



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:38 AM UTC

PDB ID : 7COQ / pdb_00007coq
Title : Hexameric Ring Complex of Engineered V1-ATPase bound to AMP-PNP:
A3(De)3_(ANP)1cat
Authors : Kosugi, T.; Tanabe, M.; Koga, N.
Deposited on : 2020-08-05
Resolution : 3.44 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:

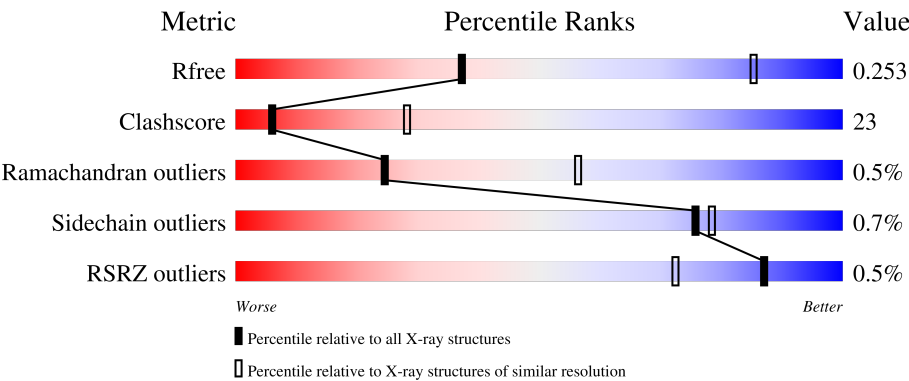
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	596	70%28%.
1	B	596	57%40%..
1	C	596	62%36%.
2	D	458	% 53%40%. 6%
2	E	458	% 50%46%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	458	% 51% 46% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24060 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	B	586	Total	C	N	O	S	0	0	0
			4562	2866	766	904	26			
1	C	584	Total	C	N	O	S	0	0	0
			4549	2858	764	901	26			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3369	2134	576	646	13			
2	E	449	Total	C	N	O	S	0	0	0
			3509	2224	601	670	14			
2	F	445	Total	C	N	O	S	0	0	0
			3477	2204	597	662	14			

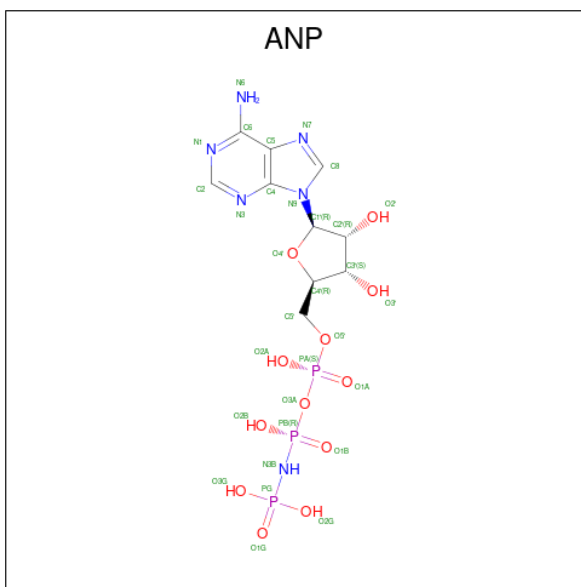
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLY	SER	engineered mutation	UNP Q08637
D	152	PRO	GLY	engineered mutation	UNP Q08637
D	153	PRO	SER	engineered mutation	UNP Q08637
D	155	ALA	LEU	engineered mutation	UNP Q08637
D	156	GLY	PRO	engineered mutation	UNP Q08637
D	157	LYS	HIS	engineered mutation	UNP Q08637
D	158	SER	LYS	engineered mutation	UNP Q08637
D	159	ALA	GLU	engineered mutation	UNP Q08637
D	248	GLU	THR	engineered mutation	UNP Q08637
D	339	SER	GLN	engineered mutation	UNP Q08637
E	151	GLY	SER	engineered mutation	UNP Q08637
E	152	PRO	GLY	engineered mutation	UNP Q08637
E	153	PRO	SER	engineered mutation	UNP Q08637
E	155	ALA	LEU	engineered mutation	UNP Q08637
E	156	GLY	PRO	engineered mutation	UNP Q08637
E	157	LYS	HIS	engineered mutation	UNP Q08637
E	158	SER	LYS	engineered mutation	UNP Q08637
E	159	ALA	GLU	engineered mutation	UNP Q08637
E	248	GLU	THR	engineered mutation	UNP Q08637
E	339	SER	GLN	engineered mutation	UNP Q08637
F	151	GLY	SER	engineered mutation	UNP Q08637
F	152	PRO	GLY	engineered mutation	UNP Q08637
F	153	PRO	SER	engineered mutation	UNP Q08637
F	155	ALA	LEU	engineered mutation	UNP Q08637
F	156	GLY	PRO	engineered mutation	UNP Q08637
F	157	LYS	HIS	engineered mutation	UNP Q08637
F	158	SER	LYS	engineered mutation	UNP Q08637
F	159	ALA	GLU	engineered mutation	UNP Q08637
F	248	GLU	THR	engineered mutation	UNP Q08637
F	339	SER	GLN	engineered mutation	UNP Q08637

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

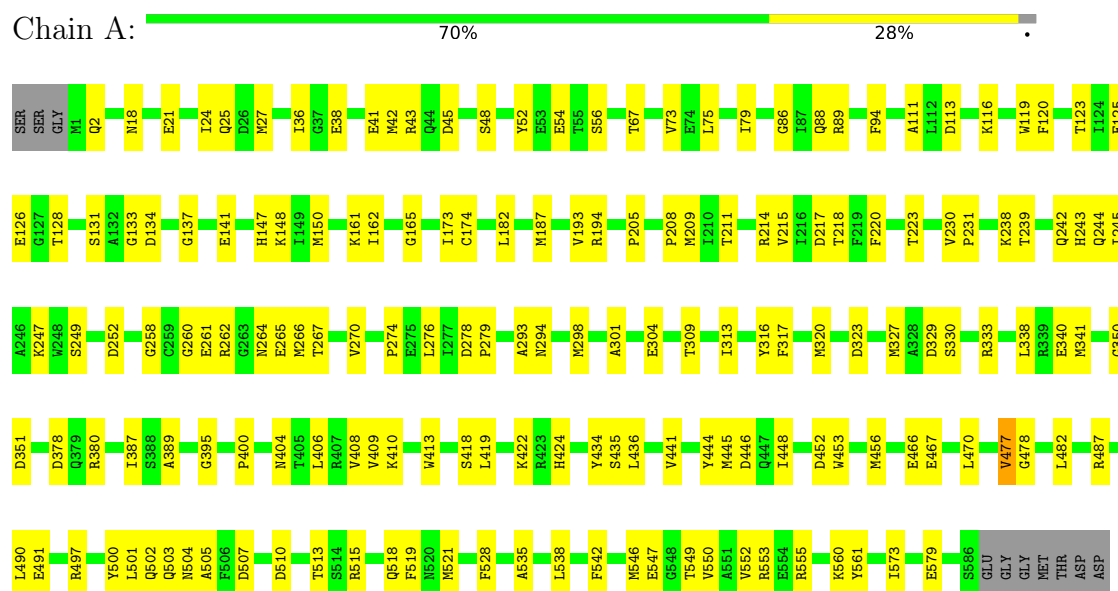


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

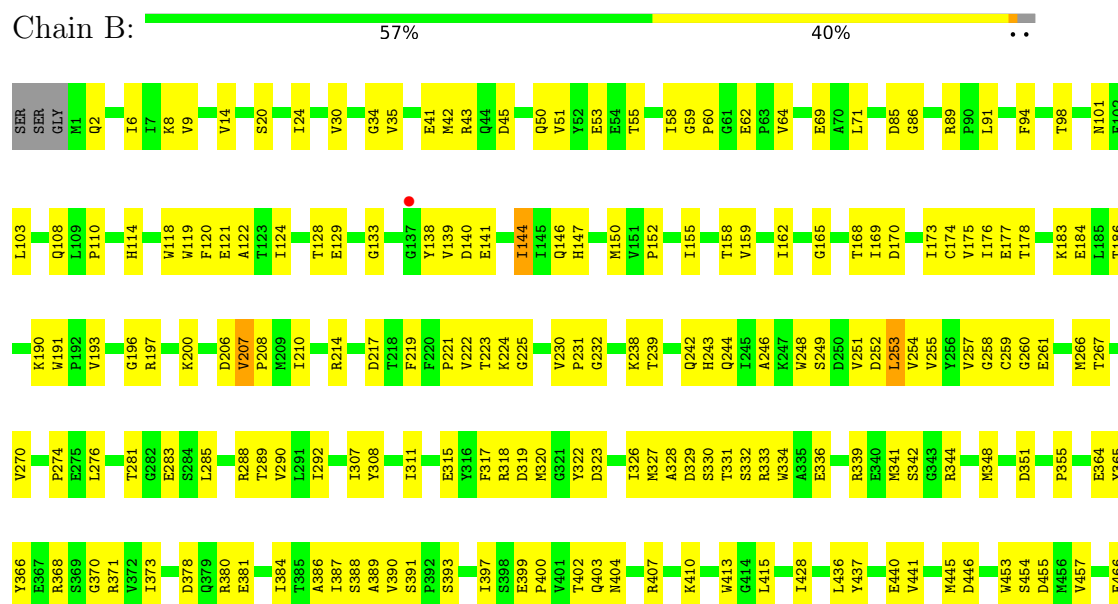
3 Residue-property plots

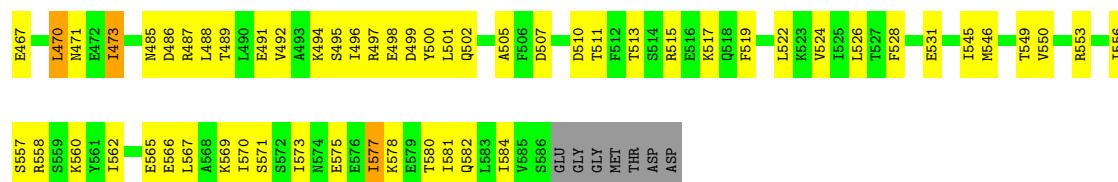
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: V-type sodium ATPase catalytic subunit A



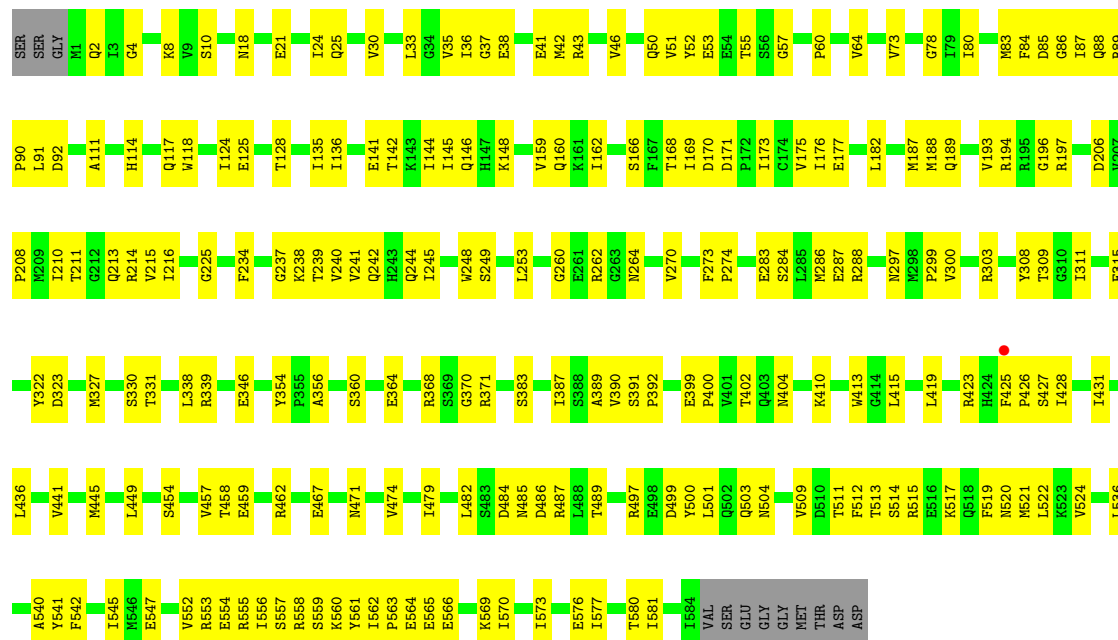
• Molecule 1: V-type sodium ATPase catalytic subunit A





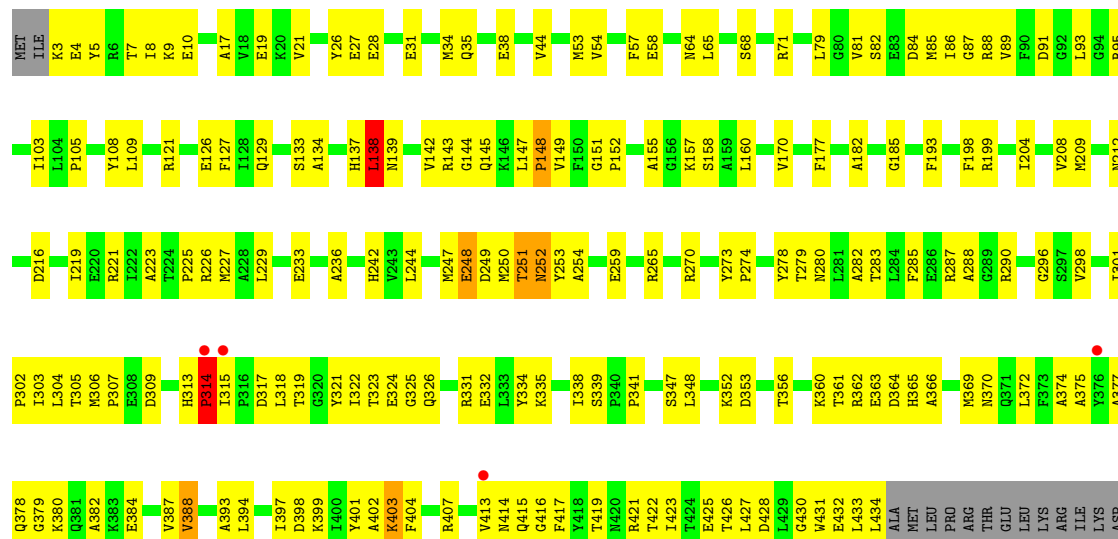
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C: 62% 36% .



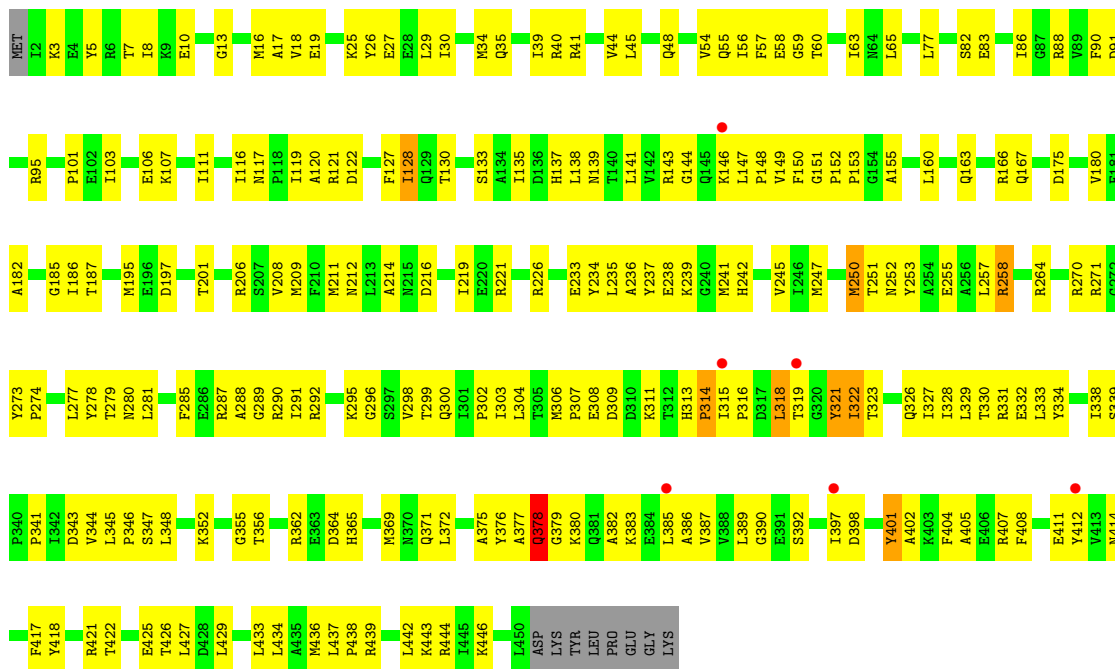
• Molecule 2: V-type sodium ATPase subunit B

Chain D: 53% 40% 6% .

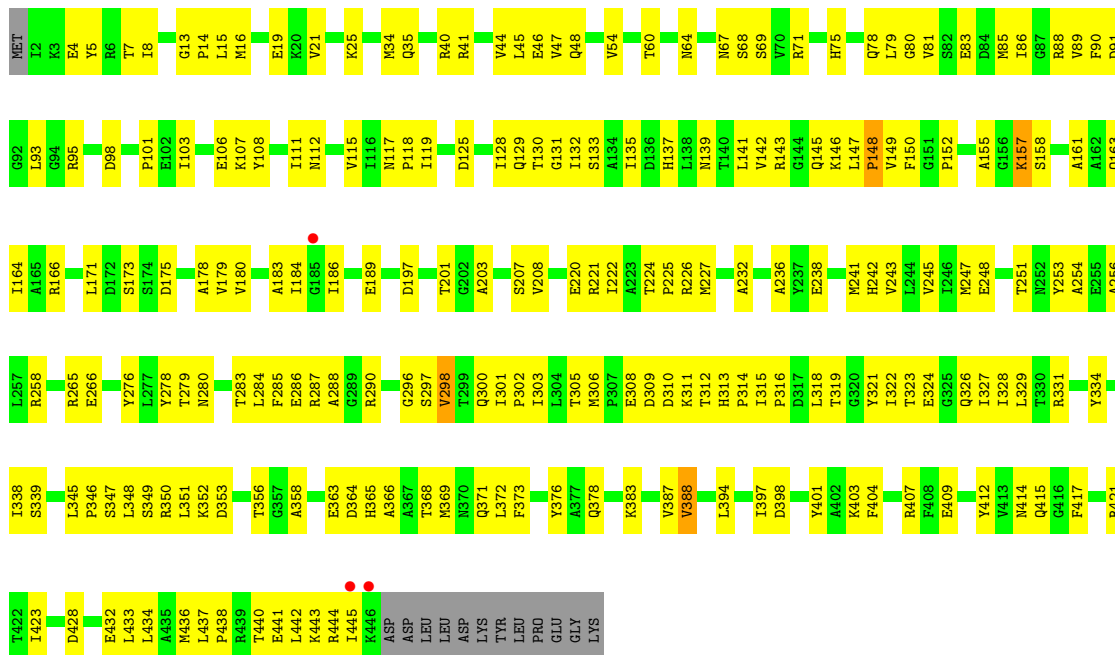


ASP
LEU
LEU
ASP
LYS
TYR
LEU
PRO
GLU
GLY
LYS

• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.44Å 124.49Å 131.34Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	46.34 – 3.44 46.34 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.34-3.44) 99.7 (46.34-3.44)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.18_3845)	Depositor
R, R_{free}	0.213 , 0.248 0.216 , 0.253	Depositor DCC
R_{free} test set	2383 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	101.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24060	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: ANP, MG

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	0.22	0/4638	0.46	0/6275
1	B	0.25	0/4638	0.51	1/6275 (0.0%)
1	C	0.27	0/4625	0.56	0/6257
2	D	0.45	2/3429 (0.1%)	0.76	9/4637 (0.2%)
2	E	0.40	2/3570 (0.1%)	0.71	7/4826 (0.1%)
2	F	0.34	1/3538 (0.0%)	0.63	0/4782
All	All	0.32	5/24438 (0.0%)	0.60	17/33052 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	252	ASN	CG-ND2	11.71	1.57	1.33
2	D	252	ASN	CA-C	-5.65	1.44	1.52
2	E	378	GLN	CD-NE2	-5.55	1.21	1.33
2	F	157	LYS	CG-CD	-5.17	1.36	1.52
2	E	322	ILE	CG1-CD1	-5.06	1.32	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	138	LEU	CB-CG-CD2	9.31	138.64	110.70
2	D	251	THR	CA-C-N	-8.83	106.12	121.66
2	D	251	THR	C-N-CA	-8.83	106.12	121.66
2	E	378	GLN	CB-CG-CD	-8.05	98.91	112.60
2	D	252	ASN	N-CA-CB	7.13	121.56	110.44
2	D	403	LYS	CB-CG-CD	7.08	127.58	111.30
2	D	248	GLU	CA-C-N	6.68	133.02	122.93
2	D	248	GLU	C-N-CA	6.68	133.02	122.93
2	D	314	PRO	CA-N-CD	-6.13	103.42	112.00
1	B	253	LEU	CB-CG-CD1	-5.86	93.12	110.70
2	D	252	ASN	N-CA-C	-5.84	105.99	113.23
2	E	321	TYR	CA-CB-CG	-5.48	104.03	113.90
2	E	258	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	E	258	ARG	CB-CG-CD	-5.45	98.77	111.30
2	E	314	PRO	CA-C-N	5.20	123.52	120.24
2	E	314	PRO	C-N-CA	5.20	123.52	120.24
2	E	318	LEU	CA-CB-CG	-5.07	98.57	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	363	GLU	Peptide
2	E	378	GLN	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4562	0	4528	127	2
1	B	4562	0	4528	213	1
1	C	4549	0	4513	184	0
2	D	3369	0	3377	188	0
2	E	3509	0	3537	235	1
2	F	3477	0	3507	190	0
3	C	1	0	0	0	0
4	C	31	0	13	8	0
All	All	24060	0	24003	1090	2

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 23.

All (1090) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:LEU:HB3	2:E:338:ILE:HD11	1.30	1.12
1:B:403:GLN:NE2	2:F:308:GLU:OE2	1.87	1.06
2:D:185:GLY:O	2:D:252:ASN:ND2	1.96	0.98
1:B:470:LEU:HD23	1:B:470:LEU:H	1.30	0.94
2:E:251:THR:HG23	2:E:304:LEU:HB2	1.49	0.94
2:D:307:PRO:HG3	2:D:313:HIS:HB2	1.48	0.94
2:D:157:LYS:NZ	2:D:305:THR:OG1	2.02	0.93
1:B:281:THR:HG23	1:B:283:GLU:H	1.37	0.89
2:D:177:PHE:HE2	2:D:244:LEU:HB2	1.39	0.88
1:C:426:PRO:HG3	1:C:503:GLN:H	1.39	0.88
1:B:122:ALA:HB1	1:B:162:ILE:HD12	1.55	0.86
2:E:285:PHE:HD2	2:E:322:ILE:CD1	1.89	0.86
2:D:382:ALA:HB2	2:D:401:TYR:HB3	1.58	0.86
2:E:389:LEU:HD12	2:E:392:SER:HB2	1.57	0.85
2:F:131:GLY:O	2:F:415:GLN:NE2	2.09	0.85
1:C:521:MET:HE2	1:C:556:ILE:HB	1.58	0.84
2:D:251:THR:HG23	2:D:314:PRO:HG2	1.59	0.84
2:E:278:TYR:HB3	2:E:318:LEU:HD21	1.60	0.84
1:A:351:ASP:OD1	2:E:258:ARG:NH2	2.10	0.83
2:E:55:GLN:OE1	2:E:264:ARG:NH1	2.11	0.83
1:A:549:THR:HG23	1:A:553:ARG:HD3	1.62	0.82
2:E:270:ARG:NH1	2:E:278:TYR:OH	2.12	0.82
2:E:328:ILE:HG12	2:E:347:SER:HB3	1.58	0.81
1:B:528:PHE:HA	1:B:577:ILE:HD13	1.62	0.80
1:B:232:GLY:HA3	1:B:238:LYS:HD2	1.63	0.80
1:B:214:ARG:NH2	1:B:510:ASP:OD1	2.14	0.80
1:C:160:GLN:NE2	1:C:177:GLU:OE1	2.15	0.80
2:E:437:LEU:HD22	2:E:438:PRO:HD2	1.63	0.80
2:E:379:GLY:HA3	2:E:405:ALA:HB2	1.63	0.80
2:D:382:ALA:CB	2:D:401:TYR:HB3	2.12	0.80
2:E:195:MET:HE2	2:E:211:MET:HG3	1.64	0.79
2:F:313:HIS:CD2	2:F:316:PRO:HD2	2.17	0.79
2:E:412:TYR:HA	2:E:421:ARG:HH12	1.47	0.79
2:E:13:GLY:O	2:E:60:THR:OG1	2.01	0.79
2:E:338:ILE:HG22	2:E:414:ASN:HB2	1.65	0.79
1:B:144:ILE:HD11	1:B:281:THR:HG21	1.66	0.79
1:B:467:GLU:O	1:B:471:ASN:ND2	2.15	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:PHE:CE1	2:D:433:LEU:HB3	2.18	0.78
2:E:365:HIS:HB2	2:E:427:LEU:HD21	1.65	0.78
2:F:34:MET:SD	2:F:40:ARG:NH1	2.57	0.78
2:D:365:HIS:HB2	2:D:427:LEU:HD11	1.66	0.78
2:F:288:ALA:HB2	2:F:300:GLN:HG3	1.65	0.78
1:C:210:ILE:HD11	1:C:515:ARG:HH21	1.49	0.78
2:F:4:GLU:OE2	2:F:71:ARG:NH2	2.17	0.77
2:F:356:THR:OG1	2:F:365:HIS:ND1	2.16	0.77
2:F:183:ALA:HB1	2:F:186:ILE:HD11	1.65	0.77
2:D:399:LYS:HA	2:D:402:ALA:HB3	1.67	0.77
1:B:206:ASP:OD1	1:B:371:ARG:NH1	2.18	0.76
1:C:208:PRO:HG3	1:C:441:VAL:HG22	1.68	0.76
1:B:566:GLU:OE1	1:B:569:LYS:NZ	2.18	0.76
1:A:133:GLY:O	1:A:380:ARG:NH2	2.18	0.76
2:E:166:ARG:O	2:E:206:ARG:NH1	2.17	0.76
1:A:214:ARG:NH2	1:A:510:ASP:OD1	2.16	0.76
1:C:542:PHE:HA	1:C:545:ILE:HB	1.67	0.76
1:B:159:VAL:HA	1:B:176:ILE:HG22	1.68	0.75
2:D:356:THR:HG23	2:D:365:HIS:CD2	2.21	0.75
1:B:507:ASP:HB3	1:B:510:ASP:HB3	1.68	0.75
1:B:545:ILE:O	1:B:549:THR:OG1	2.04	0.75
2:D:143:ARG:NH2	2:D:170:VAL:HG21	2.02	0.75
2:F:146:LYS:HE3	2:F:288:ALA:HB3	1.68	0.75
2:F:89:VAL:HB	2:F:98:ASP:HB3	1.68	0.75
1:B:549:THR:HG22	1:B:553:ARG:HG3	1.68	0.75
2:E:411:GLU:O	2:E:421:ARG:NH2	2.20	0.75
1:C:390:VAL:HG21	1:C:402:THR:HG22	1.68	0.74
2:E:285:PHE:HD2	2:E:322:ILE:HD13	1.51	0.74
2:E:322:ILE:HD12	2:E:322:ILE:C	2.12	0.74
2:F:141:LEU:HD11	2:F:301:ILE:HD11	1.68	0.74
2:E:160:LEU:O	2:E:163:GLN:HB3	1.88	0.74
2:E:285:PHE:CD2	2:E:322:ILE:HD11	2.23	0.73
1:B:253:LEU:HD11	1:B:317:PHE:CD2	2.24	0.73
1:C:238:LYS:NZ	4:C:602:ANP:O1B	2.21	0.73
2:D:199:ARG:HG2	2:D:204:ILE:HD12	1.70	0.73
1:B:85:ASP:OD1	1:B:86:GLY:N	2.21	0.73
1:C:245:ILE:HD11	1:C:387:ILE:HG13	1.71	0.73
2:F:137:HIS:HE2	2:F:368:THR:HG1	0.73	0.73
2:E:429:LEU:O	2:E:433:LEU:HB2	1.89	0.73
1:B:522:LEU:HG	1:B:526:LEU:HD11	1.70	0.72
1:C:560:LYS:HE2	1:C:560:LYS:HA	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:SER:OG	2:F:421:ARG:NH1	2.23	0.72
2:F:254:ALA:HB3	2:F:315:ILE:HD11	1.72	0.72
2:D:254:ALA:HB3	2:D:314:PRO:HG3	1.71	0.72
2:F:137:HIS:ND1	2:F:412:TYR:OH	2.23	0.72
2:F:401:TYR:OH	2:F:441:GLU:HG2	1.90	0.72
2:E:313:HIS:HB3	2:E:314:PRO:HD2	1.71	0.72
1:B:155:ILE:HD11	1:B:183:LYS:HG3	1.71	0.72
2:E:375:ALA:HA	2:E:378:GLN:OE1	1.88	0.72
2:F:338:ILE:HG13	2:F:414:ASN:HB3	1.72	0.72
1:A:258:GLY:HA2	1:A:329:ASP:O	1.90	0.71
2:E:146:LYS:HE3	2:E:302:PRO:HG3	1.71	0.71
1:B:9:VAL:HG23	1:B:14:VAL:HG22	1.71	0.71
1:C:400:PRO:O	1:C:404:ASN:ND2	2.18	0.71
2:D:380:LYS:HA	2:D:384:GLU:HB2	1.72	0.71
1:C:264:ASN:ND2	2:F:324:GLU:OE2	2.22	0.71
1:C:425:PHE:HB3	4:C:602:ANP:C5	2.20	0.71
2:E:86:ILE:HA	2:E:208:VAL:HG23	1.72	0.71
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.08	0.71
1:B:168:THR:HG23	1:B:170:ASP:H	1.54	0.71
2:F:44:VAL:HG22	2:F:54:VAL:HG12	1.72	0.71
1:C:330:SER:H	1:C:389:ALA:HB3	1.55	0.71
2:D:147:LEU:O	2:D:301:ILE:HA	1.90	0.71
2:F:64:ASN:OD1	2:F:67:ASN:ND2	2.23	0.71
2:F:434:LEU:HD12	2:F:437:LEU:HD23	1.71	0.71
1:C:536:LEU:HA	1:C:540:ALA:HB3	1.71	0.71
2:E:151:GLY:O	2:E:306:MET:N	2.23	0.71
1:B:244:GLN:OE1	1:B:248:TRP:NE1	2.23	0.70
2:F:306:MET:HG3	2:F:316:PRO:HG3	1.73	0.70
2:D:198:PHE:HB3	2:D:204:ILE:HG13	1.73	0.70
2:F:184:ILE:HD11	2:F:225:PRO:HD3	1.73	0.70
1:A:238:LYS:NZ	1:A:329:ASP:OD2	2.22	0.70
1:A:445:MET:HE2	1:A:445:MET:HA	1.74	0.70
2:D:315:ILE:HB	2:D:318:LEU:HB2	1.72	0.70
1:B:207:VAL:HG13	1:B:224:LYS:HB2	1.72	0.70
1:C:297:ASN:HD21	2:F:286:GLU:HB3	1.57	0.70
2:E:107:LYS:NZ	2:E:238:GLU:OE1	2.16	0.70
1:C:146:GLN:O	1:C:322:TYR:OH	2.09	0.70
1:C:214:ARG:HG3	1:C:503:GLN:OE1	1.91	0.70
1:C:399:GLU:OE1	1:C:402:THR:HG23	1.92	0.70
2:D:393:ALA:O	2:D:394:LEU:HG	1.92	0.70
2:D:148:PRO:HD2	2:D:326:GLN:HA	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:146:LYS:HD3	2:E:300:GLN:HG3	1.73	0.70
2:F:112:ASN:O	2:F:287:ARG:NH1	2.25	0.70
1:B:524:VAL:HG11	1:B:573:ILE:HD12	1.74	0.69
1:C:262:ARG:NH1	2:F:323:THR:O	2.25	0.69
1:B:242:GLN:NE2	1:B:329:ASP:OD1	2.24	0.69
2:D:352:LYS:HD2	2:D:369:MET:HE1	1.75	0.69
2:E:150:PHE:CE2	2:E:304:LEU:HD11	2.28	0.69
2:E:285:PHE:CD2	2:E:322:ILE:CD1	2.75	0.69
2:E:386:ALA:HA	2:E:389:LEU:HB3	1.73	0.69
1:B:467:GLU:HA	1:B:470:LEU:HD11	1.72	0.69
2:E:141:LEU:HD21	2:E:299:THR:HG21	1.74	0.69
2:D:339:SER:H	2:D:414:ASN:CB	2.06	0.69
1:A:218:THR:OG1	1:A:500:TYR:OH	2.08	0.68
2:E:106:GLU:OE2	2:E:234:TYR:OH	2.09	0.68
1:A:555:ARG:HD3	1:A:573:ILE:HG12	1.76	0.68
2:E:383:LYS:O	2:E:387:VAL:HG23	1.93	0.68
2:F:125:ASP:OD1	2:F:290:ARG:NH1	2.26	0.68
2:D:221:ARG:O	2:D:225:PRO:HD2	1.93	0.68
2:D:248:GLU:OE1	2:D:249:ASP:HB2	1.93	0.68
2:D:339:SER:H	2:D:414:ASN:HB3	1.58	0.68
1:A:262:ARG:NH1	1:A:265:GLU:OE1	2.26	0.68
1:A:445:MET:HE1	1:A:515:ARG:HD3	1.75	0.68
1:B:214:ARG:HB3	1:B:500:TYR:CE1	2.28	0.68
2:D:319:THR:O	2:D:323:THR:HG23	1.93	0.68
2:E:285:PHE:HD2	2:E:322:ILE:HD11	1.59	0.68
2:F:221:ARG:O	2:F:225:PRO:HD2	1.94	0.68
1:B:466:GLU:C	1:B:470:LEU:HD21	2.18	0.68
1:C:514:SER:H	1:C:560:LYS:NZ	1.91	0.67
1:C:234:PHE:HB3	2:F:321:TYR:CD1	2.29	0.67
2:E:29:LEU:HD21	2:E:77:LEU:HD13	1.76	0.67
1:A:148:LYS:H	1:A:320:MET:HE1	1.59	0.67
1:C:410:LYS:HB3	1:C:436:LEU:HB2	1.77	0.67
1:C:78:GLY:N	1:C:141:GLU:OE1	2.17	0.67
2:D:428:ASP:HA	2:D:431:TRP:HD1	1.59	0.66
2:E:362:ARG:HB3	2:E:364:ASP:OD1	1.95	0.66
1:C:346:GLU:O	2:D:265:ARG:NH2	2.25	0.66
1:A:214:ARG:NH1	1:A:513:THR:OG1	2.28	0.66
1:B:246:ALA:HB2	1:B:327:MET:HE1	1.77	0.66
1:C:513:THR:HG23	1:C:517:LYS:HD2	1.77	0.66
2:D:177:PHE:CE2	2:D:244:LEU:HB2	2.27	0.66
1:C:552:VAL:HA	1:C:555:ARG:HD3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:OE1	1:B:190:LYS:NZ	2.28	0.66
1:B:147:HIS:CD2	1:B:320:MET:HE1	2.30	0.66
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.76	0.66
2:F:132:ILE:HB	2:F:135:ILE:HB	1.78	0.66
2:F:148:PRO:HD2	2:F:326:GLN:HA	1.77	0.66
1:B:2:GLN:HE22	1:B:20:SER:H	1.44	0.66
1:C:30:VAL:HG23	1:C:64:VAL:HG22	1.77	0.66
2:D:253:TYR:OH	2:D:280:ASN:OD1	2.14	0.65
1:A:491:GLU:HG2	1:A:546:MET:HE1	1.76	0.65
1:A:173:ILE:HD13	1:A:187:MET:HG2	1.77	0.65
4:C:602:ANP:O2G	4:C:602:ANP:O2B	2.15	0.65
2:E:371:GLN:OE1	2:E:443:LYS:N	2.17	0.65
2:F:4:GLU:OE1	2:F:69:SER:OG	2.14	0.65
1:B:129:GLU:N	1:B:129:GLU:OE1	2.27	0.65
1:B:528:PHE:HD1	1:B:577:ILE:HD12	1.61	0.65
1:B:176:ILE:HD11	1:B:183:LYS:HB2	1.77	0.65
1:C:114:HIS:ND1	1:C:170:ASP:OD1	2.20	0.65
1:C:297:ASN:HD22	2:F:115:VAL:HG13	1.61	0.65
2:E:137:HIS:HE1	2:E:372:LEU:HD23	1.61	0.65
1:B:85:ASP:OD2	1:B:89:ARG:NH2	2.29	0.65
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.77	0.65
2:F:394:LEU:HA	2:F:398:ASP:HB2	1.78	0.65
2:D:148:PRO:HB3	2:D:302:PRO:HG2	1.80	0.64
2:E:236:ALA:O	2:E:296:GLY:HA3	1.97	0.64
2:F:13:GLY:O	2:F:60:THR:OG1	2.13	0.64
1:B:366:TYR:OH	1:B:388:SER:OG	2.07	0.64
2:D:387:VAL:O	2:D:388:VAL:HG12	1.98	0.64
1:C:449:LEU:HD13	1:C:519:PHE:HD2	1.63	0.64
1:B:244:GLN:NE2	1:B:505:ALA:O	2.31	0.64
2:D:338:ILE:HA	2:D:414:ASN:HB3	1.80	0.64
2:D:138:LEU:HD22	2:D:139:ASN:H	1.63	0.64
2:D:398:ASP:O	2:D:401:TYR:HB2	1.98	0.64
2:E:40:ARG:NH1	2:E:59:GLY:O	2.29	0.64
2:F:179:VAL:O	2:F:207:SER:OG	2.13	0.64
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.79	0.63
1:C:262:ARG:NH2	4:C:602:ANP:O1G	2.31	0.63
1:C:499:ASP:OD1	1:C:553:ARG:HB3	1.98	0.63
1:C:10:SER:HB2	2:F:46:GLU:HG3	1.79	0.63
2:D:356:THR:HG22	2:D:366:ALA:HB2	1.79	0.63
2:E:251:THR:HG22	2:E:315:ILE:HD12	1.79	0.63
2:E:137:HIS:CE1	2:E:372:LEU:HD23	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:332:GLU:OE2	2:E:332:GLU:N	2.29	0.63
2:F:143:ARG:HD3	2:F:242:HIS:CD2	2.33	0.63
1:B:307:ILE:HB	1:B:365:TYR:CE2	2.33	0.63
1:B:318:ARG:HD3	1:B:384:ILE:HG13	1.79	0.63
2:E:377:ALA:O	2:E:380:LYS:HB3	1.99	0.63
2:F:148:PRO:HG3	2:F:323:THR:HG21	1.80	0.63
1:B:62:GLU:OE2	2:E:25:LYS:NZ	2.31	0.63
1:C:426:PRO:HG3	1:C:503:GLN:N	2.11	0.63
2:F:353:ASP:HA	2:F:356:THR:HG22	1.80	0.63
2:E:10:GLU:HG2	2:E:17:ALA:HB3	1.81	0.63
1:A:504:ASN:OD1	1:A:507:ASP:N	2.31	0.62
1:B:30:VAL:HA	1:B:64:VAL:HG22	1.81	0.62
1:A:487:ARG:HG2	1:A:542:PHE:CE2	2.34	0.62
1:B:208:PRO:HA	1:B:223:THR:HA	1.79	0.62
2:E:7:THR:OG1	2:E:19:GLU:O	2.17	0.62
1:B:575:GLU:N	1:B:575:GLU:OE1	2.32	0.62
2:E:111:ILE:O	2:E:287:ARG:NH2	2.31	0.62
1:C:117:GLN:OE1	1:C:166:SER:OG	2.16	0.62
2:E:148:PRO:HB3	2:E:302:PRO:HG2	1.82	0.62
1:A:141:GLU:OE1	1:A:147:HIS:ND1	2.25	0.62
1:B:214:ARG:HB3	1:B:500:TYR:HE1	1.63	0.62
2:D:134:ALA:C	2:D:138:LEU:HD11	2.25	0.62
1:B:327:MET:HA	1:B:387:ILE:O	1.99	0.62
1:B:550:VAL:HG22	1:B:553:ARG:HH22	1.65	0.62
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.81	0.62
1:C:562:ILE:HG22	1:C:563:PRO:HD2	1.82	0.62
2:F:371:GLN:HE21	2:F:443:LYS:HG3	1.65	0.62
1:C:237:GLY:HA3	4:C:602:ANP:H2	1.80	0.61
1:C:467:GLU:CD	1:C:497:ARG:HH22	2.08	0.61
2:D:362:ARG:NH2	2:D:364:ASP:OD2	2.20	0.61
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.81	0.61
1:C:514:SER:OG	1:C:560:LYS:NZ	2.32	0.61
1:B:333:ARG:NH1	1:B:391:SER:OG	2.34	0.61
1:A:120:PHE:HE2	1:A:162:ILE:HD11	1.64	0.61
2:D:339:SER:HB2	2:D:417:PHE:CD1	2.35	0.61
2:F:313:HIS:HE2	2:F:315:ILE:HB	1.66	0.61
1:B:230:VAL:HG13	1:B:238:LYS:HZ1	1.66	0.61
1:B:437:TYR:OH	2:F:189:GLU:OE1	2.15	0.61
2:D:397:ILE:HA	2:D:399:LYS:HE3	1.82	0.61
2:D:404:PHE:HE1	2:D:433:LEU:HB3	1.61	0.60
1:B:399:GLU:O	1:B:403:GLN:HG2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:ALA:O	2:D:296:GLY:HA3	2.01	0.60
2:F:132:ILE:HA	2:F:415:GLN:NE2	2.16	0.60
2:F:166:ARG:NH1	2:F:197:ASP:OD2	2.35	0.60
1:A:266:MET:SD	1:A:293:ALA:HB1	2.41	0.60
2:D:212:ASN:HD21	2:D:216:ASP:HB2	1.66	0.60
2:F:339:SER:HB3	2:F:417:PHE:CE2	2.37	0.60
1:B:413:TRP:HB3	1:B:428:ILE:HD13	1.83	0.60
2:E:16:MET:HE1	2:E:56:ILE:HD11	1.83	0.60
2:E:185:GLY:O	2:E:252:ASN:ND2	2.35	0.60
2:E:330:THR:HB	2:E:333:LEU:HD13	1.82	0.60
2:F:86:ILE:HD12	2:F:86:ILE:H	1.67	0.60
1:B:495:SER:O	1:B:499:ASP:HB2	2.01	0.60
1:C:159:VAL:HG12	1:C:176:ILE:HD12	1.84	0.60
1:C:160:GLN:HB3	1:C:175:VAL:HG13	1.83	0.60
2:E:41:ARG:H	2:E:41:ARG:HD2	1.67	0.60
2:F:155:ALA:HB3	2:F:334:TYR:OH	2.01	0.60
1:B:565:GLU:N	1:B:565:GLU:OE1	2.33	0.60
2:E:333:LEU:CB	2:E:338:ILE:HD11	2.19	0.60
2:F:288:ALA:HA	2:F:298:VAL:HG13	1.84	0.59
1:B:257:VAL:HG12	1:B:292:ILE:HB	1.85	0.59
1:B:348:MET:HE3	2:F:265:ARG:HA	1.83	0.59
2:D:121:ARG:NH1	2:D:288:ALA:O	2.35	0.59
2:E:57:PHE:HD1	2:E:219:ILE:HD12	1.66	0.59
1:C:283:GLU:HG2	1:C:287:GLU:HG3	1.83	0.59
2:D:226:ARG:NH2	2:D:253:TYR:OH	2.36	0.59
2:F:313:HIS:ND1	2:F:314:PRO:HD2	2.18	0.59
1:C:2:GLN:NE2	1:C:18:ASN:OD1	2.34	0.59
2:E:163:GLN:NE2	2:E:417:PHE:O	2.34	0.59
2:E:247:MET:SD	2:E:250:MET:HE2	2.42	0.59
2:F:387:VAL:O	2:F:388:VAL:HG22	2.03	0.59
1:A:294:ASN:HB3	1:A:298:MET:HE2	1.83	0.59
2:F:221:ARG:HD3	2:F:256:ALA:HB2	1.85	0.59
2:F:345:LEU:HB2	2:F:346:PRO:HD3	1.84	0.59
1:C:573:ILE:O	1:C:577:ILE:HG13	2.02	0.59
2:E:226:ARG:NH2	2:E:280:ASN:OD1	2.35	0.59
2:D:422:THR:HB	2:D:425:GLU:HG3	1.83	0.59
1:B:400:PRO:HA	1:B:403:GLN:HG3	1.85	0.59
1:C:517:LYS:NZ	1:C:560:LYS:HB2	2.18	0.59
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.84	0.58
2:E:130:THR:HG21	2:E:135:ILE:HG21	1.85	0.58
2:E:401:TYR:CE1	2:E:437:LEU:HD21	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:OE2	1:A:43:ARG:NH1	2.35	0.58
1:B:50:GLN:NE2	1:B:341:MET:SD	2.68	0.58
2:F:376:TYR:OH	2:F:409:GLU:OE1	2.16	0.58
2:E:437:LEU:HD13	2:E:438:PRO:N	2.18	0.58
2:F:285:PHE:HE2	2:F:319:THR:HG23	1.69	0.58
2:E:401:TYR:CE1	2:E:437:LEU:HD11	2.39	0.58
2:E:408:PHE:HD2	2:E:433:LEU:HD23	1.66	0.58
2:F:131:GLY:HA2	2:F:421:ARG:O	2.02	0.58
2:D:382:ALA:O	2:D:394:LEU:HD22	2.02	0.58
2:E:313:HIS:HB3	2:E:314:PRO:CD	2.33	0.58
2:F:442:LEU:HD12	2:F:442:LEU:H	1.68	0.58
2:D:315:ILE:HD12	2:D:315:ILE:H	1.68	0.58
2:E:146:LYS:HE2	2:E:285:PHE:CG	2.39	0.58
1:A:546:MET:O	1:A:550:VAL:HG23	2.03	0.58
2:D:372:LEU:HA	2:D:375:ALA:HB3	1.85	0.58
2:E:352:LYS:O	2:E:356:THR:HG22	2.04	0.58
2:E:422:THR:O	2:E:426:THR:HG23	2.02	0.58
1:B:270:VAL:O	1:B:274:PRO:HD2	2.04	0.58
1:C:51:VAL:HG21	1:C:55:THR:CG2	2.34	0.58
2:D:309:ASP:N	2:D:309:ASP:OD1	2.34	0.58
2:F:371:GLN:NE2	2:F:443:LYS:HG3	2.19	0.58
1:A:79:ILE:HD11	1:A:313:ILE:HD13	1.85	0.58
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.19	0.58
1:B:446:ASP:OD1	1:B:453:TRP:N	2.37	0.57
1:C:300:VAL:HA	1:C:303:ARG:HG3	1.85	0.57
2:E:212:ASN:OD1	2:E:221:ARG:HA	2.03	0.57
1:A:528:PHE:HE2	1:A:549:THR:OG1	1.87	0.57
1:C:514:SER:H	1:C:560:LYS:HZ1	1.50	0.57
2:E:407:ARG:NE	2:E:411:GLU:OE2	2.29	0.57
2:F:428:ASP:O	2:F:432:GLU:HG3	2.03	0.57
1:B:214:ARG:NH2	1:B:560:LYS:HB2	2.19	0.57
2:E:116:ILE:HG21	2:E:121:ARG:HE	1.69	0.57
2:E:315:ILE:HG13	2:E:316:PRO:HD3	1.86	0.57
2:D:149:VAL:CG1	2:D:303:ILE:HG13	2.35	0.57
2:F:117:ASN:OD1	2:F:119:ILE:HG12	2.03	0.57
1:A:43:ARG:HG3	2:E:10:GLU:HB2	1.86	0.57
1:B:467:GLU:OE1	1:B:497:ARG:NH2	2.34	0.57
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.86	0.57
2:F:183:ALA:HB1	2:F:186:ILE:CD1	2.34	0.57
1:A:350:GLY:C	2:E:258:ARG:HH21	2.12	0.57
1:A:406:LEU:HA	1:A:409:VAL:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:HIS:CE1	2:D:369:MET:HA	2.39	0.57
1:B:128:THR:H	1:B:159:VAL:HG22	1.70	0.57
2:F:139:ASN:ND2	2:F:347:SER:HB3	2.20	0.57
1:B:147:HIS:HD2	1:B:320:MET:HE1	1.69	0.57
2:D:127:PHE:HA	2:D:142:VAL:HA	1.87	0.57
2:D:280:ASN:O	2:D:283:THR:OG1	2.22	0.57
2:F:145:GLN:HG3	2:F:351:LEU:HD12	1.87	0.57
2:F:147:LEU:O	2:F:301:ILE:HA	2.03	0.57
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.70	0.56
1:C:415:LEU:HB3	1:C:427:SER:OG	2.05	0.56
1:B:571:SER:O	1:B:575:GLU:OE1	2.23	0.56
2:D:58:GLU:OE2	2:D:58:GLU:N	2.36	0.56
2:D:338:ILE:HA	2:D:414:ASN:HD22	1.70	0.56
2:E:57:PHE:CD1	2:E:219:ILE:HD12	2.40	0.56
2:F:157:LYS:HE3	2:F:305:THR:HG21	1.87	0.56
2:D:270:ARG:NH1	2:D:270:ARG:HB2	2.19	0.56
2:D:338:ILE:HG12	2:D:341:PRO:HA	1.86	0.56
2:F:175:ASP:N	2:F:175:ASP:OD1	2.37	0.56
1:C:315:GLU:OE2	1:C:368:ARG:NE	2.39	0.56
1:C:471:ASN:O	1:C:474:VAL:HG12	2.05	0.56
1:C:484:ASP:HB3	1:C:542:PHE:HE2	1.70	0.56
2:E:364:ASP:OD1	2:E:364:ASP:N	2.37	0.56
2:F:150:PHE:HB3	2:F:306:MET:SD	2.45	0.56
1:A:205:PRO:C	1:A:223:THR:HG21	2.31	0.56
2:D:334:TYR:HA	2:D:338:ILE:HG23	1.85	0.56
2:F:88:ARG:NH1	2:F:101:PRO:O	2.39	0.56
1:A:86:GLY:N	1:A:294:ASN:OD1	2.39	0.56
2:E:152:PRO:HB2	2:E:153:PRO:HD2	1.88	0.56
2:E:153:PRO:HG2	2:E:331:ARG:HH12	1.71	0.56
1:C:273:PHE:HB3	1:C:286:MET:HG2	1.88	0.56
2:D:126:GLU:OE1	2:D:126:GLU:N	2.33	0.56
2:D:31:GLU:OE1	2:D:71:ARG:NH1	2.35	0.56
2:E:437:LEU:HD13	2:E:438:PRO:CD	2.36	0.56
1:B:8:LYS:HB2	2:E:48:GLN:HB2	1.87	0.56
1:B:124:ILE:O	1:B:162:ILE:HD11	2.06	0.56
1:C:482:LEU:O	1:C:487:ARG:NH2	2.39	0.56
1:B:24:ILE:HD11	1:B:42:MET:HB3	1.88	0.55
1:B:333:ARG:NH1	1:B:391:SER:HG	2.04	0.55
2:D:82:SER:OG	2:D:84:ASP:OD2	2.24	0.55
2:E:378:GLN:NE2	2:E:401:TYR:CZ	2.74	0.55
1:C:485:ASN:O	1:C:489:THR:OG1	2.18	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:ASP:O	2:D:432:GLU:HG2	2.06	0.55
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.39	0.55
1:B:403:GLN:HE22	2:F:308:GLU:CD	2.03	0.55
2:E:386:ALA:HA	2:E:389:LEU:CB	2.37	0.55
1:C:520:ASN:O	1:C:524:VAL:HG13	2.07	0.55
2:E:128:ILE:HG13	2:E:143:ARG:HG3	1.88	0.55
2:D:34:MET:HE2	2:D:38:GLU:HB3	1.88	0.55
2:D:144:GLY:HA2	2:D:298:VAL:O	2.06	0.55
2:E:133:SER:HB3	2:E:412:TYR:CE2	2.41	0.55
2:F:251:THR:CG2	2:F:315:ILE:HG21	2.37	0.55
2:E:122:ASP:N	2:E:290:ARG:O	2.27	0.55
1:B:251:VAL:O	1:B:288:ARG:NH1	2.40	0.55
1:B:365:TYR:HD1	1:B:366:TYR:CD1	2.24	0.55
1:C:264:ASN:HD21	2:F:146:LYS:NZ	2.05	0.55
2:D:133:SER:CB	2:D:421:ARG:HH11	2.20	0.55
2:D:364:ASP:OD1	2:D:364:ASP:N	2.37	0.55
1:A:482:LEU:HD23	1:A:482:LEU:H	1.72	0.54
1:A:209:MET:HE3	1:A:211:THR:HG22	1.89	0.54
1:B:341:MET:HA	1:B:344:ARG:HD3	1.90	0.54
2:E:304:LEU:HD12	2:E:304:LEU:C	2.32	0.54
1:B:581:ILE:HG13	1:B:582:GLN:N	2.22	0.54
1:C:33:LEU:H	1:C:33:LEU:HD12	1.71	0.54
2:F:313:HIS:NE2	2:F:315:ILE:HB	2.21	0.54
1:A:446:ASP:OD1	1:A:453:TRP:N	2.39	0.54
1:A:560:LYS:HG2	1:A:561:TYR:CD1	2.43	0.54
1:C:211:THR:HG23	1:C:245:ILE:HG22	1.88	0.54
2:D:87:GLY:HA2	2:D:204:ILE:O	2.07	0.54
2:D:133:SER:OG	2:D:421:ARG:NH1	2.40	0.54
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.88	0.54
1:A:211:THR:OG1	1:A:217:ASP:OD1	2.18	0.54
1:B:378:ASP:HB2	1:B:380:ARG:HD2	1.89	0.54
2:E:147:LEU:HD11	2:E:327:ILE:HG13	1.89	0.54
1:B:110:PRO:HB3	1:B:114:HIS:CE1	2.43	0.54
1:B:281:THR:HG23	1:B:283:GLU:N	2.14	0.54
2:F:403:LYS:HD2	2:F:403:LYS:N	2.23	0.54
2:F:254:ALA:HB3	2:F:315:ILE:CD1	2.35	0.54
1:B:410:LYS:HE3	1:B:437:TYR:OH	2.08	0.54
1:B:158:THR:HG23	1:B:177:GLU:HB3	1.90	0.54
1:B:415:LEU:HD23	1:B:428:ILE:HG12	1.89	0.54
1:C:214:ARG:HD3	1:C:513:THR:HG21	1.90	0.54
2:D:282:ALA:HB2	2:D:322:ILE:HD13	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:OE2	1:C:194:ARG:NH2	2.41	0.53
2:D:127:PHE:HE1	2:D:360:LYS:O	1.90	0.53
2:E:216:ASP:O	2:E:221:ARG:NH1	2.41	0.53
2:E:233:GLU:OE2	2:E:287:ARG:HG2	2.07	0.53
1:B:494:LYS:O	1:B:498:GLU:HB2	2.08	0.53
2:E:285:PHE:CE2	2:E:322:ILE:HD11	2.44	0.53
1:B:221:PRO:HB2	1:B:441:VAL:HG21	1.90	0.53
1:B:244:GLN:NE2	1:B:505:ALA:HB1	2.22	0.53
1:B:410:LYS:HB3	1:B:436:LEU:HB3	1.90	0.53
2:D:382:ALA:HB1	2:D:401:TYR:C	2.32	0.53
2:E:345:LEU:HD23	2:E:346:PRO:HD3	1.90	0.53
1:C:53:GLU:HA	1:C:299:PRO:HG2	1.91	0.53
1:C:85:ASP:OD1	1:C:86:GLY:N	2.41	0.53
1:C:169:ILE:HG22	1:C:188:MET:HB2	1.91	0.53
1:C:560:LYS:HE2	1:C:560:LYS:CA	2.35	0.53
2:F:137:HIS:HD2	2:F:365:HIS:HD2	1.57	0.53
1:B:248:TRP:CZ2	1:B:511:THR:HG23	2.43	0.53
1:B:528:PHE:CD1	1:B:577:ILE:HD12	2.43	0.53
1:B:562:ILE:HD11	1:B:570:ILE:HG12	1.91	0.53
2:D:134:ALA:O	2:D:138:LEU:HD11	2.08	0.53
2:E:401:TYR:CD1	2:E:437:LEU:HD21	2.44	0.53
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.44	0.53
1:B:267:THR:HG21	2:E:121:ARG:HG2	1.91	0.53
4:C:602:ANP:O3'	2:F:348:LEU:HD21	2.09	0.53
2:F:279:THR:O	2:F:283:THR:HG23	2.09	0.53
1:A:148:LYS:H	1:A:320:MET:CE	2.20	0.53
1:B:404:ASN:OD1	1:B:407:ARG:NH1	2.42	0.53
1:C:323:ASP:OD2	1:C:383:SER:OG	2.27	0.53
1:C:484:ASP:HB3	1:C:542:PHE:CE2	2.44	0.53
2:D:143:ARG:HH11	2:D:242:HIS:CE1	2.25	0.53
2:E:237:TYR:OH	2:E:289:GLY:O	2.26	0.53
2:F:319:THR:O	2:F:323:THR:HG23	2.08	0.53
1:A:125:GLU:O	1:A:128:THR:OG1	2.24	0.53
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.91	0.53
1:A:123:THR:HG23	1:A:137:GLY:HA2	1.91	0.52
1:C:83:MET:HG2	1:C:91:LEU:HD12	1.91	0.52
1:C:173:ILE:HD13	1:C:187:MET:HG2	1.90	0.52
2:E:397:ILE:O	2:E:401:TYR:HB2	2.10	0.52
1:B:41:GLU:OE1	1:B:43:ARG:NH2	2.43	0.52
1:B:71:LEU:HD22	1:B:193:VAL:HG11	1.91	0.52
1:B:371:ARG:NH2	1:B:381:GLU:OE1	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HD2	1:A:94:PHE:HE2	1.75	0.52
1:C:565:GLU:N	1:C:565:GLU:OE2	2.42	0.52
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.43	0.52
2:E:34:MET:HE2	2:E:63:ILE:HG12	1.90	0.52
1:B:326:ILE:HG23	1:B:386:ALA:HA	1.91	0.52
2:D:148:PRO:HG3	2:D:323:THR:OG1	2.10	0.52
2:D:332:GLU:O	2:D:335:LYS:HG2	2.09	0.52
2:F:5:TYR:CD2	2:F:21:VAL:HG12	2.45	0.52
1:B:152:PRO:O	1:B:155:ILE:HG22	2.09	0.52
2:D:212:ASN:ND2	2:D:216:ASP:HB2	2.24	0.52
2:E:422:THR:OG1	2:E:425:GLU:HG3	2.10	0.52
2:F:35:GLN:OE1	2:F:35:GLN:N	2.38	0.52
2:F:157:LYS:HD3	2:F:305:THR:HG22	1.91	0.52
2:F:222:ILE:HA	2:F:253:TYR:HE1	1.75	0.52
1:B:332:SER:O	1:B:336:GLU:HG3	2.09	0.52
1:C:214:ARG:NH1	1:C:513:THR:OG1	2.43	0.52
2:E:209:MET:HE2	2:E:211:MET:HE2	1.89	0.52
2:D:138:LEU:CG	2:D:139:ASN:H	2.23	0.52
1:A:477:VAL:HG12	1:A:478:GLY:H	1.75	0.52
1:C:504:ASN:HB3	1:C:511:THR:HA	1.91	0.52
1:A:252:ASP:OD2	1:A:323:ASP:N	2.31	0.52
1:C:283:GLU:N	1:C:283:GLU:OE1	2.42	0.52
1:C:524:VAL:HG12	1:C:573:ILE:HG12	1.91	0.52
2:F:372:LEU:HD23	2:F:404:PHE:HZ	1.74	0.52
1:B:562:ILE:HD11	1:B:570:ILE:CG1	2.40	0.51
1:C:425:PHE:HB3	4:C:602:ANP:C4	2.39	0.51
1:C:517:LYS:HZ1	1:C:560:LYS:HB2	1.73	0.51
2:E:257:LEU:HD12	2:E:277:LEU:HD13	1.92	0.51
2:E:245:VAL:O	2:E:300:GLN:HA	2.10	0.51
1:A:270:VAL:O	1:A:274:PRO:HD2	2.11	0.51
1:B:91:LEU:HB3	2:E:119:ILE:HD13	1.91	0.51
1:B:485:ASN:O	1:B:488:LEU:HG	2.10	0.51
2:F:349:SER:O	2:F:352:LYS:NZ	2.36	0.51
2:E:39:ILE:HD12	2:E:39:ILE:O	2.10	0.51
2:F:334:TYR:HD1	2:F:334:TYR:O	1.92	0.51
1:B:258:GLY:HA2	1:B:329:ASP:O	2.09	0.51
1:C:360:SER:OG	2:D:259:GLU:OE1	2.25	0.51
2:D:285:PHE:HE2	2:D:319:THR:HG1	1.58	0.51
2:E:146:LYS:HE2	2:E:285:PHE:CD1	2.46	0.51
1:C:91:LEU:HD13	2:F:118:PRO:HD2	1.92	0.51
1:C:142:THR:HG1	1:C:145:ILE:H	1.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ASN:O	2:D:68:SER:OG	2.23	0.51
1:C:4:GLY:O	1:C:64:VAL:N	2.42	0.51
1:C:125:GLU:O	1:C:128:THR:OG1	2.24	0.51
2:E:83:GLU:HG3	2:E:239:LYS:HE2	1.92	0.51
1:A:497:ARG:HA	1:A:501:LEU:HB2	1.93	0.51
1:B:497:ARG:HA	1:B:501:LEU:HB2	1.92	0.51
2:D:79:LEU:HB2	2:D:227:MET:SD	2.51	0.51
2:D:137:HIS:O	2:D:365:HIS:HE1	1.94	0.51
2:E:58:GLU:N	2:E:58:GLU:OE1	2.43	0.51
2:E:278:TYR:CD1	2:E:279:THR:HG23	2.46	0.51
2:F:137:HIS:HD2	2:F:365:HIS:CD2	2.29	0.51
2:F:150:PHE:O	2:F:328:ILE:HA	2.11	0.51
1:B:174:CYS:SG	1:B:175:VAL:N	2.84	0.50
1:B:486:ASP:OD1	1:B:486:ASP:N	2.37	0.50
2:E:250:MET:O	2:E:253:TYR:HB3	2.11	0.50
2:E:258:ARG:HB2	2:E:273:TYR:CD1	2.46	0.50
1:A:261:GLU:HB2	1:A:266:MET:HE2	1.93	0.50
1:B:51:VAL:HG21	1:B:55:THR:HG22	1.93	0.50
1:C:245:ILE:O	1:C:249:SER:OG	2.25	0.50
2:D:339:SER:HB2	2:D:417:PHE:CE1	2.46	0.50
2:E:234:TYR:HD1	2:E:235:LEU:HD23	1.76	0.50
2:F:148:PRO:HB3	2:F:302:PRO:HG2	1.93	0.50
1:A:18:ASN:N	1:A:45:ASP:OD1	2.42	0.50
1:A:126:GLU:OE2	1:A:161:LYS:HA	2.11	0.50
1:B:470:LEU:HA	1:B:473:ILE:HD12	1.92	0.50
1:C:37:GLY:HA2	1:C:51:VAL:HA	1.93	0.50
2:D:270:ARG:HB2	2:D:270:ARG:HH11	1.77	0.50
2:D:339:SER:O	2:D:414:ASN:HA	2.12	0.50
1:A:466:GLU:O	1:A:470:LEU:HG	2.12	0.50
1:B:580:THR:O	1:B:584:ILE:HG13	2.12	0.50
1:C:43:ARG:O	1:C:46:VAL:HG12	2.12	0.50
2:E:30:ILE:HD13	2:E:54:VAL:HG11	1.94	0.50
1:C:144:ILE:HB	1:C:145:ILE:HD12	1.92	0.50
1:C:509:VAL:HG12	1:C:557:SER:O	2.12	0.50
2:D:273:TYR:HB3	2:D:274:PRO:HD2	1.93	0.50
2:F:366:ALA:HA	2:F:369:MET:HE2	1.94	0.50
1:B:35:VAL:HG21	1:B:58:ILE:HD11	1.93	0.50
1:C:211:THR:HG21	1:C:216:ILE:HD12	1.94	0.50
1:C:559:SER:OG	1:C:569:LYS:NZ	2.26	0.50
1:C:560:LYS:C	1:C:560:LYS:HD3	2.37	0.50
2:E:338:ILE:HD12	2:E:338:ILE:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:371:GLN:HG2	2:E:434:LEU:HD21	1.93	0.50
1:A:262:ARG:NE	2:D:321:TYR:O	2.45	0.50
1:B:210:ILE:O	1:B:249:SER:HA	2.12	0.50
1:C:364:GLU:O	1:C:368:ARG:HG3	2.12	0.50
2:D:317:ASP:O	2:D:321:TYR:HD1	1.94	0.50
2:F:150:PHE:HB2	2:F:328:ILE:HG22	1.94	0.50
1:B:122:ALA:CB	1:B:162:ILE:HD12	2.37	0.49
1:C:124:ILE:HG22	1:C:162:ILE:HD13	1.94	0.49
2:D:81:VAL:HA	2:D:85:MET:CE	2.42	0.49
2:E:88:ARG:NH2	2:E:101:PRO:O	2.43	0.49
2:E:155:ALA:HA	2:E:334:TYR:CD2	2.47	0.49
2:E:338:ILE:CG2	2:E:414:ASN:HB2	2.39	0.49
2:F:93:LEU:C	2:F:227:MET:HE3	2.37	0.49
2:F:236:ALA:HB2	2:F:243:VAL:HG23	1.94	0.49
1:A:54:GLU:HG3	1:A:56:SER:H	1.76	0.49
1:B:124:ILE:HG22	1:B:162:ILE:CD1	2.42	0.49
1:B:239:THR:O	1:B:243:HIS:ND1	2.45	0.49
2:D:307:PRO:HG3	2:D:313:HIS:CB	2.32	0.49
2:D:364:ASP:CG	2:D:427:LEU:HD13	2.37	0.49
2:D:377:ALA:O	2:D:380:LYS:HE2	2.11	0.49
1:B:94:PHE:O	1:B:98:THR:OG1	2.29	0.49
1:B:553:ARG:HA	1:B:556:ILE:HD12	1.94	0.49
1:C:474:VAL:HG23	1:C:482:LEU:HD11	1.94	0.49
2:F:404:PHE:CD1	2:F:437:LEU:HD21	2.47	0.49
1:B:365:TYR:HD1	1:B:366:TYR:HD1	1.60	0.49
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.94	0.49
1:C:423:ARG:HG2	1:C:425:PHE:CE1	2.48	0.49
2:E:278:TYR:CB	2:E:318:LEU:HD21	2.38	0.49
1:B:453:TRP:O	1:B:457:VAL:HG23	2.13	0.49
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.30	0.49
1:C:262:ARG:NH2	2:F:350:ARG:HH12	2.11	0.49
2:D:428:ASP:HA	2:D:431:TRP:CD1	2.43	0.49
1:A:419:LEU:HB3	1:A:424:HIS:HB3	1.94	0.49
1:A:507:ASP:HB3	1:A:510:ASP:HB3	1.95	0.49
2:D:91:ASP:OD1	2:D:91:ASP:N	2.38	0.49
2:D:325:GLY:HA2	2:D:348:LEU:CD1	2.43	0.49
2:E:319:THR:O	2:E:323:THR:N	2.46	0.49
1:B:531:GLU:OE2	1:B:581:ILE:HD13	2.13	0.49
2:D:129:GLN:OE1	2:D:422:THR:HA	2.13	0.49
2:D:185:GLY:C	2:D:252:ASN:HD22	2.19	0.49
1:B:133:GLY:O	1:B:380:ARG:NH2	2.22	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TRP:NE1	1:B:197:ARG:HG3	2.28	0.49
1:C:24:ILE:HG22	1:C:25:GLN:HG3	1.94	0.49
2:E:26:TYR:CD2	2:E:27:GLU:HG3	2.48	0.49
2:F:91:ASP:OD2	2:F:95:ARG:NH2	2.43	0.49
2:F:8:ILE:HG21	2:F:16:MET:HE3	1.93	0.49
2:E:380:LYS:HD3	2:E:380:LYS:C	2.37	0.49
2:F:171:LEU:HD12	2:F:171:LEU:HA	1.64	0.49
2:F:251:THR:HG23	2:F:315:ILE:HG21	1.94	0.49
1:B:470:LEU:H	1:B:470:LEU:CD2	2.06	0.48
1:C:454:SER:O	1:C:458:THR:HG23	2.13	0.48
2:D:79:LEU:HD21	2:D:85:MET:HE1	1.95	0.48
2:D:138:LEU:CD2	2:D:139:ASN:H	2.24	0.48
2:E:29:LEU:HD11	2:E:77:LEU:N	2.28	0.48
2:E:138:LEU:HA	2:E:369:MET:HG3	1.94	0.48
1:C:576:GLU:O	1:C:580:THR:OG1	2.31	0.48
2:E:65:LEU:HD12	2:E:65:LEU:H	1.78	0.48
2:E:127:PHE:HB2	2:E:355:GLY:O	2.13	0.48
2:F:266:GLU:OE2	2:F:276:TYR:OH	2.10	0.48
1:C:445:MET:SD	1:C:515:ARG:NH1	2.86	0.48
2:E:398:ASP:N	2:E:398:ASP:OD1	2.43	0.48
2:F:364:ASP:O	2:F:368:THR:HG23	2.13	0.48
2:D:138:LEU:HD22	2:D:139:ASN:CG	2.39	0.48
2:E:83:GLU:H	2:E:83:GLU:CD	2.18	0.48
2:E:278:TYR:HA	2:E:318:LEU:HD22	1.96	0.48
1:B:311:ILE:HG12	1:B:326:ILE:HD13	1.95	0.48
1:C:524:VAL:HG12	1:C:573:ILE:CG1	2.43	0.48
2:D:88:ARG:HH12	2:D:103:ILE:HD11	1.78	0.48
2:D:307:PRO:CG	2:D:313:HIS:HB2	2.34	0.48
2:D:380:LYS:CA	2:D:384:GLU:HB2	2.42	0.48
2:E:364:ASP:OD1	2:E:365:HIS:N	2.46	0.48
2:F:433:LEU:O	2:F:436:MET:HG3	2.14	0.48
1:B:224:LYS:NZ	1:B:323:ASP:OD2	2.40	0.48
1:C:241:VAL:O	1:C:245:ILE:HG23	2.13	0.48
2:E:163:GLN:O	2:E:167:GLN:HG3	2.14	0.48
2:E:182:ALA:O	2:E:247:MET:HA	2.13	0.48
2:E:327:ILE:HA	2:E:347:SER:HB2	1.96	0.48
2:F:318:LEU:O	2:F:322:ILE:HG13	2.13	0.48
1:A:487:ARG:HG2	1:A:542:PHE:HE2	1.79	0.48
1:C:459:GLU:OE2	1:C:462:ARG:NH2	2.47	0.48
2:D:379:GLY:O	2:D:382:ALA:HB3	2.13	0.48
1:A:477:VAL:HG12	1:A:478:GLY:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:HIS:HB3	1:B:276:LEU:HD11	1.94	0.48
1:B:254:VAL:HB	1:B:289:THR:HG22	1.96	0.48
1:C:547:GLU:HA	1:C:547:GLU:OE1	2.13	0.48
2:E:288:ALA:HB2	2:E:300:GLN:HG2	1.96	0.48
2:F:34:MET:HA	2:F:68:SER:OG	2.14	0.48
1:A:113:ASP:OD2	1:A:116:LYS:HB2	2.14	0.48
1:B:200:LYS:HB3	1:B:373:ILE:HG22	1.96	0.48
1:B:498:GLU:OE1	1:B:502:GLN:NE2	2.47	0.48
1:C:193:VAL:HG12	1:C:308:TYR:HB3	1.96	0.48
2:D:44:VAL:HA	2:D:54:VAL:HG12	1.94	0.48
1:B:567:LEU:HG	1:B:570:ILE:HD12	1.96	0.48
1:C:517:LYS:HD3	1:C:521:MET:HE3	1.95	0.48
2:E:436:MET:SD	2:E:436:MET:N	2.71	0.48
2:E:442:LEU:HD12	2:E:442:LEU:HA	1.74	0.48
1:A:400:PRO:O	1:A:404:ASN:ND2	2.46	0.47
1:C:30:VAL:HG13	1:C:35:VAL:HG23	1.96	0.47
2:D:8:ILE:HD12	2:D:68:SER:HB2	1.95	0.47
1:A:513:THR:HG22	1:A:518:GLN:HG2	1.96	0.47
2:E:26:TYR:CE2	2:E:27:GLU:HG3	2.49	0.47
2:E:143:ARG:HH11	2:E:242:HIS:CE1	2.32	0.47
2:E:382:ALA:HB1	2:E:402:ALA:HB2	1.95	0.47
1:B:150:MET:HE1	1:B:319:ASP:C	2.39	0.47
1:B:315:GLU:OE1	1:B:368:ARG:NH2	2.45	0.47
2:D:82:SER:O	2:D:85:MET:HG3	2.13	0.47
2:D:89:VAL:HG22	2:D:209:MET:HG3	1.97	0.47
2:D:278:TYR:HA	2:D:318:LEU:HD21	1.95	0.47
2:D:105:PRO:HG2	2:D:108:TYR:CZ	2.49	0.47
2:D:313:HIS:O	2:D:314:PRO:C	2.57	0.47
2:E:82:SER:CB	2:E:103:ILE:HD11	2.44	0.47
1:A:162:ILE:HD13	1:A:174:CYS:HB3	1.96	0.47
1:B:255:VAL:HG23	1:B:290:VAL:HB	1.97	0.47
1:B:492:VAL:O	1:B:496:ILE:HG13	2.15	0.47
1:C:2:GLN:OE1	1:C:21:GLU:HB2	2.14	0.47
1:C:8:LYS:HG3	2:F:48:GLN:HB3	1.97	0.47
2:E:444:ARG:O	2:E:444:ARG:HG3	2.14	0.47
1:A:42:MET:HG2	2:E:65:LEU:HD13	1.95	0.47
1:A:340:GLU:OE2	2:D:279:THR:OG1	2.32	0.47
1:B:169:ILE:O	1:B:186:THR:OG1	2.32	0.47
1:B:150:MET:HE3	1:B:320:MET:HG2	1.97	0.47
1:B:206:ASP:HA	1:B:440:GLU:OE1	2.15	0.47
2:E:8:ILE:HD13	2:E:16:MET:SD	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:ARG:HD3	2:E:242:HIS:ND1	2.29	0.47
2:E:258:ARG:NH1	2:E:273:TYR:CE2	2.83	0.47
2:E:311:LYS:HD3	2:E:311:LYS:HA	1.62	0.47
2:E:401:TYR:HE1	2:E:437:LEU:HD11	1.77	0.47
1:B:261:GLU:OE1	1:B:330:SER:N	2.48	0.47
1:B:365:TYR:CD1	1:B:366:TYR:CD1	3.02	0.47
1:C:41:GLU:OE1	1:C:43:ARG:NH1	2.45	0.47
2:D:143:ARG:HH21	2:D:170:VAL:HG21	1.77	0.47
2:E:180:VAL:HA	2:E:208:VAL:O	2.15	0.47
2:E:281:LEU:HD13	2:E:319:THR:CG2	2.45	0.47
2:F:401:TYR:O	2:F:404:PHE:HB3	2.15	0.47
1:B:259:CYS:HB3	1:B:334:TRP:HB2	1.96	0.47
1:B:261:GLU:OE1	1:B:333:ARG:HG3	2.15	0.47
1:B:500:TYR:CE2	1:B:522:LEU:HD13	2.50	0.47
1:C:196:GLY:HA2	1:C:368:ARG:NH2	2.29	0.47
2:E:307:PRO:O	2:E:308:GLU:HB3	2.15	0.47
2:D:142:VAL:HG22	2:D:145:GLN:HB2	1.97	0.47
2:F:152:PRO:HD3	2:F:329:LEU:O	2.15	0.47
1:A:243:HIS:O	1:A:247:LYS:HG2	2.16	0.46
1:B:150:MET:HE2	1:B:380:ARG:HH21	1.80	0.46
1:C:60:PRO:HD3	2:F:47:VAL:HG21	1.97	0.46
1:C:509:VAL:HG11	1:C:558:ARG:HA	1.97	0.46
2:E:315:ILE:HG13	2:E:316:PRO:CD	2.45	0.46
2:E:386:ALA:HA	2:E:389:LEU:CD2	2.45	0.46
2:E:404:PHE:HE1	2:E:433:LEU:O	1.98	0.46
2:F:161:ALA:HB2	2:F:303:ILE:HD12	1.97	0.46
1:A:244:GLN:NE2	1:A:505:ALA:HB1	2.31	0.46
1:A:467:GLU:OE2	1:A:497:ARG:NE	2.30	0.46
1:B:261:GLU:HB2	1:B:266:MET:HE2	1.97	0.46
1:B:339:ARG:HD3	2:E:270:ARG:HH12	1.79	0.46
1:C:274:PRO:HD3	1:C:286:MET:HG3	1.96	0.46
2:D:152:PRO:HG2	2:D:155:ALA:HB2	1.97	0.46
2:E:44:VAL:HA	2:E:54:VAL:HG12	1.98	0.46
2:E:148:PRO:HG3	2:E:323:THR:HG21	1.96	0.46
2:E:338:ILE:HD13	2:E:341:PRO:HA	1.97	0.46
1:B:121:GLU:HB2	1:B:138:TYR:CE2	2.51	0.46
2:D:254:ALA:CB	2:D:314:PRO:HG3	2.41	0.46
2:D:362:ARG:HE	2:D:364:ASP:CG	2.24	0.46
2:E:258:ARG:HA	2:E:274:PRO:HG3	1.98	0.46
2:F:112:ASN:C	2:F:287:ARG:HH12	2.23	0.46
2:F:278:TYR:HB2	2:F:318:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:HE1	1:B:319:ASP:O	2.16	0.46
2:D:93:LEU:C	2:D:227:MET:HE3	2.41	0.46
2:D:233:GLU:OE2	2:D:287:ARG:NE	2.37	0.46
2:F:157:LYS:HG3	2:F:158:SER:N	2.30	0.46
1:B:320:MET:HB2	1:B:322:TYR:CD2	2.50	0.46
1:B:380:ARG:CD	1:B:380:ARG:H	2.27	0.46
1:C:245:ILE:HG13	1:C:327:MET:HE1	1.96	0.46
2:D:133:SER:HB3	2:D:421:ARG:HD2	1.98	0.46
2:D:138:LEU:HD13	2:D:138:LEU:H	1.80	0.46
2:F:285:PHE:CE2	2:F:319:THR:HG23	2.49	0.46
1:A:327:MET:HE2	1:A:327:MET:HB3	1.85	0.46
1:A:546:MET:HE3	1:A:553:ARG:NH1	2.30	0.46
1:B:120:PHE:CZ	1:B:173:ILE:HD11	2.50	0.46
1:C:327:MET:HB3	1:C:387:ILE:HB	1.96	0.46
2:E:34:MET:CE	2:E:63:ILE:HG12	2.46	0.46
2:E:343:ASP:OD1	2:E:345:LEU:HD23	2.16	0.46
2:F:88:ARG:HA	2:F:98:ASP:OD2	2.15	0.46
1:C:168:THR:OG1	1:C:171:ASP:OD2	2.31	0.46
1:C:331:THR:OG1	1:C:390:VAL:HG12	2.16	0.46
2:F:107:LYS:NZ	2:F:238:GLU:OE2	2.38	0.46
1:B:497:ARG:HB3	1:B:501:LEU:HD12	1.98	0.46
1:B:522:LEU:O	1:B:526:LEU:HG	2.16	0.46
1:B:569:LYS:H	1:B:569:LYS:HD3	1.81	0.46
1:C:560:LYS:HG3	1:C:561:TYR:CD2	2.51	0.46
2:E:40:ARG:HD3	2:E:58:GLU:HB2	1.97	0.46
2:F:438:PRO:HB2	2:F:440:THR:HG22	1.98	0.46
1:A:301:ALA:HA	1:A:341:MET:HE1	1.98	0.46
1:A:491:GLU:HG2	1:A:546:MET:CE	2.46	0.46
1:B:399:GLU:OE2	1:B:402:THR:HG23	2.16	0.46
1:C:159:VAL:HG12	1:C:176:ILE:CD1	2.46	0.46
2:D:160:LEU:N	2:D:417:PHE:HE2	2.13	0.46
2:E:149:VAL:HB	2:E:303:ILE:HG12	1.97	0.46
1:C:242:GLN:HG2	1:C:327:MET:HB2	1.98	0.46
1:C:356:ALA:HB1	2:D:259:GLU:HA	1.98	0.46
2:D:375:ALA:HB1	2:D:404:PHE:CE2	2.50	0.46
2:E:91:ASP:OD2	2:E:95:ARG:NH1	2.49	0.46
2:F:178:ALA:HB2	2:F:241:MET:HE2	1.98	0.46
2:F:222:ILE:HD12	2:F:222:ILE:H	1.81	0.46
1:B:491:GLU:O	1:B:494:LYS:HG3	2.16	0.45
2:D:86:ILE:HA	2:D:208:VAL:CG2	2.46	0.45
2:E:116:ILE:HD11	2:E:291:ILE:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:MET:HB3	2:F:208:VAL:HG21	1.99	0.45
1:A:452:ASP:O	1:A:456:MET:HG3	2.16	0.45
1:B:380:ARG:H	1:B:380:ARG:HD3	1.80	0.45
1:B:445:MET:HE1	1:B:515:ARG:HD3	1.97	0.45
1:C:311:ILE:O	1:C:315:GLU:HG3	2.17	0.45
2:D:57:PHE:CD1	2:D:219:ILE:HG21	2.51	0.45
2:F:315:ILE:HB	2:F:316:PRO:CD	2.45	0.45
1:A:75:LEU:HD13	1:A:316:TYR:HB2	1.98	0.45
1:A:444:TYR:O	1:A:448:ILE:HG22	2.15	0.45
1:B:34:GLY:O	1:B:108:GLN:NE2	2.50	0.45
1:B:528:PHE:HA	1:B:577:ILE:CD1	2.41	0.45
1:C:253:LEU:HD23	1:C:288:ARG:O	2.17	0.45
2:D:331:ARG:HB3	2:D:331:ARG:NH1	2.32	0.45
2:D:415:GLN:NE2	2:D:419:THR:O	2.50	0.45
2:D:425:GLU:O	2:D:428:ASP:N	2.49	0.45
2:E:255:GLU:HA	2:E:273:TYR:HE1	1.81	0.45
2:E:383:LYS:HA	2:E:386:ALA:HB3	1.98	0.45
2:F:201:THR:HG23	2:F:203:ALA:H	1.81	0.45
2:D:81:VAL:HA	2:D:85:MET:HE3	1.98	0.45
2:D:139:ASN:ND2	2:D:347:SER:C	2.75	0.45
2:D:338:ILE:HD11	2:D:413:VAL:HG11	1.97	0.45
2:E:44:VAL:HG22	2:E:54:VAL:HG12	1.98	0.45
2:F:75:HIS:ND1	2:F:78:GLN:OE1	2.49	0.45
1:A:329:ASP:HA	1:A:330:SER:HA	1.60	0.45
1:B:248:TRP:HA	1:B:248:TRP:CE3	2.51	0.45
1:C:240:VAL:O	1:C:244:GLN:NE2	2.46	0.45
2:D:382:ALA:HB1	2:D:401:TYR:HB3	1.95	0.45
2:E:197:ASP:O	2:E:201:THR:HG23	2.16	0.45
2:F:34:MET:SD	2:F:40:ARG:HD2	2.57	0.45
1:C:560:LYS:HG3	1:C:561:TYR:HD2	1.81	0.45
2:E:146:LYS:CD	2:E:300:GLN:HG3	2.44	0.45
2:E:433:LEU:C	2:E:436:MET:SD	3.00	0.45
1:A:120:PHE:CE2	1:A:162:ILE:HD11	2.49	0.45
1:A:131:SER:N	1:A:134:ASP:OD2	2.30	0.45
1:B:71:LEU:O	1:B:193:VAL:HG12	2.16	0.45
2:D:364:ASP:OD2	2:D:427:LEU:HD13	2.17	0.45
2:E:60:THR:HG22	2:E:63:ILE:HD12	1.97	0.45
2:E:425:GLU:O	2:E:429:LEU:HG	2.17	0.45
2:F:222:ILE:HA	2:F:253:TYR:CE1	2.51	0.45
1:A:245:ILE:O	1:A:249:SER:OG	2.23	0.45
1:B:35:VAL:HG13	1:B:53:GLU:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:LYS:HD3	1:C:560:LYS:O	2.17	0.45
2:E:383:LYS:O	2:E:387:VAL:N	2.50	0.45
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.99	0.45
1:B:342:SER:HB2	1:B:355:PRO:HG3	1.99	0.45
2:D:53:MET:HB2	2:D:53:MET:HE3	1.72	0.45
2:D:416:GLY:O	2:D:419:THR:OG1	2.35	0.45
2:F:226:ARG:NH2	2:F:280:ASN:OD1	2.49	0.45
2:F:358:ALA:HB2	2:F:363:GLU:HB3	1.98	0.45
1:A:408:VAL:HA	2:E:187:THR:HG21	1.99	0.45
1:B:371:ARG:HH21	1:B:381:GLU:CD	2.22	0.45
1:B:391:SER:OG	1:B:391:SER:O	2.31	0.45
2:D:133:SER:HB2	2:D:426:THR:HG23	1.99	0.45
2:F:306:MET:HG3	2:F:316:PRO:CG	2.46	0.45
1:B:242:GLN:HE22	1:B:329:ASP:CG	2.22	0.44
2:D:331:ARG:HB3	2:D:331:ARG:CZ	2.47	0.44
1:A:445:MET:HE1	1:A:515:ARG:CD	2.44	0.44
1:C:124:ILE:HB	1:C:136:ILE:HA	1.98	0.44
1:C:142:THR:HG21	1:C:287:GLU:O	2.17	0.44
1:C:206:ASP:OD1	1:C:371:ARG:NH1	2.50	0.44
1:C:390:VAL:CG2	1:C:402:THR:HG22	2.42	0.44
1:C:454:SER:O	1:C:457:VAL:HG22	2.17	0.44
2:E:195:MET:CE	2:E:211:MET:HG3	2.43	0.44
1:B:124:ILE:HG22	1:B:162:ILE:HD11	1.99	0.44
1:B:219:PHE:C	1:B:221:PRO:HD3	2.43	0.44
1:B:549:THR:CG2	1:B:553:ARG:HG3	2.44	0.44
2:D:374:ALA:O	2:D:378:GLN:HB2	2.18	0.44
2:E:139:ASN:OD1	2:E:348:LEU:HA	2.17	0.44
2:F:434:LEU:HA	2:F:437:LEU:HD23	1.98	0.44
1:A:243:HIS:ND1	1:A:276:LEU:HD11	2.33	0.44
1:A:317:PHE:HA	1:A:320:MET:HG3	1.99	0.44
1:A:333:ARG:HA	1:A:333:ARG:HD2	1.89	0.44
2:F:88:ARG:NH2	2:F:101:PRO:HG2	2.31	0.44
1:C:146:GLN:H	1:C:146:GLN:HG2	1.53	0.44
1:C:413:TRP:HB3	1:C:428:ILE:HG12	2.00	0.44
1:C:419:LEU:HD12	1:C:419:LEU:HA	1.82	0.44
2:D:5:TYR:CD2	2:D:21:VAL:HG12	2.53	0.44
2:D:65:LEU:HD12	2:D:65:LEU:H	1.83	0.44
2:F:88:ARG:NH1	2:F:103:ILE:HG12	2.32	0.44
1:A:150:MET:CE	1:A:320:MET:HG2	2.47	0.44
1:B:307:ILE:HD11	1:B:334:TRP:CE2	2.52	0.44
2:E:255:GLU:HG2	2:E:273:TYR:OH	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:ARG:HD3	2:F:242:HIS:HD2	1.81	0.44
1:B:244:GLN:OE1	1:B:248:TRP:CD1	2.70	0.44
1:B:531:GLU:OE1	1:B:578:LYS:HG3	2.18	0.44
2:D:366:ALA:O	2:D:370:ASN:ND2	2.47	0.44
2:F:64:ASN:O	2:F:68:SER:HB2	2.18	0.44
1:A:230:VAL:O	1:A:389:ALA:HA	2.18	0.44
1:B:193:VAL:HG22	1:B:308:TYR:HB3	1.99	0.44
1:C:38:GLU:N	1:C:50:GLN:O	2.42	0.44
1:C:92:ASP:HA	2:F:119:ILE:CD1	2.48	0.44
1:A:88:GLN:HG2	1:A:111:ALA:HB1	2.00	0.44
2:D:7:THR:OG1	2:D:19:GLU:O	2.33	0.44
2:E:371:GLN:CG	2:E:434:LEU:HD21	2.47	0.44
2:E:436:MET:HB3	2:E:436:MET:HE3	1.76	0.44
2:F:132:ILE:HA	2:F:415:GLN:CD	2.42	0.44
1:A:490:LEU:HA	1:A:490:LEU:HD22	1.77	0.43
1:B:176:ILE:HD13	1:B:178:THR:HG23	1.99	0.43
2:E:135:ILE:HG13	2:E:327:ILE:CD1	2.48	0.43
2:E:439:ARG:HD3	2:E:439:ARG:N	2.33	0.43
1:B:6:ILE:HG22	1:B:60:PRO:HA	2.00	0.43
2:D:9:LYS:CG	2:D:19:GLU:HG3	2.48	0.43
2:D:129:GLN:OE1	2:D:423:ILE:N	2.43	0.43
2:D:403:LYS:HG3	2:D:407:ARG:HD3	2.00	0.43
2:F:142:VAL:HG21	2:F:351:LEU:O	2.18	0.43
2:F:318:LEU:HD13	2:F:318:LEU:HA	1.87	0.43
1:A:36:ILE:HD12	1:A:36:ILE:HA	1.91	0.43
1:C:38:GLU:HB2	1:C:52:TYR:HE1	1.84	0.43
2:D:35:GLN:OE1	2:D:35:GLN:N	2.38	0.43
2:E:3:LYS:HD3	2:E:5:TYR:HE1	1.83	0.43
2:E:16:MET:CE	2:E:56:ILE:HD11	2.48	0.43
2:E:185:GLY:HA3	2:E:221:ARG:HD2	1.99	0.43
2:E:339:SER:HB3	2:E:417:PHE:CE2	2.52	0.43
2:E:389:LEU:HD12	2:E:392:SER:CB	2.36	0.43
2:F:242:HIS:ND1	2:F:296:GLY:HA2	2.33	0.43
1:B:140:ASP:OD1	1:B:146:GLN:HG2	2.17	0.43
1:B:257:VAL:HG23	1:B:328:ALA:HB2	2.01	0.43
1:C:42:MET:HG2	2:D:65:LEU:HD13	2.00	0.43
2:D:304:LEU:HD12	2:D:304:LEU:HA	1.69	0.43
2:F:147:LEU:HD23	2:F:147:LEU:HA	1.91	0.43
2:F:306:MET:HE2	2:F:310:ASP:HB3	2.01	0.43
1:A:260:GLY:O	1:A:333:ARG:HG3	2.18	0.43
1:C:339:ARG:HB2	1:C:354:TYR:HD1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:MET:HE3	2:D:250:MET:HB3	1.92	0.43
2:F:7:THR:OG1	2:F:19:GLU:O	2.36	0.43
1:A:238:LYS:O	1:A:242:GLN:HG3	2.18	0.43
1:C:118:TRP:CH2	1:C:141:GLU:HG3	2.53	0.43
2:D:85:MET:O	2:D:88:ARG:HB2	2.18	0.43
2:E:143:ARG:HH11	2:E:242:HIS:HE1	1.65	0.43
2:F:14:PRO:HD2	2:F:15:LEU:HD12	2.00	0.43
2:F:225:PRO:HB3	2:F:247:MET:HE2	2.00	0.43
1:A:267:THR:HG21	2:D:121:ARG:HB3	2.01	0.43
1:B:252:ASP:OD2	1:B:322:TYR:HA	2.19	0.43
2:E:148:PRO:HD2	2:E:326:GLN:HA	2.01	0.43
2:F:128:ILE:HG22	2:F:141:LEU:HB3	2.00	0.43
2:F:163:GLN:OE1	2:F:417:PHE:HA	2.18	0.43
2:F:356:THR:HG1	2:F:365:HIS:CE1	2.30	0.43
1:A:27:MET:O	1:A:67:THR:OG1	2.29	0.43
1:A:261:GLU:OE1	1:A:330:SER:N	2.52	0.43
1:C:565:GLU:O	1:C:569:LYS:HB2	2.18	0.43
2:D:414:ASN:OD1	2:D:414:ASN:O	2.37	0.43
1:A:119:TRP:CZ3	1:A:165:GLY:HA2	2.54	0.43
1:C:30:VAL:HG23	1:C:64:VAL:CG2	2.48	0.43
1:C:248:TRP:HB3	1:C:512:PHE:CD1	2.54	0.43
2:D:138:LEU:HD13	2:D:138:LEU:N	2.34	0.43
2:E:308:GLU:O	2:E:309:ASP:HB2	2.19	0.43
2:F:157:LYS:HD3	2:F:305:THR:CG2	2.49	0.43
1:A:194:ARG:NH2	1:A:304:GLU:OE2	2.47	0.43
1:B:120:PHE:HB2	1:B:139:VAL:HG22	2.01	0.43
1:B:191:TRP:CD1	1:B:197:ARG:HG3	2.54	0.43
1:B:453:TRP:CZ3	1:B:519:PHE:HA	2.53	0.43
1:C:84:PHE:HB3	1:C:88:GLN:HA	2.01	0.43
2:D:139:ASN:CG	2:D:348:LEU:HA	2.44	0.43
2:E:137:HIS:HD2	2:E:365:HIS:CD2	2.37	0.43
1:C:297:ASN:OD1	2:F:286:GLU:HB2	2.19	0.42
2:D:91:ASP:OD1	2:D:95:ARG:N	2.37	0.42
2:D:223:ALA:O	2:D:227:MET:HG2	2.19	0.42
2:E:119:ILE:O	2:E:292:ARG:NH1	2.51	0.42
2:E:322:ILE:HD12	2:E:323:THR:N	2.34	0.42
2:F:35:GLN:NE2	2:F:64:ASN:H	2.15	0.42
2:F:81:VAL:O	2:F:106:GLU:N	2.52	0.42
1:B:59:GLY:N	2:E:25:LYS:HG3	2.34	0.42
1:B:267:THR:HG21	2:E:121:ARG:O	2.19	0.42
1:C:519:PHE:CD1	1:C:519:PHE:C	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:PHE:CD2	2:D:193:PHE:C	2.97	0.42
2:D:339:SER:H	2:D:414:ASN:HB2	1.82	0.42
2:E:29:LEU:HD11	2:E:77:LEU:HA	2.01	0.42
2:E:376:TYR:C	2:E:378:GLN:N	2.73	0.42
1:B:252:ASP:OD2	1:B:322:TYR:HD1	2.02	0.42
1:B:253:LEU:HD23	1:B:288:ARG:O	2.20	0.42
1:C:80:ILE:HG13	1:C:141:GLU:OE2	2.19	0.42
2:E:281:LEU:HD13	2:E:319:THR:HG23	2.01	0.42
2:F:394:LEU:CA	2:F:398:ASP:HB2	2.46	0.42
1:A:73:VAL:HG13	1:A:193:VAL:HG22	2.01	0.42
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.83	0.42
1:B:9:VAL:HG11	1:B:58:ILE:O	2.19	0.42
1:B:225:GLY:O	1:B:370:GLY:HA2	2.19	0.42
1:C:169:ILE:CG2	1:C:188:MET:HB2	2.49	0.42
1:C:211:THR:HG22	1:C:213:GLN:HB2	2.00	0.42
1:C:577:ILE:O	1:C:581:ILE:HG12	2.19	0.42
2:F:88:ARG:HH11	2:F:103:ILE:HG12	1.85	0.42
1:A:208:PRO:HB3	1:A:441:VAL:HG22	2.01	0.42
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.88	0.42
1:B:455:ASP:N	1:B:455:ASP:OD1	2.51	0.42
1:B:486:ASP:HA	1:B:489:THR:OG1	2.19	0.42
1:C:262:ARG:H	1:C:262:ARG:HG3	1.56	0.42
1:C:553:ARG:O	1:C:556:ILE:HG12	2.19	0.42
2:D:427:LEU:HA	2:D:427:LEU:HD23	1.69	0.42
2:E:130:THR:O	2:E:167:GLN:HB2	2.20	0.42
2:F:149:VAL:HA	2:F:327:ILE:O	2.19	0.42
2:F:312:THR:O	2:F:312:THR:HG22	2.18	0.42
2:F:371:GLN:CD	2:F:442:LEU:HA	2.44	0.42
1:B:196:GLY:HA2	1:B:368:ARG:NH2	2.34	0.42
1:C:517:LYS:HE3	1:C:560:LYS:CE	2.50	0.42
2:E:144:GLY:HA2	2:E:298:VAL:O	2.20	0.42
2:E:166:ARG:NH2	2:E:418:TYR:HD1	2.17	0.42
2:F:111:ILE:HB	2:F:226:ARG:HB3	2.02	0.42
2:F:243:VAL:N	2:F:297:SER:O	2.52	0.42
2:F:383:LYS:HB2	2:F:383:LYS:HE2	1.88	0.42
1:C:514:SER:CB	1:C:560:LYS:NZ	2.83	0.42
2:E:16:MET:HB2	2:E:16:MET:HE3	1.79	0.42
2:F:79:LEU:HB2	2:F:227:MET:SD	2.60	0.42
2:F:137:HIS:NE2	2:F:368:THR:OG1	2.12	0.42
1:A:327:MET:HE3	1:A:387:ILE:HG21	2.02	0.42
1:A:378:ASP:OD1	1:A:378:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:TRP:CH2	1:B:141:GLU:HG3	2.55	0.42
1:B:217:ASP:OD1	1:B:217:ASP:N	2.53	0.42
1:C:189:GLN:NE2	1:C:197:ARG:HH12	2.17	0.42
2:D:147:LEU:O	2:D:302:PRO:HD2	2.19	0.42
2:E:7:THR:OG1	2:E:7:THR:O	2.36	0.42
2:E:60:THR:O	2:E:63:ILE:HG13	2.19	0.42
2:F:130:THR:OG1	2:F:132:ILE:HG12	2.20	0.42
1:A:2:GLN:OE1	1:A:21:GLU:N	2.52	0.42
2:D:109:LEU:HD23	2:D:109:LEU:HA	1.86	0.42
2:D:177:PHE:HE2	2:D:244:LEU:CB	2.20	0.42
2:D:430:GLY:O	2:D:434:LEU:HG	2.19	0.42
2:E:35:GLN:H	2:E:35:GLN:CD	2.23	0.42
1:C:57:GLY:O	2:F:25:LYS:HD3	2.20	0.42
1:C:239:THR:OG1	4:C:602:ANP:O2B	2.38	0.42
1:C:391:SER:HB3	2:F:321:TYR:CZ	2.55	0.42
1:C:564:GLU:O	1:C:564:GLU:HG2	2.20	0.42
2:D:86:ILE:HA	2:D:208:VAL:HG22	2.01	0.42
2:D:361:THR:HG21	2:D:365:HIS:HD2	1.85	0.42
2:F:444:ARG:HD2	2:F:445:ILE:H	1.84	0.42
1:A:73:VAL:HG11	1:A:309:THR:HG23	2.01	0.41
1:A:214:ARG:NH2	1:A:503:GLN:HG3	2.35	0.41
1:C:234:PHE:HB3	2:F:321:TYR:CE1	2.55	0.41
1:C:260:GLY:O	2:F:278:TYR:OH	2.31	0.41
1:C:467:GLU:OE1	1:C:497:ARG:NH1	2.50	0.41
2:D:26:TYR:CZ	2:D:27:GLU:HG3	2.55	0.41
2:D:247:MET:HE3	2:D:247:MET:HB2	1.94	0.41
2:D:318:LEU:O	2:D:322:ILE:HG13	2.20	0.41
2:E:175:ASP:OD2	2:E:295:LYS:NZ	2.44	0.41
2:F:90:PHE:HZ	2:F:103:ILE:HD11	1.84	0.41
1:B:351:ASP:OD1	2:F:258:ARG:NH1	2.53	0.41
1:B:550:VAL:HA	1:B:553:ARG:CZ	2.50	0.41
1:C:73:VAL:HG11	1:C:309:THR:HG23	2.01	0.41
1:C:225:GLY:O	1:C:370:GLY:HA2	2.19	0.41
2:D:28:GLU:O	2:D:44:VAL:HG23	2.20	0.41
2:E:138:LEU:CD1	2:E:344:VAL:HG11	2.50	0.41
2:E:236:ALA:HA	2:E:241:MET:O	2.20	0.41
2:F:141:LEU:HD23	2:F:142:VAL:N	2.34	0.41
2:F:232:ALA:HA	2:F:243:VAL:HG11	2.02	0.41
1:A:220:PHE:HA	1:A:435:SER:HB3	2.03	0.41
1:C:124:ILE:HD12	1:C:124:ILE:HA	1.95	0.41
1:C:500:TYR:CE1	1:C:522:LEU:HB2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:GLY:O	2:D:305:THR:HA	2.21	0.41
2:F:83:GLU:H	2:F:83:GLU:HG2	1.68	0.41
2:F:327:ILE:HA	2:F:347:SER:OG	2.20	0.41
1:A:550:VAL:HG22	1:A:553:ARG:NH2	2.35	0.41
1:B:248:TRP:HZ2	1:B:511:THR:HG23	1.86	0.41
1:C:87:ILE:HG13	1:C:89:ARG:HG3	2.02	0.41
2:E:362:ARG:NH2	2:E:364:ASP:OD2	2.47	0.41
2:E:372:LEU:HD21	2:E:408:PHE:HE2	1.85	0.41
1:B:119:TRP:HA	1:B:165:GLY:O	2.21	0.41
1:B:393:SER:HA	2:E:321:TYR:CE1	2.56	0.41
1:B:446:ASP:OD2	1:B:454:SER:OG	2.27	0.41
1:B:546:MET:HE3	1:B:553:ARG:NH1	2.35	0.41
1:C:521:MET:O	1:C:524:VAL:HG22	2.20	0.41
2:E:385:LEU:HD23	2:E:385:LEU:HA	1.89	0.41
2:F:45:LEU:HD23	2:F:45:LEU:HA	1.88	0.41
2:F:226:ARG:CZ	2:F:284:LEU:HD21	2.50	0.41
1:A:231:PRO:HD2	1:A:413:TRP:O	2.20	0.41
1:A:351:ASP:OD1	2:E:258:ARG:CZ	2.67	0.41
1:B:378:ASP:OD1	1:B:378:ASP:N	2.53	0.41
1:C:36:ILE:HG23	1:C:52:TYR:HB2	2.03	0.41
1:C:234:PHE:HB3	2:F:321:TYR:HD1	1.83	0.41
1:C:245:ILE:CD1	1:C:387:ILE:HG13	2.46	0.41
2:D:339:SER:HB2	2:D:417:PHE:HD1	1.83	0.41
2:E:255:GLU:HA	2:E:273:TYR:CE1	2.55	0.41
2:E:271:ARG:NH2	2:E:271:ARG:HB2	2.35	0.41
2:E:383:LYS:O	2:E:383:LYS:HG3	2.20	0.41
2:E:404:PHE:CE1	2:E:433:LEU:O	2.73	0.41
2:F:93:LEU:CD2	2:F:220:GLU:HG2	2.51	0.41
1:A:350:GLY:C	2:E:258:ARG:NH2	2.78	0.41
1:A:549:THR:HA	1:A:552:VAL:HG12	2.02	0.41
1:B:285:LEU:O	1:B:289:THR:HG23	2.20	0.41
1:B:342:SER:CB	1:B:355:PRO:HG3	2.50	0.41
2:D:88:ARG:HD2	2:D:88:ARG:HA	1.82	0.41
2:D:339:SER:N	2:D:414:ASN:HB3	2.29	0.41
2:D:398:ASP:O	2:D:401:TYR:N	2.53	0.41
2:E:39:ILE:HD13	2:E:41:ARG:HH11	1.85	0.41
2:F:164:ILE:HD13	2:F:164:ILE:HA	1.92	0.41
1:A:351:ASP:N	2:E:258:ARG:NH2	2.68	0.41
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.88	0.41
1:B:144:ILE:HD13	1:B:144:ILE:HG21	1.87	0.41
1:B:364:GLU:O	1:B:368:ARG:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ASP:OD2	1:B:557:SER:HA	2.20	0.41
2:D:3:LYS:HE2	2:D:3:LYS:HB2	1.87	0.41
2:D:4:GLU:OE2	2:D:71:ARG:NH2	2.54	0.41
2:D:84:ASP:HB2	2:D:103:ILE:HD12	2.02	0.41
2:F:141:LEU:HD23	2:F:142:VAL:H	1.86	0.41
1:A:89:ARG:HD2	1:A:94:PHE:CE2	2.55	0.41
1:A:497:ARG:O	1:A:502:GLN:HG3	2.20	0.41
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.84	0.41
1:A:560:LYS:HE2	1:A:561:TYR:CE1	2.55	0.41
1:B:45:ASP:OD2	1:B:45:ASP:N	2.41	0.41
1:B:575:GLU:N	1:B:575:GLU:CD	2.78	0.41
1:C:308:TYR:HD1	1:C:308:TYR:HA	1.80	0.41
2:E:45:LEU:HD23	2:E:45:LEU:HA	1.80	0.41
2:E:90:PHE:O	2:E:211:MET:N	2.53	0.41
2:E:319:THR:O	2:E:323:THR:HG23	2.20	0.41
2:E:376:TYR:CD1	2:E:408:PHE:CD1	3.09	0.41
2:F:224:THR:HB	2:F:225:PRO:CD	2.50	0.41
2:F:309:ASP:O	2:F:311:LYS:N	2.54	0.41
1:A:406:LEU:HD22	1:A:434:TYR:OH	2.21	0.41
1:B:231:PRO:HB3	1:B:390:VAL:HG23	2.03	0.41
2:E:117:ASN:OD1	2:E:119:ILE:HG12	2.21	0.41
2:E:186:ILE:O	2:E:214:ALA:N	2.53	0.41
2:E:257:LEU:HD23	2:E:257:LEU:HA	1.96	0.41
1:A:239:THR:HG22	1:A:243:HIS:HE2	1.86	0.40
1:A:264:ASN:HB2	2:D:324:GLU:OE2	2.20	0.40
1:A:418:SER:O	1:A:422:LYS:HG3	2.21	0.40
1:A:560:LYS:HE2	1:A:561:TYR:HE1	1.85	0.40
1:B:487:ARG:O	1:B:487:ARG:HD3	2.21	0.40
1:C:211:THR:HG22	1:C:213:GLN:H	1.87	0.40
2:D:151:GLY:O	2:D:306:MET:N	2.49	0.40
2:D:353:ASP:OD1	2:D:353:ASP:N	2.54	0.40
2:F:373:PHE:CD1	2:F:373:PHE:C	2.99	0.40
2:F:397:ILE:HG23	2:F:398:ASP:OD1	2.21	0.40
1:A:535:ALA:HA	1:A:538:LEU:HB2	2.03	0.40
2:D:225:PRO:O	2:D:229:LEU:HD12	2.21	0.40
2:E:250:MET:O	2:E:253:TYR:N	2.54	0.40
2:E:444:ARG:HH21	2:E:446:LYS:HB3	1.86	0.40
2:F:137:HIS:CE1	2:F:368:THR:HG1	2.27	0.40
1:A:182:LEU:H	1:A:182:LEU:HD23	1.86	0.40
1:A:215:VAL:HB	1:A:501:LEU:HD22	2.03	0.40
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:SER:HB3	1:A:333:ARG:HG2	2.02	0.40
1:B:173:ILE:HG22	1:B:186:THR:HA	2.04	0.40
1:B:331:THR:OG1	1:B:389:ALA:O	2.38	0.40
1:C:274:PRO:HA	1:C:284:SER:HB2	2.03	0.40
1:C:338:LEU:HD12	1:C:338:LEU:HA	1.90	0.40
1:C:486:ASP:OD1	1:C:486:ASP:N	2.54	0.40
1:C:541:TYR:O	1:C:545:ILE:HG13	2.20	0.40
1:C:554:GLU:OE1	1:C:558:ARG:NH2	2.55	0.40
1:C:566:GLU:O	1:C:570:ILE:HG12	2.22	0.40
2:D:427:LEU:O	2:D:431:TRP:CD1	2.73	0.40
2:E:41:ARG:NH2	2:E:95:ARG:HE	2.18	0.40
2:E:322:ILE:CD1	2:E:322:ILE:C	2.87	0.40
2:F:80:GLY:HA2	2:F:108:TYR:HD1	1.86	0.40
2:F:129:GLN:OE1	2:F:423:ILE:N	2.46	0.40
2:F:248:GLU:OE1	2:F:248:GLU:HA	2.21	0.40
1:A:521:MET:HE2	1:A:521:MET:HB3	1.90	0.40
1:B:101:ASN:HB3	2:E:120:ALA:HB1	2.03	0.40
1:B:487:ARG:HD3	1:B:487:ARG:C	2.47	0.40
1:C:135:ILE:HD12	1:C:148:LYS:HB3	2.03	0.40
2:D:244:LEU:HD11	2:D:301:ILE:CD1	2.51	0.40
2:E:329:LEU:HA	2:E:341:PRO:O	2.21	0.40
2:F:139:ASN:HD22	2:F:347:SER:HB3	1.84	0.40
2:F:180:VAL:O	2:F:245:VAL:HA	2.21	0.40
1:A:88:GLN:HG2	1:A:111:ALA:CB	2.52	0.40
1:B:184:GLU:H	1:B:184:GLU:HG2	1.69	0.40
1:C:327:MET:HA	1:C:387:ILE:O	2.22	0.40
2:E:83:GLU:CG	2:E:239:LYS:HE2	2.51	0.40
2:E:146:LYS:CE	2:E:302:PRO:HG3	2.45	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:GLU:OE1	1:B:558:ARG:NH2[2_555]	2.14	0.06
1:A:547:GLU:OE1	2:E:446:LYS:NZ[2_555]	2.17	0.03

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	584/596 (98%)	568 (97%)	14 (2%)	2 (0%)	36	66
1	B	584/596 (98%)	565 (97%)	16 (3%)	3 (0%)	24	56
1	C	582/596 (98%)	559 (96%)	20 (3%)	3 (0%)	24	56
2	D	430/458 (94%)	405 (94%)	22 (5%)	3 (1%)	18	50
2	E	447/458 (98%)	422 (94%)	24 (5%)	1 (0%)	43	73
2	F	443/458 (97%)	418 (94%)	22 (5%)	3 (1%)	18	50
All	All	3070/3162 (97%)	2937 (96%)	118 (4%)	15 (0%)	24	56

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ILE
1	C	392	PRO
1	C	431	ILE
2	D	314	PRO
1	A	477	VAL
2	F	173	SER
1	B	260	GLY
2	D	388	VAL
2	D	148	PRO
2	F	388	VAL
1	C	479	ILE
1	A	395	GLY
1	B	397	ILE
2	F	148	PRO
2	E	390	GLY

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	502/509 (99%)	502 (100%)	0	100	100
1	B	502/509 (99%)	497 (99%)	5 (1%)	68	75
1	C	500/509 (98%)	497 (99%)	3 (1%)	78	80
2	D	356/380 (94%)	354 (99%)	2 (1%)	78	80
2	E	372/380 (98%)	368 (99%)	4 (1%)	65	74
2	F	368/380 (97%)	363 (99%)	5 (1%)	59	71
All	All	2600/2667 (98%)	2581 (99%)	19 (1%)	76	78

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	VAL
1	B	222	VAL
1	B	470	LEU
1	B	473	ILE
1	B	577	ILE
1	C	182	LEU
1	C	215	VAL
1	C	270	VAL
2	D	138	LEU
2	D	158	SER
2	E	18	VAL
2	E	128	ILE
2	E	250	MET
2	E	401	TYR
2	F	41	ARG
2	F	298	VAL
2	F	331	ARG
2	F	378	GLN
2	F	407	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	242	GLN
1	C	50	GLN
1	C	101	ASN
1	C	108	GLN
1	C	160	GLN
1	C	204	ASN
1	C	243	HIS
1	C	264	ASN
1	C	297	ASN
1	C	403	GLN
1	C	429	ASN
2	D	139	ASN
2	D	212	ASN
2	D	365	HIS
2	D	410	ASN
2	D	414	ASN
2	E	64	ASN
2	E	78	GLN
2	E	137	HIS
2	E	242	HIS
2	E	300	GLN
2	F	215	ASN
2	F	371	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	ANP	C	602	3	33,33,33	1.25	6 (18%)	45,52,52	1.43	5 (11%)

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	ANP	C	602	3	-	8/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ANP	PG-O1G	2.64	1.50	1.46
4	C	602	ANP	C4-N3	-2.56	1.29	1.34
4	C	602	ANP	PB-O1B	2.42	1.49	1.46
4	C	602	ANP	PB-O3A	-2.39	1.56	1.59
4	C	602	ANP	PG-N3B	2.35	1.69	1.63
4	C	602	ANP	C8-N9	-2.11	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	ANP	C5-C4-N9	-5.20	100.14	105.81
4	C	602	ANP	C4-C5-N7	4.54	115.77	110.58
4	C	602	ANP	C6-C5-C4	-2.87	113.26	117.18
4	C	602	ANP	C4-N9-C8	2.78	108.66	105.74
4	C	602	ANP	C5-C4-N3	2.49	130.14	126.72

There are no chirality outliers.

All (8) torsion outliers are listed below:

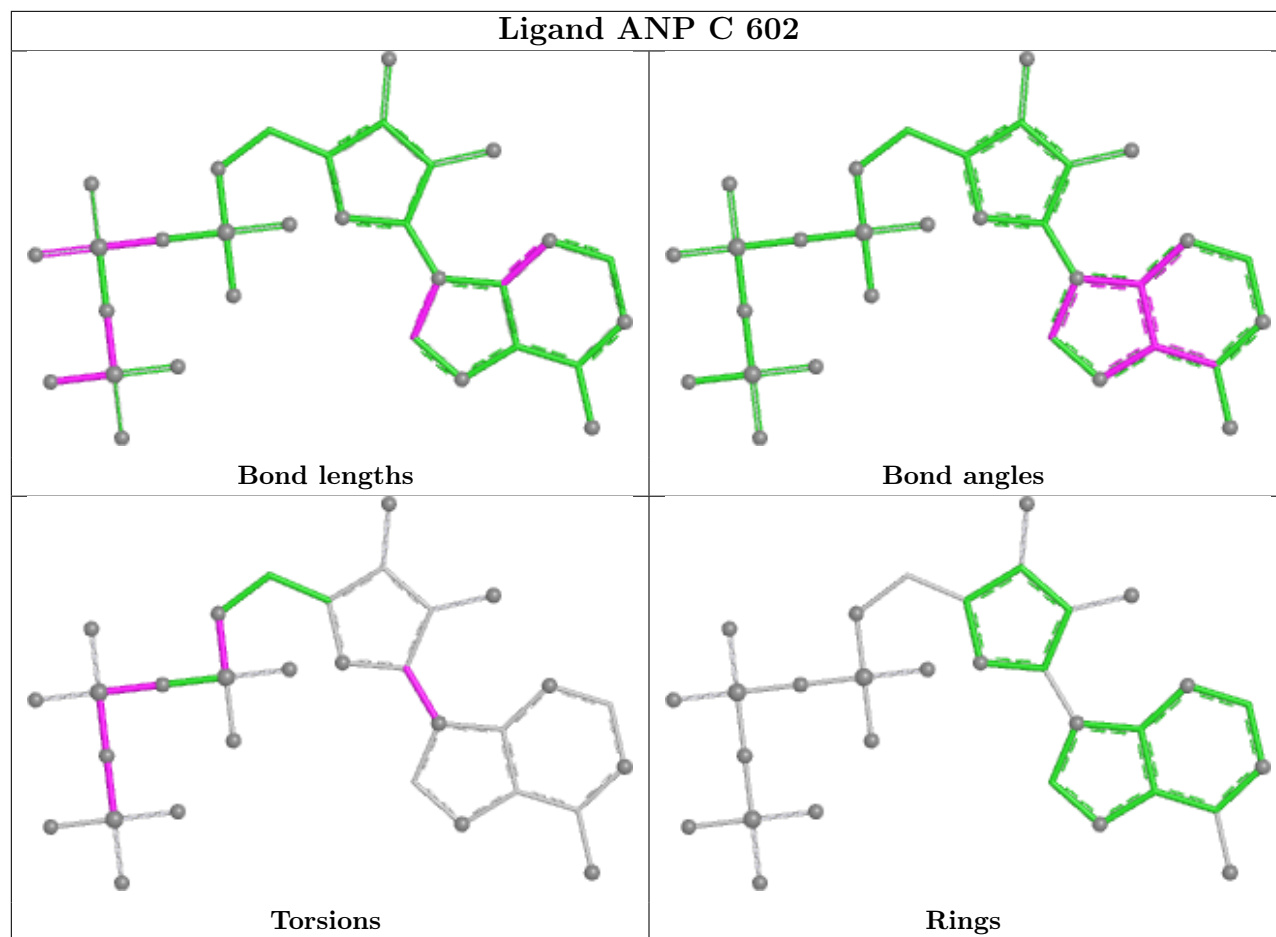
Mol	Chain	Res	Type	Atoms
4	C	602	ANP	PB-N3B-PG-O1G
4	C	602	ANP	PG-N3B-PB-O1B
4	C	602	ANP	PA-O3A-PB-O2B
4	C	602	ANP	C5'-O5'-PA-O1A
4	C	602	ANP	O4'-C1'-N9-C4
4	C	602	ANP	O4'-C1'-N9-C8
4	C	602	ANP	C5'-O5'-PA-O2A
4	C	602	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	602	ANP	8	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	586/596 (98%)	-0.47	0 100 100	50, 73, 117, 139	0
1	B	586/596 (98%)	-0.27	1 (0%) 91 84	69, 107, 156, 174	0
1	C	584/596 (97%)	-0.36	1 (0%) 91 84	61, 83, 141, 167	0
2	D	432/458 (94%)	-0.21	4 (0%) 81 62	54, 85, 172, 196	0
2	E	449/458 (98%)	-0.21	6 (1%) 75 55	57, 95, 162, 179	0
2	F	445/458 (97%)	-0.26	3 (0%) 84 67	63, 96, 142, 168	0
All	All	3082/3162 (97%)	-0.31	15 (0%) 87 72	50, 90, 151, 196	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	315	ILE	4.2
2	E	319	THR	3.9
1	B	137	GLY	3.1
2	D	314	PRO	2.8
2	D	413	VAL	2.8
2	F	445	ILE	2.6
2	D	376	TYR	2.5
2	E	146	LYS	2.4
2	F	446	LYS	2.4
1	C	425	PHE	2.4
2	F	185	GLY	2.3
2	D	315	ILE	2.3
2	E	412	TYR	2.1
2	E	385	LEU	2.1
2	E	397	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

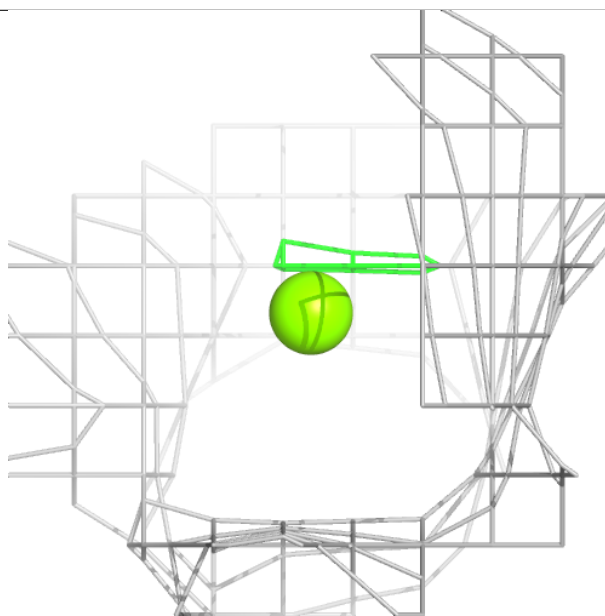
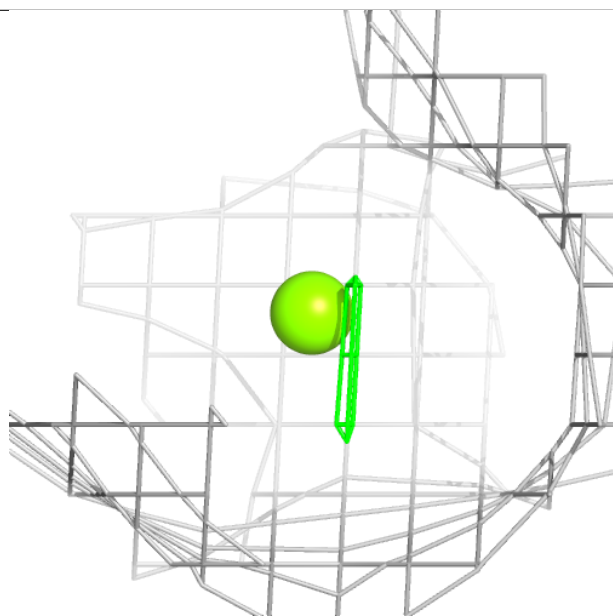
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

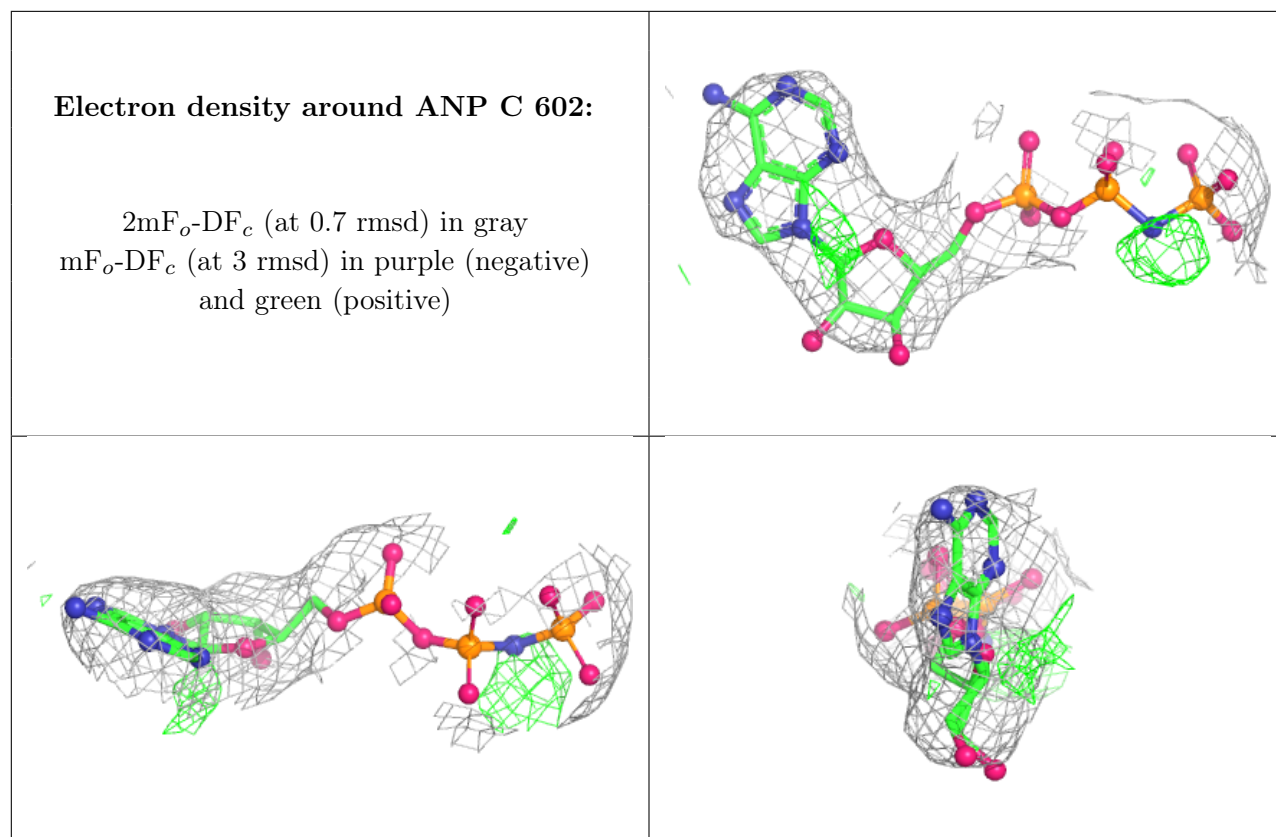
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	601	1/1	0.95	0.11	68,68,68,68	0
4	ANP	C	602	31/31	0.95	0.08	76,90,103,112	0

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 MG C 601:

$2mF_o-DF_c$ (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.