



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:37 PM UTC

PDB ID : 2QKY / pdb_00002qky
Title : complex structure of dipeptidyl peptidase IV and a oxadiazolyl ketone
Authors : Kim, K.-H.; Hong, S.Y.; Koo, K.D.; Lee, C.-S.; Kim, G.T.; Han, H.O.
Deposited on : 2007-07-12
Resolution : 3.10 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 types of validation reports are described at

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

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

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

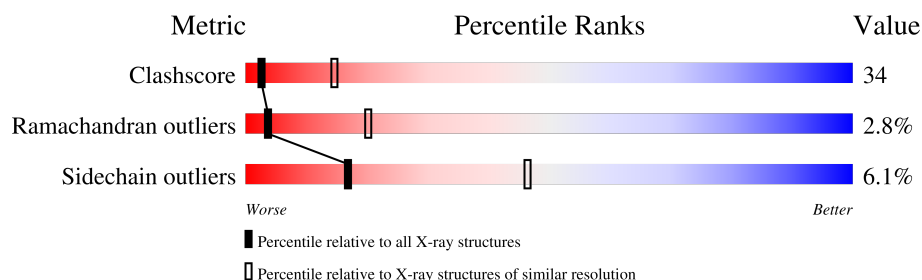
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 of 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	728	42% 49% 9%
1	B	728	42% 50% 7%
1	C	728	42% 50% 7%
1	D	728	43% 49% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24275 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.

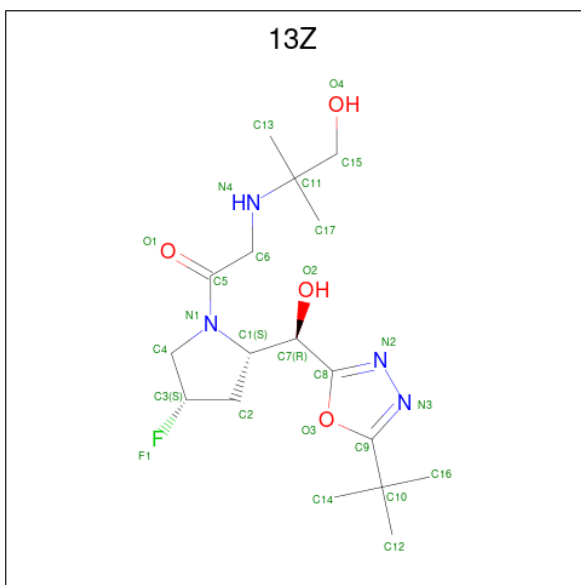
- Molecule 1 is a protein called Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	C	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	D	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	-	expression tag	UNP P27487
B	39	THR	-	expression tag	UNP P27487
C	39	THR	-	expression tag	UNP P27487
D	39	THR	-	expression tag	UNP P27487

- Molecule 2 is 2-[(2-{(2S,4S)-2-[(R)-(5-tert-butyl-1,3,4-oxadiazol-2-yl)(hydroxy)methyl]-4-fluoropyrrolidin-1-yl}-2-oxoethyl)amino]-2-methylpropan-1-ol (CCD ID: 13Z) (formula: C₁₇H₂₉FN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	B	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	C	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	D	1	Total 26	C 17	F 1	N 4	O 4	0	0

- Molecule 3 is water.

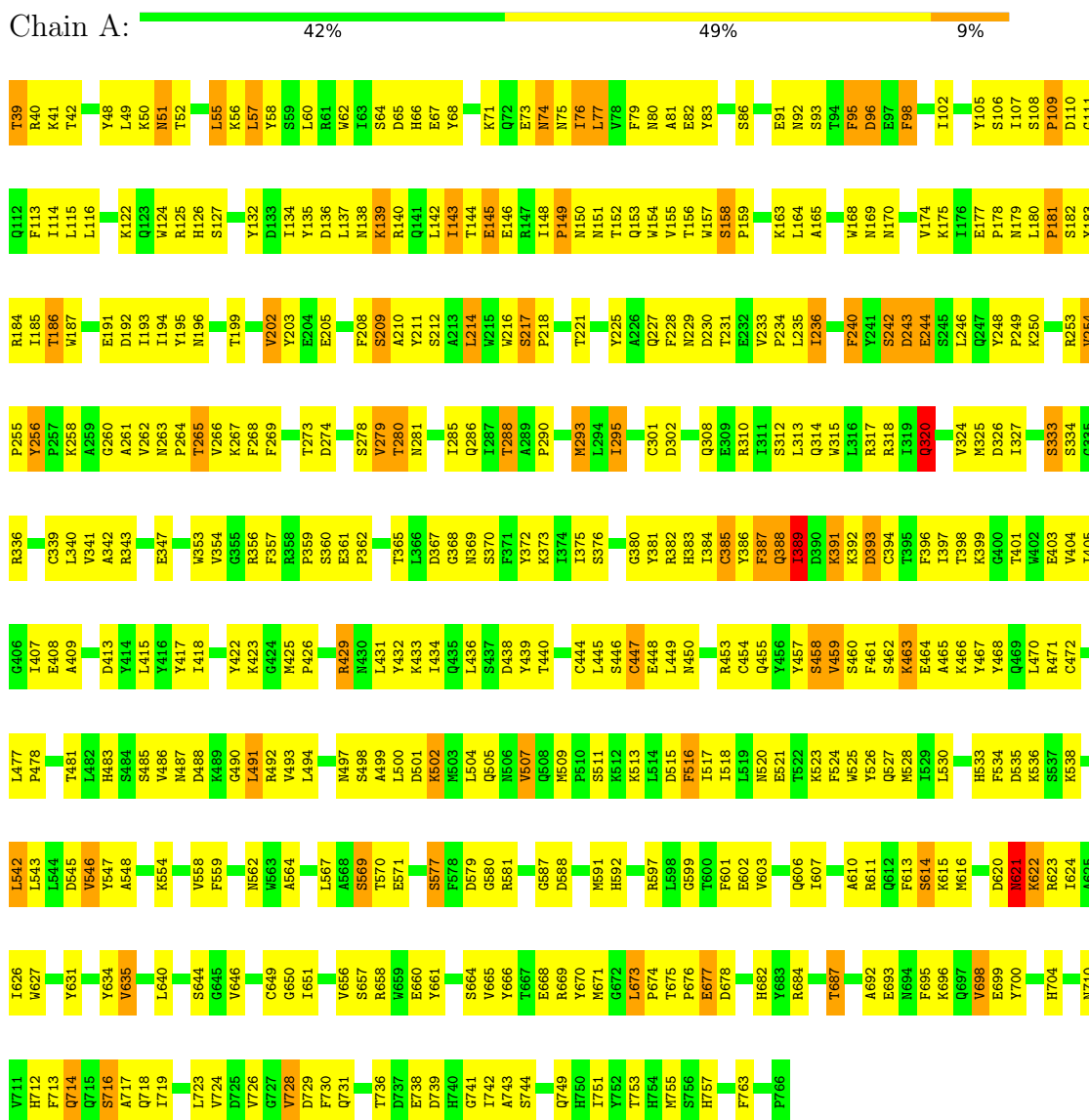
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	72	Total	O	0	0
			72	72		
3	C	66	Total	O	0	0
			66	66		
3	D	92	Total	O	0	0
			92	92		

3 Residue-property plots

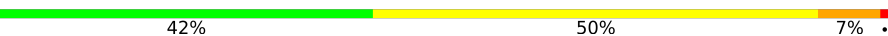
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

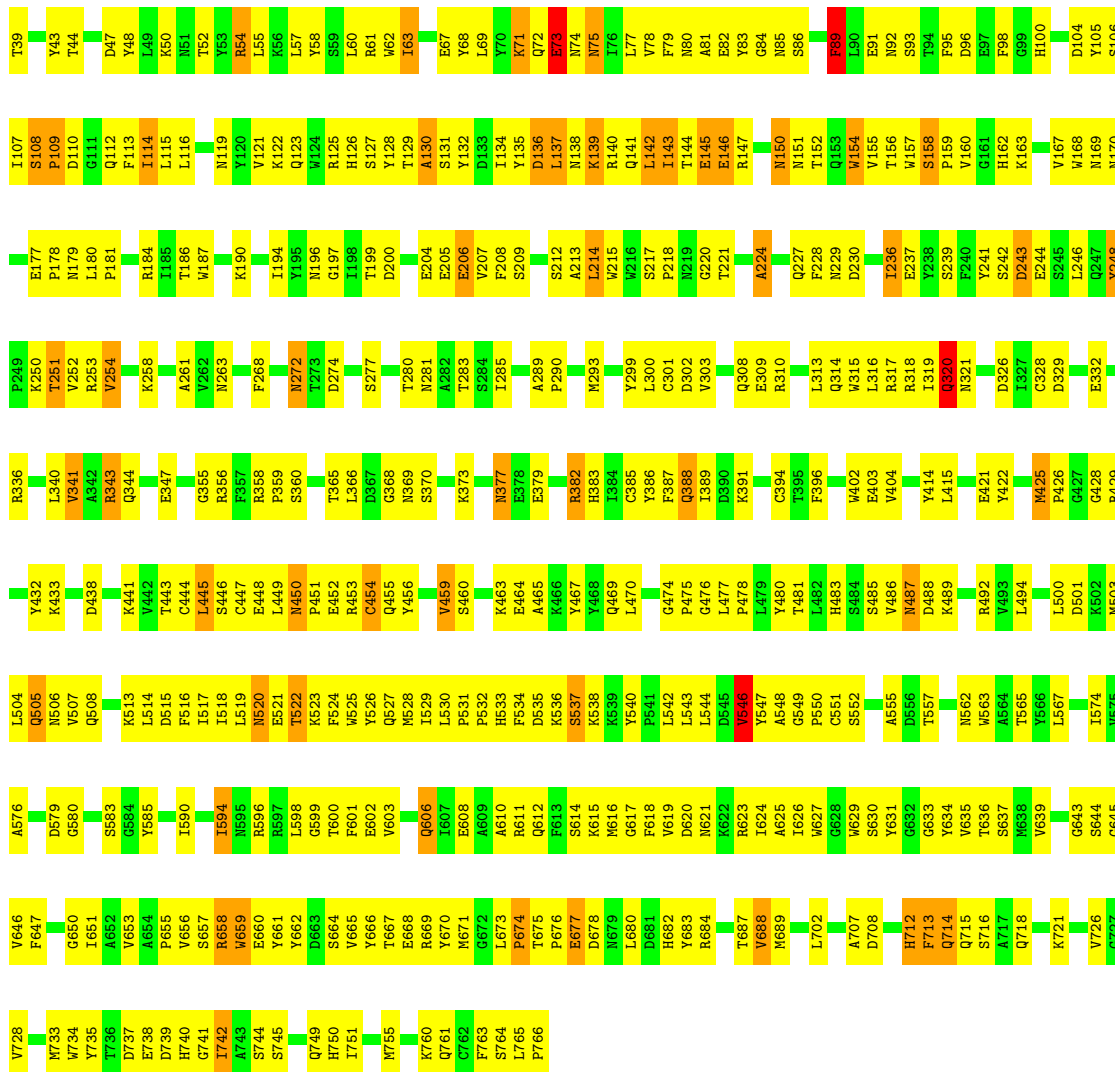
Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

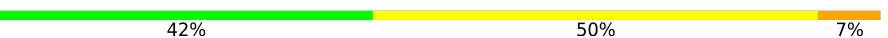


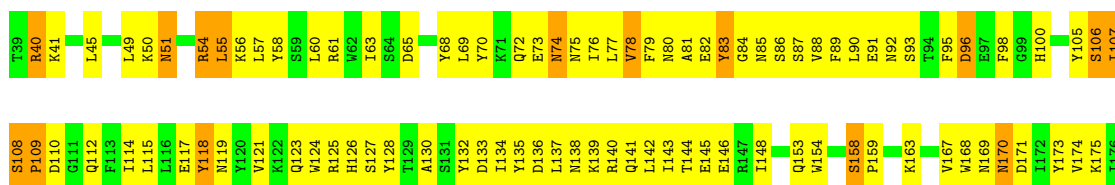
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

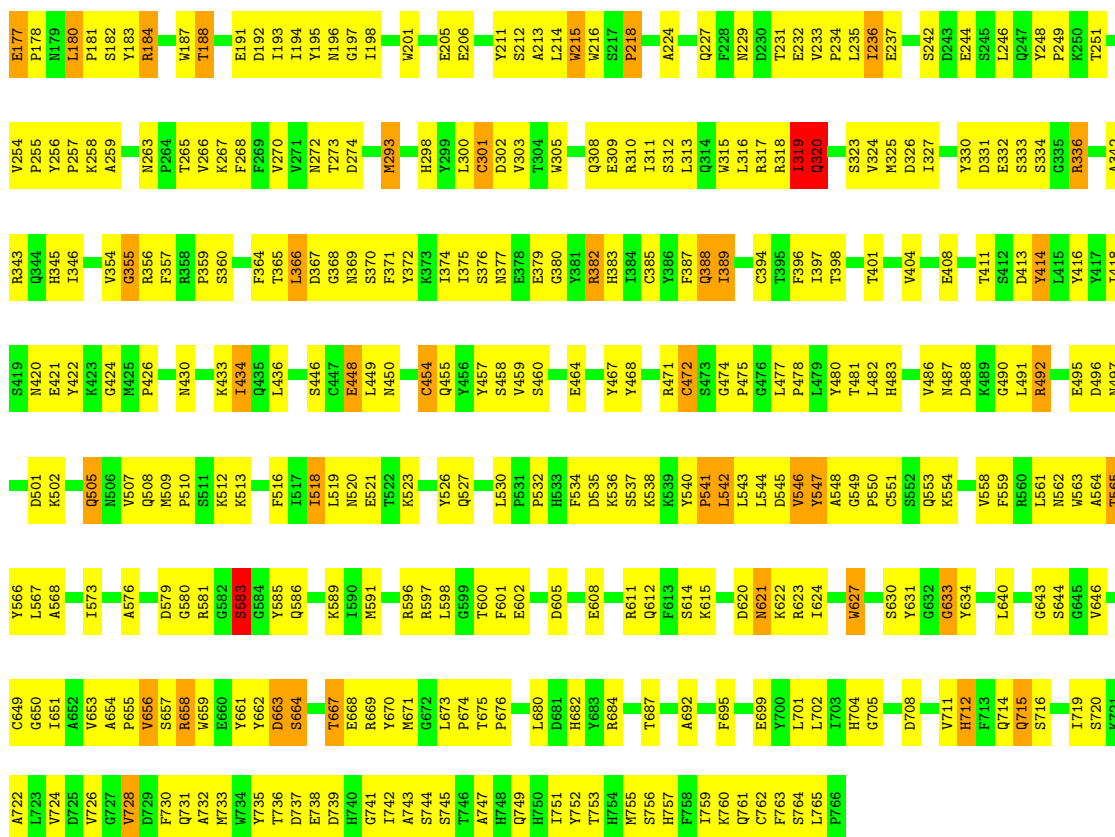
Chain B: 



- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

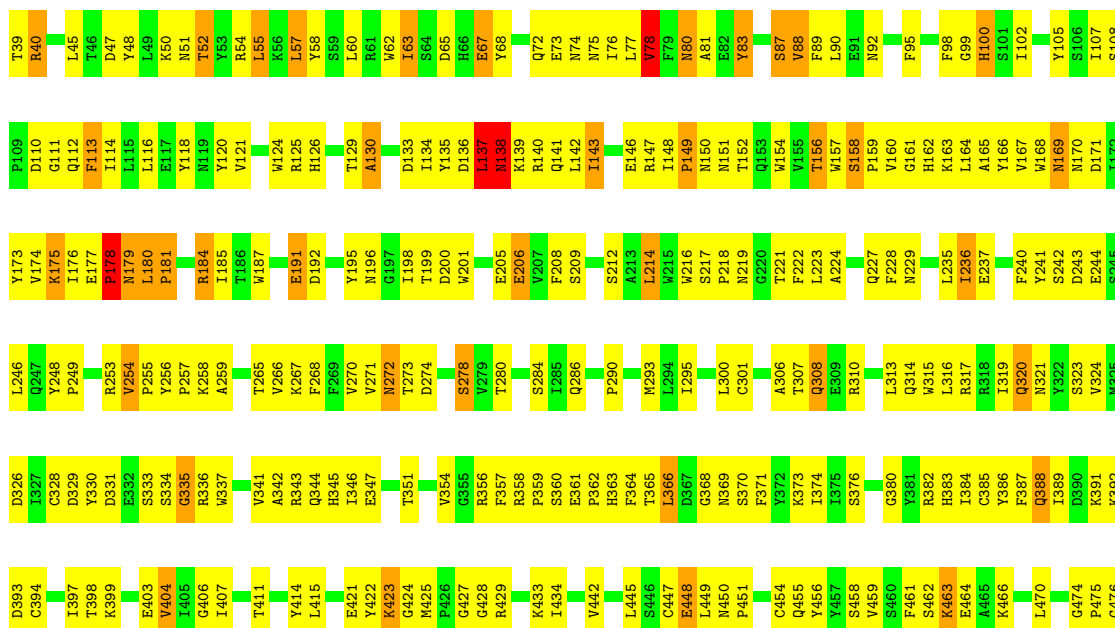
Chain C: 





- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

Chain D: 43% 49% 8% .



M733	S642	W563	T481
W734	G643	L567	L482
D737	F647	E571	H483
D739	C649	N572	S484
H740	G650	I573	S485
G741			H486
I742	V653	S577	M487
A743	A654		L491
S744	P655	R581	R492
S745	V656	Y585	V493
Q749	S657	Q586	L494
H750	R658		
I751	M659	K589	D501
Y752	E660	T590	L504
	Y661	M591	Q605
M755	D663		N506
I759	S664	T594	V507
K760	V665	N595	Q608
Q761	V666	R596	M509
Q762	T667	R597	P510
F763	E668	L598	S511
S764	R669		K512
L765	E677	F601	K513
P766	D678	E602	L514
	N679		D515
	L680	D605	F516
	D681	Q606	I517
	H682	I607	
	Y683	R611	N520
	R684	O612	E521
	N685	F613	T522
		S614	K523
	M689	K615	
	V698	M616	Y526
	E699	G617	Q527
			L530
	T703	D620	P531
	H704	M621	P532
		R622	H533
		K623	
	D708	L624	P541
	D709	A625	
	N710	T626	L544
	H711	M627	D545
	V712	G628	V546
	F713	M629	Y547
	Q714	S630	A548
	Q715	Y631	G549
		G632	P550
	I719	G633	C551
	S720	F634	S552
	K721	V635	
		T636	T557
	V724		
	A725	L640	L561
		M641	N562

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.18Å 106.11Å 132.05Å 76.30° 78.62° 80.11°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	86.7 (20.00-3.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24275	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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:
13Z

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	0.67	0/6137	1.09	35/8346 (0.4%)
1	B	0.67	0/6137	1.11	47/8346 (0.6%)
1	C	0.66	2/6137 (0.0%)	1.06	29/8346 (0.3%)
1	D	0.69	0/6137	1.10	47/8346 (0.6%)
All	All	0.67	2/24548 (0.0%)	1.09	158/33384 (0.5%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	319	ILE	CA-CB	6.30	1.60	1.53
1	C	107	ILE	CA-CB	5.41	1.59	1.54

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	335	GLY	N-CA-C	-8.79	103.04	115.43
1	B	415	LEU	N-CA-C	-8.61	95.89	109.50
1	A	546	VAL	N-CA-C	8.57	120.83	108.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	CYS	N-CA-C	8.42	122.14	108.34
1	D	546	VAL	N-CA-C	8.36	119.73	108.27
1	B	454	CYS	N-CA-C	8.19	122.36	108.02
1	D	357	PHE	N-CA-C	-8.01	105.49	114.62
1	C	298	HIS	N-CA-C	7.91	118.42	108.45
1	A	569	SER	N-CA-C	7.90	119.89	111.28
1	B	158	SER	N-CA-C	-7.81	99.30	110.08
1	B	450	ASN	CA-C-N	7.78	127.41	119.56
1	B	450	ASN	C-N-CA	7.78	127.41	119.56
1	C	388	GLN	N-CA-C	-7.75	96.60	109.24
1	C	40	ARG	N-CA-C	7.71	120.54	110.43
1	C	633	GLY	N-CA-C	-7.57	103.72	112.50
1	D	530	LEU	CA-C-N	7.50	125.06	119.66
1	D	530	LEU	C-N-CA	7.50	125.06	119.66
1	C	206	GLU	N-CA-C	7.30	122.19	113.28
1	B	71	LYS	N-CA-C	-7.25	98.78	110.32
1	B	162	HIS	N-CA-C	7.22	118.92	110.41
1	A	603	VAL	N-CA-C	-7.03	104.34	110.74
1	A	459	VAL	N-CA-C	7.02	118.82	108.65
1	B	388	GLN	N-CA-C	-6.95	97.20	108.52
1	D	206	GLU	N-CA-C	6.91	121.99	112.04
1	B	713	PHE	N-CA-C	-6.90	103.84	111.36
1	A	392	LYS	N-CA-C	6.89	119.64	111.71
1	D	458	SER	N-CA-C	-6.89	98.84	109.24
1	C	450	ASN	CA-C-N	6.86	128.41	119.84
1	C	450	ASN	C-N-CA	6.86	128.41	119.84
1	A	278	SER	N-CA-C	-6.86	104.39	112.89
1	B	594	ILE	CB-CA-C	-6.84	103.36	112.46
1	B	248	TYR	CA-C-N	6.82	127.23	119.93
1	B	248	TYR	C-N-CA	6.82	127.23	119.93
1	B	179	ASN	N-CA-C	6.81	120.48	112.72
1	D	40	ARG	N-CA-C	6.81	119.52	110.53
1	A	102	ILE	N-CA-C	6.80	117.02	107.37
1	D	463	LYS	N-CA-C	6.80	118.69	111.28
1	B	610	ALA	N-CA-C	-6.79	103.81	111.14
1	B	505	GLN	N-CA-C	-6.78	103.95	111.82
1	D	388	GLN	N-CA-C	-6.67	97.64	108.52
1	C	643	GLY	N-CA-C	-6.60	105.94	114.85
1	A	158	SER	N-CA-C	-6.56	99.38	109.41
1	B	459	VAL	N-CA-C	6.51	119.69	108.95
1	D	631	TYR	N-CA-C	-6.50	104.03	112.23
1	D	660	GLU	N-CA-C	-6.50	105.32	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	LEU	N-CA-C	6.45	120.09	107.57
1	D	659	TRP	N-CA-C	6.45	120.25	112.38
1	C	673	LEU	N-CA-C	6.41	117.73	109.65
1	B	328	CYS	N-CA-C	6.41	119.35	108.90
1	B	451	PRO	N-CA-C	6.41	121.87	113.86
1	A	324	VAL	N-CA-C	6.39	117.23	107.77
1	A	687	THR	N-CA-C	6.39	119.74	110.28
1	C	320	GLN	N-CA-C	6.33	124.27	110.80
1	D	617	GLY	N-CA-C	6.31	124.07	115.30
1	B	529	ILE	N-CA-C	-6.24	98.76	107.80
1	A	217	SER	N-CA-C	-6.22	102.26	110.40
1	D	719	ILE	N-CA-C	-6.21	104.80	110.82
1	A	240	PHE	N-CA-C	-6.20	98.28	108.76
1	B	425	MET	CA-C-N	6.18	125.91	119.05
1	B	425	MET	C-N-CA	6.18	125.91	119.05
1	B	463	LYS	N-CA-C	6.18	119.66	111.75
1	D	485	SER	N-CA-C	6.17	117.81	111.14
1	B	206	GLU	N-CA-C	6.14	120.78	113.16
1	C	547	TYR	N-CA-C	-6.14	105.70	113.43
1	D	308	GLN	N-CA-C	-6.13	105.76	113.18
1	B	150	ASN	N-CA-C	-6.12	102.03	110.35
1	A	244	GLU	N-CA-C	-6.10	105.87	113.38
1	C	659	TRP	N-CA-C	6.04	120.12	112.87
1	C	546	VAL	N-CA-C	6.01	117.41	108.46
1	B	89	PHE	N-CA-C	-6.00	105.62	113.12
1	C	55	LEU	N-CA-C	-6.00	101.40	110.28
1	D	450	ASN	CA-C-N	5.96	125.58	119.56
1	D	450	ASN	C-N-CA	5.96	125.58	119.56
1	A	622	LYS	N-CA-C	-5.96	105.19	112.88
1	A	357	PHE	N-CA-C	-5.95	107.01	114.56
1	A	320	GLN	N-CA-C	5.94	123.45	110.80
1	D	591	MET	N-CA-C	5.93	117.83	111.36
1	B	130	ALA	N-CA-C	5.92	116.92	108.74
1	C	448	GLU	N-CA-C	5.89	120.63	113.38
1	B	63	ILE	N-CA-C	-5.89	107.01	112.43
1	C	158	SER	N-CA-C	-5.89	101.47	110.01
1	B	656	VAL	N-CA-C	-5.88	100.11	108.58
1	B	546	VAL	N-CA-C	5.88	118.33	108.81
1	B	643	GLY	N-CA-C	-5.87	106.64	115.32
1	B	139	LYS	N-CA-C	-5.85	106.00	113.02
1	A	98	PHE	N-CA-C	-5.84	104.83	111.14
1	D	425	MET	CA-C-N	5.84	125.53	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	425	MET	C-N-CA	5.84	125.53	119.05
1	A	698	VAL	N-CA-C	5.83	116.04	108.35
1	B	617	GLY	N-CA-C	5.81	124.12	115.64
1	D	177	GLU	CA-C-N	5.79	127.07	119.84
1	D	177	GLU	C-N-CA	5.79	127.07	119.84
1	C	505	GLN	N-CA-C	-5.78	105.49	112.54
1	D	665	VAL	N-CA-C	5.76	116.50	110.62
1	A	450	ASN	CA-C-N	5.76	125.45	119.05
1	A	450	ASN	C-N-CA	5.76	125.45	119.05
1	B	485	SER	N-CA-C	5.73	117.61	111.36
1	D	421	GLU	N-CA-C	5.71	117.98	111.02
1	A	236	ILE	N-CA-C	-5.71	100.21	108.71
1	A	606	GLN	N-CA-C	-5.69	105.00	111.14
1	B	688	VAL	N-CA-C	-5.65	104.84	111.00
1	C	177	GLU	CA-C-N	5.63	126.88	119.84
1	C	177	GLU	C-N-CA	5.63	126.88	119.84
1	B	404	VAL	N-CA-C	-5.62	101.47	108.89
1	C	389	ILE	N-CA-C	5.61	121.00	109.34
1	B	224	ALA	N-CA-C	-5.60	102.47	110.59
1	D	632	GLY	N-CA-C	-5.57	105.94	113.24
1	A	393	ASP	N-CA-C	5.55	118.86	109.76
1	D	607	ILE	N-CA-C	-5.51	105.35	110.53
1	D	87	SER	N-CA-C	5.50	116.90	107.28
1	D	745	SER	N-CA-C	5.50	117.98	111.33
1	B	715	GLN	N-CA-C	5.49	118.19	111.82
1	B	154	TRP	N-CA-C	5.49	116.86	108.52
1	D	178	PRO	N-CA-C	5.46	123.73	112.47
1	D	271	VAL	N-CA-C	5.46	116.84	108.71
1	C	54	ARG	N-CA-C	5.46	117.62	108.73
1	A	463	LYS	N-CA-C	5.43	120.28	111.37
1	D	545	ASP	N-CA-C	-5.41	101.15	109.76
1	A	635	VAL	N-CA-C	-5.41	105.10	111.00
1	B	537	SER	N-CA-C	-5.41	106.72	113.38
1	D	100	HIS	N-CA-C	-5.39	99.32	110.80
1	B	659	TRP	N-CA-C	5.37	119.55	112.89
1	A	365	THR	N-CA-C	-5.36	102.95	110.35
1	D	78	VAL	N-CA-C	-5.36	102.00	109.45
1	C	342	ALA	N-CA-C	-5.34	106.54	113.16
1	C	180	LEU	CA-C-N	5.33	125.23	119.85
1	C	180	LEU	C-N-CA	5.33	125.23	119.85
1	D	548	ALA	N-CA-C	5.32	122.13	110.80
1	B	236	ILE	N-CA-C	-5.31	101.99	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	LEU	N-CA-C	-5.30	105.42	111.14
1	A	716	SER	N-CA-C	-5.29	104.95	111.40
1	D	150	ASN	N-CA-C	-5.28	103.51	110.43
1	C	78	VAL	N-CA-C	-5.26	100.91	108.48
1	C	454	CYS	N-CA-C	5.25	117.64	108.76
1	A	518	ILE	N-CA-C	5.25	116.31	108.54
1	A	673	LEU	N-CA-C	5.25	116.69	110.07
1	D	179	ASN	N-CA-C	5.24	119.95	113.50
1	D	328	CYS	N-CA-C	5.24	117.50	109.07
1	D	392	LYS	N-CA-C	5.23	119.14	112.34
1	D	278	SER	N-CA-C	-5.21	107.31	113.97
1	A	516	PHE	N-CA-C	5.20	115.92	108.74
1	C	518	ILE	N-CA-C	5.19	115.33	107.80
1	A	448	GLU	N-CA-C	5.17	119.45	113.20
1	A	301	CYS	N-CA-C	5.16	119.58	113.28
1	B	343	ARG	N-CA-C	-5.14	103.95	111.30
1	D	83	TYR	N-CA-C	5.14	117.67	111.40
1	D	470	LEU	N-CA-C	-5.13	102.88	110.48
1	D	45	LEU	N-CA-C	-5.13	105.77	111.36
1	B	300	LEU	N-CA-C	-5.10	100.41	108.73
1	B	320	GLN	N-CA-C	5.09	121.63	110.80
1	C	656	VAL	N-CA-C	-5.05	101.19	108.71
1	A	76	ILE	CB-CA-C	-5.05	105.17	111.08
1	B	383	HIS	N-CA-C	5.04	116.86	109.24
1	C	414	TYR	N-CA-C	5.03	116.72	109.07
1	A	389	ILE	N-CA-C	5.03	119.79	109.34
1	B	86	SER	N-CA-C	5.02	116.16	108.52
1	D	404	VAL	N-CA-C	-5.02	101.11	108.54
1	A	387	PHE	N-CA-C	5.01	117.07	108.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	700	TYR	Sidechain
1	B	128	TYR	Sidechain
1	C	83	TYR	Sidechain
1	D	752	TYR	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	5965	0	5686	410	0
1	B	5965	0	5686	411	0
1	C	5965	0	5686	390	0
1	D	5965	0	5686	408	0
2	A	26	0	28	2	0
2	B	26	0	28	2	0
2	C	26	0	28	1	0
2	D	26	0	28	3	0
3	A	81	0	0	2	0
3	B	72	0	0	5	0
3	C	66	0	0	2	0
3	D	92	0	0	9	0
All	All	24275	0	22856	1587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1587) 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:D:173:TYR:HE2	1:D:184:ARG:HG2	1.07	1.12
1:D:173:TYR:CE2	1:D:184:ARG:HG2	1.89	1.06
1:A:253:ARG:HH21	1:B:253:ARG:NH1	1.55	1.05
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.41	1.03
1:A:154:TRP:CZ3	1:A:214:LEU:HD21	1.95	1.02
1:C:651:ILE:HG21	1:C:755:MET:HE3	1.43	0.99
1:A:429:ARG:HG2	1:A:429:ARG:HH11	1.31	0.95
1:D:180:LEU:HB2	1:D:181:PRO:HD2	1.49	0.94
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.49	0.94
1:D:481:THR:HG1	1:D:483:HIS:HE2	1.07	0.93
1:D:143:ILE:HG23	1:D:179:ASN:OD1	1.67	0.93
1:A:286:GLN:HE21	1:A:288:THR:HG23	1.34	0.92
1:B:54:ARG:H	1:B:54:ARG:CD	1.83	0.92
1:A:154:TRP:HZ3	1:A:214:LEU:HD21	1.30	0.91
1:D:75:ASN:HD22	1:D:92:ASN:ND2	1.68	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASP:OD1	1:A:464:GLU:N	2.04	0.90
1:A:693:GLU:HG3	1:A:696:LYS:NZ	1.86	0.90
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.55	0.89
1:C:325:MET:HE1	1:C:371:PHE:CE2	2.07	0.89
1:B:518:ILE:O	1:B:519:LEU:HD23	1.74	0.88
1:D:134:ILE:HD11	1:D:157:TRP:CH2	2.09	0.87
1:A:253:ARG:HH21	1:B:253:ARG:HH11	1.16	0.87
1:C:98:PHE:HE2	1:C:100:HIS:HB2	1.39	0.86
1:C:621:ASN:HD22	1:C:622:LYS:H	1.22	0.86
1:A:295:ILE:HD11	1:A:317:ARG:HH21	1.38	0.86
1:A:382:ARG:H	1:A:403:GLU:HG2	1.39	0.85
1:C:369:ASN:C	1:C:389:ILE:HG23	2.01	0.85
1:B:765:LEU:HB2	1:B:766:PRO:C	2.02	0.85
1:A:693:GLU:HG3	1:A:696:LYS:HZ1	1.40	0.84
1:C:621:ASN:ND2	1:C:622:LYS:HG3	1.92	0.84
1:D:114:ILE:HG22	1:D:137:LEU:HD21	1.59	0.84
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.26	0.84
1:C:54:ARG:HG2	1:C:54:ARG:HH11	1.44	0.83
1:C:354:VAL:CG1	1:C:359:PRO:HG3	2.08	0.82
1:B:54:ARG:NH2	1:B:503:MET:HE1	1.95	0.82
1:D:272:ASN:HD22	1:D:272:ASN:C	1.88	0.82
1:D:621:ASN:HA	1:D:624:ILE:HD11	1.62	0.82
1:C:258:LYS:HZ1	1:C:712:HIS:HD2	1.25	0.81
1:B:84:GLY:HA3	1:B:492:ARG:NH1	1.95	0.81
1:B:109:PRO:HG2	1:B:158:SER:O	1.81	0.81
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.62	0.81
1:B:433:LYS:HD3	1:B:445:LEU:HD11	1.62	0.80
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.63	0.80
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.82	0.80
1:A:718:GLN:NE2	1:B:244:GLU:HA	1.96	0.80
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.83	0.79
1:C:542:LEU:C	1:C:542:LEU:HD23	2.06	0.79
1:D:134:ILE:HD11	1:D:157:TRP:HH2	1.47	0.79
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.18	0.79
1:D:549:GLY:O	1:D:552:SER:HB3	1.83	0.79
1:B:139:LYS:O	1:B:141:GLN:HG3	1.82	0.78
1:C:622:LYS:O	1:C:623:ARG:HG3	1.83	0.78
1:B:75:ASN:O	1:B:77:LEU:HD13	1.83	0.78
1:D:571:GLU:CD	1:D:760:LYS:HD3	2.08	0.78
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.18	0.77
1:D:133:ASP:CG	1:D:147:ARG:HH21	1.91	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ARG:HG3	1:D:337:TRP:H	1.49	0.77
1:A:295:ILE:HD11	1:A:317:ARG:NH2	1.99	0.77
1:C:119:ASN:O	1:C:130:ALA:HA	1.84	0.77
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.20	0.77
1:D:143:ILE:HG13	3:D:822:HOH:O	1.84	0.77
1:C:722:ALA:O	1:C:726:VAL:HG22	1.85	0.76
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.21	0.76
1:A:405:ILE:HG13	1:A:429:ARG:HD3	1.67	0.76
1:D:387:PHE:CE1	1:D:394:CYS:HB3	2.21	0.76
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.68	0.76
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.01	0.76
1:C:658:ARG:NH2	1:C:684:ARG:HD3	2.01	0.75
1:D:134:ILE:HD13	1:D:178:PRO:HB3	1.68	0.75
1:D:110:ASP:O	1:D:112:GLN:N	2.19	0.75
1:C:325:MET:HE1	1:C:371:PHE:CZ	2.22	0.75
1:D:765:LEU:HB2	1:D:766:PRO:O	1.87	0.75
1:B:54:ARG:H	1:B:54:ARG:HD3	1.50	0.75
1:C:631:TYR:O	1:C:634:TYR:HB3	1.87	0.75
1:B:71:LYS:HE3	1:B:105:TYR:HE1	1.51	0.74
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.20	0.74
1:C:627:TRP:CE3	1:C:755:MET:HE1	2.22	0.74
1:D:47:ASP:OD2	1:D:52:THR:HG21	1.87	0.74
1:B:134:ILE:HB	1:B:143:ILE:HD12	1.69	0.74
1:A:214:LEU:HD23	1:A:214:LEU:O	1.88	0.74
1:A:651:ILE:HG21	1:A:755:MET:HE3	1.69	0.74
1:D:310:ARG:HG3	1:D:329:ASP:OD1	1.87	0.73
1:A:50:LYS:O	1:A:51:ASN:HB2	1.86	0.73
1:D:598:LEU:HD22	1:D:631:TYR:OH	1.87	0.73
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.23	0.73
1:A:55:LEU:HD12	1:A:500:LEU:HD22	1.69	0.73
1:A:159:PRO:HG3	1:A:217:SER:O	1.87	0.73
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.69	0.73
1:D:293:MET:HE1	1:D:317:ARG:HG3	1.70	0.73
1:C:621:ASN:HD22	1:C:622:LYS:N	1.85	0.73
1:D:369:ASN:O	1:D:389:ILE:HG23	1.89	0.73
1:A:397:ILE:HD12	1:A:434:ILE:HG21	1.70	0.73
1:C:121:VAL:O	1:C:128:TYR:HB2	1.89	0.73
1:C:354:VAL:HG12	1:C:359:PRO:HG3	1.71	0.73
1:D:235:LEU:HD23	1:D:255:PRO:HA	1.71	0.73
1:B:329:ASP:OD1	1:B:343:ARG:NH1	2.21	0.73
1:B:369:ASN:O	1:B:389:ILE:HG23	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.69	0.72
1:B:123:GLN:HB3	1:B:127:SER:OG	1.89	0.72
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.24	0.72
1:C:114:ILE:HG22	1:C:137:LEU:HD21	1.71	0.72
1:C:79:PHE:CE1	1:C:86:SER:HB3	2.25	0.72
1:A:150:ASN:O	1:A:151:ASN:HB2	1.90	0.72
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.70	0.72
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:D:135:TYR:OH	1:D:140:ARG:HG2	1.90	0.71
1:D:272:ASN:HD22	1:D:273:THR:N	1.87	0.71
1:D:293:MET:CE	1:D:317:ARG:HG3	2.20	0.71
1:B:487:ASN:HD22	1:B:489:LYS:H	1.38	0.71
1:D:158:SER:CB	1:D:163:LYS:HB2	2.19	0.71
1:A:376:SER:HA	1:A:381:TYR:O	1.89	0.71
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.55	0.71
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.71	0.71
1:A:415:LEU:HB2	1:A:436:LEU:HD21	1.71	0.71
1:C:146:GLU:OE1	1:C:181:PRO:HB3	1.90	0.71
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.71	0.71
1:A:134:ILE:HD11	1:A:164:LEU:HD11	1.72	0.71
1:C:516:PHE:CD2	1:C:523:LYS:HB2	2.26	0.71
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.73	0.71
1:D:272:ASN:ND2	1:D:274:ASP:H	1.88	0.71
1:C:137:LEU:O	1:C:140:ARG:HD2	1.90	0.71
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.89	0.70
1:C:420:ASN:HD22	1:C:426:PRO:HA	1.56	0.70
1:C:458:SER:HB3	1:C:471:ARG:HB3	1.71	0.70
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.73	0.70
1:C:596:ARG:O	1:C:597:ARG:HD2	1.91	0.70
1:B:603:VAL:HG22	1:B:635:VAL:HG13	1.73	0.70
1:B:519:LEU:O	1:B:522:THR:N	2.24	0.70
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.72	0.70
1:C:55:LEU:CD1	1:C:561:LEU:HD12	2.21	0.70
1:C:65:ASP:OD1	1:C:464:GLU:N	2.24	0.70
1:A:429:ARG:HG2	1:A:429:ARG:NH1	2.06	0.70
1:D:134:ILE:CG2	1:D:143:ILE:HD12	2.21	0.70
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.27	0.69
1:B:93:SER:HA	1:B:96:ASP:OD1	1.92	0.69
1:C:139:LYS:O	1:C:139:LYS:HG3	1.91	0.69
1:D:138:ASN:OD1	1:D:139:LYS:N	2.25	0.69
1:C:258:LYS:NZ	1:C:712:HIS:HD2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ARG:HB3	1:D:506:ASN:O	1.93	0.69
1:A:286:GLN:NE2	1:A:288:THR:HG23	2.05	0.69
1:A:218:PRO:HB2	1:A:308:GLN:CD	2.18	0.69
1:C:658:ARG:HE	1:C:687:THR:HG21	1.56	0.69
1:A:248:TYR:CE2	1:B:258:LYS:HD2	2.28	0.69
1:A:258:LYS:NZ	1:A:712:HIS:CD2	2.61	0.69
1:A:477:LEU:HD13	1:A:500:LEU:HD23	1.74	0.69
1:B:674:PRO:O	1:B:680:LEU:HD13	1.93	0.69
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.23	0.69
1:C:633:GLY:HA3	1:C:655:PRO:HB3	1.73	0.69
1:D:95:PHE:CE1	1:D:116:LEU:HD11	2.28	0.69
1:B:487:ASN:ND2	1:B:489:LYS:H	1.90	0.68
1:B:602:GLU:N	1:B:602:GLU:OE2	2.26	0.68
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.09	0.68
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.23	0.68
1:A:127:SER:HB3	1:A:211:TYR:CG	2.28	0.68
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.75	0.68
1:C:365:THR:O	1:C:368:GLY:N	2.26	0.68
1:C:369:ASN:O	1:C:389:ILE:HG23	1.93	0.68
1:C:654:ALA:HA	1:C:704:HIS:ND1	2.09	0.68
1:D:235:LEU:HD23	1:D:255:PRO:CA	2.24	0.68
1:B:388:GLN:HG2	1:B:391:LYS:HE3	1.76	0.68
1:A:459:VAL:HG22	1:A:460:SER:H	1.58	0.68
1:C:258:LYS:HD2	1:D:248:TYR:CE2	2.28	0.68
1:B:667:THR:O	1:B:671:MET:HB2	1.93	0.68
1:D:62:TRP:CE3	1:D:462:SER:HB3	2.29	0.68
1:D:195:TYR:O	1:D:227:GLN:HA	1.94	0.68
1:A:621:ASN:HA	1:A:624:ILE:HD11	1.77	0.67
1:B:702:LEU:HD21	1:B:716:SER:HB3	1.76	0.67
1:B:745:SER:O	1:B:749:GLN:HG3	1.94	0.67
1:C:458:SER:CB	1:C:471:ARG:HD3	2.23	0.67
1:C:542:LEU:HD23	1:C:543:LEU:N	2.08	0.67
1:D:134:ILE:HG23	1:D:143:ILE:HD12	1.76	0.67
1:A:244:GLU:HA	1:B:718:GLN:NE2	2.10	0.67
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.09	0.67
1:A:263:ASN:ND2	1:A:318:ARG:CZ	2.58	0.67
1:B:516:PHE:HE2	1:B:518:ILE:HD11	1.59	0.67
1:B:534:PHE:HE1	1:B:574:ILE:HD11	1.58	0.67
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.30	0.67
1:C:720:SER:O	1:C:724:VAL:HG23	1.95	0.67
1:B:425:MET:HE1	1:B:455:GLN:OE1	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLU:HB2	1:C:132:TYR:CE2	2.30	0.67
1:D:108:SER:HB3	1:D:157:TRP:CE2	2.30	0.67
1:D:319:ILE:O	1:D:321:ASN:N	2.28	0.67
1:A:502:LYS:O	1:A:505:GLN:HG2	1.95	0.67
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.30	0.67
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.77	0.67
1:B:635:VAL:O	1:B:639:VAL:HG23	1.95	0.67
1:C:507:VAL:HG13	1:C:509:MET:HG2	1.76	0.67
1:D:139:LYS:HG2	1:D:141:GLN:HB2	1.77	0.67
1:D:214:LEU:HD12	1:D:223:LEU:HD11	1.77	0.66
1:C:93:SER:O	1:C:96:ASP:HB2	1.95	0.66
1:D:763:PHE:HB2	1:D:765:LEU:HD21	1.77	0.66
1:B:54:ARG:CZ	1:B:503:MET:HE1	2.26	0.66
1:B:145:GLU:O	1:B:146:GLU:C	2.38	0.66
1:C:74:ASN:O	1:C:92:ASN:HA	1.95	0.66
1:D:745:SER:O	1:D:749:GLN:HG3	1.94	0.66
1:D:125:ARG:NH2	1:D:205:GLU:OE2	2.27	0.66
1:B:242:SER:CB	1:B:246:LEU:HD23	2.25	0.66
1:B:671:MET:HE1	1:B:682:HIS:HD2	1.60	0.66
1:C:235:LEU:HD23	1:C:255:PRO:HA	1.77	0.66
1:C:761:GLN:NE2	1:C:762:CYS:HA	2.11	0.66
1:D:492:ARG:HB3	1:D:492:ARG:NH1	2.11	0.66
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.11	0.66
1:A:138:ASN:C	1:A:140:ARG:H	2.03	0.66
1:A:175:LYS:CG	1:A:182:SER:HB3	2.23	0.66
1:B:518:ILE:CD1	1:B:523:LYS:HB3	2.25	0.66
1:A:263:ASN:HD22	1:A:318:ARG:CZ	2.09	0.65
1:C:72:GLN:O	1:C:75:ASN:HB2	1.97	0.65
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.31	0.65
1:A:156:THR:HG23	1:A:165:ALA:HB3	1.78	0.65
1:A:240:PHE:HB3	1:A:250:LYS:HG3	1.77	0.65
1:B:741:GLY:O	1:B:742:ILE:C	2.39	0.65
1:C:702:LEU:HD11	1:C:716:SER:OG	1.95	0.65
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.31	0.65
1:B:242:SER:HB3	1:B:246:LEU:HD23	1.79	0.65
1:B:514:LEU:HD22	1:B:557:THR:HG22	1.78	0.65
1:B:644:SER:O	1:B:646:VAL:HG23	1.97	0.65
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.32	0.65
1:A:64:SER:O	1:A:463:LYS:HG2	1.97	0.65
1:C:65:ASP:OD2	1:C:464:GLU:HB2	1.96	0.65
1:D:365:THR:O	1:D:368:GLY:N	2.24	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:LYS:O	1:C:527:GLN:HA	1.96	0.65
1:C:458:SER:HB3	1:C:471:ARG:HD3	1.77	0.65
1:C:507:VAL:HG22	1:C:508:GLN:N	2.12	0.65
1:C:125:ARG:HG2	1:C:126:HIS:CE1	2.32	0.65
1:A:511:SER:OG	1:A:530:LEU:HB2	1.96	0.64
1:C:114:ILE:CG2	1:C:137:LEU:HD21	2.26	0.64
1:D:397:ILE:HD12	1:D:434:ILE:HD13	1.77	0.64
1:C:535:ASP:OD1	1:C:538:LYS:HE2	1.96	0.64
1:D:57:LEU:HD12	1:D:57:LEU:H	1.62	0.64
1:D:110:ASP:C	1:D:112:GLN:H	2.05	0.64
1:A:381:TYR:CE2	1:A:401:THR:HA	2.32	0.64
1:C:73:GLU:C	1:C:75:ASN:H	2.06	0.64
1:C:581:ARG:HB2	1:C:605:ASP:OD2	1.97	0.64
1:A:459:VAL:HG22	1:A:460:SER:N	2.11	0.64
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.31	0.64
1:C:244:GLU:HG3	1:D:689:MET:CE	2.27	0.64
1:D:146:GLU:HB2	1:D:179:ASN:O	1.96	0.64
1:D:571:GLU:O	1:D:573:ILE:HG13	1.97	0.64
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.95	0.64
1:C:745:SER:O	1:C:749:GLN:HG3	1.98	0.64
1:C:75:ASN:HD21	1:C:92:ASN:ND2	1.95	0.64
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.79	0.64
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.78	0.64
1:C:127:SER:HB3	1:C:211:TYR:CD1	2.33	0.64
1:D:159:PRO:HG3	1:D:217:SER:O	1.97	0.64
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.27	0.64
1:D:515:ASP:OD2	1:D:516:PHE:N	2.30	0.64
1:A:260:GLY:HA3	1:A:674:PRO:HG3	1.79	0.63
1:D:765:LEU:HB2	1:D:766:PRO:C	2.22	0.63
1:B:513:LYS:HZ3	1:B:515:ASP:HB2	1.63	0.63
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.80	0.63
1:D:492:ARG:HB3	1:D:492:ARG:HH11	1.63	0.63
1:D:743:ALA:O	1:D:744:SER:C	2.39	0.63
1:B:446:SER:O	1:B:449:LEU:HG	1.98	0.63
1:A:58:TYR:CE2	1:A:494:LEU:HD13	2.33	0.63
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.34	0.63
1:C:90:LEU:HD21	1:C:95:PHE:HE2	1.63	0.63
1:B:130:ALA:HB3	1:B:132:TYR:CE1	2.33	0.63
1:C:336:ARG:HG3	1:C:336:ARG:HH11	1.64	0.63
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.81	0.63
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:C	1:A:389:ILE:HG23	2.23	0.63
1:B:426:PRO:HG3	1:B:525:TRP:CD1	2.33	0.63
1:C:127:SER:HB3	1:C:211:TYR:CG	2.34	0.63
1:C:702:LEU:HD21	1:C:716:SER:HB3	1.81	0.63
1:D:173:TYR:HE2	1:D:184:ARG:CG	1.98	0.63
1:D:217:SER:HB2	1:D:222:PHE:HB2	1.80	0.63
1:D:633:GLY:C	1:D:655:PRO:HB3	2.24	0.63
1:A:192:ASP:O	1:A:193:ILE:HD13	1.99	0.63
1:B:71:LYS:HE3	1:B:105:TYR:CE1	2.31	0.63
1:C:54:ARG:HG2	1:C:54:ARG:NH1	2.11	0.63
1:C:383:HIS:HB3	1:C:398:THR:OG1	1.97	0.63
1:D:74:ASN:C	1:D:92:ASN:HB3	2.24	0.62
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.34	0.62
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.00	0.62
1:C:170:ASN:N	1:C:170:ASN:HD22	1.97	0.62
1:C:354:VAL:HG11	1:C:359:PRO:HG3	1.80	0.62
1:D:370:SER:HB2	1:D:387:PHE:O	2.00	0.62
1:B:54:ARG:CD	1:B:54:ARG:N	2.60	0.62
1:B:513:LYS:NZ	1:B:515:ASP:HB2	2.14	0.62
1:C:135:TYR:CD1	1:C:141:GLN:O	2.52	0.62
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.82	0.62
1:A:62:TRP:CG	1:A:462:SER:HA	2.34	0.62
1:D:75:ASN:HD22	1:D:92:ASN:HD22	1.45	0.62
1:B:272:ASN:C	1:B:272:ASN:HD22	2.08	0.62
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.34	0.62
1:D:596:ARG:O	1:D:597:ARG:HD2	2.00	0.62
1:A:168:TRP:O	1:A:169:ASN:HB2	1.99	0.62
1:A:415:LEU:HD23	1:A:415:LEU:C	2.25	0.62
1:A:673:LEU:HB2	1:A:678:ASP:OD2	2.00	0.62
1:C:376:SER:HA	1:C:382:ARG:HA	1.82	0.62
1:A:461:PHE:CE2	1:A:468:TYR:HB3	2.35	0.62
1:C:118:TYR:O	1:C:130:ALA:HB1	1.99	0.62
1:D:75:ASN:ND2	1:D:92:ASN:ND2	2.44	0.62
1:D:40:ARG:HG3	1:D:40:ARG:HH11	1.65	0.61
1:D:504:LEU:HD22	1:D:509:MET:HE2	1.81	0.61
1:B:75:ASN:HD22	1:B:92:ASN:ND2	1.98	0.61
1:C:492:ARG:HB3	1:C:492:ARG:HH11	1.65	0.61
1:D:336:ARG:HG3	1:D:337:TRP:N	2.14	0.61
1:A:675:THR:HB	1:A:676:PRO:HD2	1.81	0.61
1:C:73:GLU:O	1:C:75:ASN:N	2.34	0.61
1:C:550:PRO:HD3	1:C:631:TYR:CE2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:VAL:HG13	1:B:487:ASN:N	2.15	0.61
1:A:81:ALA:O	1:A:491:LEU:HD13	2.01	0.61
1:A:453:ARG:HG2	1:A:454:CYS:SG	2.41	0.61
1:B:268:PHE:CE2	1:B:313:LEU:HD21	2.35	0.61
1:D:133:ASP:OD2	1:D:147:ARG:NH2	2.32	0.61
1:D:272:ASN:C	1:D:272:ASN:ND2	2.55	0.61
1:D:433:LYS:HB2	1:D:445:LEU:HD11	1.81	0.61
1:A:580:GLY:O	1:A:581:ARG:C	2.43	0.61
1:B:528:MET:HG2	1:B:576:ALA:HB2	1.82	0.61
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.35	0.61
1:A:76:ILE:HD11	1:A:105:TYR:CE1	2.36	0.61
1:B:92:ASN:OD1	1:B:93:SER:N	2.33	0.61
1:A:71:LYS:HG3	1:A:76:ILE:HG12	1.83	0.61
1:B:658:ARG:HH22	1:B:684:ARG:HD3	1.66	0.61
1:C:455:GLN:HB2	1:C:475:PRO:HD3	1.82	0.61
1:C:658:ARG:HH22	1:C:684:ARG:HD3	1.66	0.61
1:D:293:MET:HE3	1:D:324:VAL:HG23	1.81	0.61
1:B:414:TYR:CD2	1:B:433:LYS:HG2	2.36	0.61
1:C:541:PRO:HB2	1:C:763:PHE:CE2	2.36	0.61
1:D:136:ASP:OD1	1:D:138:ASN:HB3	2.00	0.61
1:D:167:VAL:HA	1:D:171:ASP:O	2.01	0.61
1:A:253:ARG:NH2	1:B:253:ARG:HH11	1.94	0.61
1:A:730:PHE:HD1	1:A:731:GLN:O	1.84	0.61
1:D:235:LEU:HD21	1:D:255:PRO:HG3	1.82	0.61
1:D:414:TYR:CE2	1:D:433:LYS:HE3	2.36	0.61
1:C:218:PRO:HB2	1:C:308:GLN:NE2	2.16	0.60
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.36	0.60
1:B:75:ASN:ND2	1:B:92:ASN:ND2	2.49	0.60
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.01	0.60
1:A:403:GLU:OE2	1:A:587:GLY:N	2.34	0.60
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.32	0.60
1:D:241:TYR:O	1:D:246:LEU:HD23	2.01	0.60
1:D:751:ILE:HG23	1:D:752:TYR:N	2.16	0.60
1:A:95:PHE:CB	1:A:98:PHE:HB2	2.31	0.60
1:A:438:ASP:O	1:A:440:THR:N	2.35	0.60
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.16	0.60
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.37	0.60
1:C:134:ILE:HD13	1:C:178:PRO:HB3	1.83	0.60
1:C:542:LEU:C	1:C:542:LEU:CD2	2.73	0.60
1:D:208:PHE:HE1	1:D:300:LEU:O	1.84	0.60
1:B:150:ASN:O	1:B:151:ASN:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:THR:HG23	1:B:167:VAL:O	2.01	0.60
1:C:105:TYR:O	1:C:106:SER:HB2	2.02	0.60
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.31	0.60
1:D:134:ILE:HG21	1:D:178:PRO:HB2	1.81	0.60
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.83	0.60
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.83	0.60
1:C:82:GLU:HG2	1:C:83:TYR:CZ	2.37	0.60
1:C:258:LYS:NZ	1:C:712:HIS:CD2	2.70	0.60
1:A:75:ASN:N	1:A:92:ASN:HB3	2.17	0.60
1:A:248:TYR:CZ	1:B:258:LYS:HD2	2.36	0.60
1:B:122:LYS:HG2	1:B:123:GLN:N	2.16	0.60
1:B:199:THR:HA	1:B:228:PHE:CE2	2.37	0.60
1:A:42:THR:HB	1:A:569:SER:OG	2.03	0.59
1:A:432:TYR:CE2	1:A:444:CYS:HB2	2.38	0.59
1:A:631:TYR:O	1:A:634:TYR:HB3	2.01	0.59
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.37	0.59
1:B:159:PRO:O	1:B:160:VAL:HG23	2.02	0.59
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.37	0.59
1:A:148:ILE:HD12	1:A:148:ILE:H	1.67	0.59
1:A:227:GLN:O	1:A:266:VAL:HA	2.01	0.59
1:A:611:ARG:O	1:A:614:SER:HB3	2.03	0.59
1:B:52:THR:O	1:B:54:ARG:NH1	2.31	0.59
1:B:206:GLU:OE1	2:B:767:13Z:H15	2.02	0.59
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.99	0.59
1:C:49:LEU:CD2	1:C:749:GLN:HA	2.31	0.59
1:C:580:GLY:O	1:C:583:SER:OG	2.20	0.59
1:C:658:ARG:HE	1:C:687:THR:CG2	2.15	0.59
1:C:720:SER:HB2	1:C:730:PHE:HZ	1.67	0.59
1:D:235:LEU:CD2	1:D:255:PRO:HG3	2.32	0.59
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.38	0.59
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.82	0.59
1:D:708:ASP:OD2	1:D:740:HIS:HA	2.02	0.59
1:A:286:GLN:HE21	1:A:288:THR:CG2	2.11	0.59
1:B:671:MET:HE1	1:B:682:HIS:CD2	2.38	0.59
1:D:602:GLU:OE2	1:D:602:GLU:N	2.32	0.59
1:D:614:SER:HB2	1:D:621:ASN:OD1	2.03	0.59
1:D:741:GLY:O	1:D:742:ILE:C	2.45	0.59
1:A:57:LEU:N	1:A:57:LEU:HD12	2.17	0.59
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.36	0.59
1:B:555:ALA:HB3	1:B:579:ASP:OD2	2.02	0.59
1:C:75:ASN:ND2	1:C:92:ASN:CG	2.60	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:ASN:H	1:D:487:ASN:HD22	1.49	0.59
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.38	0.59
1:A:644:SER:HB2	1:A:646:VAL:HG23	1.85	0.59
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.21	0.59
1:D:316:LEU:HD21	1:D:320:GLN:HG2	1.85	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.03	0.59
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.83	0.59
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.85	0.59
1:B:611:ARG:O	1:B:615:LYS:HG2	2.03	0.59
1:C:597:ARG:HH12	1:C:682:HIS:HB2	1.68	0.59
1:C:621:ASN:ND2	1:C:622:LYS:H	1.98	0.59
1:C:634:TYR:HD1	1:C:656:VAL:O	1.85	0.59
1:D:370:SER:HG	1:D:386:TYR:HE1	1.49	0.59
1:B:765:LEU:H	1:B:765:LEU:HD22	1.68	0.59
1:C:244:GLU:HG3	1:D:689:MET:HE3	1.85	0.59
1:D:664:SER:HB2	1:D:668:GLU:OE2	2.02	0.59
1:B:355:GLY:HA2	1:B:382:ARG:HH12	1.68	0.59
1:A:142:LEU:O	1:A:143:ILE:C	2.45	0.58
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.03	0.58
1:C:174:VAL:O	1:C:183:TYR:HD2	1.84	0.58
1:B:293:MET:HE1	1:B:317:ARG:HG3	1.84	0.58
1:C:658:ARG:HB2	1:C:687:THR:CG2	2.29	0.58
1:D:118:TYR:O	1:D:130:ALA:HB1	2.02	0.58
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.28	0.58
1:C:58:TYR:HD2	1:C:58:TYR:O	1.86	0.58
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.85	0.58
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.85	0.58
1:A:472:CYS:O	1:A:478:PRO:HA	2.04	0.58
1:A:524:PHE:HD2	1:A:580:GLY:HA2	1.69	0.58
1:D:513:LYS:O	1:D:527:GLN:HA	2.02	0.58
1:D:422:TYR:CE2	1:D:423:LYS:HE2	2.39	0.58
1:A:468:TYR:CE2	1:A:483:HIS:HB2	2.38	0.58
1:B:135:TYR:CE2	1:B:140:ARG:HA	2.37	0.58
1:D:113:PHE:N	1:D:113:PHE:CD2	2.71	0.58
1:D:114:ILE:HG22	1:D:137:LEU:CD2	2.31	0.58
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.18	0.58
1:D:191:GLU:O	1:D:192:ASP:HB2	2.03	0.58
1:A:260:GLY:HA3	1:A:674:PRO:CG	2.34	0.58
1:B:54:ARG:H	1:B:54:ARG:HD2	1.65	0.58
1:B:60:LEU:C	1:B:60:LEU:HD12	2.29	0.58
1:C:516:PHE:HD2	1:C:523:LYS:HB2	1.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.85	0.58
1:A:75:ASN:OD1	1:A:91:GLU:HA	2.03	0.57
1:B:125:ARG:NH2	1:B:205:GLU:OE2	2.37	0.57
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.84	0.57
1:C:621:ASN:HD21	1:C:622:LYS:HG3	1.68	0.57
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.04	0.57
1:D:486:VAL:HG13	1:D:487:ASN:N	2.19	0.57
1:B:122:LYS:CG	1:B:123:GLN:N	2.67	0.57
1:A:74:ASN:C	1:A:92:ASN:HB3	2.29	0.57
1:A:458:SER:HB3	1:A:471:ARG:HD3	1.85	0.57
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.39	0.57
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.39	0.57
1:B:751:ILE:O	1:B:755:MET:HG3	2.04	0.57
1:C:644:SER:HB2	1:C:646:VAL:HG23	1.85	0.57
1:C:751:ILE:O	1:C:755:MET:HG3	2.03	0.57
1:D:455:GLN:NE2	1:D:475:PRO:HG3	2.19	0.57
1:D:765:LEU:N	1:D:765:LEU:HD22	2.20	0.57
1:B:113:PHE:CD1	1:B:136:ASP:HA	2.40	0.57
1:B:208:PHE:O	1:B:209:SER:HB2	2.03	0.57
1:C:77:LEU:HD22	1:C:87:SER:O	2.05	0.57
1:C:671:MET:HE1	1:C:682:HIS:CD2	2.39	0.57
1:D:314:GLN:NE2	1:D:362:PRO:HD3	2.20	0.57
1:B:443:THR:HG22	1:B:445:LEU:HD23	1.86	0.57
1:D:266:VAL:O	1:D:267:LYS:HG2	2.04	0.57
1:D:374:ILE:CD1	1:D:404:VAL:HG12	2.35	0.57
1:A:627:TRP:CZ3	1:A:755:MET:HE1	2.39	0.57
1:B:301:CYS:O	1:B:358:ARG:NH1	2.37	0.57
1:B:459:VAL:HG22	1:B:460:SER:N	2.18	0.57
1:C:56:LYS:HD3	1:C:495:GLU:OE1	2.05	0.57
1:C:63:ILE:HG21	1:C:69:LEU:HG	1.84	0.57
1:C:236:ILE:HD12	1:C:237:GLU:H	1.67	0.57
1:D:73:GLU:N	1:D:73:GLU:CD	2.62	0.57
1:D:336:ARG:CG	1:D:337:TRP:N	2.68	0.57
1:C:73:GLU:C	1:C:75:ASN:N	2.63	0.57
1:A:524:PHE:CD2	1:A:580:GLY:HA2	2.40	0.57
1:A:627:TRP:CE3	1:A:755:MET:HE1	2.40	0.57
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.86	0.57
1:C:60:LEU:C	1:C:60:LEU:HD12	2.30	0.57
1:C:387:PHE:CE1	1:C:394:CYS:HB3	2.39	0.57
1:C:621:ASN:HD22	1:C:621:ASN:N	2.01	0.57
1:D:360:SER:O	1:D:373:LYS:NZ	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:O	1:A:209:SER:C	2.48	0.57
1:D:180:LEU:HB2	1:D:181:PRO:CD	2.30	0.57
1:D:516:PHE:CD2	1:D:523:LYS:HB2	2.38	0.57
1:D:544:LEU:HD21	1:D:606:GLN:HG3	1.87	0.57
1:A:175:LYS:HG3	1:A:182:SER:CB	2.25	0.57
1:B:146:GLU:OE1	1:B:181:PRO:HB3	2.05	0.57
1:D:75:ASN:ND2	1:D:92:ASN:HD22	2.01	0.57
1:D:658:ARG:O	1:D:661:TYR:HB2	2.04	0.57
1:B:464:GLU:O	1:B:465:ALA:HB3	2.04	0.56
1:A:143:ILE:HD13	1:A:178:PRO:HB2	1.87	0.56
1:C:545:ASP:OD1	1:C:554:LYS:NZ	2.35	0.56
1:A:163:LYS:NZ	1:A:273:THR:OG1	2.37	0.56
1:A:293:MET:HG2	1:A:315:TRP:CB	2.36	0.56
1:A:433:LYS:HD3	1:A:445:LEU:HD21	1.87	0.56
1:C:41:LYS:HG3	1:C:507:VAL:HG23	1.87	0.56
1:C:397:ILE:HD12	1:C:434:ILE:HD13	1.88	0.56
1:C:620:ASP:OD2	1:C:623:ARG:HD3	2.05	0.56
1:C:657:SER:HB3	1:C:719:ILE:HD11	1.86	0.56
1:D:124:TRP:HA	1:D:124:TRP:CE3	2.41	0.56
1:A:736:THR:HG22	1:B:721:LYS:HD3	1.86	0.56
1:B:61:ARG:NH1	1:B:105:TYR:CE2	2.73	0.56
1:B:242:SER:OG	1:B:243:ASP:N	2.38	0.56
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.87	0.56
1:B:54:ARG:HD3	1:B:54:ARG:N	2.20	0.56
1:B:57:LEU:HA	1:B:480:TYR:CZ	2.41	0.56
1:B:63:ILE:HG21	1:B:69:LEU:HG	1.86	0.56
1:B:535:ASP:O	1:B:537:SER:N	2.38	0.56
1:C:535:ASP:C	1:C:537:SER:H	2.14	0.56
1:B:487:ASN:HD22	1:B:489:LYS:N	2.03	0.56
1:A:116:LEU:O	1:A:132:TYR:HA	2.06	0.56
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.05	0.56
1:B:119:ASN:O	1:B:121:VAL:HG23	2.06	0.56
1:D:236:ILE:HG23	1:D:254:VAL:HG13	1.88	0.56
1:C:459:VAL:HG22	1:C:460:SER:N	2.20	0.56
1:C:711:VAL:HG12	1:C:715:GLN:HG3	1.87	0.56
1:D:169:ASN:N	1:D:169:ASN:HD22	2.03	0.56
1:D:253:ARG:HB2	1:D:253:ARG:HH11	1.71	0.56
1:D:422:TYR:CE2	1:D:423:LYS:HG3	2.41	0.56
1:D:765:LEU:H	1:D:766:PRO:HA	1.70	0.56
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.87	0.56
1:A:724:VAL:HG22	1:B:750:HIS:CD2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ARG:HG3	1:D:310:ARG:HH11	1.71	0.56
1:D:376:SER:OG	1:D:380:GLY:HA2	2.05	0.56
1:A:242:SER:OG	1:A:243:ASP:N	2.39	0.56
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.41	0.56
1:C:621:ASN:ND2	1:C:622:LYS:N	2.54	0.56
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.41	0.55
1:A:422:TYR:CZ	1:A:423:LYS:HE3	2.41	0.55
1:C:596:ARG:C	1:C:597:ARG:HD2	2.31	0.55
1:D:114:ILE:CG2	1:D:137:LEU:HD21	2.34	0.55
1:A:148:ILE:HD12	1:A:148:ILE:N	2.21	0.55
1:A:184:ARG:HD3	1:A:186:THR:O	2.07	0.55
1:D:267:LYS:HD2	1:D:286:GLN:HE22	1.71	0.55
1:D:484:SER:HB3	1:D:487:ASN:HD21	1.71	0.55
1:A:325:MET:CE	1:A:362:PRO:HG3	2.35	0.55
1:B:518:ILE:HD13	1:B:523:LYS:HB3	1.87	0.55
1:C:611:ARG:HG2	1:C:615:LYS:NZ	2.20	0.55
1:D:60:LEU:HD12	1:D:60:LEU:C	2.31	0.55
1:D:146:GLU:OE1	1:D:181:PRO:HA	2.06	0.55
1:D:415:LEU:C	1:D:415:LEU:HD23	2.31	0.55
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.88	0.55
1:C:55:LEU:HD11	1:C:561:LEU:HD12	1.87	0.55
1:D:67:GLU:OE1	1:D:78:VAL:HG21	2.06	0.55
1:A:263:ASN:HD22	1:A:318:ARG:NH1	2.03	0.55
1:D:124:TRP:HA	1:D:124:TRP:HE3	1.71	0.55
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.87	0.55
1:D:765:LEU:N	1:D:766:PRO:HA	2.21	0.55
1:A:280:THR:HG22	1:A:281:ASN:H	1.71	0.55
1:B:379:GLU:HG3	3:B:809:HOH:O	2.06	0.55
1:D:241:TYR:O	1:D:242:SER:HB3	2.07	0.55
1:B:168:TRP:O	1:B:169:ASN:HB2	2.07	0.55
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.75	0.55
1:C:377:ASN:OD1	1:C:379:GLU:N	2.39	0.55
1:C:486:VAL:HG13	1:C:487:ASN:H	1.71	0.55
1:B:135:TYR:C	1:B:135:TYR:CD2	2.85	0.55
1:A:122:LYS:NZ	1:A:124:TRP:O	2.31	0.55
1:A:458:SER:CB	1:A:471:ARG:HD3	2.37	0.55
1:B:657:SER:HB2	1:B:689:MET:SD	2.47	0.55
1:B:658:ARG:HD2	1:B:661:TYR:CZ	2.42	0.55
1:D:40:ARG:HD2	1:D:506:ASN:HA	1.88	0.55
1:A:408:GLU:HG3	1:A:418:ILE:HG13	1.88	0.55
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LYS:O	1:B:618:PHE:HA	2.05	0.54
1:C:507:VAL:HG22	1:C:508:GLN:H	1.73	0.54
1:D:47:ASP:HA	1:D:52:THR:CG2	2.38	0.54
1:A:360:SER:O	1:A:373:LYS:NZ	2.37	0.54
1:A:542:LEU:HD23	1:A:542:LEU:C	2.32	0.54
1:B:115:LEU:HD21	1:B:132:TYR:CD2	2.41	0.54
1:C:372:TYR:OH	1:C:436:LEU:HD22	2.07	0.54
1:C:732:ALA:HB1	1:D:734:TRP:CZ3	2.42	0.54
1:D:174:VAL:HG23	1:D:185:ILE:CG1	2.38	0.54
1:A:142:LEU:O	1:A:144:THR:HG23	2.08	0.54
1:A:158:SER:HA	1:A:216:TRP:CE2	2.43	0.54
1:B:75:ASN:HB3	1:B:92:ASN:N	2.22	0.54
1:B:627:TRP:HA	1:B:651:ILE:O	2.08	0.54
1:C:420:ASN:HD22	1:C:426:PRO:CA	2.20	0.54
1:D:158:SER:OG	1:D:163:LYS:HB2	2.07	0.54
1:D:611:ARG:O	1:D:615:LYS:HG2	2.06	0.54
1:A:340:LEU:O	1:A:343:ARG:N	2.38	0.54
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.43	0.54
1:A:154:TRP:CH2	1:A:156:THR:HB	2.43	0.54
1:A:258:LYS:HZ1	1:A:712:HIS:CD2	2.13	0.54
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.33	0.54
1:C:195:TYR:HB3	1:C:198:ILE:O	2.07	0.54
1:A:108:SER:O	1:A:111:GLY:N	2.39	0.54
1:A:242:SER:O	1:A:243:ASP:O	2.26	0.54
1:B:218:PRO:HB2	1:B:308:GLN:HE22	1.72	0.54
1:C:167:VAL:HA	1:C:171:ASP:O	2.08	0.54
1:C:370:SER:HA	1:C:387:PHE:O	2.08	0.54
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.06	0.54
1:A:154:TRP:CZ3	1:A:214:LEU:CD2	2.82	0.54
1:B:134:ILE:CB	1:B:143:ILE:HD12	2.37	0.54
1:B:136:ASP:O	1:B:138:ASN:N	2.40	0.54
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.42	0.54
1:C:58:TYR:O	1:C:58:TYR:CD2	2.60	0.54
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.90	0.54
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.05	0.54
1:D:74:ASN:O	1:D:92:ASN:HB3	2.08	0.54
1:D:657:SER:HB2	1:D:689:MET:SD	2.48	0.54
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.90	0.54
1:A:736:THR:CG2	1:B:721:LYS:HD3	2.37	0.54
1:B:535:ASP:C	1:B:537:SER:H	2.16	0.54
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ILE:HG23	1:D:407:ILE:HD11	1.90	0.54
1:B:75:ASN:HB3	1:B:92:ASN:H	1.73	0.53
1:C:357:PHE:O	1:C:669:ARG:NH1	2.41	0.53
1:B:272:ASN:ND2	1:B:274:ASP:H	2.07	0.53
1:C:491:LEU:O	1:C:492:ARG:HB3	2.08	0.53
1:D:346:ILE:CG2	1:D:347:GLU:N	2.71	0.53
1:A:634:TYR:HD1	1:A:656:VAL:O	1.90	0.53
1:B:631:TYR:O	1:B:634:TYR:HB3	2.09	0.53
1:C:520:ASN:O	1:C:521:GLU:HB2	2.07	0.53
1:A:397:ILE:CD1	1:A:434:ILE:HG21	2.37	0.53
1:C:195:TYR:O	1:C:227:GLN:HA	2.09	0.53
1:D:65:ASP:OD2	1:D:466:LYS:HD2	2.08	0.53
1:D:321:ASN:HA	1:D:354:VAL:HG23	1.91	0.53
1:D:627:TRP:CZ3	1:D:755:MET:HE1	2.44	0.53
1:D:760:LYS:HD2	1:D:766:PRO:O	2.08	0.53
1:B:74:ASN:HB3	1:B:92:ASN:HB2	1.91	0.53
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.09	0.53
1:C:674:PRO:O	1:C:680:LEU:HD13	2.09	0.53
1:D:629:TRP:O	1:D:630:SER:HB3	2.08	0.53
1:A:170:ASN:OD1	1:A:194:ILE:O	2.26	0.53
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.08	0.53
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.39	0.53
1:B:708:ASP:OD2	1:B:740:HIS:HA	2.09	0.53
1:C:621:ASN:ND2	1:C:621:ASN:N	2.55	0.53
1:A:370:SER:HA	1:A:387:PHE:O	2.09	0.53
1:C:661:TYR:HB2	1:C:715:GLN:NE2	2.24	0.53
1:D:81:ALA:O	1:D:491:LEU:HD13	2.09	0.53
1:D:482:LEU:HD13	1:D:494:LEU:HD11	1.91	0.53
1:A:73:GLU:C	1:A:75:ASN:H	2.15	0.53
1:A:515:ASP:OD1	1:A:516:PHE:N	2.38	0.53
1:A:724:VAL:HA	1:B:750:HIS:HD2	1.74	0.53
1:B:89:PHE:CD1	1:B:89:PHE:C	2.87	0.53
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.09	0.53
1:B:658:ARG:NH2	1:B:684:ARG:HD3	2.23	0.53
1:B:666:TYR:CD1	1:B:666:TYR:C	2.86	0.53
1:C:127:SER:O	1:C:128:TYR:HB3	2.08	0.53
1:C:316:LEU:HD12	1:C:323:SER:HB3	1.90	0.53
1:A:545:ASP:OD1	1:A:554:LYS:NZ	2.42	0.53
1:C:266:VAL:HG22	1:C:267:LYS:N	2.23	0.53
1:C:334:SER:OG	1:C:336:ARG:HG2	2.09	0.53
1:D:129:THR:O	1:D:130:ALA:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:C	1:A:336:ARG:H	2.16	0.52
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.52
1:C:110:ASP:OD2	1:C:112:GLN:HB2	2.10	0.52
1:D:77:LEU:HD12	1:D:77:LEU:N	2.24	0.52
1:D:199:THR:HA	1:D:228:PHE:CE2	2.45	0.52
1:B:428:GLY:O	1:B:429:ARG:HG2	2.09	0.52
1:D:219:ASN:OD1	1:D:219:ASN:C	2.53	0.52
1:D:487:ASN:H	1:D:487:ASN:ND2	2.07	0.52
1:A:235:LEU:HD23	1:A:255:PRO:CA	2.39	0.52
1:A:385:CYS:HB3	1:A:387:PHE:HE2	1.74	0.52
1:A:615:LYS:O	1:A:616:MET:C	2.52	0.52
1:B:516:PHE:CE2	1:B:518:ILE:HD11	2.43	0.52
1:B:664:SER:O	1:B:668:GLU:HB2	2.09	0.52
1:B:763:PHE:HB2	1:B:765:LEU:HD21	1.90	0.52
1:A:49:LEU:HD13	1:A:749:GLN:HA	1.92	0.52
1:A:354:VAL:CG1	1:A:359:PRO:HG3	2.39	0.52
1:A:684:ARG:HG3	1:A:684:ARG:HH11	1.74	0.52
1:B:155:VAL:HG12	1:B:156:THR:N	2.24	0.52
1:B:237:GLU:HA	1:B:252:VAL:O	2.09	0.52
1:B:487:ASN:HD22	1:B:487:ASN:C	2.17	0.52
1:B:765:LEU:HD22	1:B:765:LEU:N	2.25	0.52
1:C:324:VAL:HG22	1:C:346:ILE:HG12	1.90	0.52
1:D:241:TYR:O	1:D:242:SER:CB	2.57	0.52
1:D:640:LEU:HD22	1:D:698:VAL:HG21	1.91	0.52
1:A:39:THR:HG23	1:A:40:ARG:H	1.72	0.52
1:A:431:LEU:CD2	1:A:445:LEU:HD12	2.39	0.52
1:A:445:LEU:HD22	1:A:488:ASP:OD1	2.08	0.52
1:A:610:ALA:O	1:A:613:PHE:N	2.42	0.52
1:C:74:ASN:C	1:C:92:ASN:HB3	2.35	0.52
1:C:170:ASN:O	1:C:196:ASN:HB2	2.10	0.52
1:C:300:LEU:HD13	1:C:315:TRP:CH2	2.44	0.52
1:C:312:SER:O	1:C:313:LEU:HD12	2.09	0.52
1:A:621:ASN:N	1:A:621:ASN:HD22	2.08	0.52
1:C:75:ASN:HD21	1:C:92:ASN:CG	2.18	0.52
1:C:80:ASN:O	1:C:84:GLY:N	2.39	0.52
1:D:218:PRO:HB2	1:D:308:GLN:OE1	2.09	0.52
1:D:541:PRO:HG2	1:D:573:ILE:HA	1.91	0.52
1:A:517:ILE:HG13	1:A:517:ILE:O	2.09	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:B:459:VAL:CG2	1:B:460:SER:N	2.73	0.52
1:D:301:CYS:SG	1:D:359:PRO:HD2	2.50	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:TYR:OH	1:D:616:MET:HE1	2.09	0.52
1:B:369:ASN:C	1:B:389:ILE:HG23	2.34	0.52
1:C:191:GLU:O	1:C:193:ILE:HG12	2.09	0.52
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.44	0.52
1:A:51:ASN:O	1:A:52:THR:C	2.51	0.52
1:A:293:MET:HE3	1:A:315:TRP:O	2.10	0.52
1:A:486:VAL:HG13	1:A:487:ASN:N	2.25	0.52
1:C:224:ALA:HA	1:C:270:VAL:HA	1.91	0.52
1:D:520:ASN:C	1:D:522:THR:H	2.16	0.52
1:D:703:ILE:HG23	1:D:733:MET:O	2.09	0.52
1:A:718:GLN:HE22	1:B:244:GLU:HA	1.72	0.52
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.45	0.52
1:B:429:ARG:HG3	1:B:456:TYR:CE1	2.45	0.52
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.91	0.51
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.45	0.51
1:A:499:ALA:O	1:A:500:LEU:C	2.53	0.51
1:C:382:ARG:HG2	1:C:382:ARG:NH1	2.23	0.51
1:C:589:LYS:HB3	3:C:782:HOH:O	2.10	0.51
1:C:733:MET:HG3	1:C:735:TYR:CE1	2.45	0.51
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.45	0.51
1:D:268:PHE:CE2	1:D:313:LEU:HD21	2.45	0.51
1:B:208:PHE:CD1	1:B:208:PHE:N	2.76	0.51
1:B:629:TRP:O	1:B:630:SER:HB3	2.10	0.51
1:C:266:VAL:CG2	1:C:267:LYS:N	2.72	0.51
1:C:482:LEU:C	1:C:483:HIS:CD2	2.87	0.51
1:D:236:ILE:HG12	1:D:712:HIS:ND1	2.25	0.51
1:D:571:GLU:O	1:D:572:ASN:C	2.53	0.51
1:A:742:ILE:HG22	1:A:742:ILE:O	2.10	0.51
1:B:459:VAL:HG23	1:B:469:GLN:O	2.10	0.51
1:B:620:ASP:O	1:B:621:ASN:C	2.53	0.51
1:C:173:TYR:HA	1:C:183:TYR:O	2.10	0.51
1:A:177:GLU:HB2	1:A:180:LEU:CG	2.40	0.51
1:B:57:LEU:HA	1:B:480:TYR:CE1	2.45	0.51
1:B:134:ILE:CG2	1:B:143:ILE:HD12	2.41	0.51
1:B:293:MET:CE	1:B:317:ARG:HG3	2.39	0.51
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.92	0.51
1:D:174:VAL:HG23	1:D:185:ILE:HD11	1.93	0.51
1:B:108:SER:HB3	1:B:157:TRP:CE3	2.44	0.51
1:C:184:ARG:HB3	1:C:187:TRP:CZ2	2.46	0.51
1:C:336:ARG:HH11	1:C:336:ARG:CG	2.22	0.51
1:D:134:ILE:HD13	1:D:178:PRO:CB	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:HA	1:D:389:ILE:O	2.11	0.51
1:D:343:ARG:O	1:D:345:HIS:ND1	2.43	0.51
1:A:382:ARG:N	1:A:403:GLU:HG2	2.17	0.51
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.92	0.51
1:B:552:SER:O	1:B:583:SER:HB2	2.09	0.51
1:C:148:ILE:H	1:C:148:ILE:HD12	1.76	0.51
1:C:258:LYS:HZ1	1:C:712:HIS:CD2	2.15	0.51
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.46	0.51
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.41	0.51
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.59	0.51
1:B:115:LEU:HD11	1:B:132:TYR:HB3	1.93	0.51
1:B:242:SER:HB2	1:B:246:LEU:HD23	1.93	0.51
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.46	0.51
1:D:146:GLU:HG3	1:D:181:PRO:N	2.26	0.51
1:D:163:LYS:NZ	1:D:273:THR:OG1	2.44	0.51
1:D:331:ASP:HB3	1:D:334:SER:OG	2.10	0.51
1:A:146:GLU:HB2	1:A:179:ASN:O	2.11	0.51
1:B:217:SER:O	1:B:220:GLY:N	2.37	0.51
1:C:180:LEU:HB3	1:C:181:PRO:HD2	1.91	0.51
1:D:272:ASN:HD21	1:D:274:ASP:H	1.59	0.51
1:A:139:LYS:HE2	1:D:333:SER:OG	2.11	0.51
1:B:534:PHE:CE1	1:B:574:ILE:HD11	2.43	0.51
1:B:673:LEU:O	1:B:678:ASP:HB3	2.11	0.51
1:C:236:ILE:HD12	1:C:237:GLU:N	2.25	0.51
1:A:409:ALA:HB2	1:A:461:PHE:CD1	2.46	0.50
1:B:360:SER:O	1:B:373:LYS:HE2	2.11	0.50
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.11	0.50
1:C:168:TRP:O	1:C:169:ASN:HB2	2.12	0.50
1:C:231:THR:HG22	1:C:232:GLU:HG3	1.93	0.50
1:C:508:GLN:O	1:C:532:PRO:HG2	2.11	0.50
1:D:341:VAL:O	1:D:344:GLN:HB2	2.11	0.50
1:D:532:PRO:O	1:D:533:HIS:C	2.55	0.50
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.26	0.50
1:A:530:LEU:HD13	1:A:534:PHE:CD2	2.46	0.50
1:B:105:TYR:HD2	1:B:107:ILE:HD12	1.75	0.50
1:B:317:ARG:O	1:B:318:ARG:C	2.54	0.50
1:C:736:THR:HB	1:D:721:LYS:HB2	1.93	0.50
1:D:474:GLY:HA2	1:D:476:GLY:O	2.11	0.50
1:A:313:LEU:O	1:A:325:MET:HA	2.10	0.50
1:B:547:TYR:HD1	1:B:549:GLY:H	1.54	0.50
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASN:ND2	1:D:274:ASP:N	2.59	0.50
1:A:383:HIS:CD2	1:A:399:LYS:HA	2.46	0.50
1:A:558:VAL:HG12	1:A:559:PHE:N	2.26	0.50
1:A:610:ALA:O	1:A:611:ARG:C	2.53	0.50
1:C:195:TYR:N	1:C:195:TYR:CD1	2.79	0.50
1:C:761:GLN:NE2	1:C:762:CYS:CA	2.74	0.50
1:A:533:HIS:O	1:A:534:PHE:C	2.55	0.50
1:A:692:ALA:O	1:A:695:PHE:HB2	2.11	0.50
1:C:258:LYS:HD2	1:D:248:TYR:CD2	2.46	0.50
1:D:649:CYS:HA	1:D:699:GLU:O	2.11	0.50
1:A:607:ILE:O	1:A:610:ALA:HB3	2.11	0.50
1:B:207:VAL:HG12	1:B:208:PHE:HD1	1.76	0.50
1:D:243:ASP:HB3	3:D:796:HOH:O	2.11	0.50
1:D:709:ASP:O	1:D:712:HIS:CE1	2.65	0.50
1:A:76:ILE:CD1	1:A:105:TYR:CZ	2.95	0.50
1:B:633:GLY:C	1:B:655:PRO:HB3	2.36	0.50
1:D:175:LYS:HD3	1:D:178:PRO:HA	1.93	0.50
1:A:93:SER:O	1:A:96:ASP:HB2	2.11	0.50
1:B:614:SER:HA	1:B:619:VAL:HB	1.92	0.50
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.94	0.50
1:C:518:ILE:O	1:C:519:LEU:HD23	2.11	0.50
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.92	0.50
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.47	0.50
1:A:60:LEU:HD12	1:A:60:LEU:C	2.37	0.50
1:A:71:LYS:HG3	1:A:76:ILE:CG1	2.42	0.50
1:A:676:PRO:HG2	1:A:677:GLU:H	1.77	0.50
1:B:341:VAL:O	1:B:344:GLN:HB2	2.11	0.50
1:A:664:SER:O	1:A:668:GLU:HG3	2.12	0.49
1:B:547:TYR:HE1	1:B:549:GLY:HA3	1.77	0.49
1:C:701:LEU:HD13	1:C:731:GLN:CB	2.37	0.49
1:B:377:ASN:OD1	1:B:379:GLU:N	2.44	0.49
1:D:236:ILE:CG2	1:D:254:VAL:HG13	2.42	0.49
1:D:681:ASP:HB3	3:D:852:HOH:O	2.12	0.49
1:D:763:PHE:O	1:D:764:SER:C	2.55	0.49
1:A:429:ARG:NH1	1:A:429:ARG:CG	2.70	0.49
1:B:316:LEU:CD2	1:B:320:GLN:HG2	2.42	0.49
1:C:68:TYR:CE1	1:C:79:PHE:CD2	3.01	0.49
1:C:385:CYS:HA	1:C:396:PHE:HA	1.93	0.49
1:D:214:LEU:CD1	1:D:223:LEU:HD11	2.41	0.49
1:D:751:ILE:CG2	1:D:752:TYR:N	2.75	0.49
1:A:490:GLY:O	1:A:491:LEU:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:O	1:C:63:ILE:HG23	2.12	0.49
1:C:316:LEU:CD1	1:C:323:SER:HB3	2.42	0.49
1:C:408:GLU:N	1:C:416:TYR:O	2.39	0.49
1:C:512:LYS:HD3	3:C:818:HOH:O	2.12	0.49
1:D:98:PHE:HE1	1:D:142:LEU:HD21	1.76	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.49
1:A:138:ASN:C	1:A:140:ARG:N	2.70	0.49
1:A:588:ASP:O	1:A:592:HIS:HB2	2.12	0.49
1:B:60:LEU:HD12	1:B:60:LEU:O	2.12	0.49
1:B:73:GLU:O	1:B:75:ASN:ND2	2.46	0.49
1:B:134:ILE:O	1:B:142:LEU:HD12	2.12	0.49
1:B:199:THR:HA	1:B:228:PHE:CD2	2.47	0.49
1:B:388:GLN:HG2	1:B:391:LYS:CE	2.42	0.49
1:B:534:PHE:HA	1:B:540:TYR:OH	2.12	0.49
1:C:175:LYS:NZ	1:C:180:LEU:O	2.46	0.49
1:A:613:PHE:O	1:A:615:LYS:N	2.46	0.49
1:B:486:VAL:CG1	1:B:487:ASN:N	2.75	0.49
1:B:542:LEU:HD23	1:B:543:LEU:N	2.28	0.49
1:C:597:ARG:HA	1:C:682:HIS:CD2	2.47	0.49
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.94	0.49
1:C:728:VAL:HG22	1:C:728:VAL:O	2.12	0.49
1:D:370:SER:OG	1:D:386:TYR:HE1	1.95	0.49
1:A:142:LEU:O	1:A:143:ILE:O	2.31	0.49
1:A:175:LYS:HD2	3:A:812:HOH:O	2.12	0.49
1:A:293:MET:HE3	1:A:315:TRP:C	2.38	0.49
1:A:716:SER:O	1:A:719:ILE:N	2.45	0.49
1:B:636:THR:HG21	1:B:651:ILE:O	2.13	0.49
1:D:51:ASN:O	1:D:54:ARG:HD3	2.13	0.49
1:D:159:PRO:HD3	1:D:216:TRP:CG	2.47	0.49
1:D:631:TYR:HB2	2:D:767:13Z:F1	2.03	0.49
1:B:438:ASP:HB3	1:B:441:LYS:HG3	1.95	0.49
1:B:535:ASP:C	1:B:535:ASP:OD2	2.54	0.49
1:C:345:HIS:HE1	1:C:389:ILE:O	1.95	0.49
1:C:471:ARG:HG3	1:C:471:ARG:HH11	1.77	0.49
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.27	0.49
1:D:146:GLU:HB3	1:D:180:LEU:O	2.13	0.49
1:A:64:SER:C	1:A:463:LYS:HG2	2.38	0.49
1:A:626:ILE:HG23	1:A:626:ILE:O	2.12	0.49
1:C:755:MET:O	1:C:759:ILE:HG12	2.12	0.49
1:D:257:PRO:O	1:D:663:ASP:HA	2.12	0.49
1:A:225:TYR:CZ	1:A:269:PHE:HB2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:O	1:B:137:LEU:C	2.56	0.49
1:B:184:ARG:HD3	1:B:186:THR:O	2.12	0.49
1:B:241:TYR:O	1:B:242:SER:HB3	2.13	0.49
1:B:289:ALA:HB2	1:B:315:TRP:CZ3	2.48	0.49
1:C:272:ASN:C	1:C:272:ASN:OD1	2.56	0.49
1:C:454:CYS:HA	1:C:474:GLY:O	2.13	0.49
1:D:562:ASN:HB2	3:D:845:HOH:O	2.13	0.49
1:D:704:HIS:NE2	1:D:711:VAL:O	2.45	0.49
1:A:242:SER:HB3	1:A:246:LEU:HD22	1.94	0.48
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.59	0.48
1:C:61:ARG:O	1:C:68:TYR:HA	2.12	0.48
1:C:300:LEU:HD13	1:C:315:TRP:CZ3	2.48	0.48
1:C:487:ASN:O	1:C:488:ASP:C	2.55	0.48
1:C:654:ALA:HA	1:C:704:HIS:CE1	2.47	0.48
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.48
1:A:199:THR:HG21	1:A:208:PHE:HD2	1.78	0.48
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.95	0.48
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.42	0.48
1:B:80:ASN:OD1	1:B:82:GLU:N	2.46	0.48
1:B:169:ASN:N	1:B:169:ASN:HD22	2.10	0.48
1:B:208:PHE:N	1:B:208:PHE:HD1	2.11	0.48
1:B:428:GLY:C	1:B:429:ARG:HG2	2.38	0.48
1:B:644:SER:C	1:B:646:VAL:H	2.21	0.48
1:C:249:PRO:HD3	1:D:714:GLN:NE2	2.27	0.48
1:A:138:ASN:O	1:A:140:ARG:HG2	2.12	0.48
1:A:478:PRO:HB2	1:A:497:ASN:HD21	1.77	0.48
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.94	0.48
1:C:312:SER:C	1:C:313:LEU:HD12	2.37	0.48
1:C:374:ILE:HD11	1:C:404:VAL:HG12	1.95	0.48
1:D:68:TYR:CD1	1:D:68:TYR:C	2.91	0.48
1:D:108:SER:HB3	1:D:157:TRP:CZ2	2.48	0.48
1:D:169:ASN:O	1:D:170:ASN:HB2	2.12	0.48
1:A:60:LEU:HD12	1:A:60:LEU:O	2.13	0.48
1:A:347:GLU:OE1	1:A:373:LYS:HE3	2.13	0.48
1:B:156:THR:HG21	1:B:214:LEU:CD1	2.43	0.48
1:D:73:GLU:CD	1:D:73:GLU:H	2.20	0.48
1:D:224:ALA:CB	1:D:270:VAL:HG22	2.44	0.48
1:D:501:ASP:O	1:D:505:GLN:HG2	2.14	0.48
1:D:620:ASP:OD2	1:D:623:ARG:HD3	2.12	0.48
1:A:498:SER:O	1:A:501:ASP:HB3	2.13	0.48
1:A:558:VAL:CG1	1:A:559:PHE:N	2.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:HIS:C	1:A:714:GLN:N	2.67	0.48
1:A:738:GLU:CD	1:A:744:SER:OG	2.56	0.48
1:B:84:GLY:HA3	1:B:492:ARG:HH12	1.71	0.48
1:B:207:VAL:HG12	1:B:208:PHE:CD1	2.49	0.48
1:B:370:SER:HB2	1:B:387:PHE:O	2.13	0.48
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.48
1:B:657:SER:O	1:B:688:VAL:HG23	2.13	0.48
1:C:301:CYS:SG	1:C:316:LEU:HB2	2.54	0.48
1:C:486:VAL:HG13	1:C:487:ASN:N	2.28	0.48
1:D:175:LYS:HE3	1:D:180:LEU:O	2.13	0.48
1:D:382:ARG:HD2	1:D:403:GLU:OE2	2.13	0.48
1:A:48:TYR:CD2	1:A:49:LEU:HD23	2.48	0.48
1:A:367:ASP:OD1	1:A:369:ASN:N	2.43	0.48
1:A:481:THR:HG22	1:A:493:VAL:HG22	1.96	0.48
1:B:131:SER:C	1:B:132:TYR:CD1	2.92	0.48
1:C:73:GLU:O	1:C:75:ASN:ND2	2.43	0.48
1:C:472:CYS:O	1:C:478:PRO:HA	2.14	0.48
1:A:554:LYS:H	1:A:579:ASP:CG	2.21	0.48
1:B:733:MET:HG3	1:B:735:TYR:CE2	2.49	0.48
1:C:413:ASP:C	1:C:414:TYR:CD1	2.92	0.48
1:D:259:ALA:HB3	1:D:660:GLU:HA	1.96	0.48
1:D:293:MET:HG3	1:D:315:TRP:HB2	1.95	0.48
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.30	0.48
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.94	0.48
1:B:562:ASN:HB2	3:B:830:HOH:O	2.14	0.48
1:C:553:GLN:HA	1:C:579:ASP:OD1	2.14	0.48
1:C:675:THR:HB	1:C:676:PRO:HD2	1.95	0.48
1:D:68:TYR:CD1	1:D:68:TYR:O	2.66	0.48
1:D:581:ARG:HB2	1:D:605:ASP:OD2	2.14	0.48
1:A:528:MET:HE3	1:A:613:PHE:CE1	2.49	0.48
1:B:55:LEU:HD11	1:B:478:PRO:HD2	1.96	0.48
1:B:422:TYR:CD1	1:B:447:CYS:SG	3.07	0.48
1:B:644:SER:O	1:B:646:VAL:N	2.47	0.48
1:C:45:LEU:HD13	1:C:566:TYR:CD2	2.48	0.48
1:C:135:TYR:HD1	1:C:142:LEU:HD13	1.78	0.48
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.95	0.48
1:B:47:ASP:CG	1:B:52:THR:HG1	2.20	0.48
1:B:170:ASN:O	1:B:196:ASN:HB2	2.14	0.48
1:C:107:ILE:CD1	1:C:114:ILE:HD12	2.44	0.48
1:D:341:VAL:HG13	1:D:342:ALA:N	2.28	0.48
1:D:755:MET:O	1:D:759:ILE:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:OD1	1:A:80:ASN:C	2.57	0.47
1:C:233:VAL:HG12	1:C:234:PRO:O	2.14	0.47
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.14	0.47
1:C:627:TRP:HB2	1:C:651:ILE:HB	1.96	0.47
1:D:99:GLY:O	1:D:100:HIS:CG	2.67	0.47
1:D:516:PHE:CD2	1:D:523:LYS:HD3	2.49	0.47
1:A:67:GLU:HA	1:A:79:PHE:O	2.14	0.47
1:A:150:ASN:O	1:A:151:ASN:CB	2.59	0.47
1:A:154:TRP:CZ3	1:A:156:THR:CG2	2.98	0.47
1:A:546:VAL:HG12	1:A:627:TRP:O	2.13	0.47
1:B:113:PHE:CD2	1:B:178:PRO:HG2	2.48	0.47
1:B:445:LEU:HD23	1:B:445:LEU:N	2.29	0.47
1:B:500:LEU:HG	1:B:504:LEU:HD12	1.96	0.47
1:B:763:PHE:HB2	1:B:765:LEU:CD2	2.44	0.47
1:C:107:ILE:HG22	1:C:108:SER:O	2.14	0.47
1:D:75:ASN:OD1	1:D:77:LEU:HD11	2.14	0.47
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.47
1:A:468:TYR:O	1:A:483:HIS:N	2.36	0.47
1:A:753:THR:O	1:A:757:HIS:CD2	2.67	0.47
1:B:319:ILE:O	1:B:321:ASN:N	2.43	0.47
1:C:309:GLU:HB3	1:C:330:TYR:HB3	1.96	0.47
1:D:146:GLU:HG3	1:D:180:LEU:C	2.40	0.47
1:A:712:HIS:O	1:A:713:PHE:C	2.57	0.47
1:B:136:ASP:HB3	1:B:139:LYS:HG2	1.96	0.47
1:C:510:PRO:HB2	1:C:530:LEU:O	2.14	0.47
1:D:156:THR:HG23	1:D:165:ALA:O	2.15	0.47
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.97	0.47
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.48	0.47
1:A:613:PHE:C	1:A:615:LYS:N	2.72	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.50	0.47
1:B:39:THR:O	1:B:39:THR:HG22	2.13	0.47
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.49	0.47
1:B:358:ARG:O	1:B:359:PRO:C	2.58	0.47
1:B:454:CYS:HA	1:B:474:GLY:O	2.15	0.47
1:B:477:LEU:HD12	1:B:501:ASP:HB2	1.97	0.47
1:C:317:ARG:O	1:C:318:ARG:C	2.55	0.47
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.79	0.47
1:D:487:ASN:HD22	1:D:487:ASN:N	2.09	0.47
1:A:293:MET:HE3	1:A:315:TRP:HB2	1.95	0.47
1:A:465:ALA:O	1:A:485:SER:OG	2.21	0.47
1:A:526:TYR:CD1	1:A:526:TYR:C	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HB3	1:B:480:TYR:OH	2.15	0.47
1:B:206:GLU:OE2	1:B:666:TYR:HB2	2.15	0.47
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.49	0.47
1:C:50:LYS:HE3	1:C:749:GLN:OE1	2.15	0.47
1:C:124:TRP:HA	1:C:124:TRP:CE3	2.50	0.47
1:C:159:PRO:HD3	1:C:216:TRP:HB2	1.95	0.47
1:C:319:ILE:O	1:C:319:ILE:HG13	2.15	0.47
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.14	0.47
1:C:369:ASN:HA	1:C:389:ILE:CG2	2.44	0.47
1:D:173:TYR:CD2	1:D:184:ARG:HA	2.50	0.47
1:D:356:ARG:HD3	1:D:551:CYS:SG	2.54	0.47
1:D:484:SER:HB2	1:D:491:LEU:HD21	1.96	0.47
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.50	0.47
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.49	0.47
1:D:154:TRP:NE1	1:D:212:SER:HB2	2.30	0.47
1:A:135:TYR:OH	1:A:140:ARG:NE	2.48	0.47
1:A:634:TYR:CD1	1:A:656:VAL:O	2.68	0.47
1:B:317:ARG:C	1:B:319:ILE:N	2.72	0.47
1:B:453:ARG:HG2	1:B:454:CYS:SG	2.55	0.47
1:B:519:LEU:O	1:B:520:ASN:C	2.58	0.47
1:D:208:PHE:O	1:D:209:SER:HB3	2.14	0.47
1:A:154:TRP:CZ3	1:A:156:THR:HB	2.50	0.47
1:A:333:SER:OG	1:A:334:SER:N	2.41	0.47
1:A:404:VAL:HG13	1:A:417:TYR:HD1	1.80	0.47
1:A:751:ILE:HG12	1:A:751:ILE:O	2.15	0.47
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.30	0.47
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.47
1:D:306:ALA:HB3	1:D:310:ARG:O	2.15	0.47
1:B:285:ILE:HG21	1:B:336:ARG:HA	1.95	0.46
1:A:279:VAL:HG12	1:A:280:THR:OG1	2.15	0.46
1:A:543:LEU:HD11	1:A:627:TRP:HD1	1.80	0.46
1:A:620:ASP:OD1	1:A:620:ASP:C	2.58	0.46
1:B:519:LEU:O	1:B:522:THR:HG23	2.15	0.46
1:B:535:ASP:C	1:B:537:SER:N	2.72	0.46
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.46
1:C:256:TYR:C	1:C:256:TYR:CD1	2.93	0.46
1:C:411:THR:OG1	1:C:414:TYR:N	2.47	0.46
1:D:320:GLN:OE1	1:D:669:ARG:HD3	2.15	0.46
1:D:463:LYS:HB3	1:D:464:GLU:OE2	2.14	0.46
1:D:764:SER:O	1:D:764:SER:OG	2.32	0.46
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:HG2	1:A:325:MET:HB2	1.97	0.46
1:B:105:TYR:HD2	1:B:107:ILE:CD1	2.29	0.46
1:B:263:ASN:ND2	1:B:318:ARG:CZ	2.78	0.46
1:C:81:ALA:O	1:C:492:ARG:NH2	2.47	0.46
1:C:310:ARG:NH1	1:C:368:GLY:O	2.48	0.46
1:C:374:ILE:HD11	1:C:404:VAL:CG1	2.45	0.46
1:C:375:ILE:O	1:C:382:ARG:HA	2.16	0.46
1:D:530:LEU:HA	1:D:531:PRO:HD3	1.81	0.46
1:A:631:TYR:HB2	2:A:767:13Z:F1	2.05	0.46
1:A:664:SER:OG	1:A:665:VAL:N	2.48	0.46
1:B:105:TYR:CD2	1:B:107:ILE:CD1	2.99	0.46
1:B:187:TRP:CH2	1:B:281:ASN:OD1	2.69	0.46
1:C:69:LEU:HD23	1:C:78:VAL:HA	1.96	0.46
1:C:105:TYR:HA	1:C:115:LEU:O	2.16	0.46
1:C:118:TYR:N	1:C:118:TYR:CD1	2.83	0.46
1:C:701:LEU:CD1	1:C:731:GLN:HB2	2.37	0.46
1:D:374:ILE:HD11	1:D:404:VAL:HG12	1.97	0.46
1:D:586:GLN:HB2	3:D:843:HOH:O	2.15	0.46
1:A:542:LEU:O	1:A:624:ILE:HA	2.15	0.46
1:B:170:ASN:OD1	1:B:170:ASN:N	2.48	0.46
1:B:508:GLN:HB3	1:B:532:PRO:HG2	1.97	0.46
1:B:519:LEU:O	1:B:521:GLU:N	2.49	0.46
1:D:72:GLN:NE2	1:D:77:LEU:HD22	2.30	0.46
1:A:325:MET:HE1	1:A:362:PRO:HG3	1.96	0.46
1:A:500:LEU:O	1:A:501:ASP:C	2.59	0.46
1:B:107:ILE:HA	1:B:114:ILE:HA	1.98	0.46
1:B:527:GLN:O	1:B:527:GLN:HG3	2.16	0.46
1:B:550:PRO:O	1:B:551:CYS:HB3	2.16	0.46
1:D:55:LEU:CD2	1:D:561:LEU:HD12	2.46	0.46
1:A:157:TRP:O	1:A:216:TRP:NE1	2.49	0.46
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.15	0.46
1:B:500:LEU:HG	1:B:504:LEU:CD1	2.46	0.46
1:C:201:TRP:CH2	1:C:205:GLU:HG2	2.51	0.46
1:C:216:TRP:HZ3	1:C:273:THR:HG21	1.80	0.46
1:C:621:ASN:ND2	1:C:621:ASN:H	2.14	0.46
1:A:68:TYR:CE1	1:A:79:PHE:CB	2.98	0.46
1:A:230:ASP:O	1:A:233:VAL:HB	2.16	0.46
1:A:312:SER:HA	1:A:326:ASP:O	2.15	0.46
1:B:115:LEU:HB2	1:B:157:TRP:HZ2	1.81	0.46
1:B:317:ARG:O	1:B:319:ILE:N	2.48	0.46
1:C:215:TRP:CE3	1:C:215:TRP:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:LEU:HD13	1:C:534:PHE:CD2	2.51	0.46
1:D:80:ASN:OD1	1:D:83:TYR:N	2.49	0.46
1:D:206:GLU:CD	1:D:666:TYR:HB2	2.41	0.46
1:D:307:THR:OG1	1:D:310:ARG:N	2.49	0.46
1:A:77:LEU:N	1:A:77:LEU:HD23	2.31	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.50	0.46
1:A:425:MET:HE1	1:A:455:GLN:OE1	2.16	0.46
1:A:728:VAL:HG23	1:A:729:ASP:O	2.15	0.46
1:B:532:PRO:O	1:B:533:HIS:HB2	2.15	0.46
1:B:658:ARG:HB3	1:B:689:MET:HE1	1.96	0.46
1:D:224:ALA:HB2	1:D:270:VAL:HG22	1.98	0.46
1:D:258:LYS:O	1:D:259:ALA:C	2.59	0.46
1:D:422:TYR:C	1:D:424:GLY:H	2.24	0.46
1:D:520:ASN:C	1:D:522:THR:N	2.74	0.46
1:D:709:ASP:OD1	1:D:709:ASP:N	2.48	0.46
1:A:228:PHE:HA	1:A:265:THR:O	2.16	0.46
1:B:246:LEU:HD11	1:B:248:TYR:O	2.15	0.46
1:C:109:PRO:HG2	1:C:158:SER:O	2.16	0.46
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.46
1:D:253:ARG:NH1	1:D:253:ARG:CB	2.79	0.46
1:D:411:THR:HG1	1:D:414:TYR:H	1.64	0.46
1:A:742:ILE:HD13	1:A:751:ILE:HD12	1.97	0.45
1:B:43:TYR:CD2	1:B:565:THR:CG2	2.99	0.45
1:B:81:ALA:HB3	1:B:467:TYR:CE2	2.50	0.45
1:B:598:LEU:O	1:B:682:HIS:NE2	2.44	0.45
1:B:644:SER:C	1:B:646:VAL:N	2.74	0.45
1:D:47:ASP:HA	1:D:52:THR:HG23	1.99	0.45
1:D:139:LYS:HG2	1:D:141:GLN:CB	2.46	0.45
1:D:173:TYR:CE2	1:D:184:ARG:CG	2.80	0.45
1:A:208:PHE:O	1:A:210:ALA:N	2.49	0.45
1:A:381:TYR:CE2	1:A:401:THR:CA	2.98	0.45
1:A:739:ASP:C	1:A:741:GLY:H	2.23	0.45
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.16	0.45
1:B:237:GLU:CG	1:B:253:ARG:HG2	2.46	0.45
1:B:506:ASN:CG	1:B:506:ASN:O	2.59	0.45
1:C:244:GLU:OE2	1:D:658:ARG:NH2	2.48	0.45
1:C:248:TYR:O	1:C:249:PRO:C	2.59	0.45
1:C:622:LYS:C	1:C:623:ARG:HG3	2.41	0.45
1:B:308:GLN:C	1:B:309:GLU:HG3	2.41	0.45
1:D:146:GLU:HB3	1:D:180:LEU:C	2.42	0.45
1:D:148:ILE:O	1:D:149:PRO:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:TYR:CD2	1:D:433:LYS:CG	3.00	0.45
1:D:597:ARG:HA	1:D:682:HIS:CD2	2.51	0.45
1:A:256:TYR:O	1:B:248:TYR:OH	2.28	0.45
1:A:302:ASP:OD1	1:A:302:ASP:C	2.59	0.45
1:A:314:GLN:HE22	1:A:361:GLU:HA	1.80	0.45
1:B:422:TYR:CE1	1:B:447:CYS:HB3	2.51	0.45
1:C:197:GLY:C	1:C:213:ALA:HB3	2.42	0.45
1:C:360:SER:OG	1:C:374:ILE:O	2.32	0.45
1:D:57:LEU:HD12	1:D:57:LEU:N	2.28	0.45
1:D:76:ILE:O	1:D:89:PHE:N	2.49	0.45
1:A:341:VAL:C	1:A:343:ARG:H	2.24	0.45
1:A:676:PRO:HG2	1:A:677:GLU:N	2.31	0.45
1:B:52:THR:HG22	3:B:816:HOH:O	2.16	0.45
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.99	0.45
1:C:507:VAL:CG2	1:C:508:GLN:N	2.79	0.45
1:C:540:TYR:C	1:C:541:PRO:O	2.55	0.45
1:D:72:GLN:O	1:D:73:GLU:C	2.58	0.45
1:A:114:ILE:HG22	1:A:137:LEU:HG	1.99	0.45
1:A:126:HIS:CD2	1:A:209:SER:C	2.95	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.16	0.45
1:B:250:LYS:HG2	1:B:251:THR:N	2.31	0.45
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.51	0.45
1:C:364:PHE:HA	1:C:371:PHE:CB	2.47	0.45
1:D:331:ASP:O	1:D:335:GLY:N	2.37	0.45
1:A:290:PRO:HD3	1:A:326:ASP:OD2	2.17	0.45
1:A:415:LEU:C	1:A:415:LEU:CD2	2.89	0.45
1:C:741:GLY:O	1:C:742:ILE:C	2.59	0.45
1:D:87:SER:O	1:D:88:VAL:C	2.59	0.45
1:D:95:PHE:CD1	1:D:116:LEU:HD11	2.52	0.45
1:A:49:LEU:HB3	1:A:749:GLN:HG2	1.98	0.45
1:A:83:TYR:C	1:A:492:ARG:NH2	2.75	0.45
1:A:113:PHE:CE1	1:A:143:ILE:HD11	2.52	0.45
1:A:738:GLU:OE2	1:A:744:SER:OG	2.34	0.45
1:B:516:PHE:HA	1:B:526:TYR:HD2	1.82	0.45
1:C:743:ALA:O	1:C:744:SER:C	2.60	0.45
1:D:343:ARG:NE	1:D:389:ILE:HD12	2.32	0.45
1:D:459:VAL:CG1	1:D:461:PHE:HE1	2.30	0.45
1:D:642:SER:O	1:D:643:GLY:C	2.60	0.45
1:A:76:ILE:HD11	1:A:105:TYR:CZ	2.51	0.45
1:A:233:VAL:HG22	1:A:262:VAL:O	2.17	0.45
1:A:426:PRO:HD2	1:A:525:TRP:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ASP:C	1:A:741:GLY:N	2.75	0.45
1:B:58:TYR:CE2	1:B:494:LEU:HB3	2.52	0.45
1:B:547:TYR:CE1	1:B:549:GLY:HA3	2.50	0.45
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.97	0.45
1:C:367:ASP:OD1	1:C:369:ASN:N	2.50	0.45
1:D:164:LEU:HD23	1:D:164:LEU:HA	1.80	0.45
1:A:285:ILE:HG23	1:A:336:ARG:HE	1.82	0.45
1:B:215:TRP:CH2	1:B:303:VAL:HG21	2.52	0.45
1:B:742:ILE:HD12	1:B:751:ILE:HD12	1.99	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:D:110:ASP:C	1:D:112:GLN:N	2.71	0.45
1:D:422:TYR:C	1:D:424:GLY:N	2.74	0.45
1:D:422:TYR:CD2	1:D:423:LYS:HG3	2.52	0.45
1:A:202:VAL:CG1	1:A:203:TYR:N	2.80	0.44
1:A:562:ASN:OD1	1:A:564:ALA:N	2.50	0.44
1:A:620:ASP:OD2	1:A:623:ARG:CD	2.64	0.44
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.17	0.44
1:B:316:LEU:HD21	1:B:320:GLN:HB3	1.99	0.44
1:B:662:TYR:CE2	2:B:767:13Z:H4	2.52	0.44
1:C:148:ILE:HD12	1:C:148:ILE:N	2.31	0.44
1:C:480:TYR:C	1:C:481:THR:HG23	2.41	0.44
1:C:581:ARG:CZ	1:C:601:PHE:CD1	3.00	0.44
1:C:602:GLU:OE2	1:C:602:GLU:N	2.48	0.44
1:D:39:THR:HB	3:D:768:HOH:O	2.16	0.44
1:D:60:LEU:HD12	1:D:60:LEU:O	2.16	0.44
1:D:110:ASP:C	1:D:110:ASP:OD2	2.60	0.44
1:D:160:VAL:HG12	1:D:161:GLY:N	2.32	0.44
1:A:288:THR:HG22	3:A:815:HOH:O	2.16	0.44
1:B:377:ASN:OD1	1:B:377:ASN:C	2.60	0.44
1:C:175:LYS:HG3	1:C:182:SER:HA	2.00	0.44
1:C:272:ASN:OD1	1:C:274:ASP:N	2.50	0.44
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.86	0.44
1:C:544:LEU:HD12	1:C:576:ALA:O	2.17	0.44
1:D:451:PRO:HA	3:D:859:HOH:O	2.16	0.44
1:A:417:TYR:CE2	1:A:432:TYR:HB2	2.51	0.44
1:B:113:PHE:CE1	1:B:136:ASP:HA	2.52	0.44
1:C:257:PRO:HG2	1:C:664:SER:OG	2.17	0.44
1:C:364:PHE:HA	1:C:371:PHE:HB3	2.00	0.44
1:C:747:ALA:O	1:C:751:ILE:HG22	2.17	0.44
1:D:662:TYR:CE2	2:D:767:13Z:H4	2.52	0.44
1:B:662:TYR:HB3	1:B:667:THR:OG1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:O	1:C:140:ARG:CD	2.62	0.44
1:C:490:GLY:O	1:C:491:LEU:C	2.60	0.44
1:C:653:VAL:C	1:C:655:PRO:HD3	2.42	0.44
1:D:63:ILE:HG22	1:D:67:GLU:O	2.16	0.44
1:D:72:GLN:O	1:D:74:ASN:N	2.50	0.44
1:D:137:LEU:CD2	1:D:137:LEU:N	2.79	0.44
1:D:258:LYS:NZ	1:D:712:HIS:HD2	2.16	0.44
1:D:636:THR:HG22	1:D:640:LEU:HD12	2.00	0.44
1:D:740:HIS:NE2	2:D:767:13Z:N2	2.66	0.44
1:A:372:TYR:CD2	1:A:415:LEU:HD12	2.52	0.44
1:A:477:LEU:HD22	1:A:500:LEU:HD23	1.98	0.44
1:A:723:LEU:HD22	1:A:728:VAL:HG11	1.99	0.44
1:B:73:GLU:O	1:B:74:ASN:HB2	2.17	0.44
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.16	0.44
1:C:302:ASP:OD1	1:C:303:VAL:N	2.51	0.44
1:D:594:ILE:CG2	1:D:601:PHE:HB2	2.47	0.44
1:A:82:GLU:OE1	1:A:467:TYR:CE1	2.70	0.44
1:A:477:LEU:CD1	1:A:500:LEU:HD23	2.44	0.44
1:B:85:ASN:OD1	1:B:85:ASN:N	2.50	0.44
1:B:115:LEU:CG	1:B:132:TYR:HD2	2.31	0.44
1:B:268:PHE:CD2	1:B:313:LEU:HD11	2.52	0.44
1:B:744:SER:O	1:B:745:SER:C	2.59	0.44
1:C:310:ARG:HH21	1:C:343:ARG:HH12	1.66	0.44
1:C:630:SER:O	1:C:655:PRO:HA	2.18	0.44
1:D:102:ILE:HD13	1:D:116:LEU:HD22	2.00	0.44
1:D:208:PHE:O	1:D:209:SER:CB	2.66	0.44
1:A:235:LEU:HD21	1:A:255:PRO:HG3	2.00	0.44
1:B:115:LEU:HB2	1:B:157:TRP:CZ2	2.51	0.44
1:C:124:TRP:HA	1:C:124:TRP:HE3	1.82	0.44
1:D:112:GLN:HB3	1:D:113:PHE:CE2	2.52	0.44
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.17	0.44
1:A:125:ARG:NH2	1:A:205:GLU:OE2	2.51	0.44
1:A:446:SER:O	1:A:447:CYS:C	2.61	0.44
1:B:627:TRP:O	1:B:627:TRP:CG	2.69	0.44
1:C:418:ILE:HA	1:C:430:ASN:O	2.18	0.44
1:C:526:TYR:CD1	1:C:526:TYR:C	2.96	0.44
1:D:266:VAL:HG22	1:D:267:LYS:N	2.33	0.44
1:D:761:GLN:HE21	1:D:761:GLN:HB3	1.57	0.44
1:A:280:THR:HG22	1:A:281:ASN:N	2.33	0.44
1:A:622:LYS:C	1:A:623:ARG:HG3	2.42	0.44
1:A:730:PHE:CD1	1:A:731:GLN:O	2.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:OD2	1:B:230:ASP:OD2	2.36	0.44
1:B:546:VAL:HB	1:B:606:GLN:OE1	2.18	0.44
1:B:600:THR:O	1:B:601:PHE:C	2.59	0.44
1:C:68:TYR:CD1	1:C:68:TYR:C	2.95	0.44
1:C:75:ASN:OD1	1:C:92:ASN:OD1	2.36	0.44
1:C:107:ILE:HD11	1:C:114:ILE:HD12	1.99	0.44
1:C:658:ARG:HH22	1:C:684:ARG:CD	2.30	0.44
1:C:711:VAL:O	1:C:712:HIS:C	2.60	0.44
1:D:76:ILE:O	1:D:89:PHE:HB3	2.18	0.44
1:A:79:PHE:CE1	1:A:86:SER:HB3	2.52	0.43
1:A:267:LYS:HB3	1:A:269:PHE:CE1	2.53	0.43
1:A:658:ARG:CB	1:A:687:THR:HG22	2.48	0.43
1:C:608:GLU:O	1:C:612:GLN:HG3	2.17	0.43
1:C:751:ILE:HG23	1:C:752:TYR:N	2.33	0.43
1:D:715:GLN:O	1:D:719:ILE:HG13	2.18	0.43
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.83	0.43
1:B:487:ASN:HD22	1:B:488:ASP:N	2.17	0.43
1:B:543:LEU:HD12	1:B:625:ALA:O	2.18	0.43
1:C:175:LYS:HG3	1:C:182:SER:CA	2.48	0.43
1:C:627:TRP:CZ3	1:C:755:MET:HE1	2.52	0.43
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.17	0.43
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.53	0.43
1:D:546:VAL:HG21	1:D:606:GLN:HG2	2.00	0.43
1:D:631:TYR:O	1:D:634:TYR:HB3	2.18	0.43
1:B:658:ARG:CB	1:B:687:THR:HG22	2.42	0.43
1:C:40:ARG:NH1	1:C:505:GLN:O	2.48	0.43
1:C:331:ASP:HB3	1:C:334:SER:HB3	2.00	0.43
1:C:662:TYR:CE2	2:C:767:13Z:H4	2.53	0.43
1:D:143:ILE:CG2	1:D:179:ASN:OD1	2.53	0.43
1:D:640:LEU:CD2	1:D:698:VAL:HG21	2.48	0.43
1:A:68:TYR:CD1	1:A:68:TYR:C	2.97	0.43
1:A:98:PHE:HE1	1:A:142:LEU:HD11	1.83	0.43
1:A:170:ASN:HD22	1:A:170:ASN:N	2.15	0.43
1:A:244:GLU:HA	1:B:718:GLN:HE22	1.82	0.43
1:A:623:ARG:NH2	1:A:763:PHE:O	2.45	0.43
1:B:520:ASN:O	1:B:521:GLU:HB2	2.18	0.43
1:C:138:ASN:C	1:C:140:ARG:H	2.26	0.43
1:C:224:ALA:HB2	1:C:270:VAL:HG13	1.99	0.43
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.53	0.43
1:C:535:ASP:C	1:C:537:SER:N	2.76	0.43
1:D:174:VAL:CG2	1:D:185:ILE:HD11	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:THR:CG2	1:D:208:PHE:CD2	3.02	0.43
1:D:244:GLU:C	1:D:246:LEU:H	2.25	0.43
1:D:256:TYR:CD1	1:D:256:TYR:C	2.96	0.43
1:D:520:ASN:O	1:D:522:THR:N	2.52	0.43
1:A:113:PHE:CD1	1:A:136:ASP:HA	2.53	0.43
1:A:486:VAL:CG1	1:A:487:ASN:N	2.82	0.43
1:B:272:ASN:C	1:B:272:ASN:ND2	2.75	0.43
1:B:516:PHE:HA	1:B:526:TYR:CD2	2.54	0.43
1:C:76:ILE:O	1:C:89:PHE:N	2.45	0.43
1:C:114:ILE:HG22	1:C:137:LEU:CD2	2.46	0.43
1:C:471:ARG:HG3	1:C:471:ARG:NH1	2.34	0.43
1:C:562:ASN:O	1:C:563:TRP:C	2.60	0.43
1:D:120:TYR:HA	1:D:130:ALA:HB2	1.99	0.43
1:D:310:ARG:HG3	1:D:310:ARG:NH1	2.33	0.43
1:D:662:TYR:HE1	1:D:710:ASN:OD1	2.02	0.43
1:A:325:MET:HE1	1:A:362:PRO:HB3	2.00	0.43
1:A:464:GLU:O	1:A:465:ALA:C	2.61	0.43
1:A:547:TYR:CE1	2:A:767:13Z:H14A	2.53	0.43
1:A:741:GLY:C	1:A:743:ALA:N	2.74	0.43
1:C:457:TYR:CE1	1:C:472:CYS:HB2	2.52	0.43
1:C:600:THR:OG1	1:C:601:PHE:N	2.51	0.43
1:D:149:PRO:HB2	1:D:168:TRP:NE1	2.33	0.43
1:D:170:ASN:O	1:D:196:ASN:HB2	2.18	0.43
1:D:180:LEU:C	1:D:181:PRO:O	2.60	0.43
1:D:195:TYR:HB3	1:D:198:ILE:O	2.18	0.43
1:D:653:VAL:CG2	1:D:755:MET:HE3	2.49	0.43
1:A:55:LEU:CD1	1:A:500:LEU:HD22	2.46	0.43
1:A:666:TYR:O	1:A:669:ARG:HB3	2.19	0.43
1:B:481:THR:OG1	1:B:483:HIS:NE2	2.51	0.43
1:B:680:LEU:O	1:B:683:TYR:HB2	2.18	0.43
1:C:611:ARG:O	1:C:614:SER:HB3	2.19	0.43
1:C:661:TYR:CB	1:C:715:GLN:NE2	2.81	0.43
1:D:162:HIS:HD2	1:D:176:ILE:O	2.01	0.43
1:D:244:GLU:C	1:D:246:LEU:N	2.75	0.43
1:D:668:GLU:O	1:D:669:ARG:C	2.62	0.43
1:D:711:VAL:O	1:D:712:HIS:C	2.61	0.43
1:A:138:ASN:O	1:A:140:ARG:N	2.51	0.43
1:A:148:ILE:HG22	1:A:152:THR:OG1	2.18	0.43
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.53	0.43
1:A:356:ARG:HA	1:A:591:MET:HE1	2.00	0.43
1:A:446:SER:HB2	1:A:457:TYR:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.53	0.43
1:B:272:ASN:HD22	1:B:274:ASP:H	1.64	0.43
1:B:426:PRO:C	1:B:428:GLY:H	2.26	0.43
1:C:88:VAL:HG11	1:C:91:GLU:OE2	2.19	0.43
1:C:564:ALA:O	1:C:565:THR:C	2.62	0.43
1:C:653:VAL:O	1:C:654:ALA:C	2.62	0.43
1:C:756:SER:O	1:C:760:LYS:HG3	2.19	0.43
1:D:58:TYR:CE2	1:D:494:LEU:HB3	2.53	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HD12	2.00	0.43
1:B:104:ASP:OD1	1:B:105:TYR:N	2.50	0.43
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.34	0.43
1:B:177:GLU:O	1:B:178:PRO:C	2.62	0.43
1:B:624:ILE:HG22	1:B:647:PHE:CD1	2.54	0.43
1:C:244:GLU:HG3	1:D:689:MET:HE2	1.98	0.43
1:D:253:ARG:HH11	1:D:253:ARG:CB	2.31	0.43
1:D:365:THR:O	1:D:366:LEU:C	2.61	0.43
1:A:76:ILE:HD13	1:A:105:TYR:CZ	2.54	0.43
1:B:73:GLU:OE2	1:B:73:GLU:N	2.52	0.43
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.88	0.43
1:B:190:LYS:HA	3:B:811:HOH:O	2.18	0.43
1:B:365:THR:O	1:B:366:LEU:C	2.60	0.43
1:D:447:CYS:C	1:D:448:GLU:OE1	2.62	0.43
1:A:139:LYS:HB2	1:D:334:SER:HB3	2.00	0.42
1:A:174:VAL:HG23	1:A:185:ILE:CG1	2.48	0.42
1:A:256:TYR:CD1	1:A:256:TYR:C	2.96	0.42
1:A:310:ARG:NH1	1:A:368:GLY:O	2.52	0.42
1:A:380:GLY:O	1:A:587:GLY:HA2	2.19	0.42
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.01	0.42
1:A:516:PHE:CE2	1:A:523:LYS:HE3	2.53	0.42
1:A:716:SER:C	1:A:718:GLN:N	2.77	0.42
1:B:154:TRP:CG	1:B:155:VAL:N	2.87	0.42
1:B:199:THR:HG22	1:B:228:PHE:CE2	2.54	0.42
1:B:546:VAL:CG2	1:B:547:TYR:N	2.82	0.42
1:B:608:GLU:O	1:B:612:GLN:HG2	2.19	0.42
1:B:637:SER:HB3	1:B:688:VAL:HG11	2.01	0.42
1:B:651:ILE:HG21	1:B:755:MET:CE	2.48	0.42
1:B:675:THR:C	1:B:680:LEU:HB2	2.44	0.42
1:B:676:PRO:HD2	1:B:677:GLU:OE2	2.18	0.42
1:C:127:SER:CB	1:C:211:TYR:CG	3.02	0.42
1:C:369:ASN:HA	1:C:389:ILE:HG21	2.01	0.42
1:C:558:VAL:HG12	1:C:559:PHE:N	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:ILE:HD11	1:C:765:LEU:CD1	2.49	0.42
1:C:598:LEU:HD21	1:C:670:TYR:HB3	2.00	0.42
1:C:742:ILE:HG21	1:C:751:ILE:HD12	2.00	0.42
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.44	0.42
1:A:581:ARG:NH1	1:A:601:PHE:CD1	2.88	0.42
1:B:150:ASN:O	1:B:151:ASN:CB	2.64	0.42
1:B:713:PHE:O	1:B:714:GLN:C	2.61	0.42
1:C:123:GLN:HB3	1:C:124:TRP:H	1.69	0.42
1:C:235:LEU:HD21	1:C:255:PRO:HG3	2.00	0.42
1:D:105:TYR:C	1:D:105:TYR:CD2	2.96	0.42
1:D:135:TYR:HA	3:D:822:HOH:O	2.18	0.42
1:D:201:TRP:CH2	1:D:205:GLU:HG2	2.53	0.42
1:A:310:ARG:HD3	1:A:327:ILE:CG2	2.49	0.42
1:B:44:THR:O	1:B:47:ASP:HB2	2.19	0.42
1:B:765:LEU:H	1:B:765:LEU:CD2	2.29	0.42
1:C:376:SER:OG	1:C:380:GLY:HA2	2.19	0.42
1:C:422:TYR:C	1:C:424:GLY:N	2.77	0.42
1:C:482:LEU:HA	1:C:482:LEU:HD12	1.66	0.42
1:C:518:ILE:C	1:C:519:LEU:HD23	2.45	0.42
1:C:692:ALA:HB1	1:C:726:VAL:HG21	2.00	0.42
1:A:158:SER:HA	1:A:216:TRP:CD2	2.54	0.42
1:A:459:VAL:CG2	1:A:460:SER:N	2.80	0.42
1:B:115:LEU:HG	1:B:132:TYR:HD2	1.84	0.42
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.01	0.42
1:B:197:GLY:C	1:B:213:ALA:HB3	2.45	0.42
1:B:204:GLU:O	1:B:204:GLU:HG2	2.20	0.42
1:B:310:ARG:NH1	1:B:329:ASP:OD2	2.52	0.42
1:C:55:LEU:HD11	1:C:561:LEU:CD1	2.50	0.42
1:C:649:CYS:CB	1:C:699:GLU:HB2	2.48	0.42
1:D:139:LYS:O	1:D:140:ARG:C	2.61	0.42
1:D:142:LEU:HD12	1:D:142:LEU:HA	1.73	0.42
1:D:514:LEU:HD12	1:D:526:TYR:O	2.19	0.42
1:A:459:VAL:CG2	1:A:460:SER:H	2.29	0.42
1:B:138:ASN:C	1:B:140:ARG:H	2.27	0.42
1:B:194:ILE:HD13	1:B:229:ASN:HA	2.01	0.42
1:B:464:GLU:O	1:B:465:ALA:CB	2.67	0.42
1:B:514:LEU:CD2	1:B:557:THR:HG22	2.48	0.42
1:C:242:SER:HB3	1:C:246:LEU:HD23	2.02	0.42
1:C:249:PRO:HG3	1:D:714:GLN:NE2	2.34	0.42
1:C:519:LEU:HD21	1:C:612:GLN:HE22	1.82	0.42
1:C:621:ASN:HA	1:C:624:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:HB3	1:D:92:ASN:H	1.83	0.42
1:D:157:TRP:CE3	1:D:164:LEU:HD23	2.54	0.42
1:D:383:HIS:CE1	1:D:399:LYS:HA	2.55	0.42
1:D:384:ILE:CG1	1:D:404:VAL:HG11	2.50	0.42
1:D:594:ILE:HD12	1:D:598:LEU:HD23	2.00	0.42
1:D:682:HIS:O	1:D:683:TYR:C	2.63	0.42
1:A:75:ASN:CA	1:A:92:ASN:HB3	2.48	0.42
1:B:517:ILE:HD12	1:B:612:GLN:HG3	2.01	0.42
1:C:234:PRO:HB2	1:D:248:TYR:CE1	2.54	0.42
1:C:651:ILE:HD13	1:C:755:MET:HE3	2.00	0.42
1:C:738:GLU:OE1	1:C:742:ILE:HA	2.20	0.42
1:D:229:ASN:HB3	1:D:265:THR:OG1	2.20	0.42
1:D:301:CYS:O	1:D:358:ARG:NH1	2.53	0.42
1:D:374:ILE:HD13	1:D:404:VAL:HG12	2.02	0.42
1:D:739:ASP:HB2	1:D:740:HIS:H	1.58	0.42
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.45	0.42
1:A:125:ARG:HH21	1:A:710:ASN:HD21	1.66	0.42
1:A:240:PHE:CE2	1:A:242:SER:HA	2.54	0.42
1:A:266:VAL:HG22	1:A:267:LYS:N	2.34	0.42
1:A:422:TYR:OH	1:A:423:LYS:HE3	2.20	0.42
1:B:677:GLU:CD	1:B:677:GLU:H	2.28	0.42
1:C:75:ASN:ND2	1:C:92:ASN:ND2	2.63	0.42
1:D:526:TYR:HB2	1:D:577:SER:O	2.19	0.42
1:A:60:LEU:HD22	1:A:68:TYR:CD2	2.55	0.42
1:A:110:ASP:OD2	1:A:111:GLY:N	2.53	0.42
1:B:110:ASP:OD2	1:B:112:GLN:HB2	2.20	0.42
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.55	0.42
1:C:705:GLY:O	1:C:708:ASP:HB2	2.20	0.42
1:D:449:LEU:HA	1:D:449:LEU:HD23	1.73	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.20	0.42
1:B:50:LYS:HD3	1:B:50:LYS:HA	1.82	0.42
1:B:168:TRP:CZ2	1:B:169:ASN:OD1	2.73	0.42
1:B:229:ASN:OD1	1:B:229:ASN:C	2.63	0.42
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.85	0.42
1:B:474:GLY:HA2	1:B:476:GLY:O	2.20	0.42
1:C:562:ASN:O	1:C:565:THR:N	2.52	0.42
1:D:323:SER:OG	1:D:347:GLU:HB3	2.20	0.42
1:D:361:GLU:OE2	1:D:363:HIS:NE2	2.50	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:A:192:ASP:HA	1:A:195:TYR:OH	2.19	0.42
1:A:599:GLY:N	1:A:602:GLU:OE1	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:GLU:CD	1:A:744:SER:HG	2.28	0.42
1:B:236:ILE:HG23	1:B:254:VAL:HG13	2.02	0.42
1:B:385:CYS:HA	1:B:396:PHE:HA	2.02	0.42
1:B:546:VAL:HA	3:B:826:HOH:O	2.20	0.42
1:C:188:THR:HB	1:C:194:ILE:HG21	2.02	0.42
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.42
1:C:433:LYS:O	1:C:433:LYS:HG3	2.19	0.42
1:C:496:ASP:O	1:C:497:ASN:C	2.63	0.42
1:D:634:TYR:HD1	1:D:656:VAL:O	2.02	0.42
1:D:678:ASP:CG	1:D:679:ASN:N	2.78	0.42
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.50	0.41
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.02	0.41
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.20	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:742:ILE:CD1	1:B:751:ILE:HD12	2.50	0.41
1:C:263:ASN:HD21	1:C:664:SER:HB2	1.84	0.41
1:C:446:SER:HA	1:C:449:LEU:HG	2.02	0.41
1:C:468:TYR:O	1:C:482:LEU:HD12	2.20	0.41
1:C:547:TYR:O	1:C:549:GLY:N	2.53	0.41
1:C:551:CYS:HB2	1:C:591:MET:SD	2.59	0.41
1:C:714:GLN:NE2	1:D:249:PRO:HD3	2.35	0.41
1:C:739:ASP:C	1:C:741:GLY:N	2.78	0.41
1:D:138:ASN:CG	1:D:139:LYS:N	2.74	0.41
1:A:535:ASP:OD1	1:A:538:LYS:HE2	2.20	0.41
1:A:620:ASP:OD2	1:A:623:ARG:HD2	2.20	0.41
1:B:425:MET:HA	1:B:426:PRO:HD2	1.90	0.41
1:B:433:LYS:HB2	1:B:445:LEU:HD21	2.02	0.41
1:B:629:TRP:HA	1:B:653:VAL:O	2.20	0.41
1:B:707:ALA:HB2	1:B:737:ASP:HA	2.02	0.41
1:C:477:LEU:CD1	1:C:501:ASP:HB2	2.50	0.41
1:C:510:PRO:CB	1:C:530:LEU:O	2.68	0.41
1:C:585:TYR:C	1:C:586:GLN:HG3	2.45	0.41
1:D:51:ASN:OD1	1:D:54:ARG:HD2	2.20	0.41
1:D:167:VAL:HG13	1:D:171:ASP:O	2.20	0.41
1:A:148:ILE:HA	1:A:149:PRO:HD2	1.79	0.41
1:A:248:TYR:CD2	1:B:258:LYS:HD2	2.54	0.41
1:B:136:ASP:CB	1:B:139:LYS:HG2	2.51	0.41
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.56	0.41
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.90	0.41
1:C:177:GLU:HB2	1:C:180:LEU:HD12	2.01	0.41
1:C:336:ARG:CG	1:C:336:ARG:NH1	2.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:ARG:NH2	1:D:679:ASN:HB2	2.35	0.41
1:A:108:SER:O	1:A:109:PRO:C	2.63	0.41
1:A:446:SER:HA	1:A:449:LEU:HD12	2.02	0.41
1:A:543:LEU:HD23	1:A:567:LEU:HD13	2.03	0.41
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.20	0.41
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.41
1:B:734:TRP:CD1	1:B:734:TRP:C	2.98	0.41
1:C:136:ASP:C	1:C:136:ASP:OD1	2.63	0.41
1:D:105:TYR:HD2	1:D:107:ILE:HD12	1.86	0.41
1:D:160:VAL:CG1	1:D:161:GLY:N	2.84	0.41
1:D:195:TYR:CE2	1:D:200:ASP:HA	2.56	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.03	0.41
1:D:434:ILE:HG13	1:D:442:VAL:HG22	2.02	0.41
1:D:482:LEU:HD12	1:D:482:LEU:HA	1.90	0.41
1:A:375:ILE:HD11	1:A:396:PHE:CZ	2.55	0.41
1:A:438:ASP:C	1:A:440:THR:H	2.28	0.41
1:B:340:LEU:HD23	1:B:340:LEU:HA	1.88	0.41
1:C:422:TYR:C	1:C:424:GLY:H	2.29	0.41
1:D:229:ASN:OD1	1:D:229:ASN:C	2.62	0.41
1:D:240:PHE:CE1	1:D:737:ASP:HB3	2.55	0.41
1:D:330:TYR:HD1	1:D:337:TRP:CE2	2.38	0.41
1:D:475:PRO:HD3	1:D:557:THR:HB	2.01	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.93	0.41
1:A:124:TRP:HA	1:A:124:TRP:HE3	1.84	0.41
1:A:620:ASP:O	1:A:622:LYS:N	2.54	0.41
1:A:673:LEU:HD23	1:A:674:PRO:HD2	2.02	0.41
1:B:80:ASN:OD1	1:B:80:ASN:C	2.63	0.41
1:B:187:TRP:CZ3	1:B:281:ASN:OD1	2.73	0.41
1:B:347:GLU:OE1	1:B:373:LYS:NZ	2.52	0.41
1:D:374:ILE:CD1	1:D:406:GLY:HA2	2.50	0.41
1:A:340:LEU:C	1:A:342:ALA:N	2.79	0.41
1:A:383:HIS:HA	1:A:404:VAL:HG23	2.03	0.41
1:A:457:TYR:CE1	1:A:472:CYS:HB2	2.56	0.41
1:B:563:TRP:CZ3	1:B:567:LEU:HD11	2.55	0.41
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.83	0.41
1:C:325:MET:HE3	1:C:327:ILE:HD11	2.02	0.41
1:D:107:ILE:HD12	1:D:107:ILE:N	2.35	0.41
1:D:125:ARG:HG2	1:D:126:HIS:CD2	2.56	0.41
1:D:629:TRP:O	1:D:630:SER:CB	2.69	0.41
1:A:227:GLN:N	1:A:267:LYS:O	2.54	0.41
1:A:353:TRP:CZ2	1:A:670:TYR:HE1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:MET:HB3	1:A:509:MET:HE3	1.75	0.41
1:B:135:TYR:O	1:B:137:LEU:N	2.54	0.41
1:B:660:GLU:OE2	1:B:684:ARG:NE	2.53	0.41
1:B:738:GLU:OE2	1:B:744:SER:HB2	2.21	0.41
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.20	0.41
1:C:175:LYS:HG3	1:C:182:SER:HB3	2.02	0.41
1:C:293:MET:HG2	1:C:315:TRP:CB	2.51	0.41
1:C:397:ILE:O	1:C:397:ILE:HG13	2.20	0.41
1:C:568:ALA:HA	1:C:573:ILE:O	2.21	0.41
1:D:256:TYR:HA	1:D:257:PRO:HD3	1.92	0.41
1:D:428:GLY:C	1:D:429:ARG:HG2	2.46	0.41
1:A:73:GLU:C	1:A:75:ASN:N	2.79	0.41
1:A:132:TYR:CZ	1:A:155:VAL:HG12	2.56	0.41
1:A:343:ARG:HG2	1:A:389:ILE:HD12	2.02	0.41
1:A:381:TYR:CE2	1:A:401:THR:C	2.99	0.41
1:A:387:PHE:CE2	1:A:394:CYS:CB	3.04	0.41
1:A:513:LYS:HE2	1:A:515:ASP:CB	2.51	0.41
1:A:640:LEU:HB3	1:A:698:VAL:HG21	2.02	0.41
1:B:67:GLU:HA	1:B:79:PHE:O	2.20	0.41
1:B:524:PHE:CD2	1:B:580:GLY:HA2	2.56	0.41
1:B:599:GLY:N	1:B:602:GLU:OE1	2.46	0.41
1:C:110:ASP:OD2	1:C:110:ASP:C	2.62	0.41
1:C:188:THR:O	1:C:194:ILE:CG2	2.69	0.41
1:C:192:ASP:HA	1:C:195:TYR:OH	2.21	0.41
1:D:105:TYR:CD2	1:D:107:ILE:CD1	3.03	0.41
1:D:154:TRP:O	1:D:166:TYR:HA	2.21	0.41
1:D:387:PHE:CZ	1:D:394:CYS:SG	3.14	0.41
1:D:448:GLU:O	1:D:449:LEU:C	2.63	0.41
1:D:563:TRP:CZ3	1:D:567:LEU:HD11	2.56	0.41
1:D:581:ARG:NE	1:D:605:ASP:OD2	2.49	0.41
1:D:624:ILE:O	1:D:647:PHE:HA	2.21	0.41
1:D:732:ALA:O	1:D:733:MET:HB2	2.20	0.41
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.21	0.41
1:B:366:LEU:C	1:B:368:GLY:H	2.29	0.41
1:C:82:GLU:HG2	1:C:83:TYR:CE1	2.56	0.41
1:C:365:THR:O	1:C:366:LEU:C	2.64	0.41
1:A:180:LEU:O	1:A:181:PRO:O	2.39	0.40
1:A:438:ASP:C	1:A:438:ASP:OD1	2.63	0.40
1:B:501:ASP:O	1:B:505:GLN:HG2	2.21	0.40
1:B:594:ILE:CG2	1:B:601:PHE:HB2	2.51	0.40
1:B:659:TRP:O	1:B:667:THR:HG21	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ASP:HB2	1:B:740:HIS:H	1.74	0.40
1:C:56:LYS:C	1:C:57:LEU:HD12	2.47	0.40
1:C:169:ASN:HD22	1:C:169:ASN:N	2.19	0.40
1:D:51:ASN:O	1:D:54:ARG:CD	2.69	0.40
1:D:136:ASP:N	3:D:822:HOH:O	2.54	0.40
1:D:258:LYS:NZ	1:D:661:TYR:O	2.52	0.40
1:D:623:ARG:HB3	1:D:763:PHE:CD1	2.56	0.40
1:D:763:PHE:C	1:D:765:LEU:HD22	2.46	0.40
1:A:82:GLU:O	1:A:492:ARG:NH2	2.54	0.40
1:A:107:ILE:HA	1:A:114:ILE:HA	2.02	0.40
1:A:158:SER:HB2	1:A:159:PRO:HD2	2.04	0.40
1:A:242:SER:CB	1:A:246:LEU:HD22	2.50	0.40
1:A:372:TYR:CZ	1:A:386:TYR:CE1	3.08	0.40
1:A:716:SER:O	1:A:717:ALA:C	2.64	0.40
1:B:289:ALA:HB2	1:B:315:TRP:CE3	2.55	0.40
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.22	0.40
1:B:446:SER:HA	1:B:449:LEU:HG	2.01	0.40
1:B:450:ASN:CG	1:B:453:ARG:HB3	2.46	0.40
1:B:550:PRO:O	1:B:551:CYS:CB	2.69	0.40
1:B:760:LYS:HD2	1:B:766:PRO:O	2.22	0.40
1:C:139:LYS:O	1:C:140:ARG:C	2.65	0.40
1:C:611:ARG:HG2	1:C:615:LYS:HZ2	1.85	0.40
1:C:651:ILE:CD1	1:C:755:MET:HE3	2.51	0.40
1:D:148:ILE:O	1:D:149:PRO:O	2.38	0.40
1:D:427:GLY:O	1:D:557:THR:HG23	2.21	0.40
1:D:720:SER:O	1:D:724:VAL:HG23	2.21	0.40
1:A:671:MET:SD	1:A:682:HIS:HD2	2.44	0.40
1:B:144:THR:O	1:B:147:ARG:HD2	2.21	0.40
1:B:356:ARG:HD3	1:B:585:TYR:HE1	1.85	0.40
1:B:433:LYS:HE2	1:B:488:ASP:OD1	2.21	0.40
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.93	0.40
1:B:480:TYR:CD1	1:B:480:TYR:N	2.90	0.40
1:B:629:TRP:O	1:B:630:SER:CB	2.66	0.40
1:C:70:TYR:HB3	1:C:79:PHE:HE2	1.87	0.40
1:C:369:ASN:CA	1:C:389:ILE:HG23	2.51	0.40
1:A:602:GLU:OE2	1:A:602:GLU:N	2.50	0.40
1:B:82:GLU:HA	1:B:82:GLU:OE1	2.22	0.40
1:C:558:VAL:CG1	1:C:559:PHE:N	2.85	0.40
1:C:633:GLY:CA	1:C:655:PRO:HB3	2.46	0.40
1:C:753:THR:O	1:C:757:HIS:CD2	2.75	0.40
1:C:761:GLN:NE2	1:C:762:CYS:N	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HD12	1:D:90:LEU:HA	1.89	0.40
1:D:266:VAL:C	1:D:267:LYS:HG2	2.46	0.40
1:D:581:ARG:HH21	1:D:605:ASP:CG	2.27	0.40
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.01	0.40
1:B:121:VAL:HB	1:B:129:THR:OG1	2.22	0.40
1:B:199:THR:HG23	1:B:213:ALA:HB2	2.03	0.40
1:B:658:ARG:HE	1:B:687:THR:HG21	1.87	0.40
1:C:50:LYS:O	1:C:51:ASN:C	2.64	0.40
1:C:355:GLY:O	1:C:356:ARG:C	2.65	0.40
1:C:566:TYR:O	1:C:567:LEU:C	2.62	0.40
1:C:657:SER:HB3	1:C:719:ILE:CD1	2.51	0.40
1:D:50:LYS:HD3	1:D:50:LYS:HA	1.80	0.40
1:D:77:LEU:N	1:D:77:LEU:CD1	2.84	0.40
1:D:383:HIS:HB3	1:D:398:THR:OG1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	726/728 (100%)	593 (82%)	112 (15%)	21 (3%)	3	19
1	B	726/728 (100%)	622 (86%)	84 (12%)	20 (3%)	4	20
1	C	726/728 (100%)	620 (85%)	86 (12%)	20 (3%)	4	20
1	D	726/728 (100%)	634 (87%)	73 (10%)	19 (3%)	4	21
All	All	2904/2912 (100%)	2469 (85%)	355 (12%)	80 (3%)	4	20

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	320	GLN
1	A	439	TYR
1	B	137	LEU
1	B	320	GLN
1	B	520	ASN
1	B	712	HIS
1	C	74	ASN
1	C	106	SER
1	C	143	ILE
1	C	548	ALA
1	D	88	VAL
1	D	111	GLY
1	D	320	GLN
1	A	139	LYS
1	A	143	ILE
1	A	181	PRO
1	A	209	SER
1	A	261	ALA
1	A	389	ILE
1	A	614	SER
1	A	621	ASN
1	B	73	GLU
1	B	146	GLU
1	B	280	THR
1	B	536	LYS
1	B	764	SER
1	C	712	HIS
1	D	138	ASN
1	D	764	SER
1	A	231	THR
1	A	242	SER
1	A	577	SER
1	B	377	ASN
1	B	616	MET
1	C	583	SER
1	C	668	GLU
1	D	149	PRO
1	D	366	LEU
1	D	521	GLU
1	D	710	ASN
1	D	712	HIS
1	A	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	ASN
1	A	149	PRO
1	A	333	SER
1	A	491	LEU
1	B	261	ALA
1	C	366	LEU
1	C	536	LYS
1	C	695	PHE
1	D	178	PRO
1	D	423	LYS
1	D	683	TYR
1	A	191	GLU
1	A	447	CYS
1	B	136	ASP
1	B	143	ILE
1	B	548	ALA
1	C	51	ASN
1	C	218	PRO
1	C	259	ALA
1	C	320	GLN
1	C	664	SER
1	C	667	THR
1	C	715	GLN
1	C	737	ASP
1	D	130	ALA
1	D	714	GLN
1	B	645	GLY
1	B	714	GLN
1	D	143	ILE
1	D	280	THR
1	B	109	PRO
1	B	674	PRO
1	B	742	ILE
1	D	742	ILE
1	C	355	GLY
1	C	541	PRO
1	D	181	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	653/653 (100%)	611 (94%)	42 (6%)	16	44
1	B	653/653 (100%)	620 (95%)	33 (5%)	21	52
1	C	653/653 (100%)	611 (94%)	42 (6%)	16	44
1	D	653/653 (100%)	610 (93%)	43 (7%)	15	43
All	All	2612/2612 (100%)	2452 (94%)	160 (6%)	17	46

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	55	LEU
1	A	57	LEU
1	A	77	LEU
1	A	95	PHE
1	A	96	ASP
1	A	106	SER
1	A	109	PRO
1	A	145	GLU
1	A	186	THR
1	A	202	VAL
1	A	214	LEU
1	A	254	VAL
1	A	256	TYR
1	A	265	THR
1	A	279	VAL
1	A	280	THR
1	A	288	THR
1	A	293	MET
1	A	295	ILE
1	A	339	CYS
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	391	LYS
1	A	393	ASP
1	A	413	ASP
1	A	429	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	458	SER
1	A	502	LYS
1	A	507	VAL
1	A	536	LYS
1	A	542	LEU
1	A	570	THR
1	A	577	SER
1	A	597	ARG
1	A	621	ASN
1	A	657	SER
1	A	677	GLU
1	A	704	HIS
1	A	714	GLN
1	A	728	VAL
1	B	54	ARG
1	B	72	GLN
1	B	73	GLU
1	B	75	ASN
1	B	78	VAL
1	B	89	PHE
1	B	91	GLU
1	B	108	SER
1	B	114	ILE
1	B	145	GLU
1	B	214	LEU
1	B	221	THR
1	B	239	SER
1	B	243	ASP
1	B	251	THR
1	B	254	VAL
1	B	272	ASN
1	B	277	SER
1	B	283	THR
1	B	332	GLU
1	B	341	VAL
1	B	382	ARG
1	B	445	LEU
1	B	448	GLU
1	B	452	GLU
1	B	487	ASN
1	B	522	THR
1	B	546	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	590	ILE
1	B	606	GLN
1	B	658	ARG
1	B	677	GLU
1	B	761	GLN
1	C	96	ASP
1	C	108	SER
1	C	109	PRO
1	C	118	TYR
1	C	133	ASP
1	C	144	THR
1	C	145	GLU
1	C	170	ASN
1	C	184	ARG
1	C	188	THR
1	C	214	LEU
1	C	215	TRP
1	C	236	ILE
1	C	251	THR
1	C	254	VAL
1	C	293	MET
1	C	301	CYS
1	C	319	ILE
1	C	326	ASP
1	C	332	GLU
1	C	333	SER
1	C	336	ARG
1	C	382	ARG
1	C	388	GLN
1	C	401	THR
1	C	421	GLU
1	C	434	ILE
1	C	448	GLU
1	C	472	CYS
1	C	492	ARG
1	C	502	LYS
1	C	542	LEU
1	C	546	VAL
1	C	565	THR
1	C	583	SER
1	C	621	ASN
1	C	627	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	658	ARG
1	C	663	ASP
1	C	667	THR
1	C	728	VAL
1	C	764	SER
1	D	52	THR
1	D	55	LEU
1	D	57	LEU
1	D	63	ILE
1	D	67	GLU
1	D	78	VAL
1	D	80	ASN
1	D	113	PHE
1	D	121	VAL
1	D	137	LEU
1	D	138	ASN
1	D	151	ASN
1	D	152	THR
1	D	156	THR
1	D	158	SER
1	D	169	ASN
1	D	175	LYS
1	D	180	LEU
1	D	184	ARG
1	D	191	GLU
1	D	214	LEU
1	D	221	THR
1	D	236	ILE
1	D	254	VAL
1	D	272	ASN
1	D	278	SER
1	D	284	SER
1	D	295	ILE
1	D	351	THR
1	D	385	CYS
1	D	393	ASP
1	D	448	GLU
1	D	487	ASN
1	D	507	VAL
1	D	511	SER
1	D	546	VAL
1	D	589	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	590	ILE
1	D	606	GLN
1	D	677	GLU
1	D	685	ASN
1	D	761	GLN
1	D	765	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	286	GLN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	505	GLN
1	A	572	ASN
1	A	621	ASN
1	A	710	ASN
1	A	712	HIS
1	A	731	GLN
1	A	748	HIS
1	A	749	GLN
1	A	757	HIS
1	B	51	ASN
1	B	66	HIS
1	B	74	ASN
1	B	75	ASN
1	B	150	ASN
1	B	169	ASN
1	B	272	ASN
1	B	298	HIS
1	B	435	GLN
1	B	487	ASN
1	B	506	ASN
1	B	508	GLN
1	B	685	ASN
1	B	712	HIS
1	B	731	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	748	HIS
1	B	750	HIS
1	B	761	GLN
1	C	75	ASN
1	C	100	HIS
1	C	103	ASN
1	C	126	HIS
1	C	138	ASN
1	C	169	ASN
1	C	170	ASN
1	C	345	HIS
1	C	450	ASN
1	C	508	GLN
1	C	572	ASN
1	C	621	ASN
1	C	712	HIS
1	C	731	GLN
1	C	754	HIS
1	C	757	HIS
1	C	761	GLN
1	D	72	GLN
1	D	74	ASN
1	D	85	ASN
1	D	92	ASN
1	D	150	ASN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	388	GLN
1	D	455	GLN
1	D	487	ASN
1	D	506	ASN
1	D	595	ASN
1	D	606	GLN
1	D	685	ASN
1	D	712	HIS
1	D	714	GLN
1	D	731	GLN
1	D	757	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	761	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	13Z	C	767	1	25,27,27	1.54	3 (12%)	31,41,41	1.18	2 (6%)
2	13Z	D	767	1	25,27,27	1.01	2 (8%)	31,41,41	1.11	2 (6%)
2	13Z	B	767	1	25,27,27	1.46	3 (12%)	31,41,41	1.08	3 (9%)
2	13Z	A	767	1	25,27,27	1.58	5 (20%)	31,41,41	1.15	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	13Z	C	767	1	-	6/26/39/39	0/2/2/2
2	13Z	D	767	1	-	9/26/39/39	0/2/2/2
2	13Z	B	767	1	-	7/26/39/39	0/2/2/2
2	13Z	A	767	1	-	9/26/39/39	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	767	13Z	C9-N3	5.26	1.33	1.28
2	C	767	13Z	C9-N3	5.14	1.33	1.28
2	A	767	13Z	C9-N3	4.35	1.32	1.28
2	A	767	13Z	C11-N4	3.94	1.53	1.49
2	C	767	13Z	C8-N2	2.96	1.31	1.28
2	D	767	13Z	C9-N3	2.64	1.31	1.28
2	A	767	13Z	C1-N1	2.57	1.50	1.46
2	A	767	13Z	C8-N2	2.53	1.30	1.28
2	C	767	13Z	C5-N1	2.34	1.42	1.35
2	B	767	13Z	C8-N2	2.30	1.30	1.28
2	D	767	13Z	C1-N1	2.27	1.49	1.46
2	B	767	13Z	C5-N1	2.27	1.41	1.35
2	A	767	13Z	C5-N1	2.18	1.41	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	767	13Z	C3-C4-N1	2.75	107.16	103.13
2	B	767	13Z	C3-C4-N1	2.56	106.88	103.13
2	D	767	13Z	C4-N1-C5	-2.54	124.37	129.13
2	C	767	13Z	C4-N1-C5	-2.52	124.42	129.13
2	D	767	13Z	C3-C4-N1	2.42	106.68	103.13
2	A	767	13Z	F1-C3-C4	2.39	111.85	108.41
2	B	767	13Z	F1-C3-C4	2.23	111.63	108.41
2	B	767	13Z	C4-N1-C5	-2.15	125.09	129.13
2	A	767	13Z	C3-C4-N1	2.15	106.28	103.13
2	A	767	13Z	C2-C1-N1	2.12	104.77	101.67

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	767	13Z	C5-C6-N4-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	767	13Z	O2-C7-C8-O3
2	A	767	13Z	C13-C11-N4-C6
2	A	767	13Z	C15-C11-N4-C6
2	A	767	13Z	C17-C11-N4-C6
2	A	767	13Z	N4-C11-C15-O4
2	A	767	13Z	C13-C11-C15-O4
2	A	767	13Z	C17-C11-C15-O4
2	B	767	13Z	C15-C11-N4-C6
2	C	767	13Z	O2-C7-C8-O3
2	C	767	13Z	C13-C11-N4-C6
2	C	767	13Z	C15-C11-N4-C6
2	C	767	13Z	C17-C11-N4-C6
2	D	767	13Z	O2-C7-C8-O3
2	D	767	13Z	C13-C11-N4-C6
2	D	767	13Z	C15-C11-N4-C6
2	D	767	13Z	C17-C11-N4-C6
2	D	767	13Z	N4-C11-C15-O4
2	D	767	13Z	C13-C11-C15-O4
2	D	767	13Z	C17-C11-C15-O4
2	A	767	13Z	C1-C7-C8-O3
2	C	767	13Z	C1-C7-C8-O3
2	D	767	13Z	C1-C7-C8-O3
2	B	767	13Z	O1-C5-C6-N4
2	B	767	13Z	N1-C5-C6-N4
2	B	767	13Z	O2-C7-C8-O3
2	B	767	13Z	C5-C6-N4-C11
2	C	767	13Z	C5-C6-N4-C11
2	D	767	13Z	C5-C6-N4-C11
2	B	767	13Z	C17-C11-N4-C6
2	B	767	13Z	C1-C7-C8-O3

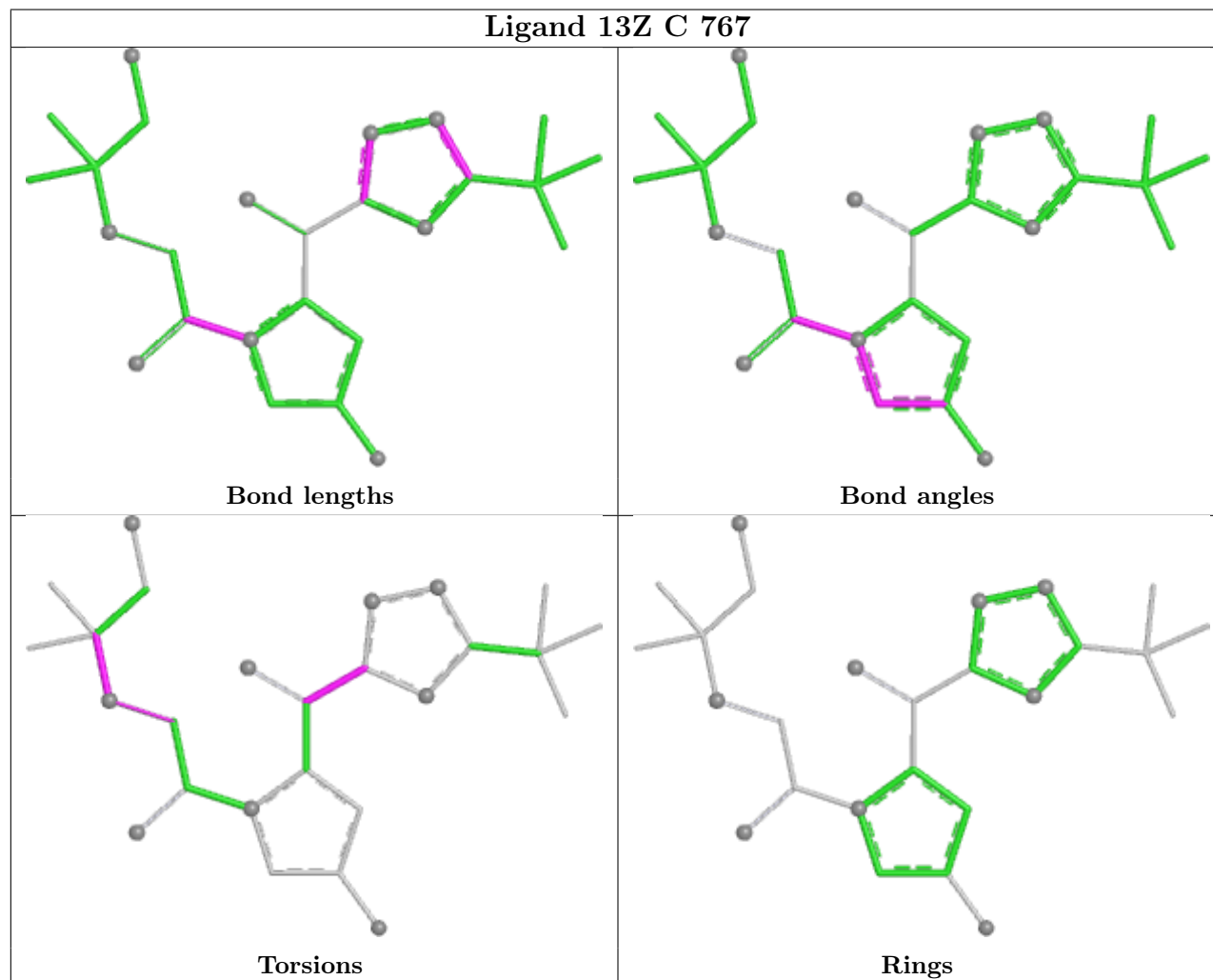
There are no ring outliers.

4 monomers are involved in 8 short contacts:

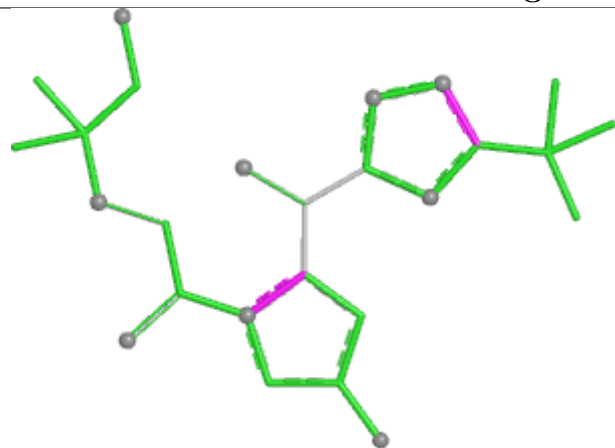
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	767	13Z	1	0
2	D	767	13Z	3	0
2	B	767	13Z	2	0
2	A	767	13Z	2	0

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

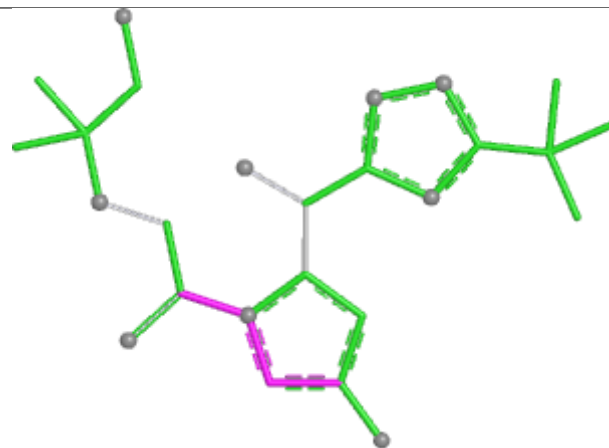
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



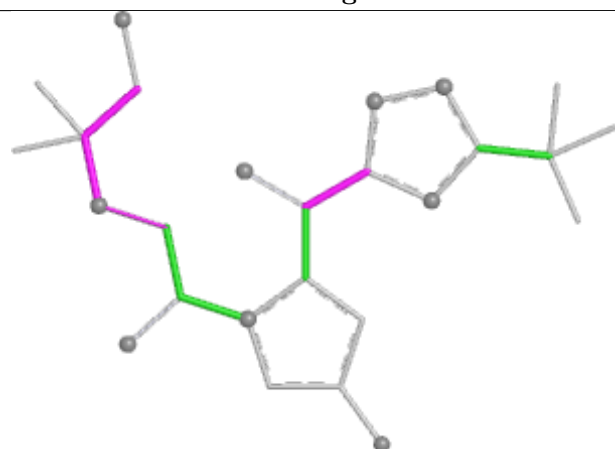
Ligand 13Z D 767



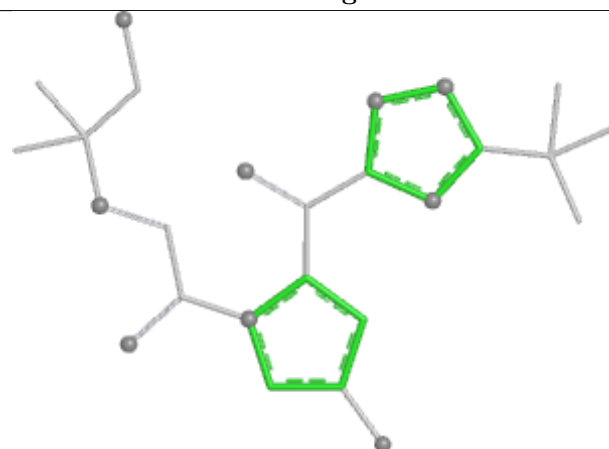
Bond lengths



Bond angles

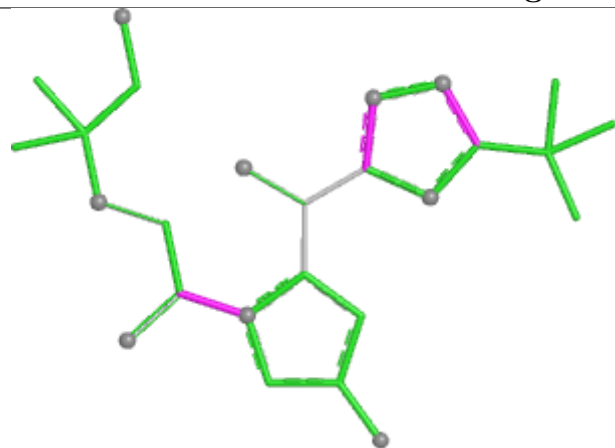


Torsions

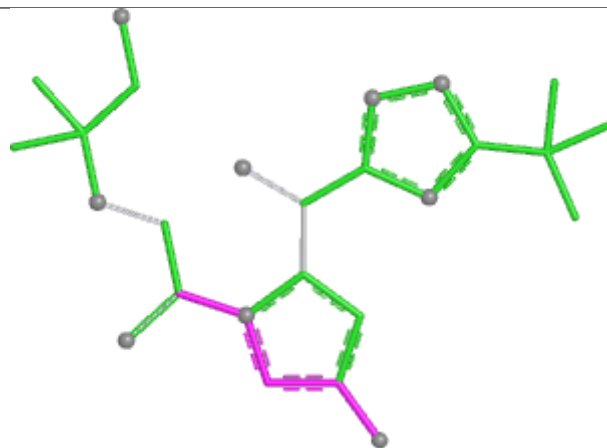


Rings

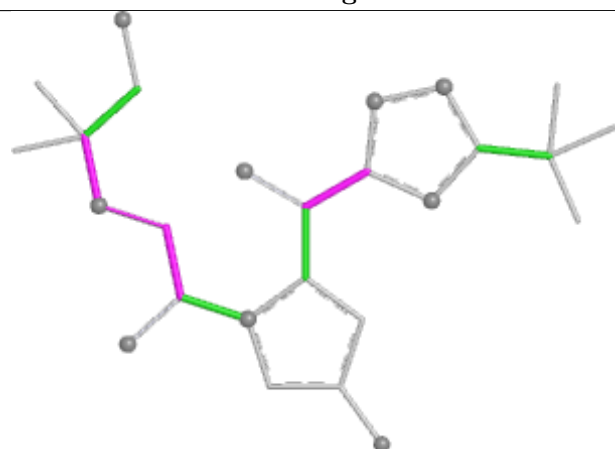
Ligand 13Z B 767



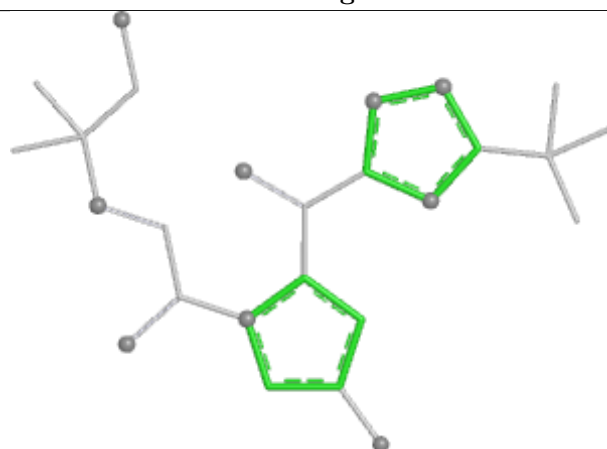
Bond lengths



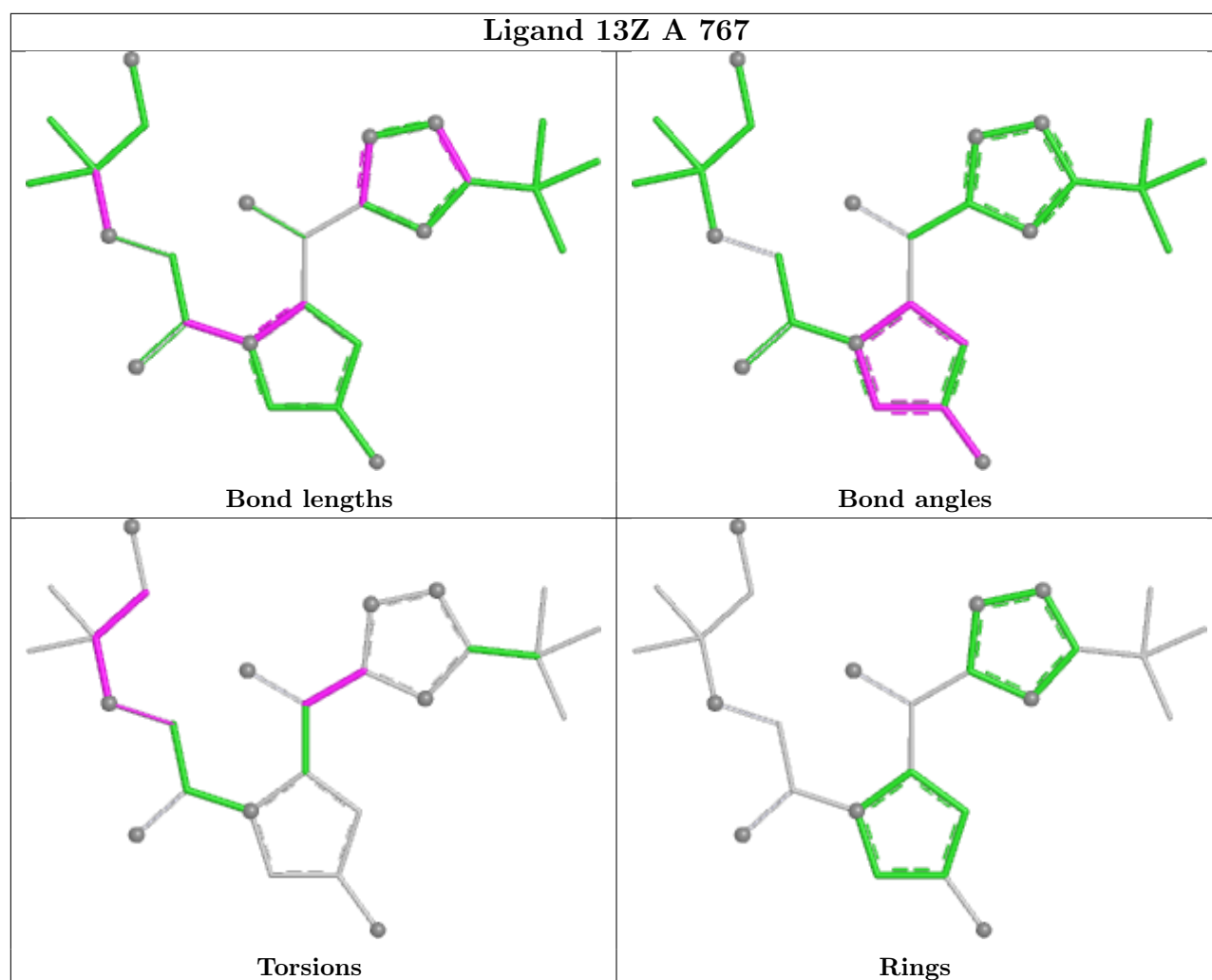
Bond angles



Torsions



Rings



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.