ILE:HG23	2.01	0.61
1:D:325:MET:HG2	1:D:330:MET:HB3	1.83	0.61
1:D:409:ARG:O	1:D:413:GLN:HG3	2.01	0.61
1:A:371:ASP:O	1:A:375:ILE:HG13	2.01	0.61
1:D:448:LYS:HZ2	1:D:449:LYS:HG2	1.66	0.61
1:A:370:LEU:HD11	1:A:426:LEU:HD21	1.81	0.61
1:B:292:LYS:CE	2:F:696:LYS:HG2	2.31	0.61
1:B:463:ILE:O	1:B:464:TYR:CD1	2.54	0.61
1:C:384:CYS:O	1:C:401:GLN:HB2	2.01	0.61
1:C:288:THR:HA	1:C:309:LEU:HD11	1.81	0.61
1:B:355:MET:HE2	3:B:776:471:HCE1	1.82	0.60
1:C:325:MET:HG2	1:C:330:MET:HB3	1.83	0.60
1:A:257:LYS:HE2	1:A:261:ASN:HD22	1.63	0.60
1:B:457:HIS:C	1:B:459:LEU:N	2.54	0.60
1:A:412:LEU:HD22	1:A:422:LEU:HD23	1.84	0.60
1:B:343:PHE:O	1:B:347:LEU:CD1	2.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD13	1:C:263:ILE:HG21	1.82	0.60
2:H:685:LEU:HA	4:H:243:HOH:O	2.01	0.60
1:C:463:ILE:HG23	1:C:463:ILE:O	2.02	0.60
1:B:292:LYS:NZ	2:F:696:LYS:CG	2.65	0.60
1:A:244:MET:SD	1:A:268:ALA:CB	2.90	0.60
1:D:348:ARG:C	1:D:349:LYS:CG	2.66	0.60
2:F:686:GLU:OE2	2:F:690:ARG:NH1	2.34	0.60
1:D:343:PHE:O	1:D:346:SER:OG	2.19	0.59
1:B:353:ASP:O	1:B:443:LEU:HD21	2.02	0.59
1:D:446:ILE:C	1:D:447:ILE:HD12	2.22	0.59
1:A:459:LEU:HD23	1:A:460:LEU:N	2.17	0.59
1:D:280:SER:O	1:D:284:VAL:HG23	2.03	0.59
1:A:268:ALA:HA	1:A:271:ARG:HE	1.67	0.59
1:C:235:ASN:CG	1:C:236:ASN:N	2.55	0.59
1:D:302:LEU:O	1:D:306:VAL:HG23	2.02	0.59
1:B:314:TYR:CE1	3:B:776:471:H4A2	2.37	0.59
1:C:247:LEU:HD21	1:C:268:ALA:HB1	1.85	0.59
1:C:393:ASN:HB3	1:C:396:HIS:CE1	2.37	0.59
1:A:396:HIS:ND1	1:A:396:HIS:N	2.50	0.59
1:C:297:PHE:HA	1:C:300:LEU:CD1	2.32	0.59
1:D:297:PHE:O	1:D:300:LEU:HD13	2.03	0.59
1:B:454:ALA:O	1:B:455:ALA:CB	2.51	0.59
2:F:686:GLU:O	2:F:690:ARG:HB2	2.03	0.59
1:B:445:GLN:C	1:B:447:ILE:H	2.05	0.58
1:C:268:ALA:O	1:C:271:ARG:N	2.36	0.58
1:C:443:LEU:O	1:C:443:LEU:HG	2.03	0.58
1:C:460:LEU:CD2	1:C:464:TYR:CE2	2.86	0.58
1:D:288:THR:HA	1:D:309:LEU:HD11	1.84	0.58
1:C:299:ASN:HA	2:F:697:TYR:HB2	1.85	0.58
1:A:412:LEU:HD11	1:A:426:LEU:CD1	2.33	0.58
1:A:412:LEU:CD1	1:A:426:LEU:HD12	2.32	0.58
1:B:270:VAL:CG1	1:B:454:ALA:HB2	2.33	0.58
1:C:423:PHE:CZ	1:C:427:LEU:HD21	2.39	0.58
1:A:318:PHE:HA	1:A:321:LEU:HB2	1.85	0.58
1:D:308:LEU:HD11	1:D:397:ILE:HD13	1.84	0.58
2:F:690:ARG:O	2:F:694:MET:HE3	2.02	0.58
2:F:683:MET:HG3	2:F:684:GLY:H	1.69	0.58
1:A:301:ASP:C	1:A:301:ASP:OD1	2.42	0.58
1:B:445:GLN:HA	1:B:445:GLN:NE2	2.12	0.58
1:A:269:GLU:CG	1:A:348:ARG:NH1	2.53	0.58
1:A:244:MET:CE	1:A:268:ALA:HB2	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:O	1:B:324:VAL:HG13	2.04	0.58
1:B:423:PHE:CZ	1:B:427:LEU:HD21	2.38	0.58
1:D:270:VAL:CG2	1:D:348:ARG:HH21	2.16	0.58
2:G:688:ILE:O	2:G:691:LYS:HG3	2.03	0.57
1:A:217:ASN:O	1:A:286:GLU:HB3	2.05	0.57
1:A:230:SER:HB3	4:A:799:HOH:O	2.04	0.57
1:B:292:LYS:CE	2:F:696:LYS:HE2	2.34	0.57
1:A:259:VAL:O	1:A:259:VAL:HG13	2.03	0.57
1:B:213:ALA:HB1	1:B:293:ALA:HB3	1.85	0.57
1:C:268:ALA:O	1:C:270:VAL:N	2.38	0.57
1:C:457:HIS:CD2	1:C:458:PRO:CD	2.87	0.57
1:D:209:ARG:CD	2:H:700:TRP:CZ3	2.83	0.57
1:B:450:THR:HG22	1:B:451:GLU:N	2.19	0.57
1:D:270:VAL:HG12	1:D:270:VAL:O	2.05	0.57
1:A:399:LYS:CG	1:A:400:MET:N	2.68	0.57
1:B:460:LEU:CD2	1:B:460:LEU:N	2.55	0.57
1:C:315:GLU:OE2	1:C:434:ARG:HG2	2.05	0.57
1:D:457:HIS:O	1:D:460:LEU:CD1	2.52	0.57
1:D:358:LYS:N	1:D:358:LYS:HD2	2.20	0.57
2:G:688:ILE:O	2:G:691:LYS:CG	2.53	0.57
1:A:333:ALA:C	1:A:334:TYR:CD2	2.78	0.56
1:B:251:GLU:N	1:B:251:GLU:OE1	2.38	0.56
1:D:301:ASP:HB3	1:D:303:ASN:H	1.70	0.56
1:A:263:ILE:H	1:A:263:ILE:CD1	2.17	0.56
1:C:214:TYR:C	1:C:216:LYS:H	2.09	0.56
1:C:297:PHE:O	1:C:300:LEU:CD1	2.52	0.56
1:A:263:ILE:HG22	1:A:266:LYS:HZ3	1.69	0.56
1:C:218:PHE:HZ	1:C:287:LEU:HD23	1.70	0.56
1:A:276:CYS:O	1:A:280:SER:HB2	2.05	0.56
1:B:230:SER:C	1:B:232:LYS:HG3	2.26	0.56
1:B:459:LEU:HD11	1:B:463:ILE:HD11	1.86	0.56
1:C:453:ASP:CG	1:C:454:ALA:N	2.59	0.56
1:B:251:GLU:OE1	1:B:252:LYS:N	2.37	0.56
1:B:278:CYS:C	1:B:280:SER:H	2.08	0.56
1:C:457:HIS:CG	1:C:458:PRO:HD3	2.40	0.56
1:D:270:VAL:HG23	1:D:348:ARG:HH21	1.68	0.56
1:B:456:LEU:CD2	1:B:456:LEU:H	1.93	0.56
3:D:778:471:H4A1	4:D:779:HOH:O	2.05	0.56
2:E:683:MET:HG3	2:E:684:GLY:N	2.19	0.56
2:G:685:LEU:HD23	2:G:685:LEU:H	1.70	0.56
1:C:461:GLN:HE22	1:C:465:ARG:HH11	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:LEU:C	1:D:461:GLN:H	2.09	0.56
1:A:238:PRO:HA	1:A:336:ASN:O	2.05	0.56
1:C:467:MET:O	1:C:468:TYR:CG	2.59	0.55
2:H:683:MET:HG3	2:H:684:GLY:N	2.21	0.55
1:A:232:LYS:O	1:A:233:ALA:HB3	2.07	0.55
1:C:269:GLU:HB2	1:C:351:PHE:CD2	2.42	0.55
2:H:686:GLU:HA	2:H:689:ILE:HG23	1.88	0.55
1:B:201:ALA:HA	1:B:204:LYS:CD	2.37	0.55
1:D:252:LYS:HA	1:D:258:LEU:HD13	1.89	0.55
1:A:277:GLN:C	1:A:279:THR:N	2.59	0.55
1:B:247:LEU:O	1:B:251:GLU:HG3	2.07	0.55
1:B:427:LEU:CD2	1:B:430:MET:HE2	2.37	0.55
1:A:374:ASP:OD2	1:A:416:HIS:CE1	2.54	0.55
1:C:242:HIS:CE1	1:C:243:ASP:OD2	2.60	0.55
1:C:396:HIS:O	1:C:400:MET:HB2	2.07	0.55
1:A:247:LEU:HG	1:A:247:LEU:O	2.04	0.55
1:C:280:SER:C	1:C:282:GLU:N	2.60	0.55
1:D:259:VAL:O	1:D:260:ALA:HB2	2.06	0.55
1:B:209:ARG:HD2	2:F:700:TRP:CZ3	2.42	0.55
1:C:235:ASN:O	1:C:236:ASN:HB3	2.06	0.55
1:D:244:MET:HE3	1:D:268:ALA:HB3	1.87	0.55
1:A:340:THR:O	1:A:344:LEU:HD12	2.07	0.55
1:B:462:GLU:C	1:B:464:TYR:H	2.10	0.55
1:C:277:GLN:C	1:C:279:THR:H	2.06	0.55
1:D:351:PHE:O	1:D:354:ILE:N	2.31	0.55
1:A:269:GLU:HB2	1:A:351:PHE:CE2	2.42	0.54
1:C:346:SER:O	1:C:347:LEU:HD23	2.07	0.54
1:D:394:VAL:O	1:D:394:VAL:CG1	2.53	0.54
1:A:422:LEU:O	1:A:425:LYS:HB2	2.07	0.54
1:D:235:ASN:C	1:D:235:ASN:HD22	2.10	0.54
1:D:370:LEU:HD11	1:D:426:LEU:HD21	1.88	0.54
1:A:409:ARG:HG2	1:A:413:GLN:NE2	2.22	0.54
1:A:448:LYS:O	1:A:452:SER:OG	2.19	0.54
2:E:697:TYR:CD1	2:E:697:TYR:O	2.55	0.54
1:D:300:LEU:HD23	1:D:397:ILE:HD11	1.90	0.54
1:B:235:ASN:OD1	1:B:236:ASN:N	2.40	0.54
1:B:457:HIS:O	1:B:459:LEU:N	2.41	0.54
1:B:423:PHE:HB3	1:B:424:PRO:CD	2.38	0.54
1:B:292:LYS:NZ	2:F:696:LYS:HG2	2.22	0.54
1:A:263:ILE:CG2	1:A:266:LYS:NZ	2.71	0.54
1:A:263:ILE:N	1:A:263:ILE:HD13	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:HIS:ND1	1:A:458:PRO:HD2	2.22	0.54
1:B:251:GLU:CD	1:B:252:LYS:N	2.61	0.54
1:B:257:LYS:O	1:B:257:LYS:HG2	2.07	0.54
1:C:209:ARG:HH22	1:C:293:ALA:CB	2.12	0.54
1:D:350:PRO:O	1:D:353:ASP:OD2	2.26	0.54
1:B:355:MET:HE1	3:B:776:471:HCE1	1.89	0.54
1:D:444:VAL:O	1:D:446:ILE:N	2.33	0.54
1:A:257:LYS:CG	1:A:257:LYS:O	2.56	0.54
1:B:280:SER:O	1:B:284:VAL:HG23	2.08	0.54
1:C:363:MET:HA	1:C:363:MET:CE	2.38	0.54
1:C:421:PHE:O	1:C:425:LYS:HB2	2.08	0.54
1:D:271:ARG:C	1:D:273:PHE:H	2.10	0.54
2:F:689:ILE:HG13	2:F:693:LEU:HD22	1.90	0.54
2:E:682:ASN:O	2:E:683:MET:CB	2.56	0.54
1:B:279:THR:HG22	1:B:279:THR:O	2.08	0.53
1:C:345:LYS:C	1:C:352:CYS:HB2	2.28	0.53
1:D:445:GLN:O	1:D:446:ILE:HG13	2.08	0.53
1:A:300:LEU:HD11	1:A:400:MET:HE3	1.90	0.53
1:C:348:ARG:O	1:C:351:PHE:HB2	2.07	0.53
1:C:460:LEU:HD23	1:C:464:TYR:CD2	2.43	0.53
1:C:209:ARG:NH2	1:C:293:ALA:C	2.62	0.53
1:C:211:TYR:CZ	1:C:215:LEU:HD11	2.43	0.53
1:C:393:ASN:C	1:C:395:GLY:H	2.12	0.53
1:A:379:VAL:O	1:A:383:ILE:HG13	2.08	0.53
1:B:201:ALA:C	1:B:204:LYS:HE2	2.28	0.53
1:C:300:LEU:CD1	1:C:300:LEU:H	1.94	0.53
1:C:370:LEU:HD11	1:C:426:LEU:HD21	1.90	0.53
1:A:279:THR:HG21	4:A:798:HOH:O	2.08	0.53
1:A:345:LYS:O	1:A:345:LYS:CG	2.56	0.53
1:C:463:ILE:O	1:C:464:TYR:HD2	1.92	0.53
1:D:457:HIS:CD2	1:D:459:LEU:N	2.77	0.53
1:A:344:LEU:O	1:A:347:LEU:HG	2.09	0.53
1:C:209:ARG:NH2	1:C:293:ALA:O	2.42	0.53
1:C:247:LEU:CD1	1:C:272:ILE:HD11	2.39	0.53
1:B:292:LYS:HZ1	2:F:696:LYS:HE3	1.72	0.53
1:B:439:GLU:O	1:B:443:LEU:HB3	2.08	0.53
1:D:457:HIS:HD2	1:D:459:LEU:CA	2.22	0.53
1:C:288:THR:CG2	2:G:693:LEU:HD13	2.39	0.53
1:C:237:PRO:HB2	1:C:238:PRO:CD	2.30	0.52
1:C:420:ILE:HD13	1:C:420:ILE:C	2.29	0.52
1:A:467:MET:CE	1:A:467:MET:HA	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:O	1:B:303:ASN:N	2.42	0.52
1:B:258:LEU:HD22	1:B:263:ILE:HB	1.90	0.52
1:D:255:VAL:N	1:D:258:LEU:HD11	2.17	0.52
1:B:302:LEU:C	1:B:302:LEU:HD23	2.30	0.52
1:A:354:ILE:O	1:A:357:PRO:HD2	2.09	0.52
1:C:280:SER:O	1:C:282:GLU:N	2.43	0.52
1:D:351:PHE:C	1:D:353:ASP:N	2.62	0.52
1:B:269:GLU:OE1	1:B:348:ARG:N	2.43	0.52
1:D:269:GLU:HB3	1:D:347:LEU:HD22	1.90	0.52
2:F:695:GLY:HA2	4:F:242:HOH:O	2.09	0.52
1:A:388:ARG:O	1:A:391:LEU:HG	2.10	0.52
1:C:420:ILE:HD11	1:C:421:PHE:CD2	2.45	0.52
1:B:459:LEU:C	1:B:460:LEU:HD23	2.29	0.52
1:A:275:CYS:O	1:A:278:CYS:N	2.42	0.52
2:H:686:GLU:O	2:H:690:ARG:HB2	2.10	0.52
1:A:257:LYS:O	1:A:261:ASN:HB2	2.09	0.52
1:C:247:LEU:HD13	1:C:272:ILE:HD11	1.92	0.52
1:C:279:THR:HG22	1:C:279:THR:O	2.09	0.51
1:D:412:LEU:HD11	1:D:426:LEU:CD1	2.40	0.51
1:D:448:LYS:HZ2	1:D:449:LYS:CG	2.24	0.51
1:B:235:ASN:ND2	4:B:880:HOH:O	2.43	0.51
1:B:301:ASP:C	1:B:303:ASN:N	2.62	0.51
1:C:306:VAL:HA	2:G:689:ILE:HD11	1.92	0.51
1:B:370:LEU:HD11	1:B:426:LEU:HD21	1.92	0.51
1:C:231:GLY:C	1:C:233:ALA:N	2.63	0.51
1:D:255:VAL:HB	1:D:258:LEU:CD1	2.40	0.51
2:H:685:LEU:HD23	2:H:685:LEU:N	2.26	0.51
1:B:412:LEU:HG	1:B:422:LEU:HD13	1.93	0.51
1:D:230:SER:O	1:D:232:LYS:HD3	2.09	0.51
1:A:312:GLY:O	1:A:382:ILE:HD11	2.11	0.51
1:B:255:VAL:HG11	1:B:258:LEU:HG	1.91	0.51
1:B:340:THR:HG22	1:B:343:PHE:H	1.75	0.51
1:C:276:CYS:SG	3:C:777:471:H3A1	2.51	0.51
1:D:255:VAL:O	1:D:258:LEU:HD12	2.10	0.51
1:D:356:GLU:N	1:D:357:PRO:CD	2.74	0.51
1:B:270:VAL:HG11	1:B:454:ALA:HB2	1.92	0.51
1:C:269:GLU:HB2	1:C:351:PHE:CE2	2.45	0.51
1:B:412:LEU:CD2	1:B:426:LEU:HD12	2.39	0.51
1:C:358:LYS:HZ1	1:C:440:HIS:HB2	1.76	0.51
1:D:262:GLY:O	1:D:266:LYS:HE3	2.11	0.51
1:A:301:ASP:OD1	1:A:303:ASN:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:O	1:A:379:VAL:HG23	2.11	0.50
1:A:422:LEU:HA	1:A:425:LYS:HD2	1.93	0.50
1:C:363:MET:HA	1:C:363:MET:HE2	1.92	0.50
1:D:447:ILE:O	1:D:447:ILE:HG22	2.11	0.50
1:D:288:THR:CG2	2:H:693:LEU:HD13	2.41	0.50
1:B:338:PHE:O	1:B:338:PHE:HD1	1.95	0.50
1:C:207:ALA:HB2	1:C:407:VAL:HG13	1.93	0.50
1:D:373:SER:HG	1:D:411:HIS:CE1	2.29	0.50
1:D:309:LEU:O	1:D:313:VAL:HB	2.11	0.50
1:A:420:ILE:CD1	1:A:421:PHE:N	2.71	0.50
1:A:429:LYS:C	1:A:431:ALA:N	2.65	0.50
1:B:269:GLU:OE1	1:B:347:LEU:HB3	2.11	0.50
1:B:355:MET:HG2	3:B:776:471:HC1L	1.93	0.50
1:B:276:CYS:SG	3:B:776:471:H3A1	2.51	0.50
1:C:378:PHE:HE1	1:C:430:MET:HG3	1.76	0.50
1:C:412:LEU:CD1	1:C:422:LEU:HG	2.41	0.50
1:D:248:CYS:O	1:D:252:LYS:HB2	2.11	0.50
1:D:409:ARG:CB	1:D:409:ARG:NH1	2.74	0.50
1:A:279:THR:O	1:A:279:THR:HG22	2.12	0.50
1:A:457:HIS:CE1	1:A:458:PRO:HD2	2.47	0.50
1:C:394:VAL:O	1:C:394:VAL:CG1	2.59	0.50
1:D:358:LYS:HD2	1:D:358:LYS:H	1.76	0.50
1:D:409:ARG:HB2	1:D:409:ARG:NH1	2.27	0.50
1:B:434:ARG:NH2	4:B:805:HOH:O	2.29	0.50
1:B:460:LEU:O	1:B:462:GLU:O	2.30	0.50
1:C:438:THR:CG2	1:C:439:GLU:N	2.75	0.50
1:C:462:GLU:O	1:C:463:ILE:HG22	2.11	0.50
1:D:349:LYS:HA	1:D:350:PRO:C	2.28	0.50
1:A:244:MET:HE1	1:A:268:ALA:CB	2.35	0.50
2:H:683:MET:CG	2:H:684:GLY:H	2.25	0.50
1:C:276:CYS:SG	3:C:777:471:HC1M	2.51	0.49
1:D:297:PHE:HA	1:D:300:LEU:CD1	2.41	0.49
2:G:686:GLU:O	2:G:690:ARG:HB2	2.12	0.49
1:A:270:VAL:O	1:A:270:VAL:HG12	2.11	0.49
1:A:275:CYS:O	1:A:277:GLN:N	2.45	0.49
1:C:354:ILE:O	1:C:357:PRO:HD2	2.12	0.49
1:D:251:GLU:O	1:D:258:LEU:HD13	2.12	0.49
1:A:258:LEU:HD23	1:A:258:LEU:N	2.27	0.49
1:C:391:LEU:HB2	1:C:394:VAL:HG23	1.94	0.49
1:A:351:PHE:O	1:A:353:ASP:N	2.46	0.49
1:B:244:MET:O	1:B:248:CYS:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:LEU:CD1	1:D:426:LEU:HD12	2.40	0.49
1:A:356:GLU:N	1:A:357:PRO:CD	2.76	0.49
1:D:309:LEU:CB	2:H:689:ILE:HD12	2.43	0.49
1:D:457:HIS:HD2	1:D:459:LEU:N	2.10	0.49
1:D:460:LEU:N	1:D:460:LEU:HD12	2.18	0.49
1:A:385:CYS:SG	1:A:388:ARG:NE	2.85	0.49
1:B:434:ARG:O	1:B:437:VAL:HG12	2.13	0.49
1:C:355:MET:HB2	4:C:806:HOH:O	2.11	0.49
1:D:420:ILE:HD11	1:D:421:PHE:CZ	2.47	0.49
1:B:230:SER:O	1:B:232:LYS:CE	2.57	0.49
1:C:225:ALA:O	1:C:229:LEU:HD12	2.13	0.49
1:A:273:PHE:C	1:A:273:PHE:CD2	2.86	0.49
1:D:396:HIS:O	1:D:400:MET:N	2.44	0.49
1:C:446:ILE:O	1:C:446:ILE:CG2	2.60	0.49
1:D:257:LYS:HG2	1:D:257:LYS:O	2.11	0.49
1:D:351:PHE:C	1:D:353:ASP:H	2.16	0.49
1:A:244:MET:SD	1:A:268:ALA:HB3	2.52	0.49
1:B:338:PHE:O	1:B:338:PHE:CD1	2.66	0.49
1:C:299:ASN:O	1:C:300:LEU:C	2.51	0.49
1:D:251:GLU:O	1:D:258:LEU:CD1	2.61	0.49
1:D:382:ILE:C	1:D:382:ILE:HD12	2.32	0.49
1:A:209:ARG:HD3	2:E:700:TRP:CH2	2.47	0.48
2:H:683:MET:O	2:H:685:LEU:HD23	2.13	0.48
1:A:459:LEU:C	1:A:459:LEU:HD23	2.33	0.48
1:B:343:PHE:CD1	1:B:343:PHE:O	2.66	0.48
1:C:412:LEU:HD11	1:C:422:LEU:HG	1.95	0.48
1:D:272:ILE:HG22	1:D:272:ILE:O	2.13	0.48
1:A:263:ILE:HG23	1:A:266:LYS:NZ	2.28	0.48
1:C:229:LEU:HD22	1:C:326:ASN:ND2	2.28	0.48
1:C:247:LEU:CD2	1:C:272:ILE:HD11	2.43	0.48
2:E:691:LYS:O	2:E:691:LYS:HG2	2.13	0.48
1:B:391:LEU:HB2	1:B:394:VAL:HG23	1.96	0.48
1:D:409:ARG:HB3	1:D:409:ARG:HH11	1.79	0.48
1:C:299:ASN:O	1:C:300:LEU:O	2.31	0.48
1:D:420:ILE:HD11	1:D:421:PHE:CD1	2.49	0.48
2:F:690:ARG:O	2:F:694:MET:CE	2.62	0.48
1:A:237:PRO:HB2	1:A:238:PRO:HD2	1.95	0.48
1:B:437:VAL:CG1	1:B:438:THR:N	2.76	0.48
1:D:311:TYR:CZ	1:D:389:PRO:HG2	2.48	0.48
2:F:685:LEU:N	2:F:685:LEU:HD23	2.29	0.48
1:A:457:HIS:CG	1:A:458:PRO:CD	2.92	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:O	1:B:261:ASN:HB2	2.14	0.48
1:B:453:ASP:CG	1:B:454:ALA:H	2.17	0.48
1:A:209:ARG:HD3	2:E:700:TRP:CZ3	2.49	0.48
1:B:446:ILE:CG2	1:B:446:ILE:O	2.59	0.48
1:C:358:LYS:HZ1	1:C:440:HIS:CD2	2.32	0.48
1:D:205:SER:O	1:D:209:ARG:HB2	2.13	0.48
1:D:274:HIS:O	1:D:277:GLN:N	2.31	0.48
1:D:460:LEU:N	1:D:460:LEU:CD1	2.76	0.48
1:D:409:ARG:CB	1:D:409:ARG:HH11	2.26	0.48
1:B:209:ARG:HD2	2:F:700:TRP:HZ3	1.77	0.48
1:A:237:PRO:CB	1:A:238:PRO:HD2	2.44	0.47
1:C:280:SER:C	1:C:282:GLU:H	2.17	0.47
1:C:301:ASP:O	1:C:304:ASP:N	2.47	0.47
1:D:446:ILE:HG22	1:D:446:ILE:O	2.12	0.47
1:B:242:HIS:NE2	1:B:246:THR:HG21	2.29	0.47
1:B:287:LEU:HD22	1:B:383:ILE:HD11	1.97	0.47
1:C:258:LEU:HD13	1:C:263:ILE:CG2	2.45	0.47
1:C:288:THR:HG23	1:C:309:LEU:CD1	2.43	0.47
1:C:289:GLU:HA	1:C:289:GLU:OE1	2.14	0.47
1:D:331:LEU:HD23	1:D:338:PHE:HD2	1.79	0.47
1:D:384:CYS:SG	1:D:400:MET:CE	3.03	0.47
2:E:700:TRP:CG	2:E:700:TRP:O	2.67	0.47
1:A:393:ASN:HB3	1:A:396:HIS:ND1	2.29	0.47
1:B:230:SER:O	1:B:232:LYS:CG	2.55	0.47
1:B:292:LYS:HZ1	2:F:696:LYS:HE2	1.76	0.47
1:B:348:ARG:O	1:B:351:PHE:HD2	1.96	0.47
1:C:242:HIS:HB3	1:C:340:THR:HG21	1.95	0.47
1:C:396:HIS:O	1:C:400:MET:CB	2.62	0.47
1:C:423:PHE:HB3	1:C:424:PRO:CD	2.44	0.47
1:D:396:HIS:CG	4:D:838:HOH:O	2.66	0.47
1:B:338:PHE:C	1:B:338:PHE:CD1	2.88	0.47
1:C:422:LEU:HA	1:C:425:LYS:HB2	1.97	0.47
1:D:443:LEU:O	1:D:443:LEU:HD12	2.14	0.47
1:A:212:GLU:OE1	2:E:700:TRP:CH2	2.67	0.47
1:B:349:LYS:HG3	1:B:350:PRO:HA	1.95	0.47
1:B:427:LEU:HD22	1:B:430:MET:CE	2.45	0.47
1:C:207:ALA:HB2	1:C:407:VAL:CG1	2.44	0.47
1:C:463:ILE:HG23	1:C:464:TYR:HD2	1.79	0.47
1:C:465:ARG:HG3	1:C:465:ARG:HH11	1.79	0.47
1:A:301:ASP:O	1:A:304:ASP:N	2.45	0.47
1:B:268:ALA:HB1	1:B:271:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:VAL:HG12	1:B:438:THR:N	2.29	0.47
1:C:444:VAL:C	1:C:446:ILE:H	2.17	0.47
1:A:435:GLN:O	1:A:439:GLU:HG3	2.15	0.47
1:B:254:LEU:CD2	3:B:776:471:HC3M	2.44	0.47
1:B:457:HIS:ND1	1:B:459:LEU:N	2.62	0.47
1:C:214:TYR:C	1:C:216:LYS:N	2.68	0.47
1:D:462:GLU:O	1:D:463:ILE:HG13	2.14	0.47
1:B:270:VAL:CG1	1:B:454:ALA:HB3	2.42	0.47
1:C:208:LYS:O	1:C:208:LYS:HG2	2.11	0.47
1:D:264:GLN:H	1:D:264:GLN:NE2	2.12	0.47
1:D:271:ARG:C	1:D:273:PHE:N	2.67	0.47
1:A:267:GLU:OE1	1:A:348:ARG:NH1	2.48	0.47
1:B:288:THR:HA	1:B:309:LEU:HD11	1.96	0.47
1:C:293:ALA:O	1:C:294:ILE:C	2.53	0.47
1:D:230:SER:O	1:D:232:LYS:N	2.47	0.47
1:C:282:GLU:HA	1:C:282:GLU:OE1	2.15	0.46
1:C:457:HIS:O	1:C:460:LEU:HD12	2.15	0.46
1:D:290:PHE:HE2	1:D:379:VAL:HG12	1.80	0.46
1:A:315:GLU:CB	1:A:382:ILE:HD13	2.43	0.46
1:B:349:LYS:HA	1:B:351:PHE:H	1.80	0.46
1:D:242:HIS:HE1	1:D:243:ASP:OD2	1.94	0.46
1:A:461:GLN:N	1:A:461:GLN:NE2	2.63	0.46
1:B:230:SER:O	1:B:231:GLY:C	2.53	0.46
1:C:247:LEU:HD12	1:C:247:LEU:O	2.16	0.46
1:D:425:LYS:O	1:D:429:LYS:HG2	2.15	0.46
1:C:263:ILE:HG12	1:C:266:LYS:NZ	2.30	0.46
1:D:259:VAL:HG13	1:D:259:VAL:O	2.15	0.46
1:C:396:HIS:CE1	4:C:785:HOH:O	2.68	0.46
1:A:222:LYS:O	1:A:226:ARG:HG2	2.15	0.46
1:A:421:PHE:C	1:A:424:PRO:HD2	2.36	0.46
1:C:300:LEU:N	1:C:300:LEU:CD1	2.63	0.46
1:A:269:GLU:OE1	1:A:348:ARG:HG2	2.16	0.46
1:A:273:PHE:HZ	1:A:454:ALA:O	1.90	0.46
1:A:467:MET:HA	1:A:467:MET:HE3	1.98	0.46
1:D:235:ASN:ND2	1:D:237:PRO:HD3	2.30	0.46
2:E:685:LEU:C	2:E:687:ALA:N	2.69	0.46
1:A:298:ALA:HA	1:A:305:GLN:NE2	2.31	0.46
1:C:244:MET:HA	1:C:247:LEU:HB3	1.98	0.46
1:C:248:CYS:O	1:C:252:LYS:HB2	2.16	0.46
1:C:450:THR:CG2	1:C:450:THR:O	2.64	0.46
2:E:685:LEU:CD2	2:E:685:LEU:H	1.89	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HB3	2:F:689:ILE:HD12	1.97	0.46
1:A:460:LEU:CD2	2:E:688:ILE:HD11	2.46	0.46
1:D:229:LEU:CD2	1:D:338:PHE:HE2	2.29	0.46
1:D:465:ARG:NH1	1:D:465:ARG:HG3	2.29	0.46
1:A:252:LYS:HD3	1:A:259:VAL:HG23	1.98	0.46
1:B:201:ALA:O	1:B:204:LYS:CE	2.60	0.46
1:B:246:THR:C	1:B:248:CYS:N	2.68	0.46
1:B:259:VAL:O	1:B:259:VAL:HG22	2.16	0.46
1:B:348:ARG:NH2	1:B:351:PHE:CE2	2.75	0.46
1:C:391:LEU:HD22	1:C:397:ILE:CD1	2.46	0.46
1:D:248:CYS:O	1:D:252:LYS:CB	2.64	0.46
1:A:299:ASN:O	1:A:300:LEU:C	2.53	0.45
1:A:429:LYS:C	1:A:431:ALA:H	2.19	0.45
1:C:209:ARG:NH2	1:C:293:ALA:CB	2.75	0.45
1:C:301:ASP:O	1:C:302:LEU:C	2.55	0.45
1:C:460:LEU:HA	1:C:462:GLU:O	2.17	0.45
1:D:457:HIS:C	1:D:459:LEU:N	2.68	0.45
2:E:694:MET:HE3	2:E:694:MET:HB3	1.83	0.45
2:F:696:LYS:CD	2:F:696:LYS:C	2.82	0.45
1:A:396:HIS:O	1:A:400:MET:HB2	2.16	0.45
1:B:447:ILE:O	1:B:447:ILE:HG22	2.15	0.45
1:C:358:LYS:NZ	1:C:440:HIS:HD2	2.14	0.45
1:C:378:PHE:CE1	1:C:430:MET:HG3	2.51	0.45
1:D:393:ASN:C	1:D:395:GLY:H	2.20	0.45
1:D:432:ASP:O	1:D:435:GLN:HB3	2.16	0.45
1:D:465:ARG:O	1:D:465:ARG:HD3	2.16	0.45
2:E:683:MET:O	2:E:685:LEU:CD2	2.64	0.45
1:B:348:ARG:HH11	1:B:348:ARG:HG2	1.80	0.45
1:B:427:LEU:HD22	1:B:430:MET:HE2	1.97	0.45
1:C:307:THR:HA	1:C:310:LYS:HD3	1.98	0.45
1:D:294:ILE:O	1:D:296:GLY:N	2.50	0.45
1:C:255:VAL:HB	1:C:258:LEU:HG	1.98	0.45
1:D:274:HIS:O	1:D:277:GLN:CB	2.61	0.45
2:E:697:TYR:O	2:E:698:ASP:CB	2.57	0.45
1:C:252:LYS:NZ	1:C:259:VAL:HG23	2.31	0.45
1:D:348:ARG:CG	1:D:349:LYS:H	2.28	0.45
2:G:688:ILE:CD1	2:G:689:ILE:HG22	2.46	0.45
1:B:255:VAL:HG12	1:B:257:LYS:H	1.81	0.45
1:C:280:SER:O	1:C:283:THR:N	2.50	0.45
1:B:221:ASN:OD1	1:B:224:LYS:HG3	2.16	0.45
1:C:245:GLU:O	1:C:248:CYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ILE:CG2	1:C:464:TYR:HD2	2.29	0.45
1:C:247:LEU:CD2	1:C:268:ALA:HB1	2.47	0.45
1:D:231:GLY:O	1:D:232:LYS:C	2.54	0.45
1:A:257:LYS:HE2	1:A:261:ASN:HD21	1.75	0.45
1:B:325:MET:HG2	1:B:330:MET:CB	2.46	0.45
1:C:462:GLU:HG2	1:C:462:GLU:H	1.56	0.45
2:F:697:TYR:N	2:F:697:TYR:CD1	2.85	0.44
2:G:685:LEU:HD23	2:G:685:LEU:N	2.32	0.44
1:B:248:CYS:HA	1:B:251:GLU:CD	2.38	0.44
1:B:324:VAL:O	1:B:324:VAL:CG1	2.66	0.44
1:D:208:LYS:O	1:D:212:GLU:HG2	2.17	0.44
1:D:317:ILE:O	1:D:321:LEU:HB2	2.17	0.44
1:C:268:ALA:HA	1:C:271:ARG:NH1	2.33	0.44
1:D:235:ASN:O	1:D:235:ASN:CG	2.55	0.44
1:D:270:VAL:CG1	1:D:270:VAL:O	2.65	0.44
1:D:455:ALA:O	1:D:456:LEU:HD13	2.17	0.44
1:B:304:ASP:OD1	1:B:391:LEU:HA	2.16	0.44
1:C:382:ILE:HG13	1:C:383:ILE:N	2.33	0.44
1:B:248:CYS:C	1:B:251:GLU:OE1	2.55	0.44
1:B:427:LEU:HD23	1:B:430:MET:HE2	1.98	0.44
1:C:325:MET:HG2	1:C:330:MET:CB	2.48	0.44
1:A:269:GLU:HB2	1:A:351:PHE:CD2	2.53	0.44
1:B:418:ASP:HB2	4:B:849:HOH:O	2.17	0.44
1:D:353:ASP:O	1:D:357:PRO:CD	2.65	0.44
2:E:691:LYS:HB3	2:E:691:LYS:HE2	1.74	0.44
1:A:396:HIS:HB3	1:A:399:LYS:HZ3	1.77	0.44
1:C:284:VAL:HG12	1:C:284:VAL:O	2.18	0.44
1:C:363:MET:HE2	4:C:779:HOH:O	2.17	0.44
1:C:408:LEU:HD23	1:C:423:PHE:HE1	1.82	0.44
1:C:438:THR:HG22	1:C:439:GLU:HG3	2.00	0.44
1:D:455:ALA:C	1:D:456:LEU:HD13	2.38	0.44
1:C:460:LEU:HB3	1:C:464:TYR:CG	2.53	0.44
1:C:343:PHE:CG	1:C:343:PHE:O	2.71	0.44
1:D:345:LYS:C	1:D:352:CYS:HB3	2.39	0.44
1:D:354:ILE:O	1:D:357:PRO:HD2	2.17	0.44
1:B:208:LYS:HG3	1:B:208:LYS:O	2.18	0.43
1:C:426:LEU:O	1:C:429:LYS:N	2.51	0.43
1:D:223:VAL:HG23	1:D:372:ASP:OD2	2.18	0.43
1:B:309:LEU:CB	2:F:689:ILE:HD12	2.48	0.43
1:A:257:LYS:CG	1:A:261:ASN:ND2	2.81	0.43
1:A:419:ASP:CB	1:A:422:LEU:HB2	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ALA:O	1:A:445:GLN:HG3	2.18	0.43
1:B:411:HIS:O	1:B:415:ASN:HB2	2.17	0.43
1:D:307:THR:HG21	1:D:391:LEU:CD2	2.48	0.43
1:D:392:LEU:HD13	1:D:393:ASN:ND2	2.33	0.43
1:B:462:GLU:C	1:B:464:TYR:N	2.72	0.43
1:C:247:LEU:HD22	1:C:272:ILE:HD11	1.99	0.43
1:A:257:LYS:O	1:A:258:LEU:HD23	2.16	0.43
1:B:421:PHE:O	1:B:425:LYS:HG3	2.18	0.43
1:B:428:GLN:HB2	4:B:785:HOH:O	2.17	0.43
1:C:211:TYR:O	1:C:214:TYR:HB3	2.18	0.43
1:C:268:ALA:C	1:C:270:VAL:H	2.21	0.43
1:C:291:ALA:C	1:C:293:ALA:N	2.71	0.43
1:C:301:ASP:O	1:C:303:ASN:N	2.52	0.43
1:C:465:ARG:O	1:C:467:MET:N	2.51	0.43
1:D:224:LYS:O	1:D:228:ILE:HG13	2.18	0.43
1:D:254:LEU:CD2	3:D:778:471:HC3M	2.48	0.43
1:D:399:LYS:HB2	1:D:399:LYS:HE3	1.70	0.43
1:B:459:LEU:CD1	1:B:463:ILE:HD11	2.46	0.43
1:C:230:SER:C	1:C:232:LYS:N	2.69	0.43
1:C:252:LYS:HZ2	1:C:259:VAL:HG23	1.84	0.43
1:D:445:GLN:C	1:D:446:ILE:HG13	2.38	0.43
1:A:460:LEU:HD22	2:E:688:ILE:HD11	2.00	0.43
1:B:238:PRO:HA	1:B:336:ASN:O	2.19	0.43
1:C:264:GLN:O	1:C:265:ASN:HB2	2.18	0.43
2:F:690:ARG:HG2	4:F:270:HOH:O	2.18	0.43
1:D:345:LYS:HA	1:D:352:CYS:CA	2.47	0.43
1:D:393:ASN:HB3	1:D:396:HIS:CD2	2.54	0.43
1:A:258:LEU:HD13	1:A:263:ILE:HB	2.00	0.43
1:B:237:PRO:CB	1:B:238:PRO:HD2	2.49	0.43
1:B:288:THR:HG21	2:F:692:ALA:HB3	2.00	0.43
1:B:214:TYR:CD1	1:B:214:TYR:C	2.92	0.42
1:C:349:LYS:HE3	1:C:349:LYS:HB3	1.52	0.42
1:D:207:ALA:HB2	1:D:407:VAL:CG1	2.49	0.42
1:D:412:LEU:HA	1:D:412:LEU:HD23	1.88	0.42
1:A:302:LEU:C	1:A:302:LEU:HD12	2.39	0.42
1:A:364:LYS:O	1:A:367:ALA:HB3	2.19	0.42
1:B:445:GLN:O	1:B:447:ILE:N	2.48	0.42
1:C:246:THR:HA	1:C:249:MET:HE2	2.01	0.42
1:C:269:GLU:CB	1:C:351:PHE:HD2	2.33	0.42
1:C:446:ILE:C	1:C:447:ILE:HG13	2.39	0.42
1:D:351:PHE:O	1:D:352:CYS:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:N	1:A:202:ASP:OD1	2.40	0.42
1:B:281:VAL:O	1:B:281:VAL:HG12	2.19	0.42
1:B:460:LEU:HB3	1:B:464:TYR:HE2	1.84	0.42
1:C:345:LYS:O	1:C:352:CYS:HB2	2.18	0.42
1:D:255:VAL:HB	1:D:258:LEU:HD11	2.00	0.42
1:D:334:TYR:HE1	4:D:812:HOH:O	1.99	0.42
1:B:243:ASP:O	1:B:245:GLU:N	2.52	0.42
1:B:301:ASP:O	1:B:304:ASP:N	2.53	0.42
1:D:353:ASP:O	1:D:357:PRO:CG	2.67	0.42
1:A:345:LYS:HA	1:A:352:CYS:HB2	2.00	0.42
1:B:445:GLN:NE2	1:B:448:LYS:HD2	2.35	0.42
1:C:353:ASP:O	1:C:443:LEU:HD21	2.20	0.42
1:A:212:GLU:OE1	2:E:700:TRP:CZ3	2.71	0.42
2:F:697:TYR:N	2:F:697:TYR:HD1	2.18	0.42
1:B:212:GLU:OE1	2:F:700:TRP:CH2	2.73	0.42
1:A:446:ILE:O	1:A:450:THR:HB	2.19	0.42
1:C:250:ALA:O	1:C:252:LYS:N	2.53	0.42
1:A:370:LEU:HB3	1:A:374:ASP:HB2	2.01	0.42
1:A:290:PHE:O	1:A:294:ILE:HG13	2.19	0.42
1:A:308:LEU:HD11	1:A:397:ILE:HD13	2.00	0.42
1:A:412:LEU:HD22	1:A:422:LEU:CD2	2.49	0.42
1:B:247:LEU:HD21	1:B:272:ILE:HG12	2.00	0.42
1:B:301:ASP:C	1:B:303:ASN:H	2.22	0.42
1:B:313:VAL:HG11	2:F:685:LEU:HD11	2.00	0.42
1:B:463:ILE:O	1:B:464:TYR:HD1	2.03	0.42
1:C:269:GLU:CB	1:C:351:PHE:CD2	3.02	0.42
1:C:393:ASN:C	1:C:395:GLY:N	2.70	0.42
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.42
1:A:279:THR:HG22	4:A:812:HOH:O	2.19	0.42
1:B:212:GLU:O	1:B:216:LYS:HB2	2.20	0.42
1:C:457:HIS:C	1:C:459:LEU:H	2.22	0.42
1:D:293:ALA:O	1:D:295:PRO:HD3	2.20	0.42
1:D:364:LYS:HE3	4:D:835:HOH:O	2.19	0.42
1:A:313:VAL:HG13	1:A:314:TYR:H	1.84	0.42
1:D:247:LEU:HD23	1:D:268:ALA:HB1	2.02	0.42
1:B:213:ALA:HB1	1:B:293:ALA:CB	2.50	0.41
1:B:249:MET:O	1:B:252:LYS:HB3	2.20	0.41
2:E:686:GLU:OE2	2:E:690:ARG:NH1	2.52	0.41
1:C:243:ASP:OD1	1:C:245:GLU:HB3	2.21	0.41
1:B:292:LYS:HZ3	2:F:696:LYS:CG	2.33	0.41
1:B:255:VAL:HG12	1:B:257:LYS:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:CG1	1:B:258:LEU:HG	2.50	0.41
1:B:292:LYS:NZ	2:F:696:LYS:HG3	2.34	0.41
1:B:314:TYR:HB3	1:B:437:VAL:CG2	2.50	0.41
1:B:340:THR:HG22	1:B:342:GLU:N	2.35	0.41
1:C:445:GLN:O	1:C:446:ILE:HG13	2.19	0.41
1:D:255:VAL:O	1:D:257:LYS:N	2.49	0.41
2:E:684:GLY:CA	2:E:685:LEU:HD23	2.51	0.41
2:E:686:GLU:HA	2:E:689:ILE:HG12	2.02	0.41
2:G:689:ILE:HG12	2:G:690:ARG:N	2.34	0.41
1:A:313:VAL:HG13	1:A:314:TYR:N	2.35	0.41
1:B:247:LEU:HD23	1:B:343:PHE:HZ	1.84	0.41
1:B:445:GLN:C	1:B:447:ILE:N	2.73	0.41
1:D:259:VAL:HG22	1:D:259:VAL:O	2.20	0.41
1:A:320:MET:C	1:A:322:SER:N	2.73	0.41
1:A:461:GLN:CG	1:A:464:TYR:CD2	2.89	0.41
1:B:339:ILE:HG23	1:B:339:ILE:O	2.20	0.41
1:C:273:PHE:O	1:C:277:GLN:CG	2.64	0.41
1:C:282:GLU:CA	1:C:282:GLU:OE1	2.69	0.41
1:C:322:SER:HB3	1:C:366:ASN:HD21	1.85	0.41
1:D:280:SER:HB3	3:D:778:471:H4D2	2.03	0.41
1:D:288:THR:O	1:D:292:LYS:HG3	2.20	0.41
1:D:300:LEU:N	1:D:300:LEU:CD1	2.82	0.41
1:A:318:PHE:CE1	1:A:358:LYS:HE2	2.55	0.41
1:B:200:THR:O	1:B:204:LYS:CD	2.41	0.41
1:B:302:LEU:HD23	1:B:302:LEU:O	2.21	0.41
1:C:204:LYS:HA	1:C:204:LYS:HD2	1.78	0.41
1:C:394:VAL:O	1:C:394:VAL:HG13	2.20	0.41
1:A:226:ARG:NH2	1:A:325:MET:O	2.53	0.41
1:C:459:LEU:O	1:C:462:GLU:O	2.39	0.41
2:E:693:LEU:HA	2:E:693:LEU:HD12	1.74	0.41
1:C:235:ASN:O	1:C:236:ASN:CB	2.69	0.41
1:D:264:GLN:H	1:D:264:GLN:HE21	1.67	0.41
1:A:393:ASN:C	1:A:395:GLY:H	2.24	0.41
1:B:443:LEU:O	1:B:443:LEU:HG	2.20	0.41
1:C:423:PHE:N	1:C:424:PRO:HD2	2.36	0.41
1:C:363:MET:CE	4:C:779:HOH:O	2.69	0.41
1:C:463:ILE:CG2	1:C:463:ILE:O	2.67	0.41
1:D:252:LYS:CA	1:D:258:LEU:HD13	2.50	0.41
1:B:263:ILE:HA	1:B:266:LYS:HE3	2.03	0.41
1:C:220:MET:HE1	1:C:228:ILE:HD12	2.02	0.41
1:D:243:ASP:OD1	1:D:246:THR:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG21	1:A:377:LEU:HD23	2.03	0.40
1:A:457:HIS:C	1:A:459:LEU:H	2.24	0.40
1:B:265:ASN:OD1	1:B:265:ASN:O	2.38	0.40
1:B:451:GLU:C	1:B:453:ASP:OD1	2.57	0.40
1:C:254:LEU:HD12	1:C:254:LEU:HA	1.87	0.40
1:D:223:VAL:CG2	1:D:372:ASP:OD2	2.70	0.40
2:E:685:LEU:O	2:E:689:ILE:HG23	2.21	0.40
2:H:689:ILE:O	2:H:689:ILE:HG13	2.20	0.40
1:A:393:ASN:N	1:A:393:ASN:HD22	2.18	0.40
1:C:396:HIS:HE1	4:C:785:HOH:O	2.04	0.40
1:A:302:LEU:CD1	2:E:693:LEU:HD23	2.51	0.40
2:F:697:TYR:O	2:F:697:TYR:CD1	2.74	0.40
1:B:212:GLU:OE1	2:F:700:TRP:CZ3	2.74	0.40
1:A:421:PHE:O	1:A:424:PRO:HD2	2.21	0.40
1:C:247:LEU:HD22	1:C:343:PHE:HZ	1.85	0.40
1:C:248:CYS:C	1:C:250:ALA:N	2.74	0.40
1:D:257:LYS:HZ2	1:D:257:LYS:HG2	1.81	0.40
1:D:252:LYS:O	1:D:258:LEU:HD12	2.22	0.40
1:D:392:LEU:HB2	4:D:810:HOH:O	2.21	0.40
1:D:448:LYS:NZ	1:D:449:LYS:HG2	2.34	0.40
2:F:693:LEU:C	2:F:694:MET:HE2	2.41	0.40
1:A:297:PHE:O	1:A:305:GLN:NE2	2.55	0.40
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.87	0.40
1:C:244:MET:HE3	1:C:268:ALA:HB3	2.03	0.40
1:C:311:TYR:CZ	1:C:389:PRO:HG2	2.56	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	267/269 (99%)	205 (77%)	46 (17%)	16 (6%)	1 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	267/269 (99%)	222 (83%)	31 (12%)	14 (5%)	2	12
1	C	267/269 (99%)	198 (74%)	50 (19%)	19 (7%)	1	5
1	D	267/269 (99%)	214 (80%)	35 (13%)	18 (7%)	1	6
2	E	17/19 (90%)	9 (53%)	6 (35%)	2 (12%)	0	1
2	F	17/19 (90%)	11 (65%)	5 (29%)	1 (6%)	1	9
2	G	17/19 (90%)	14 (82%)	2 (12%)	1 (6%)	1	9
2	H	17/19 (90%)	14 (82%)	2 (12%)	1 (6%)	1	9
All	All	1136/1152 (99%)	887 (78%)	177 (16%)	72 (6%)	1	7

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	SER
1	A	256	ALA
1	A	346	SER
1	B	448	LYS
1	B	455	ALA
1	B	456	LEU
1	B	463	ILE
1	C	232	LYS
1	C	234	SER
1	C	269	GLU
1	C	394	VAL
1	D	260	ALA
1	D	349	LYS
1	D	352	CYS
1	D	455	ALA
2	E	683	MET
2	E	698	ASP
2	H	698	ASP
1	A	229	LEU
1	A	276	CYS
1	A	352	CYS
1	A	452	SER
1	A	462	GLU
1	A	465	ARG
1	A	466	ASP
1	B	234	SER
1	B	250	ALA
1	B	260	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	302	LEU
1	B	446	ILE
1	C	231	GLY
1	C	257	LYS
1	C	300	LEU
1	C	343	PHE
1	C	447	ILE
1	D	231	GLY
1	D	295	PRO
1	D	394	VAL
1	D	446	ILE
1	D	462	GLU
1	D	463	ILE
2	F	695	GLY
1	A	201	ALA
1	A	265	ASN
1	A	300	LEU
1	A	394	VAL
1	B	232	LYS
1	B	244	MET
1	C	265	ASN
1	D	257	LYS
1	D	267	GLU
1	D	269	GLU
1	D	445	GLN
2	G	698	ASP
1	A	260	ALA
1	B	279	THR
1	C	446	ILE
1	C	466	ASP
1	D	223	VAL
1	D	268	ALA
1	D	279	THR
1	B	264	GLN
1	C	250	ALA
1	C	251	GLU
1	C	254	LEU
1	C	463	ILE
1	D	229	LEU
1	C	302	LEU
1	B	295	PRO
1	C	281	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	VAL
1	C	458	PRO

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	234/235 (100%)	190 (81%)	44 (19%)	1	8
1	B	234/235 (100%)	193 (82%)	41 (18%)	2	10
1	C	234/235 (100%)	202 (86%)	32 (14%)	3	17
1	D	234/235 (100%)	189 (81%)	45 (19%)	1	8
2	E	12/15 (80%)	4 (33%)	8 (67%)	0	0
2	F	13/15 (87%)	7 (54%)	6 (46%)	0	0
2	G	12/15 (80%)	8 (67%)	4 (33%)	0	1
2	H	12/15 (80%)	7 (58%)	5 (42%)	0	0
All	All	985/1000 (98%)	800 (81%)	185 (19%)	1	8

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	A	204	LYS
1	A	223	VAL
1	A	230	SER
1	A	232	LYS
1	A	235	ASN
1	A	251	GLU
1	A	253	THR
1	A	258	LEU
1	A	259	VAL
1	A	263	ILE
1	A	264	GLN
1	A	265	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	269	GLU
1	A	271	ARG
1	A	273	PHE
1	A	280	SER
1	A	283	THR
1	A	301	ASP
1	A	302	LEU
1	A	304	ASP
1	A	321	LEU
1	A	334	TYR
1	A	353	ASP
1	A	355	MET
1	A	361	PHE
1	A	363	MET
1	A	371	ASP
1	A	373	SER
1	A	382	ILE
1	A	387	ASP
1	A	392	LEU
1	A	396	HIS
1	A	410	LEU
1	A	420	ILE
1	A	428	GLN
1	A	435	GLN
1	A	444	VAL
1	A	453	ASP
1	A	456	LEU
1	A	459	LEU
1	A	460	LEU
1	A	461	GLN
1	A	463	ILE
1	B	206	LEU
1	B	215	LEU
1	B	216	LYS
1	B	220	MET
1	B	232	LYS
1	B	244	MET
1	B	247	LEU
1	B	248	CYS
1	B	251	GLU
1	B	266	LYS
1	B	269	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	282	GLU
1	B	286	GLU
1	B	295	PRO
1	B	303	ASN
1	B	322	SER
1	B	324	VAL
1	B	334	TYR
1	B	350	PRO
1	B	353	ASP
1	B	358	LYS
1	B	363	MET
1	B	377	LEU
1	B	392	LEU
1	B	394	VAL
1	B	407	VAL
1	B	408	LEU
1	B	420	ILE
1	B	422	LEU
1	B	435	GLN
1	B	436	LEU
1	B	437	VAL
1	B	442	GLN
1	B	444	VAL
1	B	445	GLN
1	B	446	ILE
1	B	450	THR
1	B	453	ASP
1	B	456	LEU
1	B	459	LEU
1	B	460	LEU
1	C	208	LYS
1	C	209	ARG
1	C	220	MET
1	C	230	SER
1	C	232	LYS
1	C	236	ASN
1	C	244	MET
1	C	251	GLU
1	C	254	LEU
1	C	259	VAL
1	C	264	GLN
1	C	267	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	280	SER
1	C	282	GLU
1	C	303	ASN
1	C	310	LYS
1	C	345	LYS
1	C	363	MET
1	C	382	ILE
1	C	396	HIS
1	C	412	LEU
1	C	415	ASN
1	C	420	ILE
1	C	438	THR
1	C	452	SER
1	C	456	LEU
1	C	459	LEU
1	C	460	LEU
1	C	461	GLN
1	C	462	GLU
1	C	463	ILE
1	C	465	ARG
1	D	202	ASP
1	D	208	LYS
1	D	209	ARG
1	D	223	VAL
1	D	230	SER
1	D	235	ASN
1	D	251	GLU
1	D	253	THR
1	D	254	LEU
1	D	258	LEU
1	D	263	ILE
1	D	264	GLN
1	D	267	GLU
1	D	269	GLU
1	D	271	ARG
1	D	276	CYS
1	D	282	GLU
1	D	300	LEU
1	D	301	ASP
1	D	303	ASN
1	D	313	VAL
1	D	327	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	346	SER
1	D	350	PRO
1	D	352	CYS
1	D	363	MET
1	D	382	ILE
1	D	391	LEU
1	D	392	LEU
1	D	394	VAL
1	D	399	LYS
1	D	405	VAL
1	D	409	ARG
1	D	414	SER
1	D	420	ILE
1	D	430	MET
1	D	442	GLN
1	D	443	LEU
1	D	445	GLN
1	D	453	ASP
1	D	456	LEU
1	D	459	LEU
1	D	461	GLN
1	D	465	ARG
1	D	468	TYR
2	E	683	MET
2	E	685	LEU
2	E	688	ILE
2	E	689	ILE
2	E	693	LEU
2	E	694	MET
2	E	697	TYR
2	E	700	TRP
2	F	685	LEU
2	F	689	ILE
2	F	693	LEU
2	F	694	MET
2	F	696	LYS
2	F	697	TYR
2	G	688	ILE
2	G	689	ILE
2	G	693	LEU
2	G	700	TRP
2	H	686	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	689	ILE
2	H	690	ARG
2	H	693	LEU
2	H	698	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	261	ASN
1	A	264	GLN
1	A	277	GLN
1	A	299	ASN
1	A	305	GLN
1	A	366	ASN
1	A	411	HIS
1	A	413	GLN
1	A	415	ASN
1	A	416	HIS
1	A	442	GLN
1	B	217	ASN
1	B	264	GLN
1	B	277	GLN
1	B	336	ASN
1	B	406	HIS
1	B	411	HIS
1	B	416	HIS
1	B	445	GLN
1	C	236	ASN
1	C	242	HIS
1	C	264	GLN
1	C	299	ASN
1	C	336	ASN
1	C	366	ASN
1	C	393	ASN
1	C	435	GLN
1	C	440	HIS
1	C	445	GLN
1	C	461	GLN
1	D	235	ASN
1	D	242	HIS
1	D	261	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	264	GLN
1	D	299	ASN
1	D	303	ASN
1	D	393	ASN
1	D	401	GLN
1	D	445	GLN
1	D	457	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	471	B	776	-	44,48,48	1.98	17 (38%)	55,66,66	1.69	8 (14%)
3	471	A	775	-	44,48,48	1.95	18 (40%)	55,66,66	1.29	6 (10%)
3	471	D	778	-	44,48,48	1.95	18 (40%)	55,66,66	1.52	6 (10%)
3	471	C	777	-	44,48,48	1.99	17 (38%)	55,66,66	1.40	6 (10%)

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	471	B	776	-	-	9/36/39/39	0/4/4/4
3	471	A	775	-	-	9/36/39/39	0/4/4/4
3	471	D	778	-	-	5/36/39/39	0/4/4/4
3	471	C	777	-	-	9/36/39/39	0/4/4/4

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	777	471	C1H-C1G	-6.22	1.40	1.49
3	B	776	471	C1H-C1G	-6.10	1.40	1.49
3	A	775	471	C1H-C1G	-5.81	1.40	1.49
3	D	778	471	C1H-C1G	-5.81	1.40	1.49
3	B	776	471	C1A-N	4.53	1.39	1.33
3	C	777	471	C1A-N	4.53	1.39	1.33
3	A	775	471	C1A-N	4.49	1.39	1.33
3	D	778	471	C1A-N	4.46	1.39	1.33
3	B	776	471	C1L-C1K	-2.93	1.34	1.39
3	A	775	471	C1L-C1K	-2.93	1.34	1.39
3	D	778	471	C1J-C1K	-2.90	1.34	1.39
3	C	777	471	C1J-C1K	-2.90	1.34	1.39
3	C	777	471	C1L-C1K	-2.88	1.34	1.39
3	B	776	471	C1J-C1K	-2.88	1.34	1.39
3	D	778	471	C1L-C1K	-2.88	1.34	1.39
3	A	775	471	C1J-C1K	-2.87	1.34	1.39
3	A	775	471	C1M-C1H	-2.79	1.34	1.39
3	C	777	471	C1M-C1H	-2.78	1.34	1.39
3	D	778	471	C1M-C1H	-2.77	1.34	1.39
3	A	775	471	C1I-C1H	-2.76	1.34	1.39
3	B	776	471	C1M-C1H	-2.73	1.34	1.39
3	C	777	471	C1I-C1H	-2.71	1.34	1.39
3	B	776	471	C1I-C1H	-2.71	1.34	1.39
3	D	778	471	C1I-C1H	-2.68	1.34	1.39
3	C	777	471	C1F-C1A	-2.41	1.33	1.38
3	B	776	471	C1F-C1A	-2.38	1.33	1.38
3	A	775	471	C1F-C1A	-2.38	1.33	1.38
3	D	778	471	C1F-C1A	-2.38	1.33	1.38
3	B	776	471	CE1-CD1	-2.35	1.34	1.38
3	C	777	471	C1J-C1I	-2.33	1.34	1.38
3	A	775	471	CE2-CD2	-2.31	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	778	471	C1J-C1I	-2.31	1.34	1.38
3	A	775	471	C1J-C1I	-2.30	1.34	1.38
3	A	775	471	CE1-CD1	-2.30	1.34	1.38
3	D	778	471	C1M-C1L	-2.29	1.34	1.38
3	C	777	471	C1M-C1L	-2.29	1.34	1.38
3	C	777	471	CE2-CD2	-2.29	1.34	1.38
3	C	777	471	CE1-CD1	-2.28	1.34	1.38
3	D	778	471	CE1-CD1	-2.28	1.34	1.38
3	B	776	471	C1M-C1L	-2.28	1.34	1.38
3	B	776	471	CE2-CD2	-2.28	1.34	1.38
3	B	776	471	C1J-C1I	-2.27	1.34	1.38
3	A	775	471	C1M-C1L	-2.26	1.34	1.38
3	D	778	471	CE2-CD2	-2.26	1.34	1.38
3	B	776	471	C3N-C3I	-2.23	1.34	1.39
3	B	776	471	C1F-C1G	2.22	1.50	1.43
3	D	778	471	C3N-C3I	-2.22	1.34	1.39
3	D	778	471	C1F-C1G	2.21	1.50	1.43
3	C	777	471	C3J-C3I	-2.21	1.34	1.39
3	C	777	471	C1F-C1G	2.20	1.50	1.43
3	C	777	471	C3E-C3D	2.20	1.51	1.48
3	B	776	471	C3J-C3I	-2.20	1.34	1.39
3	A	775	471	C1F-C1G	2.20	1.50	1.43
3	D	778	471	C3J-C3I	-2.19	1.34	1.39
3	A	775	471	C3J-C3I	-2.19	1.34	1.39
3	A	775	471	C3N-C3I	-2.18	1.34	1.39
3	C	777	471	C3N-C3I	-2.18	1.34	1.39
3	D	778	471	C3E-C3D	2.17	1.51	1.48
3	B	776	471	C3E-C3D	2.15	1.51	1.48
3	A	775	471	C3E-C3D	2.12	1.51	1.48
3	B	776	471	C3K-C3J	-2.09	1.34	1.38
3	A	775	471	C3K-C3J	-2.09	1.34	1.38
3	D	778	471	C3M-C3N	-2.07	1.34	1.38
3	D	778	471	C3K-C3J	-2.06	1.34	1.38
3	B	776	471	C3M-C3N	-2.06	1.34	1.38
3	C	777	471	C3M-C3N	-2.05	1.34	1.38
3	C	777	471	C3K-C3J	-2.04	1.34	1.38
3	D	778	471	CE2-CZ	-2.03	1.34	1.38
3	A	775	471	CE1-CZ	-2.02	1.34	1.38
3	A	775	471	C3M-C3N	-2.02	1.34	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	778	471	C4A-CA-N	5.82	121.89	109.05
3	B	776	471	C1B-C1A-N	5.79	125.31	118.82
3	B	776	471	C4A-CA-N	5.78	121.82	109.05
3	B	776	471	C1F-C1A-N	-4.97	117.31	121.29
3	D	778	471	C1B-C1A-N	4.89	124.30	118.82
3	C	777	471	C1B-C1A-N	4.64	124.01	118.82
3	A	775	471	C1B-C1A-N	4.49	123.84	118.82
3	D	778	471	C1A-C1F-C1G	3.94	133.35	124.22
3	C	777	471	C3I-C3G-N3H	3.43	128.17	123.56
3	A	775	471	C3I-C3G-N3H	3.30	127.99	123.56
3	C	777	471	C4A-CA-N	3.12	115.94	109.05
3	C	777	471	C4A-CA-CB	3.05	119.54	110.40
3	B	776	471	C1H-C1G-C1F	2.90	126.02	119.80
3	D	778	471	C3I-C3G-N3H	2.86	127.40	123.56
3	B	776	471	C3I-C3G-N3H	2.77	127.28	123.56
3	B	776	471	C4A-CA-CB	2.70	118.50	110.40
3	C	777	471	C1A-C1F-C1G	2.68	130.43	124.22
3	A	775	471	CG-CB-CA	2.67	119.84	113.78
3	A	775	471	C1A-C1F-C1G	2.65	130.36	124.22
3	D	778	471	C4A-CA-CB	2.62	118.23	110.40
3	B	776	471	O1G-C1G-C1H	-2.42	115.30	119.19
3	A	775	471	C1F-C1A-N	-2.34	119.42	121.29
3	A	775	471	C1H-C1G-C1F	2.29	124.71	119.80
3	B	776	471	C1A-C1F-C1G	2.18	129.28	124.22
3	D	778	471	C1B-C1A-C1F	-2.17	115.55	120.11
3	C	777	471	C3N-C3I-C3G	2.01	123.51	120.44

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	776	471	C4A-CA-N-C1A
3	B	776	471	N4B-C4A-CA-N
3	A	775	471	N4B-C4A-CA-CB
3	D	778	471	C4A-CA-N-C1A
3	D	778	471	N4B-C4A-CA-N
3	C	777	471	N4B-C4A-CA-N
3	C	777	471	C1F-C1G-C1H-C1I
3	C	777	471	O1G-C1G-C1H-C1I
3	C	777	471	OH-C3A-C3B-C3C
3	C	777	471	O1G-C1G-C1H-C1M
3	C	777	471	C1F-C1G-C1H-C1M
3	B	776	471	O1G-C1G-C1H-C1M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	775	471	N4B-C4A-CA-N
3	B	776	471	C1F-C1G-C1H-C1M
3	B	776	471	O1G-C1G-C1H-C1I
3	B	776	471	C1F-C1G-C1H-C1I
3	C	777	471	CE1-CZ-OH-C3A
3	A	775	471	CE1-CZ-OH-C3A
3	A	775	471	CE2-CZ-OH-C3A
3	B	776	471	CE1-CZ-OH-C3A
3	D	778	471	CE1-CZ-OH-C3A
3	C	777	471	CE2-CZ-OH-C3A
3	B	776	471	CE2-CZ-OH-C3A
3	D	778	471	CE2-CZ-OH-C3A
3	B	776	471	N4B-C4A-CA-CB
3	D	778	471	N4B-C4A-CA-CB
3	C	777	471	N4B-C4A-CA-CB
3	A	775	471	N-CA-CB-CG
3	A	775	471	O1G-C1G-C1H-C1M
3	A	775	471	O1G-C1G-C1H-C1I
3	A	775	471	C1F-C1G-C1H-C1M
3	A	775	471	C1F-C1G-C1H-C1I

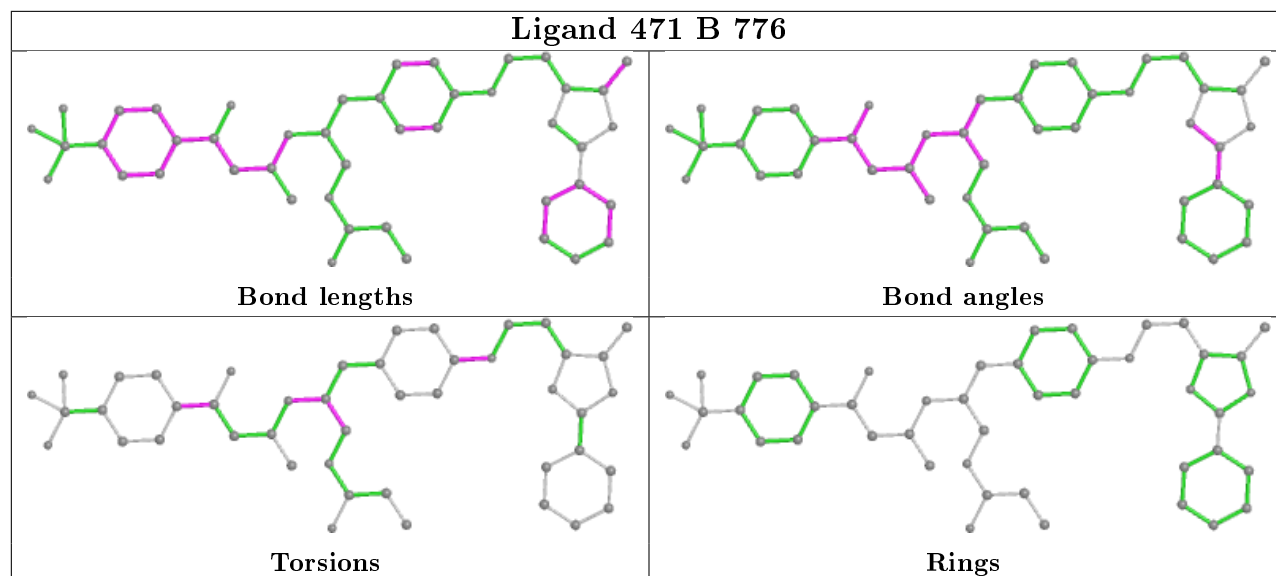
There are no ring outliers.

4 monomers are involved in 14 short contacts:

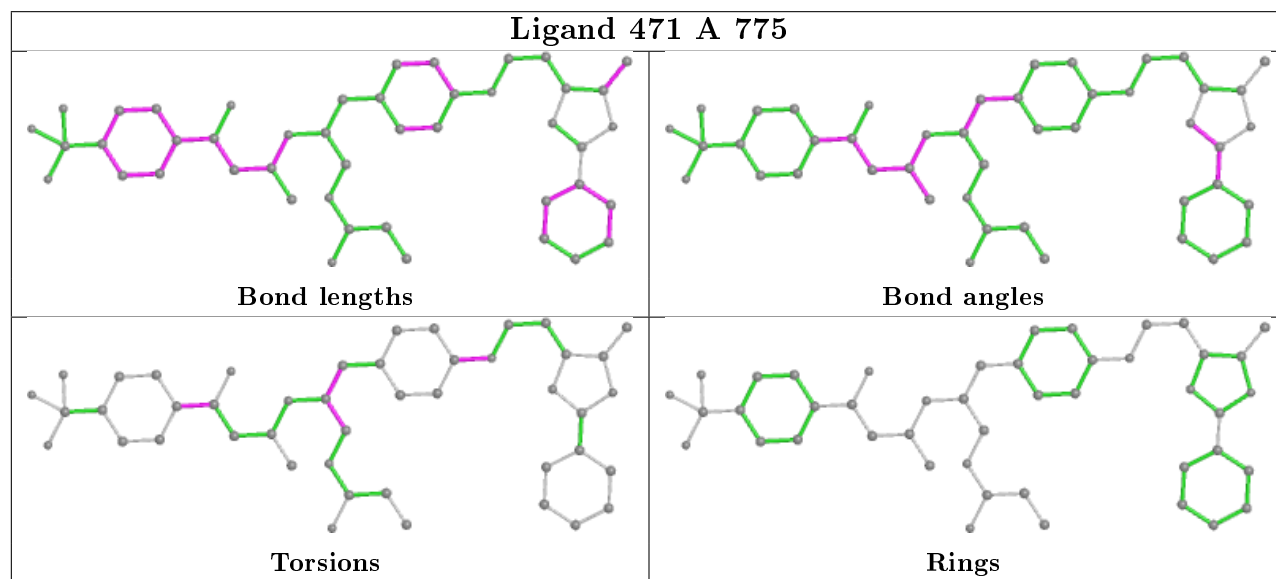
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	776	471	8	0
3	A	775	471	1	0
3	D	778	471	3	0
3	C	777	471	2	0

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.

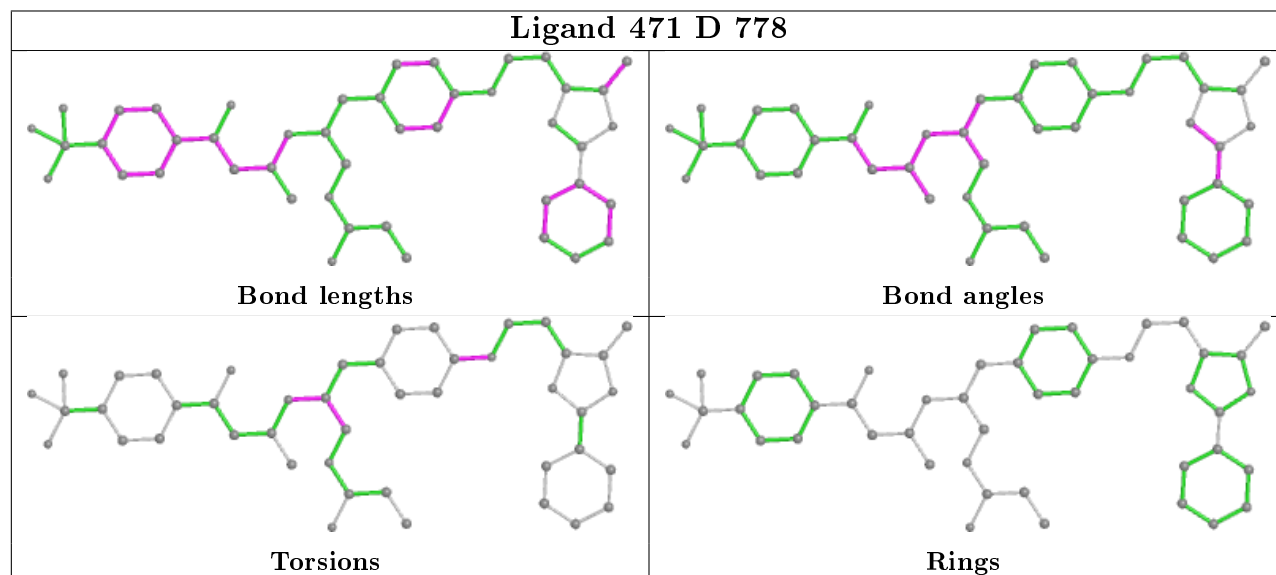
Ligand 471 B 776

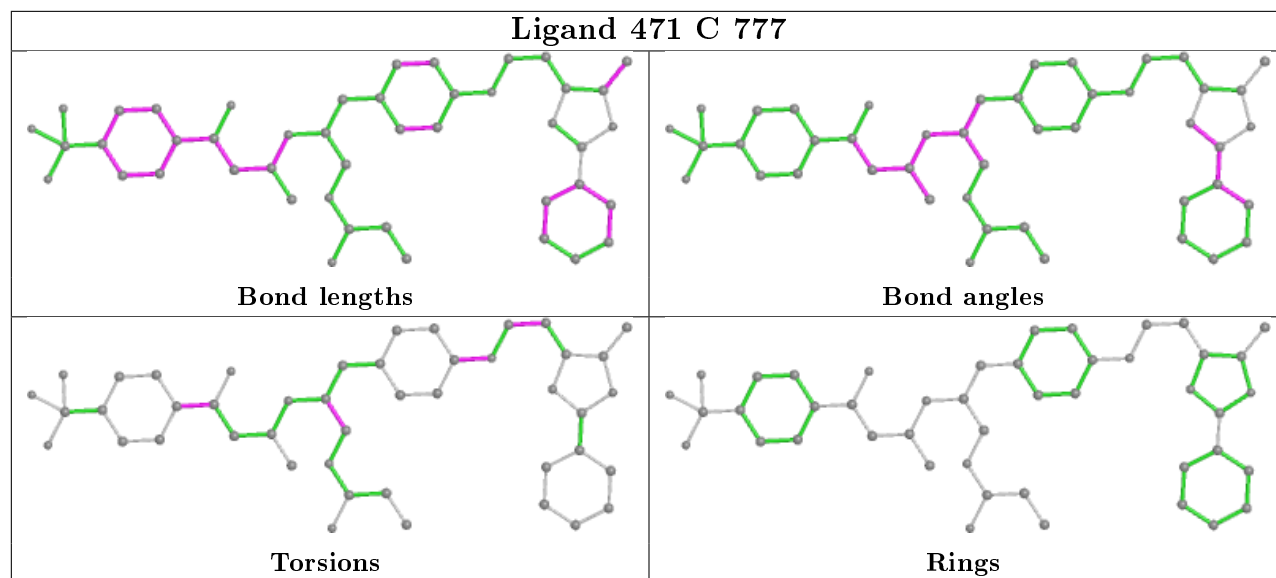


Ligand 471 A 775



Ligand 471 D 778





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.