



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:25 AM UTC

PDB ID : 1XKH / pdb_00001xkh
Title : Pyoverdine outer membrane receptor FpvA from *Pseudomonas aeruginosa* PAO1 bound to pyoverdine
Authors : Cobessi, D.; Celia, H.; Folschweiller, N.; Schalk, I.J.; Abdallah, M.A.; Pattus, F.
Deposited on : 2004-09-29
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

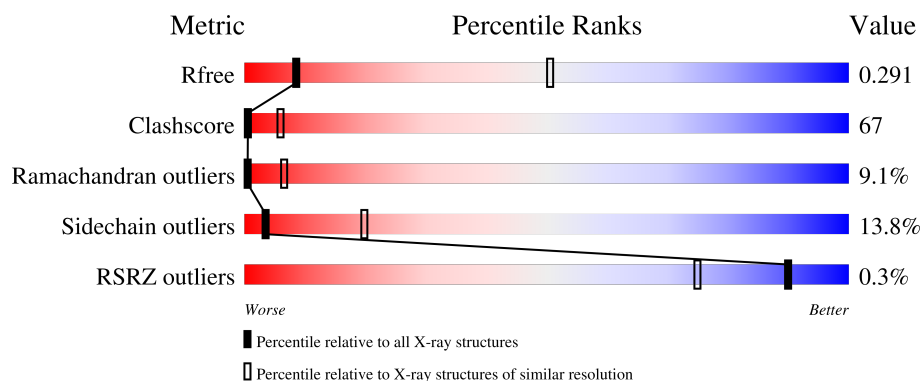
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	687	 23% 59% 17% .
1	B	687	 22% 58% 17% .
1	C	687	 23% 58% 17% .
2	I	8	 12% 38% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	8	
2	K	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	2002	-	-	X	-
4	PVE	I	1	X	-	-	-
4	PVE	J	1	X	-	-	-
4	PVE	K	1	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16719 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 Ferripyoverdine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			
1	B	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			
1	C	687	Total	C	N	O	Se	0	0	0
			5474	3449	933	1080	12			

- Molecule 2 is a protein called Pyoverdine C-E.

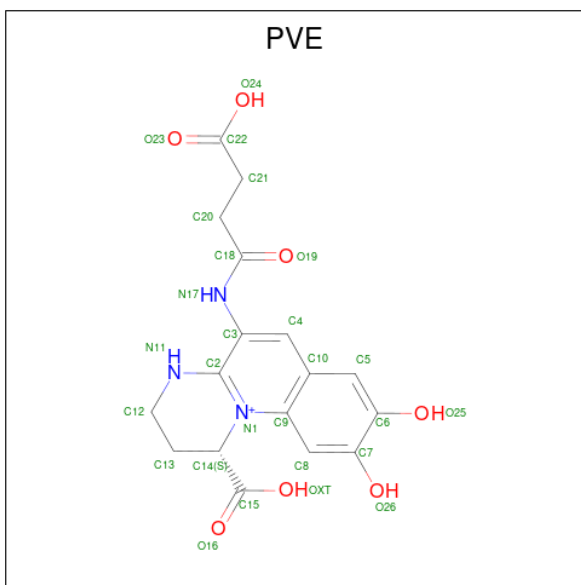
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			68	38	14	16			
2	J	8	Total	C	N	O	0	0	0
			68	38	14	16			
2	K	8	Total	C	N	O	0	0	0
			68	38	14	16			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is (1S)-1-CARBOXY-5-[(3-CARBOXYPROPANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (CCD ID: PVE) (formula: C₁₇H₁₈N₃O₇).

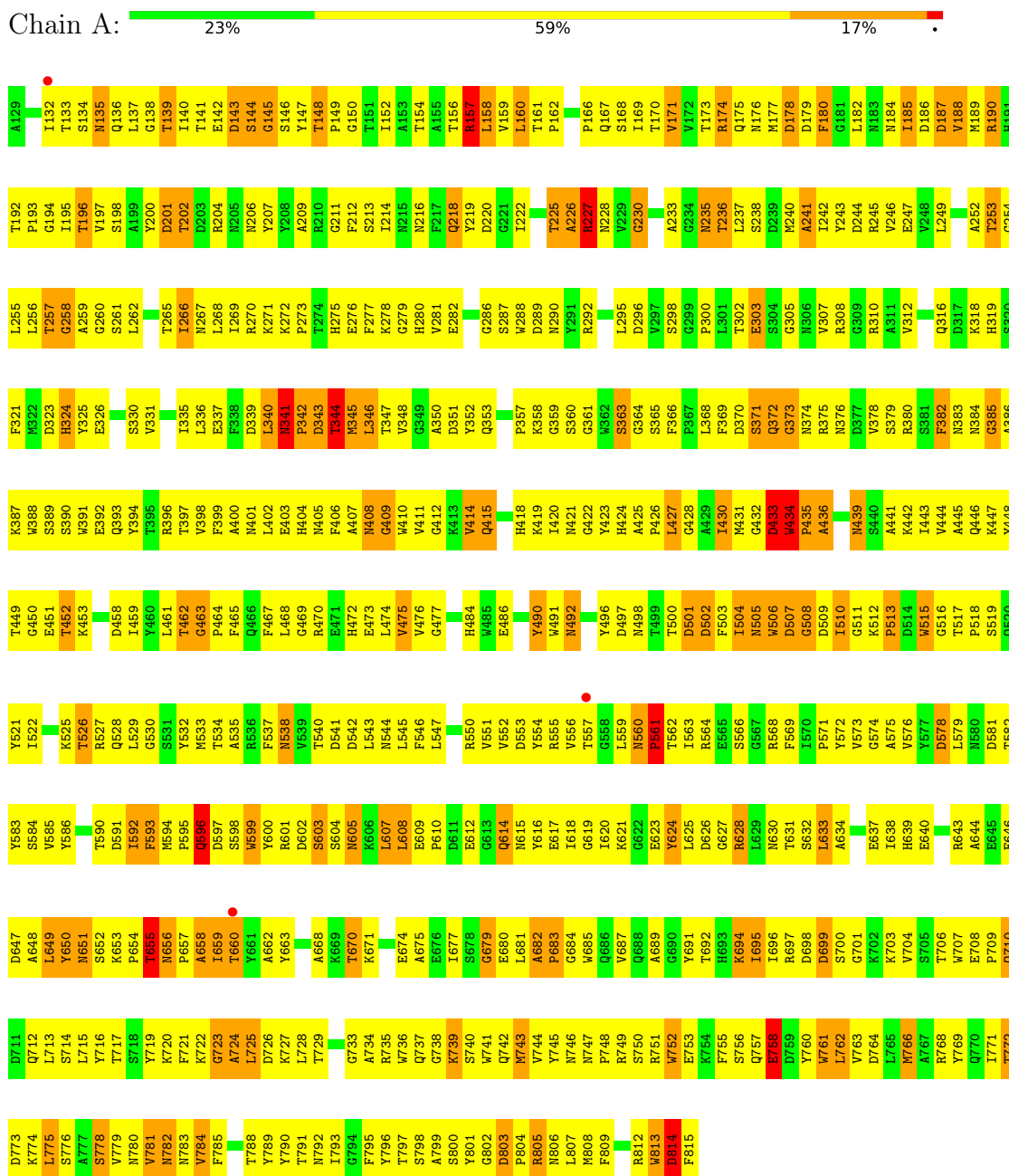


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total 26	C 17	N 3	O 6	0	0
4	J	1	Total 26	C 17	N 3	O 6	0	0
4	K	1	Total 26	C 17	N 3	O 6	0	0

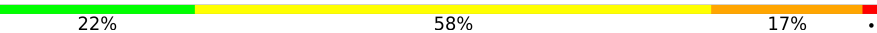
3 Residue-property plots

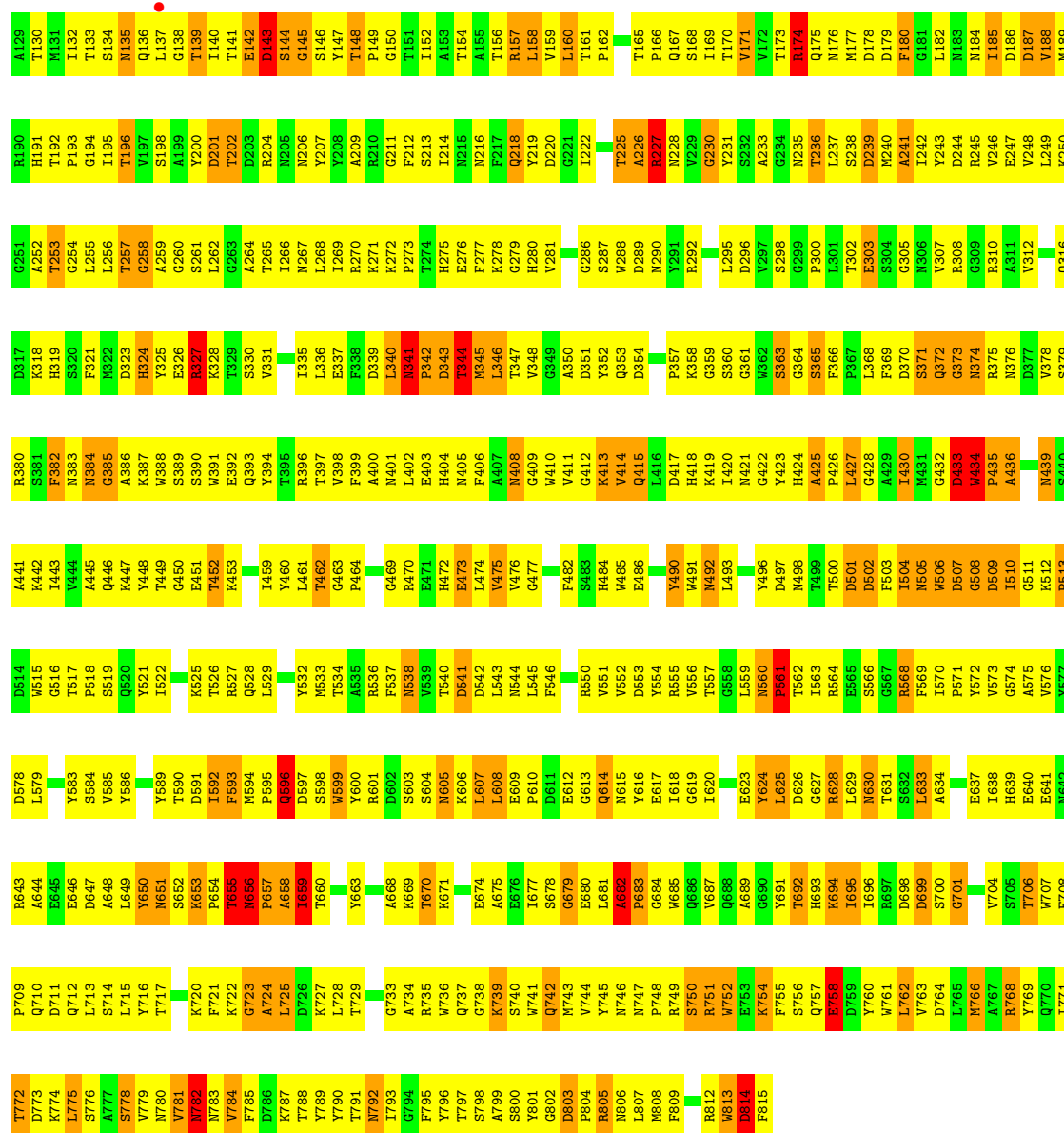
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Ferripyoverdine receptor

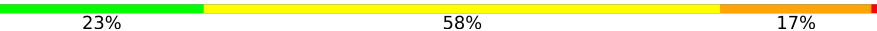


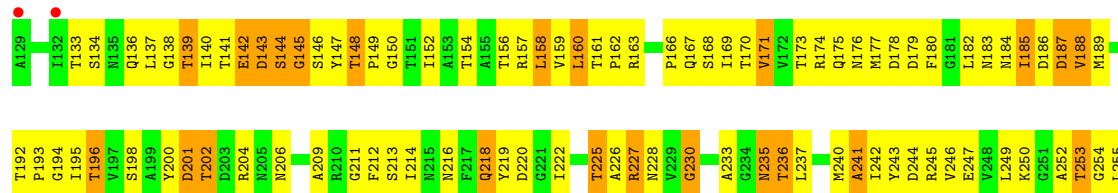
• Molecule 1: Ferripyoverdine receptor

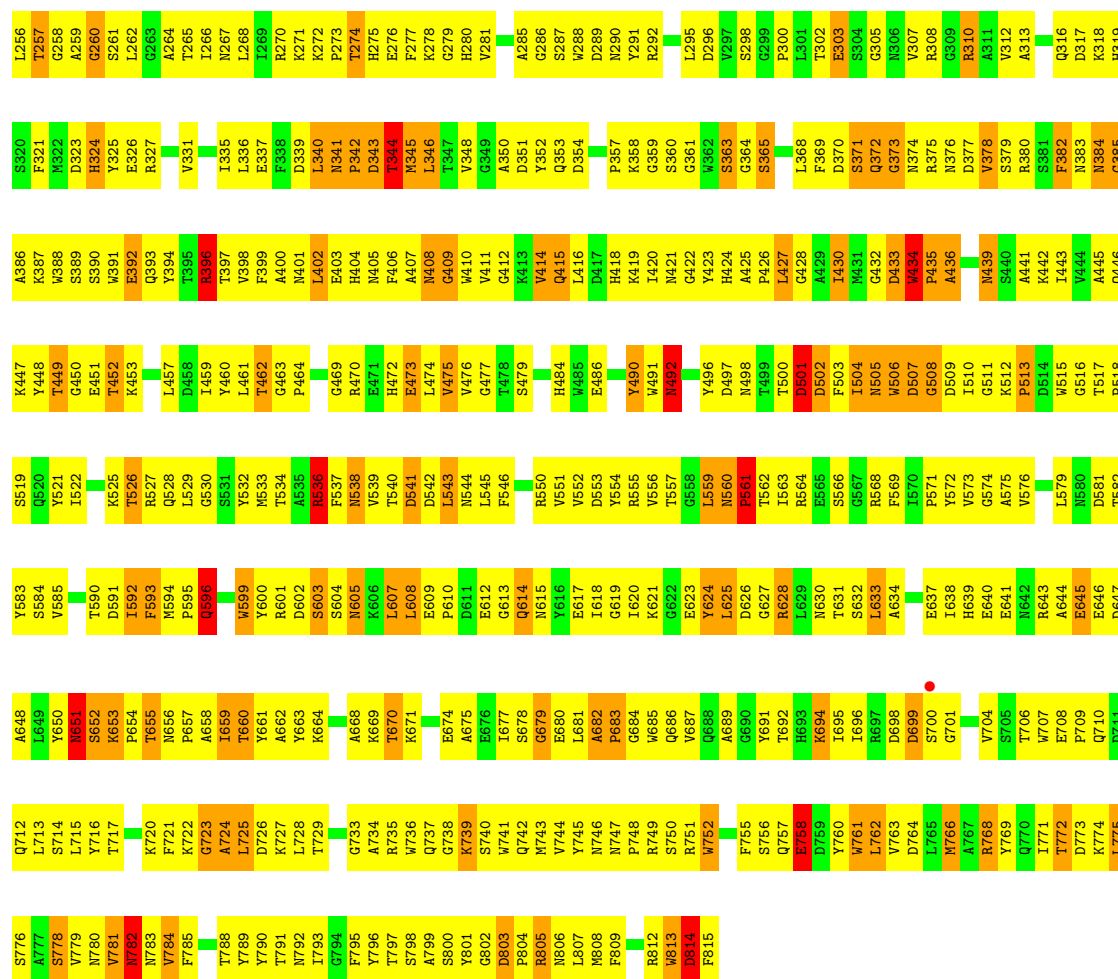
Chain B:  22% 58% 17%



• Molecule 1: Ferripyoverdine receptor

Chain C:  23% 58% 17%





● Molecule 2: Pyoverdin C-E

Chain I: 12% 38% 50%



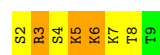
● Molecule 2: Pyoverdin C-E

Chain J: 12% 50% 38%



● Molecule 2: Pyoverdin C-E

Chain K: 12% 50% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.45Å 231.34Å 121.69Å 90.00° 104.57° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.60) 96.8 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.288 0.260 , 0.291	Depositor DCC
R_{free} test set	2105 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	16719	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.58	0/5606	1.07	37/7599 (0.5%)
1	B	0.58	1/5606 (0.0%)	1.07	45/7599 (0.6%)
1	C	0.58	0/5606	1.07	38/7599 (0.5%)
2	I	0.71	0/31	1.14	0/36
2	J	0.79	0/31	1.10	0/36
2	K	0.73	0/31	0.97	0/36
All	All	0.58	1/16911 (0.0%)	1.07	120/22905 (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	3
1	B	0	4
1	C	0	4
2	I	0	5
2	J	0	5
2	K	0	4
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	THR	CA-C	5.49	1.55	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	813	TRP	N-CA-C	12.28	125.52	110.41
1	A	813	TRP	N-CA-C	12.28	125.42	110.19
1	C	813	TRP	N-CA-C	12.19	125.40	110.41
1	A	651	ASN	N-CA-C	-10.80	98.81	113.18
1	C	782	ASN	N-CA-C	10.70	124.23	111.82
1	A	782	ASN	N-CA-C	10.62	124.14	111.82
1	B	782	ASN	N-CA-C	10.40	123.89	111.82
1	B	651	ASN	N-CA-C	-9.22	101.93	113.55
1	B	226	ALA	N-CA-C	-8.56	103.89	112.97
1	A	226	ALA	N-CA-C	-8.37	104.10	112.97
1	C	226	ALA	N-CA-C	-8.33	104.14	112.97
1	A	188	VAL	N-CA-C	-7.93	105.36	111.62
1	B	434	TRP	N-CA-C	7.76	126.96	109.81
1	C	272	LYS	CA-C-N	7.63	127.67	119.89
1	C	272	LYS	C-N-CA	7.63	127.67	119.89
1	A	434	TRP	N-CA-C	7.61	126.63	109.81
1	C	434	TRP	N-CA-C	7.60	126.61	109.81
1	C	188	VAL	N-CA-C	-7.18	105.38	111.56
1	C	372	GLN	N-CA-C	-7.05	105.86	114.75
1	A	372	GLN	N-CA-C	-7.04	105.88	114.75
1	A	272	LYS	CA-C-N	7.01	127.05	119.89
1	A	272	LYS	C-N-CA	7.01	127.05	119.89
1	B	409	GLY	N-CA-C	-6.99	105.17	115.72
1	C	409	GLY	N-CA-C	-6.99	105.17	115.72
1	A	463	GLY	CA-C-N	6.96	127.38	119.93
1	A	463	GLY	C-N-CA	6.96	127.38	119.93
1	A	148	THR	CA-C-N	6.88	127.33	120.52
1	A	148	THR	C-N-CA	6.88	127.33	120.52
1	C	148	THR	CA-C-N	6.87	127.32	120.52
1	C	148	THR	C-N-CA	6.87	127.32	120.52
1	A	409	GLY	N-CA-C	-6.80	105.45	115.72
1	B	188	VAL	N-CA-C	-6.77	105.74	111.56
1	C	652	SER	N-CA-C	-6.77	99.46	109.62
1	C	385	GLY	N-CA-C	6.75	119.76	112.33
1	B	372	GLN	N-CA-C	-6.75	106.24	114.75
1	B	344	THR	N-CA-C	6.74	120.15	110.24
1	C	344	THR	N-CA-C	6.73	120.13	110.24
1	B	385	GLY	N-CA-C	6.70	119.70	112.33
1	B	132	ILE	N-CA-C	6.62	113.30	106.21
1	C	346	LEU	N-CA-C	-6.60	95.85	107.73
1	B	346	LEU	N-CA-C	-6.55	95.95	107.73
1	A	346	LEU	N-CA-C	-6.50	96.47	108.24
1	A	344	THR	N-CA-C	6.49	119.78	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LYS	CA-C-N	6.42	126.43	119.89
1	B	272	LYS	C-N-CA	6.42	126.43	119.89
1	C	133	THR	N-CA-C	-6.26	105.68	113.38
1	A	132	ILE	N-CA-C	6.12	112.76	106.21
1	C	463	GLY	CA-C-N	6.08	127.44	119.84
1	C	463	GLY	C-N-CA	6.08	127.44	119.84
1	B	148	THR	CA-C-N	6.07	126.53	120.52
1	B	148	THR	C-N-CA	6.07	126.53	120.52
1	A	133	THR	N-CA-C	-6.04	105.95	113.38
1	B	365	SER	N-CA-C	-6.02	106.92	114.56
1	B	133	THR	N-CA-C	-5.99	106.02	113.38
1	B	679	GLY	N-CA-C	5.93	117.97	110.38
1	A	679	GLY	N-CA-C	5.92	117.96	110.38
1	C	651	ASN	N-CA-C	-5.91	98.22	110.80
1	B	434	TRP	CA-C-N	-5.88	112.49	119.84
1	B	434	TRP	C-N-CA	-5.88	112.49	119.84
1	B	463	GLY	CA-C-N	5.84	127.14	119.84
1	B	463	GLY	C-N-CA	5.84	127.14	119.84
1	A	359	GLY	N-CA-C	-5.82	106.71	115.32
1	B	701	GLY	N-CA-C	5.79	119.74	112.79
1	B	359	GLY	N-CA-C	-5.79	106.75	115.32
1	B	427	LEU	N-CA-C	5.78	118.65	110.50
1	C	253	THR	N-CA-C	5.76	119.57	112.54
1	A	253	THR	N-CA-C	5.74	119.54	112.54
1	B	682	ALA	CA-C-N	-5.69	112.72	119.84
1	B	682	ALA	C-N-CA	-5.69	112.72	119.84
1	A	382	PHE	N-CA-C	-5.69	102.87	110.55
1	C	359	GLY	N-CA-C	-5.63	106.98	115.32
1	A	434	TRP	CA-C-N	-5.62	112.81	119.84
1	A	434	TRP	C-N-CA	-5.62	112.81	119.84
1	B	230	GLY	N-CA-C	-5.61	105.89	113.24
1	C	276	GLU	N-CA-C	-5.60	103.31	110.53
1	A	427	LEU	N-CA-C	5.59	118.38	110.50
1	A	276	GLU	N-CA-C	-5.58	103.33	110.53
1	B	180	PHE	N-CA-C	5.57	119.78	113.15
1	A	180	PHE	N-CA-C	5.51	119.63	113.02
1	B	276	GLU	N-CA-C	-5.51	103.43	110.53
1	B	425	ALA	N-CA-C	5.49	120.37	109.01
1	A	655	THR	N-CA-C	5.47	122.44	110.80
1	C	382	PHE	N-CA-C	-5.42	103.23	110.55
1	A	596	GLN	N-CA-C	5.42	117.08	110.41
1	A	343	ASP	N-CA-C	-5.39	99.31	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	GLY	N-CA-C	5.39	119.47	112.25
1	A	266	ILE	CB-CA-C	-5.39	105.41	111.45
1	B	655	THR	N-CA-C	5.37	122.24	110.80
1	C	434	TRP	CA-C-N	-5.36	113.14	119.84
1	C	434	TRP	C-N-CA	-5.36	113.14	119.84
1	A	235	ASN	N-CA-C	5.35	117.55	111.02
1	A	425	ALA	N-CA-C	5.34	120.06	109.01
1	A	157	ARG	N-CA-C	-5.33	107.15	113.38
1	B	130	THR	N-CA-C	5.32	117.26	108.48
1	C	427	LEU	N-CA-C	5.32	118.00	110.50
1	B	157	ARG	N-CA-C	-5.32	107.16	113.38
1	C	596	GLN	N-CA-C	5.32	116.95	110.41
1	B	343	ASP	N-CA-C	-5.31	99.48	110.80
1	B	382	PHE	N-CA-C	-5.30	103.40	110.55
1	B	596	GLN	N-CA-C	5.29	116.92	110.41
1	B	253	THR	N-CA-C	5.29	119.00	112.54
1	C	425	ALA	N-CA-C	5.29	119.95	109.01
1	C	679	GLY	N-CA-C	5.24	117.09	110.38
1	A	230	GLY	N-CA-C	-5.24	106.38	113.24
1	B	652	SER	N-CA-C	-5.22	98.04	107.75
1	C	365	SER	N-CA-C	-5.21	107.59	114.31
1	C	230	GLY	N-CA-C	-5.19	106.44	113.24
1	C	235	ASN	N-CA-C	5.19	117.35	111.02
1	C	343	ASP	N-CA-C	-5.19	99.75	110.80
1	B	143	ASP	O-C-N	5.18	124.67	120.83
1	C	260	GLY	CA-C-N	-5.17	114.56	122.62
1	C	260	GLY	C-N-CA	-5.17	114.56	122.62
1	C	581	ASP	N-CA-C	-5.12	106.29	112.54
1	B	165	THR	CA-C-N	5.06	126.16	119.84
1	B	165	THR	C-N-CA	5.06	126.16	119.84
1	C	492	ASN	N-CA-C	-5.05	102.59	109.71
1	B	492	ASN	N-CA-C	-5.05	102.59	109.71
1	A	581	ASP	N-CA-C	-5.04	106.39	112.54
1	B	787	LYS	N-CA-C	5.03	116.87	108.23
1	C	378	VAL	N-CA-C	5.03	114.49	108.06

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	190	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	227	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	227	ARG	Sidechain
1	B	327	ARG	Sidechain
1	B	751	ARG	Sidechain
1	C	310	ARG	Sidechain
1	C	396	ARG	Sidechain
1	C	536	ARG	Sidechain
1	C	768	ARG	Sidechain
2	I	2	DSN	Peptide
2	I	3	ARG	Sidechain,Peptide
2	I	4	DSN	Peptide
2	I	5	FHO	Peptide
2	J	2	DSN	Peptide
2	J	3	ARG	Sidechain,Peptide
2	J	4	DSN	Peptide
2	J	5	FHO	Peptide
2	K	3	ARG	Sidechain,Peptide
2	K	4	DSN	Peptide
2	K	5	FHO	Peptide

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	5474	0	5154	704	0
1	B	5474	0	5154	735	0
1	C	5474	0	5154	716	0
2	I	68	0	65	3	0
2	J	68	0	65	2	0
2	K	68	0	65	2	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
4	I	26	0	13	1	0
4	J	26	0	13	3	0
4	K	26	0	13	1	0
All	All	16719	0	15696	2159	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 67.

All (2159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:ARG:HG3	1:B:778:SER:CB	1.61	1.31
1:A:189:MSE:CE	1:A:195:ILE:HD13	1.68	1.23
1:B:768:ARG:CG	1:B:778:SER:HB3	1.70	1.21
1:C:352:TYR:CD1	1:C:396:ARG:HG2	1.78	1.19
1:A:227:ARG:HD3	1:A:594:MSE:HE1	1.28	1.11
1:A:474:LEU:HD12	1:A:475:VAL:H	1.08	1.10
1:B:681:LEU:HD22	1:B:687:VAL:HG11	1.32	1.09
1:C:352:TYR:HD1	1:C:396:ARG:HG2	1.04	1.09
1:C:352:TYR:HD1	1:C:396:ARG:CG	1.66	1.09
1:A:189:MSE:HE1	1:A:195:ILE:HD13	1.09	1.08
1:B:227:ARG:HD3	1:B:594:MSE:HE1	1.30	1.08
1:C:554:TYR:CD2	1:C:595:PRO:HG3	1.89	1.08
1:B:371:SER:HB2	1:B:436:ALA:HA	1.34	1.05
1:C:370:ASP:HA	1:C:435:PRO:HD2	1.40	1.04
1:A:371:SER:HB2	1:A:436:ALA:HA	1.36	1.03
1:C:474:LEU:HD11	1:C:533:MSE:HG3	1.39	1.03
1:B:474:LEU:HD11	1:B:533:MSE:HG3	1.42	1.02
1:B:659:ILE:HG12	1:B:660:THR:H	1.21	1.02
1:A:681:LEU:HD22	1:A:687:VAL:HG11	1.38	1.01
1:C:227:ARG:HD3	1:C:594:MSE:HE1	1.06	1.01
1:C:371:SER:HB2	1:C:436:ALA:HA	1.39	1.01
1:A:370:ASP:HA	1:A:435:PRO:HD2	1.44	1.00
1:A:147:TYR:HA	1:A:173:THR:HG21	1.42	1.00
1:B:370:ASP:HA	1:B:435:PRO:HD2	1.39	1.00
1:C:768:ARG:HB2	1:C:778:SER:HB3	1.44	0.98
1:B:280:HIS:HB2	1:B:813:TRP:HB3	1.42	0.97
1:B:134:SER:HA	1:B:139:THR:HA	1.46	0.97
1:B:474:LEU:HD12	1:B:475:VAL:H	1.30	0.97
1:C:280:HIS:HB2	1:C:813:TRP:HB3	1.47	0.97
1:A:474:LEU:HD11	1:A:533:MSE:HG3	1.45	0.97
1:B:136:GLN:HG3	1:B:413:LYS:HZ1	1.25	0.96
1:B:653:LYS:H	1:B:653:LYS:HD3	1.27	0.96
1:C:536:ARG:HG3	1:C:536:ARG:O	1.62	0.96
1:B:246:VAL:HG23	1:B:268:LEU:HD23	1.45	0.96
1:B:147:TYR:HA	1:B:173:THR:HG21	1.46	0.96
1:C:134:SER:HA	1:C:139:THR:HA	1.48	0.96
1:C:339:ASP:O	1:C:340:LEU:HG	1.66	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MSE:HE1	1:A:195:ILE:CD1	1.95	0.96
1:C:147:TYR:HA	1:C:173:THR:HG21	1.46	0.96
1:C:227:ARG:CD	1:C:594:MSE:HE1	1.95	0.96
1:B:434:TRP:HB3	1:B:441:ALA:HB1	1.48	0.95
1:C:776:SER:HB2	1:C:812:ARG:HB2	1.48	0.95
1:A:182:LEU:HD22	1:A:187:ASP:O	1.66	0.95
1:A:776:SER:HB2	1:A:812:ARG:HB2	1.48	0.95
1:C:474:LEU:HD12	1:C:475:VAL:H	1.32	0.95
1:A:339:ASP:O	1:A:340:LEU:HG	1.66	0.95
1:A:782:ASN:HB2	1:A:806:ASN:HB2	1.47	0.95
1:B:776:SER:HB2	1:B:812:ARG:HB2	1.47	0.94
1:A:280:HIS:HB2	1:A:813:TRP:HB3	1.47	0.94
1:C:771:ILE:HG13	1:C:772:THR:HG23	1.49	0.94
1:A:154:THR:HB	1:A:247:GLU:OE2	1.68	0.93
1:A:246:VAL:HG23	1:A:268:LEU:HD23	1.49	0.93
1:A:542:ASP:HA	1:A:578:ASP:OD2	1.68	0.93
1:A:695:ILE:HD11	1:A:710:GLN:NE2	1.82	0.93
1:B:518:PRO:HG2	1:B:521:TYR:OH	1.67	0.93
1:C:286:GLY:HA3	1:C:808:MSE:HG3	1.50	0.93
1:B:339:ASP:O	1:B:340:LEU:HG	1.66	0.93
1:B:771:ILE:HG13	1:B:772:THR:HG23	1.50	0.93
1:C:286:GLY:CA	1:C:808:MSE:HG3	1.99	0.93
1:A:771:ILE:HG13	1:A:772:THR:HG23	1.49	0.93
1:B:154:THR:HB	1:B:247:GLU:OE2	1.68	0.92
1:A:462:THR:HB	1:A:475:VAL:HG23	1.51	0.92
1:A:134:SER:HA	1:A:139:THR:HA	1.49	0.92
1:A:218:GLN:HB3	1:A:267:ASN:OD1	1.69	0.92
1:A:467:PHE:CE2	1:A:468:LEU:HD23	2.04	0.92
1:C:154:THR:HB	1:C:247:GLU:OE2	1.68	0.91
1:A:252:ALA:HB3	1:A:590:THR:HB	1.52	0.91
1:A:434:TRP:HB3	1:A:441:ALA:HB1	1.49	0.91
1:B:518:PRO:HG2	1:B:521:TYR:CZ	2.06	0.91
1:C:341:ASN:HB3	1:C:342:PRO:CD	2.01	0.91
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.06	0.91
1:C:645:GLU:HG2	1:C:664:LYS:NZ	1.86	0.91
1:B:568:ARG:HD3	1:B:569:PHE:H	1.34	0.91
1:C:462:THR:HB	1:C:475:VAL:HG23	1.52	0.91
1:A:474:LEU:HD12	1:A:475:VAL:N	1.86	0.91
1:C:252:ALA:HB3	1:C:590:THR:HB	1.53	0.91
1:C:394:TYR:CZ	1:C:422:GLY:HA3	2.05	0.91
1:A:637:GLU:HG3	1:A:671:LYS:HB3	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:TRP:N	1:B:599:TRP:HE3	1.69	0.90
1:C:434:TRP:HB3	1:C:441:ALA:HB1	1.50	0.90
1:B:568:ARG:HD3	1:B:569:PHE:N	1.87	0.90
1:B:812:ARG:HG3	1:B:813:TRP:H	1.36	0.90
1:A:812:ARG:HG3	1:A:813:TRP:H	1.34	0.90
1:B:754:LYS:H	1:B:754:LYS:HD2	1.35	0.90
1:C:812:ARG:HG3	1:C:813:TRP:H	1.35	0.90
1:C:188:VAL:HG11	1:C:246:VAL:HG11	1.52	0.90
1:B:252:ALA:HB3	1:B:590:THR:HB	1.53	0.89
1:C:258:GLY:HA3	1:C:528:GLN:OE1	1.71	0.89
1:B:136:GLN:HG3	1:B:413:LYS:NZ	1.85	0.89
1:A:599:TRP:N	1:A:599:TRP:HE3	1.70	0.89
1:B:768:ARG:HG3	1:B:778:SER:HB3	0.90	0.89
1:C:782:ASN:HB2	1:C:806:ASN:HB2	1.55	0.88
1:B:462:THR:HB	1:B:475:VAL:HG23	1.55	0.88
1:C:236:THR:HG23	1:C:237:LEU:CD2	2.04	0.88
1:C:637:GLU:HG3	1:C:671:LYS:HB3	1.56	0.88
1:B:637:GLU:HG3	1:B:671:LYS:HB3	1.56	0.87
1:C:645:GLU:HG2	1:C:664:LYS:HZ3	1.38	0.87
1:A:599:TRP:HE3	1:A:599:TRP:H	1.19	0.87
1:B:258:GLY:HA3	1:B:528:GLN:OE1	1.75	0.87
1:C:243:TYR:CD2	1:C:268:LEU:HB3	2.09	0.87
1:C:271:LYS:HD2	1:C:310:ARG:CZ	2.04	0.87
1:B:782:ASN:HB2	1:B:806:ASN:HB2	1.57	0.86
1:B:659:ILE:HG12	1:B:660:THR:N	1.82	0.86
1:B:653:LYS:HD3	1:B:653:LYS:N	1.86	0.86
1:B:188:VAL:HG11	1:B:246:VAL:HG11	1.57	0.86
1:A:258:GLY:HA3	1:A:528:GLN:OE1	1.76	0.86
1:C:568:ARG:HE	1:C:569:PHE:H	1.23	0.85
1:C:189:MSE:HE2	1:C:266:ILE:HD11	1.59	0.85
1:B:341:ASN:HB3	1:B:342:PRO:CD	2.07	0.85
1:B:394:TYR:CZ	1:B:422:GLY:HA3	2.12	0.85
1:A:324:HIS:HE1	1:A:383:ASN:HB3	1.42	0.84
1:A:526:THR:HG23	1:A:556:VAL:HG23	1.60	0.84
1:A:360:SER:HB3	1:A:390:SER:HA	1.58	0.84
1:A:776:SER:H	1:A:812:ARG:HB3	1.43	0.84
1:B:599:TRP:HE3	1:B:599:TRP:H	1.19	0.84
1:B:357:PRO:O	1:B:390:SER:HB2	1.78	0.84
1:B:762:LEU:HD21	1:B:789:TYR:HE2	1.43	0.84
1:A:188:VAL:HG11	1:A:246:VAL:HG11	1.60	0.84
1:C:227:ARG:HD3	1:C:594:MSE:CE	2.01	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HD2	1:A:316:GLN:CD	2.03	0.84
1:C:324:HIS:HE1	1:C:383:ASN:HB3	1.43	0.84
1:C:776:SER:H	1:C:812:ARG:HB3	1.43	0.84
1:A:198:SER:HB3	1:A:206:ASN:ND2	1.93	0.84
1:B:236:THR:HG23	1:B:237:LEU:CD2	2.08	0.83
1:B:655:THR:HG23	1:B:659:ILE:HD12	1.58	0.83
1:B:779:VAL:HG21	1:B:809:PHE:CE1	2.11	0.83
1:C:764:ASP:HB3	1:C:782:ASN:O	1.78	0.83
1:B:747:ASN:HB3	1:B:748:PRO:HD3	1.61	0.83
1:C:416:LEU:CD2	1:C:457:LEU:CD1	2.56	0.83
1:B:776:SER:H	1:B:812:ARG:HB3	1.43	0.83
1:C:271:LYS:CD	1:C:310:ARG:NH2	2.41	0.83
1:C:526:THR:HG23	1:C:556:VAL:HG23	1.60	0.83
1:C:352:TYR:CD1	1:C:396:ARG:CG	2.51	0.83
1:A:568:ARG:HE	1:A:569:PHE:H	1.21	0.82
1:B:352:TYR:HD1	1:B:396:ARG:HB3	1.44	0.82
1:C:560:ASN:ND2	1:C:561:PRO:HD2	1.95	0.82
1:A:364:GLY:HA3	1:A:798:SER:HB2	1.62	0.82
1:C:659:ILE:HG23	1:C:660:THR:H	1.45	0.82
1:B:364:GLY:HA3	1:B:798:SER:HB2	1.62	0.82
1:A:681:LEU:HD22	1:A:687:VAL:CG1	2.08	0.82
1:C:360:SER:HB3	1:C:390:SER:HA	1.60	0.82
1:A:352:TYR:HD1	1:A:396:ARG:HB3	1.45	0.82
1:C:357:PRO:O	1:C:390:SER:HB2	1.80	0.82
1:B:360:SER:HB3	1:B:390:SER:HA	1.61	0.81
1:A:747:ASN:HB3	1:A:748:PRO:HD3	1.59	0.81
1:A:583:TYR:HB3	1:A:620:ILE:HD11	1.61	0.81
1:B:526:THR:HG22	1:B:556:VAL:HG23	1.61	0.81
1:B:341:ASN:HB3	1:B:342:PRO:HD2	1.62	0.81
1:B:189:MSE:HE2	1:B:266:ILE:HD11	1.59	0.81
1:A:560:ASN:ND2	1:A:561:PRO:HD2	1.96	0.81
1:B:560:ASN:ND2	1:B:561:PRO:HD2	1.96	0.81
1:A:357:PRO:O	1:A:390:SER:HB2	1.80	0.81
1:C:646:GLU:HB2	1:C:661:TYR:OH	1.81	0.80
1:C:236:THR:HG23	1:C:237:LEU:HD22	1.64	0.80
1:C:599:TRP:N	1:C:599:TRP:HE3	1.78	0.80
1:B:789:TYR:CE1	1:B:802:GLY:HA3	2.16	0.80
1:B:583:TYR:HB3	1:B:620:ILE:HD11	1.64	0.80
1:C:583:TYR:HB3	1:C:620:ILE:HD11	1.64	0.80
1:A:344:THR:HG21	1:A:405:ASN:HD21	1.47	0.80
1:C:341:ASN:HB3	1:C:342:PRO:HD2	1.62	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:TRP:N	1:B:599:TRP:CE3	2.48	0.79
1:B:779:VAL:CG2	1:B:809:PHE:CD1	2.65	0.79
1:C:601:ARG:HH11	1:C:601:ARG:HG3	1.48	0.79
1:A:764:ASP:HB3	1:A:782:ASN:O	1.83	0.79
1:B:443:ILE:HD13	1:B:510:ILE:HD12	1.64	0.79
1:C:364:GLY:HA3	1:C:798:SER:HB2	1.64	0.79
1:B:324:HIS:HE1	1:B:383:ASN:HB3	1.48	0.79
1:B:643:ARG:HH12	1:B:704:VAL:HG21	1.47	0.79
1:A:560:ASN:HD22	1:A:561:PRO:HD2	1.48	0.78
1:B:763:VAL:HG11	1:B:785:PHE:CE2	2.18	0.78
1:B:601:ARG:HH11	1:B:601:ARG:HG3	1.48	0.78
1:C:661:TYR:HD1	1:C:662:ALA:H	1.31	0.78
1:C:292:ARG:HD2	1:C:316:GLN:CD	2.09	0.78
1:A:768:ARG:HG3	1:A:778:SER:HB3	1.64	0.78
1:C:402:LEU:HD12	1:C:414:VAL:CG1	2.14	0.78
1:B:292:ARG:HD2	1:B:316:GLN:CD	2.09	0.78
1:C:271:LYS:HD2	1:C:310:ARG:NH2	1.98	0.78
1:C:560:ASN:HD22	1:C:561:PRO:HD2	1.46	0.78
1:C:189:MSE:CE	1:C:266:ILE:HD11	2.12	0.78
1:A:198:SER:HB3	1:A:206:ASN:HD21	1.47	0.77
1:C:275:HIS:O	1:C:300:PRO:HG3	1.84	0.77
1:C:584:SER:O	1:C:620:ILE:HG13	1.84	0.77
1:A:599:TRP:N	1:A:599:TRP:CE3	2.49	0.77
1:B:560:ASN:HD22	1:B:561:PRO:HD2	1.48	0.77
1:B:643:ARG:NH1	1:B:704:VAL:HG21	1.99	0.77
1:C:365:SER:C	1:C:384:ASN:HD22	1.92	0.77
1:A:344:THR:HG21	1:A:405:ASN:ND2	2.00	0.77
1:A:341:ASN:HB3	1:A:342:PRO:CD	2.14	0.76
1:B:184:ASN:OD1	1:B:186:ASP:HB2	1.86	0.76
1:C:335:ILE:C	1:C:336:LEU:HD12	2.11	0.76
1:B:681:LEU:HD22	1:B:687:VAL:CG1	2.11	0.76
1:A:601:ARG:HG3	1:A:601:ARG:HH11	1.51	0.76
1:B:391:TRP:O	1:B:391:TRP:HD1	1.68	0.76
1:A:387:LYS:HD2	1:A:509:ASP:HB3	1.67	0.76
1:A:474:LEU:CD1	1:A:475:VAL:H	1.93	0.76
1:A:763:VAL:HG13	1:A:784:VAL:HB	1.67	0.76
1:C:369:PHE:O	1:C:433:ASP:HA	1.85	0.76
1:C:763:VAL:HG13	1:C:784:VAL:HB	1.66	0.76
1:A:275:HIS:O	1:A:300:PRO:HG3	1.85	0.76
1:A:443:ILE:HD13	1:A:510:ILE:HD12	1.67	0.76
1:B:253:THR:HG21	1:B:265:THR:OG1	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HB3	1:A:342:PRO:HD2	1.67	0.76
1:A:584:SER:O	1:A:620:ILE:HG13	1.86	0.76
1:C:252:ALA:HB3	1:C:590:THR:CB	2.16	0.76
1:B:779:VAL:HG21	1:B:809:PHE:CD1	2.21	0.76
1:B:252:ALA:HB3	1:B:590:THR:CB	2.15	0.75
1:B:584:SER:O	1:B:620:ILE:HG13	1.86	0.75
1:C:331:VAL:HB	1:C:353:GLN:HG3	1.68	0.75
1:C:600:TYR:OH	2:K:2:DSN:HB3	1.86	0.75
1:A:189:MSE:HE3	1:A:195:ILE:HD13	1.67	0.75
1:A:625:LEU:HD13	1:A:628:ARG:HH12	1.50	0.75
1:A:655:THR:HG23	1:A:656:ASN:H	1.50	0.75
1:A:252:ALA:HB3	1:A:590:THR:CB	2.15	0.75
1:B:280:HIS:HB2	1:B:813:TRP:CB	2.16	0.75
1:A:762:LEU:HD21	1:A:789:TYR:HE2	1.52	0.75
1:B:335:ILE:C	1:B:336:LEU:HD12	2.12	0.75
1:B:625:LEU:O	1:B:627:GLY:N	2.18	0.75
1:A:253:THR:HG21	1:A:265:THR:OG1	1.85	0.75
1:A:643:ARG:HH12	1:A:704:VAL:HG21	1.51	0.75
1:C:599:TRP:N	1:C:599:TRP:CE3	2.53	0.75
1:B:445:ALA:O	1:B:446:GLN:HG3	1.87	0.75
1:C:253:THR:HG21	1:C:265:THR:OG1	1.87	0.75
1:A:335:ILE:C	1:A:336:LEU:HD12	2.13	0.74
1:C:559:LEU:HG	1:C:559:LEU:O	1.87	0.74
1:A:391:TRP:CE3	1:A:427:LEU:HD11	2.23	0.74
1:A:434:TRP:CE3	1:A:434:TRP:HA	2.22	0.74
1:B:331:VAL:HB	1:B:353:GLN:HG3	1.68	0.74
1:B:391:TRP:O	1:B:391:TRP:CD1	2.40	0.74
1:B:189:MSE:HE2	1:B:266:ILE:CD1	2.17	0.74
1:B:275:HIS:O	1:B:300:PRO:HG3	1.87	0.74
1:C:189:MSE:CE	1:C:266:ILE:CD1	2.65	0.74
1:C:643:ARG:HH12	1:C:704:VAL:HG21	1.52	0.74
1:C:443:ILE:HD13	1:C:510:ILE:HD12	1.69	0.74
1:A:189:MSE:CE	1:A:195:ILE:CD1	2.60	0.74
1:B:754:LYS:HD3	1:B:754:LYS:O	1.88	0.73
1:C:768:ARG:CB	1:C:778:SER:HB3	2.19	0.73
1:A:185:ILE:CD1	1:A:189:MSE:HG2	2.18	0.73
1:A:434:TRP:HB3	1:A:441:ALA:CB	2.18	0.73
1:A:369:PHE:O	1:A:433:ASP:HA	1.88	0.73
1:A:397:THR:HB	1:A:419:LYS:HG3	1.68	0.73
1:C:762:LEU:HD21	1:C:789:TYR:HE2	1.51	0.73
1:A:380:ARG:HA	1:A:801:TYR:CD2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:LEU:O	1:A:627:GLY:N	2.20	0.73
4:J:1:PVE:H11	4:J:1:PVE:H212	1.53	0.73
1:A:227:ARG:HD3	1:A:594:MSE:CE	2.13	0.73
1:A:537:PHE:HE2	1:A:547:LEU:HD12	1.53	0.73
1:B:629:LEU:HD12	1:B:630:ASN:H	1.54	0.73
1:C:340:LEU:HB2	1:C:343:ASP:HB2	1.70	0.73
1:B:189:MSE:CE	1:B:266:ILE:HD11	2.19	0.73
1:C:434:TRP:HB3	1:C:441:ALA:CB	2.18	0.73
1:A:496:TYR:CD1	1:A:513:PRO:HB3	2.24	0.73
1:A:633:LEU:HD23	1:A:633:LEU:O	1.89	0.72
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.24	0.72
1:C:445:ALA:O	1:C:446:GLN:HG3	1.88	0.72
1:A:340:LEU:HB2	1:A:343:ASP:HB2	1.69	0.72
1:A:625:LEU:C	1:A:627:GLY:H	1.98	0.72
1:B:559:LEU:HD23	1:B:559:LEU:O	1.89	0.72
1:A:194:GLY:HA2	1:A:712:GLN:OE1	1.89	0.72
1:A:763:VAL:HG11	1:A:785:PHE:CE2	2.24	0.72
1:B:434:TRP:HB3	1:B:441:ALA:CB	2.19	0.72
1:A:695:ILE:HD11	1:A:710:GLN:HE21	1.55	0.72
1:B:625:LEU:C	1:B:627:GLY:H	1.98	0.72
1:C:380:ARG:HA	1:C:801:TYR:CD2	2.25	0.72
1:C:747:ASN:HB3	1:C:748:PRO:HD3	1.70	0.72
1:A:240:MSE:O	1:A:242:ILE:N	2.23	0.72
1:B:369:PHE:O	1:B:433:ASP:HA	1.90	0.72
1:B:474:LEU:HD11	1:B:533:MSE:CG	2.20	0.72
1:B:768:ARG:CB	1:B:778:SER:HB3	2.20	0.72
1:B:340:LEU:HB2	1:B:343:ASP:HB2	1.70	0.71
1:C:352:TYR:CE1	1:C:396:ARG:HD2	2.25	0.71
1:C:271:LYS:HD3	1:C:310:ARG:NH2	2.04	0.71
1:B:376:ASN:HD21	1:B:435:PRO:HG2	1.55	0.71
1:C:496:TYR:CD1	1:C:513:PRO:HB3	2.24	0.71
1:A:192:THR:HB	1:A:195:ILE:HD12	1.73	0.71
1:B:763:VAL:HG13	1:B:784:VAL:HB	1.72	0.71
1:C:184:ASN:OD1	1:C:186:ASP:HB2	1.90	0.71
1:C:643:ARG:NH1	1:C:704:VAL:HG21	2.05	0.71
1:A:643:ARG:NH1	1:A:704:VAL:HG21	2.04	0.71
1:B:189:MSE:CE	1:B:266:ILE:CD1	2.68	0.71
1:C:397:THR:HB	1:C:419:LYS:HG3	1.73	0.71
1:C:625:LEU:O	1:C:627:GLY:N	2.22	0.71
1:A:402:LEU:HD12	1:A:402:LEU:O	1.91	0.71
1:B:218:GLN:HB3	1:B:267:ASN:OD1	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:MSE:O	1:B:242:ILE:N	2.24	0.71
1:B:273:PRO:HG3	1:B:337:GLU:HG3	1.73	0.71
1:A:342:PRO:C	1:A:344:THR:H	1.99	0.71
1:A:657:PRO:C	1:A:659:ILE:H	1.95	0.71
1:B:659:ILE:CG1	1:B:660:THR:H	2.00	0.71
1:C:554:TYR:CD2	1:C:595:PRO:CG	2.71	0.71
1:C:625:LEU:C	1:C:627:GLY:H	1.99	0.71
1:A:168:SER:HB2	1:A:617:GLU:OE2	1.91	0.71
1:B:764:ASP:HB3	1:B:782:ASN:O	1.91	0.71
1:B:169:ILE:HD13	1:B:249:LEU:HA	1.71	0.70
1:B:192:THR:HB	1:B:195:ILE:HD12	1.73	0.70
1:B:397:THR:HB	1:B:419:LYS:HG3	1.72	0.70
1:C:240:MSE:O	1:C:242:ILE:N	2.23	0.70
1:A:467:PHE:CE2	1:A:468:LEU:CD2	2.74	0.70
1:B:135:ASN:HD22	1:B:135:ASN:N	1.88	0.70
1:B:227:ARG:CD	1:B:594:MSE:HE1	2.16	0.70
1:A:652:SER:O	1:A:654:PRO:HD3	1.91	0.70
1:B:496:TYR:CD1	1:B:513:PRO:HB3	2.27	0.70
1:B:233:ALA:HB2	1:B:423:TYR:HB3	1.73	0.70
1:A:233:ALA:HB2	1:A:423:TYR:HB3	1.74	0.70
1:B:194:GLY:HA2	1:B:712:GLN:OE1	1.92	0.70
1:C:233:ALA:HB2	1:C:423:TYR:HB3	1.74	0.70
1:C:386:ALA:HB3	1:C:389:SER:HB2	1.74	0.70
1:C:601:ARG:HG3	1:C:601:ARG:NH1	2.06	0.70
1:C:683:PRO:HG2	1:C:684:GLY:H	1.57	0.70
1:C:242:ILE:O	1:C:271:LYS:HG3	1.92	0.70
1:C:552:VAL:HG22	1:C:553:ASP:N	2.05	0.70
1:B:386:ALA:HB3	1:B:389:SER:HB2	1.73	0.70
1:A:559:LEU:HD23	1:A:559:LEU:O	1.92	0.70
1:C:189:MSE:HE2	1:C:266:ILE:CD1	2.22	0.70
1:B:144:SER:O	1:B:146:SER:N	2.24	0.69
1:B:754:LYS:HD2	1:B:754:LYS:N	2.03	0.69
1:A:768:ARG:CB	1:A:778:SER:HB3	2.23	0.69
1:B:552:VAL:HG22	1:B:553:ASP:N	2.07	0.69
1:C:763:VAL:HG11	1:C:785:PHE:CE2	2.27	0.69
1:C:169:ILE:HD13	1:C:249:LEU:HA	1.73	0.69
1:A:376:ASN:HD21	1:A:435:PRO:HG2	1.57	0.69
1:B:720:LYS:HG3	1:B:729:THR:OG1	1.92	0.69
1:C:506:TRP:CZ2	1:C:508:GLY:HA2	2.28	0.69
1:C:246:VAL:HG23	1:C:268:LEU:HD23	1.74	0.69
1:B:352:TYR:CD1	1:B:396:ARG:HB3	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASN:OD1	1:B:658:ALA:HB2	1.93	0.69
1:C:342:PRO:C	1:C:344:THR:H	2.00	0.69
1:C:720:LYS:HG3	1:C:729:THR:OG1	1.92	0.69
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.57	0.69
1:A:331:VAL:HB	1:A:353:GLN:HG3	1.73	0.69
1:A:552:VAL:HG22	1:A:553:ASP:N	2.07	0.69
1:B:447:LYS:HE2	3:B:2002:SO4:O4	1.93	0.69
1:B:492:ASN:HB2	1:B:519:SER:OG	1.92	0.69
1:A:169:ILE:HD13	1:A:249:LEU:HA	1.74	0.68
1:C:538:ASN:CB	1:C:544:ASN:ND2	2.56	0.68
1:B:342:PRO:C	1:B:344:THR:H	2.00	0.68
1:C:140:ILE:HG22	1:C:141:THR:N	2.08	0.68
1:C:470:ARG:HG2	1:C:470:ARG:HH11	1.59	0.68
1:A:439:ASN:OD1	1:A:502:ASP:HB2	1.93	0.68
1:A:659:ILE:HG12	1:A:660:THR:H	1.58	0.68
1:B:762:LEU:HD21	1:B:789:TYR:CE2	2.28	0.68
1:C:169:ILE:CD1	1:C:249:LEU:HA	2.23	0.68
1:C:340:LEU:O	1:C:341:ASN:HB2	1.93	0.68
1:A:140:ILE:HG22	1:A:141:THR:N	2.09	0.68
1:A:506:TRP:CZ2	1:A:508:GLY:HA2	2.29	0.68
1:A:647:ASP:H	1:A:663:TYR:HA	1.59	0.68
1:B:654:PRO:O	1:B:656:ASN:N	2.24	0.68
1:C:271:LYS:CD	1:C:310:ARG:CZ	2.72	0.68
1:C:402:LEU:HD12	1:C:414:VAL:HG13	1.74	0.68
1:B:601:ARG:HG3	1:B:601:ARG:NH1	2.07	0.68
1:A:601:ARG:HG3	1:A:601:ARG:NH1	2.08	0.68
1:C:192:THR:HB	1:C:195:ILE:HD12	1.75	0.68
1:C:218:GLN:HB3	1:C:267:ASN:OD1	1.92	0.68
1:C:652:SER:O	1:C:654:PRO:HD3	1.94	0.68
1:A:646:GLU:HA	1:A:663:TYR:CD2	2.27	0.68
1:B:625:LEU:HD13	1:B:628:ARG:HH12	1.58	0.68
1:B:174:ARG:HD2	1:B:177:MSE:HE3	1.76	0.68
1:C:169:ILE:HD11	1:C:249:LEU:CD1	2.24	0.68
1:A:238:SER:HA	1:A:353:GLN:HE22	1.57	0.67
1:A:720:LYS:HG3	1:A:729:THR:OG1	1.94	0.67
1:B:140:ILE:HG22	1:B:141:THR:N	2.07	0.67
1:B:158:LEU:HD21	1:B:473:GLU:HG3	1.76	0.67
1:A:697:ARG:NH2	1:A:703:LYS:HZ2	1.92	0.67
1:B:776:SER:CB	1:B:812:ARG:HB2	2.23	0.67
1:B:403:GLU:HB3	1:B:413:LYS:HG3	1.76	0.67
1:B:779:VAL:HG23	1:B:809:PHE:CD1	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:ASN:HD21	1:C:749:ARG:CG	2.07	0.67
1:A:352:TYR:CD1	1:A:396:ARG:HB3	2.28	0.67
1:A:412:GLY:HA3	1:A:461:LEU:HD23	1.76	0.67
1:A:271:LYS:NZ	1:A:310:ARG:NH2	2.42	0.67
1:B:402:LEU:O	1:B:402:LEU:HD12	1.95	0.67
1:A:169:ILE:HD11	1:A:249:LEU:CD1	2.24	0.67
1:B:168:SER:HB2	1:B:617:GLU:OE2	1.94	0.67
1:A:189:MSE:HE3	1:A:195:ILE:HG21	1.77	0.67
1:C:638:ILE:N	1:C:670:THR:O	2.21	0.67
1:A:492:ASN:HB2	1:A:519:SER:OG	1.95	0.67
1:A:445:ALA:O	1:A:446:GLN:HG3	1.94	0.67
1:A:746:ASN:HD22	1:A:749:ARG:HB2	1.59	0.67
1:B:280:HIS:CE1	1:B:812:ARG:HH21	2.12	0.67
1:B:345:MSE:O	1:B:402:LEU:HA	1.94	0.67
1:B:421:ASN:O	1:B:452:THR:HG22	1.95	0.66
1:B:517:THR:HB	1:B:518:PRO:HD2	1.77	0.66
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.30	0.66
1:A:683:PRO:HG2	1:A:684:GLY:H	1.60	0.66
1:A:194:GLY:CA	1:A:712:GLN:OE1	2.44	0.66
1:B:169:ILE:CD1	1:B:249:LEU:HA	2.25	0.66
1:B:412:GLY:HA3	1:B:461:LEU:HD23	1.77	0.66
1:B:647:ASP:H	1:B:663:TYR:HA	1.60	0.66
1:C:144:SER:O	1:C:146:SER:N	2.26	0.66
1:C:647:ASP:H	1:C:663:TYR:HA	1.58	0.66
1:A:638:ILE:N	1:A:670:THR:O	2.21	0.66
1:C:345:MSE:O	1:C:402:LEU:HA	1.95	0.66
1:C:412:GLY:HA3	1:C:461:LEU:HD23	1.77	0.66
1:A:266:ILE:HG22	1:A:267:ASN:N	2.10	0.66
1:A:768:ARG:CG	1:A:778:SER:HB3	2.25	0.66
1:A:776:SER:CB	1:A:812:ARG:HB2	2.25	0.66
1:B:791:THR:HG22	1:B:800:SER:O	1.95	0.66
1:C:280:HIS:HB2	1:C:813:TRP:CB	2.25	0.66
1:C:554:TYR:CG	1:C:595:PRO:HG3	2.30	0.66
1:A:682:ALA:CB	1:A:683:PRO:CD	2.73	0.66
1:B:194:GLY:CA	1:B:712:GLN:OE1	2.44	0.66
1:B:774:LYS:HD3	1:B:814:ASP:OD2	1.96	0.66
1:A:227:ARG:CD	1:A:594:MSE:HE1	2.17	0.66
1:B:422:GLY:HA2	1:B:451:GLU:HA	1.78	0.66
1:C:319:HIS:CG	1:C:326:GLU:HG2	2.31	0.66
1:C:416:LEU:HD23	1:C:457:LEU:HD12	1.78	0.66
1:C:605:ASN:OD1	1:C:658:ALA:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ILE:HD11	1:C:710:GLN:HE21	1.60	0.65
1:B:474:LEU:CD1	1:B:475:VAL:H	2.06	0.65
1:B:683:PRO:HG2	1:B:684:GLY:H	1.61	0.65
1:B:695:ILE:HD11	1:B:710:GLN:HE21	1.61	0.65
1:B:376:ASN:ND2	1:B:435:PRO:HG2	2.12	0.65
1:A:422:GLY:HA2	1:A:451:GLU:HA	1.77	0.65
1:B:185:ILE:O	1:B:185:ILE:HD13	1.96	0.65
1:B:474:LEU:HD12	1:B:475:VAL:N	2.08	0.65
1:C:474:LEU:CD1	1:C:475:VAL:H	2.08	0.65
1:C:682:ALA:CB	1:C:683:PRO:CD	2.74	0.65
1:A:719:TYR:CE2	1:A:721:PHE:HD1	2.13	0.65
1:C:134:SER:HB3	1:C:139:THR:HB	1.79	0.65
1:C:434:TRP:HA	1:C:434:TRP:CE3	2.32	0.65
1:C:625:LEU:HD13	1:C:628:ARG:HH12	1.61	0.65
1:C:813:TRP:O	1:C:814:ASP:HB2	1.97	0.65
1:A:184:ASN:OD1	1:A:186:ASP:HB2	1.96	0.65
1:A:746:ASN:ND2	1:A:749:ARG:HB2	2.12	0.65
1:B:387:LYS:HG3	1:B:509:ASP:HA	1.78	0.65
1:B:434:TRP:HA	1:B:434:TRP:CE3	2.32	0.65
1:C:185:ILE:CD1	1:C:189:MSE:HG2	2.27	0.65
1:A:190:ARG:NH1	1:A:197:VAL:HG11	2.11	0.64
1:A:387:LYS:HG3	1:A:509:ASP:HA	1.78	0.64
1:B:629:LEU:HD12	1:B:630:ASN:N	2.13	0.64
1:C:185:ILE:HD13	1:C:185:ILE:O	1.97	0.64
1:C:209:ALA:HB2	1:C:214:ILE:HD11	1.78	0.64
1:B:682:ALA:CB	1:B:683:PRO:CD	2.75	0.64
1:C:387:LYS:HD2	1:C:509:ASP:HB3	1.79	0.64
1:C:402:LEU:HD12	1:C:402:LEU:O	1.97	0.64
1:A:209:ALA:HB2	1:A:214:ILE:HD11	1.78	0.64
1:B:136:GLN:CG	1:B:413:LYS:NZ	2.60	0.64
1:C:474:LEU:HD12	1:C:475:VAL:N	2.10	0.64
1:C:776:SER:CB	1:C:812:ARG:HB2	2.26	0.64
1:C:439:ASN:OD1	1:C:502:ASP:HB2	1.97	0.64
1:A:657:PRO:O	1:A:659:ILE:HG22	1.97	0.64
1:A:391:TRP:CZ3	1:A:427:LEU:HD11	2.33	0.64
1:B:233:ALA:HA	1:B:393:GLN:OE1	1.98	0.64
1:C:736:TRP:HA	1:C:760:TYR:O	1.98	0.64
1:A:319:HIS:CG	1:A:326:GLU:HG2	2.33	0.64
1:B:746:ASN:HD22	1:B:749:ARG:HB2	1.62	0.64
1:C:492:ASN:HB2	1:C:519:SER:OG	1.96	0.64
1:A:350:ALA:HB2	1:A:398:VAL:HG22	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MSE:HA	1:B:182:LEU:HD12	1.80	0.64
1:B:185:ILE:CD1	1:B:189:MSE:HG2	2.28	0.64
1:B:741:TRP:HA	1:B:755:PHE:O	1.97	0.64
1:C:169:ILE:HD11	1:C:249:LEU:HD12	1.80	0.64
1:C:365:SER:C	1:C:384:ASN:ND2	2.56	0.63
1:A:147:TYR:HA	1:A:173:THR:CG2	2.25	0.63
1:A:421:ASN:O	1:A:452:THR:HG22	1.98	0.63
1:A:467:PHE:HD2	1:A:468:LEU:HG	1.62	0.63
1:B:169:ILE:HD11	1:B:249:LEU:CD1	2.28	0.63
1:A:370:ASP:O	1:A:372:GLN:N	2.31	0.63
1:C:416:LEU:HD22	1:C:457:LEU:CD1	2.28	0.63
1:C:538:ASN:HB2	1:C:544:ASN:ND2	2.13	0.63
1:A:376:ASN:ND2	1:A:435:PRO:HG2	2.13	0.63
1:B:134:SER:CA	1:B:139:THR:HA	2.25	0.63
1:B:136:GLN:HG2	1:B:137:LEU:H	1.64	0.63
1:A:345:MSE:O	1:A:402:LEU:HA	1.99	0.63
1:B:134:SER:HB3	1:B:139:THR:HB	1.79	0.63
1:A:434:TRP:HA	1:A:434:TRP:HE3	1.63	0.63
1:B:236:THR:HG23	1:B:237:LEU:HD22	1.79	0.63
1:C:422:GLY:HA2	1:C:451:GLU:HA	1.79	0.63
1:C:568:ARG:HE	1:C:569:PHE:N	1.95	0.63
1:A:287:SER:O	1:A:290:ASN:HB2	1.99	0.63
1:A:364:GLY:HA3	1:A:798:SER:CB	2.28	0.63
1:B:246:VAL:CG2	1:B:268:LEU:HD23	2.26	0.63
1:B:364:GLY:HA3	1:B:798:SER:CB	2.28	0.63
1:C:432:GLY:O	1:C:433:ASP:C	2.42	0.63
1:C:370:ASP:O	1:C:372:GLN:N	2.31	0.63
1:C:783:ASN:HB3	1:C:805:ARG:HA	1.81	0.63
1:A:774:LYS:HD3	1:A:814:ASP:OD2	1.98	0.62
1:B:768:ARG:HG3	1:B:778:SER:OG	1.97	0.62
1:A:169:ILE:CD1	1:A:249:LEU:HA	2.29	0.62
1:A:655:THR:HG23	1:A:656:ASN:N	2.14	0.62
1:B:166:PRO:HG3	1:B:546:PHE:CD2	2.34	0.62
1:B:236:THR:HG23	1:B:237:LEU:HD23	1.78	0.62
1:C:134:SER:CA	1:C:139:THR:HA	2.26	0.62
1:C:387:LYS:HG3	1:C:509:ASP:HA	1.81	0.62
1:C:791:THR:HG22	1:C:800:SER:O	1.99	0.62
1:A:240:MSE:HE2	1:A:240:MSE:HA	1.81	0.62
1:B:350:ALA:HB2	1:B:398:VAL:HG22	1.79	0.62
1:B:432:GLY:O	1:B:433:ASP:C	2.42	0.62
1:C:593:PHE:HB3	1:C:612:GLU:HG3	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:ILE:N	1:B:670:THR:O	2.21	0.62
1:C:364:GLY:HA3	1:C:798:SER:CB	2.30	0.62
1:A:370:ASP:O	1:A:371:SER:C	2.43	0.62
1:A:625:LEU:HD13	1:A:628:ARG:NH1	2.13	0.62
1:A:646:GLU:HA	1:A:663:TYR:HD2	1.64	0.62
1:B:754:LYS:HD3	1:B:754:LYS:C	2.24	0.62
1:B:813:TRP:O	1:B:814:ASP:HB2	1.99	0.62
1:C:216:ASN:HD21	1:C:261:SER:H	1.45	0.62
1:C:402:LEU:CD1	1:C:414:VAL:CG1	2.78	0.62
1:A:169:ILE:HD11	1:A:249:LEU:HD12	1.81	0.62
1:C:421:ASN:O	1:C:452:THR:HG22	1.99	0.62
1:C:546:PHE:O	1:C:573:VAL:HA	1.99	0.62
1:C:661:TYR:CD1	1:C:662:ALA:N	2.67	0.62
1:C:774:LYS:HD3	1:C:814:ASP:OD2	2.00	0.62
1:B:589:TYR:HE1	1:B:614:GLN:HB3	1.64	0.62
1:A:136:GLN:HG2	1:A:137:LEU:H	1.63	0.62
1:A:136:GLN:HG2	1:A:137:LEU:N	2.15	0.62
1:A:174:ARG:HD2	1:A:177:MSE:HE3	1.82	0.62
1:A:538:ASN:H	1:A:538:ASN:HD22	1.48	0.62
1:B:209:ALA:HB2	1:B:214:ILE:HD11	1.82	0.62
1:B:554:TYR:CG	1:B:595:PRO:HG3	2.35	0.62
1:A:682:ALA:HB1	1:A:683:PRO:CD	2.30	0.62
1:A:791:THR:HG22	1:A:800:SER:O	1.99	0.62
1:C:370:ASP:O	1:C:371:SER:C	2.42	0.62
1:A:273:PRO:HG3	1:A:337:GLU:HG3	1.82	0.61
1:A:596:GLN:HG2	1:A:600:TYR:HD2	1.65	0.61
1:B:475:VAL:O	1:B:475:VAL:HG22	2.00	0.61
1:C:554:TYR:CE2	1:C:595:PRO:HG3	2.35	0.61
1:C:682:ALA:HB1	1:C:683:PRO:CD	2.30	0.61
1:C:698:ASP:O	1:C:701:GLY:N	2.33	0.61
1:C:782:ASN:HB3	1:C:806:ASN:HD22	1.65	0.61
1:B:167:GLN:NE2	1:B:572:TYR:CE1	2.69	0.61
1:B:650:TYR:CE1	1:B:654:PRO:HD2	2.35	0.61
1:C:380:ARG:HH11	1:C:380:ARG:HG3	1.65	0.61
1:A:656:ASN:O	1:A:659:ILE:HB	2.00	0.61
1:A:783:ASN:HB3	1:A:805:ARG:HA	1.82	0.61
1:B:538:ASN:HB3	1:B:544:ASN:OD1	2.00	0.61
1:B:546:PHE:O	1:B:573:VAL:HA	2.00	0.61
1:A:281:VAL:HG13	1:A:281:VAL:O	1.99	0.61
1:A:568:ARG:HE	1:A:569:PHE:N	1.95	0.61
1:A:657:PRO:C	1:A:659:ILE:N	2.57	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:VAL:HB	1:A:807:LEU:CD1	2.31	0.61
1:B:698:ASP:O	1:B:699:ASP:C	2.43	0.61
1:A:540:THR:C	1:A:542:ASP:H	2.09	0.61
1:B:287:SER:O	1:B:290:ASN:HB2	2.01	0.61
1:B:391:TRP:CE3	1:B:427:LEU:HD11	2.35	0.61
1:B:655:THR:HA	1:B:659:ILE:HD12	1.82	0.61
1:C:273:PRO:HG3	1:C:337:GLU:HG3	1.81	0.61
1:C:416:LEU:HD22	1:C:457:LEU:HD13	1.81	0.61
1:C:540:THR:C	1:C:542:ASP:H	2.09	0.61
1:C:698:ASP:O	1:C:699:ASP:C	2.43	0.61
1:A:216:ASN:HD21	1:A:261:SER:H	1.47	0.61
1:A:262:LEU:CD1	1:A:640:GLU:HG3	2.31	0.61
1:B:538:ASN:HD22	1:B:538:ASN:H	1.48	0.61
1:B:706:THR:OG1	1:B:741:TRP:CD1	2.53	0.61
1:C:166:PRO:HG3	1:C:546:PHE:CD2	2.35	0.61
1:A:432:GLY:O	1:A:433:ASP:C	2.42	0.61
1:A:736:TRP:HA	1:A:760:TYR:O	2.00	0.61
1:B:340:LEU:O	1:B:341:ASN:HB2	1.99	0.61
1:B:600:TYR:O	1:B:607:LEU:HA	1.99	0.61
1:B:698:ASP:O	1:B:701:GLY:N	2.33	0.61
1:A:593:PHE:HB3	1:A:612:GLU:HG3	1.82	0.61
1:B:593:PHE:HB3	1:B:612:GLU:HG3	1.83	0.61
1:C:183:ASN:HD21	1:C:808:MSE:HE1	1.65	0.61
1:C:240:MSE:HE2	1:C:240:MSE:HA	1.83	0.61
1:C:262:LEU:CD1	1:C:640:GLU:HG3	2.30	0.61
1:C:596:GLN:HG2	1:C:600:TYR:HD2	1.65	0.61
1:A:166:PRO:HG3	1:A:546:PHE:CD2	2.35	0.61
1:A:340:LEU:CB	1:A:343:ASP:HB2	2.30	0.61
1:A:434:TRP:CB	1:A:441:ALA:HB1	2.29	0.61
1:A:600:TYR:O	1:A:607:LEU:HA	2.00	0.61
1:C:677:ILE:HG12	1:C:678:SER:N	2.13	0.61
1:C:771:ILE:HG13	1:C:772:THR:CG2	2.28	0.61
1:A:144:SER:O	1:A:146:SER:N	2.29	0.61
1:A:467:PHE:CD2	1:A:468:LEU:HD23	2.35	0.61
1:C:552:VAL:CG1	1:C:593:PHE:HZ	2.13	0.61
1:B:262:LEU:CD1	1:B:640:GLU:HG3	2.31	0.60
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.66	0.60
1:B:694:LYS:O	1:B:694:LYS:HD3	2.01	0.60
1:C:782:ASN:CB	1:C:806:ASN:HD22	2.14	0.60
1:B:540:THR:C	1:B:542:ASP:H	2.09	0.60
1:C:348:VAL:HG12	1:C:400:ALA:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:HIS:CG	1:B:326:GLU:HG2	2.37	0.60
1:B:736:TRP:HA	1:B:760:TYR:O	2.00	0.60
1:B:746:ASN:ND2	1:B:749:ARG:HB2	2.17	0.60
1:B:771:ILE:HG13	1:B:772:THR:CG2	2.29	0.60
1:A:280:HIS:HB2	1:A:813:TRP:CB	2.26	0.60
1:A:280:HIS:O	1:A:295:LEU:HD12	2.00	0.60
1:A:386:ALA:HB3	1:A:389:SER:HB2	1.81	0.60
1:B:281:VAL:O	1:B:281:VAL:HG13	1.98	0.60
1:C:506:TRP:CH2	1:C:508:GLY:HA2	2.36	0.60
1:A:540:THR:CG2	1:A:542:ASP:OD2	2.49	0.60
1:A:134:SER:CA	1:A:139:THR:HA	2.28	0.60
1:A:659:ILE:HG12	1:A:660:THR:N	2.17	0.60
1:C:158:LEU:HD21	1:C:473:GLU:HG3	1.84	0.60
1:C:271:LYS:HB3	1:C:310:ARG:NH1	2.17	0.60
1:A:344:THR:CG2	1:A:405:ASN:ND2	2.64	0.60
1:C:746:ASN:ND2	1:C:749:ARG:CG	2.65	0.60
1:B:655:THR:HG23	1:B:659:ILE:CD1	2.28	0.60
1:B:677:ILE:HG12	1:B:678:SER:N	2.15	0.60
1:C:776:SER:H	1:C:812:ARG:CB	2.15	0.60
1:A:506:TRP:CH2	1:A:508:GLY:HA2	2.36	0.60
1:A:648:ALA:O	1:A:649:LEU:C	2.44	0.60
1:A:682:ALA:HB1	1:A:683:PRO:HD3	1.84	0.60
1:A:134:SER:HB3	1:A:139:THR:HB	1.84	0.60
1:B:260:GLY:O	1:B:594:MSE:HB2	2.01	0.60
1:B:391:TRP:CD1	1:B:393:GLN:HG3	2.36	0.60
1:B:783:ASN:HB3	1:B:805:ARG:HA	1.82	0.60
1:C:536:ARG:O	1:C:536:ARG:CG	2.42	0.60
1:A:596:GLN:HG2	1:A:600:TYR:CD2	2.37	0.59
1:B:246:VAL:O	1:B:246:VAL:HG13	2.01	0.59
1:C:741:TRP:HA	1:C:755:PHE:O	2.02	0.59
1:A:554:TYR:CG	1:A:595:PRO:HG3	2.36	0.59
1:B:391:TRP:HD1	1:B:393:GLN:HG3	1.67	0.59
1:C:340:LEU:CB	1:C:343:ASP:HB2	2.32	0.59
1:C:596:GLN:HG2	1:C:600:TYR:CD2	2.37	0.59
1:C:600:TYR:O	1:C:607:LEU:HA	2.01	0.59
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.67	0.59
1:B:340:LEU:CB	1:B:343:ASP:HB2	2.32	0.59
1:A:698:ASP:O	1:A:701:GLY:N	2.35	0.59
1:B:370:ASP:O	1:B:371:SER:C	2.44	0.59
1:A:697:ARG:NH2	1:A:703:LYS:NZ	2.50	0.59
1:B:350:ALA:CB	1:B:398:VAL:HG22	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:SER:H	1:B:812:ARG:CB	2.15	0.59
1:B:782:ASN:HB3	1:B:806:ASN:HD22	1.67	0.59
1:C:216:ASN:HA	1:C:227:ARG:HH21	1.66	0.59
1:C:681:LEU:HD22	1:C:687:VAL:HG11	1.84	0.59
1:C:689:ALA:HB2	1:C:715:LEU:HD12	1.83	0.59
1:B:136:GLN:HG2	1:B:137:LEU:N	2.16	0.59
1:C:200:TYR:HD1	1:C:795:PHE:CZ	2.21	0.59
1:A:698:ASP:O	1:A:699:ASP:C	2.46	0.59
1:C:177:MSE:HA	1:C:182:LEU:HD12	1.83	0.59
4:J:1:PVE:H212	4:J:1:PVE:N11	2.16	0.59
1:A:185:ILE:O	1:A:185:ILE:HD13	2.03	0.59
1:A:260:GLY:O	1:A:594:MSE:HB2	2.03	0.59
1:A:813:TRP:O	1:A:814:ASP:HB2	2.01	0.59
1:B:434:TRP:CB	1:B:441:ALA:HB1	2.30	0.59
1:B:543:LEU:HA	1:B:576:VAL:O	2.02	0.59
1:C:529:LEU:HB2	1:C:553:ASP:OD2	2.03	0.59
1:C:607:LEU:O	1:C:608:LEU:C	2.44	0.59
1:A:341:ASN:C	1:A:343:ASP:N	2.61	0.59
1:B:447:LYS:HD2	1:B:515:TRP:CD1	2.38	0.59
1:B:596:GLN:HG2	1:B:600:TYR:HD2	1.68	0.59
1:B:682:ALA:HB1	1:B:683:PRO:CD	2.32	0.59
1:C:346:LEU:HA	1:C:402:LEU:HB3	1.83	0.59
1:C:655:THR:OG1	1:C:659:ILE:HD12	2.01	0.59
1:A:745:TYR:HB2	1:A:752:TRP:HE1	1.67	0.59
1:B:341:ASN:C	1:B:343:ASP:N	2.61	0.59
1:C:287:SER:O	1:C:290:ASN:HB2	2.03	0.59
1:C:682:ALA:HB1	1:C:683:PRO:HD3	1.85	0.59
1:A:344:THR:HG1	1:A:404:HIS:HA	1.66	0.58
1:B:240:MSE:HA	1:B:240:MSE:HE2	1.85	0.58
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.35	0.58
1:C:243:TYR:CE2	1:C:268:LEU:HB3	2.37	0.58
1:A:546:PHE:O	1:A:573:VAL:HA	2.03	0.58
1:A:768:ARG:HB2	1:A:778:SER:HB3	1.85	0.58
1:C:236:THR:HG23	1:C:237:LEU:HD23	1.80	0.58
1:C:474:LEU:CD1	1:C:533:MSE:HG3	2.25	0.58
1:C:745:TYR:HB2	1:C:752:TRP:HE1	1.68	0.58
1:A:324:HIS:CE1	1:A:383:ASN:HB3	2.31	0.58
1:A:771:ILE:HG13	1:A:772:THR:CG2	2.29	0.58
1:B:766:MSE:SE	1:B:766:MSE:C	2.96	0.58
1:C:350:ALA:HB2	1:C:398:VAL:HG22	1.84	0.58
1:C:511:GLY:O	1:C:513:PRO:HD3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:LEU:O	1:B:608:LEU:C	2.47	0.58
1:A:607:LEU:O	1:A:608:LEU:C	2.46	0.58
1:A:776:SER:H	1:A:812:ARG:CB	2.15	0.58
1:A:538:ASN:HD22	1:A:538:ASN:N	2.01	0.58
1:C:189:MSE:HE1	1:C:266:ILE:CD1	2.32	0.58
1:C:342:PRO:C	1:C:344:THR:N	2.61	0.58
1:C:394:TYR:CE1	1:C:422:GLY:HA3	2.38	0.58
1:C:691:TYR:HA	1:C:712:GLN:O	2.04	0.58
1:A:342:PRO:C	1:A:344:THR:N	2.61	0.58
1:B:370:ASP:O	1:B:372:GLN:N	2.36	0.58
1:B:185:ILE:HG23	1:B:186:ASP:N	2.19	0.58
1:C:228:ASN:HA	2:K:3:ARG:HH11	1.66	0.58
1:A:619:GLY:HA3	1:A:634:ALA:HB2	1.86	0.58
1:C:185:ILE:HG23	1:C:186:ASP:N	2.18	0.58
1:C:416:LEU:CD2	1:C:457:LEU:HD12	2.32	0.58
1:C:447:LYS:HD2	1:C:515:TRP:CD1	2.39	0.58
1:C:358:LYS:HA	1:C:390:SER:HB3	1.86	0.58
1:B:691:TYR:HA	1:B:712:GLN:O	2.03	0.57
1:C:218:GLN:OE1	1:C:265:THR:HG21	2.04	0.57
1:A:357:PRO:HD2	1:A:392:GLU:HA	1.85	0.57
1:B:342:PRO:C	1:B:344:THR:N	2.61	0.57
1:B:655:THR:HG22	1:B:655:THR:O	2.03	0.57
1:C:552:VAL:HG11	1:C:593:PHE:CZ	2.39	0.57
1:C:683:PRO:HG2	1:C:684:GLY:N	2.18	0.57
1:A:350:ALA:CB	1:A:398:VAL:HG22	2.35	0.57
1:B:169:ILE:HD11	1:B:249:LEU:HD12	1.86	0.57
1:B:446:GLN:HG2	1:B:491:TRP:HB3	1.86	0.57
1:C:339:ASP:C	1:C:340:LEU:HG	2.28	0.57
1:A:741:TRP:HA	1:A:755:PHE:O	2.03	0.57
1:B:764:ASP:HB2	1:B:782:ASN:HA	1.85	0.57
1:A:218:GLN:OE1	1:A:265:THR:HG21	2.03	0.57
1:B:560:ASN:O	1:B:562:THR:N	2.37	0.57
1:C:352:TYR:HD1	1:C:396:ARG:CB	2.16	0.57
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.40	0.57
1:A:540:THR:HG22	1:A:542:ASP:OD2	2.05	0.57
1:B:554:TYR:CD2	1:B:595:PRO:HG3	2.38	0.57
1:C:147:TYR:HA	1:C:173:THR:CG2	2.28	0.57
1:C:443:ILE:HG13	1:C:443:ILE:O	2.04	0.57
1:C:538:ASN:HB3	1:C:544:ASN:ND2	2.18	0.57
1:B:682:ALA:HB1	1:B:683:PRO:HD3	1.87	0.57
1:C:186:ASP:C	1:C:188:VAL:H	2.13	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:C	1:A:188:VAL:H	2.13	0.57
1:A:246:VAL:HG13	1:A:246:VAL:O	2.03	0.57
1:A:401:ASN:HB3	1:A:415:GLN:HB3	1.86	0.57
1:B:619:GLY:HA3	1:B:634:ALA:HB2	1.87	0.57
1:C:434:TRP:CB	1:C:441:ALA:HB1	2.31	0.57
1:B:216:ASN:HD21	1:B:261:SER:H	1.51	0.57
1:C:281:VAL:O	1:C:281:VAL:HG13	2.05	0.57
1:C:554:TYR:CE2	1:C:595:PRO:CG	2.88	0.57
1:A:167:GLN:NE2	1:A:572:TYR:CE1	2.73	0.57
1:A:339:ASP:C	1:A:340:LEU:HG	2.29	0.57
1:A:543:LEU:HA	1:A:576:VAL:O	2.04	0.57
1:C:352:TYR:CE1	1:C:396:ARG:HG2	2.37	0.57
1:A:233:ALA:HA	1:A:393:GLN:OE1	2.05	0.56
1:A:719:TYR:HE2	1:A:721:PHE:HD1	1.54	0.56
1:A:768:ARG:HG3	1:A:778:SER:CB	2.33	0.56
1:A:802:GLY:O	1:A:803:ASP:C	2.48	0.56
1:B:140:ILE:HG22	1:B:141:THR:H	1.68	0.56
1:B:404:HIS:O	1:B:411:VAL:HG23	2.05	0.56
1:B:506:TRP:CH2	1:B:508:GLY:HA2	2.39	0.56
1:B:596:GLN:HG2	1:B:600:TYR:CD2	2.40	0.56
1:B:631:THR:HG22	1:B:677:ILE:HG13	1.86	0.56
1:C:341:ASN:C	1:C:343:ASP:N	2.61	0.56
1:C:401:ASN:HB3	1:C:415:GLN:HB3	1.87	0.56
1:C:503:PHE:O	1:C:506:TRP:HB3	2.05	0.56
1:C:543:LEU:HA	1:C:576:VAL:O	2.05	0.56
1:A:145:GLY:CA	1:A:175:GLN:HG2	2.35	0.56
1:A:145:GLY:HA2	1:A:175:GLN:HG2	1.87	0.56
1:A:240:MSE:C	1:A:242:ILE:H	2.13	0.56
1:A:391:TRP:O	1:A:391:TRP:HD1	1.88	0.56
1:A:467:PHE:HE2	1:A:468:LEU:CD2	2.16	0.56
1:A:496:TYR:CE1	1:A:513:PRO:HB3	2.40	0.56
1:A:511:GLY:O	1:A:513:PRO:HD3	2.04	0.56
1:A:790:TYR:CE1	1:A:801:TYR:CE1	2.93	0.56
1:B:196:THR:HG21	1:B:709:PRO:HD2	1.87	0.56
1:B:401:ASN:HB3	1:B:415:GLN:HB3	1.87	0.56
1:B:477:GLY:HA3	1:B:532:TYR:CE1	2.40	0.56
1:B:511:GLY:O	1:B:513:PRO:HD3	2.05	0.56
1:C:341:ASN:O	1:C:342:PRO:C	2.48	0.56
1:C:391:TRP:CZ3	1:C:427:LEU:HD11	2.40	0.56
1:C:707:TRP:O	1:C:709:PRO:HD3	2.05	0.56
1:C:762:LEU:HD21	1:C:789:TYR:CE2	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:O	1:A:550:ARG:HD2	2.06	0.56
1:A:467:PHE:HE2	1:A:468:LEU:HD23	1.67	0.56
1:A:683:PRO:HG2	1:A:684:GLY:N	2.21	0.56
1:B:191:HIS:CD2	1:B:716:TYR:CZ	2.93	0.56
1:B:723:GLY:O	1:B:724:ALA:C	2.49	0.56
1:C:246:VAL:HG13	1:C:246:VAL:O	2.05	0.56
1:C:538:ASN:H	1:C:538:ASN:HD22	1.51	0.56
1:A:631:THR:HG22	1:A:677:ILE:HG22	1.88	0.56
1:A:774:LYS:O	1:A:775:LEU:HB2	2.06	0.56
1:B:554:TYR:O	1:B:564:ARG:HB2	2.06	0.56
1:A:247:GLU:HG3	1:A:267:ASN:HB3	1.86	0.56
1:B:242:ILE:O	1:B:271:LYS:HG3	2.06	0.56
1:B:339:ASP:C	1:B:340:LEU:HG	2.31	0.56
1:B:392:GLU:HB3	1:B:424:HIS:HB3	1.86	0.56
1:B:745:TYR:HE1	1:B:750:SER:O	1.86	0.56
1:B:802:GLY:O	1:B:803:ASP:C	2.48	0.56
1:A:140:ILE:HG22	1:A:141:THR:H	1.70	0.56
1:A:185:ILE:HG23	1:A:186:ASP:N	2.20	0.56
1:A:774:LYS:O	1:A:775:LEU:CB	2.53	0.56
1:B:280:HIS:C	1:B:280:HIS:CD2	2.83	0.56
1:B:358:LYS:HA	1:B:390:SER:HB3	1.88	0.56
1:B:538:ASN:HD22	1:B:538:ASN:N	2.02	0.56
1:C:280:HIS:O	1:C:295:LEU:HD12	2.05	0.56
1:C:568:ARG:NE	1:C:568:ARG:HA	2.20	0.56
1:C:391:TRP:O	1:C:391:TRP:CD1	2.59	0.56
1:C:554:TYR:O	1:C:564:ARG:HB2	2.06	0.56
1:C:689:ALA:HB1	1:C:714:SER:O	2.05	0.56
1:A:190:ARG:NH1	1:A:197:VAL:CG1	2.69	0.56
1:A:220:ASP:OD2	1:A:270:ARG:HG3	2.05	0.56
1:A:560:ASN:O	1:A:562:THR:N	2.39	0.56
1:A:723:GLY:O	1:A:724:ALA:C	2.48	0.56
1:C:653:LYS:O	1:C:655:THR:N	2.38	0.56
1:C:725:LEU:C	1:C:727:LYS:H	2.13	0.56
1:A:694:LYS:O	1:A:694:LYS:HD3	2.05	0.56
1:B:341:ASN:O	1:B:343:ASP:N	2.39	0.56
1:B:387:LYS:N	1:B:508:GLY:O	2.29	0.56
1:B:689:ALA:HB2	1:B:715:LEU:HA	1.88	0.56
1:C:394:TYR:OH	1:C:422:GLY:HA3	2.05	0.56
1:C:802:GLY:O	1:C:803:ASP:C	2.48	0.56
1:B:657:PRO:C	1:B:659:ILE:H	2.14	0.55
1:B:725:LEU:C	1:B:727:LYS:H	2.12	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:HG22	1:C:141:THR:H	1.70	0.55
1:C:233:ALA:HA	1:C:393:GLN:OE1	2.05	0.55
1:A:323:ASP:O	1:A:325:TYR:N	2.39	0.55
1:A:358:LYS:HA	1:A:390:SER:HB3	1.87	0.55
1:A:443:ILE:O	1:A:443:ILE:HG13	2.06	0.55
1:A:529:LEU:HB2	1:A:553:ASP:OD2	2.06	0.55
1:B:240:MSE:C	1:B:242:ILE:H	2.14	0.55
1:B:503:PHE:O	1:B:506:TRP:HB3	2.06	0.55
1:B:689:ALA:HB2	1:B:715:LEU:CD1	2.36	0.55
1:C:185:ILE:HD13	1:C:185:ILE:C	2.31	0.55
1:A:185:ILE:HD13	1:A:189:MSE:HG2	1.89	0.55
1:A:503:PHE:O	1:A:506:TRP:HB3	2.07	0.55
1:B:486:GLU:HA	1:B:522:ILE:O	2.06	0.55
1:C:375:ARG:NH1	1:C:755:PHE:HE1	2.04	0.55
1:A:719:TYR:CE2	1:A:721:PHE:CD1	2.94	0.55
1:B:201:ASP:HB3	1:B:363:SER:N	2.22	0.55
1:B:653:LYS:H	1:B:653:LYS:CD	2.12	0.55
1:C:689:ALA:HB2	1:C:715:LEU:HA	1.88	0.55
1:C:766:MSE:SE	1:C:766:MSE:C	2.99	0.55
1:B:253:THR:CG2	1:B:265:THR:OG1	2.54	0.55
1:B:394:TYR:CE1	1:B:422:GLY:HA3	2.41	0.55
1:B:706:THR:OG1	1:B:741:TRP:CE2	2.58	0.55
1:C:391:TRP:O	1:C:391:TRP:HD1	1.88	0.55
1:C:526:THR:HG22	1:C:554:TYR:HE1	1.71	0.55
1:C:716:TYR:CD1	1:C:733:GLY:HA3	2.42	0.55
1:A:246:VAL:CG2	1:A:268:LEU:HD23	2.30	0.55
1:A:689:ALA:HB2	1:A:715:LEU:HA	1.89	0.55
1:B:185:ILE:HD13	1:B:185:ILE:C	2.31	0.55
1:B:538:ASN:CB	1:B:544:ASN:OD1	2.54	0.55
1:C:352:TYR:CD1	1:C:396:ARG:CD	2.89	0.55
1:C:694:LYS:HD3	1:C:710:GLN:HA	1.89	0.55
1:A:375:ARG:NH1	1:A:755:PHE:HE1	2.05	0.55
1:A:552:VAL:CG2	1:A:553:ASP:N	2.70	0.55
1:A:658:ALA:O	1:A:659:ILE:O	2.24	0.55
1:C:220:ASP:OD2	1:C:270:ARG:NE	2.40	0.55
1:C:552:VAL:CG2	1:C:553:ASP:N	2.69	0.55
1:C:560:ASN:O	1:C:562:THR:N	2.40	0.55
1:A:707:TRP:O	1:A:709:PRO:HD3	2.07	0.55
1:C:240:MSE:C	1:C:242:ILE:H	2.13	0.55
1:C:552:VAL:HG11	1:C:593:PHE:HZ	1.72	0.55
1:C:689:ALA:CB	1:C:715:LEU:HA	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:HG22	1:A:475:VAL:O	2.07	0.55
1:A:725:LEU:C	1:A:727:LYS:H	2.15	0.55
1:C:216:ASN:HA	1:C:227:ARG:NH2	2.22	0.55
1:C:357:PRO:HD2	1:C:392:GLU:HA	1.88	0.55
1:C:475:VAL:O	1:C:475:VAL:HG22	2.06	0.55
1:C:496:TYR:CE1	1:C:513:PRO:HB3	2.42	0.55
1:C:709:PRO:HG2	1:C:737:GLN:HB2	1.89	0.55
1:A:391:TRP:O	1:A:391:TRP:CD1	2.59	0.55
1:A:568:ARG:NE	1:A:568:ARG:HA	2.21	0.55
1:A:595:PRO:HA	1:A:610:PRO:HB3	1.89	0.55
1:B:141:THR:C	1:B:143:ASP:H	2.15	0.55
1:B:552:VAL:CG2	1:B:553:ASP:N	2.69	0.55
1:C:341:ASN:O	1:C:343:ASP:N	2.40	0.55
1:C:694:LYS:HE2	1:C:708:GLU:O	2.06	0.55
1:A:423:TYR:O	1:A:423:TYR:CD1	2.60	0.54
1:A:554:TYR:O	1:A:564:ARG:HB2	2.07	0.54
1:A:625:LEU:C	1:A:627:GLY:N	2.65	0.54
1:B:683:PRO:HG2	1:B:684:GLY:N	2.21	0.54
1:C:404:HIS:O	1:C:411:VAL:HG23	2.08	0.54
1:A:691:TYR:HA	1:A:712:GLN:O	2.07	0.54
1:B:375:ARG:NH1	1:B:755:PHE:HE1	2.05	0.54
1:B:721:PHE:HD2	1:B:725:LEU:HD12	1.72	0.54
1:C:386:ALA:O	1:C:389:SER:N	2.37	0.54
1:A:341:ASN:O	1:A:343:ASP:N	2.40	0.54
1:A:348:VAL:HG12	1:A:400:ALA:HA	1.88	0.54
1:B:538:ASN:HA	1:B:544:ASN:HA	1.89	0.54
1:B:764:ASP:HA	1:B:784:VAL:HG23	1.88	0.54
1:C:200:TYR:CE2	1:C:206:ASN:HB3	2.41	0.54
1:C:774:LYS:O	1:C:775:LEU:CB	2.56	0.54
1:C:812:ARG:HG3	1:C:813:TRP:N	2.15	0.54
1:A:510:ILE:CG2	1:A:511:GLY:N	2.70	0.54
1:A:542:ASP:HA	1:A:578:ASP:CG	2.30	0.54
1:A:769:TYR:HD2	1:A:771:ILE:HG22	1.73	0.54
1:A:783:ASN:C	1:A:783:ASN:HD22	2.15	0.54
1:B:348:VAL:HG12	1:B:400:ALA:HA	1.88	0.54
1:C:141:THR:C	1:C:143:ASP:H	2.15	0.54
1:C:538:ASN:HD22	1:C:538:ASN:N	2.05	0.54
1:A:341:ASN:O	1:A:342:PRO:C	2.48	0.54
1:B:341:ASN:O	1:B:342:PRO:C	2.48	0.54
1:B:484:HIS:ND1	1:B:525:LYS:HG2	2.22	0.54
1:B:589:TYR:CE1	1:B:614:GLN:HB3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:TYR:HE1	1:B:654:PRO:HD2	1.71	0.54
1:C:298:SER:HB2	1:C:310:ARG:HG3	1.90	0.54
1:C:350:ALA:CB	1:C:398:VAL:HG22	2.38	0.54
1:B:184:ASN:OD1	1:B:186:ASP:N	2.41	0.54
1:A:689:ALA:HB1	1:A:714:SER:O	2.08	0.54
1:B:173:THR:OG1	1:B:174:ARG:N	2.40	0.54
1:B:191:HIS:HD2	1:B:716:TYR:CZ	2.26	0.54
1:B:200:TYR:CE2	1:B:206:ASN:HB3	2.43	0.54
1:B:569:PHE:CE2	1:B:571:PRO:HB3	2.43	0.54
1:B:597:ASP:HB3	1:B:599:TRP:CE3	2.42	0.54
1:C:220:ASP:OD2	1:C:270:ARG:HG3	2.08	0.54
1:C:253:THR:OG1	1:C:257:THR:CG2	2.56	0.54
1:C:255:LEU:O	1:C:550:ARG:HD2	2.08	0.54
1:C:595:PRO:HA	1:C:610:PRO:HB3	1.90	0.54
1:C:484:HIS:ND1	1:C:525:LYS:HG2	2.22	0.54
1:C:631:THR:HG22	1:C:677:ILE:HG13	1.90	0.54
1:A:271:LYS:HB3	1:A:310:ARG:CZ	2.38	0.54
1:A:340:LEU:O	1:A:341:ASN:HB2	2.07	0.54
1:A:597:ASP:HB3	1:A:599:TRP:CE3	2.43	0.54
1:C:657:PRO:C	1:C:659:ILE:H	2.14	0.54
1:C:769:TYR:HD2	1:C:771:ILE:HG22	1.73	0.54
1:A:689:ALA:CB	1:A:715:LEU:HA	2.38	0.54
1:B:755:PHE:HB3	1:B:793:ILE:HG21	1.89	0.54
1:C:167:GLN:NE2	1:C:572:TYR:CE1	2.76	0.54
1:C:271:LYS:HB3	1:C:310:ARG:CZ	2.38	0.54
1:C:434:TRP:C	1:C:436:ALA:H	2.16	0.54
1:C:723:GLY:O	1:C:724:ALA:C	2.50	0.54
1:C:746:ASN:HD21	1:C:749:ARG:HG2	1.71	0.54
1:A:446:GLN:HB3	1:A:448:TYR:HE1	1.73	0.53
1:B:186:ASP:C	1:B:188:VAL:H	2.16	0.53
1:B:220:ASP:OD2	1:B:270:ARG:NE	2.41	0.53
1:B:754:LYS:N	1:B:754:LYS:CD	2.71	0.53
1:C:158:LEU:HD13	1:C:475:VAL:HB	1.89	0.53
1:C:442:LYS:HA	1:C:498:ASN:O	2.07	0.53
1:C:592:ILE:HG12	1:C:593:PHE:N	2.23	0.53
1:A:366:PHE:HB3	1:A:382:PHE:HD2	1.73	0.53
1:A:447:LYS:HD2	1:A:515:TRP:CD1	2.43	0.53
1:A:681:LEU:HB2	1:A:687:VAL:HG12	1.91	0.53
1:C:170:THR:HG21	1:C:193:PRO:HG2	1.91	0.53
1:A:184:ASN:OD1	1:A:186:ASP:N	2.41	0.53
1:B:596:GLN:OE1	1:B:644:ALA:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ALA:CB	1:B:715:LEU:HA	2.38	0.53
1:B:689:ALA:HB1	1:B:714:SER:O	2.07	0.53
1:C:324:HIS:CE1	1:C:383:ASN:HB3	2.33	0.53
1:A:434:TRP:C	1:A:436:ALA:H	2.16	0.53
1:A:651:ASN:O	1:A:653:LYS:HG3	2.09	0.53
1:B:218:GLN:OE1	1:B:265:THR:HG21	2.07	0.53
1:B:323:ASP:O	1:B:325:TYR:N	2.42	0.53
1:B:689:ALA:HB2	1:B:715:LEU:HD12	1.89	0.53
1:B:769:TYR:HD2	1:B:771:ILE:HG22	1.73	0.53
1:C:375:ARG:CZ	1:C:755:PHE:CE1	2.91	0.53
1:C:774:LYS:O	1:C:775:LEU:HB2	2.09	0.53
1:A:394:TYR:OH	1:A:422:GLY:HA3	2.07	0.53
1:A:689:ALA:HB2	1:A:715:LEU:CD1	2.38	0.53
1:A:740:SER:O	1:A:756:SER:HA	2.09	0.53
1:B:231:TYR:CE2	1:B:485:TRP:HH2	2.27	0.53
1:B:241:ALA:HB2	1:B:292:ARG:NH2	2.24	0.53
1:B:325:TYR:C	1:B:326:GLU:HG3	2.34	0.53
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.43	0.53
1:A:378:VAL:HG22	1:A:382:PHE:HB2	1.91	0.53
1:A:387:LYS:N	1:A:508:GLY:O	2.30	0.53
1:B:296:ASP:OD2	1:B:310:ARG:NH2	2.42	0.53
1:B:446:GLN:HB3	1:B:448:TYR:HE1	1.74	0.53
1:B:707:TRP:O	1:B:709:PRO:HD3	2.08	0.53
1:C:281:VAL:HB	1:C:295:LEU:HD13	1.91	0.53
1:C:372:GLN:N	1:C:372:GLN:OE1	2.42	0.53
1:C:538:ASN:HA	1:C:544:ASN:HA	1.90	0.53
1:C:638:ILE:HD12	1:C:670:THR:HG21	1.91	0.53
1:A:152:ILE:HD13	1:A:169:ILE:HG21	1.91	0.53
1:A:366:PHE:HB3	1:A:382:PHE:CD2	2.44	0.53
1:A:375:ARG:CZ	1:A:755:PHE:CE1	2.91	0.53
1:A:655:THR:O	1:A:659:ILE:HB	2.09	0.53
1:B:157:ARG:HD3	1:B:460:TYR:CD2	2.43	0.53
1:C:539:VAL:HB	1:C:543:LEU:CD2	2.39	0.53
1:A:201:ASP:OD1	1:A:201:ASP:N	2.41	0.53
1:C:538:ASN:CB	1:C:544:ASN:HD22	2.21	0.53
1:C:683:PRO:CG	1:C:684:GLY:H	2.21	0.53
1:C:740:SER:O	1:C:756:SER:HA	2.09	0.53
1:A:242:ILE:O	1:A:271:LYS:HG3	2.09	0.53
1:A:551:VAL:HG22	1:A:552:VAL:H	1.73	0.53
1:A:592:ILE:HG12	1:A:593:PHE:N	2.22	0.53
1:B:189:MSE:HE1	1:B:266:ILE:CD1	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HG3	1:B:420:ILE:HD11	1.90	0.53
1:B:774:LYS:O	1:B:775:LEU:HB2	2.09	0.53
1:C:266:ILE:HG22	1:C:267:ASN:N	2.24	0.53
1:C:506:TRP:CE2	1:C:508:GLY:HA2	2.44	0.53
1:C:783:ASN:HD22	1:C:783:ASN:C	2.15	0.53
1:A:477:GLY:HA3	1:A:532:TYR:CE1	2.44	0.53
1:A:484:HIS:ND1	1:A:525:LYS:HG2	2.24	0.53
1:B:247:GLU:CG	1:B:267:ASN:HD22	2.22	0.53
1:B:344:THR:HG21	1:B:405:ASN:ND2	2.24	0.53
1:B:434:TRP:C	1:B:436:ALA:H	2.17	0.53
1:B:625:LEU:HD13	1:B:628:ARG:NH1	2.23	0.53
1:C:246:VAL:CG2	1:C:268:LEU:HD23	2.39	0.53
1:C:596:GLN:OE1	1:C:644:ALA:HB2	2.08	0.53
1:A:372:GLN:N	1:A:372:GLN:OE1	2.42	0.52
1:A:670:THR:O	1:A:670:THR:HG22	2.08	0.52
1:B:496:TYR:CE1	1:B:513:PRO:HB3	2.43	0.52
1:B:738:GLY:O	1:B:739:LYS:O	2.28	0.52
1:C:157:ARG:NH1	1:C:532:TYR:OH	2.42	0.52
1:C:201:ASP:OD2	1:C:204:ARG:NE	2.41	0.52
1:C:378:VAL:HG22	1:C:382:PHE:HB2	1.92	0.52
1:A:241:ALA:HB2	1:A:292:ARG:NH2	2.24	0.52
1:A:743:MSE:SE	1:A:753:GLU:O	2.77	0.52
1:B:372:GLN:N	1:B:372:GLN:OE1	2.41	0.52
1:B:619:GLY:HA3	1:B:634:ALA:CB	2.39	0.52
1:C:145:GLY:CA	1:C:175:GLN:HG2	2.38	0.52
1:C:211:GLY:N	1:C:708:GLU:OE1	2.43	0.52
1:A:404:HIS:O	1:A:411:VAL:HG23	2.10	0.52
1:A:599:TRP:HE1	2:I:4:DSN:HA	1.73	0.52
1:B:372:GLN:HA	1:B:748:PRO:HB3	1.91	0.52
1:B:658:ALA:O	1:B:659:ILE:O	2.27	0.52
1:B:706:THR:OG1	1:B:741:TRP:CG	2.62	0.52
1:C:446:GLN:HB3	1:C:448:TYR:CE1	2.45	0.52
1:C:625:LEU:C	1:C:627:GLY:N	2.66	0.52
1:A:470:ARG:HG2	1:A:470:ARG:NH1	2.23	0.52
1:B:158:LEU:HD13	1:B:475:VAL:HB	1.91	0.52
1:C:157:ARG:HD3	1:C:460:TYR:CD2	2.44	0.52
1:A:441:ALA:H	1:A:500:THR:HG22	1.75	0.52
1:A:590:THR:OG1	1:A:615:ASN:HB3	2.10	0.52
1:B:266:ILE:HG22	1:B:267:ASN:N	2.24	0.52
1:B:443:ILE:HG13	1:B:443:ILE:O	2.09	0.52
1:B:763:VAL:HG11	1:B:785:PHE:CD2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:THR:HB	1:C:679:GLY:HA2	1.91	0.52
1:C:194:GLY:HA3	1:C:250:LYS:NZ	2.24	0.52
1:C:694:LYS:HD3	1:C:694:LYS:O	2.09	0.52
1:A:271:LYS:HD3	1:A:310:ARG:NH2	2.25	0.52
1:A:486:GLU:HA	1:A:522:ILE:O	2.10	0.52
1:A:619:GLY:HA3	1:A:634:ALA:CB	2.39	0.52
1:B:589:TYR:HE1	1:B:614:GLN:CB	2.23	0.52
1:B:745:TYR:HB2	1:B:752:TRP:HE1	1.74	0.52
1:C:185:ILE:O	1:C:188:VAL:HB	2.10	0.52
1:C:439:ASN:HD21	1:C:504:ILE:HG22	1.75	0.52
1:C:446:GLN:HG2	1:C:491:TRP:CB	2.39	0.52
1:C:527:ARG:HH11	1:C:529:LEU:CD1	2.23	0.52
1:A:201:ASP:HB3	1:A:363:SER:N	2.25	0.52
1:A:439:ASN:HD21	1:A:504:ILE:HG22	1.75	0.52
1:B:595:PRO:HA	1:B:610:PRO:HB3	1.91	0.52
1:B:740:SER:O	1:B:756:SER:HA	2.10	0.52
1:B:749:ARG:C	1:B:751:ARG:H	2.18	0.52
1:C:325:TYR:C	1:C:326:GLU:HG3	2.33	0.52
1:A:185:ILE:O	1:A:186:ASP:C	2.51	0.52
1:A:517:THR:O	1:A:518:PRO:C	2.53	0.52
1:A:527:ARG:HH11	1:A:529:LEU:CD1	2.23	0.52
1:A:766:MSE:SE	1:A:766:MSE:C	3.03	0.52
1:B:135:ASN:ND2	1:B:138:GLY:O	2.43	0.52
1:B:325:TYR:CE1	1:B:327:ARG:HB3	2.44	0.52
1:B:529:LEU:HB2	1:B:553:ASP:OD2	2.10	0.52
1:B:790:TYR:CE1	1:B:801:TYR:CE1	2.96	0.52
1:C:645:GLU:HG2	1:C:664:LYS:HZ2	1.68	0.52
1:A:185:ILE:O	1:A:188:VAL:N	2.39	0.52
1:B:148:THR:HB	1:B:679:GLY:HA2	1.92	0.52
1:B:625:LEU:C	1:B:627:GLY:N	2.65	0.52
1:C:200:TYR:CD1	1:C:795:PHE:CZ	2.97	0.52
1:C:551:VAL:HG22	1:C:552:VAL:H	1.74	0.52
1:C:625:LEU:HD13	1:C:628:ARG:NH1	2.24	0.52
1:C:681:LEU:HB2	1:C:687:VAL:HG12	1.91	0.52
1:A:192:THR:CB	1:A:195:ILE:HD12	2.39	0.52
1:A:506:TRP:CE2	1:A:508:GLY:HA2	2.45	0.52
1:B:247:GLU:HG3	1:B:267:ASN:HB3	1.91	0.52
1:B:357:PRO:HG2	1:B:391:TRP:H	1.75	0.52
1:B:446:GLN:HB3	1:B:448:TYR:CE1	2.45	0.52
1:B:681:LEU:HB2	1:B:687:VAL:HG12	1.92	0.52
1:C:749:ARG:C	1:C:751:ARG:H	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:CD1	1:A:169:ILE:HG21	2.40	0.51
1:A:189:MSE:CE	1:A:195:ILE:HG21	2.39	0.51
1:A:812:ARG:CG	1:A:813:TRP:H	2.13	0.51
1:B:185:ILE:CG2	1:B:186:ASP:N	2.74	0.51
1:B:270:ARG:NH1	1:B:351:ASP:OD2	2.44	0.51
1:B:341:ASN:O	1:B:344:THR:N	2.43	0.51
1:B:357:PRO:HD2	1:B:392:GLU:HA	1.91	0.51
1:C:357:PRO:HG2	1:C:391:TRP:H	1.74	0.51
1:A:211:GLY:N	1:A:708:GLU:OE1	2.41	0.51
1:A:288:TRP:O	1:A:319:HIS:HB2	2.09	0.51
1:A:446:GLN:HG2	1:A:491:TRP:CB	2.40	0.51
1:A:726:ASP:OD1	1:A:726:ASP:N	2.41	0.51
1:A:762:LEU:HD21	1:A:789:TYR:CE2	2.38	0.51
1:B:709:PRO:HG2	1:B:737:GLN:HB2	1.92	0.51
1:C:152:ILE:CD1	1:C:169:ILE:HG21	2.41	0.51
1:C:185:ILE:CG2	1:C:186:ASP:N	2.73	0.51
1:C:225:THR:C	1:C:227:ARG:H	2.17	0.51
1:C:372:GLN:HA	1:C:748:PRO:HB3	1.91	0.51
1:C:624:TYR:CD1	1:C:624:TYR:N	2.79	0.51
1:A:158:LEU:HD13	1:A:475:VAL:HB	1.92	0.51
1:B:145:GLY:HA2	1:B:175:GLN:HG2	1.92	0.51
1:B:220:ASP:OD2	1:B:270:ARG:HG3	2.09	0.51
1:B:423:TYR:O	1:B:423:TYR:CD1	2.63	0.51
1:B:812:ARG:HG3	1:B:813:TRP:N	2.16	0.51
1:C:152:ILE:HD13	1:C:169:ILE:HG21	1.92	0.51
1:C:323:ASP:O	1:C:325:TYR:N	2.44	0.51
1:C:486:GLU:HA	1:C:522:ILE:O	2.09	0.51
1:C:518:PRO:HB2	1:C:521:TYR:CZ	2.45	0.51
1:A:281:VAL:HB	1:A:295:LEU:HD13	1.92	0.51
1:B:140:ILE:HG22	1:B:142:GLU:H	1.76	0.51
1:B:279:GLY:O	1:B:280:HIS:HB3	2.10	0.51
1:B:510:ILE:CG2	1:B:511:GLY:N	2.73	0.51
1:B:774:LYS:O	1:B:775:LEU:CB	2.58	0.51
1:C:365:SER:CA	1:C:384:ASN:ND2	2.74	0.51
1:C:446:GLN:HB3	1:C:448:TYR:HE1	1.74	0.51
1:C:590:THR:OG1	1:C:615:ASN:HB3	2.11	0.51
1:A:228:ASN:OD1	1:A:230:GLY:N	2.43	0.51
1:A:253:THR:OG1	1:A:257:THR:CG2	2.59	0.51
1:A:357:PRO:HG2	1:A:391:TRP:H	1.75	0.51
1:A:360:SER:HB3	1:A:390:SER:CA	2.38	0.51
1:A:697:ARG:HH21	1:A:703:LYS:HZ2	1.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.46	0.51
1:B:194:GLY:HA3	1:B:250:LYS:NZ	2.25	0.51
1:C:201:ASP:HB3	1:C:363:SER:N	2.26	0.51
1:C:618:ILE:CG2	1:C:618:ILE:O	2.57	0.51
1:A:396:ARG:HG3	1:A:420:ILE:HD11	1.91	0.51
1:A:624:TYR:N	1:A:624:TYR:CD1	2.79	0.51
1:A:640:GLU:OE2	1:A:643:ARG:HG3	2.10	0.51
1:A:749:ARG:C	1:A:751:ARG:H	2.19	0.51
1:B:375:ARG:CZ	1:B:755:PHE:CE1	2.93	0.51
1:C:192:THR:CB	1:C:195:ILE:HD12	2.40	0.51
1:C:510:ILE:CG2	1:C:511:GLY:N	2.73	0.51
1:A:141:THR:C	1:A:143:ASP:H	2.18	0.51
1:A:225:THR:C	1:A:227:ARG:H	2.19	0.51
1:A:387:LYS:HG3	1:A:509:ASP:CA	2.41	0.51
1:A:749:ARG:HH11	1:A:751:ARG:HH21	1.57	0.51
1:B:145:GLY:CA	1:B:175:GLN:HG2	2.40	0.51
1:B:646:GLU:HG3	1:B:646:GLU:O	2.09	0.51
1:B:734:ALA:HA	1:B:762:LEU:O	2.11	0.51
1:C:376:ASN:ND2	1:C:435:PRO:HG2	2.25	0.51
1:C:414:VAL:CB	1:C:459:ILE:HG22	2.41	0.51
1:A:220:ASP:OD2	1:A:270:ARG:NE	2.44	0.51
1:A:414:VAL:CB	1:A:459:ILE:HG22	2.41	0.51
1:B:170:THR:HG21	1:B:193:PRO:HG2	1.93	0.51
1:B:378:VAL:HG22	1:B:382:PHE:HB2	1.92	0.51
1:B:446:GLN:HG2	1:B:491:TRP:CB	2.39	0.51
1:B:655:THR:CG2	1:B:659:ILE:HD12	2.34	0.51
1:B:670:THR:O	1:B:670:THR:HG22	2.09	0.51
1:C:196:THR:HG21	1:C:709:PRO:HD2	1.91	0.51
1:A:218:GLN:HA	1:A:222:ILE:O	2.10	0.51
1:A:538:ASN:HA	1:A:544:ASN:HA	1.92	0.51
1:B:646:GLU:HA	1:B:663:TYR:CD2	2.46	0.51
1:C:790:TYR:CE1	1:C:801:TYR:CE1	2.98	0.51
1:A:140:ILE:HG22	1:A:142:GLU:H	1.74	0.51
1:A:185:ILE:HD13	1:A:185:ILE:C	2.35	0.51
1:A:372:GLN:HA	1:A:748:PRO:HB3	1.92	0.51
1:A:446:GLN:HB3	1:A:448:TYR:CE1	2.46	0.51
1:B:592:ILE:HG12	1:B:593:PHE:N	2.25	0.51
1:C:211:GLY:HA2	1:C:708:GLU:OE1	2.11	0.51
1:C:695:ILE:CD1	1:C:710:GLN:HE21	2.24	0.51
1:A:157:ARG:NH2	1:A:458:ASP:OD2	2.44	0.50
1:B:277:PHE:CG	1:B:278:LYS:N	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LYS:HG3	1:B:509:ASP:CA	2.41	0.50
1:A:201:ASP:OD2	1:A:204:ARG:NE	2.42	0.50
1:A:446:GLN:HG2	1:A:491:TRP:HB3	1.93	0.50
1:B:157:ARG:NH1	1:B:532:TYR:OH	2.43	0.50
1:B:179:ASP:OD1	1:B:768:ARG:NH2	2.45	0.50
1:B:473:GLU:HG2	1:B:536:ARG:HB3	1.93	0.50
1:B:682:ALA:HB3	1:B:685:TRP:HB2	1.94	0.50
1:C:640:GLU:OE2	1:C:643:ARG:HG3	2.10	0.50
1:A:266:ILE:CG2	1:A:267:ASN:N	2.74	0.50
1:A:341:ASN:O	1:A:344:THR:N	2.45	0.50
1:A:527:ARG:HH11	1:A:529:LEU:HD11	1.77	0.50
1:A:553:ASP:HA	1:A:566:SER:HA	1.93	0.50
1:A:683:PRO:CG	1:A:684:GLY:H	2.24	0.50
1:B:185:ILE:O	1:B:186:ASP:C	2.54	0.50
1:B:225:THR:C	1:B:227:ARG:H	2.18	0.50
1:B:434:TRP:O	1:B:441:ALA:HB2	2.12	0.50
1:B:647:ASP:OD1	1:B:648:ALA:N	2.45	0.50
1:B:653:LYS:HG2	1:B:659:ILE:HG13	1.92	0.50
1:B:706:THR:OG1	1:B:741:TRP:CD2	2.64	0.50
1:C:241:ALA:HB2	1:C:292:ARG:NH2	2.27	0.50
1:C:317:ASP:C	1:C:317:ASP:OD1	2.54	0.50
1:C:619:GLY:HA3	1:C:634:ALA:HB2	1.93	0.50
1:A:709:PRO:HG2	1:A:737:GLN:HB2	1.93	0.50
1:A:789:TYR:CE1	1:A:802:GLY:HA3	2.46	0.50
1:B:253:THR:OG1	1:B:257:THR:CG2	2.59	0.50
1:B:275:HIS:CE1	1:B:308:ARG:HH11	2.30	0.50
1:B:475:VAL:O	1:B:476:VAL:C	2.53	0.50
1:B:650:TYR:CZ	1:B:653:LYS:HB2	2.46	0.50
1:B:754:LYS:C	1:B:754:LYS:CD	2.84	0.50
1:C:168:SER:HB2	1:C:617:GLU:OE2	2.11	0.50
1:A:298:SER:HB2	1:A:310:ARG:HG3	1.94	0.50
1:A:341:ASN:CB	1:A:342:PRO:CD	2.86	0.50
1:A:388:TRP:CH2	1:A:428:GLY:HA3	2.46	0.50
1:A:503:PHE:O	1:A:504:ILE:C	2.53	0.50
1:A:749:ARG:NH1	1:A:751:ARG:HH21	2.08	0.50
1:B:156:THR:C	1:B:158:LEU:H	2.18	0.50
1:B:255:LEU:O	1:B:550:ARG:HD2	2.11	0.50
1:B:305:GLY:C	1:B:307:VAL:N	2.68	0.50
1:B:517:THR:O	1:B:518:PRO:C	2.53	0.50
1:B:551:VAL:HG22	1:B:552:VAL:H	1.76	0.50
1:A:467:PHE:CD2	1:A:468:LEU:CD2	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:PHE:CE2	1:A:571:PRO:HB3	2.47	0.50
1:A:653:LYS:O	1:A:653:LYS:HD2	2.12	0.50
1:B:201:ASP:OD2	1:B:204:ARG:NE	2.43	0.50
1:C:412:GLY:CA	1:C:461:LEU:HD23	2.42	0.50
1:C:414:VAL:HB	1:C:459:ILE:HG22	1.93	0.50
1:C:728:LEU:HB2	1:C:769:TYR:CD1	2.46	0.50
1:C:755:PHE:HB3	1:C:793:ILE:HG21	1.93	0.50
1:A:648:ALA:O	1:A:650:TYR:N	2.45	0.50
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.47	0.50
1:B:624:TYR:N	1:B:624:TYR:CD1	2.79	0.50
1:B:657:PRO:O	1:B:659:ILE:HG22	2.11	0.50
1:B:683:PRO:CG	1:B:684:GLY:H	2.25	0.50
1:B:746:ASN:O	1:B:747:ASN:C	2.55	0.50
1:C:189:MSE:HE1	1:C:266:ILE:HD11	1.92	0.50
1:C:218:GLN:HA	1:C:222:ILE:O	2.11	0.50
1:C:734:ALA:HA	1:C:762:LEU:O	2.12	0.50
1:A:148:THR:OG1	1:A:149:PRO:HD2	2.11	0.50
1:A:277:PHE:CG	1:A:278:LYS:N	2.80	0.50
1:A:545:LEU:HD12	1:A:575:ALA:HB2	1.93	0.50
1:A:596:GLN:OE1	1:A:644:ALA:HB2	2.11	0.50
1:A:789:TYR:C	1:A:789:TYR:CD1	2.90	0.50
1:B:192:THR:CB	1:B:195:ILE:HD12	2.39	0.50
1:B:509:ASP:CG	1:B:509:ASP:O	2.54	0.50
1:B:553:ASP:HA	1:B:566:SER:HA	1.94	0.50
1:B:600:TYR:HD1	1:B:663:TYR:CD1	2.30	0.50
1:C:296:ASP:OD2	1:C:310:ARG:NH2	2.42	0.50
1:C:341:ASN:O	1:C:344:THR:N	2.45	0.50
1:C:441:ALA:H	1:C:500:THR:HG22	1.77	0.50
1:C:783:ASN:O	1:C:784:VAL:C	2.55	0.50
1:B:201:ASP:CG	1:B:204:ARG:HE	2.20	0.50
1:B:442:LYS:HA	1:B:498:ASN:O	2.11	0.50
1:B:604:SER:O	1:B:605:ASN:HB2	2.11	0.50
1:C:140:ILE:CG2	1:C:141:THR:N	2.75	0.50
1:C:145:GLY:HA2	1:C:175:GLN:HG2	1.92	0.50
1:C:247:GLU:CG	1:C:267:ASN:HD22	2.24	0.50
1:A:170:THR:HG21	1:A:193:PRO:HG2	1.94	0.49
1:A:772:THR:O	1:A:773:ASP:C	2.55	0.49
1:A:783:ASN:C	1:A:783:ASN:ND2	2.69	0.49
1:A:812:ARG:HG3	1:A:813:TRP:N	2.15	0.49
1:B:247:GLU:HG3	1:B:267:ASN:HD22	1.76	0.49
1:B:262:LEU:HD23	1:B:592:ILE:CG2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HA	1:B:402:LEU:HB3	1.93	0.49
1:B:646:GLU:HA	1:B:663:TYR:HD2	1.76	0.49
1:C:288:TRP:O	1:C:319:HIS:HB2	2.12	0.49
1:A:185:ILE:CG2	1:A:186:ASP:N	2.75	0.49
1:A:412:GLY:CA	1:A:461:LEU:HD23	2.42	0.49
1:A:414:VAL:HB	1:A:459:ILE:HG22	1.94	0.49
1:A:556:VAL:O	1:A:556:VAL:HG13	2.12	0.49
1:A:755:PHE:HB3	1:A:793:ILE:HG21	1.94	0.49
1:B:763:VAL:HG11	1:B:785:PHE:HE2	1.75	0.49
1:C:140:ILE:HG22	1:C:142:GLU:H	1.76	0.49
1:C:434:TRP:O	1:C:436:ALA:N	2.45	0.49
4:I:1:PVE:H202	4:I:1:PVE:H11	1.78	0.49
1:A:308:ARG:NH2	1:A:339:ASP:OD2	2.45	0.49
1:A:391:TRP:HD1	1:A:393:GLN:HG3	1.77	0.49
1:B:204:ARG:HD3	1:B:391:TRP:CH2	2.46	0.49
1:B:370:ASP:HB2	1:B:435:PRO:HB2	1.93	0.49
1:B:372:GLN:CD	1:B:373:GLY:N	2.70	0.49
1:B:738:GLY:O	1:B:739:LYS:C	2.55	0.49
1:C:253:THR:OG1	1:C:257:THR:HG23	2.12	0.49
1:C:370:ASP:HB2	1:C:435:PRO:HB2	1.94	0.49
1:C:423:TYR:CD1	1:C:423:TYR:O	2.66	0.49
1:A:154:THR:O	1:A:256:LEU:HD12	2.12	0.49
1:A:325:TYR:C	1:A:326:GLU:HG3	2.36	0.49
1:A:392:GLU:HB3	1:A:424:HIS:HB3	1.93	0.49
1:A:396:ARG:HD3	1:A:420:ILE:HD11	1.95	0.49
1:A:804:PRO:O	1:A:805:ARG:C	2.54	0.49
1:B:288:TRP:O	1:B:319:HIS:HB2	2.12	0.49
1:B:388:TRP:CH2	1:B:428:GLY:HA3	2.47	0.49
1:B:783:ASN:O	1:B:784:VAL:C	2.55	0.49
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.25	0.49
1:C:569:PHE:CE2	1:C:571:PRO:HB3	2.47	0.49
1:C:738:GLY:O	1:C:739:LYS:O	2.31	0.49
1:A:305:GLY:C	1:A:307:VAL:N	2.69	0.49
1:A:658:ALA:C	1:A:659:ILE:O	2.53	0.49
1:A:694:LYS:HD3	1:A:710:GLN:HA	1.95	0.49
1:B:230:GLY:HA2	4:J:1:PVE:O25	2.12	0.49
1:C:553:ASP:HA	1:C:566:SER:HA	1.94	0.49
1:C:751:ARG:HG3	1:C:751:ARG:O	2.12	0.49
1:A:196:THR:HG21	1:A:709:PRO:HD2	1.93	0.49
1:A:302:THR:O	1:A:303:GLU:C	2.55	0.49
1:A:604:SER:O	1:A:605:ASN:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:SER:HB2	1:B:310:ARG:HG3	1.94	0.49
1:B:386:ALA:O	1:B:389:SER:N	2.44	0.49
1:B:441:ALA:H	1:B:500:THR:HG22	1.76	0.49
1:B:628:ARG:HB2	1:B:628:ARG:HH11	1.78	0.49
1:C:383:ASN:C	1:C:385:GLY:N	2.70	0.49
1:C:387:LYS:N	1:C:508:GLY:O	2.34	0.49
1:C:604:SER:O	1:C:605:ASN:HB2	2.13	0.49
1:C:624:TYR:O	1:C:625:LEU:HB2	2.13	0.49
1:A:764:ASP:HA	1:A:784:VAL:HG23	1.94	0.49
1:B:140:ILE:CG2	1:B:141:THR:N	2.74	0.49
1:B:189:MSE:CE	1:B:266:ILE:HD12	2.41	0.49
1:B:590:THR:OG1	1:B:615:ASN:HB3	2.11	0.49
1:B:618:ILE:O	1:B:618:ILE:CG2	2.60	0.49
1:C:173:THR:OG1	1:C:174:ARG:N	2.46	0.49
1:C:504:ILE:O	1:C:505:ASN:C	2.56	0.49
1:A:292:ARG:HD2	1:A:316:GLN:OE1	2.12	0.49
1:A:783:ASN:O	1:A:784:VAL:C	2.55	0.49
1:B:182:LEU:HD22	1:B:187:ASP:O	2.13	0.49
1:C:670:THR:O	1:C:670:THR:HG22	2.11	0.49
1:A:598:SER:N	1:A:599:TRP:CE3	2.81	0.49
1:A:682:ALA:HB3	1:A:683:PRO:HD2	1.95	0.49
1:B:211:GLY:N	1:B:708:GLU:OE1	2.43	0.49
1:B:412:GLY:CA	1:B:461:LEU:HD23	2.43	0.49
1:B:546:PHE:N	1:B:574:GLY:O	2.43	0.49
1:B:556:VAL:O	1:B:556:VAL:HG13	2.11	0.49
1:B:698:ASP:O	1:B:699:ASP:O	2.30	0.49
1:C:179:ASP:OD1	1:C:768:ARG:NH2	2.46	0.49
1:C:244:ASP:OD2	1:C:245:ARG:NH1	2.45	0.49
1:C:383:ASN:O	1:C:385:GLY:N	2.46	0.49
1:C:647:ASP:HB3	1:C:662:ALA:O	2.13	0.49
1:A:474:LEU:HD11	1:A:533:MSE:CG	2.31	0.49
1:A:599:TRP:NE1	2:I:4:DSN:HA	2.28	0.49
1:B:152:ILE:HD13	1:B:169:ILE:HG21	1.94	0.49
1:B:605:ASN:ND2	1:B:605:ASN:O	2.46	0.49
1:C:136:GLN:CD	1:C:136:GLN:H	2.21	0.49
1:C:538:ASN:HB2	1:C:544:ASN:HD22	1.78	0.49
1:C:698:ASP:O	1:C:699:ASP:O	2.31	0.49
1:A:148:THR:HB	1:A:679:GLY:HA2	1.94	0.48
1:A:262:LEU:HD23	1:A:592:ILE:CG2	2.43	0.48
1:A:657:PRO:O	1:A:659:ILE:N	2.46	0.48
1:A:735:ARG:HG3	1:A:736:TRP:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ASN:CB	1:A:806:ASN:HD22	2.25	0.48
1:B:147:TYR:HA	1:B:173:THR:CG2	2.29	0.48
1:B:394:TYR:OH	1:B:422:GLY:HA3	2.13	0.48
1:B:423:TYR:N	1:B:450:GLY:O	2.44	0.48
1:B:561:PRO:O	1:B:563:ILE:HG23	2.13	0.48
1:B:728:LEU:HB2	1:B:769:TYR:CD1	2.48	0.48
1:B:735:ARG:HG3	1:B:736:TRP:N	2.28	0.48
1:C:201:ASP:OD1	1:C:201:ASP:N	2.45	0.48
1:C:262:LEU:HD23	1:C:592:ILE:CG2	2.43	0.48
1:C:740:SER:O	1:C:757:GLN:N	2.38	0.48
1:A:561:PRO:O	1:A:563:ILE:HG23	2.13	0.48
1:A:659:ILE:CG1	1:A:660:THR:H	2.24	0.48
1:A:740:SER:O	1:A:757:GLN:N	2.37	0.48
1:B:302:THR:O	1:B:303:GLU:C	2.56	0.48
1:B:418:HIS:HE1	1:B:453:LYS:HD3	1.78	0.48
1:B:537:PHE:O	1:B:545:LEU:N	2.39	0.48
1:C:185:ILE:O	1:C:188:VAL:N	2.41	0.48
1:C:370:ASP:OD2	1:C:373:GLY:HA3	2.13	0.48
1:C:372:GLN:CD	1:C:373:GLY:N	2.71	0.48
1:C:545:LEU:HD12	1:C:575:ALA:HB2	1.95	0.48
1:A:442:LYS:HA	1:A:498:ASN:O	2.13	0.48
1:A:695:ILE:HD11	1:A:710:GLN:HE22	1.74	0.48
1:B:598:SER:N	1:B:599:TRP:CE3	2.81	0.48
1:C:277:PHE:CG	1:C:278:LYS:N	2.81	0.48
1:C:376:ASN:HD21	1:C:435:PRO:HG2	1.77	0.48
1:C:441:ALA:O	1:C:500:THR:HG22	2.13	0.48
1:C:527:ARG:HH11	1:C:529:LEU:HD11	1.77	0.48
1:C:561:PRO:O	1:C:563:ILE:HG23	2.13	0.48
1:C:764:ASP:HA	1:C:784:VAL:HG23	1.95	0.48
1:A:200:TYR:HB3	1:A:201:ASP:OD1	2.14	0.48
1:A:518:PRO:HB2	1:A:521:TYR:CZ	2.49	0.48
1:A:689:ALA:HB2	1:A:715:LEU:HD12	1.95	0.48
1:B:135:ASN:N	1:B:135:ASN:ND2	2.57	0.48
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.77	0.48
1:B:599:TRP:HE1	2:J:4:DSN:HA	1.78	0.48
1:C:185:ILE:O	1:C:186:ASP:C	2.55	0.48
1:C:646:GLU:HA	1:C:663:TYR:CD2	2.48	0.48
1:C:746:ASN:O	1:C:747:ASN:C	2.56	0.48
1:C:804:PRO:O	1:C:805:ARG:C	2.56	0.48
1:A:173:THR:OG1	1:A:174:ARG:N	2.46	0.48
1:A:624:TYR:O	1:A:625:LEU:HB2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:OD2	1:B:373:GLY:HA3	2.14	0.48
1:B:391:TRP:CZ3	1:B:427:LEU:HD11	2.48	0.48
1:B:637:GLU:HG3	1:B:671:LYS:CB	2.38	0.48
1:C:200:TYR:HB3	1:C:201:ASP:OD1	2.13	0.48
1:C:298:SER:HB2	1:C:310:ARG:CG	2.43	0.48
1:C:305:GLY:C	1:C:307:VAL:N	2.68	0.48
1:C:352:TYR:HB2	1:C:396:ARG:HB3	1.95	0.48
1:C:789:TYR:CE1	1:C:802:GLY:HA3	2.49	0.48
1:A:140:ILE:CG2	1:A:141:THR:N	2.75	0.48
1:A:149:PRO:HB3	1:A:171:VAL:HG11	1.96	0.48
1:A:475:VAL:O	1:A:476:VAL:C	2.56	0.48
1:A:698:ASP:O	1:A:699:ASP:O	2.31	0.48
1:B:286:GLY:CA	1:B:808:MSE:HG3	2.43	0.48
1:B:341:ASN:HD22	1:B:342:PRO:HD3	1.78	0.48
1:C:149:PRO:HB3	1:C:171:VAL:HG11	1.95	0.48
1:C:529:LEU:O	1:C:552:VAL:HG23	2.13	0.48
1:A:418:HIS:HE1	1:A:453:LYS:HD3	1.78	0.48
1:A:687:VAL:HG23	1:A:717:THR:HB	1.96	0.48
1:B:185:ILE:O	1:B:188:VAL:HB	2.13	0.48
1:B:414:VAL:CB	1:B:459:ILE:HG22	2.43	0.48
1:B:518:PRO:HG2	1:B:521:TYR:CE2	2.46	0.48
1:C:681:LEU:HD22	1:C:687:VAL:CG1	2.43	0.48
1:A:156:THR:C	1:A:158:LEU:H	2.21	0.48
1:A:345:MSE:HE3	1:A:403:GLU:CD	2.38	0.48
1:A:375:ARG:CZ	1:A:755:PHE:HE1	2.27	0.48
1:B:200:TYR:CZ	1:B:206:ASN:HB3	2.49	0.48
1:B:694:LYS:HD3	1:B:710:GLN:HA	1.95	0.48
1:C:260:GLY:O	1:C:594:MSE:HB2	2.13	0.48
1:A:277:PHE:O	1:A:278:LYS:HB2	2.14	0.48
1:A:391:TRP:CD1	1:A:393:GLN:HG3	2.49	0.48
1:A:738:GLY:O	1:A:739:LYS:C	2.56	0.48
1:A:746:ASN:O	1:A:747:ASN:C	2.56	0.48
1:B:218:GLN:HA	1:B:222:ILE:O	2.14	0.48
1:B:228:ASN:C	1:B:228:ASN:OD1	2.56	0.48
1:B:804:PRO:O	1:B:805:ARG:C	2.55	0.48
1:C:233:ALA:HA	1:C:393:GLN:CG	2.44	0.48
1:C:270:ARG:NH1	1:C:351:ASP:OD2	2.47	0.48
1:C:386:ALA:O	1:C:387:LYS:C	2.55	0.48
1:A:158:LEU:O	1:A:160:LEU:HG	2.14	0.48
1:A:253:THR:O	1:A:255:LEU:N	2.47	0.48
1:A:386:ALA:O	1:A:387:LYS:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ALA:HB1	1:A:537:PHE:CE1	2.49	0.48
1:B:152:ILE:CD1	1:B:169:ILE:HG21	2.44	0.48
1:B:271:LYS:HB3	1:B:310:ARG:CZ	2.44	0.48
1:B:763:VAL:CG1	1:B:785:PHE:CD2	2.96	0.48
1:C:154:THR:O	1:C:256:LEU:HD12	2.14	0.48
1:C:247:GLU:HG3	1:C:267:ASN:HB3	1.96	0.48
1:C:253:THR:CG2	1:C:265:THR:OG1	2.58	0.48
1:C:387:LYS:HG3	1:C:509:ASP:CA	2.44	0.48
1:C:434:TRP:HA	1:C:434:TRP:HE3	1.79	0.48
1:C:517:THR:O	1:C:518:PRO:C	2.57	0.48
1:C:619:GLY:HA3	1:C:634:ALA:CB	2.44	0.48
1:C:683:PRO:CG	1:C:684:GLY:N	2.77	0.48
1:C:781:VAL:HB	1:C:807:LEU:CD2	2.44	0.48
1:A:200:TYR:CE2	1:A:206:ASN:HB3	2.49	0.47
1:A:227:ARG:NH1	1:A:260:GLY:HA2	2.29	0.47
1:A:253:THR:CG2	1:A:265:THR:OG1	2.57	0.47
1:A:319:HIS:HA	1:A:326:GLU:HA	1.95	0.47
1:B:148:THR:OG1	1:B:149:PRO:HD2	2.14	0.47
1:B:396:ARG:CG	1:B:420:ILE:HD11	2.44	0.47
1:B:418:HIS:CE1	1:B:453:LYS:HD3	2.48	0.47
1:B:722:LYS:O	1:B:723:GLY:C	2.57	0.47
1:B:740:SER:HB2	1:B:757:GLN:HB3	1.96	0.47
1:C:156:THR:C	1:C:158:LEU:H	2.22	0.47
1:C:406:PHE:HB3	1:C:408:ASN:OD1	2.14	0.47
1:C:764:ASP:HB3	1:C:782:ASN:C	2.38	0.47
1:A:185:ILE:O	1:A:188:VAL:HB	2.14	0.47
1:A:376:ASN:HD21	1:A:435:PRO:CG	2.26	0.47
1:A:738:GLY:O	1:A:739:LYS:O	2.32	0.47
1:C:136:GLN:HG2	1:C:137:LEU:H	1.78	0.47
1:C:285:ALA:CB	1:C:291:TYR:HD1	2.27	0.47
1:C:526:THR:CG2	1:C:554:TYR:HE1	2.26	0.47
1:C:628:ARG:HG2	1:C:680:GLU:OE1	2.13	0.47
1:A:271:LYS:HZ3	1:A:310:ARG:NH2	2.11	0.47
1:A:396:ARG:HG3	1:A:420:ILE:CG1	2.44	0.47
1:B:386:ALA:O	1:B:387:LYS:C	2.56	0.47
1:B:434:TRP:HA	1:B:434:TRP:HE3	1.77	0.47
1:B:503:PHE:O	1:B:504:ILE:C	2.57	0.47
1:B:783:ASN:C	1:B:783:ASN:HD22	2.20	0.47
1:C:230:GLY:HA2	4:K:1:PVE:O25	2.13	0.47
1:C:738:GLY:O	1:C:739:LYS:C	2.56	0.47
1:A:372:GLN:CD	1:A:373:GLY:N	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:PHE:O	1:A:504:ILE:O	2.33	0.47
1:A:655:THR:O	1:A:656:ASN:O	2.31	0.47
1:A:728:LEU:HB2	1:A:769:TYR:CD1	2.50	0.47
1:B:286:GLY:HA2	1:B:808:MSE:HA	1.97	0.47
1:B:504:ILE:O	1:B:505:ASN:C	2.55	0.47
1:B:638:ILE:HD12	1:B:670:THR:HG21	1.95	0.47
1:C:279:GLY:O	1:C:280:HIS:HB3	2.14	0.47
1:C:296:ASP:CG	1:C:310:ARG:HH21	2.22	0.47
1:C:484:HIS:CE1	1:C:525:LYS:HE2	2.48	0.47
1:A:500:THR:O	1:A:501:ASP:C	2.58	0.47
1:A:745:TYR:HB2	1:A:752:TRP:NE1	2.29	0.47
1:A:779:VAL:HG23	1:A:809:PHE:HA	1.96	0.47
1:B:391:TRP:CD1	1:B:391:TRP:C	2.92	0.47
1:B:779:VAL:HG23	1:B:809:PHE:HA	1.96	0.47
1:C:259:ALA:HB1	1:C:595:PRO:HD2	1.95	0.47
1:C:503:PHE:O	1:C:504:ILE:C	2.57	0.47
1:C:552:VAL:CG1	1:C:593:PHE:CZ	2.95	0.47
1:A:209:ALA:HB2	1:A:214:ILE:CD1	2.43	0.47
1:A:396:ARG:CG	1:A:420:ILE:HD11	2.45	0.47
1:A:399:PHE:CD1	1:A:399:PHE:C	2.92	0.47
1:A:474:LEU:CD1	1:A:475:VAL:N	2.66	0.47
1:B:239:ASP:OD2	1:B:292:ARG:NH2	2.40	0.47
1:B:376:ASN:HD21	1:B:435:PRO:CG	2.25	0.47
1:B:396:ARG:HG3	1:B:420:ILE:CG1	2.45	0.47
1:B:430:ILE:HD11	1:B:441:ALA:HB3	1.96	0.47
1:B:540:THR:HG22	1:B:542:ASP:OD1	2.15	0.47
1:B:545:LEU:HD12	1:B:575:ALA:HB2	1.96	0.47
1:C:375:ARG:HG3	1:C:375:ARG:HH11	1.79	0.47
1:A:273:PRO:HG2	1:A:337:GLU:OE1	2.14	0.47
1:A:281:VAL:O	1:A:281:VAL:CG1	2.62	0.47
1:A:346:LEU:HA	1:A:402:LEU:HB3	1.96	0.47
1:A:434:TRP:O	1:A:436:ALA:N	2.47	0.47
1:B:271:LYS:HD3	1:B:310:ARG:NH2	2.30	0.47
1:B:281:VAL:O	1:B:281:VAL:CG1	2.63	0.47
1:B:307:VAL:HG13	1:B:307:VAL:O	2.14	0.47
1:B:399:PHE:CD1	1:B:399:PHE:C	2.93	0.47
1:B:484:HIS:CE1	1:B:525:LYS:HE2	2.50	0.47
1:B:527:ARG:HH11	1:B:529:LEU:CD1	2.28	0.47
1:B:782:ASN:CB	1:B:806:ASN:HD22	2.28	0.47
1:C:158:LEU:O	1:C:160:LEU:HG	2.15	0.47
1:C:182:LEU:HD22	1:C:187:ASP:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ARG:CZ	1:C:755:PHE:HE1	2.28	0.47
1:C:399:PHE:C	1:C:399:PHE:CD1	2.92	0.47
1:C:410:TRP:CZ3	1:C:464:PRO:O	2.68	0.47
1:C:477:GLY:HA3	1:C:532:TYR:CE1	2.50	0.47
1:C:546:PHE:N	1:C:574:GLY:O	2.46	0.47
1:C:628:ARG:CB	1:C:628:ARG:HH11	2.28	0.47
1:C:646:GLU:HA	1:C:663:TYR:HD2	1.78	0.47
1:C:722:LYS:O	1:C:723:GLY:C	2.58	0.47
1:A:286:GLY:CA	1:A:808:MSE:HG3	2.44	0.47
1:A:292:ARG:HG3	1:A:316:GLN:HB2	1.96	0.47
1:A:386:ALA:O	1:A:389:SER:N	2.47	0.47
1:A:655:THR:O	1:A:656:ASN:C	2.58	0.47
1:B:158:LEU:O	1:B:160:LEU:HG	2.14	0.47
1:B:441:ALA:O	1:B:500:THR:HG22	2.15	0.47
1:B:527:ARG:HH21	1:B:555:ARG:HD2	1.80	0.47
1:B:601:ARG:HD3	1:B:607:LEU:N	2.30	0.47
1:B:628:ARG:HH11	1:B:628:ARG:CB	2.27	0.47
1:B:640:GLU:OE2	1:B:643:ARG:HG3	2.14	0.47
1:B:812:ARG:HG2	1:B:812:ARG:HH11	1.80	0.47
1:C:159:VAL:C	1:C:160:LEU:HG	2.40	0.47
1:C:360:SER:HB3	1:C:390:SER:CA	2.40	0.47
1:A:296:ASP:OD2	1:A:310:ARG:NH2	2.48	0.47
1:A:370:ASP:HB2	1:A:435:PRO:HB2	1.97	0.47
1:A:375:ARG:HH11	1:A:375:ARG:HG3	1.79	0.47
1:B:781:VAL:HB	1:B:807:LEU:CD2	2.44	0.47
1:C:253:THR:O	1:C:255:LEU:N	2.48	0.47
1:C:318:LYS:HE2	1:C:327:ARG:HH21	1.80	0.47
1:C:814:ASP:HB3	1:C:815:PHE:H	1.62	0.47
1:B:280:HIS:O	1:B:295:LEU:HD12	2.15	0.47
1:B:387:LYS:HD2	1:B:509:ASP:HB3	1.97	0.47
1:A:335:ILE:O	1:A:336:LEU:HD12	2.15	0.46
1:A:423:TYR:N	1:A:450:GLY:O	2.40	0.46
1:A:430:ILE:HD11	1:A:441:ALA:HB3	1.97	0.46
1:A:465:PHE:CZ	1:A:467:PHE:HB2	2.50	0.46
1:B:211:GLY:HA2	1:B:708:GLU:OE1	2.15	0.46
1:B:233:ALA:HA	1:B:393:GLN:CG	2.44	0.46
1:B:240:MSE:C	1:B:242:ILE:N	2.73	0.46
1:B:383:ASN:C	1:B:385:GLY:N	2.73	0.46
1:B:633:LEU:O	1:B:633:LEU:HD23	2.15	0.46
1:B:687:VAL:HG23	1:B:717:THR:HB	1.97	0.46
1:B:766:MSE:HB2	1:B:780:ASN:ND2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ASN:C	1:B:783:ASN:ND2	2.73	0.46
1:C:302:THR:O	1:C:303:GLU:C	2.57	0.46
1:C:391:TRP:HD1	1:C:393:GLN:HG3	1.79	0.46
1:C:475:VAL:O	1:C:476:VAL:C	2.55	0.46
1:C:600:TYR:HD1	1:C:663:TYR:CD1	2.32	0.46
1:C:737:GLN:HG2	1:C:760:TYR:CB	2.45	0.46
1:A:212:PHE:CD2	1:A:262:LEU:HB2	2.50	0.46
1:A:734:ALA:HA	1:A:762:LEU:O	2.16	0.46
1:B:253:THR:O	1:B:255:LEU:N	2.48	0.46
1:B:295:LEU:O	1:B:312:VAL:HG23	2.15	0.46
1:B:500:THR:O	1:B:501:ASP:C	2.58	0.46
1:C:319:HIS:HA	1:C:326:GLU:HA	1.96	0.46
1:C:344:THR:HB	1:C:403:GLU:HG3	1.97	0.46
1:C:360:SER:CB	1:C:390:SER:HA	2.40	0.46
1:C:789:TYR:CD1	1:C:789:TYR:C	2.93	0.46
1:A:156:THR:C	1:A:158:LEU:N	2.74	0.46
1:A:418:HIS:CE1	1:A:453:LYS:HD3	2.50	0.46
1:A:434:TRP:O	1:A:441:ALA:HB2	2.16	0.46
1:A:484:HIS:CE1	1:A:525:LYS:HE2	2.50	0.46
1:A:546:PHE:N	1:A:574:GLY:O	2.45	0.46
1:A:618:ILE:O	1:A:618:ILE:CG2	2.64	0.46
1:B:159:VAL:C	1:B:160:LEU:HG	2.40	0.46
1:B:209:ALA:HB2	1:B:214:ILE:CD1	2.45	0.46
1:B:246:VAL:O	1:B:246:VAL:CG1	2.63	0.46
1:B:308:ARG:NH2	1:B:339:ASP:OD2	2.49	0.46
1:B:375:ARG:CZ	1:B:755:PHE:HE1	2.29	0.46
1:B:396:ARG:HD3	1:B:420:ILE:HD11	1.95	0.46
1:B:713:LEU:O	1:B:735:ARG:HA	2.16	0.46
1:C:220:ASP:OD2	1:C:270:ARG:CD	2.64	0.46
1:C:247:GLU:HG3	1:C:267:ASN:HD22	1.79	0.46
1:C:385:GLY:O	1:C:508:GLY:HA3	2.16	0.46
1:C:740:SER:HB2	1:C:757:GLN:HB3	1.97	0.46
1:C:757:GLN:O	1:C:758:GLU:O	2.33	0.46
1:A:135:ASN:ND2	1:A:138:GLY:O	2.49	0.46
1:A:289:ASP:O	1:A:318:LYS:HA	2.15	0.46
1:A:396:ARG:CD	1:A:420:ILE:HD11	2.45	0.46
1:B:385:GLY:O	1:B:508:GLY:HA3	2.15	0.46
1:B:414:VAL:HB	1:B:459:ILE:HG22	1.97	0.46
1:B:518:PRO:HG2	1:B:521:TYR:HH	1.77	0.46
1:B:796:TYR:O	1:B:797:THR:HB	2.15	0.46
1:C:392:GLU:HB3	1:C:424:HIS:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:VAL:HG23	1:C:717:THR:HB	1.97	0.46
1:C:812:ARG:HH11	1:C:812:ARG:HG2	1.81	0.46
1:A:159:VAL:C	1:A:160:LEU:HG	2.41	0.46
1:A:179:ASP:HB3	1:A:766:MSE:HE3	1.98	0.46
1:A:694:LYS:HE2	1:A:708:GLU:O	2.16	0.46
1:B:324:HIS:CE1	1:B:383:ASN:HD22	2.33	0.46
1:B:527:ARG:HH11	1:B:529:LEU:HD11	1.81	0.46
1:C:209:ALA:HB2	1:C:214:ILE:CD1	2.43	0.46
1:C:289:ASP:O	1:C:318:LYS:HA	2.16	0.46
1:C:388:TRP:CH2	1:C:428:GLY:HA3	2.50	0.46
1:C:423:TYR:N	1:C:450:GLY:O	2.44	0.46
1:C:435:PRO:O	1:C:436:ALA:O	2.33	0.46
1:C:500:THR:O	1:C:501:ASP:C	2.57	0.46
1:C:502:ASP:C	1:C:502:ASP:OD1	2.58	0.46
1:C:682:ALA:HB3	1:C:683:PRO:HD2	1.97	0.46
1:A:621:LYS:HG2	1:A:632:SER:HB2	1.97	0.46
1:A:682:ALA:HB3	1:A:685:TRP:HB2	1.98	0.46
1:B:434:TRP:O	1:B:436:ALA:N	2.49	0.46
1:B:655:THR:C	1:B:656:ASN:O	2.58	0.46
1:C:335:ILE:O	1:C:336:LEU:HD12	2.15	0.46
1:C:670:THR:OG1	1:C:696:ILE:HD12	2.15	0.46
1:C:725:LEU:C	1:C:727:LYS:N	2.74	0.46
1:C:783:ASN:C	1:C:783:ASN:ND2	2.70	0.46
1:A:148:THR:HB	1:A:679:GLY:CA	2.46	0.46
1:A:152:ILE:O	1:A:152:ILE:HG13	2.14	0.46
1:A:341:ASN:C	1:A:343:ASP:H	2.23	0.46
1:A:812:ARG:HG2	1:A:812:ARG:HH11	1.81	0.46
1:B:156:THR:C	1:B:158:LEU:N	2.71	0.46
1:B:319:HIS:HA	1:B:326:GLU:HA	1.98	0.46
1:B:789:TYR:CD1	1:B:789:TYR:C	2.94	0.46
1:C:156:THR:C	1:C:158:LEU:N	2.74	0.46
1:C:526:THR:HG22	1:C:554:TYR:CE1	2.50	0.46
1:C:596:GLN:HE21	1:C:596:GLN:HB2	1.54	0.46
1:C:735:ARG:HG3	1:C:736:TRP:N	2.29	0.46
1:A:260:GLY:C	1:A:592:ILE:HD11	2.41	0.46
1:A:683:PRO:CG	1:A:684:GLY:N	2.79	0.46
1:A:772:THR:OG1	1:A:775:LEU:HB3	2.16	0.46
1:B:235:ASN:C	1:B:237:LEU:H	2.24	0.46
1:B:502:ASP:C	1:B:502:ASP:OD1	2.59	0.46
1:C:198:SER:HB3	1:C:206:ASN:ND2	2.31	0.46
1:C:628:ARG:HH11	1:C:628:ARG:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:PHE:C	1:C:797:THR:N	2.73	0.46
1:A:441:ALA:O	1:A:500:THR:HG22	2.15	0.46
1:A:706:THR:HB	1:A:741:TRP:CE2	2.50	0.46
1:B:233:ALA:CA	1:B:393:GLN:OE1	2.63	0.46
1:C:235:ASN:C	1:C:237:LEU:H	2.24	0.46
1:C:383:ASN:C	1:C:385:GLY:H	2.23	0.46
1:C:464:PRO:HA	1:C:472:HIS:O	2.16	0.46
1:C:490:TYR:CD1	1:C:490:TYR:N	2.83	0.46
1:C:556:VAL:HG13	1:C:556:VAL:O	2.16	0.46
1:C:747:ASN:CB	1:C:748:PRO:HD3	2.42	0.46
1:B:490:TYR:N	1:B:490:TYR:CD1	2.84	0.46
1:B:633:LEU:HB2	1:B:675:ALA:HB2	1.98	0.46
1:C:746:ASN:HD21	1:C:749:ARG:HG3	1.81	0.46
1:C:772:THR:O	1:C:773:ASP:C	2.59	0.46
1:A:184:ASN:ND2	1:A:187:ASP:OD2	2.49	0.45
1:A:383:ASN:C	1:A:385:GLY:N	2.72	0.45
1:A:383:ASN:O	1:A:385:GLY:N	2.48	0.45
1:A:504:ILE:O	1:A:505:ASN:C	2.58	0.45
1:A:561:PRO:O	1:A:562:THR:C	2.59	0.45
1:B:216:ASN:OD1	1:B:227:ARG:NH2	2.48	0.45
1:B:591:ASP:OD1	1:B:614:GLN:HG3	2.16	0.45
1:B:792:ASN:ND2	1:B:792:ASN:C	2.74	0.45
1:C:661:TYR:HD1	1:C:662:ALA:N	2.01	0.45
2:I:7:FHO:HZ	2:I:7:FHO:HG1C	1.79	0.45
1:A:351:ASP:OD2	1:A:397:THR:HG23	2.17	0.45
1:A:795:PHE:C	1:A:797:THR:N	2.73	0.45
1:B:368:LEU:HD21	1:B:799:ALA:HB2	1.97	0.45
1:C:186:ASP:C	1:C:188:VAL:N	2.74	0.45
1:C:289:ASP:OD1	1:C:289:ASP:N	2.49	0.45
1:C:341:ASN:C	1:C:343:ASP:H	2.24	0.45
1:C:434:TRP:O	1:C:441:ALA:HB2	2.16	0.45
1:C:609:GLU:HB3	1:C:610:PRO:HD2	1.98	0.45
1:C:682:ALA:HB3	1:C:685:TRP:HB2	1.97	0.45
1:A:182:LEU:HD13	1:A:187:ASP:O	2.16	0.45
1:A:370:ASP:OD2	1:A:373:GLY:HA3	2.16	0.45
1:A:490:TYR:N	1:A:490:TYR:CD1	2.84	0.45
1:B:178:ASP:O	1:B:179:ASP:C	2.59	0.45
1:B:189:MSE:CE	1:B:195:ILE:HD13	2.45	0.45
1:B:288:TRP:CZ2	1:B:321:PHE:HB3	2.52	0.45
1:B:344:THR:HB	1:B:403:GLU:HG3	1.97	0.45
1:B:421:ASN:O	1:B:452:THR:CG2	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD12	1:B:534:THR:O	2.17	0.45
1:B:699:ASP:O	1:B:700:SER:C	2.59	0.45
1:C:142:GLU:HG2	1:C:142:GLU:O	2.16	0.45
1:C:169:ILE:CG2	1:C:170:THR:N	2.80	0.45
1:C:593:PHE:CD1	1:C:593:PHE:C	2.94	0.45
1:C:651:ASN:ND2	1:C:652:SER:H	2.15	0.45
1:C:745:TYR:HB2	1:C:752:TRP:NE1	2.30	0.45
1:A:275:HIS:CE1	1:A:308:ARG:HH11	2.34	0.45
1:A:537:PHE:CE2	1:A:547:LEU:HD12	2.42	0.45
1:A:601:ARG:HH11	1:A:601:ARG:CG	2.24	0.45
1:B:154:THR:O	1:B:256:LEU:HD12	2.16	0.45
1:B:281:VAL:HB	1:B:295:LEU:HD13	1.98	0.45
1:B:365:SER:N	1:B:799:ALA:O	2.48	0.45
1:B:396:ARG:CD	1:B:420:ILE:HD11	2.46	0.45
1:B:601:ARG:HD3	1:B:607:LEU:CA	2.46	0.45
1:B:725:LEU:C	1:B:727:LYS:N	2.74	0.45
1:B:751:ARG:O	1:B:751:ARG:HG3	2.16	0.45
1:C:169:ILE:CD1	1:C:249:LEU:HD12	2.45	0.45
1:C:216:ASN:ND2	1:C:261:SER:H	2.13	0.45
1:C:307:VAL:O	1:C:307:VAL:HG13	2.16	0.45
1:C:418:HIS:HE1	1:C:453:LYS:HD3	1.81	0.45
1:C:624:TYR:O	1:C:625:LEU:CB	2.64	0.45
1:A:169:ILE:HD11	1:A:249:LEU:HD13	1.96	0.45
1:A:344:THR:HB	1:A:403:GLU:HG3	1.98	0.45
1:B:292:ARG:HG3	1:B:316:GLN:HB2	1.98	0.45
1:B:772:THR:O	1:B:773:ASP:C	2.59	0.45
1:C:394:TYR:C	1:C:394:TYR:CD1	2.95	0.45
1:A:233:ALA:HA	1:A:393:GLN:CG	2.47	0.45
1:A:235:ASN:C	1:A:237:LEU:H	2.25	0.45
1:A:298:SER:HB2	1:A:310:ARG:CG	2.47	0.45
1:A:502:ASP:C	1:A:502:ASP:OD1	2.60	0.45
1:A:591:ASP:OD1	1:A:614:GLN:HG3	2.17	0.45
1:A:601:ARG:HD3	1:A:607:LEU:N	2.32	0.45
1:A:713:LEU:O	1:A:735:ARG:HA	2.17	0.45
1:A:740:SER:HB2	1:A:757:GLN:HB3	1.97	0.45
1:B:243:TYR:HB3	1:B:269:ILE:O	2.17	0.45
1:B:682:ALA:HB3	1:B:683:PRO:HD2	1.99	0.45
1:B:683:PRO:CG	1:B:684:GLY:N	2.79	0.45
1:C:540:THR:C	1:C:542:ASP:N	2.75	0.45
1:A:628:ARG:HH11	1:A:628:ARG:HB2	1.82	0.45
1:B:277:PHE:O	1:B:278:LYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HD11	1:C:249:LEU:HD13	1.98	0.45
1:A:638:ILE:HD12	1:A:670:THR:HG21	1.99	0.45
1:B:231:TYR:CD2	1:B:485:TRP:CH2	3.05	0.45
1:B:561:PRO:O	1:B:562:THR:C	2.60	0.45
1:B:694:LYS:HD3	1:B:694:LYS:C	2.41	0.45
1:B:742:GLN:OE1	1:B:742:GLN:HA	2.16	0.45
1:C:633:LEU:HD23	1:C:633:LEU:O	2.17	0.45
1:C:681:LEU:HD23	1:C:685:TRP:CD2	2.52	0.45
1:A:351:ASP:OD2	1:A:397:THR:CG2	2.64	0.45
1:A:540:THR:C	1:A:542:ASP:N	2.75	0.45
1:A:699:ASP:O	1:A:700:SER:C	2.59	0.45
1:A:797:THR:HG22	1:A:797:THR:O	2.17	0.45
1:C:148:THR:HB	1:C:679:GLY:CA	2.46	0.45
1:C:391:TRP:CD1	1:C:393:GLN:HG3	2.51	0.45
1:C:418:HIS:CE1	1:C:453:LYS:HD3	2.51	0.45
1:A:751:ARG:HG3	1:A:751:ARG:O	2.16	0.45
1:B:335:ILE:O	1:B:336:LEU:HD12	2.17	0.45
1:B:757:GLN:O	1:B:758:GLU:O	2.34	0.45
1:A:271:LYS:NZ	1:A:310:ARG:HH22	2.14	0.44
1:A:279:GLY:O	1:A:280:HIS:HB3	2.17	0.44
1:A:410:TRP:CZ3	1:A:464:PRO:O	2.69	0.44
1:A:601:ARG:HD3	1:A:607:LEU:CA	2.47	0.44
1:A:637:GLU:HG3	1:A:671:LYS:CB	2.35	0.44
1:A:764:ASP:HB3	1:A:782:ASN:C	2.41	0.44
1:B:212:PHE:CD2	1:B:262:LEU:HB2	2.52	0.44
1:B:649:LEU:O	1:B:651:ASN:N	2.45	0.44
1:C:273:PRO:HG2	1:C:337:GLU:OE1	2.17	0.44
1:C:728:LEU:HB2	1:C:769:TYR:CE1	2.52	0.44
1:A:255:LEU:HD22	1:A:572:TYR:CG	2.52	0.44
1:A:503:PHE:C	1:A:504:ILE:O	2.61	0.44
1:A:546:PHE:HB2	1:A:574:GLY:O	2.18	0.44
1:A:628:ARG:HH11	1:A:628:ARG:CB	2.30	0.44
1:A:682:ALA:CB	1:A:683:PRO:HD2	2.48	0.44
1:B:383:ASN:O	1:B:385:GLY:N	2.50	0.44
1:B:707:TRP:CH2	1:B:793:ILE:HB	2.52	0.44
1:C:274:THR:HG22	1:C:298:SER:OG	2.16	0.44
1:C:706:THR:HB	1:C:741:TRP:CE2	2.53	0.44
1:A:169:ILE:CD1	1:A:249:LEU:HD12	2.45	0.44
1:A:280:HIS:CE1	1:A:296:ASP:HB3	2.52	0.44
1:A:402:LEU:HD12	1:A:402:LEU:C	2.41	0.44
1:A:628:ARG:HG2	1:A:680:GLU:OE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:THR:C	1:B:542:ASP:N	2.75	0.44
1:C:184:ASN:ND2	1:C:187:ASP:OD2	2.51	0.44
1:C:537:PHE:O	1:C:545:LEU:N	2.40	0.44
1:A:243:TYR:HA	1:A:270:ARG:HA	2.00	0.44
1:A:270:ARG:NH1	1:A:351:ASP:OD2	2.50	0.44
1:A:271:LYS:HZ2	1:A:310:ARG:NH2	2.12	0.44
1:A:515:TRP:CD1	1:A:515:TRP:H	2.36	0.44
1:A:621:LYS:HG2	1:A:632:SER:CB	2.46	0.44
1:A:796:TYR:O	1:A:797:THR:HB	2.18	0.44
1:B:169:ILE:CG2	1:B:170:THR:N	2.79	0.44
1:B:226:ALA:HB3	1:B:235:ASN:HD21	1.83	0.44
1:C:180:PHE:HA	1:C:780:ASN:ND2	2.33	0.44
1:C:308:ARG:NH2	1:C:339:ASP:OD2	2.50	0.44
1:C:351:ASP:OD2	1:C:397:THR:CG2	2.66	0.44
1:C:368:LEU:HD21	1:C:799:ALA:HB2	2.00	0.44
1:A:414:VAL:HG23	1:A:459:ILE:CG2	2.48	0.44
1:A:430:ILE:HB	1:A:443:ILE:HG22	2.00	0.44
1:B:275:HIS:CE1	1:B:308:ARG:NH1	2.86	0.44
1:B:740:SER:O	1:B:757:GLN:N	2.40	0.44
1:C:391:TRP:CE3	1:C:427:LEU:HD11	2.53	0.44
1:C:561:PRO:O	1:C:562:THR:C	2.60	0.44
1:C:682:ALA:HB2	1:C:685:TRP:HE3	1.83	0.44
1:C:779:VAL:HG23	1:C:809:PHE:HA	1.98	0.44
1:A:616:TYR:HE2	1:A:639:HIS:ND1	2.16	0.44
1:B:148:THR:HB	1:B:679:GLY:CA	2.47	0.44
1:B:198:SER:HB3	1:B:206:ASN:ND2	2.33	0.44
1:B:220:ASP:OD2	1:B:270:ARG:CD	2.66	0.44
1:B:341:ASN:CB	1:B:342:PRO:CD	2.87	0.44
1:B:461:LEU:HB2	1:B:476:VAL:HG13	1.99	0.44
1:B:507:ASP:O	1:B:508:GLY:C	2.60	0.44
1:B:698:ASP:O	1:B:701:GLY:HA3	2.17	0.44
1:B:706:THR:OG1	1:B:741:TRP:NE1	2.51	0.44
1:C:189:MSE:CE	1:C:266:ILE:HD12	2.44	0.44
1:C:280:HIS:CE1	1:C:296:ASP:HB3	2.53	0.44
1:C:651:ASN:ND2	1:C:652:SER:N	2.65	0.44
1:A:204:ARG:HD3	1:A:391:TRP:CH2	2.53	0.44
1:A:216:ASN:ND2	1:A:261:SER:H	2.15	0.44
1:B:144:SER:C	1:B:146:SER:N	2.76	0.44
1:B:247:GLU:O	1:B:267:ASN:HB3	2.17	0.44
1:B:298:SER:HB2	1:B:310:ARG:CG	2.47	0.44
1:C:419:LYS:HG2	1:C:420:ILE:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ILE:HD11	1:C:441:ALA:HB3	2.00	0.44
1:C:507:ASP:O	1:C:508:GLY:C	2.61	0.44
1:C:511:GLY:O	1:C:513:PRO:CD	2.65	0.44
1:C:637:GLU:HA	1:C:671:LYS:HA	2.00	0.44
1:A:434:TRP:CE3	1:A:434:TRP:CA	2.96	0.44
1:A:529:LEU:HB3	1:A:530:GLY:H	1.71	0.44
1:A:707:TRP:CH2	1:A:793:ILE:HB	2.53	0.44
1:B:341:ASN:C	1:B:343:ASP:H	2.23	0.44
1:B:435:PRO:O	1:B:436:ALA:O	2.34	0.44
1:B:781:VAL:HB	1:B:807:LEU:HD21	1.99	0.44
1:C:290:ASN:HA	1:C:318:LYS:CB	2.48	0.44
1:C:414:VAL:HG23	1:C:459:ILE:CG2	2.48	0.44
1:C:781:VAL:HB	1:C:807:LEU:HD21	2.00	0.44
1:B:366:PHE:HB3	1:B:382:PHE:CD2	2.53	0.44
1:B:674:GLU:HB2	1:B:692:THR:HG23	1.99	0.44
1:C:216:ASN:HD21	1:C:261:SER:N	2.11	0.44
1:C:237:LEU:HD23	1:C:237:LEU:N	2.32	0.44
1:C:601:ARG:HD3	1:C:607:LEU:N	2.33	0.44
1:B:149:PRO:HB3	1:B:171:VAL:HG11	1.99	0.43
1:B:185:ILE:O	1:B:188:VAL:N	2.44	0.43
1:B:682:ALA:HB2	1:B:685:TRP:HE3	1.82	0.43
1:B:781:VAL:HA	1:B:807:LEU:HD23	2.00	0.43
1:C:204:ARG:HD3	1:C:391:TRP:CH2	2.53	0.43
1:C:496:TYR:CZ	1:C:513:PRO:HD3	2.53	0.43
1:C:526:THR:HA	1:C:555:ARG:O	2.18	0.43
1:C:633:LEU:HB2	1:C:675:ALA:HB2	1.99	0.43
1:A:219:TYR:N	1:A:222:ILE:O	2.49	0.43
1:B:141:THR:C	1:B:143:ASP:N	2.75	0.43
1:B:351:ASP:OD2	1:B:397:THR:HG23	2.18	0.43
1:B:375:ARG:HH11	1:B:375:ARG:HG3	1.83	0.43
1:C:275:HIS:CE1	1:C:308:ARG:HH11	2.36	0.43
1:C:591:ASP:OD1	1:C:614:GLN:HG3	2.18	0.43
1:C:601:ARG:HD3	1:C:607:LEU:CA	2.49	0.43
1:C:709:PRO:CG	1:C:737:GLN:HB2	2.47	0.43
1:C:721:PHE:CD2	1:C:728:LEU:HD23	2.53	0.43
1:A:527:ARG:HH21	1:A:555:ARG:HD2	1.84	0.43
1:A:719:TYR:HE2	1:A:721:PHE:CD1	2.31	0.43
1:B:173:THR:CG2	1:B:176:ASN:HB2	2.48	0.43
1:B:461:LEU:HB2	1:B:476:VAL:CG1	2.48	0.43
1:B:578:ASP:HA	1:B:584:SER:OG	2.18	0.43
1:B:609:GLU:HB3	1:B:610:PRO:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:CG2	1:C:141:THR:H	2.31	0.43
1:C:247:GLU:O	1:C:267:ASN:HB3	2.18	0.43
1:C:262:LEU:HD21	1:C:613:GLY:HA3	2.00	0.43
1:C:774:LYS:HB3	1:C:814:ASP:OD2	2.18	0.43
1:A:410:TRP:HE1	1:A:462:THR:N	2.16	0.43
1:A:507:ASP:O	1:A:508:GLY:C	2.62	0.43
1:A:608:LEU:O	1:A:609:GLU:C	2.61	0.43
1:A:721:PHE:CD2	1:A:728:LEU:HD23	2.54	0.43
1:B:260:GLY:C	1:B:592:ILE:HD11	2.43	0.43
1:B:482:PHE:CE1	1:B:527:ARG:CG	3.01	0.43
1:B:628:ARG:HG2	1:B:680:GLU:OE1	2.18	0.43
1:C:194:GLY:HA3	1:C:250:LYS:HZ1	1.81	0.43
1:C:200:TYR:HD1	1:C:795:PHE:CE1	2.36	0.43
1:C:576:VAL:HA	1:C:585:VAL:O	2.17	0.43
1:C:721:PHE:HD2	1:C:725:LEU:HD12	1.83	0.43
1:A:139:THR:CG2	1:A:150:GLY:HA3	2.49	0.43
1:A:510:ILE:HG22	1:A:511:GLY:N	2.34	0.43
1:A:593:PHE:CD1	1:A:593:PHE:C	2.96	0.43
1:A:694:LYS:HD3	1:A:694:LYS:C	2.43	0.43
1:B:140:ILE:CG2	1:B:141:THR:H	2.29	0.43
1:B:419:LYS:HG2	1:B:420:ILE:N	2.33	0.43
1:B:435:PRO:HG3	1:B:503:PHE:CZ	2.53	0.43
1:B:616:TYR:HE2	1:B:639:HIS:ND1	2.17	0.43
1:B:658:ALA:C	1:B:659:ILE:O	2.61	0.43
1:C:243:TYR:CZ	1:C:268:LEU:HD13	2.53	0.43
1:C:421:ASN:O	1:C:452:THR:CG2	2.64	0.43
1:C:695:ILE:HD11	1:C:710:GLN:NE2	2.28	0.43
1:A:228:ASN:OD1	1:A:228:ASN:C	2.61	0.43
1:A:576:VAL:HA	1:A:585:VAL:O	2.17	0.43
1:A:659:ILE:CG1	1:A:660:THR:N	2.82	0.43
1:B:237:LEU:HD23	1:B:237:LEU:N	2.33	0.43
1:B:425:ALA:O	1:B:448:TYR:N	2.40	0.43
1:B:542:ASP:HB3	1:B:578:ASP:HB2	1.99	0.43
1:B:556:VAL:HG12	1:B:563:ILE:O	2.18	0.43
1:C:152:ILE:HB	1:C:154:THR:HG22	1.99	0.43
1:C:371:SER:HB3	1:C:372:GLN:OE1	2.19	0.43
1:C:621:LYS:HG2	1:C:632:SER:HB2	2.00	0.43
1:A:237:LEU:N	1:A:237:LEU:HD23	2.34	0.43
1:A:286:GLY:HA2	1:A:808:MSE:HA	2.01	0.43
1:A:342:PRO:HB3	1:A:405:ASN:O	2.19	0.43
1:A:365:SER:N	1:A:799:ALA:O	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLY:O	1:A:508:GLY:HA3	2.17	0.43
1:A:419:LYS:HG2	1:A:420:ILE:N	2.33	0.43
1:A:596:GLN:HE21	1:A:596:GLN:HB2	1.54	0.43
1:A:682:ALA:HB2	1:A:685:TRP:HE3	1.84	0.43
1:A:719:TYR:CD2	1:A:721:PHE:CD1	3.06	0.43
1:B:136:GLN:CG	1:B:413:LYS:HZ3	2.32	0.43
1:B:216:ASN:ND2	1:B:261:SER:H	2.17	0.43
1:B:365:SER:HB2	1:B:799:ALA:O	2.19	0.43
1:C:674:GLU:HB2	1:C:692:THR:HG23	1.99	0.43
1:C:713:LEU:O	1:C:735:ARG:HA	2.18	0.43
1:C:781:VAL:HA	1:C:807:LEU:HD23	2.00	0.43
1:A:271:LYS:HZ3	1:A:310:ARG:HH22	1.67	0.43
1:A:586:TYR:CD1	1:A:619:GLY:O	2.72	0.43
1:A:633:LEU:HB2	1:A:675:ALA:HB2	2.01	0.43
1:A:721:PHE:HD2	1:A:725:LEU:HD12	1.83	0.43
1:A:761:TRP:CE3	1:A:761:TRP:HA	2.54	0.43
1:B:179:ASP:HB3	1:B:766:MSE:HE3	2.00	0.43
1:B:695:ILE:HD13	1:B:695:ILE:HA	1.93	0.43
1:C:144:SER:C	1:C:146:SER:N	2.77	0.43
1:C:184:ASN:OD1	1:C:186:ASP:N	2.52	0.43
1:C:682:ALA:CB	1:C:683:PRO:HD2	2.49	0.43
1:C:699:ASP:O	1:C:700:SER:C	2.61	0.43
1:C:796:TYR:O	1:C:797:THR:HB	2.19	0.43
1:B:201:ASP:O	1:B:202:THR:C	2.61	0.43
1:B:289:ASP:O	1:B:318:LYS:HA	2.19	0.43
1:B:430:ILE:HB	1:B:443:ILE:HG22	2.00	0.43
1:C:430:ILE:HB	1:C:443:ILE:HG22	2.01	0.43
1:C:446:GLN:HG2	1:C:491:TRP:HB3	2.00	0.43
1:C:602:ASP:O	1:C:604:SER:N	2.52	0.43
1:C:653:LYS:H	1:C:653:LYS:HG3	1.49	0.43
1:C:659:ILE:HG23	1:C:660:THR:N	2.23	0.43
1:C:695:ILE:HD13	1:C:695:ILE:HA	1.92	0.43
1:C:797:THR:O	1:C:797:THR:HG22	2.19	0.43
1:A:423:TYR:CE1	1:A:449:THR:C	2.97	0.43
1:A:431:MSE:SE	1:A:444:VAL:HG21	2.68	0.43
1:B:189:MSE:HG3	1:B:207:TYR:CD2	2.54	0.43
1:B:410:TRP:HE1	1:B:462:THR:N	2.17	0.43
1:B:745:TYR:CE1	1:B:750:SER:HA	2.54	0.43
1:C:352:TYR:CE1	1:C:396:ARG:CD	3.01	0.43
1:C:423:TYR:CE1	1:C:449:THR:C	2.97	0.43
1:A:169:ILE:CG2	1:A:170:THR:N	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:CD2	1:A:187:ASP:O	2.52	0.42
1:A:186:ASP:O	1:A:188:VAL:N	2.52	0.42
1:A:435:PRO:HG3	1:A:503:PHE:CZ	2.54	0.42
1:A:472:HIS:CE1	1:A:538:ASN:ND2	2.87	0.42
1:B:374:ASN:HB3	1:B:375:ARG:H	1.56	0.42
1:B:410:TRP:CZ3	1:B:464:PRO:O	2.72	0.42
1:B:560:ASN:O	1:B:561:PRO:C	2.61	0.42
1:C:295:LEU:O	1:C:312:VAL:HG23	2.19	0.42
1:C:749:ARG:O	1:C:751:ARG:N	2.52	0.42
1:A:189:MSE:HG3	1:A:207:TYR:CE2	2.54	0.42
1:A:243:TYR:HB3	1:A:269:ILE:O	2.19	0.42
1:A:307:VAL:O	1:A:307:VAL:HG13	2.19	0.42
1:A:511:GLY:O	1:A:513:PRO:CD	2.67	0.42
1:A:657:PRO:C	1:A:659:ILE:HG22	2.44	0.42
1:A:728:LEU:HB2	1:A:769:TYR:CE1	2.54	0.42
1:B:342:PRO:HB3	1:B:405:ASN:O	2.19	0.42
1:B:599:TRP:NE1	2:J:4:DSN:HA	2.33	0.42
1:C:136:GLN:HG2	1:C:137:LEU:N	2.34	0.42
1:C:138:GLY:O	1:C:139:THR:C	2.62	0.42
1:C:243:TYR:HA	1:C:270:ARG:HA	2.02	0.42
1:C:286:GLY:HA2	1:C:808:MSE:HA	2.01	0.42
1:C:365:SER:N	1:C:799:ALA:O	2.49	0.42
1:A:200:TYR:CZ	1:A:206:ASN:HB3	2.54	0.42
1:A:244:ASP:OD2	1:A:245:ARG:NH1	2.53	0.42
1:B:253:THR:OG1	1:B:257:THR:HG23	2.20	0.42
1:B:383:ASN:C	1:B:385:GLY:H	2.28	0.42
1:B:472:HIS:CE1	1:B:538:ASN:ND2	2.88	0.42
1:C:179:ASP:HB3	1:C:766:MSE:HE3	2.01	0.42
1:C:435:PRO:HG3	1:C:503:PHE:CZ	2.54	0.42
1:C:529:LEU:HB3	1:C:530:GLY:H	1.71	0.42
1:C:659:ILE:O	1:C:660:THR:C	2.61	0.42
1:C:724:ALA:C	1:C:725:LEU:HD23	2.44	0.42
1:A:180:PHE:HA	1:A:780:ASN:ND2	2.35	0.42
1:A:394:TYR:CD1	1:A:394:TYR:C	2.97	0.42
1:A:406:PHE:HB3	1:A:408:ASN:OD1	2.19	0.42
1:A:651:ASN:C	1:A:653:LYS:H	2.27	0.42
1:A:695:ILE:HD13	1:A:695:ILE:HA	1.86	0.42
1:B:589:TYR:CE1	1:B:614:GLN:HG2	2.54	0.42
1:B:694:LYS:HE2	1:B:708:GLU:O	2.19	0.42
1:C:141:THR:C	1:C:143:ASP:N	2.76	0.42
1:C:212:PHE:CD2	1:C:262:LEU:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:VAL:HG22	1:A:552:VAL:N	2.35	0.42
1:A:757:GLN:O	1:A:758:GLU:O	2.38	0.42
1:A:782:ASN:HB3	1:A:806:ASN:HD22	1.84	0.42
1:B:180:PHE:HA	1:B:780:ASN:ND2	2.34	0.42
1:B:434:TRP:CE3	1:B:434:TRP:CA	3.01	0.42
1:B:640:GLU:HB3	1:B:668:ALA:HB3	2.02	0.42
1:B:807:LEU:HD23	1:B:807:LEU:HA	1.80	0.42
1:C:219:TYR:N	1:C:222:ILE:O	2.50	0.42
1:C:556:VAL:HG12	1:C:563:ILE:O	2.19	0.42
1:A:747:ASN:HB3	1:A:748:PRO:CD	2.40	0.42
1:B:141:THR:O	1:B:143:ASP:N	2.53	0.42
1:B:235:ASN:O	1:B:237:LEU:N	2.53	0.42
1:B:259:ALA:HB1	1:B:595:PRO:HD2	2.02	0.42
1:B:380:ARG:HG3	1:B:380:ARG:NH1	2.34	0.42
1:B:464:PRO:HA	1:B:472:HIS:O	2.19	0.42
1:B:596:GLN:HE21	1:B:596:GLN:HB2	1.54	0.42
1:B:797:THR:O	1:B:797:THR:HG22	2.19	0.42
1:C:434:TRP:CE3	1:C:434:TRP:CA	3.01	0.42
1:C:623:GLU:C	1:C:624:TYR:CD1	2.98	0.42
1:C:791:THR:HG23	1:C:800:SER:HB2	2.01	0.42
1:A:372:GLN:O	1:A:373:GLY:O	2.38	0.42
1:A:383:ASN:C	1:A:385:GLY:H	2.27	0.42
1:A:435:PRO:O	1:A:436:ALA:O	2.37	0.42
1:A:746:ASN:ND2	1:A:749:ARG:CB	2.82	0.42
1:B:196:THR:OG1	1:B:708:GLU:HG3	2.20	0.42
1:B:202:THR:HG21	1:B:361:GLY:H	1.84	0.42
1:B:262:LEU:HD23	1:B:592:ILE:HG23	2.02	0.42
1:B:394:TYR:CD1	1:B:394:TYR:C	2.97	0.42
1:B:402:LEU:HD12	1:B:402:LEU:C	2.43	0.42
1:B:757:GLN:O	1:B:758:GLU:C	2.63	0.42
1:B:757:GLN:NE2	1:B:757:GLN:HA	2.35	0.42
1:B:795:PHE:C	1:B:797:THR:N	2.72	0.42
1:C:143:ASP:O	1:C:145:GLY:N	2.53	0.42
1:C:277:PHE:O	1:C:278:LYS:HB2	2.19	0.42
1:C:472:HIS:CE1	1:C:538:ASN:ND2	2.88	0.42
1:C:647:ASP:OD1	1:C:648:ALA:N	2.52	0.42
1:C:698:ASP:O	1:C:701:GLY:HA3	2.19	0.42
1:A:190:ARG:HH11	1:A:190:ARG:HG2	1.84	0.42
1:A:253:THR:OG1	1:A:257:THR:HG23	2.19	0.42
1:A:591:ASP:CG	1:A:592:ILE:N	2.78	0.42
1:B:186:ASP:C	1:B:188:VAL:N	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ALA:HB2	1:B:214:ILE:CG1	2.50	0.42
1:B:231:TYR:CD2	1:B:485:TRP:HH2	2.38	0.42
1:B:292:ARG:HD2	1:B:316:GLN:OE1	2.20	0.42
1:B:401:ASN:CB	1:B:415:GLN:HB3	2.49	0.42
1:B:692:THR:O	1:B:711:ASP:HA	2.20	0.42
1:B:791:THR:HG23	1:B:800:SER:HB2	2.02	0.42
1:C:262:LEU:HD23	1:C:592:ILE:HG23	2.01	0.42
1:C:492:ASN:HD22	1:C:492:ASN:HA	1.48	0.42
1:C:560:ASN:O	1:C:561:PRO:C	2.63	0.42
1:C:621:LYS:HG2	1:C:632:SER:CB	2.49	0.42
1:C:656:ASN:O	1:C:657:PRO:C	2.62	0.42
1:A:421:ASN:O	1:A:452:THR:CG2	2.66	0.42
1:A:526:THR:HA	1:A:555:ARG:O	2.18	0.42
1:A:560:ASN:O	1:A:561:PRO:C	2.62	0.42
1:A:614:GLN:HE21	1:A:614:GLN:HB2	1.62	0.42
1:A:807:LEU:HD12	1:A:807:LEU:HA	1.93	0.42
1:B:152:ILE:HB	1:B:154:THR:HG22	2.01	0.42
1:B:391:TRP:CD1	1:B:393:GLN:CG	3.02	0.42
1:B:447:LYS:HD2	1:B:515:TRP:CG	2.55	0.42
1:B:586:TYR:CD1	1:B:619:GLY:O	2.72	0.42
1:B:723:GLY:O	1:B:725:LEU:N	2.53	0.42
1:B:814:ASP:HB3	1:B:815:PHE:H	1.61	0.42
1:C:163:ARG:NH2	1:C:584:SER:OG	2.49	0.42
1:C:211:GLY:CA	1:C:708:GLU:OE1	2.68	0.42
1:C:368:LEU:HD21	1:C:798:SER:O	2.20	0.42
1:C:474:LEU:HD12	1:C:534:THR:O	2.20	0.42
1:C:639:HIS:CD2	1:C:669:LYS:HG3	2.55	0.42
1:A:140:ILE:CG2	1:A:141:THR:H	2.31	0.42
1:A:144:SER:C	1:A:146:SER:N	2.78	0.42
1:A:177:MSE:HE2	1:A:245:ARG:HA	2.01	0.42
1:A:410:TRP:CE2	1:A:463:GLY:N	2.88	0.42
1:A:472:HIS:ND1	1:A:538:ASN:ND2	2.68	0.42
1:A:554:TYR:CD1	1:A:595:PRO:HG3	2.55	0.42
1:A:556:VAL:O	1:A:556:VAL:HG22	2.20	0.42
1:A:749:ARG:HH11	1:A:751:ARG:NH2	2.18	0.42
1:B:243:TYR:HA	1:B:270:ARG:HA	2.01	0.42
1:B:423:TYR:CE1	1:B:449:THR:C	2.98	0.42
1:B:475:VAL:CG1	1:B:534:THR:HB	2.50	0.42
1:B:749:ARG:O	1:B:751:ARG:N	2.50	0.42
1:C:351:ASP:OD2	1:C:397:THR:HG23	2.20	0.42
1:C:552:VAL:HG22	1:C:553:ASP:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ALA:O	1:C:659:ILE:C	2.63	0.42
1:A:407:ALA:C	1:A:409:GLY:N	2.76	0.41
1:A:430:ILE:CD1	1:A:441:ALA:HB3	2.50	0.41
1:A:475:VAL:CG1	1:A:534:THR:HB	2.50	0.41
1:A:637:GLU:HA	1:A:671:LYS:HA	2.02	0.41
1:A:670:THR:OG1	1:A:696:ILE:HD12	2.19	0.41
1:B:262:LEU:HD21	1:B:613:GLY:HA3	2.01	0.41
1:B:327:ARG:HG3	1:B:328:LYS:N	2.33	0.41
1:B:351:ASP:OD2	1:B:397:THR:CG2	2.68	0.41
1:B:414:VAL:HG23	1:B:459:ILE:CG2	2.50	0.41
1:C:169:ILE:HD13	1:C:169:ILE:HA	1.84	0.41
1:C:342:PRO:HB3	1:C:405:ASN:O	2.20	0.41
1:C:807:LEU:HD23	1:C:807:LEU:HA	1.83	0.41
1:A:161:THR:HB	1:A:162:PRO:CD	2.50	0.41
1:A:556:VAL:HG12	1:A:563:ILE:O	2.20	0.41
1:A:724:ALA:C	1:A:725:LEU:HD23	2.45	0.41
1:A:791:THR:HG23	1:A:800:SER:HB2	2.02	0.41
1:B:174:ARG:C	1:B:176:ASN:N	2.76	0.41
1:B:280:HIS:ND1	1:B:812:ARG:NH2	2.68	0.41
1:B:445:ALA:HB3	1:B:493:LEU:HD11	2.02	0.41
1:B:624:TYR:O	1:B:625:LEU:HB2	2.20	0.41
1:C:158:LEU:CD1	1:C:475:VAL:HB	2.50	0.41
1:C:243:TYR:CE2	1:C:268:LEU:CB	3.03	0.41
1:C:372:GLN:O	1:C:373:GLY:O	2.38	0.41
1:C:380:ARG:HG3	1:C:380:ARG:NH1	2.33	0.41
1:C:414:VAL:HG23	1:C:459:ILE:HG22	2.01	0.41
1:C:521:TYR:C	1:C:522:ILE:HG13	2.45	0.41
1:A:609:GLU:HB3	1:A:610:PRO:HD2	2.02	0.41
1:A:655:THR:CG2	1:A:656:ASN:H	2.26	0.41
1:B:401:ASN:HB3	1:B:415:GLN:CB	2.50	0.41
1:B:589:TYR:HE1	1:B:614:GLN:HG2	1.84	0.41
1:B:693:HIS:HA	1:B:710:GLN:O	2.21	0.41
1:B:724:ALA:C	1:B:725:LEU:HD23	2.46	0.41
1:B:728:LEU:HB2	1:B:769:TYR:CE1	2.55	0.41
1:C:201:ASP:O	1:C:202:THR:C	2.64	0.41
1:C:295:LEU:O	1:C:312:VAL:HA	2.19	0.41
1:C:526:THR:CG2	1:C:554:TYR:CE1	3.02	0.41
1:A:288:TRP:CZ2	1:A:321:PHE:HB3	2.55	0.41
1:A:368:LEU:HD21	1:A:799:ALA:HB2	2.01	0.41
1:A:430:ILE:HD11	1:A:441:ALA:CB	2.50	0.41
1:B:637:GLU:HA	1:B:671:LYS:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:THR:CA	1:B:659:ILE:HD12	2.47	0.41
1:B:745:TYR:HB2	1:B:752:TRP:NE1	2.35	0.41
1:C:152:ILE:O	1:C:152:ILE:HG13	2.19	0.41
1:C:202:THR:HG21	1:C:361:GLY:H	1.85	0.41
1:C:352:TYR:HE1	1:C:396:ARG:HD2	1.81	0.41
1:C:757:GLN:O	1:C:758:GLU:C	2.63	0.41
1:A:325:TYR:C	1:A:325:TYR:CD1	2.98	0.41
1:A:698:ASP:O	1:A:701:GLY:HA3	2.21	0.41
1:A:814:ASP:HB3	1:A:815:PHE:H	1.61	0.41
1:B:295:LEU:O	1:B:312:VAL:HA	2.20	0.41
1:B:384:ASN:O	1:B:430:ILE:HG22	2.19	0.41
1:B:414:VAL:HG23	1:B:459:ILE:HG22	2.01	0.41
1:B:696:ILE:O	1:B:696:ILE:HG23	2.20	0.41
1:C:174:ARG:C	1:C:176:ASN:N	2.78	0.41
1:C:201:ASP:CG	1:C:204:ARG:HE	2.26	0.41
1:C:313:ALA:HA	1:C:331:VAL:O	2.20	0.41
1:C:434:TRP:C	1:C:436:ALA:N	2.79	0.41
1:C:461:LEU:O	1:C:475:VAL:HA	2.20	0.41
1:C:461:LEU:HB2	1:C:476:VAL:CG1	2.51	0.41
1:C:503:PHE:O	1:C:504:ILE:O	2.38	0.41
1:C:591:ASP:CG	1:C:592:ILE:N	2.79	0.41
1:C:608:LEU:O	1:C:609:GLU:C	2.62	0.41
1:C:668:ALA:HA	1:C:698:ASP:HA	2.03	0.41
1:C:766:MSE:HB2	1:C:780:ASN:ND2	2.35	0.41
1:A:201:ASP:CG	1:A:204:ARG:HE	2.28	0.41
1:A:246:VAL:O	1:A:246:VAL:CG1	2.67	0.41
1:A:262:LEU:HD23	1:A:592:ILE:HG23	2.02	0.41
1:A:378:VAL:CG2	1:A:382:PHE:HB2	2.51	0.41
1:A:414:VAL:HG23	1:A:459:ILE:HG22	2.01	0.41
1:A:537:PHE:O	1:A:545:LEU:N	2.42	0.41
1:A:602:ASP:O	1:A:604:SER:N	2.53	0.41
1:B:161:THR:HB	1:B:162:PRO:CD	2.50	0.41
1:B:434:TRP:C	1:B:436:ALA:N	2.79	0.41
1:B:503:PHE:CD2	1:B:504:ILE:N	2.89	0.41
1:B:515:TRP:CD1	1:B:515:TRP:H	2.36	0.41
1:B:682:ALA:CB	1:B:683:PRO:HD2	2.51	0.41
1:C:186:ASP:O	1:C:188:VAL:N	2.53	0.41
1:C:214:ILE:HG23	1:C:264:ALA:O	2.19	0.41
1:C:292:ARG:HD2	1:C:316:GLN:OE1	2.20	0.41
1:C:439:ASN:O	1:C:502:ASP:HA	2.21	0.41
1:C:532:TYR:HD2	1:C:550:ARG:NH1	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:C	1:A:143:ASP:N	2.78	0.41
1:A:235:ASN:O	1:A:237:LEU:N	2.54	0.41
1:A:439:ASN:O	1:A:502:ASP:HA	2.20	0.41
1:A:640:GLU:HB3	1:A:668:ALA:HB3	2.03	0.41
1:B:526:THR:HA	1:B:555:ARG:O	2.20	0.41
1:B:529:LEU:O	1:B:552:VAL:HG23	2.20	0.41
1:B:532:TYR:HD2	1:B:550:ARG:NH1	2.18	0.41
1:B:639:HIS:CD2	1:B:669:LYS:HG3	2.56	0.41
1:B:682:ALA:HB3	1:B:685:TRP:CB	2.50	0.41
1:C:147:TYR:CD2	1:C:686:GLN:HB3	2.56	0.41
1:C:180:PHE:HA	1:C:780:ASN:HD21	1.86	0.41
1:C:582:THR:HG22	1:C:583:TYR:N	2.36	0.41
1:A:623:GLU:C	1:A:624:TYR:CD1	2.99	0.41
1:A:722:LYS:O	1:A:723:GLY:C	2.62	0.41
1:B:211:GLY:CA	1:B:708:GLU:OE1	2.68	0.41
1:B:219:TYR:CD1	1:B:219:TYR:N	2.89	0.41
1:B:219:TYR:N	1:B:222:ILE:O	2.51	0.41
1:B:406:PHE:HB3	1:B:408:ASN:OD1	2.21	0.41
1:B:505:ASN:O	1:B:505:ASN:CG	2.64	0.41
1:B:576:VAL:HA	1:B:585:VAL:O	2.20	0.41
1:B:593:PHE:CD1	1:B:593:PHE:C	2.97	0.41
1:C:148:THR:OG1	1:C:149:PRO:HD2	2.19	0.41
1:C:281:VAL:O	1:C:281:VAL:CG1	2.68	0.41
1:C:323:ASP:O	1:C:324:HIS:ND1	2.54	0.41
1:C:443:ILE:O	1:C:443:ILE:CG1	2.68	0.41
1:C:602:ASP:O	1:C:603:SER:C	2.63	0.41
1:C:772:THR:OG1	1:C:775:LEU:HB3	2.20	0.41
1:A:209:ALA:HB2	1:A:214:ILE:CG1	2.51	0.41
1:A:226:ALA:HB3	1:A:235:ASN:HD21	1.86	0.41
1:A:255:LEU:HD22	1:A:572:TYR:CD2	2.55	0.41
1:A:290:ASN:HA	1:A:318:LYS:CB	2.50	0.41
1:A:361:GLY:HA2	1:A:385:GLY:CA	2.51	0.41
1:A:396:ARG:HG3	1:A:420:ILE:CD1	2.51	0.41
1:A:602:ASP:O	1:A:603:SER:C	2.64	0.41
1:A:766:MSE:HG3	1:A:780:ASN:ND2	2.36	0.41
1:B:214:ILE:HG23	1:B:264:ALA:O	2.21	0.41
1:B:281:VAL:HB	1:B:295:LEU:CD1	2.50	0.41
1:B:430:ILE:HD11	1:B:441:ALA:CB	2.50	0.41
1:B:447:LYS:CE	3:B:2002:SO4:O4	2.65	0.41
1:B:461:LEU:O	1:B:475:VAL:HA	2.21	0.41
1:B:510:ILE:HG22	1:B:511:GLY:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:GLU:C	1:B:624:TYR:CD1	2.99	0.41
1:C:173:THR:CG2	1:C:176:ASN:HB2	2.50	0.41
1:C:235:ASN:O	1:C:237:LEU:N	2.53	0.41
1:C:255:LEU:HD22	1:C:572:TYR:CG	2.56	0.41
1:C:472:HIS:ND1	1:C:538:ASN:ND2	2.69	0.41
1:C:539:VAL:HB	1:C:543:LEU:HD23	2.03	0.41
1:A:275:HIS:CE1	1:A:308:ARG:NH1	2.89	0.41
1:A:357:PRO:O	1:A:390:SER:CB	2.61	0.41
1:A:582:THR:HG22	1:A:583:TYR:N	2.35	0.41
1:B:173:THR:HG23	1:B:176:ASN:HB2	2.02	0.41
1:B:347:THR:C	1:B:348:VAL:HG13	2.46	0.41
1:C:139:THR:CG2	1:C:150:GLY:HA3	2.50	0.41
1:C:503:PHE:CD2	1:C:504:ILE:N	2.89	0.41
1:C:761:TRP:CE3	1:C:761:TRP:HA	2.56	0.41
1:A:189:MSE:HE3	1:A:195:ILE:CD1	2.44	0.40
1:A:202:THR:HG21	1:A:361:GLY:H	1.85	0.40
1:A:244:ASP:N	1:A:269:ILE:O	2.49	0.40
1:A:292:ARG:CG	1:A:316:GLN:HB2	2.50	0.40
1:A:371:SER:HB3	1:A:372:GLN:OE1	2.21	0.40
1:A:647:ASP:HB3	1:A:662:ALA:O	2.22	0.40
1:A:674:GLU:HB2	1:A:692:THR:HG23	2.02	0.40
1:A:749:ARG:O	1:A:751:ARG:N	2.53	0.40
1:A:766:MSE:HB2	1:A:780:ASN:ND2	2.36	0.40
1:B:139:THR:CG2	1:B:150:GLY:HA3	2.51	0.40
1:B:143:ASP:O	1:B:145:GLY:N	2.55	0.40
1:B:169:ILE:HD13	1:B:169:ILE:HA	1.88	0.40
1:B:474:LEU:CG	1:B:475:VAL:N	2.84	0.40
1:B:670:THR:OG1	1:B:696:ILE:CG1	2.69	0.40
1:B:670:THR:OG1	1:B:696:ILE:HD12	2.21	0.40
1:C:681:LEU:HD23	1:C:685:TRP:CE2	2.57	0.40
1:C:694:LYS:HD3	1:C:694:LYS:C	2.46	0.40
1:A:178:ASP:O	1:A:179:ASP:C	2.64	0.40
1:A:200:TYR:C	1:A:201:ASP:OD1	2.64	0.40
1:B:152:ILE:O	1:B:152:ILE:HG13	2.20	0.40
1:B:472:HIS:ND1	1:B:538:ASN:ND2	2.70	0.40
1:B:496:TYR:CZ	1:B:513:PRO:HD3	2.57	0.40
1:B:556:VAL:O	1:B:556:VAL:HG22	2.21	0.40
1:B:698:ASP:O	1:B:701:GLY:CA	2.70	0.40
1:C:365:SER:HB2	1:C:799:ALA:O	2.22	0.40
1:C:515:TRP:CD1	1:C:515:TRP:H	2.39	0.40
1:C:540:THR:HG22	1:C:542:ASP:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:ASN:O	1:C:653:LYS:HG3	2.21	0.40
1:A:158:LEU:O	1:A:160:LEU:CD1	2.70	0.40
1:A:295:LEU:O	1:A:312:VAL:HA	2.21	0.40
1:A:365:SER:HB2	1:A:799:ALA:O	2.21	0.40
1:A:401:ASN:CB	1:A:415:GLN:HB3	2.49	0.40
1:A:668:ALA:HA	1:A:698:ASP:HA	2.04	0.40
1:B:511:GLY:O	1:B:513:PRO:CD	2.68	0.40
1:B:552:VAL:HG22	1:B:553:ASP:H	1.86	0.40
1:C:161:THR:HB	1:C:162:PRO:CD	2.52	0.40
1:C:174:ARG:HG3	1:C:178:ASP:OD2	2.21	0.40
1:C:288:TRP:CZ2	1:C:321:PHE:HB3	2.56	0.40
1:C:407:ALA:C	1:C:409:GLY:N	2.79	0.40
1:A:147:TYR:CE1	1:A:176:ASN:HA	2.56	0.40
1:A:259:ALA:HB1	1:A:595:PRO:HD2	2.04	0.40
1:A:323:ASP:O	1:A:324:HIS:ND1	2.54	0.40
1:B:169:ILE:CD1	1:B:249:LEU:HD12	2.49	0.40
1:B:209:ALA:CB	1:B:214:ILE:HG12	2.51	0.40
1:B:518:PRO:CG	1:B:521:TYR:CE2	3.05	0.40
1:B:762:LEU:CD2	1:B:789:TYR:HE2	2.23	0.40
1:B:789:TYR:C	1:B:789:TYR:HD1	2.29	0.40
1:C:430:ILE:CD1	1:C:441:ALA:HB3	2.52	0.40
1:A:347:THR:C	1:A:348:VAL:HG13	2.47	0.40
1:A:725:LEU:C	1:A:727:LYS:N	2.76	0.40
1:B:170:THR:O	1:B:248:VAL:HG12	2.22	0.40
1:B:207:TYR:O	1:B:214:ILE:HG13	2.22	0.40
1:B:238:SER:HA	1:B:353:GLN:OE1	2.22	0.40
1:B:244:ASP:OD2	1:B:245:ARG:NH1	2.55	0.40
1:B:766:MSE:HG3	1:B:780:ASN:ND2	2.37	0.40
1:C:378:VAL:CG2	1:C:382:PHE:HB2	2.51	0.40
1:C:552:VAL:CG2	1:C:553:ASP:H	2.34	0.40
1:C:556:VAL:O	1:C:556:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	685/687 (100%)	521 (76%)	102 (15%)	62 (9%)	0	6
1	B	685/687 (100%)	519 (76%)	103 (15%)	63 (9%)	0	6
1	C	685/687 (100%)	518 (76%)	108 (16%)	59 (9%)	0	7
2	I	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	J	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	K	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	2064/2085 (99%)	1561 (76%)	316 (15%)	187 (9%)	0	6

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	241	ALA
1	A	324	HIS
1	A	341	ASN
1	A	345	MSE
1	A	371	SER
1	A	374	ASN
1	A	436	ALA
1	A	561	PRO
1	A	605	ASN
1	A	626	ASP
1	A	650	TYR
1	A	655	THR
1	A	659	ILE
1	A	682	ALA
1	A	699	ASP
1	A	724	ALA
1	A	739	LYS
1	A	758	GLU
1	A	775	LEU
1	A	784	VAL
1	A	805	ARG
1	A	814	ASP
1	B	144	SER
1	B	241	ALA
1	B	324	HIS
1	B	341	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	345	MSE
1	B	371	SER
1	B	374	ASN
1	B	436	ALA
1	B	561	PRO
1	B	605	ASN
1	B	626	ASP
1	B	655	THR
1	B	659	ILE
1	B	682	ALA
1	B	699	ASP
1	B	724	ALA
1	B	739	LYS
1	B	758	GLU
1	B	775	LEU
1	B	784	VAL
1	B	805	ARG
1	B	814	ASP
1	C	144	SER
1	C	241	ALA
1	C	324	HIS
1	C	341	ASN
1	C	345	MSE
1	C	371	SER
1	C	374	ASN
1	C	436	ALA
1	C	561	PRO
1	C	605	ASN
1	C	626	ASP
1	C	651	ASN
1	C	659	ILE
1	C	660	THR
1	C	682	ALA
1	C	699	ASP
1	C	724	ALA
1	C	739	LYS
1	C	758	GLU
1	C	775	LEU
1	C	784	VAL
1	C	805	ARG
1	C	814	ASP
2	I	6	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	6	LYS
2	K	6	LYS
1	A	187	ASP
1	A	202	THR
1	A	236	THR
1	A	254	GLY
1	A	340	LEU
1	A	363	SER
1	A	373	GLY
1	A	501	ASP
1	A	504	ILE
1	A	508	GLY
1	A	516	GLY
1	A	579	LEU
1	A	603	SER
1	A	656	ASN
1	A	723	GLY
1	B	202	THR
1	B	236	THR
1	B	254	GLY
1	B	340	LEU
1	B	363	SER
1	B	469	GLY
1	B	501	ASP
1	B	504	ILE
1	B	508	GLY
1	B	516	GLY
1	B	579	LEU
1	B	603	SER
1	B	723	GLY
1	C	187	ASP
1	C	236	THR
1	C	254	GLY
1	C	340	LEU
1	C	363	SER
1	C	373	GLY
1	C	501	ASP
1	C	504	ILE
1	C	508	GLY
1	C	516	GLY
1	C	579	LEU
1	C	603	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	723	GLY
1	A	379	SER
1	A	469	GLY
1	A	505	ASN
1	A	649	LEU
1	A	683	PRO
1	A	750	SER
1	B	142	GLU
1	B	145	GLY
1	B	187	ASP
1	B	373	GLY
1	B	379	SER
1	B	505	ASN
1	B	650	TYR
1	B	658	ALA
1	B	683	PRO
1	B	750	SER
1	C	145	GLY
1	C	202	THR
1	C	379	SER
1	C	505	ASN
1	C	683	PRO
1	C	750	SER
1	A	541	ASP
1	A	658	ALA
1	A	660	THR
1	B	439	ASN
1	B	541	ASP
1	C	142	GLU
1	C	384	ASN
1	C	439	ASN
1	C	469	GLY
1	C	541	ASP
1	C	608	LEU
1	C	655	THR
1	A	303	GLU
1	A	384	ASN
1	A	439	ASN
1	A	608	LEU
1	A	744	VAL
1	B	303	GLU
1	B	384	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	426	PRO
1	B	433	ASP
1	B	608	LEU
1	B	744	VAL
1	C	303	GLU
1	C	592	ILE
1	C	625	LEU
1	C	744	VAL
1	A	145	GLY
1	A	426	PRO
1	A	433	ASP
1	A	435	PRO
1	A	475	VAL
1	A	592	ILE
1	B	475	VAL
1	B	592	ILE
1	B	625	LEU
1	C	426	PRO
1	C	435	PRO
1	C	475	VAL
1	C	512	LYS
1	C	513	PRO
1	B	656	ASN
1	A	258	GLY
1	A	512	LYS
1	A	513	PRO
1	B	435	PRO
1	A	803	ASP
1	B	513	PRO
1	B	803	ASP
1	C	803	ASP
1	B	258	GLY
1	B	512	LYS
1	B	657	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	582/570 (102%)	509 (88%)	73 (12%)	4	22
1	B	582/570 (102%)	498 (86%)	84 (14%)	3	18
1	C	582/570 (102%)	502 (86%)	80 (14%)	3	20
2	I	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	J	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	K	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	1758/1722 (102%)	1515 (86%)	243 (14%)	3	20

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	139	THR
1	A	143	ASP
1	A	157	ARG
1	A	158	LEU
1	A	160	LEU
1	A	171	VAL
1	A	174	ARG
1	A	178	ASP
1	A	185	ILE
1	A	196	THR
1	A	201	ASP
1	A	213	SER
1	A	218	GLN
1	A	225	THR
1	A	227	ARG
1	A	236	THR
1	A	257	THR
1	A	282	GLU
1	A	330	SER
1	A	341	ASN
1	A	342	PRO
1	A	344	THR
1	A	408	ASN
1	A	414	VAL
1	A	415	GLN
1	A	430	ILE
1	A	433	ASP
1	A	434	TRP
1	A	452	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	462	THR
1	A	473	GLU
1	A	490	TYR
1	A	492	ASN
1	A	497	ASP
1	A	502	ASP
1	A	506	TRP
1	A	507	ASP
1	A	510	ILE
1	A	515	TRP
1	A	526	THR
1	A	538	ASN
1	A	557	THR
1	A	560	ASN
1	A	561	PRO
1	A	578	ASP
1	A	593	PHE
1	A	596	GLN
1	A	599	TRP
1	A	607	LEU
1	A	614	GLN
1	A	624	TYR
1	A	628	ARG
1	A	630	ASN
1	A	633	LEU
1	A	670	THR
1	A	694	LYS
1	A	695	ILE
1	A	710	GLN
1	A	725	LEU
1	A	742	GLN
1	A	743	MSE
1	A	752	TRP
1	A	758	GLU
1	A	761	TRP
1	A	762	LEU
1	A	766	MSE
1	A	772	THR
1	A	778	SER
1	A	781	VAL
1	A	788	THR
1	A	792	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	814	ASP
1	B	135	ASN
1	B	139	THR
1	B	143	ASP
1	B	158	LEU
1	B	160	LEU
1	B	171	VAL
1	B	174	ARG
1	B	185	ILE
1	B	196	THR
1	B	201	ASP
1	B	213	SER
1	B	218	GLN
1	B	225	THR
1	B	227	ARG
1	B	239	ASP
1	B	257	THR
1	B	327	ARG
1	B	330	SER
1	B	341	ASN
1	B	342	PRO
1	B	344	THR
1	B	354	ASP
1	B	408	ASN
1	B	413	LYS
1	B	414	VAL
1	B	415	GLN
1	B	417	ASP
1	B	430	ILE
1	B	433	ASP
1	B	434	TRP
1	B	439	ASN
1	B	452	THR
1	B	462	THR
1	B	473	GLU
1	B	490	TYR
1	B	497	ASP
1	B	502	ASP
1	B	506	TRP
1	B	507	ASP
1	B	509	ASP
1	B	510	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	538	ASN
1	B	541	ASP
1	B	557	THR
1	B	560	ASN
1	B	561	PRO
1	B	568	ARG
1	B	570	ILE
1	B	593	PHE
1	B	596	GLN
1	B	599	TRP
1	B	606	LYS
1	B	607	LEU
1	B	614	GLN
1	B	624	TYR
1	B	628	ARG
1	B	630	ASN
1	B	633	LEU
1	B	641	GLU
1	B	653	LYS
1	B	656	ASN
1	B	659	ILE
1	B	670	THR
1	B	692	THR
1	B	694	LYS
1	B	695	ILE
1	B	706	THR
1	B	725	LEU
1	B	742	GLN
1	B	743	MSE
1	B	752	TRP
1	B	754	LYS
1	B	758	GLU
1	B	761	TRP
1	B	762	LEU
1	B	766	MSE
1	B	768	ARG
1	B	772	THR
1	B	778	SER
1	B	781	VAL
1	B	782	ASN
1	B	788	THR
1	B	792	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	814	ASP
1	C	139	THR
1	C	143	ASP
1	C	158	LEU
1	C	160	LEU
1	C	171	VAL
1	C	185	ILE
1	C	196	THR
1	C	201	ASP
1	C	213	SER
1	C	218	GLN
1	C	225	THR
1	C	227	ARG
1	C	257	THR
1	C	274	THR
1	C	342	PRO
1	C	344	THR
1	C	354	ASP
1	C	377	ASP
1	C	392	GLU
1	C	396	ARG
1	C	402	LEU
1	C	408	ASN
1	C	414	VAL
1	C	415	GLN
1	C	430	ILE
1	C	433	ASP
1	C	434	TRP
1	C	449	THR
1	C	452	THR
1	C	462	THR
1	C	473	GLU
1	C	479	SER
1	C	490	TYR
1	C	492	ASN
1	C	497	ASP
1	C	501	ASP
1	C	502	ASP
1	C	506	TRP
1	C	507	ASP
1	C	526	THR
1	C	536	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	538	ASN
1	C	541	ASP
1	C	543	LEU
1	C	557	THR
1	C	559	LEU
1	C	560	ASN
1	C	561	PRO
1	C	593	PHE
1	C	596	GLN
1	C	599	TRP
1	C	607	LEU
1	C	614	GLN
1	C	624	TYR
1	C	628	ARG
1	C	630	ASN
1	C	633	LEU
1	C	641	GLU
1	C	645	GLU
1	C	650	TYR
1	C	651	ASN
1	C	653	LYS
1	C	670	THR
1	C	694	LYS
1	C	725	LEU
1	C	726	ASP
1	C	742	GLN
1	C	743	MSE
1	C	752	TRP
1	C	758	GLU
1	C	761	TRP
1	C	762	LEU
1	C	766	MSE
1	C	772	THR
1	C	778	SER
1	C	781	VAL
1	C	782	ASN
1	C	788	THR
1	C	792	ASN
1	C	814	ASP
2	I	6	LYS
2	I	8	THR
2	J	6	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	8	THR
2	K	6	LYS
2	K	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	205	ASN
1	A	206	ASN
1	A	235	ASN
1	A	275	HIS
1	A	280	HIS
1	A	324	HIS
1	A	341	ASN
1	A	353	GLN
1	A	355	ASN
1	A	405	ASN
1	A	415	GLN
1	A	418	HIS
1	A	492	ASN
1	A	538	ASN
1	A	560	ASN
1	A	596	GLN
1	A	614	GLN
1	A	630	ASN
1	A	656	ASN
1	A	710	GLN
1	A	746	ASN
1	A	780	ASN
1	A	782	ASN
1	A	806	ASN
1	B	135	ASN
1	B	191	HIS
1	B	205	ASN
1	B	206	ASN
1	B	235	ASN
1	B	267	ASN
1	B	275	HIS
1	B	280	HIS
1	B	324	HIS
1	B	341	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	ASN
1	B	376	ASN
1	B	383	ASN
1	B	405	ASN
1	B	415	GLN
1	B	418	HIS
1	B	439	ASN
1	B	538	ASN
1	B	560	ASN
1	B	596	GLN
1	B	614	GLN
1	B	630	ASN
1	B	710	GLN
1	B	746	ASN
1	B	757	GLN
1	B	780	ASN
1	B	782	ASN
1	B	806	ASN
1	C	183	ASN
1	C	205	ASN
1	C	206	ASN
1	C	235	ASN
1	C	267	ASN
1	C	275	HIS
1	C	280	HIS
1	C	306	ASN
1	C	324	HIS
1	C	355	ASN
1	C	384	ASN
1	C	415	GLN
1	C	418	HIS
1	C	492	ASN
1	C	538	ASN
1	C	544	ASN
1	C	560	ASN
1	C	596	GLN
1	C	614	GLN
1	C	630	ASN
1	C	651	ASN
1	C	710	GLN
1	C	737	GLN
1	C	746	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	780	ASN
1	C	782	ASN
1	C	806	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	FHO	I	5	2	9,10,11	1.16	1 (11%)	4,11,13	1.75	1 (25%)
2	FHO	J	5	2	9,10,11	1.30	1 (11%)	4,11,13	1.84	1 (25%)
2	FHO	K	7	2	9,10,11	1.67	2 (22%)	4,11,13	1.14	0
2	FHO	I	7	2	9,10,11	1.81	3 (33%)	4,11,13	1.65	2 (50%)
2	FHO	J	7	2	9,10,11	1.94	3 (33%)	4,11,13	1.64	1 (25%)
2	FHO	K	5	2	9,10,11	1.22	1 (11%)	4,11,13	1.64	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHO	I	5	2	-	4/7/10/12	-
2	FHO	J	5	2	-	4/7/10/12	-
2	FHO	K	7	2	-	3/7/10/12	-
2	FHO	I	7	2	-	5/7/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHO	J	7	2	-	6/7/10/12	-
2	FHO	K	5	2	-	4/7/10/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	7	FHO	CB-CA	3.52	1.58	1.53
2	K	7	FHO	OZ-NE	-2.99	1.36	1.39
2	I	7	FHO	OZ-NE	-2.93	1.36	1.39
2	J	5	FHO	OZ-NE	-2.88	1.36	1.39
2	I	7	FHO	CB-CA	2.85	1.57	1.53
2	J	7	FHO	OZ-NE	-2.67	1.36	1.39
2	J	7	FHO	CD-NE	2.63	1.51	1.46
2	K	5	FHO	OZ-NE	-2.62	1.36	1.39
2	I	5	FHO	OZ-NE	-2.37	1.37	1.39
2	I	7	FHO	CZ-NE	-2.32	1.31	1.34
2	K	7	FHO	CZ-NE	-2.28	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5	FHO	OZ-NE-CD	3.18	121.18	113.81
2	I	5	FHO	OZ-NE-CD	3.08	120.93	113.81
2	K	5	FHO	OZ-NE-CD	2.96	120.66	113.81
2	J	7	FHO	CG-CD-NE	2.48	116.18	111.12
2	I	7	FHO	CG-CD-NE	2.47	116.16	111.12
2	I	7	FHO	OH-CZ-NE	-2.01	120.34	125.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	5	FHO	N-CA-CB-CG
2	I	5	FHO	C-CA-CB-CG
2	I	5	FHO	CG-CD-NE-OZ
2	I	5	FHO	CG-CD-NE-CZ
2	I	7	FHO	N-CA-CB-CG
2	I	7	FHO	C-CA-CB-CG
2	I	7	FHO	NE-CD-CG-CB
2	I	7	FHO	CG-CD-NE-OZ
2	I	7	FHO	CG-CD-NE-CZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	5	FHO	N-CA-CB-CG
2	J	5	FHO	C-CA-CB-CG
2	J	5	FHO	CG-CD-NE-OZ
2	J	5	FHO	CG-CD-NE-CZ
2	J	7	FHO	NE-CD-CG-CB
2	J	7	FHO	CG-CD-NE-OZ
2	J	7	FHO	CG-CD-NE-CZ
2	K	5	FHO	N-CA-CB-CG
2	K	5	FHO	C-CA-CB-CG
2	K	5	FHO	CG-CD-NE-OZ
2	K	5	FHO	CG-CD-NE-CZ
2	K	7	FHO	C-CA-CB-CG
2	K	7	FHO	CG-CD-NE-OZ
2	K	7	FHO	CA-CB-CG-CD
2	J	7	FHO	N-CA-CB-CG
2	J	7	FHO	CA-CB-CG-CD
2	J	7	FHO	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	7	FHO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	2002	-	4,4,4	0.44	0	6,6,6	0.10	0
3	SO4	C	2003	-	4,4,4	0.44	0	6,6,6	0.07	0
4	PVE	K	1	2	26,28,29	2.70	10 (38%)	30,40,42	4.41	1 (3%)
3	SO4	A	2001	-	4,4,4	0.41	0	6,6,6	0.09	0
4	PVE	J	1	2	26,28,29	2.58	11 (42%)	30,40,42	4.59	1 (3%)
4	PVE	I	1	2	26,28,29	2.46	9 (34%)	30,40,42	4.44	1 (3%)

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
4	PVE	J	1	2	1/1/3/6	7/10/21/23	0/2/3/3
4	PVE	K	1	2	1/1/3/6	8/10/21/23	0/2/3/3
4	PVE	I	1	2	1/1/3/6	7/10/21/23	0/2/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	PVE	C5-C6	6.69	1.43	1.37
4	J	1	PVE	C9-N1	6.41	1.46	1.39
4	J	1	PVE	C8-C7	6.32	1.43	1.37
4	K	1	PVE	C8-C7	6.26	1.43	1.37
4	K	1	PVE	C9-N1	5.96	1.45	1.39
4	I	1	PVE	C5-C6	5.88	1.43	1.37
4	I	1	PVE	C8-C7	5.80	1.43	1.37
4	I	1	PVE	C9-N1	4.94	1.44	1.39
4	J	1	PVE	C5-C6	4.92	1.42	1.37
4	K	1	PVE	C2-N1	3.53	1.44	1.36
4	J	1	PVE	C2-N1	3.38	1.43	1.36
4	I	1	PVE	C3-N17	-3.11	1.35	1.41
4	K	1	PVE	C4-C3	3.10	1.43	1.37
4	J	1	PVE	C3-N17	-2.98	1.35	1.41
4	K	1	PVE	C3-C2	2.83	1.44	1.41
4	I	1	PVE	C4-C3	2.75	1.42	1.37
4	K	1	PVE	C3-N17	-2.65	1.36	1.41
4	I	1	PVE	C2-N1	2.63	1.42	1.36
4	K	1	PVE	C8-C9	2.59	1.45	1.40
4	J	1	PVE	C8-C9	2.52	1.45	1.40
4	K	1	PVE	O24-C22	-2.46	1.22	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	PVE	O24-C22	-2.42	1.22	1.30
4	J	1	PVE	C4-C3	2.41	1.42	1.37
4	J	1	PVE	C3-C2	2.26	1.43	1.41
4	J	1	PVE	O24-C22	-2.26	1.23	1.30
4	I	1	PVE	C8-C9	2.20	1.44	1.40
4	I	1	PVE	C3-C2	2.19	1.43	1.41
4	J	1	PVE	O26-C7	-2.19	1.31	1.36
4	K	1	PVE	C12-N11	2.03	1.49	1.45
4	J	1	PVE	C21-C22	2.02	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	PVE	C15-C14-N1	24.65	144.00	111.53
4	I	1	PVE	C15-C14-N1	23.83	142.91	111.53
4	K	1	PVE	C15-C14-N1	23.55	142.55	111.53

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	I	1	PVE	C14
4	J	1	PVE	C14
4	K	1	PVE	C14

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	PVE	C20-C18-N17-C3
4	J	1	PVE	C20-C18-N17-C3
4	K	1	PVE	C20-C18-N17-C3
4	K	1	PVE	C13-C14-C15-O16
4	I	1	PVE	O19-C18-N17-C3
4	K	1	PVE	O19-C18-N17-C3
4	J	1	PVE	O19-C18-N17-C3
4	J	1	PVE	C18-C20-C21-C22
4	K	1	PVE	C18-C20-C21-C22
4	I	1	PVE	C18-C20-C21-C22
4	J	1	PVE	O19-C18-C20-C21
4	J	1	PVE	N17-C18-C20-C21
4	I	1	PVE	O19-C18-C20-C21
4	I	1	PVE	N17-C18-C20-C21
4	K	1	PVE	O19-C18-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	1	PVE	C20-C21-C22-O23
4	K	1	PVE	C20-C21-C22-O24
4	I	1	PVE	C20-C21-C22-O24
4	K	1	PVE	C20-C21-C22-O23
4	J	1	PVE	C20-C21-C22-O24
4	K	1	PVE	N17-C18-C20-C21
4	J	1	PVE	C20-C21-C22-O23

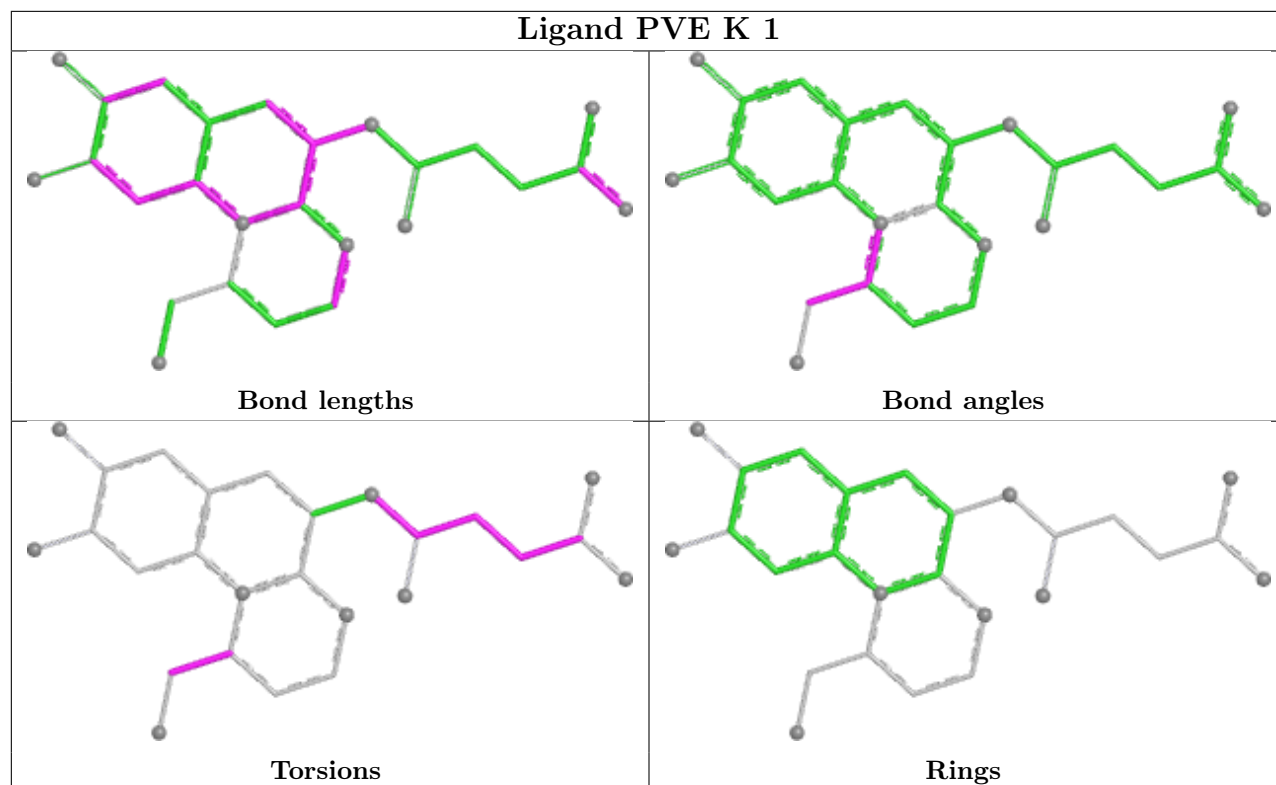
There are no ring outliers.

4 monomers are involved in 7 short contacts:

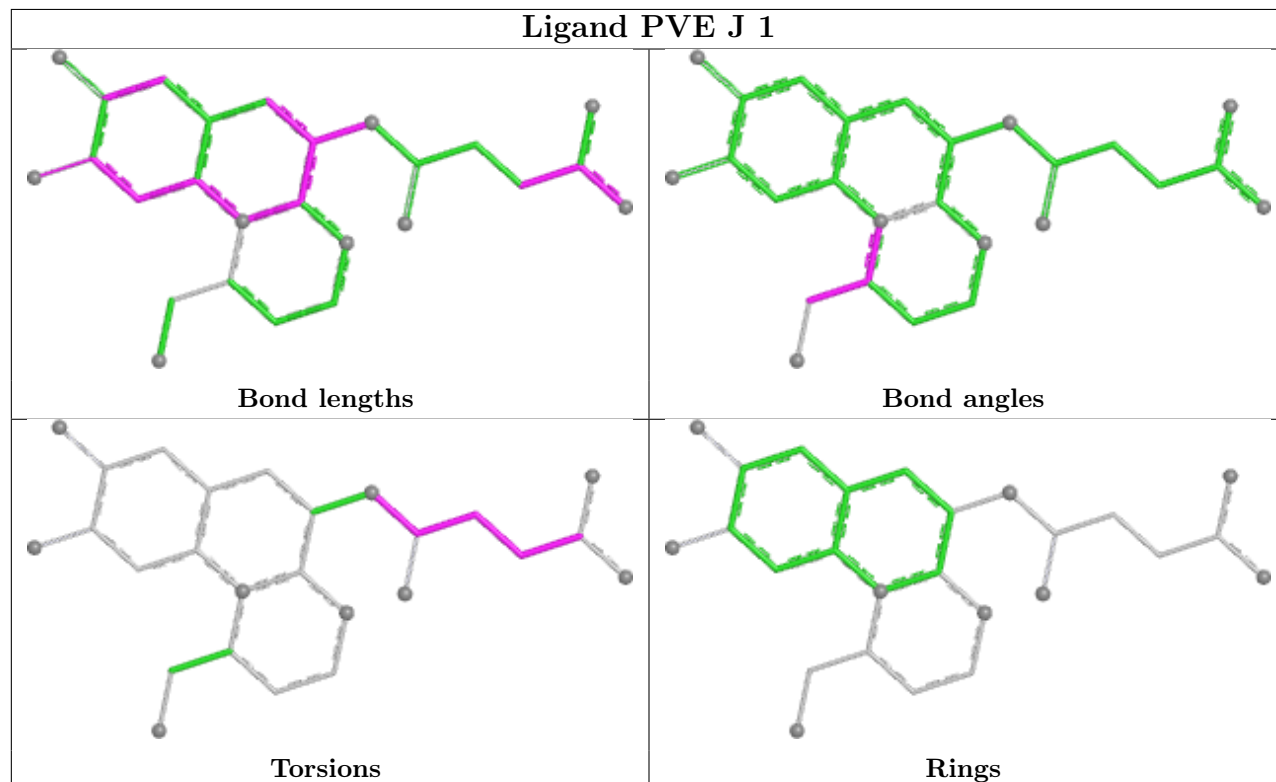
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2002	SO4	2	0
4	K	1	PVE	1	0
4	J	1	PVE	3	0
4	I	1	PVE	1	0

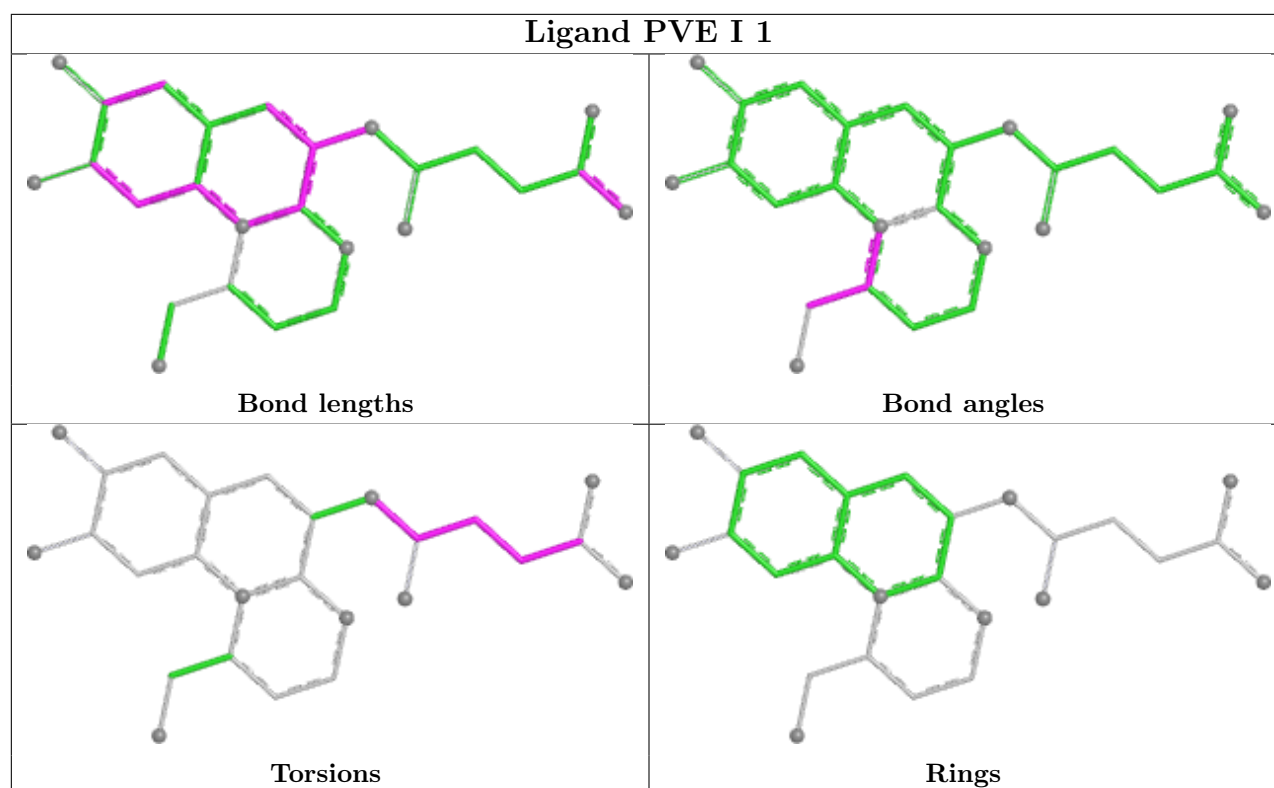
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PVE K 1



Ligand PVE J 1





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	675/687 (98%)	-0.16	3 (0%) 88 70	9, 41, 69, 111	0
1	B	675/687 (98%)	-0.21	1 (0%) 92 85	9, 41, 70, 111	0
1	C	675/687 (98%)	-0.16	3 (0%) 88 70	9, 41, 70, 118	0
2	I	4/8 (50%)	-0.11	0 100 100	56, 62, 63, 84	0
2	J	4/8 (50%)	0.02	0 100 100	65, 71, 72, 83	0
2	K	4/8 (50%)	-0.13	0 100 100	61, 66, 69, 95	0
All	All	2037/2085 (97%)	-0.18	7 (0%) 90 75	9, 41, 70, 118	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	THR	2.9
1	C	700	SER	2.8
1	A	557	THR	2.4
1	C	129	ALA	2.2
1	C	132	ILE	2.2
1	A	132	ILE	2.2
1	B	137	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FHO	I	5	11/12	0.61	0.18	66,77,89,90	0
2	DSN	K	4	6/7	0.68	0.15	87,89,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FHO	K	5	11/12	0.75	0.14	75,85,96,96	0
2	DSN	J	4	6/7	0.80	0.11	78,79,80,80	0
2	FHO	J	5	11/12	0.81	0.12	73,79,87,88	0
2	DSN	J	2	6/7	0.81	0.14	79,82,84,84	0
2	DSN	K	2	6/7	0.82	0.12	92,93,93,93	0
2	DSN	I	4	6/7	0.83	0.15	76,77,78,78	0
2	FHO	J	7	11/12	0.85	0.16	41,48,61,63	0
2	FHO	K	7	11/12	0.88	0.14	35,43,60,61	0
2	FHO	I	7	11/12	0.89	0.13	29,37,53,55	0
2	DSN	I	2	6/7	0.92	0.12	81,84,85,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

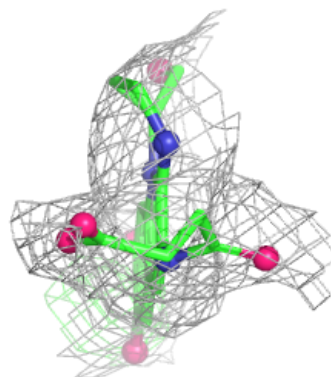
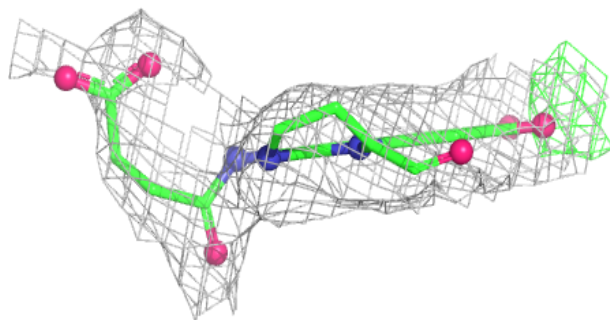
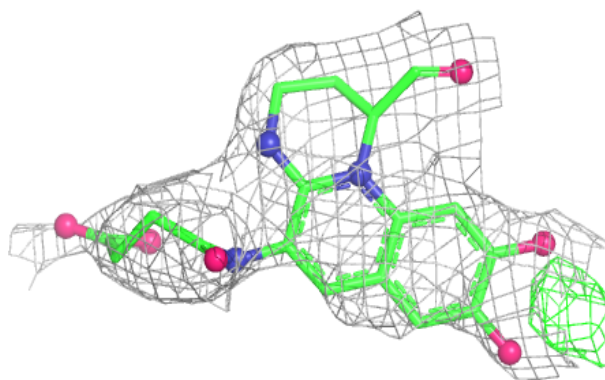
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PVE	K	1	26/27	0.83	0.15	86,88,91,92	0
4	PVE	J	1	26/27	0.85	0.16	81,86,92,92	0
4	PVE	I	1	26/27	0.86	0.14	82,85,91,91	0
3	SO4	C	2003	5/5	0.92	0.09	97,98,98,98	0
3	SO4	B	2002	5/5	0.94	0.06	67,68,68,68	0
3	SO4	A	2001	5/5	0.95	0.07	58,59,59,60	0

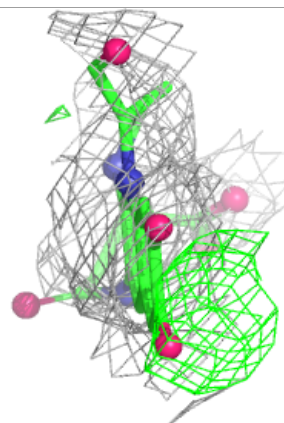
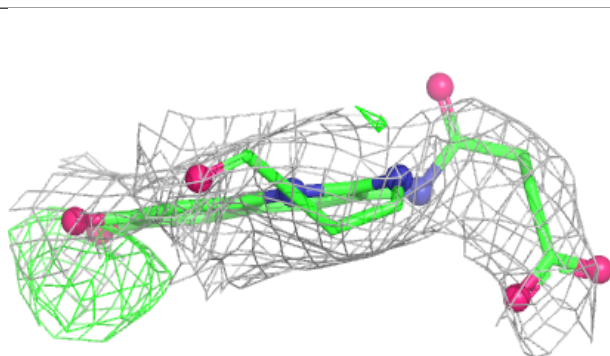
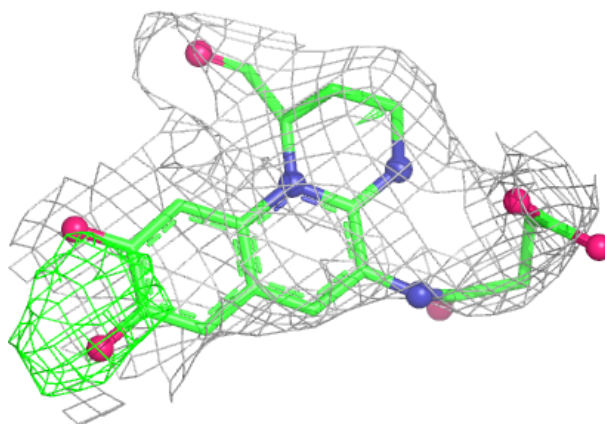
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

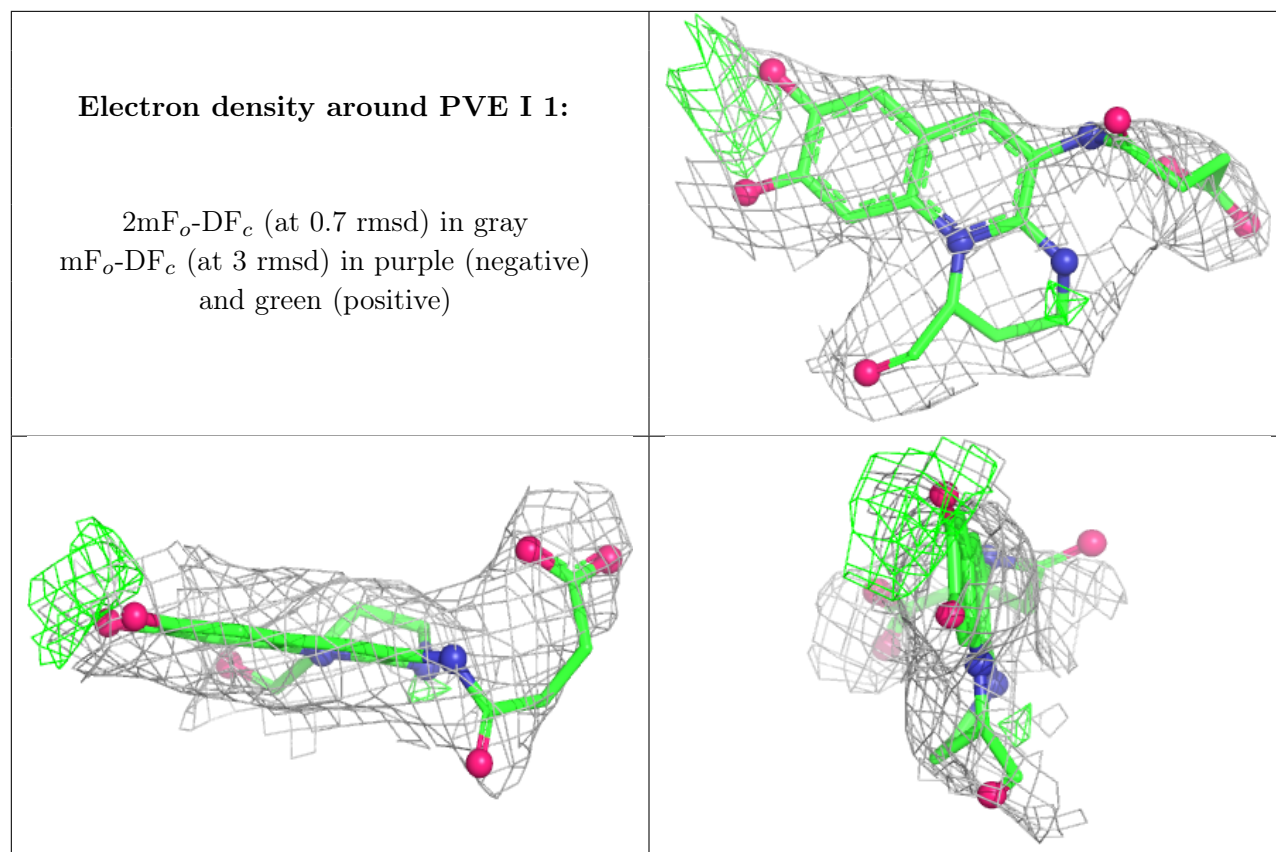
Electron density around PVE K 1:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PVE J 1:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.