



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:31 am BST

PDB ID : 1QVR
Title : Crystal Structure Analysis of ClpB
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Deposited on : 2003-08-28
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

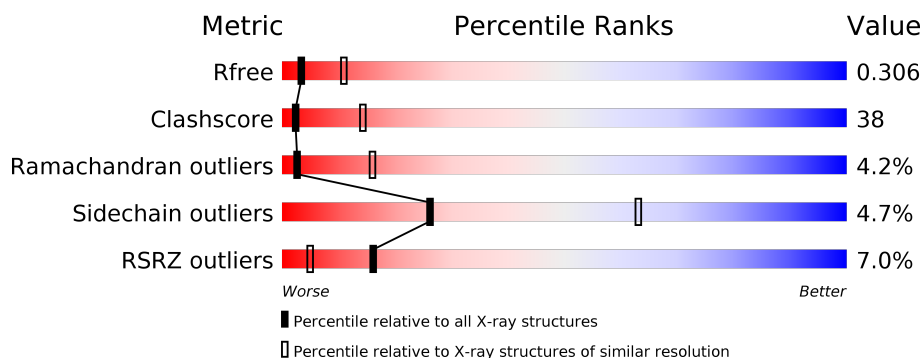
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	854	<div> <div>5%</div> <div> <div>39%</div> <div>50%</div> <div>5%</div> <div>6%</div> </div> </div>
1	B	854	<div> <div>2%</div> <div> <div>39%</div> <div>50%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	854	<div> <div>13%</div> <div> <div>41%</div> <div>48%</div> <div>•</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19496 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 ClpB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			
1	B	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			
1	C	803	Total	C	N	O	S	0	0	0
			6429	4050	1168	1204	7			

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Pt	0	0
			8	8		
2	A	8	Total	Pt	0	0
			8	8		
2	C	7	Total	Pt	0	0
			7	7		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

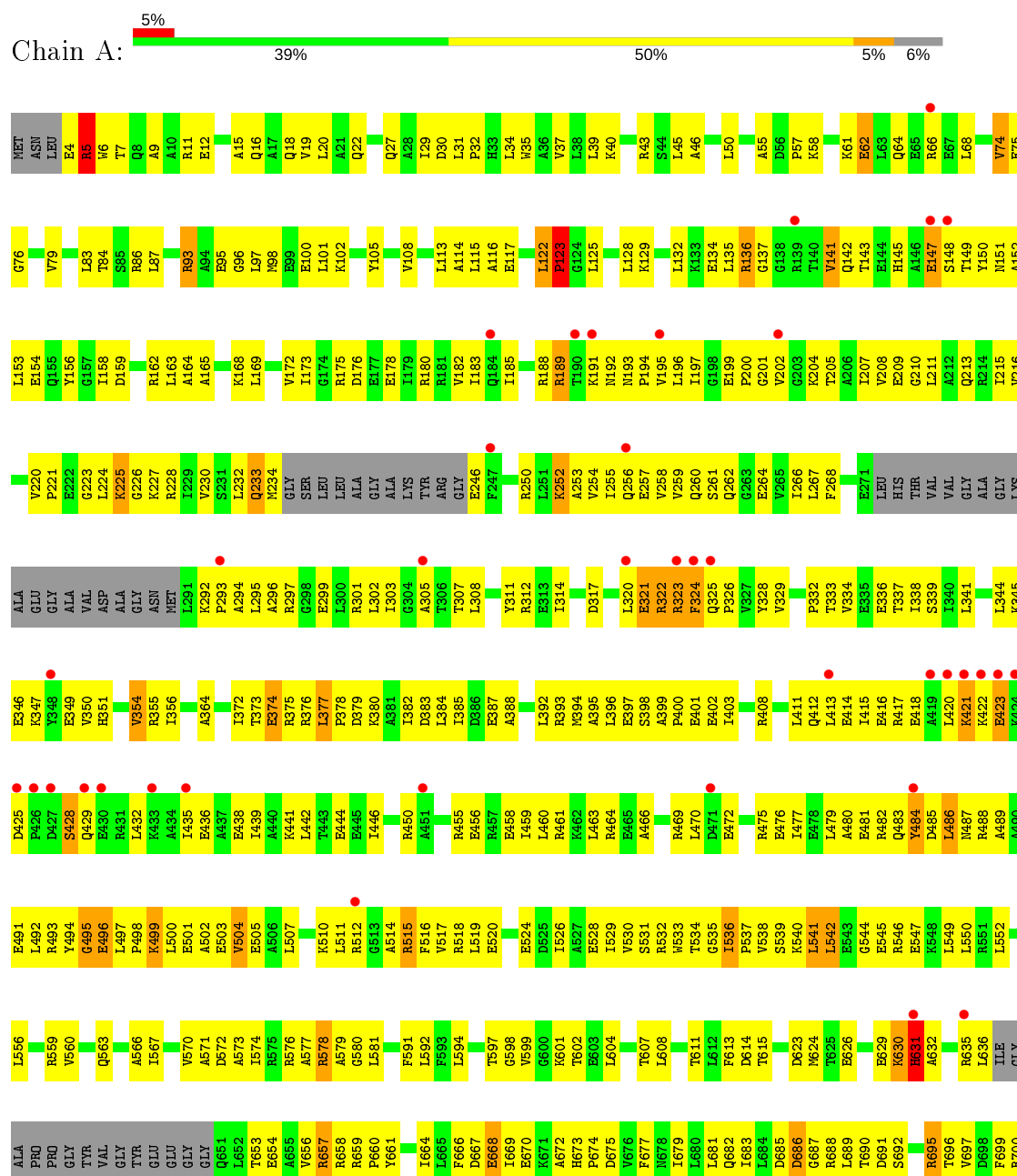


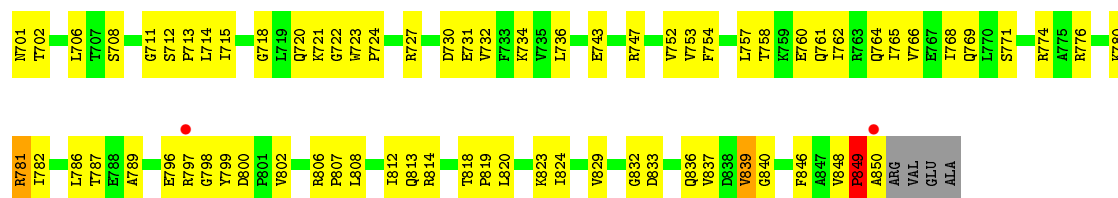
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

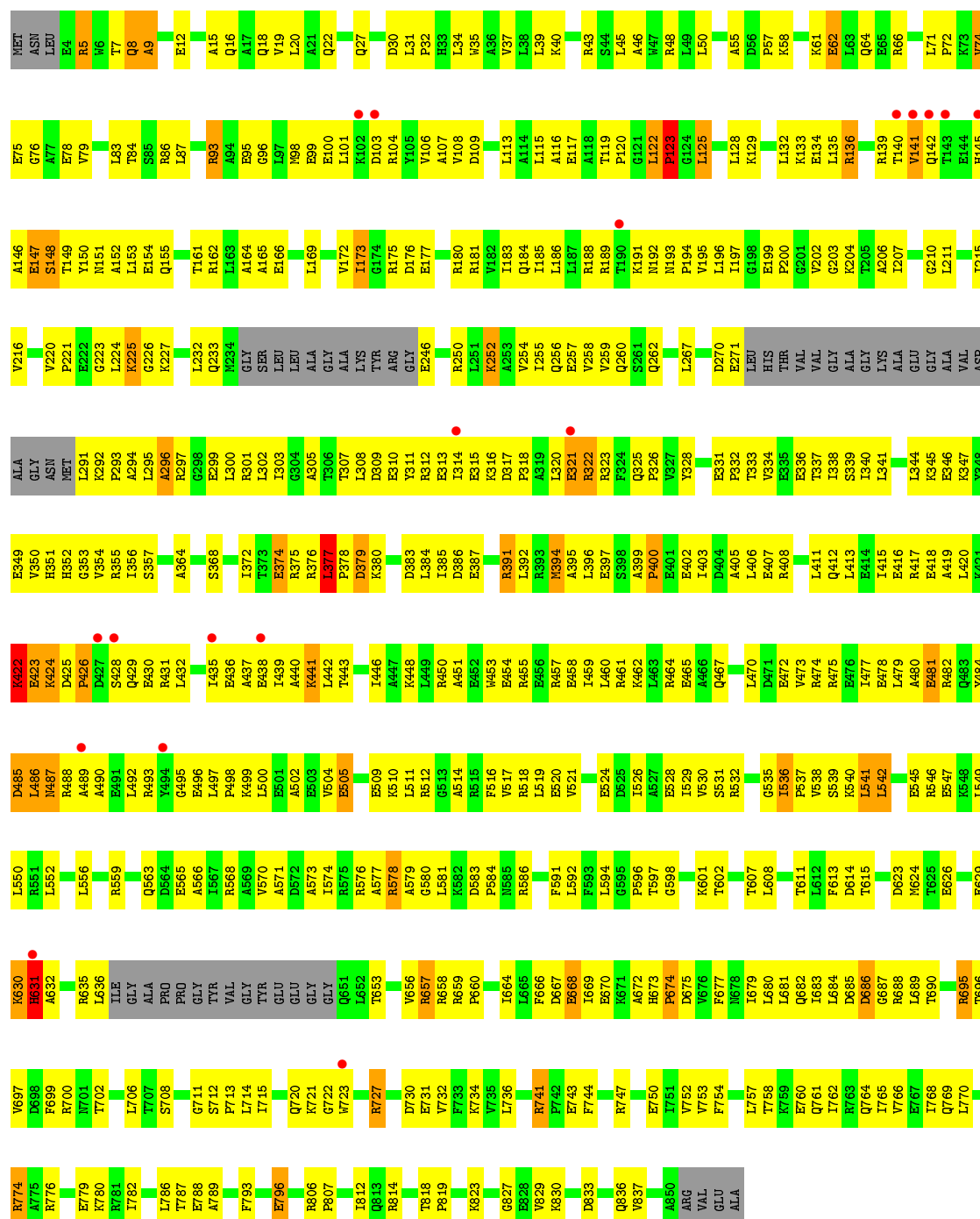
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

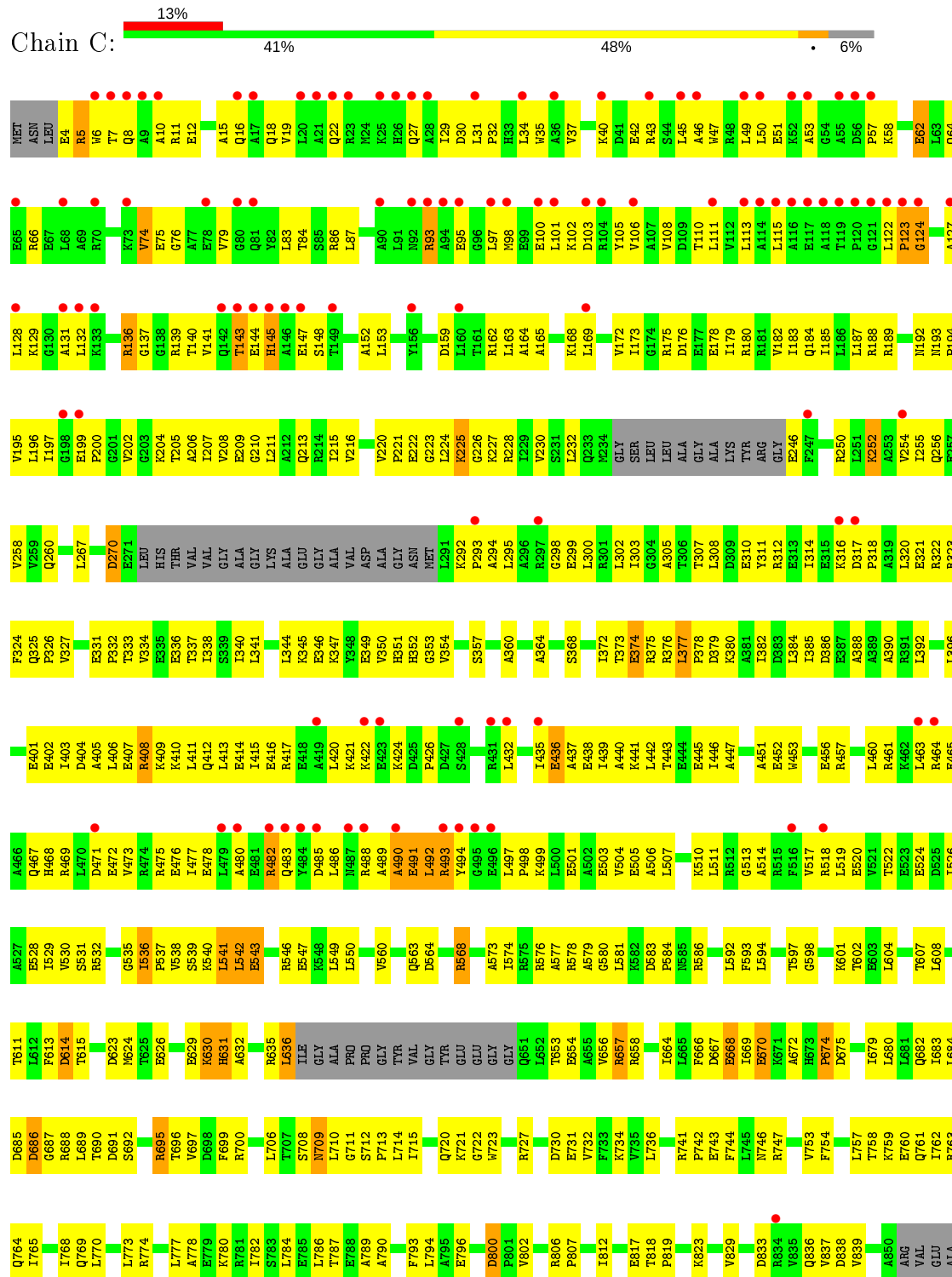




● Molecule 1: ClpB protein



● Molecule 1: ClpB protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.75Å 138.48Å 212.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 3.00 48.04 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.4 (48.04-3.00) 88.5 (48.04-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.307 0.258 , 0.306	Depositor DCC
R_{free} test set	5098 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19496	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, PT

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	0.29	0/6513	0.57	2/8778 (0.0%)
1	B	0.31	0/6513	0.60	7/8778 (0.1%)
1	C	0.28	0/6513	0.57	1/8778 (0.0%)
All	All	0.29	0/19539	0.58	10/26334 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	659	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	658	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	658	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	781	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	B	377	LEU	N-CA-C	5.32	125.37	111.00
1	B	741	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	781	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	493	ARG	N-CA-C	-5.22	96.91	111.00
1	B	741	ARG	NE-CZ-NH2	-5.21	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

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	6429	0	6642	517	0
1	B	6429	0	6643	530	0
1	C	6429	0	6642	475	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	7	0	0	0	0
3	A	62	0	26	9	0
3	B	62	0	26	5	0
3	C	62	0	26	5	0
All	All	19496	0	20005	1495	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 38.

All (1495) 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:C:165:ALA:HA	1:C:216:VAL:HG11	1.32	1.10
1:A:20:LEU:HB2	1:A:262:GLN:HE22	1.20	1.05
1:A:839:VAL:HG22	1:A:840:GLY:H	1.20	1.04
1:A:5:ARG:HD2	1:A:6:TRP:H	1.25	0.99
1:B:175:ARG:HD3	1:B:207:ILE:HD11	1.44	0.97
1:B:524:GLU:HG2	1:B:541:LEU:HD21	1.47	0.96
1:A:158:ILE:HG13	1:A:233:GLN:HE22	1.29	0.96
1:C:406:LEU:HD22	1:C:442:LEU:HD11	1.48	0.95
1:B:32:PRO:HG3	1:B:64:GLN:HE21	1.31	0.95
1:A:141:VAL:HG12	1:A:142:GLN:H	1.31	0.93
1:A:5:ARG:HD2	1:A:6:TRP:N	1.84	0.92
1:B:607:THR:O	1:B:611:THR:HG22	1.69	0.91
1:B:446:ILE:HG22	1:B:450:ARG:NH2	1.86	0.91
1:C:607:THR:O	1:C:611:THR:HG22	1.70	0.91
1:A:607:THR:O	1:A:611:THR:HG22	1.70	0.91
1:C:175:ARG:HD3	1:C:207:ILE:HD11	1.51	0.90
1:B:139:ARG:HG2	1:B:140:THR:H	1.37	0.88
1:A:323:ARG:HH11	1:A:323:ARG:HB3	1.36	0.88
1:C:489:ALA:HB1	1:C:493:ARG:HH12	1.38	0.87
1:A:175:ARG:HD3	1:A:207:ILE:HD11	1.54	0.87
1:A:32:PRO:HG3	1:A:64:GLN:HE21	1.39	0.87
1:A:396:LEU:HA	1:A:516:PHE:CE1	2.10	0.86
1:B:34:LEU:HD23	1:B:115:LEU:HD11	1.57	0.86
1:A:683:ILE:HD11	1:A:689:LEU:HD22	1.55	0.86
1:A:149:THR:HA	1:A:154:GLU:CG	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:LEU:HD11	1:C:578:ARG:HG3	1.57	0.85
1:C:392:LEU:HD11	1:C:518:ARG:HB3	1.58	0.85
1:C:255:ILE:HD11	1:C:294:ALA:HB3	1.58	0.85
1:B:441:LYS:HD3	1:B:442:LEU:N	1.92	0.85
1:A:185:ILE:HG23	1:A:325:GLN:HG3	1.57	0.85
1:C:635:ARG:HH12	1:C:679:ILE:HG21	1.40	0.84
1:A:486:LEU:HA	1:A:489:ALA:HB3	1.57	0.83
1:A:149:THR:HA	1:A:154:GLU:HG2	1.58	0.83
1:A:183:ILE:HD11	1:A:211:LEU:HD13	1.61	0.82
1:A:848:VAL:HG12	1:A:849:PRO:HD2	1.61	0.82
1:A:399:ALA:HB3	1:A:400:PRO:HD3	1.62	0.81
1:B:787:THR:HG22	1:B:789:ALA:H	1.43	0.81
1:A:34:LEU:HD23	1:A:115:LEU:HD11	1.60	0.81
1:C:492:LEU:C	1:C:494:TYR:H	1.81	0.81
1:A:602:THR:HB	3:A:911:ANP:O2A	1.79	0.81
1:C:183:ILE:HD11	1:C:211:LEU:HD13	1.61	0.81
1:A:165:ALA:HA	1:A:216:VAL:HG11	1.62	0.81
1:B:5:ARG:HE	1:B:5:ARG:HA	1.46	0.80
1:B:635:ARG:HH12	1:B:679:ILE:HG21	1.46	0.80
1:B:172:VAL:HG21	1:B:210:GLY:HA3	1.63	0.80
1:A:158:ILE:HG13	1:A:233:GLN:NE2	1.96	0.80
1:C:4:GLU:HB3	1:C:95:GLU:OE2	1.81	0.80
1:A:848:VAL:CG1	1:A:849:PRO:HD2	2.12	0.79
1:C:602:THR:HB	3:C:913:ANP:O2A	1.81	0.79
1:C:152:ALA:HB1	1:C:254:VAL:HG22	1.64	0.79
1:A:169:LEU:HD13	1:A:209:GLU:HB2	1.65	0.79
1:C:511:LEU:HD23	1:C:519:LEU:HD22	1.64	0.79
1:B:459:ILE:HG21	1:B:511:LEU:HD21	1.64	0.79
1:B:495:GLY:H	1:B:498:PRO:HG2	1.48	0.79
1:A:488:ARG:HA	1:A:491:GLU:HG2	1.66	0.78
1:B:602:THR:HB	3:B:912:ANP:O2A	1.83	0.78
1:A:492:LEU:HD23	1:A:496:GLU:HG3	1.66	0.78
1:A:787:THR:HG22	1:A:789:ALA:H	1.48	0.78
1:B:762:ILE:O	1:B:766:VAL:HG23	1.83	0.78
1:C:175:ARG:HD3	1:C:207:ILE:CD1	2.14	0.78
1:C:396:LEU:HD13	1:C:518:ARG:HB2	1.64	0.78
1:A:573:ALA:HA	1:A:576:ARG:NH1	1.99	0.77
1:C:629:GLU:HG2	1:C:630:LYS:H	1.49	0.77
1:A:259:VAL:HG23	1:A:299:GLU:HB3	1.67	0.77
1:C:629:GLU:HG2	1:C:630:LYS:HD3	1.64	0.77
1:B:460:LEU:HD21	1:B:464:ARG:CZ	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD11	1:A:578:ARG:HG3	1.65	0.76
1:B:629:GLU:HG2	1:B:630:LYS:HD3	1.65	0.76
1:A:629:GLU:HG2	1:A:630:LYS:HD3	1.67	0.76
1:B:757:LEU:HB2	1:B:762:ILE:HD11	1.67	0.76
1:A:321:GLU:C	1:A:323:ARG:H	1.89	0.76
1:B:125:LEU:H	1:B:125:LEU:HD12	1.50	0.76
1:A:441:LYS:NZ	1:A:441:LYS:HB3	2.01	0.76
1:A:818:THR:HB	1:A:819:PRO:HD3	1.68	0.76
1:A:32:PRO:HA	1:A:64:GLN:HG3	1.68	0.76
1:B:549:LEU:HD11	1:B:578:ARG:HG3	1.68	0.76
1:A:661:TYR:CE2	1:A:701:ASN:ND2	2.53	0.76
1:B:721:LYS:HD3	1:B:723:TRP:HZ3	1.50	0.76
1:C:453:TRP:O	1:C:457:ARG:HB2	1.86	0.75
1:C:564:ASP:O	1:C:568:ARG:HG3	1.86	0.75
1:B:48:ARG:HE	1:B:150:TYR:HB3	1.50	0.75
1:A:145:HIS:CE1	1:A:162:ARG:HD3	2.22	0.75
1:B:629:GLU:HG2	1:B:630:LYS:H	1.51	0.75
1:A:50:LEU:HB3	1:A:57:PRO:HG3	1.68	0.75
1:C:514:ALA:O	1:C:517:VAL:HG13	1.87	0.75
1:C:683:ILE:HD11	1:C:689:LEU:HD22	1.67	0.74
1:B:188:ARG:NH2	1:B:325:GLN:HG3	2.02	0.74
1:C:473:VAL:HG11	1:C:497:LEU:HD11	1.69	0.74
1:C:486:LEU:O	1:C:491:GLU:HB2	1.88	0.74
1:C:501:GLU:O	1:C:505:GLU:HG2	1.88	0.74
1:B:457:ARG:HB3	1:B:461:ARG:HH12	1.52	0.73
1:B:311:TYR:CZ	1:B:326:PRO:HG3	2.23	0.73
1:A:629:GLU:HG2	1:A:630:LYS:H	1.51	0.73
1:C:34:LEU:HD23	1:C:115:LEU:HD11	1.70	0.73
1:C:573:ALA:HA	1:C:576:ARG:NH1	2.03	0.73
1:B:573:ALA:HA	1:B:576:ARG:NH1	2.03	0.73
1:C:144:GLU:HG3	1:C:145:HIS:H	1.52	0.73
1:C:292:LYS:HB3	1:C:293:PRO:HD3	1.70	0.73
1:B:175:ARG:HD3	1:B:207:ILE:CD1	2.16	0.73
1:B:7:THR:HG21	1:B:107:ALA:HA	1.69	0.73
1:C:314:ILE:HG23	1:C:320:LEU:HD23	1.71	0.73
1:C:311:TYR:CE2	1:C:326:PRO:HG3	2.24	0.73
1:B:478:GLU:HG2	1:B:482:ARG:HH12	1.54	0.72
1:B:426:PRO:HA	1:B:430:GLU:HG2	1.71	0.72
1:A:632:ALA:HB2	1:A:675:ASP:OD1	1.89	0.72
1:C:764:GLN:O	1:C:768:ILE:HG22	1.89	0.72
1:B:172:VAL:HG21	1:B:210:GLY:CA	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:CZ	1:A:701:ASN:ND2	2.58	0.72
1:B:311:TYR:CE2	1:B:326:PRO:HG3	2.24	0.72
1:A:635:ARG:HH12	1:A:679:ILE:HG21	1.53	0.72
1:A:839:VAL:HG22	1:A:840:GLY:N	2.00	0.72
1:B:420:LEU:O	1:B:420:LEU:HD23	1.90	0.71
1:A:515:ARG:HD3	1:A:516:PHE:N	2.04	0.71
1:A:93:ARG:O	1:A:93:ARG:HD3	1.91	0.71
1:A:185:ILE:HD13	1:A:325:GLN:HB3	1.72	0.71
1:A:384:LEU:HG	1:A:529:ILE:HD11	1.73	0.71
1:C:93:ARG:HD3	1:C:93:ARG:O	1.90	0.71
1:A:45:LEU:HD23	1:A:108:VAL:HG23	1.73	0.71
1:B:391:ARG:HH12	1:B:528:GLU:HB3	1.54	0.71
1:C:32:PRO:HG3	1:C:64:GLN:HE21	1.56	0.71
1:A:347:LYS:HD2	1:A:351:HIS:NE2	2.05	0.70
1:C:624:MET:HG2	1:C:672:ALA:HB2	1.72	0.70
1:B:139:ARG:HG2	1:B:140:THR:N	2.06	0.70
1:B:770:LEU:HB3	1:B:774:ARG:NH1	2.07	0.70
1:C:679:ILE:H	1:C:679:ILE:HD12	1.56	0.70
1:B:93:ARG:O	1:B:93:ARG:HD3	1.90	0.70
1:C:461:ARG:HD2	1:C:461:ARG:O	1.91	0.70
1:A:317:ASP:C	1:A:321:GLU:HG2	2.12	0.70
1:B:446:ILE:HG22	1:B:450:ARG:HH21	1.56	0.70
1:C:232:LEU:HB2	1:C:267:LEU:HD11	1.73	0.70
1:B:632:ALA:HB2	1:B:675:ASP:OD1	1.91	0.70
1:C:163:LEU:HB3	1:C:168:LYS:HB3	1.74	0.70
1:C:173:ILE:HD11	1:C:340:ILE:HA	1.74	0.70
1:A:388:ALA:HB2	1:A:529:ILE:HD13	1.72	0.69
1:C:715:ILE:HD13	1:C:753:VAL:HG23	1.73	0.69
1:C:95:GLU:O	1:C:98:MET:HG2	1.93	0.69
1:A:22:GLN:HA	1:A:79:VAL:CG1	2.22	0.69
1:A:201:GLY:O	1:A:378:PRO:HB2	1.92	0.69
1:B:436:GLU:O	1:B:439:ILE:HG22	1.93	0.69
1:B:34:LEU:CD2	1:B:115:LEU:HD11	2.21	0.69
1:B:318:PRO:HA	1:B:321:GLU:HG2	1.73	0.69
1:A:193:ASN:ND2	1:A:295:LEU:HD11	2.08	0.69
1:B:27:GLN:HB2	1:B:74:VAL:HG11	1.74	0.69
1:A:344:LEU:H	1:A:344:LEU:HD12	1.58	0.69
1:C:653:THR:O	1:C:657:ARG:HB2	1.91	0.69
1:C:311:TYR:CZ	1:C:326:PRO:HG3	2.27	0.69
1:A:175:ARG:HD3	1:A:207:ILE:CD1	2.21	0.69
1:A:396:LEU:HA	1:A:516:PHE:HE1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLY:H	1:B:225:LYS:HE2	1.58	0.69
1:C:124:GLY:O	1:C:128:LEU:HD12	1.93	0.69
1:B:629:GLU:CG	1:B:630:LYS:HD3	2.23	0.68
1:C:629:GLU:CG	1:C:630:LYS:HD3	2.22	0.68
1:A:141:VAL:HG12	1:A:142:GLN:N	2.08	0.68
1:A:630:LYS:H	1:A:630:LYS:HD3	1.58	0.68
1:A:849:PRO:O	1:A:850:ALA:O	2.11	0.68
1:A:466:ALA:HB3	1:A:504:VAL:HG23	1.75	0.68
1:C:478:GLU:O	1:C:482:ARG:HB2	1.94	0.68
1:C:758:THR:OG1	1:C:761:GLN:HG3	1.94	0.68
1:B:480:ALA:CB	1:B:489:ALA:HB2	2.24	0.68
1:B:679:ILE:HD12	1:B:679:ILE:H	1.59	0.68
1:C:202:VAL:HG13	1:C:331:GLU:HA	1.74	0.68
1:A:743:GLU:O	1:A:747:ARG:HG2	1.95	0.67
1:C:223:GLY:H	1:C:225:LYS:HE2	1.59	0.67
1:A:679:ILE:HG23	1:A:689:LEU:HD11	1.76	0.67
1:A:559:ARG:HA	1:A:768:ILE:CD1	2.23	0.67
1:C:318:PRO:HA	1:C:321:GLU:HB3	1.75	0.67
1:C:350:VAL:HG22	1:C:467:GLN:HB3	1.75	0.67
1:A:223:GLY:H	1:A:225:LYS:HE2	1.58	0.67
1:B:394:MET:HG3	1:B:395:ALA:N	2.08	0.67
1:A:125:LEU:HD23	1:A:129:LYS:HE3	1.77	0.67
1:B:12:GLU:O	1:B:16:GLN:HG2	1.94	0.67
1:C:188:ARG:O	1:C:192:ASN:HB3	1.94	0.67
1:A:415:ILE:HG13	1:B:486:LEU:HG	1.76	0.67
1:A:476:GLU:HG2	1:A:488:ARG:HH21	1.60	0.67
1:B:743:GLU:O	1:B:747:ARG:HG2	1.95	0.67
1:A:172:VAL:HG21	1:A:210:GLY:CA	2.25	0.67
1:B:255:ILE:HD11	1:B:294:ALA:HB2	1.77	0.67
1:A:629:GLU:CG	1:A:630:LYS:HD3	2.24	0.67
1:C:682:GLN:NE2	1:C:689:LEU:HD12	2.10	0.67
1:B:344:LEU:H	1:B:344:LEU:HD12	1.60	0.67
1:B:715:ILE:HD13	1:B:753:VAL:HG23	1.75	0.67
1:C:7:THR:O	1:C:11:ARG:HB2	1.95	0.67
1:C:818:THR:HB	1:C:819:PRO:HD3	1.75	0.67
1:A:679:ILE:HD12	1:A:679:ILE:H	1.60	0.66
1:B:598:GLY:HA2	3:B:912:ANP:O3A	1.95	0.66
1:B:624:MET:HB3	1:B:667:ASP:O	1.95	0.66
1:C:12:GLU:O	1:C:16:GLN:HG2	1.95	0.66
1:A:758:THR:OG1	1:A:761:GLN:HG3	1.94	0.66
1:A:12:GLU:O	1:A:16:GLN:HG2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:LYS:H	1:B:630:LYS:HD3	1.60	0.66
1:A:102:LYS:O	1:A:102:LYS:HG2	1.95	0.66
1:B:32:PRO:HG3	1:B:64:GLN:NE2	2.06	0.66
1:B:478:GLU:HG2	1:B:482:ARG:NH1	2.10	0.66
1:B:425:ASP:N	1:B:426:PRO:HD3	2.11	0.66
1:B:384:LEU:HD21	1:B:530:VAL:HG22	1.78	0.66
1:B:653:THR:O	1:B:657:ARG:HB2	1.95	0.66
1:C:408:ARG:NH1	1:C:411:LEU:HD23	2.11	0.66
1:A:149:THR:HA	1:A:154:GLU:HG3	1.77	0.66
1:A:323:ARG:C	1:A:325:GLN:H	1.99	0.66
1:A:764:GLN:O	1:A:768:ILE:HG22	1.96	0.66
1:B:334:VAL:O	1:B:338:ILE:HG13	1.95	0.66
1:B:255:ILE:HD11	1:B:294:ALA:CB	2.26	0.65
1:B:412:GLN:O	1:B:415:ILE:HG22	1.95	0.65
1:C:573:ALA:HA	1:C:576:ARG:HH12	1.61	0.65
1:C:711:GLY:O	1:C:715:ILE:HG13	1.96	0.65
1:B:443:THR:HA	1:B:446:ILE:HD12	1.77	0.65
1:B:531:SER:CB	1:B:537:PRO:HG3	2.26	0.65
1:B:458:GLU:HG3	1:B:462:LYS:HE3	1.77	0.65
1:C:139:ARG:NH2	1:C:148:SER:H	1.94	0.65
1:C:172:VAL:HG21	1:C:210:GLY:CA	2.25	0.65
1:C:153:LEU:HD22	1:C:230:VAL:HG11	1.78	0.65
1:C:506:ALA:O	1:C:510:LYS:HG3	1.97	0.65
1:B:183:ILE:HD12	1:B:220:VAL:HG23	1.79	0.65
1:B:32:PRO:HA	1:B:64:GLN:HG3	1.78	0.65
1:B:419:ALA:O	1:B:422:LYS:HG3	1.95	0.65
1:C:630:LYS:H	1:C:630:LYS:HD3	1.60	0.65
1:A:176:ASP:O	1:A:180:ARG:HG3	1.97	0.65
1:B:764:GLN:O	1:B:768:ILE:HG22	1.96	0.65
1:B:153:LEU:HD23	1:B:254:VAL:HG13	1.77	0.65
1:B:271:GLU:HA	1:B:305:ALA:O	1.96	0.65
1:A:715:ILE:HD13	1:A:753:VAL:HG23	1.78	0.65
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.60	0.65
1:A:653:THR:O	1:A:657:ARG:HB2	1.97	0.65
1:B:104:ARG:HB2	1:B:139:ARG:HH21	1.61	0.65
1:C:404:ASP:HA	1:C:407:GLU:HB2	1.77	0.65
1:A:153:LEU:HD22	1:A:230:VAL:HG11	1.79	0.65
1:A:252:LYS:HA	1:A:255:ILE:HG22	1.79	0.65
1:A:432:LEU:HD23	1:A:432:LEU:H	1.61	0.65
1:B:188:ARG:O	1:B:192:ASN:HB3	1.96	0.65
1:B:46:ALA:O	1:B:50:LEU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:LEU:CD1	1:C:578:ARG:HG3	2.27	0.65
1:C:787:THR:HG22	1:C:789:ALA:H	1.61	0.65
1:C:252:LYS:HA	1:C:255:ILE:HG22	1.79	0.65
1:C:344:LEU:H	1:C:344:LEU:HD12	1.61	0.65
1:C:629:GLU:HG2	1:C:630:LYS:N	2.11	0.64
1:A:806:ARG:HB3	1:A:807:PRO:HD3	1.80	0.64
1:B:270:ASP:O	1:B:305:ALA:HB3	1.97	0.64
1:B:309:ASP:O	1:B:313:GLU:HG2	1.97	0.64
1:C:185:ILE:HG21	1:C:194:PRO:HB3	1.78	0.64
1:C:392:LEU:CD1	1:C:518:ARG:HB3	2.25	0.64
1:A:573:ALA:HA	1:A:576:ARG:HH12	1.63	0.64
1:B:295:LEU:HB3	1:B:323:ARG:HD3	1.79	0.64
1:B:311:TYR:OH	1:B:326:PRO:HG3	1.97	0.64
1:B:403:ILE:O	1:B:407:GLU:HG2	1.97	0.64
1:B:573:ALA:HA	1:B:576:ARG:HH12	1.61	0.64
1:C:316:LYS:O	1:C:318:PRO:HD3	1.98	0.64
1:B:8:GLN:H	1:B:8:GLN:NE2	1.96	0.64
1:C:417:ARG:HG3	1:C:432:LEU:CD1	2.28	0.64
1:B:344:LEU:HD11	3:B:902:ANP:H2	1.78	0.64
1:A:7:THR:O	1:A:11:ARG:HB2	1.97	0.64
1:B:818:THR:HB	1:B:819:PRO:HD3	1.80	0.64
1:B:7:THR:CG2	1:B:107:ALA:HA	2.28	0.64
1:B:514:ALA:HB3	1:B:517:VAL:O	1.97	0.64
1:C:178:GLU:HB2	1:C:207:ILE:HD12	1.80	0.64
1:C:45:LEU:HD23	1:C:108:VAL:HG23	1.80	0.64
1:C:172:VAL:HG21	1:C:210:GLY:HA2	1.78	0.63
1:A:46:ALA:O	1:A:50:LEU:HB2	1.98	0.63
1:B:195:VAL:HG13	1:B:197:ILE:HD11	1.79	0.63
1:B:629:GLU:HG2	1:B:630:LYS:N	2.12	0.63
1:C:136:ARG:HA	1:C:136:ARG:HE	1.64	0.63
1:C:159:ASP:OD2	1:C:228:ARG:HD3	1.98	0.63
1:C:46:ALA:O	1:C:50:LEU:HB2	1.98	0.63
1:C:635:ARG:HH22	1:C:679:ILE:CG1	2.11	0.63
1:B:368:SER:HA	1:B:372:ILE:HG13	1.81	0.63
1:B:460:LEU:HD21	1:B:464:ARG:NE	2.12	0.63
1:A:191:LYS:HD2	1:A:325:GLN:NE2	2.13	0.63
1:B:307:THR:HG22	1:B:308:LEU:N	2.14	0.63
1:C:51:GLU:HB2	1:C:57:PRO:HG2	1.80	0.63
1:C:5:ARG:HD3	1:C:6:TRP:H	1.63	0.63
1:A:459:ILE:HD13	1:A:510:LYS:HG3	1.81	0.63
1:C:139:ARG:HH22	1:C:148:SER:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:GLU:O	1:C:747:ARG:HG2	1.97	0.63
1:A:197:ILE:O	1:A:328:TYR:HA	1.98	0.63
1:A:472:GLU:HG3	1:A:475:ARG:HH21	1.63	0.63
1:B:165:ALA:HA	1:B:216:VAL:HG11	1.81	0.63
1:B:295:LEU:C	1:B:297:ARG:H	2.02	0.63
1:C:635:ARG:HH22	1:C:679:ILE:HG12	1.62	0.63
1:A:163:LEU:HB3	1:A:168:LYS:HB3	1.80	0.63
1:A:578:ARG:C	1:A:580:GLY:H	2.02	0.63
1:B:252:LYS:HA	1:B:255:ILE:HG22	1.79	0.63
1:C:299:GLU:O	1:C:300:LEU:HB3	1.97	0.63
1:A:4:GLU:HA	1:A:11:ARG:NH2	2.13	0.62
1:C:164:ALA:HB1	1:C:213:GLN:HA	1.81	0.62
1:C:176:ASP:O	1:C:180:ARG:HG3	1.99	0.62
1:C:5:ARG:CD	1:C:6:TRP:H	2.12	0.62
1:B:383:ASP:O	1:B:387:GLU:HB2	1.97	0.62
1:B:524:GLU:HG2	1:B:541:LEU:CD2	2.27	0.62
1:B:529:ILE:HA	1:B:532:ARG:HD3	1.81	0.62
1:B:122:LEU:HB2	1:B:123:PRO:HD2	1.80	0.62
1:B:199:GLU:HG3	1:B:200:PRO:HD2	1.80	0.62
1:A:332:PRO:HD2	1:A:378:PRO:CG	2.30	0.62
1:C:163:LEU:HD22	1:C:168:LYS:HG2	1.82	0.62
1:C:492:LEU:C	1:C:494:TYR:N	2.50	0.62
1:B:480:ALA:C	1:B:482:ARG:H	2.03	0.62
1:B:353:GLY:O	1:B:519:LEU:HD11	1.99	0.62
1:C:333:THR:OG1	1:C:336:GLU:HG3	2.00	0.62
1:C:185:ILE:O	1:C:192:ASN:HA	1.98	0.62
1:C:486:LEU:CD1	1:C:491:GLU:HG2	2.29	0.62
1:C:6:TRP:HE3	1:C:10:ALA:HB1	1.64	0.62
1:A:101:LEU:O	1:A:102:LYS:HB3	1.99	0.62
1:B:307:THR:HG22	1:B:308:LEU:H	1.64	0.62
1:C:307:THR:HG22	1:C:308:LEU:H	1.65	0.62
1:C:670:GLU:HB3	1:C:710:LEU:HD11	1.81	0.62
1:B:175:ARG:HH11	1:B:175:ARG:HG2	1.65	0.61
1:B:391:ARG:HB2	1:C:184:GLN:NE2	2.15	0.61
1:A:334:VAL:O	1:A:338:ILE:HG13	2.00	0.61
1:B:408:ARG:CZ	1:B:411:LEU:HD23	2.30	0.61
1:A:148:SER:O	1:A:154:GLU:HG2	2.00	0.61
1:B:480:ALA:HB3	1:B:489:ALA:HB2	1.82	0.61
1:B:510:LYS:C	1:B:511:LEU:HD23	2.21	0.61
1:C:446:ILE:HG22	1:C:446:ILE:O	1.99	0.61
1:A:344:LEU:HD12	1:A:344:LEU:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:O	1:A:79:VAL:HG23	2.00	0.61
1:B:510:LYS:O	1:B:511:LEU:HD23	2.01	0.61
1:A:195:VAL:HG13	1:A:197:ILE:HD11	1.81	0.61
1:A:629:GLU:HG2	1:A:630:LYS:N	2.13	0.61
1:C:806:ARG:HD2	3:C:913:ANP:O3G	2.00	0.61
1:B:352:HIS:O	1:B:354:VAL:HG13	2.01	0.61
1:C:195:VAL:HG13	1:C:197:ILE:HD11	1.81	0.61
1:C:709:ASN:ND2	1:C:709:ASN:N	2.49	0.61
1:B:75:GLU:O	1:B:79:VAL:HG23	2.00	0.61
1:B:568:ARG:HG2	1:B:568:ARG:HH11	1.65	0.60
1:C:408:ARG:O	1:C:412:GLN:HG2	2.00	0.60
1:C:447:ALA:O	1:C:451:ALA:HB2	2.00	0.60
1:A:145:HIS:NE2	1:A:147:GLU:HG2	2.16	0.60
1:B:374:GLU:HG3	1:B:375:ARG:N	2.16	0.60
1:B:721:LYS:HD3	1:B:723:TRP:CZ3	2.33	0.60
1:C:225:LYS:HD2	1:C:226:GLY:H	1.65	0.60
1:A:208:VAL:HG11	1:A:268:PHE:CD2	2.36	0.60
1:A:483:GLN:O	1:A:485:ASP:N	2.34	0.60
1:A:526:ILE:O	1:A:530:VAL:HG23	2.02	0.60
1:A:559:ARG:HA	1:A:768:ILE:HD12	1.84	0.60
1:B:185:ILE:O	1:B:192:ASN:HA	2.00	0.60
1:B:758:THR:OG1	1:B:761:GLN:HG3	2.01	0.60
1:C:100:GLU:HG3	1:C:101:LEU:N	2.15	0.60
1:C:295:LEU:HD21	1:C:324:PHE:CZ	2.37	0.60
1:C:334:VAL:O	1:C:338:ILE:HG13	2.02	0.60
1:A:27:GLN:HB2	1:A:74:VAL:HG11	1.81	0.60
1:C:598:GLY:HA2	3:C:913:ANP:O3A	2.01	0.60
1:A:425:ASP:HB3	1:A:428:SER:HB3	1.82	0.60
1:B:225:LYS:HD2	1:B:226:GLY:H	1.66	0.60
1:B:333:THR:OG1	1:B:336:GLU:HG3	2.01	0.60
1:B:806:ARG:HH21	1:C:746:ASN:ND2	1.98	0.60
1:C:30:ASP:OD1	1:C:86:ARG:NH2	2.35	0.60
1:A:225:LYS:HD2	1:A:226:GLY:H	1.66	0.60
1:A:541:LEU:HG	1:A:542:LEU:N	2.17	0.60
1:A:188:ARG:O	1:A:192:ASN:HB3	2.00	0.60
1:A:333:THR:OG1	1:A:336:GLU:HG3	2.02	0.60
1:B:173:ILE:CD1	1:B:340:ILE:HA	2.32	0.60
1:A:598:GLY:HA2	3:A:911:ANP:O3A	2.02	0.60
1:B:417:ARG:CZ	1:B:437:ALA:HB2	2.31	0.60
1:C:411:LEU:HD12	1:C:414:GLU:HB3	1.83	0.60
1:C:376:ARG:HH21	1:C:657:ARG:HD3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HG2	1:B:519:LEU:HG	1.82	0.60
1:A:199:GLU:HG2	1:A:376:ARG:HD2	1.83	0.59
1:A:497:LEU:HB3	1:A:498:PRO:HD3	1.83	0.59
1:C:344:LEU:N	1:C:344:LEU:HD12	2.17	0.59
1:C:574:ILE:O	1:C:577:ALA:HB3	2.01	0.59
1:C:75:GLU:O	1:C:79:VAL:HG23	2.01	0.59
1:B:224:LEU:HD21	1:B:301:ARG:HH22	1.65	0.59
1:B:526:ILE:O	1:B:530:VAL:HG23	2.02	0.59
1:A:682:GLN:NE2	1:A:689:LEU:HD12	2.17	0.59
1:C:199:GLU:HG3	1:C:200:PRO:HD2	1.84	0.59
1:C:541:LEU:HG	1:C:542:LEU:N	2.18	0.59
1:A:441:LYS:HZ3	1:A:441:LYS:HB3	1.67	0.59
1:B:293:PRO:HA	1:B:296:ALA:HB3	1.84	0.59
1:B:509:GLU:HG3	1:B:512:ARG:NE	2.17	0.59
1:C:368:SER:HA	1:C:372:ILE:HG13	1.85	0.59
1:A:199:GLU:HG3	1:A:200:PRO:HD2	1.84	0.59
1:A:549:LEU:CD1	1:A:578:ARG:HG3	2.32	0.59
1:B:224:LEU:HA	1:B:227:LYS:HD3	1.85	0.59
1:B:392:LEU:HD12	1:B:518:ARG:HH21	1.68	0.59
1:B:541:LEU:HG	1:B:542:LEU:N	2.17	0.59
1:A:223:GLY:N	1:A:225:LYS:HE2	2.18	0.59
1:A:224:LEU:HA	1:A:227:LYS:HD3	1.85	0.59
1:A:529:ILE:HA	1:A:532:ARG:HD3	1.85	0.59
1:B:344:LEU:N	1:B:344:LEU:HD12	2.17	0.59
1:C:105:TYR:O	1:C:140:THR:HG21	2.02	0.59
1:A:714:LEU:HD21	1:A:731:GLU:HG3	1.85	0.59
1:C:374:GLU:HG3	1:C:375:ARG:N	2.17	0.59
1:B:332:PRO:HD2	1:B:378:PRO:CG	2.33	0.59
1:C:679:ILE:N	1:C:679:ILE:HD12	2.18	0.59
1:A:191:LYS:HD2	1:A:325:GLN:HE21	1.68	0.58
1:C:298:GLY:HA2	1:C:323:ARG:NH2	2.18	0.58
1:C:332:PRO:HD2	1:C:378:PRO:CG	2.33	0.58
1:C:786:LEU:HG	1:C:837:VAL:HB	1.85	0.58
1:A:194:PRO:HA	1:A:324:PHE:O	2.03	0.58
1:B:197:ILE:O	1:B:328:TYR:HA	2.03	0.58
1:B:377:LEU:O	1:B:378:PRO:C	2.39	0.58
1:C:357:SER:HB3	1:C:520:GLU:OE1	2.03	0.58
1:C:524:GLU:O	1:C:528:GLU:HG3	2.03	0.58
1:A:354:VAL:HA	1:A:519:LEU:HD12	1.84	0.58
1:B:191:LYS:HD3	1:B:325:GLN:HE21	1.68	0.58
1:C:486:LEU:HD11	1:C:491:GLU:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:HG22	1:C:8:GLN:N	2.18	0.58
1:A:145:HIS:CE1	1:A:147:GLU:HG2	2.38	0.58
1:A:372:ILE:HD12	1:A:533:TRP:HE3	1.69	0.58
1:B:223:GLY:N	1:B:225:LYS:HE2	2.18	0.58
1:C:199:GLU:HG2	1:C:376:ARG:CZ	2.34	0.58
1:C:349:GLU:HB2	1:C:354:VAL:O	2.04	0.58
1:C:529:ILE:HA	1:C:532:ARG:HD3	1.84	0.58
1:A:20:LEU:HA	1:A:262:GLN:OE1	2.04	0.58
1:A:624:MET:HB3	1:A:667:ASP:O	2.03	0.58
1:A:34:LEU:CD2	1:A:115:LEU:HD11	2.31	0.58
1:A:441:LYS:O	1:A:444:GLU:HB3	2.04	0.58
1:B:55:ALA:HB2	1:B:123:PRO:CD	2.33	0.58
1:C:709:ASN:N	1:C:709:ASN:HD22	1.99	0.58
1:A:172:VAL:HG21	1:A:210:GLY:HA2	1.84	0.58
1:B:559:ARG:HA	1:B:768:ILE:CD1	2.34	0.58
1:B:682:GLN:HE21	1:B:689:LEU:HA	1.67	0.58
1:C:224:LEU:HA	1:C:227:LYS:HD3	1.84	0.58
1:C:197:ILE:N	1:C:197:ILE:HD12	2.18	0.58
1:A:196:LEU:O	1:A:305:ALA:HA	2.04	0.58
1:B:149:THR:HG22	1:B:155:GLN:OE1	2.03	0.58
1:B:546:ARG:O	1:B:550:LEU:HD13	2.04	0.58
1:C:193:ASN:HB2	1:C:323:ARG:O	2.04	0.58
1:C:578:ARG:C	1:C:580:GLY:H	2.07	0.58
1:C:635:ARG:NH1	1:C:679:ILE:HG21	2.16	0.58
1:A:459:ILE:HB	1:A:511:LEU:HD21	1.84	0.57
1:B:417:ARG:NH2	1:B:437:ALA:HB2	2.19	0.57
1:B:549:LEU:CD1	1:B:578:ARG:HG3	2.33	0.57
1:C:307:THR:HB	1:C:310:GLU:OE2	2.04	0.57
1:B:125:LEU:HB3	1:B:129:LYS:HE3	1.85	0.57
1:B:438:GLU:O	1:B:441:LYS:HG3	2.04	0.57
1:C:353:GLY:HA3	1:C:464:ARG:NE	2.19	0.57
1:A:125:LEU:HB3	1:A:129:LYS:HE3	1.85	0.57
1:C:49:LEU:HD12	1:C:131:ALA:HB3	1.86	0.57
1:A:163:LEU:HD22	1:A:168:LYS:HG2	1.86	0.57
1:A:526:ILE:O	1:A:529:ILE:HG12	2.04	0.57
1:B:578:ARG:C	1:B:580:GLY:H	2.08	0.57
1:A:377:LEU:O	1:A:378:PRO:C	2.41	0.57
1:A:679:ILE:N	1:A:679:ILE:HD12	2.19	0.57
1:A:205:THR:HB	3:A:901:ANP:O2A	2.04	0.57
1:B:103:ASP:HB3	1:B:140:THR:OG1	2.05	0.57
1:B:7:THR:HG22	1:B:106:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD11	1:B:211:LEU:HD13	1.84	0.57
1:C:465:GLU:HA	1:C:468:HIS:HD2	1.69	0.57
1:A:685:ASP:O	1:A:687:GLY:N	2.38	0.57
1:B:136:ARG:HB2	1:B:136:ARG:NH1	2.20	0.57
1:B:347:LYS:HB3	1:C:189:ARG:HH12	1.68	0.57
1:C:526:ILE:O	1:C:530:VAL:HG23	2.05	0.57
1:A:374:GLU:HG3	1:A:375:ARG:N	2.18	0.57
1:A:656:VAL:HG21	1:A:699:PHE:CZ	2.39	0.57
1:B:195:VAL:HG11	1:B:311:TYR:CE1	2.40	0.57
1:B:341:LEU:HD22	1:B:385:ILE:HD12	1.86	0.57
1:B:685:ASP:O	1:B:687:GLY:N	2.38	0.57
1:A:438:GLU:O	1:A:442:LEU:HD13	2.05	0.57
1:B:193:ASN:ND2	1:B:295:LEU:HD22	2.20	0.57
1:C:6:TRP:CH2	1:C:111:LEU:HD13	2.39	0.57
1:A:125:LEU:H	1:A:125:LEU:HD12	1.70	0.56
1:B:578:ARG:O	1:B:579:ALA:HB3	2.04	0.56
1:C:695:ARG:HH11	1:C:695:ARG:HG2	1.70	0.56
1:A:172:VAL:HG21	1:A:210:GLY:HA3	1.87	0.56
1:B:292:LYS:HB2	1:B:293:PRO:HD3	1.86	0.56
1:B:441:LYS:HD3	1:B:441:LYS:C	2.24	0.56
1:A:683:ILE:HD12	1:A:699:PHE:CD2	2.40	0.56
1:B:711:GLY:O	1:B:715:ILE:HG13	2.06	0.56
1:C:531:SER:HB2	1:C:537:PRO:HG3	1.86	0.56
1:B:311:TYR:O	1:B:315:GLU:HG2	2.06	0.56
1:C:53:ALA:O	1:C:127:ALA:HB1	2.05	0.56
1:C:376:ARG:NH2	1:C:657:ARG:HE	2.04	0.56
1:A:349:GLU:HB2	1:A:354:VAL:O	2.05	0.56
1:A:417:ARG:HG3	1:A:418:GLU:N	2.21	0.56
1:B:197:ILE:N	1:B:197:ILE:HD12	2.20	0.56
1:B:259:VAL:HG23	1:B:299:GLU:HB3	1.86	0.56
1:C:165:ALA:HA	1:C:216:VAL:CG1	2.20	0.56
1:C:223:GLY:N	1:C:225:LYS:HE2	2.19	0.56
1:A:780:LYS:O	1:A:782:ILE:HG13	2.06	0.56
1:B:484:TYR:O	1:B:486:LEU:N	2.39	0.56
1:B:679:ILE:HD12	1:B:679:ILE:N	2.21	0.56
1:C:101:LEU:HD12	1:C:110:THR:HG22	1.87	0.56
1:A:197:ILE:HD12	1:A:197:ILE:N	2.21	0.56
1:A:495:GLY:C	1:A:498:PRO:HD2	2.26	0.56
1:A:95:GLU:O	1:A:98:MET:HG2	2.05	0.56
1:B:113:LEU:O	1:B:117:GLU:HG3	2.05	0.56
1:A:682:GLN:HE21	1:A:689:LEU:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HD2	1:A:117:GLU:OE1	2.06	0.56
1:B:509:GLU:O	1:B:512:ARG:HG3	2.05	0.56
1:C:377:LEU:N	1:C:380:LYS:HE2	2.19	0.56
1:C:6:TRP:CZ3	1:C:111:LEU:HD13	2.40	0.56
1:A:223:GLY:CA	1:A:225:LYS:HE2	2.36	0.56
1:C:37:VAL:O	1:C:40:LYS:HE3	2.06	0.56
1:B:437:ALA:O	1:B:440:ALA:HB3	2.06	0.56
1:B:526:ILE:O	1:B:529:ILE:HG12	2.06	0.56
1:C:417:ARG:HG3	1:C:432:LEU:HD11	1.87	0.56
1:C:252:LYS:HA	1:C:255:ILE:CG2	2.36	0.55
1:A:317:ASP:O	1:A:321:GLU:HG2	2.06	0.55
1:A:484:TYR:CG	1:A:484:TYR:O	2.59	0.55
1:B:45:LEU:HD23	1:B:108:VAL:HG23	1.87	0.55
1:A:535:GLY:O	1:A:540:LYS:HD3	2.06	0.55
1:B:653:THR:HB	1:B:697:VAL:HG21	1.89	0.55
1:C:682:GLN:HE21	1:C:689:LEU:HA	1.72	0.55
1:A:321:GLU:C	1:A:323:ARG:N	2.59	0.55
1:A:524:GLU:O	1:A:528:GLU:HG3	2.06	0.55
1:A:541:LEU:HG	1:A:542:LEU:H	1.71	0.55
1:B:223:GLY:CA	1:B:225:LYS:HE2	2.37	0.55
1:B:346:GLU:O	1:B:350:VAL:HG23	2.07	0.55
1:A:415:ILE:HA	1:B:486:LEU:HG	1.87	0.55
1:B:546:ARG:HG3	1:B:547:GLU:H	1.71	0.55
1:A:760:GLU:O	1:A:764:GLN:HG3	2.06	0.55
1:A:252:LYS:HA	1:A:255:ILE:CG2	2.37	0.55
1:A:769:GLN:HG2	1:A:812:ILE:HD12	1.89	0.55
1:B:295:LEU:HB2	1:B:323:ARG:HH11	1.71	0.55
1:B:318:PRO:HA	1:B:321:GLU:CG	2.37	0.55
1:C:499:LYS:O	1:C:503:GLU:HG3	2.07	0.55
1:A:377:LEU:N	1:A:380:LYS:HE2	2.21	0.55
1:A:382:ILE:CD1	3:A:901:ANP:H1'	2.37	0.55
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.72	0.55
1:C:472:GLU:O	1:C:475:ARG:HB3	2.06	0.55
1:C:538:VAL:O	1:C:542:LEU:HB3	2.07	0.55
1:C:546:ARG:HG3	1:C:547:GLU:H	1.70	0.55
1:B:153:LEU:HD21	1:B:258:VAL:HG22	1.89	0.55
1:B:50:LEU:HB3	1:B:57:PRO:HG3	1.89	0.55
1:B:95:GLU:HA	1:B:98:MET:HG2	1.88	0.55
1:C:169:LEU:HD13	1:C:209:GLU:HB2	1.89	0.55
1:C:223:GLY:CA	1:C:225:LYS:HE2	2.37	0.55
1:C:377:LEU:O	1:C:378:PRO:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:ASP:O	1:C:687:GLY:N	2.39	0.55
1:B:307:THR:HB	1:B:310:GLU:HG3	1.88	0.55
1:A:105:TYR:CZ	1:A:143:THR:HB	2.42	0.55
1:A:151:ASN:HB2	1:A:257:GLU:OE2	2.06	0.55
1:A:485:ASP:C	1:A:487:ASN:H	2.10	0.55
1:A:495:GLY:N	1:A:498:PRO:HG2	2.21	0.55
1:A:5:ARG:CD	1:A:6:TRP:N	2.67	0.55
1:B:185:ILE:HG21	1:B:325:GLN:HB2	1.88	0.55
1:B:232:LEU:HD23	1:B:233:GLN:N	2.22	0.55
1:C:408:ARG:CZ	1:C:411:LEU:HD23	2.37	0.55
1:C:683:ILE:HD12	1:C:699:PHE:CD2	2.41	0.55
1:A:43:ARG:HH21	1:A:253:ALA:HB1	1.72	0.54
1:A:414:GLU:O	1:A:417:ARG:HG2	2.07	0.54
1:C:632:ALA:HB2	1:C:675:ASP:OD1	2.08	0.54
1:A:232:LEU:HD23	1:A:233:GLN:N	2.22	0.54
1:A:538:VAL:O	1:A:542:LEU:HB3	2.07	0.54
1:B:252:LYS:HA	1:B:255:ILE:CG2	2.36	0.54
1:B:769:GLN:HG2	1:B:812:ILE:HD12	1.88	0.54
1:A:480:ALA:C	1:A:482:ARG:H	2.11	0.54
1:B:34:LEU:HD23	1:B:115:LEU:CD1	2.33	0.54
1:C:526:ILE:O	1:C:529:ILE:HG12	2.08	0.54
1:A:185:ILE:O	1:A:192:ASN:HA	2.07	0.54
1:A:37:VAL:O	1:A:40:LYS:HE3	2.07	0.54
1:A:518:ARG:O	1:A:518:ARG:HG2	2.08	0.54
1:B:199:GLU:HG2	1:B:376:ARG:HD2	1.88	0.54
1:C:653:THR:HB	1:C:697:VAL:HG21	1.90	0.54
1:A:714:LEU:HD21	1:A:731:GLU:CG	2.38	0.54
1:B:173:ILE:HD11	1:B:339:SER:C	2.27	0.54
1:B:541:LEU:O	1:B:542:LEU:C	2.46	0.54
1:B:695:ARG:HG2	1:B:695:ARG:HH11	1.72	0.54
1:C:292:LYS:O	1:C:295:LEU:HB3	2.08	0.54
1:B:132:LEU:C	1:B:132:LEU:HD23	2.28	0.54
1:C:629:GLU:CG	1:C:630:LYS:H	2.16	0.54
1:A:255:ILE:HD11	1:A:294:ALA:HB3	1.90	0.54
1:A:458:GLU:O	1:A:461:ARG:HB3	2.08	0.54
1:A:597:THR:HG22	3:A:911:ANP:HNB1	1.72	0.54
1:C:439:ILE:HG23	1:C:440:ALA:N	2.23	0.54
1:A:208:VAL:HG21	1:A:268:PHE:CE1	2.42	0.54
1:A:613:PHE:O	1:A:615:THR:HG22	2.08	0.54
1:C:341:LEU:HD22	1:C:385:ILE:HD12	1.88	0.54
1:A:470:LEU:HA	1:A:500:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:LEU:HA	1:A:761:GLN:OE1	2.08	0.54
1:B:199:GLU:HG2	1:B:376:ARG:CZ	2.38	0.54
1:B:475:ARG:HH12	1:B:479:LEU:HD22	1.73	0.54
1:A:470:LEU:HD13	1:A:500:LEU:HB2	1.89	0.54
1:A:488:ARG:HA	1:A:491:GLU:CG	2.38	0.54
1:A:848:VAL:HG12	1:A:849:PRO:CD	2.36	0.54
1:B:151:ASN:OD1	1:B:153:LEU:N	2.39	0.54
1:B:806:ARG:HH21	1:C:746:ASN:HD21	1.56	0.54
1:C:541:LEU:O	1:C:542:LEU:C	2.46	0.54
1:C:6:TRP:HZ3	1:C:111:LEU:HD22	1.72	0.54
1:A:320:LEU:HG	1:A:324:PHE:CE1	2.44	0.53
1:A:354:VAL:HG12	1:A:518:ARG:O	2.07	0.53
1:B:232:LEU:C	1:B:232:LEU:HD23	2.28	0.53
1:B:314:ILE:HG23	1:B:320:LEU:HD23	1.89	0.53
1:C:769:GLN:HG2	1:C:812:ILE:HD12	1.89	0.53
1:A:45:LEU:CD2	1:A:108:VAL:HG23	2.38	0.53
1:A:16:GLN:HE22	1:A:261:SER:CB	2.21	0.53
1:B:37:VAL:O	1:B:40:LYS:HE3	2.08	0.53
1:C:624:MET:CG	1:C:672:ALA:HB2	2.38	0.53
1:C:679:ILE:HG23	1:C:689:LEU:HD21	1.91	0.53
1:A:152:ALA:HB1	1:A:254:VAL:HG22	1.89	0.53
1:B:48:ARG:NE	1:B:150:TYR:HB3	2.21	0.53
1:A:191:LYS:CD	1:A:325:GLN:HE21	2.22	0.53
1:A:432:LEU:O	1:A:435:ILE:HG22	2.07	0.53
1:C:196:LEU:HD23	1:C:327:VAL:HB	1.91	0.53
1:A:132:LEU:C	1:A:132:LEU:HD23	2.29	0.53
1:A:307:THR:HG22	1:A:308:LEU:N	2.23	0.53
1:A:393:ARG:HH11	1:A:393:ARG:HG2	1.74	0.53
1:A:501:GLU:O	1:A:505:GLU:HB2	2.09	0.53
1:A:96:GLY:O	1:A:100:GLU:HG3	2.08	0.53
1:B:624:MET:HG2	1:B:672:ALA:HB2	1.91	0.53
1:A:364:ALA:HA	1:A:384:LEU:HD23	1.91	0.53
1:B:113:LEU:HD11	1:B:132:LEU:HD12	1.91	0.53
1:B:151:ASN:HB3	1:B:154:GLU:HG3	1.90	0.53
1:B:8:GLN:N	1:B:8:GLN:NE2	2.56	0.53
1:C:440:ALA:O	1:C:443:THR:HB	2.08	0.53
1:C:465:GLU:HA	1:C:468:HIS:CD2	2.44	0.53
1:C:823:LYS:HB3	1:C:829:VAL:HG23	1.90	0.53
1:A:344:LEU:HD11	3:A:901:ANP:H2	1.91	0.53
1:B:416:GLU:O	1:B:420:LEU:HB2	2.08	0.53
1:B:98:MET:HE3	1:B:103:ASP:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ARG:HA	1:B:315:GLU:HB2	1.91	0.53
1:B:481:GLU:OE2	1:B:493:ARG:NH2	2.42	0.53
1:B:216:VAL:HG12	1:B:482:ARG:HE	1.74	0.53
1:C:531:SER:CB	1:C:537:PRO:HG3	2.39	0.53
1:C:43:ARG:HH11	1:C:43:ARG:HG3	1.74	0.53
1:B:541:LEU:HG	1:B:542:LEU:H	1.73	0.52
1:C:113:LEU:CD2	1:C:128:LEU:HB3	2.40	0.52
1:C:199:GLU:HG2	1:C:376:ARG:HD2	1.91	0.52
1:B:776:ARG:HG3	1:C:580:GLY:O	2.09	0.52
1:A:337:THR:HG21	1:A:377:LEU:HD22	1.90	0.52
1:B:173:ILE:HD11	1:B:340:ILE:HA	1.90	0.52
1:B:45:LEU:HD21	1:B:109:ASP:HB3	1.91	0.52
1:C:42:GLU:HA	1:C:47:TRP:CD2	2.44	0.52
1:B:337:THR:HG21	1:B:377:LEU:HD22	1.90	0.52
1:C:205:THR:O	1:C:209:GLU:HG2	2.09	0.52
1:C:320:LEU:HG	1:C:324:PHE:HE2	1.74	0.52
1:C:578:ARG:O	1:C:579:ALA:HB3	2.10	0.52
1:C:635:ARG:NH1	1:C:635:ARG:HB2	2.24	0.52
1:C:410:LYS:HG3	1:C:439:ILE:HG13	1.92	0.52
1:C:773:LEU:HD13	1:C:817:GLU:OE2	2.09	0.52
1:C:93:ARG:HH11	1:C:93:ARG:HG3	1.75	0.52
1:B:175:ARG:NH1	1:B:175:ARG:HG2	2.24	0.52
1:B:379:ASP:CG	1:C:322:ARG:HH12	2.12	0.52
1:B:776:ARG:HD2	1:B:779:GLU:OE1	2.09	0.52
1:C:759:LYS:O	1:C:763:ARG:HG3	2.09	0.52
1:A:20:LEU:HB2	1:A:262:GLN:NE2	2.04	0.52
1:A:546:ARG:HG3	1:A:547:GLU:H	1.75	0.52
1:B:15:ALA:O	1:B:19:VAL:HG23	2.10	0.52
1:C:15:ALA:O	1:C:19:VAL:HG23	2.09	0.52
1:A:323:ARG:HH11	1:A:323:ARG:CB	2.17	0.52
1:B:480:ALA:HB1	1:B:489:ALA:HB2	1.91	0.52
1:B:357:SER:HB3	1:B:520:GLU:OE1	2.09	0.52
1:A:5:ARG:HH11	1:A:5:ARG:HG2	1.75	0.52
1:A:653:THR:HB	1:A:697:VAL:HG21	1.92	0.52
1:B:20:LEU:HB2	1:B:262:GLN:HE22	1.74	0.52
1:B:93:ARG:HH11	1:B:93:ARG:HG3	1.75	0.52
1:C:806:ARG:N	1:C:807:PRO:CD	2.73	0.52
1:B:666:PHE:HB2	1:B:706:LEU:HD23	1.92	0.52
1:B:715:ILE:HG12	1:B:732:VAL:HG21	1.92	0.52
1:B:93:ARG:HD2	1:B:117:GLU:OE1	2.10	0.52
1:C:139:ARG:HH12	1:C:148:SER:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:THR:HG21	1:C:377:LEU:HD22	1.92	0.52
1:C:452:GLU:O	1:C:456:GLU:HB2	2.10	0.52
1:A:781:ARG:O	1:A:832:GLY:HA2	2.09	0.51
1:B:199:GLU:HG2	1:B:376:ARG:NE	2.25	0.51
1:B:349:GLU:HB2	1:B:354:VAL:O	2.10	0.51
1:B:386:ASP:OD2	1:C:188:ARG:NE	2.37	0.51
1:B:384:LEU:O	1:B:529:ILE:CD1	2.58	0.51
1:C:690:THR:HA	1:C:696:THR:HG22	1.91	0.51
1:B:428:SER:O	1:B:432:LEU:HD12	2.10	0.51
1:C:302:LEU:HD12	1:C:303:ILE:H	1.75	0.51
1:C:354:VAL:HA	1:C:519:LEU:HD12	1.92	0.51
1:C:654:GLU:HB3	1:C:658:ARG:NH1	2.25	0.51
1:A:15:ALA:O	1:A:19:VAL:HG23	2.11	0.51
1:B:535:GLY:O	1:B:540:LYS:HD3	2.10	0.51
1:C:34:LEU:CD2	1:C:115:LEU:HD11	2.39	0.51
1:C:364:ALA:HA	1:C:384:LEU:HD23	1.92	0.51
1:A:320:LEU:HG	1:A:324:PHE:HE1	1.75	0.51
1:A:341:LEU:HD22	1:A:385:ILE:HD12	1.93	0.51
1:A:43:ARG:HH11	1:A:43:ARG:HG3	1.74	0.51
1:B:384:LEU:HD21	1:B:530:VAL:CG2	2.41	0.51
1:C:144:GLU:CG	1:C:145:HIS:H	2.19	0.51
1:C:539:SER:O	1:C:540:LYS:C	2.49	0.51
1:C:541:LEU:HG	1:C:542:LEU:H	1.76	0.51
1:A:456:GLU:HG3	1:A:514:ALA:HB1	1.91	0.51
1:C:255:ILE:CD1	1:C:294:ALA:HB3	2.38	0.51
1:C:513:GLY:N	1:C:517:VAL:HG21	2.25	0.51
1:C:360:ALA:HB2	1:C:522:THR:HA	1.92	0.51
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.75	0.51
1:B:364:ALA:HA	1:B:384:LEU:HD23	1.93	0.51
1:B:683:ILE:HD12	1:B:699:PHE:CD2	2.46	0.51
1:B:757:LEU:CB	1:B:762:ILE:HD11	2.38	0.51
1:C:712:SER:N	1:C:713:PRO:HD2	2.26	0.51
1:A:323:ARG:O	1:A:325:GLN:N	2.44	0.51
1:A:629:GLU:CG	1:A:630:LYS:H	2.17	0.51
1:B:539:SER:O	1:B:540:LYS:C	2.49	0.51
1:B:565:GLU:OE1	1:B:753:VAL:HG12	2.10	0.51
1:B:566:ALA:HA	1:B:752:VAL:CG1	2.41	0.51
1:B:635:ARG:HH22	1:B:679:ILE:CG1	2.23	0.51
1:C:513:GLY:H	1:C:517:VAL:HG21	1.75	0.51
1:C:714:LEU:HD21	1:C:731:GLU:HG3	1.93	0.51
1:A:307:THR:HG22	1:A:308:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ARG:C	1:C:636:LEU:HD23	2.31	0.51
1:A:408:ARG:O	1:A:412:GLN:HG2	2.11	0.51
1:A:45:LEU:HD23	1:A:108:VAL:CG2	2.41	0.51
1:A:376:ARG:NH2	1:A:657:ARG:HE	2.08	0.51
1:B:297:ARG:HD2	1:B:299:GLU:OE1	2.11	0.51
1:B:524:GLU:O	1:B:528:GLU:HG3	2.11	0.51
1:B:688:ARG:HH12	1:B:700:ARG:HD3	1.76	0.51
1:C:42:GLU:HA	1:C:47:TRP:CE3	2.46	0.51
1:A:541:LEU:O	1:A:542:LEU:C	2.49	0.51
1:B:152:ALA:HB1	1:B:254:VAL:HG22	1.93	0.51
1:B:181:ARG:O	1:B:185:ILE:HG13	2.11	0.51
1:B:453:TRP:CZ2	1:B:457:ARG:HD2	2.46	0.51
1:C:469:ARG:O	1:C:473:VAL:HG23	2.10	0.51
1:A:539:SER:O	1:A:540:LYS:C	2.48	0.50
1:A:664:ILE:HG22	1:A:666:PHE:CE1	2.45	0.50
1:A:839:VAL:CG2	1:A:840:GLY:H	2.02	0.50
1:B:431:ARG:O	1:B:435:ILE:HG22	2.11	0.50
1:C:535:GLY:O	1:C:540:LYS:HD3	2.11	0.50
1:A:145:HIS:ND1	1:A:162:ARG:HD3	2.26	0.50
1:A:373:THR:HG22	1:A:658:ARG:O	2.12	0.50
1:A:411:LEU:HA	1:A:414:GLU:HB3	1.92	0.50
1:A:470:LEU:HA	1:A:500:LEU:CD1	2.41	0.50
1:B:351:HIS:HE1	1:C:187:LEU:O	1.93	0.50
1:B:431:ARG:NH1	1:B:432:LEU:HD23	2.26	0.50
1:B:690:THR:HA	1:B:696:THR:HG22	1.93	0.50
1:B:270:ASP:OD1	1:B:271:GLU:HG3	2.10	0.50
1:B:570:VAL:O	1:B:574:ILE:HG13	2.11	0.50
1:C:293:PRO:C	1:C:295:LEU:H	2.15	0.50
1:C:800:ASP:OD1	1:C:802:VAL:N	2.44	0.50
1:A:31:LEU:HD22	1:A:115:LEU:HD22	1.93	0.50
1:A:185:ILE:HG21	1:A:194:PRO:HB3	1.92	0.50
1:A:420:LEU:HB2	1:A:432:LEU:HD13	1.93	0.50
1:A:476:GLU:O	1:A:479:LEU:HB3	2.12	0.50
1:B:192:ASN:O	1:B:194:PRO:HD3	2.11	0.50
1:B:302:LEU:HD12	1:B:303:ILE:H	1.76	0.50
1:B:683:ILE:HD11	1:B:689:LEU:HD22	1.93	0.50
1:C:460:LEU:HD23	1:C:460:LEU:C	2.31	0.50
1:A:183:ILE:CD1	1:A:211:LEU:HD13	2.37	0.50
1:A:30:ASP:OD1	1:A:86:ARG:NH2	2.44	0.50
1:B:103:ASP:OD1	1:B:140:THR:HG23	2.12	0.50
1:B:256:GLN:O	1:B:260:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ILE:O	1:B:577:ALA:HB3	2.10	0.50
1:C:438:GLU:O	1:C:441:LYS:HB3	2.11	0.50
1:C:542:LEU:O	1:C:543:GLU:C	2.50	0.50
1:A:320:LEU:C	1:A:322:ARG:H	2.15	0.50
1:A:463:LEU:N	1:A:507:LEU:HD13	2.27	0.50
1:A:685:ASP:C	1:A:687:GLY:H	2.14	0.50
1:B:457:ARG:HB3	1:B:461:ARG:NH1	2.24	0.50
1:C:477:ILE:HG13	1:C:478:GLU:N	2.26	0.50
1:C:679:ILE:CG2	1:C:689:LEU:HD21	2.41	0.50
1:C:765:ILE:HA	1:C:768:ILE:CG2	2.42	0.50
1:B:148:SER:HB2	1:B:150:TYR:HE1	1.76	0.50
1:B:199:GLU:HG3	1:B:200:PRO:CD	2.42	0.50
1:B:8:GLN:H	1:B:8:GLN:HE21	1.60	0.50
1:C:175:ARG:HG2	1:C:175:ARG:HH11	1.77	0.50
1:C:27:GLN:HB2	1:C:74:VAL:HG11	1.93	0.50
1:C:714:LEU:HD21	1:C:731:GLU:CG	2.42	0.50
1:A:403:ILE:HG21	1:A:450:ARG:HH21	1.77	0.50
1:A:435:ILE:O	1:A:439:ILE:HD13	2.12	0.50
1:A:495:GLY:H	1:A:498:PRO:HG2	1.76	0.50
1:A:504:VAL:O	1:A:504:VAL:HG13	2.11	0.50
1:A:594:LEU:HD11	1:A:736:LEU:HD11	1.94	0.50
1:B:407:GLU:OE2	1:B:446:ILE:HG23	2.12	0.50
1:B:470:LEU:O	1:B:474:ARG:HG3	2.11	0.50
1:B:758:THR:O	1:B:762:ILE:HG12	2.11	0.50
1:C:199:GLU:HG2	1:C:376:ARG:NE	2.27	0.50
1:A:116:ALA:HB1	1:A:128:LEU:HD11	1.93	0.50
1:B:147:GLU:O	1:B:149:THR:N	2.45	0.50
1:B:408:ARG:NH1	1:B:411:LEU:HD23	2.26	0.50
1:B:806:ARG:N	1:B:807:PRO:CD	2.74	0.50
1:C:172:VAL:HG21	1:C:210:GLY:HA3	1.92	0.50
1:C:256:GLN:O	1:C:260:GLN:HG3	2.12	0.50
1:A:320:LEU:O	1:A:322:ARG:N	2.41	0.49
1:B:113:LEU:HD11	1:B:132:LEU:CD1	2.42	0.49
1:B:233:GLN:NE2	1:B:233:GLN:HA	2.27	0.49
1:C:147:GLU:O	1:C:148:SER:HB3	2.12	0.49
1:C:350:VAL:HG11	1:C:471:ASP:OD1	2.11	0.49
1:A:292:LYS:O	1:A:296:ALA:N	2.44	0.49
1:A:323:ARG:C	1:A:325:GLN:N	2.66	0.49
1:B:666:PHE:HB2	1:B:706:LEU:CD2	2.42	0.49
1:C:420:LEU:O	1:C:420:LEU:HD23	2.13	0.49
1:A:256:GLN:O	1:A:260:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:O	1:A:396:LEU:HD23	2.11	0.49
1:A:688:ARG:HH12	1:A:700:ARG:HD3	1.77	0.49
1:B:113:LEU:O	1:B:116:ALA:HB3	2.12	0.49
1:B:211:LEU:HD12	1:B:211:LEU:O	2.13	0.49
1:B:232:LEU:HB2	1:B:267:LEU:HD11	1.93	0.49
1:C:254:VAL:O	1:C:258:VAL:HG23	2.13	0.49
1:C:307:THR:HG22	1:C:308:LEU:N	2.26	0.49
1:A:211:LEU:HD12	1:A:211:LEU:O	2.13	0.49
1:A:476:GLU:CG	1:A:488:ARG:HH21	2.23	0.49
1:A:537:PRO:O	1:A:541:LEU:HB3	2.13	0.49
1:B:104:ARG:HB2	1:B:139:ARG:NH2	2.25	0.49
1:B:186:LEU:HD11	1:B:303:ILE:HD11	1.94	0.49
1:B:577:ALA:C	1:B:578:ARG:O	2.50	0.49
1:B:685:ASP:C	1:B:687:GLY:H	2.16	0.49
1:B:559:ARG:HA	1:B:768:ILE:HD12	1.94	0.49
1:A:117:GLU:OE2	1:A:125:LEU:HD11	2.12	0.49
1:B:254:VAL:O	1:B:258:VAL:HG23	2.12	0.49
1:B:34:LEU:HD23	1:B:115:LEU:HD21	1.93	0.49
1:B:377:LEU:N	1:B:380:LYS:HE2	2.28	0.49
1:B:566:ALA:HA	1:B:752:VAL:HG13	1.93	0.49
1:C:216:VAL:O	1:C:482:ARG:HD3	2.12	0.49
1:C:679:ILE:CD1	1:C:679:ILE:H	2.24	0.49
1:C:715:ILE:HG12	1:C:732:VAL:HG21	1.95	0.49
1:A:122:LEU:HB2	1:A:123:PRO:HD2	1.95	0.49
1:A:188:ARG:NH1	1:A:325:GLN:HE22	2.10	0.49
1:A:32:PRO:HB2	1:A:68:LEU:HD21	1.94	0.49
1:A:58:LYS:O	1:A:62:GLU:HB2	2.12	0.49
1:A:5:ARG:HD3	1:A:6:TRP:CD1	2.48	0.49
1:A:720:GLN:C	1:A:722:GLY:H	2.14	0.49
1:B:233:GLN:HE21	1:B:233:GLN:HA	1.78	0.49
1:B:384:LEU:HG	1:B:529:ILE:HD11	1.95	0.49
1:B:592:LEU:HG	1:B:594:LEU:HD21	1.95	0.49
1:A:806:ARG:HD2	3:A:911:ANP:O1G	2.12	0.49
1:B:199:GLU:HG2	1:B:376:ARG:CD	2.43	0.49
1:B:597:THR:HG22	1:B:598:GLY:N	2.27	0.49
1:C:43:ARG:NE	1:C:226:GLY:HA3	2.27	0.49
1:A:636:LEU:C	1:A:692:SER:HB2	2.33	0.49
1:C:32:PRO:HA	1:C:64:GLN:HG3	1.93	0.49
1:B:353:GLY:HA2	1:B:467:GLN:OE1	2.13	0.49
1:B:660:PRO:O	1:B:702:THR:HG22	2.13	0.49
1:C:413:LEU:C	1:C:415:ILE:H	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:PHE:O	1:C:615:THR:HG22	2.11	0.49
1:B:151:ASN:HB3	1:B:154:GLU:CG	2.43	0.49
1:B:436:GLU:OE2	1:B:436:GLU:HA	2.13	0.49
1:B:720:GLN:C	1:B:722:GLY:H	2.16	0.49
1:B:84:THR:HG22	1:B:86:ARG:H	1.78	0.49
1:C:113:LEU:HD23	1:C:128:LEU:HB3	1.94	0.49
1:A:39:LEU:O	1:A:61:LYS:HD2	2.12	0.48
1:B:391:ARG:HH12	1:B:528:GLU:CB	2.25	0.48
1:B:806:ARG:HB3	1:B:807:PRO:HD3	1.95	0.48
1:A:578:ARG:O	1:A:580:GLY:N	2.46	0.48
1:B:196:LEU:O	1:B:305:ALA:HA	2.11	0.48
1:B:570:VAL:HA	1:B:591:PHE:CE2	2.48	0.48
1:C:250:ARG:O	1:C:254:VAL:HG23	2.12	0.48
1:C:635:ARG:CB	1:C:635:ARG:HH11	2.26	0.48
1:A:635:ARG:HH22	1:A:679:ILE:CG1	2.26	0.48
1:B:250:ARG:O	1:B:254:VAL:HG23	2.13	0.48
1:B:352:HIS:HB2	1:B:354:VAL:HG22	1.95	0.48
1:B:454:GLU:OE2	1:B:454:GLU:HA	2.13	0.48
1:B:99:GLU:C	1:B:101:LEU:H	2.16	0.48
1:C:292:LYS:HE2	1:C:293:PRO:CD	2.43	0.48
1:C:332:PRO:HG2	1:C:378:PRO:HG3	1.94	0.48
1:C:37:VAL:O	1:C:40:LYS:HG3	2.14	0.48
1:C:5:ARG:HD3	1:C:6:TRP:N	2.28	0.48
1:A:16:GLN:HE22	1:A:261:SER:HB3	1.77	0.48
1:A:344:LEU:H	1:A:344:LEU:CD1	2.25	0.48
1:A:455:ARG:HG2	1:A:459:ILE:HD11	1.94	0.48
1:A:577:ALA:C	1:A:578:ARG:O	2.51	0.48
1:B:191:LYS:CD	1:B:325:GLN:HE21	2.27	0.48
1:B:568:ARG:HG2	1:B:568:ARG:NH1	2.28	0.48
1:B:712:SER:N	1:B:713:PRO:HD2	2.29	0.48
1:C:140:THR:O	1:C:140:THR:HG22	2.13	0.48
1:C:211:LEU:O	1:C:211:LEU:HD12	2.14	0.48
1:C:417:ARG:HH21	1:C:421:LYS:NZ	2.10	0.48
1:A:679:ILE:CD1	1:A:679:ILE:H	2.26	0.48
1:A:97:LEU:O	1:A:101:LEU:HG	2.13	0.48
1:B:204:LYS:NZ	1:B:204:LYS:HB2	2.28	0.48
1:B:31:LEU:HD22	1:B:115:LEU:HD22	1.95	0.48
1:B:492:LEU:HA	1:B:496:GLU:HB2	1.96	0.48
1:C:806:ARG:HB3	1:C:807:PRO:HD3	1.94	0.48
1:A:712:SER:N	1:A:713:PRO:HD2	2.29	0.48
1:B:317:ASP:CG	1:B:320:LEU:HD13	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG13	1:B:331:GLU:HA	1.94	0.48
1:B:332:PRO:HD2	1:B:378:PRO:HG3	1.96	0.48
1:B:787:THR:HG22	1:B:789:ALA:N	2.21	0.48
1:C:123:PRO:CB	1:C:127:ALA:HB3	2.44	0.48
1:C:472:GLU:O	1:C:476:GLU:HG3	2.14	0.48
1:C:497:LEU:N	1:C:498:PRO:CD	2.76	0.48
1:A:456:GLU:OE2	1:A:456:GLU:N	2.46	0.48
1:A:546:ARG:O	1:A:550:LEU:HD13	2.12	0.48
1:A:175:ARG:HG2	1:A:175:ARG:HH11	1.79	0.48
1:A:254:VAL:O	1:A:258:VAL:HG23	2.13	0.48
1:A:695:ARG:HH11	1:A:695:ARG:HG2	1.77	0.48
1:C:713:PRO:HG2	1:C:714:LEU:H	1.78	0.48
1:A:37:VAL:O	1:A:40:LYS:HG3	2.14	0.48
1:B:473:VAL:HG21	1:B:500:LEU:HD12	1.96	0.48
1:B:594:LEU:HD11	1:B:736:LEU:HD11	1.96	0.48
1:B:723:TRP:CD1	1:B:727:ARG:HB3	2.49	0.48
1:C:105:TYR:H	1:C:140:THR:HG21	1.77	0.48
1:C:332:PRO:HD2	1:C:378:PRO:HD3	1.96	0.48
1:C:84:THR:HG22	1:C:86:ARG:H	1.79	0.48
1:A:189:ARG:HA	1:A:189:ARG:HE	1.78	0.48
1:A:250:ARG:O	1:A:254:VAL:HG23	2.13	0.48
1:A:232:LEU:HB2	1:A:267:LEU:HD11	1.94	0.48
1:A:421:LYS:HE3	1:A:422:LYS:HG2	1.94	0.48
1:A:635:ARG:NH1	1:A:635:ARG:HB2	2.28	0.48
1:A:624:MET:HG2	1:A:672:ALA:HB2	1.96	0.48
1:A:84:THR:HG22	1:A:86:ARG:H	1.78	0.48
1:B:623:ASP:CG	1:C:742:PRO:HD2	2.34	0.48
1:A:311:TYR:HA	1:A:314:ILE:HD12	1.95	0.47
1:A:346:GLU:O	1:A:350:VAL:HG23	2.14	0.47
1:A:806:ARG:N	1:A:807:PRO:CD	2.77	0.47
1:B:495:GLY:C	1:B:498:PRO:HD2	2.34	0.47
1:C:656:VAL:HG21	1:C:699:PHE:CZ	2.49	0.47
1:A:178:GLU:O	1:A:182:VAL:HG23	2.14	0.47
1:A:302:LEU:HD12	1:A:303:ILE:H	1.79	0.47
1:A:690:THR:HA	1:A:696:THR:HG22	1.95	0.47
1:A:559:ARG:HA	1:A:768:ILE:HD11	1.96	0.47
1:B:116:ALA:CB	1:B:128:LEU:HD13	2.44	0.47
1:B:252:LYS:O	1:B:256:GLN:HG2	2.14	0.47
1:C:252:LYS:O	1:C:256:GLN:HG2	2.14	0.47
1:C:308:LEU:HD23	1:C:695:ARG:H	1.79	0.47
1:C:624:MET:HB3	1:C:667:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:ILE:HG23	1:C:689:LEU:HD11	1.96	0.47
1:A:188:ARG:NH1	1:A:325:GLN:NE2	2.62	0.47
1:B:202:VAL:O	1:B:378:PRO:HG2	2.14	0.47
1:B:432:LEU:HA	1:B:435:ILE:HG22	1.97	0.47
1:C:6:TRP:CE3	1:C:10:ALA:HB1	2.47	0.47
1:C:97:LEU:O	1:C:100:GLU:HG2	2.14	0.47
1:A:191:LYS:HD3	1:A:323:ARG:HB2	1.96	0.47
1:A:488:ARG:HG2	1:A:488:ARG:HH11	1.79	0.47
1:A:515:ARG:HG2	1:A:515:ARG:NH1	2.29	0.47
1:A:563:GLN:NE2	1:A:754:PHE:HB3	2.29	0.47
1:B:45:LEU:CD2	1:B:108:VAL:HG23	2.45	0.47
1:C:129:LYS:HE3	1:C:132:LEU:HD22	1.96	0.47
1:A:4:GLU:CA	1:A:11:ARG:HH22	2.27	0.47
1:A:578:ARG:O	1:A:579:ALA:HB3	2.15	0.47
1:A:721:LYS:HD3	1:A:723:TRP:CZ3	2.49	0.47
1:A:394:MET:HB2	1:B:184:GLN:NE2	2.29	0.47
1:B:347:LYS:O	1:B:350:VAL:HB	2.14	0.47
1:B:37:VAL:O	1:B:40:LYS:HG3	2.14	0.47
1:B:423:GLU:O	1:B:424:LYS:O	2.32	0.47
1:B:487:ASN:O	1:B:490:ALA:HB3	2.14	0.47
1:C:325:GLN:HA	1:C:325:GLN:NE2	2.30	0.47
1:C:384:LEU:HG	1:C:529:ILE:HD11	1.97	0.47
1:C:482:ARG:HD2	1:C:482:ARG:O	2.15	0.47
1:A:4:GLU:HA	1:A:11:ARG:HH22	1.77	0.47
1:A:392:LEU:O	1:A:395:ALA:HB3	2.15	0.47
1:A:487:ASN:ND2	1:A:487:ASN:N	2.62	0.47
1:B:162:ARG:O	1:B:166:GLU:HG2	2.14	0.47
1:B:164:ALA:HB2	1:B:169:LEU:HD12	1.95	0.47
1:B:307:THR:HB	1:B:310:GLU:CG	2.45	0.47
1:B:408:ARG:HH11	1:B:412:GLN:NE2	2.13	0.47
1:C:105:TYR:H	1:C:140:THR:CG2	2.28	0.47
1:B:347:LYS:HB3	1:C:189:ARG:NH1	2.30	0.47
1:C:336:GLU:O	1:C:340:ILE:HG13	2.14	0.47
1:A:711:GLY:O	1:A:715:ILE:HG13	2.13	0.47
1:B:431:ARG:HG3	1:B:432:LEU:N	2.28	0.47
1:B:43:ARG:NH1	1:B:43:ARG:HG3	2.27	0.47
1:C:144:GLU:HG3	1:C:145:HIS:N	2.25	0.47
1:A:175:ARG:NH1	1:A:329:VAL:HG13	2.30	0.47
1:A:159:ASP:OD2	1:A:228:ARG:HD3	2.15	0.47
1:A:531:SER:CB	1:A:537:PRO:HG3	2.45	0.47
1:A:574:ILE:O	1:A:577:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LYS:HB3	1:A:829:VAL:HG23	1.97	0.47
1:B:664:ILE:HG22	1:B:666:PHE:CE1	2.50	0.47
1:C:43:ARG:NH1	1:C:43:ARG:HG3	2.30	0.47
1:C:58:LYS:O	1:C:62:GLU:HB2	2.15	0.47
1:C:770:LEU:HB3	1:C:774:ARG:NH1	2.30	0.47
1:A:323:ARG:HB3	1:A:323:ARG:NH1	2.16	0.47
1:A:578:ARG:C	1:A:580:GLY:N	2.67	0.47
1:B:667:ASP:O	1:B:668:GLU:C	2.52	0.47
1:C:152:ALA:CB	1:C:254:VAL:HG22	2.41	0.47
1:A:164:ALA:HB1	1:A:213:GLN:HA	1.96	0.47
1:A:32:PRO:HA	1:A:64:GLN:CG	2.42	0.47
1:A:487:ASN:N	1:A:487:ASN:HD22	2.11	0.47
1:A:592:LEU:HD21	1:A:594:LEU:HD21	1.96	0.47
1:A:83:LEU:HG	1:A:87:LEU:HD23	1.97	0.47
1:C:635:ARG:NH1	1:C:635:ARG:CB	2.77	0.47
1:C:670:GLU:HB3	1:C:710:LEU:CD1	2.45	0.47
1:A:32:PRO:HG3	1:A:64:GLN:NE2	2.20	0.47
1:A:415:ILE:HA	1:B:486:LEU:CD2	2.44	0.47
1:A:43:ARG:HG3	1:A:43:ARG:NH1	2.30	0.47
1:A:441:LYS:CB	1:A:441:LYS:NZ	2.76	0.47
1:A:566:ALA:CB	1:A:752:VAL:HG11	2.46	0.47
1:B:146:ALA:O	1:B:147:GLU:HB3	2.15	0.47
1:B:332:PRO:HG2	1:B:378:PRO:HG3	1.96	0.47
1:B:455:ARG:HH11	1:B:455:ARG:HG2	1.78	0.47
1:B:472:GLU:OE1	1:B:472:GLU:HA	2.15	0.47
1:B:580:GLY:C	1:B:581:LEU:HD12	2.36	0.47
1:B:653:THR:HG22	1:B:689:LEU:HD23	1.96	0.47
1:C:445:GLU:C	1:C:447:ALA:H	2.18	0.47
1:C:715:ILE:HD13	1:C:753:VAL:CG2	2.45	0.47
1:A:597:THR:HG22	1:A:598:GLY:N	2.30	0.46
1:A:635:ARG:HH11	1:A:635:ARG:CB	2.28	0.46
1:B:332:PRO:HD2	1:B:378:PRO:HD3	1.96	0.46
1:B:591:PHE:HD2	1:B:750:GLU:HB2	1.80	0.46
1:B:714:LEU:HD21	1:B:731:GLU:HG3	1.96	0.46
1:B:770:LEU:HB3	1:B:774:ARG:HH11	1.80	0.46
1:C:535:GLY:C	1:C:536:ILE:HG12	2.35	0.46
1:C:623:ASP:O	1:C:626:GLU:HG2	2.15	0.46
1:C:685:ASP:C	1:C:687:GLY:H	2.17	0.46
1:C:708:SER:C	1:C:709:ASN:HD22	2.17	0.46
1:A:195:VAL:HG11	1:A:311:TYR:CE1	2.50	0.46
1:A:383:ASP:O	1:A:387:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:GLY:H	3:A:911:ANP:HNB1	1.63	0.46
1:B:173:ILE:HD11	1:B:340:ILE:N	2.30	0.46
1:B:679:ILE:HG23	1:B:689:LEU:HD11	1.97	0.46
1:B:680:LEU:O	1:B:684:LEU:HD12	2.15	0.46
1:B:786:LEU:HG	1:B:837:VAL:HB	1.97	0.46
1:B:145:HIS:HE1	1:C:299:GLU:HG2	1.79	0.46
1:C:413:LEU:HD13	1:C:435:ILE:HD11	1.97	0.46
1:C:396:LEU:O	1:C:453:TRP:HH2	1.98	0.46
1:A:113:LEU:CD2	1:A:128:LEU:HB3	2.46	0.46
1:A:172:VAL:O	1:A:172:VAL:HG23	2.15	0.46
1:A:252:LYS:O	1:A:256:GLN:HG2	2.16	0.46
1:A:373:THR:HG21	1:A:659:ARG:NH2	2.30	0.46
1:A:514:ALA:O	1:A:517:VAL:HG13	2.16	0.46
1:A:517:VAL:HG23	1:A:517:VAL:O	2.14	0.46
1:A:635:ARG:HH22	1:A:679:ILE:HG12	1.80	0.46
1:A:32:PRO:HB2	1:A:68:LEU:CD2	2.45	0.46
1:B:504:VAL:HG13	1:B:505:GLU:N	2.30	0.46
1:C:178:GLU:CB	1:C:207:ILE:HD12	2.44	0.46
1:C:255:ILE:HG13	1:C:300:LEU:HD22	1.97	0.46
1:C:420:LEU:C	1:C:420:LEU:HD23	2.36	0.46
1:C:98:MET:SD	1:C:106:VAL:HG22	2.55	0.46
1:A:185:ILE:HD13	1:A:325:GLN:CB	2.43	0.46
1:A:399:ALA:HB3	1:A:400:PRO:CD	2.40	0.46
1:A:635:ARG:NH1	1:A:635:ARG:CB	2.78	0.46
1:B:516:PHE:O	1:B:517:VAL:HG23	2.15	0.46
1:B:635:ARG:C	1:B:636:LEU:HD23	2.35	0.46
1:B:83:LEU:HG	1:B:87:LEU:HD23	1.96	0.46
1:C:491:GLU:OE2	1:C:492:LEU:HD13	2.15	0.46
1:C:666:PHE:HB2	1:C:706:LEU:HD23	1.97	0.46
1:A:45:LEU:HD13	1:A:150:TYR:CE2	2.50	0.46
1:A:173:ILE:HD11	1:A:339:SER:O	2.14	0.46
1:B:581:LEU:HD12	1:B:581:LEU:N	2.30	0.46
1:C:196:LEU:O	1:C:305:ALA:HA	2.15	0.46
1:B:397:GLU:HB3	1:C:222:GLU:HB2	1.97	0.46
1:A:232:LEU:C	1:A:232:LEU:HD23	2.36	0.46
1:A:541:LEU:CG	1:A:542:LEU:H	2.28	0.46
1:A:786:LEU:HG	1:A:837:VAL:HB	1.97	0.46
1:B:113:LEU:CD2	1:B:128:LEU:HB3	2.46	0.46
1:B:123:PRO:HB2	1:B:128:LEU:HD21	1.97	0.46
1:B:125:LEU:H	1:B:125:LEU:CD1	2.24	0.46
1:B:151:ASN:O	1:B:155:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:O	1:B:405:ALA:HB3	2.16	0.46
1:B:459:ILE:CG2	1:B:511:LEU:HD21	2.40	0.46
1:B:541:LEU:CG	1:B:542:LEU:N	2.78	0.46
1:B:765:ILE:HA	1:B:768:ILE:CG2	2.45	0.46
1:B:8:GLN:CG	1:B:9:ALA:N	2.79	0.46
1:C:192:ASN:O	1:C:194:PRO:HD3	2.16	0.46
1:C:347:LYS:HB3	1:C:351:HIS:NE2	2.31	0.46
1:C:667:ASP:O	1:C:668:GLU:C	2.53	0.46
1:A:4:GLU:CA	1:A:11:ARG:NH2	2.79	0.46
1:A:518:ARG:HG2	1:A:518:ARG:HH11	1.80	0.46
1:B:297:ARG:O	1:B:299:GLU:HG3	2.14	0.46
1:B:629:GLU:CG	1:B:630:LYS:H	2.17	0.46
1:C:83:LEU:HG	1:C:87:LEU:HD23	1.97	0.46
1:B:215:ILE:HA	1:B:220:VAL:CG1	2.46	0.46
1:B:402:GLU:O	1:B:406:LEU:HG	2.15	0.46
1:B:439:ILE:C	1:B:441:LYS:H	2.19	0.46
1:B:457:ARG:HE	1:B:461:ARG:HH12	1.63	0.46
1:B:695:ARG:O	1:B:695:ARG:HG2	2.16	0.46
1:B:99:GLU:C	1:B:101:LEU:N	2.69	0.46
1:C:103:ASP:HB3	1:C:140:THR:HB	1.97	0.46
1:C:205:THR:HG22	1:C:209:GLU:OE2	2.16	0.46
1:A:113:LEU:HD11	1:A:132:LEU:HD13	1.97	0.46
1:A:667:ASP:O	1:A:668:GLU:C	2.52	0.46
1:B:35:TRP:CE3	1:B:35:TRP:HA	2.51	0.46
1:B:760:GLU:O	1:B:764:GLN:HG3	2.16	0.46
1:C:7:THR:HG23	1:C:143:THR:CB	2.46	0.46
1:C:344:LEU:HD11	3:C:903:ANP:H2	1.96	0.46
1:A:480:ALA:O	1:A:482:ARG:N	2.49	0.46
1:A:715:ILE:HG12	1:A:732:VAL:HG21	1.98	0.46
1:A:798:GLY:O	1:A:807:PRO:HB2	2.16	0.46
1:B:119:THR:HA	1:B:120:PRO:HD3	1.84	0.46
1:B:462:LYS:O	1:B:465:GLU:HB3	2.16	0.46
1:B:480:ALA:O	1:B:482:ARG:N	2.49	0.46
1:B:713:PRO:HG2	1:B:714:LEU:H	1.81	0.46
1:C:173:ILE:HD11	1:C:340:ILE:CA	2.45	0.46
1:C:199:GLU:HG3	1:C:200:PRO:CD	2.45	0.46
1:C:760:GLU:O	1:C:764:GLN:HG3	2.16	0.46
1:A:456:GLU:CG	1:A:514:ALA:HB1	2.46	0.45
1:B:172:VAL:HG21	1:B:210:GLY:HA2	1.98	0.45
1:C:31:LEU:HD22	1:C:115:LEU:HD22	1.98	0.45
1:C:5:ARG:HD3	1:C:5:ARG:HA	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:TRP:N	1:C:6:TRP:CD1	2.84	0.45
1:C:688:ARG:HH12	1:C:700:ARG:HD3	1.81	0.45
1:A:101:LEU:O	1:A:102:LYS:CB	2.63	0.45
1:A:677:PHE:O	1:A:681:LEU:HB2	2.16	0.45
1:A:683:ILE:O	1:A:687:GLY:HA2	2.16	0.45
1:B:96:GLY:O	1:B:100:GLU:HG3	2.17	0.45
1:B:714:LEU:HD21	1:B:731:GLU:CG	2.46	0.45
1:C:215:ILE:HA	1:C:220:VAL:HG12	1.98	0.45
1:A:399:ALA:HA	1:A:515:ARG:NH2	2.31	0.45
1:B:441:LYS:C	1:B:443:THR:N	2.70	0.45
1:C:22:GLN:HA	1:C:79:VAL:CG1	2.46	0.45
1:C:435:ILE:HD12	1:C:438:GLU:HB3	1.97	0.45
1:C:436:GLU:HA	1:C:439:ILE:HG22	1.98	0.45
1:C:546:ARG:O	1:C:550:LEU:HD13	2.16	0.45
1:C:770:LEU:HD13	1:C:774:ARG:HH22	1.81	0.45
1:A:485:ASP:C	1:A:487:ASN:N	2.70	0.45
1:A:515:ARG:C	1:A:515:ARG:HD3	2.37	0.45
1:A:635:ARG:C	1:A:636:LEU:HD23	2.36	0.45
1:A:713:PRO:HG2	1:A:714:LEU:H	1.81	0.45
1:B:295:LEU:HB2	1:B:323:ARG:NH1	2.30	0.45
1:B:679:ILE:CD1	1:B:679:ILE:H	2.26	0.45
1:C:199:GLU:HG2	1:C:376:ARG:CD	2.47	0.45
1:C:541:LEU:CG	1:C:542:LEU:N	2.79	0.45
1:C:629:GLU:N	1:C:629:GLU:OE2	2.50	0.45
1:A:483:GLN:C	1:A:485:ASP:H	2.20	0.45
1:A:660:PRO:O	1:A:702:THR:HG22	2.17	0.45
1:A:798:GLY:HA2	1:A:808:LEU:HA	1.98	0.45
1:B:295:LEU:C	1:B:297:ARG:N	2.70	0.45
1:B:314:ILE:C	1:B:316:LYS:H	2.20	0.45
1:B:314:ILE:HG23	1:B:320:LEU:CD2	2.46	0.45
1:B:331:GLU:OE1	1:B:377:LEU:HB2	2.17	0.45
1:C:193:ASN:O	1:C:324:PHE:HA	2.17	0.45
1:C:413:LEU:HA	1:C:416:GLU:CB	2.47	0.45
1:C:45:LEU:HD23	1:C:108:VAL:CG2	2.46	0.45
1:C:794:LEU:HA	1:C:794:LEU:HD23	1.77	0.45
1:A:132:LEU:HD23	1:A:132:LEU:O	2.16	0.45
1:A:43:ARG:NH2	1:A:253:ALA:HB1	2.32	0.45
1:B:552:LEU:HD23	1:B:571:ALA:HA	1.99	0.45
1:B:677:PHE:O	1:B:681:LEU:HB2	2.17	0.45
1:B:682:GLN:NE2	1:B:689:LEU:HD12	2.32	0.45
1:C:308:LEU:CD2	1:C:695:ARG:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:GLN:NE2	1:C:754:PHE:HD2	2.14	0.45
1:A:185:ILE:CD1	1:A:325:GLN:HB3	2.45	0.45
1:A:199:GLU:HG2	1:A:376:ARG:CD	2.46	0.45
1:B:32:PRO:HA	1:B:64:GLN:CG	2.44	0.45
1:B:55:ALA:HB2	1:B:123:PRO:HD2	1.98	0.45
1:B:58:LYS:O	1:B:62:GLU:HB2	2.16	0.45
1:B:8:GLN:OE1	1:B:142:GLN:NE2	2.50	0.45
1:C:6:TRP:CG	1:C:106:VAL:HB	2.52	0.45
1:C:31:LEU:HB2	1:C:32:PRO:HD3	1.98	0.45
1:C:403:ILE:HG22	1:C:407:GLU:HG3	1.98	0.45
1:C:594:LEU:HD11	1:C:736:LEU:HD11	1.99	0.45
1:C:664:ILE:HG22	1:C:666:PHE:CE1	2.52	0.45
1:A:4:GLU:N	1:A:11:ARG:NH2	2.64	0.45
1:A:199:GLU:HG3	1:A:200:PRO:CD	2.46	0.45
1:A:158:ILE:CG1	1:A:233:GLN:HE22	2.13	0.45
1:A:31:LEU:HB2	1:A:32:PRO:HD3	1.98	0.45
1:B:148:SER:HB2	1:B:150:TYR:CE1	2.51	0.45
1:B:541:LEU:CG	1:B:542:LEU:H	2.29	0.45
1:B:8:GLN:CD	1:B:9:ALA:H	2.20	0.45
1:C:597:THR:HG22	1:C:598:GLY:N	2.31	0.45
1:C:780:LYS:O	1:C:782:ILE:HG13	2.17	0.45
1:A:113:LEU:HD23	1:A:128:LEU:HB3	1.99	0.45
1:B:215:ILE:HA	1:B:220:VAL:HG12	1.98	0.45
1:B:535:GLY:C	1:B:536:ILE:HG12	2.38	0.45
1:C:185:ILE:CG2	1:C:194:PRO:HB3	2.46	0.45
1:C:35:TRP:CE3	1:C:35:TRP:HA	2.51	0.45
1:C:486:LEU:HG	1:C:491:GLU:HG2	1.98	0.45
1:C:741:ARG:O	1:C:744:PHE:HB3	2.17	0.45
1:A:215:ILE:HA	1:A:220:VAL:CG1	2.46	0.45
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.52	0.45
1:A:695:ARG:O	1:A:695:ARG:HG2	2.17	0.45
1:B:517:VAL:CG1	1:B:518:ARG:N	2.80	0.45
1:C:332:PRO:HD2	1:C:378:PRO:CD	2.47	0.45
1:C:463:LEU:CD1	1:C:504:VAL:HA	2.48	0.45
1:A:423:GLU:HA	1:A:429:GLN:NE2	2.31	0.44
1:A:416:GLU:HB3	1:A:435:ILE:HD11	1.99	0.44
1:A:656:VAL:HG21	1:A:699:PHE:CE2	2.51	0.44
1:B:140:THR:O	1:B:141:VAL:HG23	2.16	0.44
1:A:394:MET:HB2	1:B:184:GLN:HE22	1.81	0.44
1:B:185:ILE:HD13	1:B:325:GLN:HB3	1.99	0.44
1:B:8:GLN:HG2	1:B:9:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB2	1:A:204:LYS:NZ	2.32	0.44
1:A:355:ARG:O	1:A:520:GLU:HA	2.18	0.44
1:B:74:VAL:HG23	1:B:75:GLU:N	2.32	0.44
1:C:307:THR:HB	1:C:310:GLU:OE1	2.17	0.44
1:C:535:GLY:O	1:C:536:ILE:HG12	2.18	0.44
1:A:463:LEU:HA	1:A:507:LEU:CD1	2.48	0.44
1:B:485:ASP:OD1	1:B:487:ASN:HB3	2.18	0.44
1:B:629:GLU:N	1:B:629:GLU:OE2	2.50	0.44
1:C:204:LYS:HB2	1:C:204:LYS:NZ	2.32	0.44
1:C:215:ILE:HA	1:C:220:VAL:CG1	2.47	0.44
1:B:535:GLY:O	1:B:540:LYS:NZ	2.48	0.44
1:B:635:ARG:NH1	1:B:635:ARG:HB2	2.33	0.44
1:C:344:LEU:H	1:C:344:LEU:CD1	2.29	0.44
1:C:457:ARG:O	1:C:457:ARG:HD2	2.18	0.44
1:A:125:LEU:HD23	1:A:129:LYS:CE	2.45	0.44
1:A:227:LYS:HE3	1:A:264:GLU:HA	1.99	0.44
1:A:354:VAL:HB	1:A:519:LEU:O	2.18	0.44
1:A:460:LEU:CD1	1:A:464:ARG:HG3	2.48	0.44
1:A:839:VAL:HG13	1:A:840:GLY:N	2.33	0.44
1:B:103:ASP:CG	1:B:140:THR:HG23	2.38	0.44
1:B:499:LYS:O	1:B:502:ALA:N	2.46	0.44
1:B:730:ASP:O	1:B:734:LYS:HG3	2.17	0.44
1:C:635:ARG:O	1:C:653:THR:HG23	2.17	0.44
1:A:597:THR:CG2	3:A:911:ANP:HNB1	2.31	0.44
1:B:18:GLN:HG2	1:B:22:GLN:HE21	1.83	0.44
1:C:352:HIS:NE2	1:C:386:ASP:OD1	2.50	0.44
1:C:546:ARG:HG3	1:C:547:GLU:N	2.32	0.44
1:A:225:LYS:HD2	1:A:225:LYS:N	2.33	0.44
1:A:413:LEU:O	1:A:435:ILE:HD11	2.18	0.44
1:A:432:LEU:CD2	1:A:432:LEU:H	2.28	0.44
1:B:320:LEU:HD12	1:B:320:LEU:N	2.33	0.44
1:B:500:LEU:O	1:B:504:VAL:HG12	2.18	0.44
1:B:546:ARG:HG3	1:B:547:GLU:N	2.32	0.44
1:C:270:ASP:O	1:C:305:ALA:O	2.35	0.44
1:C:410:LYS:HB2	1:C:442:LEU:HD23	1.99	0.44
1:A:135:LEU:HD22	1:A:150:TYR:OH	2.18	0.44
1:A:266:ILE:HD11	1:A:301:ARG:CZ	2.48	0.44
1:A:666:PHE:HB2	1:A:706:LEU:CD2	2.48	0.44
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.73	0.44
1:B:455:ARG:NH1	1:B:455:ARG:HG2	2.31	0.44
1:B:477:ILE:O	1:B:480:ALA:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:LYS:HE2	1:C:723:TRP:HE1	1.82	0.44
1:A:215:ILE:HA	1:A:220:VAL:HG12	1.99	0.44
1:A:156:TYR:CE2	1:A:250:ARG:HD3	2.52	0.44
1:A:30:ASP:HB3	1:A:32:PRO:HD2	2.00	0.44
1:A:392:LEU:HB3	1:A:518:ARG:HA	1.99	0.44
1:A:413:LEU:HB3	1:A:435:ILE:HG13	2.00	0.44
1:A:458:GLU:HA	1:A:458:GLU:OE2	2.18	0.44
1:B:206:ALA:O	1:B:210:GLY:N	2.47	0.44
1:B:537:PRO:O	1:B:541:LEU:HB3	2.18	0.44
1:C:463:LEU:HD13	1:C:507:LEU:HD23	1.99	0.44
1:A:332:PRO:HD2	1:A:378:PRO:HG3	1.99	0.43
1:A:546:ARG:HG3	1:A:547:GLU:N	2.33	0.43
1:A:623:ASP:O	1:A:626:GLU:HG2	2.17	0.43
1:B:318:PRO:O	1:B:322:ARG:HB3	2.18	0.43
1:B:438:GLU:O	1:B:441:LYS:N	2.48	0.43
1:B:492:LEU:O	1:B:496:GLU:HB2	2.17	0.43
1:B:497:LEU:HB3	1:B:498:PRO:HD3	1.98	0.43
1:B:556:LEU:CD2	1:B:611:THR:HG21	2.48	0.43
1:B:623:ASP:O	1:B:626:GLU:HG2	2.17	0.43
1:C:18:GLN:HG2	1:C:22:GLN:HE21	1.83	0.43
1:A:502:ALA:HA	1:A:505:GLU:HB2	1.99	0.43
1:B:291:LEU:HD12	1:B:300:LEU:CD2	2.48	0.43
1:B:418:GLU:CG	1:C:492:LEU:HD23	2.48	0.43
1:A:415:ILE:CG1	1:B:486:LEU:HG	2.47	0.43
1:C:531:SER:OG	1:C:537:PRO:HD3	2.19	0.43
1:C:74:VAL:HG23	1:C:75:GLU:N	2.33	0.43
1:A:311:TYR:CE2	1:A:326:PRO:HG3	2.53	0.43
1:A:377:LEU:H	1:A:380:LYS:HE2	1.83	0.43
1:B:117:GLU:OE2	1:B:125:LEU:HD21	2.18	0.43
1:B:225:LYS:HD2	1:B:225:LYS:N	2.33	0.43
1:B:27:GLN:HG3	1:B:78:GLU:O	2.18	0.43
1:B:394:MET:CE	1:C:180:ARG:HH22	2.31	0.43
1:B:431:ARG:HH11	1:B:431:ARG:HG3	1.84	0.43
1:B:384:LEU:HD11	1:B:530:VAL:HG22	2.00	0.43
1:B:814:ARG:HH11	1:B:814:ARG:HG3	1.83	0.43
1:C:720:GLN:C	1:C:722:GLY:H	2.21	0.43
1:B:344:LEU:H	1:B:344:LEU:CD1	2.30	0.43
1:B:392:LEU:HD12	1:B:518:ARG:NH2	2.33	0.43
1:B:408:ARG:O	1:B:412:GLN:HG2	2.18	0.43
1:A:415:ILE:HD11	1:B:489:ALA:CB	2.48	0.43
1:B:514:ALA:HB1	1:B:517:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:LYS:O	1:B:782:ILE:HG13	2.19	0.43
1:C:307:THR:HB	1:C:310:GLU:CD	2.38	0.43
1:C:30:ASP:CG	1:C:86:ARG:HH21	2.21	0.43
1:C:409:LYS:O	1:C:412:GLN:HB2	2.17	0.43
1:A:344:LEU:O	1:A:345:LYS:C	2.56	0.43
1:A:412:GLN:O	1:A:415:ILE:HG22	2.17	0.43
1:A:469:ARG:HH11	1:A:469:ARG:HG2	1.82	0.43
1:A:494:TYR:O	1:A:496:GLU:N	2.51	0.43
1:A:635:ARG:HH11	1:A:635:ARG:HB3	1.83	0.43
1:B:31:LEU:HB2	1:B:32:PRO:HD3	1.99	0.43
1:B:635:ARG:HH11	1:B:635:ARG:CB	2.32	0.43
1:C:402:GLU:O	1:C:405:ALA:HB3	2.19	0.43
1:C:413:LEU:HA	1:C:416:GLU:HB3	2.00	0.43
1:C:480:ALA:CB	1:C:490:ALA:HB3	2.48	0.43
1:C:577:ALA:C	1:C:578:ARG:O	2.52	0.43
1:C:636:LEU:HB2	1:C:691:ASP:HA	1.99	0.43
1:C:668:GLU:OE2	1:C:709:ASN:ND2	2.50	0.43
1:C:656:VAL:HG11	1:C:699:PHE:CE1	2.53	0.43
1:C:773:LEU:O	1:C:777:LEU:HG	2.18	0.43
1:A:16:GLN:NE2	1:A:261:SER:HA	2.34	0.43
1:A:411:LEU:O	1:A:415:ILE:HG22	2.19	0.43
1:A:455:ARG:HG2	1:A:459:ILE:CD1	2.48	0.43
1:B:485:ASP:OD1	1:B:488:ARG:HG3	2.19	0.43
1:B:203:GLY:HA2	3:B:902:ANP:PA	2.58	0.43
1:B:95:GLU:O	1:B:99:GLU:HG3	2.19	0.43
1:C:43:ARG:CD	1:C:226:GLY:HA3	2.48	0.43
1:C:318:PRO:O	1:C:322:ARG:HG2	2.19	0.43
1:C:332:PRO:HA	1:C:336:GLU:OE1	2.18	0.43
1:C:345:LYS:O	1:C:349:GLU:HG2	2.18	0.43
1:A:18:GLN:HG2	1:A:22:GLN:HE21	1.83	0.43
1:A:292:LYS:N	1:A:293:PRO:CD	2.82	0.43
1:B:344:LEU:O	1:B:345:LYS:C	2.57	0.43
1:C:123:PRO:HB3	1:C:127:ALA:HB3	2.01	0.43
1:C:30:ASP:HB3	1:C:32:PRO:HD2	2.00	0.43
1:C:499:LYS:HE3	1:C:503:GLU:OE2	2.18	0.43
1:C:535:GLY:O	1:C:536:ILE:CG1	2.67	0.43
1:C:730:ASP:O	1:C:734:LYS:HG3	2.18	0.43
1:A:311:TYR:CZ	1:A:326:PRO:HG3	2.54	0.43
1:B:181:ARG:O	1:B:184:GLN:HB3	2.18	0.43
1:B:578:ARG:C	1:B:580:GLY:N	2.72	0.43
1:B:635:ARG:NH1	1:B:635:ARG:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ARG:O	1:B:744:PHE:HB3	2.19	0.43
1:C:680:LEU:O	1:C:684:LEU:HD12	2.19	0.43
1:A:560:VAL:HG21	1:A:604:LEU:HA	2.01	0.43
1:A:654:GLU:HB3	1:A:658:ARG:NH1	2.34	0.43
1:A:29:ILE:HD12	1:A:83:LEU:CD1	2.49	0.43
1:B:391:ARG:HB2	1:C:184:GLN:HE21	1.82	0.43
1:B:431:ARG:HH12	1:B:432:LEU:HD23	1.82	0.43
1:B:448:LYS:O	1:B:451:ALA:HB3	2.18	0.43
1:B:583:ASP:HB3	1:B:586:ARG:CD	2.49	0.43
1:B:657:ARG:HG3	1:B:657:ARG:NH1	2.33	0.43
1:B:673:HIS:O	1:B:675:ASP:N	2.52	0.43
1:C:317:ASP:O	1:C:321:GLU:N	2.49	0.43
1:C:463:LEU:HD11	1:C:504:VAL:HG13	2.01	0.43
1:C:497:LEU:C	1:C:499:LYS:N	2.72	0.43
1:A:195:VAL:O	1:A:197:ILE:HD12	2.19	0.43
1:A:531:SER:HB2	1:A:537:PRO:HG3	2.01	0.43
1:A:636:LEU:HB2	1:A:691:ASP:HA	2.01	0.43
1:B:332:PRO:HD2	1:B:378:PRO:CD	2.49	0.43
1:B:420:LEU:HD11	1:B:432:LEU:HB3	2.00	0.43
1:B:635:ARG:HH22	1:B:679:ILE:HG12	1.83	0.43
1:C:139:ARG:CZ	1:C:148:SER:H	2.31	0.43
1:C:193:ASN:ND2	1:C:295:LEU:HD11	2.33	0.43
1:C:592:LEU:HG	1:C:594:LEU:HD21	2.00	0.43
1:A:114:ALA:HA	1:A:117:GLU:OE1	2.19	0.42
1:A:401:GLU:HB2	1:B:180:ARG:HH22	1.84	0.42
1:B:173:ILE:HG12	1:B:340:ILE:HA	2.00	0.42
1:B:497:LEU:N	1:B:498:PRO:CD	2.82	0.42
1:B:355:ARG:N	1:B:519:LEU:O	2.52	0.42
1:B:583:ASP:HB3	1:B:586:ARG:HD2	2.01	0.42
1:C:175:ARG:NH1	1:C:175:ARG:HG2	2.34	0.42
1:C:178:GLU:O	1:C:182:VAL:HG23	2.19	0.42
1:A:185:ILE:CG2	1:A:325:GLN:HG3	2.39	0.42
1:A:74:VAL:HG23	1:A:75:GLU:N	2.34	0.42
1:A:820:LEU:O	1:A:824:ILE:HG13	2.20	0.42
1:B:30:ASP:HB3	1:B:32:PRO:HD2	2.00	0.42
1:B:457:ARG:CB	1:B:461:ARG:HH22	2.32	0.42
1:C:325:GLN:HA	1:C:325:GLN:HE21	1.83	0.42
1:C:560:VAL:HG21	1:C:604:LEU:HA	2.01	0.42
1:C:778:ALA:C	1:C:780:LYS:N	2.72	0.42
1:A:35:TRP:CD1	1:A:64:GLN:HG2	2.54	0.42
1:A:492:LEU:C	1:A:494:TYR:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HA	1:A:496:GLU:HB2	2.00	0.42
1:A:837:VAL:HG22	1:A:846:PHE:CD2	2.54	0.42
1:B:116:ALA:HB1	1:B:128:LEU:CD1	2.49	0.42
1:B:133:LYS:O	1:B:135:LEU:N	2.52	0.42
1:B:753:VAL:HG13	1:B:753:VAL:O	2.19	0.42
1:B:22:GLN:HA	1:B:79:VAL:CG1	2.48	0.42
1:C:541:LEU:CG	1:C:542:LEU:H	2.31	0.42
1:C:578:ARG:C	1:C:580:GLY:N	2.72	0.42
1:A:34:LEU:HD23	1:A:115:LEU:CD1	2.41	0.42
1:A:518:ARG:HG2	1:A:518:ARG:NH1	2.34	0.42
1:A:552:LEU:HD23	1:A:571:ALA:HA	2.00	0.42
1:A:762:ILE:HD11	1:A:799:TYR:CD1	2.55	0.42
1:B:473:VAL:HG21	1:B:500:LEU:CD1	2.49	0.42
1:B:356:ILE:HA	1:B:521:VAL:HB	2.00	0.42
1:C:185:ILE:CD1	1:C:194:PRO:HB3	2.50	0.42
1:C:346:GLU:O	1:C:350:VAL:HG23	2.19	0.42
1:C:670:GLU:CB	1:C:710:LEU:HD11	2.49	0.42
1:A:178:GLU:HB2	1:A:207:ILE:HD12	2.01	0.42
1:A:294:ALA:HA	1:A:297:ARG:NH2	2.35	0.42
1:A:503:GLU:C	1:A:505:GLU:H	2.23	0.42
1:B:495:GLY:H	1:B:498:PRO:CG	2.26	0.42
1:C:225:LYS:HD2	1:C:225:LYS:N	2.33	0.42
1:C:757:LEU:HB2	1:C:762:ILE:HD11	2.01	0.42
1:A:18:GLN:HG3	1:A:29:ILE:HD11	2.01	0.42
1:A:492:LEU:C	1:A:494:TYR:H	2.23	0.42
1:A:556:LEU:CD2	1:A:611:THR:HG21	2.49	0.42
1:B:416:GLU:O	1:B:420:LEU:N	2.52	0.42
1:B:425:ASP:N	1:B:426:PRO:CD	2.79	0.42
1:B:453:TRP:CH2	1:B:457:ARG:HD2	2.55	0.42
1:B:480:ALA:C	1:B:482:ARG:N	2.70	0.42
1:B:556:LEU:HD23	1:B:607:THR:HG22	2.02	0.42
1:C:486:LEU:CG	1:C:491:GLU:HG2	2.49	0.42
1:A:136:ARG:HA	1:A:136:ARG:HD3	1.88	0.42
1:A:499:LYS:O	1:A:500:LEU:C	2.57	0.42
1:A:765:ILE:HA	1:A:768:ILE:CG2	2.49	0.42
1:A:776:ARG:NH2	1:B:584:PRO:HG3	2.35	0.42
1:B:151:ASN:OD1	1:B:257:GLU:OE1	2.37	0.42
1:B:307:THR:CG2	1:B:308:LEU:N	2.82	0.42
1:B:431:ARG:HG3	1:B:431:ARG:NH1	2.35	0.42
1:C:320:LEU:HG	1:C:324:PHE:CE2	2.53	0.42
1:C:592:LEU:HA	1:C:706:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LEU:CD1	1:C:784:LEU:HD22	2.49	0.42
1:C:7:THR:CG2	1:C:8:GLN:N	2.82	0.42
1:C:98:MET:O	1:C:102:LYS:N	2.52	0.42
1:A:321:GLU:O	1:A:323:ARG:N	2.50	0.42
1:A:463:LEU:C	1:A:463:LEU:HD23	2.40	0.42
1:A:544:GLY:O	1:A:545:GLU:C	2.58	0.42
1:A:814:ARG:HH11	1:A:814:ARG:HG3	1.85	0.42
1:B:827:GLY:O	1:B:830:LYS:HE2	2.20	0.42
1:C:292:LYS:HE2	1:C:293:PRO:HD3	2.02	0.42
1:C:790:ALA:O	1:C:793:PHE:HB3	2.20	0.42
1:A:317:ASP:O	1:A:320:LEU:N	2.48	0.42
1:B:113:LEU:HD23	1:B:128:LEU:HB3	2.02	0.42
1:B:55:ALA:HB2	1:B:123:PRO:HD3	2.02	0.42
1:B:592:LEU:CG	1:B:594:LEU:HD21	2.49	0.42
1:B:656:VAL:HG21	1:B:699:PHE:CZ	2.55	0.42
1:B:71:LEU:HA	1:B:72:PRO:HD3	1.75	0.42
1:C:152:ALA:HB1	1:C:254:VAL:CG2	2.43	0.42
1:C:347:LYS:O	1:C:350:VAL:HB	2.18	0.42
1:C:583:ASP:HB3	1:C:586:ARG:HD2	2.02	0.42
1:C:635:ARG:HH11	1:C:635:ARG:HB3	1.85	0.42
1:A:192:ASN:O	1:A:194:PRO:HD3	2.19	0.42
1:A:541:LEU:CG	1:A:542:LEU:N	2.78	0.42
1:A:572:ASP:O	1:A:576:ARG:HB2	2.20	0.42
1:A:656:VAL:HG11	1:A:699:PHE:CE1	2.55	0.42
1:B:151:ASN:HB3	1:B:154:GLU:OE2	2.20	0.42
1:A:415:ILE:HD11	1:B:489:ALA:HB1	2.02	0.42
1:B:39:LEU:O	1:B:61:LYS:HD2	2.20	0.42
1:C:206:ALA:O	1:C:210:GLY:N	2.52	0.42
1:C:408:ARG:HA	1:C:408:ARG:HD3	1.79	0.42
1:C:670:GLU:CD	1:C:670:GLU:H	2.23	0.42
1:B:312:ARG:O	1:B:315:GLU:HB2	2.20	0.41
1:B:538:VAL:O	1:B:542:LEU:HB3	2.20	0.41
1:C:473:VAL:O	1:C:477:ILE:HG23	2.19	0.41
1:B:173:ILE:HD11	1:B:340:ILE:CA	2.50	0.41
1:B:195:VAL:O	1:B:197:ILE:HD12	2.20	0.41
1:A:813:GLN:HG3	1:B:576:ARG:CD	2.50	0.41
1:B:774:ARG:CG	1:B:774:ARG:HH11	2.33	0.41
1:C:581:LEU:HD12	1:C:581:LEU:N	2.35	0.41
1:C:631:HIS:O	1:C:632:ALA:C	2.57	0.41
1:A:151:ASN:ND2	1:A:153:LEU:HB2	2.35	0.41
1:A:356:ILE:HD13	1:A:385:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LEU:HB2	1:A:435:ILE:HG22	2.01	0.41
1:A:435:ILE:HG23	1:A:436:GLU:N	2.35	0.41
1:A:720:GLN:C	1:A:722:GLY:N	2.73	0.41
1:B:613:PHE:O	1:B:615:THR:HG22	2.20	0.41
1:B:683:ILE:O	1:B:687:GLY:HA2	2.19	0.41
1:C:373:THR:HG22	1:C:658:ARG:O	2.20	0.41
1:C:413:LEU:C	1:C:415:ILE:N	2.74	0.41
1:C:636:LEU:C	1:C:692:SER:HB2	2.41	0.41
1:A:567:ILE:N	1:A:567:ILE:HD12	2.34	0.41
1:A:797:ARG:HH21	1:A:814:ARG:NH2	2.18	0.41
3:B:902:ANP:O3G	1:C:318:PRO:HB3	2.20	0.41
1:C:376:ARG:NH2	1:C:657:ARG:NE	2.69	0.41
1:C:683:ILE:HD12	1:C:699:PHE:CE2	2.55	0.41
1:A:134:GLU:O	1:A:135:LEU:HG	2.20	0.41
1:A:162:ARG:O	1:A:165:ALA:HB3	2.21	0.41
1:A:432:LEU:HB2	1:A:435:ILE:CG2	2.50	0.41
1:A:485:ASP:O	1:A:487:ASN:N	2.53	0.41
1:C:318:PRO:C	1:C:320:LEU:H	2.23	0.41
1:C:374:GLU:HG3	1:C:375:ARG:H	1.82	0.41
1:C:388:ALA:C	1:C:390:ALA:H	2.24	0.41
1:C:401:GLU:O	1:C:401:GLU:HG3	2.21	0.41
1:C:411:LEU:HA	1:C:414:GLU:HB3	2.02	0.41
1:C:499:LYS:HG3	1:C:503:GLU:OE2	2.19	0.41
1:C:753:VAL:O	1:C:753:VAL:HG13	2.20	0.41
1:A:458:GLU:O	1:A:461:ARG:N	2.54	0.41
1:B:417:ARG:O	1:B:420:LEU:N	2.53	0.41
1:B:535:GLY:O	1:B:536:ILE:HG12	2.20	0.41
1:C:172:VAL:O	1:C:172:VAL:HG23	2.20	0.41
1:C:175:ARG:O	1:C:179:ILE:HG13	2.21	0.41
1:C:593:PHE:N	1:C:706:LEU:O	2.47	0.41
1:A:4:GLU:N	1:A:11:ARG:HH22	2.18	0.41
1:A:308:LEU:O	1:A:312:ARG:HG3	2.20	0.41
1:A:345:LYS:O	1:A:349:GLU:HG2	2.20	0.41
1:A:442:LEU:O	1:A:446:ILE:HG13	2.21	0.41
1:A:477:ILE:HG21	1:A:493:ARG:HH21	1.86	0.41
1:A:597:THR:O	1:A:599:VAL:HG13	2.20	0.41
1:B:787:THR:HG22	1:B:788:GLU:N	2.36	0.41
1:B:793:PHE:O	1:B:796:GLU:HB2	2.21	0.41
1:C:460:LEU:HD23	1:C:460:LEU:O	2.21	0.41
1:A:202:VAL:HA	1:A:378:PRO:HG2	2.02	0.41
1:A:332:PRO:HD2	1:A:378:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:HD2	1:A:378:PRO:HD3	2.02	0.41
1:A:536:ILE:HG13	1:A:536:ILE:O	2.20	0.41
1:A:631:HIS:O	1:A:632:ALA:C	2.59	0.41
1:A:730:ASP:O	1:A:734:LYS:HG3	2.19	0.41
1:B:477:ILE:HG12	1:B:492:LEU:HB2	2.01	0.41
1:B:532:ARG:HH11	1:B:532:ARG:HG2	1.84	0.41
1:C:45:LEU:CD2	1:C:108:VAL:HG23	2.50	0.41
1:C:298:GLY:O	1:C:299:GLU:HB2	2.21	0.41
1:C:404:ASP:O	1:C:408:ARG:HB2	2.21	0.41
1:C:583:ASP:HA	1:C:584:PRO:HD3	1.96	0.41
1:C:695:ARG:O	1:C:695:ARG:HG2	2.20	0.41
1:C:721:LYS:HB2	1:C:723:TRP:NE1	2.36	0.41
1:A:570:VAL:HA	1:A:591:PHE:CE2	2.56	0.41
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.86	0.41
1:C:669:ILE:HG22	1:C:708:SER:HB2	2.03	0.41
1:C:206:ALA:N	3:C:903:ANP:O1A	2.54	0.41
1:A:420:LEU:CB	1:A:432:LEU:HD13	2.51	0.41
1:A:515:ARG:HD3	1:A:516:PHE:CB	2.51	0.41
1:B:396:LEU:HD22	1:B:517:VAL:HG13	2.03	0.41
1:B:536:ILE:HG13	1:B:536:ILE:O	2.21	0.41
1:B:669:ILE:HG22	1:B:708:SER:HB2	2.03	0.41
1:C:122:LEU:O	1:C:123:PRO:O	2.39	0.41
1:C:51:GLU:HB2	1:C:57:PRO:CG	2.49	0.41
1:A:322:ARG:HD3	1:A:322:ARG:HA	1.90	0.41
1:A:460:LEU:HD11	1:A:464:ARG:HG3	2.03	0.41
1:A:479:LEU:O	1:A:482:ARG:HB2	2.21	0.41
1:A:581:LEU:N	1:A:581:LEU:HD12	2.35	0.41
1:A:718:GLY:HA2	1:A:723:TRP:CE2	2.56	0.41
1:B:461:ARG:HG3	1:B:461:ARG:HH11	1.85	0.41
1:B:563:GLN:NE2	1:B:754:PHE:HB3	2.36	0.41
1:B:823:LYS:HB3	1:B:829:VAL:HG23	2.02	0.41
1:C:208:VAL:O	1:C:211:LEU:HB3	2.21	0.41
1:C:47:TRP:CE2	1:C:57:PRO:HB2	2.56	0.41
1:C:486:LEU:HG	1:C:491:GLU:CG	2.51	0.41
1:A:332:PRO:HG2	1:A:378:PRO:HG3	2.01	0.40
1:A:415:ILE:HA	1:B:486:LEU:CG	2.51	0.40
1:A:55:ALA:O	1:A:57:PRO:HD3	2.21	0.40
1:B:545:GLU:OE1	1:B:545:GLU:HA	2.22	0.40
1:C:162:ARG:O	1:C:165:ALA:HB3	2.20	0.40
1:A:152:ALA:HB1	1:A:254:VAL:CG2	2.52	0.40
1:A:723:TRP:HB2	1:A:724:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HD12	1:A:83:LEU:HD12	2.02	0.40
1:B:166:GLU:O	1:B:475:ARG:HD2	2.21	0.40
1:B:425:ASP:H	1:B:426:PRO:HD3	1.85	0.40
1:B:446:ILE:CG2	1:B:450:ARG:HH21	2.29	0.40
1:C:18:GLN:HG3	1:C:29:ILE:HD11	2.03	0.40
1:C:267:LEU:O	1:C:302:LEU:HD12	2.21	0.40
1:A:486:LEU:HA	1:A:489:ALA:CB	2.41	0.40
1:A:515:ARG:HD3	1:A:516:PHE:HB2	2.04	0.40
1:A:534:THR:HB	1:A:540:LYS:HE2	2.02	0.40
1:A:673:HIS:O	1:A:675:ASP:N	2.55	0.40
1:A:800:ASP:OD1	1:A:802:VAL:N	2.54	0.40
1:B:345:LYS:O	1:B:349:GLU:HG2	2.22	0.40
1:B:535:GLY:O	1:B:536:ILE:CG1	2.69	0.40
1:C:378:PRO:O	1:C:382:ILE:HG13	2.21	0.40
1:A:141:VAL:CG1	1:A:142:GLN:N	2.76	0.40
1:A:398:SER:O	1:A:402:GLU:HG3	2.21	0.40
1:A:4:GLU:HA	1:A:11:ARG:CZ	2.52	0.40
1:A:4:GLU:C	1:A:5:ARG:HG3	2.42	0.40
1:A:669:ILE:HG22	1:A:708:SER:HB2	2.03	0.40
1:A:762:ILE:O	1:A:766:VAL:HG23	2.22	0.40
1:A:771:SER:O	1:A:774:ARG:HB2	2.21	0.40
1:B:399:ALA:HA	1:B:400:PRO:HD3	1.95	0.40
1:B:413:LEU:HD13	1:B:439:ILE:HD13	2.04	0.40
1:B:631:HIS:O	1:B:632:ALA:C	2.59	0.40
1:C:312:ARG:HG2	1:C:312:ARG:HH11	1.86	0.40
1:C:377:LEU:H	1:C:380:LYS:HE2	1.85	0.40
1:C:436:GLU:HA	1:C:439:ILE:CG2	2.50	0.40
1:C:537:PRO:O	1:C:541:LEU:HB3	2.21	0.40
1:C:614:ASP:O	1:C:615:THR:HB	2.21	0.40
1:C:838:ASP:CG	1:C:839:VAL:H	2.25	0.40
1:C:93:ARG:O	1:C:97:LEU:HG	2.22	0.40
1:A:814:ARG:HD2	1:A:814:ARG:C	2.42	0.40
1:B:488:ARG:O	1:B:492:LEU:HG	2.21	0.40
1:C:132:LEU:C	1:C:132:LEU:HD23	2.41	0.40
1:C:435:ILE:C	1:C:437:ALA:N	2.75	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	795/854 (93%)	666 (84%)	93 (12%)	36 (4%)	2	14
1	B	795/854 (93%)	655 (82%)	104 (13%)	36 (4%)	2	14
1	C	795/854 (93%)	659 (83%)	108 (14%)	28 (4%)	3	20
All	All	2385/2562 (93%)	1980 (83%)	305 (13%)	100 (4%)	3	16

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLY
1	A	123	PRO
1	A	141	VAL
1	A	374	GLU
1	A	377	LEU
1	A	484	TYR
1	A	512	ARG
1	A	542	LEU
1	A	686	ASP
1	A	849	PRO
1	B	76	GLY
1	B	147	GLU
1	B	374	GLU
1	B	377	LEU
1	B	424	LYS
1	B	542	LEU
1	B	686	ASP
1	C	76	GLY
1	C	123	PRO
1	C	145	HIS
1	C	374	GLU
1	C	377	LEU
1	C	422	LYS
1	C	488	ARG

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Mol	Chain	Res	Type
1	C	542	LEU
1	C	686	ASP
1	A	5	ARG
1	A	74	VAL
1	A	136	ARG
1	A	137	GLY
1	A	321	GLU
1	A	324	PHE
1	A	481	GLU
1	A	496	GLU
1	A	541	LEU
1	B	74	VAL
1	B	141	VAL
1	B	148	SER
1	B	177	GLU
1	B	487	ASN
1	C	74	VAL
1	C	270	ASP
1	C	490	ALA
1	A	221	PRO
1	A	379	ASP
1	A	486	LEU
1	A	495	GLY
1	A	839	VAL
1	B	123	PRO
1	B	134	GLU
1	B	221	PRO
1	B	379	ASP
1	B	400	PRO
1	B	422	LYS
1	B	541	LEU
1	B	601	LYS
1	C	137	GLY
1	C	221	PRO
1	C	424	LYS
1	C	483	GLN
1	C	541	LEU
1	C	601	LYS
1	A	428	SER
1	A	536	ILE
1	B	125	LEU
1	B	296	ALA

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Mol	Chain	Res	Type
1	B	321	GLU
1	B	423	GLU
1	B	426	PRO
1	B	481	GLU
1	B	536	ILE
1	C	124	GLY
1	C	568	ARG
1	A	322	ARG
1	A	499	LYS
1	A	578	ARG
1	A	601	LYS
1	A	668	GLU
1	A	674	PRO
1	A	796	GLU
1	B	9	ALA
1	B	391	ARG
1	B	485	ASP
1	B	578	ARG
1	B	668	GLU
1	B	674	PRO
1	B	796	GLU
1	C	379	ASP
1	C	485	ASP
1	C	536	ILE
1	C	668	GLU
1	C	796	GLU
1	A	9	ALA
1	A	354	VAL
1	A	631	HIS
1	B	631	HIS
1	C	141	VAL
1	B	596	PRO
1	C	674	PRO
1	C	426	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	675/706 (96%)	644 (95%)	31 (5%)	27	64
1	B	675/706 (96%)	641 (95%)	34 (5%)	24	60
1	C	675/706 (96%)	645 (96%)	30 (4%)	28	65
All	All	2025/2118 (96%)	1930 (95%)	95 (5%)	26	63

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	62	GLU
1	A	66	ARG
1	A	93	ARG
1	A	122	LEU
1	A	123	PRO
1	A	147	GLU
1	A	189	ARG
1	A	225	LYS
1	A	233	GLN
1	A	234	MET
1	A	246	GLU
1	A	252	LYS
1	A	323	ARG
1	A	397	GLU
1	A	421	LYS
1	A	423	GLU
1	A	504	VAL
1	A	515	ARG
1	A	608	LEU
1	A	614	ASP
1	A	630	LYS
1	A	631	HIS
1	A	657	ARG
1	A	670	GLU
1	A	686	ASP
1	A	695	ARG
1	A	727	ARG
1	A	833	ASP
1	A	836	GLN
1	A	849	PRO
1	B	5	ARG
1	B	8	GLN
1	B	62	GLU

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Mol	Chain	Res	Type
1	B	66	ARG
1	B	93	ARG
1	B	122	LEU
1	B	123	PRO
1	B	136	ARG
1	B	161	THR
1	B	173	ILE
1	B	176	ASP
1	B	225	LYS
1	B	246	GLU
1	B	252	LYS
1	B	322	ARG
1	B	394	MET
1	B	422	LYS
1	B	429	GLN
1	B	441	LYS
1	B	486	LEU
1	B	505	GLU
1	B	608	LEU
1	B	614	ASP
1	B	630	LYS
1	B	631	HIS
1	B	657	ARG
1	B	670	GLU
1	B	674	PRO
1	B	686	ASP
1	B	695	ARG
1	B	727	ARG
1	B	774	ARG
1	B	833	ASP
1	B	836	GLN
1	C	5	ARG
1	C	62	GLU
1	C	66	ARG
1	C	93	ARG
1	C	136	ARG
1	C	143	THR
1	C	225	LYS
1	C	246	GLU
1	C	252	LYS
1	C	408	ARG
1	C	436	GLU

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Mol	Chain	Res	Type
1	C	482	ARG
1	C	491	GLU
1	C	492	LEU
1	C	543	GLU
1	C	608	LEU
1	C	614	ASP
1	C	630	LYS
1	C	631	HIS
1	C	636	LEU
1	C	657	ARG
1	C	670	GLU
1	C	674	PRO
1	C	686	ASP
1	C	695	ARG
1	C	709	ASN
1	C	727	ARG
1	C	800	ASP
1	C	833	ASP
1	C	836	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	22	GLN
1	A	27	GLN
1	A	64	GLN
1	A	92	ASN
1	A	256	GLN
1	A	429	GLN
1	A	487	ASN
1	A	682	GLN
1	A	746	ASN
1	A	764	GLN
1	B	8	GLN
1	B	16	GLN
1	B	22	GLN
1	B	27	GLN
1	B	64	GLN
1	B	92	ASN
1	B	142	GLN
1	B	145	HIS

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Mol	Chain	Res	Type
1	B	233	GLN
1	B	256	GLN
1	B	262	GLN
1	B	325	GLN
1	B	351	HIS
1	B	369	HIS
1	B	412	GLN
1	B	429	GLN
1	B	682	GLN
1	B	746	ASN
1	C	22	GLN
1	C	64	GLN
1	C	92	ASN
1	C	142	GLN
1	C	233	GLN
1	C	256	GLN
1	C	468	HIS
1	C	682	GLN
1	C	746	ASN
1	C	764	GLN
1	C	813	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 23 are monoatomic - leaving 6 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
3	ANP	C	913	-	29,33,33	1.87	8 (27%)	31,52,52	2.30	8 (25%)
3	ANP	C	903	-	29,33,33	2.02	8 (27%)	31,52,52	2.23	8 (25%)
3	ANP	B	902	-	29,33,33	2.06	7 (24%)	31,52,52	2.21	7 (22%)
3	ANP	A	911	-	29,33,33	1.92	7 (24%)	31,52,52	2.22	8 (25%)
3	ANP	A	901	-	29,33,33	2.18	8 (27%)	31,52,52	2.30	8 (25%)
3	ANP	B	912	-	29,33,33	1.91	8 (27%)	31,52,52	2.32	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	913	-	-	5/14/38/38	0/3/3/3
3	ANP	C	903	-	-	3/14/38/38	0/3/3/3
3	ANP	B	902	-	-	2/14/38/38	0/3/3/3
3	ANP	A	911	-	-	4/14/38/38	0/3/3/3
3	ANP	A	901	-	-	3/14/38/38	0/3/3/3
3	ANP	B	912	-	-	7/14/38/38	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ANP	PB-O3A	7.61	1.68	1.59
3	C	903	ANP	PB-O3A	6.76	1.67	1.59
3	A	911	ANP	PB-O3A	6.34	1.67	1.59
3	B	902	ANP	PB-O3A	6.30	1.67	1.59
3	C	913	ANP	PB-O3A	5.68	1.66	1.59
3	B	912	ANP	PB-O3A	5.49	1.66	1.59
3	C	903	ANP	PB-O2B	-4.14	1.45	1.56
3	B	902	ANP	PB-O2B	-4.07	1.45	1.56
3	B	902	ANP	C2'-C1'	-3.95	1.47	1.53
3	A	901	ANP	PB-O2B	-3.81	1.46	1.56
3	B	912	ANP	PB-O2B	-3.66	1.46	1.56
3	A	911	ANP	PB-O2B	-3.38	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	912	ANP	C2'-C1'	-3.33	1.48	1.53
3	A	901	ANP	PG-N3B	3.28	1.71	1.63
3	A	901	ANP	C2'-C1'	-3.24	1.48	1.53
3	C	903	ANP	C2'-C1'	-3.23	1.48	1.53
3	C	913	ANP	C2'-C1'	-3.21	1.48	1.53
3	C	913	ANP	PB-O2B	-3.13	1.48	1.56
3	A	901	ANP	C2-N3	3.13	1.37	1.32
3	C	913	ANP	C2-N3	3.12	1.37	1.32
3	C	903	ANP	C2-N3	2.90	1.36	1.32
3	A	911	ANP	PG-N3B	2.89	1.70	1.63
3	B	902	ANP	C2-N3	2.86	1.36	1.32
3	A	911	ANP	C2'-C1'	-2.86	1.49	1.53
3	B	902	ANP	PG-N3B	2.77	1.70	1.63
3	B	912	ANP	PG-N3B	2.72	1.70	1.63
3	B	912	ANP	C2-N3	2.69	1.36	1.32
3	B	912	ANP	PG-O3G	-2.68	1.49	1.56
3	C	913	ANP	PG-O3G	-2.65	1.49	1.56
3	C	903	ANP	PG-O3G	-2.60	1.49	1.56
3	B	902	ANP	PG-O3G	-2.56	1.49	1.56
3	A	901	ANP	PG-O3G	-2.54	1.49	1.56
3	A	911	ANP	PG-O3G	-2.54	1.49	1.56
3	A	911	ANP	C2-N3	2.51	1.36	1.32
3	A	901	ANP	O4'-C1'	2.49	1.44	1.41
3	C	903	ANP	PG-N3B	2.47	1.69	1.63
3	C	913	ANP	PG-N3B	2.43	1.69	1.63
3	A	901	ANP	C2-N1	2.38	1.38	1.33
3	B	902	ANP	C2-N1	2.37	1.38	1.33
3	B	912	ANP	C2-N1	2.28	1.38	1.33
3	C	903	ANP	C2-N1	2.24	1.38	1.33
3	C	913	ANP	O4'-C1'	2.22	1.44	1.41
3	B	912	ANP	O4'-C1'	2.15	1.44	1.41
3	C	903	ANP	C4-N3	2.08	1.38	1.35
3	C	913	ANP	C2-N1	2.03	1.37	1.33
3	A	911	ANP	O4'-C1'	2.00	1.43	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	ANP	O1B-PB-N3B	-6.91	101.59	111.77
3	A	901	ANP	O1B-PB-N3B	-6.71	101.89	111.77
3	B	912	ANP	O1B-PB-N3B	-6.47	102.25	111.77
3	C	903	ANP	O1B-PB-N3B	-6.38	102.38	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	913	ANP	O1B-PB-N3B	-6.22	102.60	111.77
3	A	911	ANP	O1B-PB-N3B	-5.77	103.28	111.77
3	C	913	ANP	C3'-C2'-C1'	5.64	109.47	100.98
3	B	912	ANP	C3'-C2'-C1'	5.23	108.86	100.98
3	A	901	ANP	O3A-PB-N3B	4.96	120.35	106.59
3	C	903	ANP	C3'-C2'-C1'	4.93	108.40	100.98
3	A	911	ANP	C3'-C2'-C1'	4.76	108.14	100.98
3	A	911	ANP	O4'-C1'-C2'	-4.76	99.97	106.93
3	B	912	ANP	O3A-PB-N3B	4.70	119.62	106.59
3	A	901	ANP	C3'-C2'-C1'	4.61	107.92	100.98
3	B	912	ANP	O4'-C1'-C2'	-4.57	100.24	106.93
3	B	902	ANP	O3A-PB-N3B	4.48	119.02	106.59
3	A	911	ANP	O3A-PB-N3B	4.34	118.62	106.59
3	C	913	ANP	O4'-C1'-C2'	-4.29	100.66	106.93
3	B	902	ANP	C3'-C2'-C1'	4.26	107.39	100.98
3	A	901	ANP	O4'-C1'-C2'	-4.26	100.70	106.93
3	C	903	ANP	O3A-PB-N3B	4.25	118.37	106.59
3	C	913	ANP	O3A-PB-N3B	4.18	118.20	106.59
3	B	902	ANP	O4'-C1'-C2'	-3.96	101.14	106.93
3	C	903	ANP	O4'-C1'-C2'	-3.91	101.21	106.93
3	B	912	ANP	O1G-PG-N3B	-3.65	106.39	111.77
3	C	913	ANP	O1G-PG-N3B	-3.60	106.46	111.77
3	A	901	ANP	O1G-PG-N3B	-3.40	106.77	111.77
3	B	902	ANP	O1G-PG-N3B	-3.30	106.90	111.77
3	C	903	ANP	O1G-PG-N3B	-3.29	106.92	111.77
3	A	911	ANP	O1G-PG-N3B	-3.13	107.17	111.77
3	C	903	ANP	N3-C2-N1	-3.12	123.80	128.68
3	A	911	ANP	N3-C2-N1	-3.11	123.82	128.68
3	A	911	ANP	O4'-C4'-C3'	-3.06	99.06	105.11
3	C	913	ANP	N3-C2-N1	-3.05	123.92	128.68
3	B	902	ANP	N3-C2-N1	-3.02	123.96	128.68
3	B	912	ANP	N3-C2-N1	-3.00	124.00	128.68
3	B	902	ANP	O4'-C4'-C3'	-2.96	99.25	105.11
3	A	901	ANP	O4'-C4'-C3'	-2.89	99.39	105.11
3	A	901	ANP	N3-C2-N1	-2.89	124.17	128.68
3	B	912	ANP	O4'-C4'-C3'	-2.79	99.59	105.11
3	C	903	ANP	PA-O3A-PB	2.69	142.09	132.62
3	C	903	ANP	O4'-C4'-C3'	-2.50	100.17	105.11
3	C	913	ANP	PA-O3A-PB	2.49	141.37	132.62
3	A	901	ANP	PA-O3A-PB	2.45	141.23	132.62
3	C	913	ANP	O4'-C4'-C3'	-2.43	100.30	105.11
3	A	911	ANP	PA-O3A-PB	2.31	140.77	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	912	ANP	O3'-C3'-C4'	-2.07	105.05	111.05
3	B	912	ANP	PA-O3A-PB	2.05	139.84	132.62

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	912	ANP	PB-N3B-PG-O1G
3	B	912	ANP	PG-N3B-PB-O1B
3	B	912	ANP	PA-O3A-PB-O1B
3	B	912	ANP	PA-O3A-PB-O2B
3	C	903	ANP	PB-N3B-PG-O1G
3	C	903	ANP	PG-N3B-PB-O1B
3	C	913	ANP	PB-N3B-PG-O1G
3	C	913	ANP	PG-N3B-PB-O1B
3	B	902	ANP	PB-N3B-PG-O1G
3	A	901	ANP	PB-N3B-PG-O1G
3	A	901	ANP	PG-N3B-PB-O1B
3	B	912	ANP	O4'-C4'-C5'-O5'
3	C	913	ANP	O4'-C4'-C5'-O5'
3	A	911	ANP	O4'-C4'-C5'-O5'
3	C	913	ANP	C3'-C4'-C5'-O5'
3	A	911	ANP	C3'-C4'-C5'-O5'
3	B	912	ANP	PB-O3A-PA-O2A
3	C	903	ANP	PB-O3A-PA-O2A
3	C	913	ANP	PB-O3A-PA-O2A
3	B	902	ANP	PB-O3A-PA-O2A
3	A	911	ANP	PB-O3A-PA-O2A
3	A	901	ANP	PB-O3A-PA-O2A
3	B	912	ANP	C3'-C4'-C5'-O5'
3	A	911	ANP	PB-N3B-PG-O1G

There are no ring outliers.

6 monomers are involved in 19 short contacts:

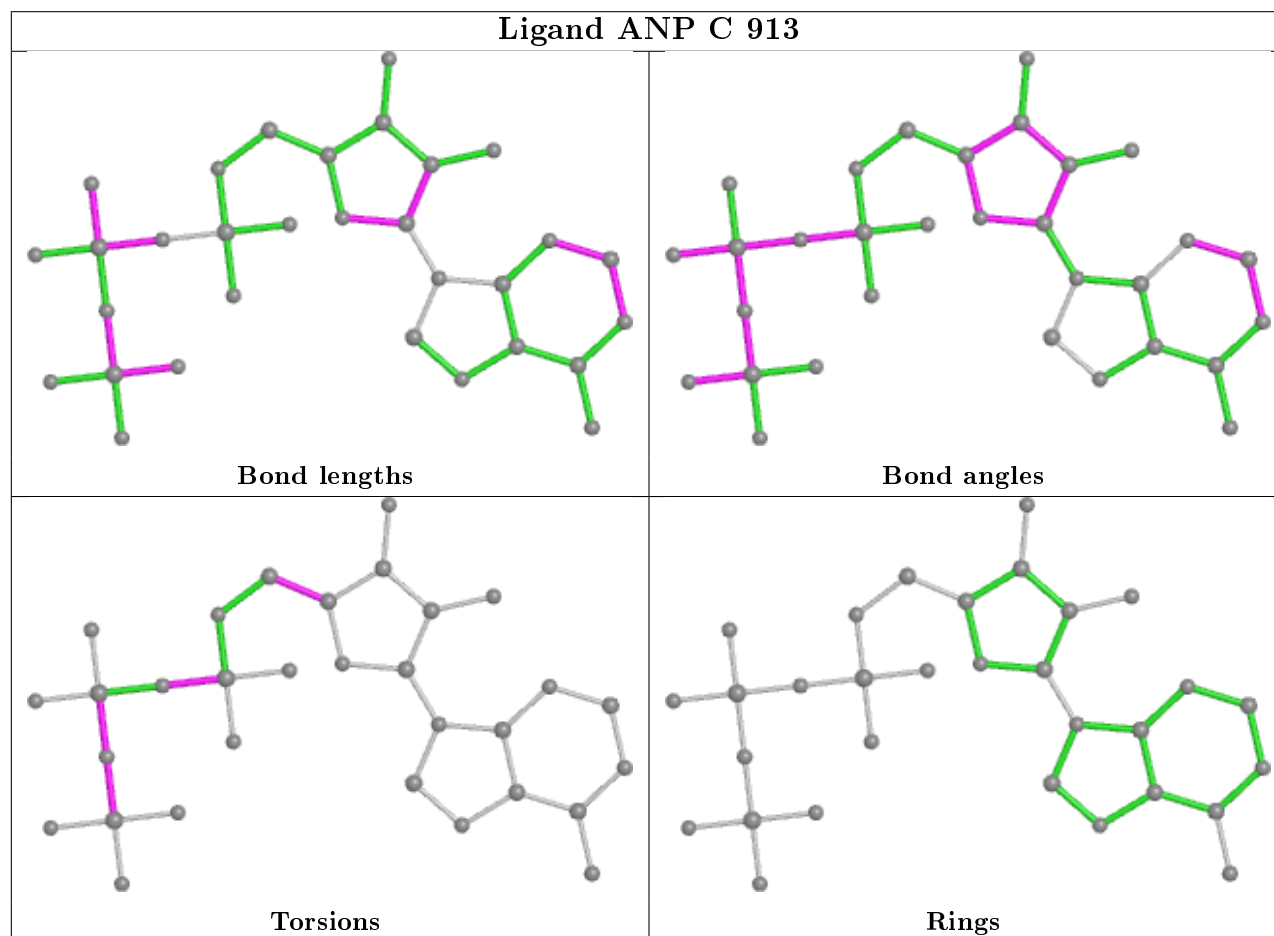
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	913	ANP	3	0
3	C	903	ANP	2	0
3	B	902	ANP	3	0
3	A	911	ANP	6	0
3	A	901	ANP	3	0

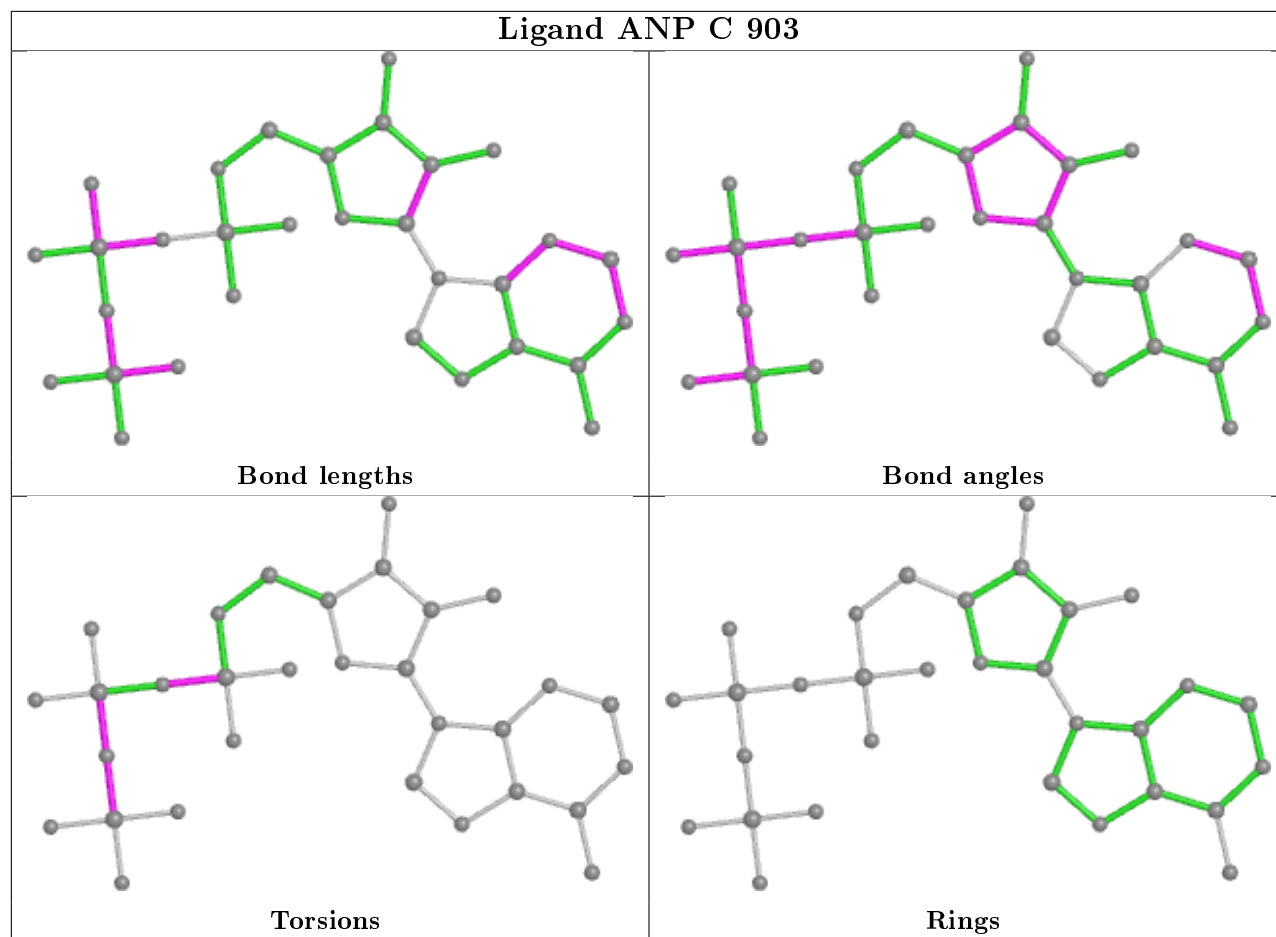
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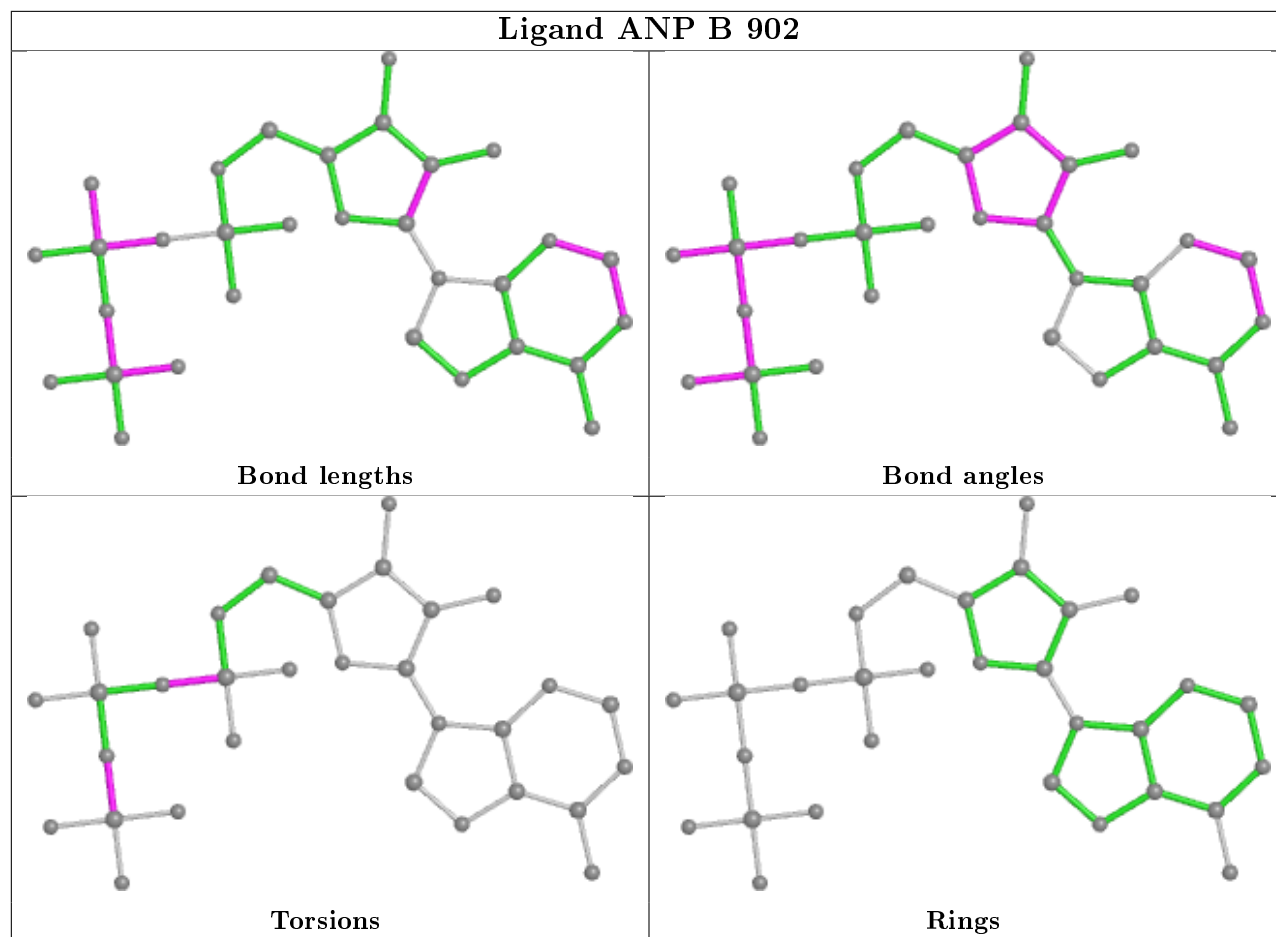
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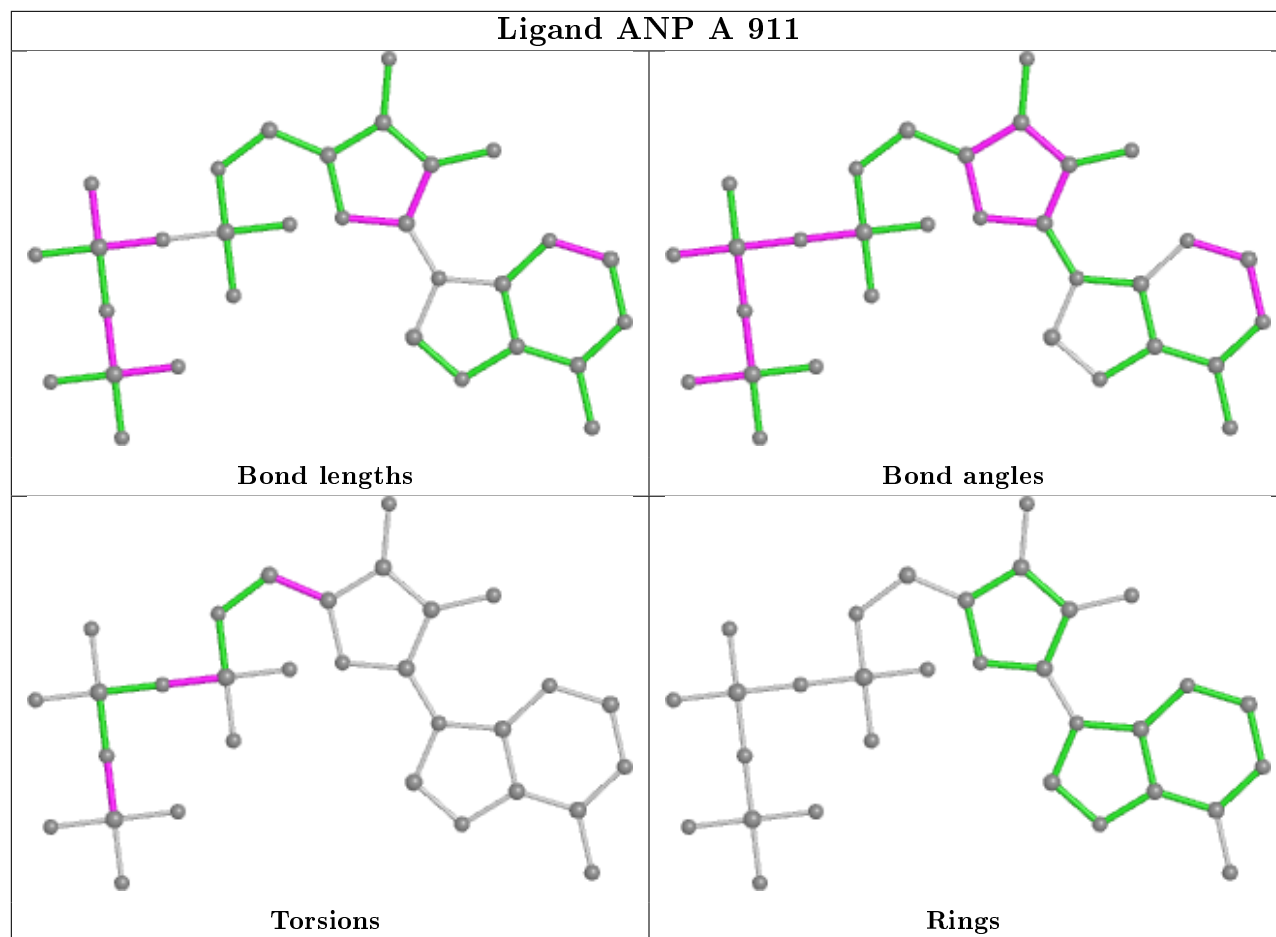
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	912	ANP	2	0

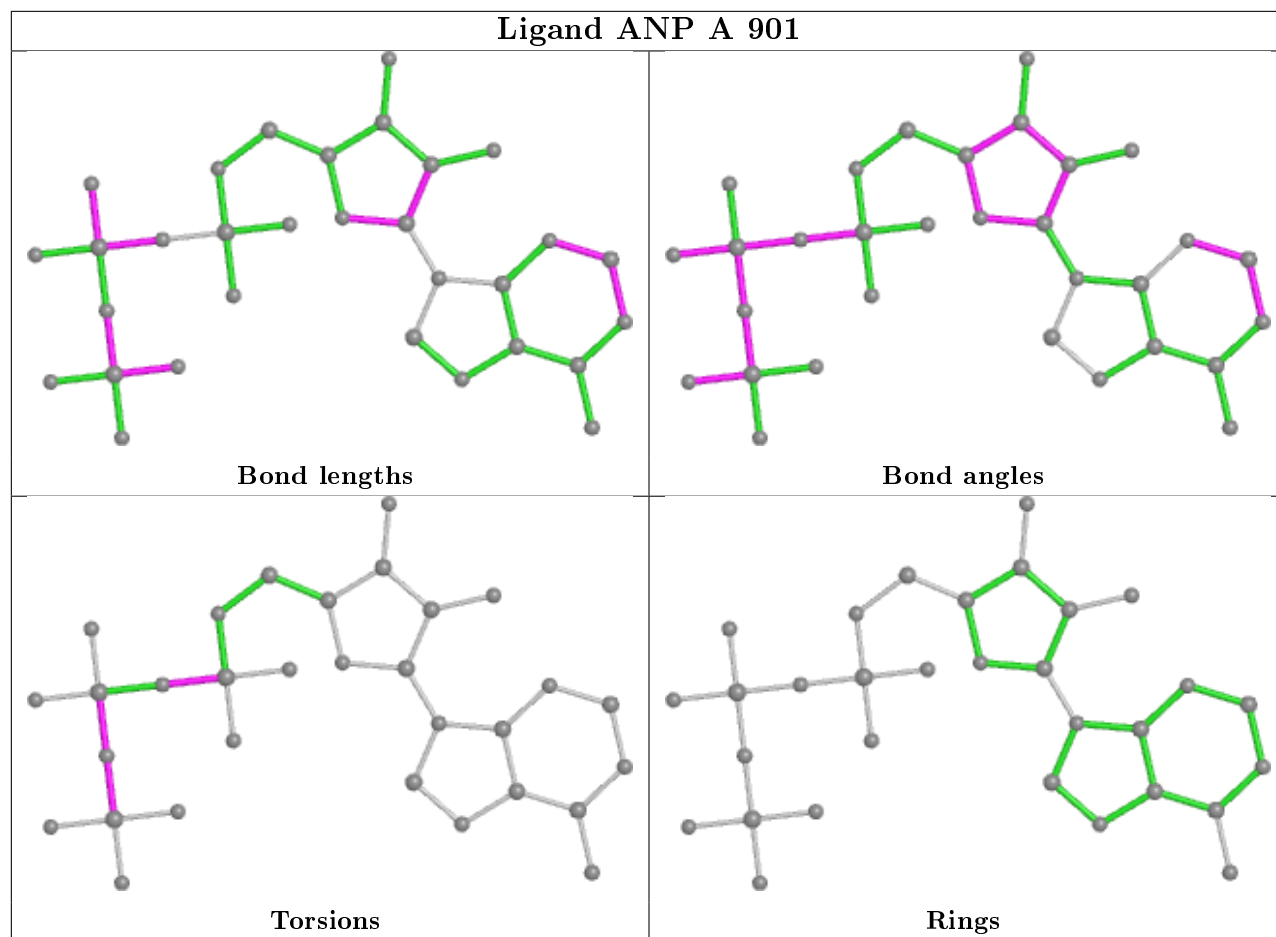
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

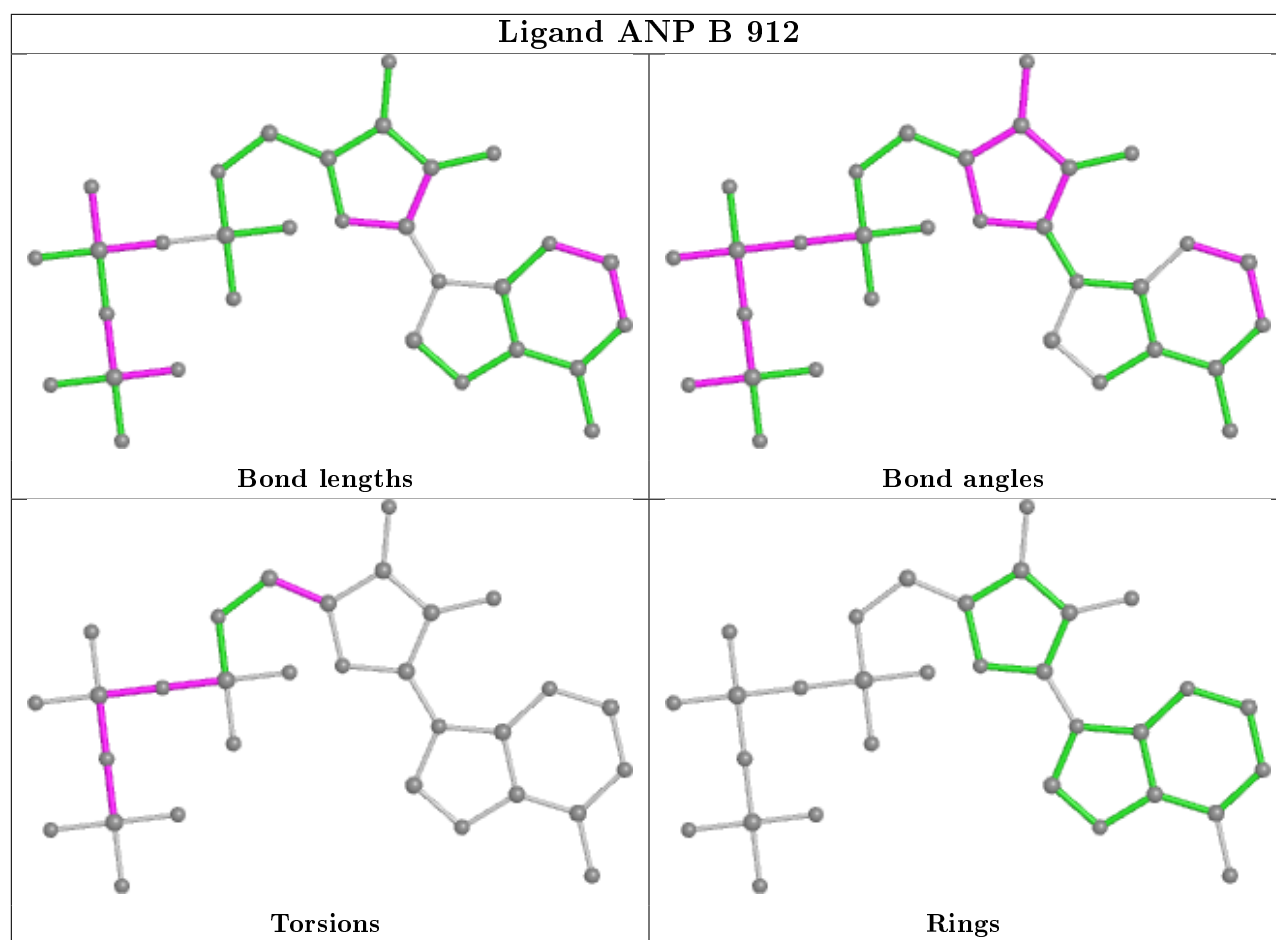












5.7 Other polymers [i](#)

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	803/854 (94%)	0.21	40 (4%) 28 10	32, 93, 142, 187	0
1	B	803/854 (94%)	0.11	18 (2%) 62 33	33, 82, 134, 176	0
1	C	803/854 (94%)	0.69	110 (13%) 3 1	37, 108, 171, 192	0
All	All	2409/2562 (94%)	0.34	168 (6%) 16 5	32, 92, 162, 192	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124	GLY	10.4
1	C	46	ALA	9.8
1	C	25	LYS	8.4
1	C	50	LEU	7.7
1	C	123	PRO	7.1
1	A	850	ALA	7.1
1	B	143	THR	6.2
1	C	94	ALA	6.1
1	C	26	HIS	6.0
1	C	27	GLN	6.0
1	B	140	THR	5.7
1	C	487	ASN	5.7
1	C	45	LEU	5.7
1	A	191	LYS	5.6
1	C	118	ALA	5.5
1	C	142	GLN	5.4
1	C	432	LEU	5.3
1	C	144	GLU	5.3
1	A	427	ASP	5.0
1	C	55	ALA	4.7
1	A	484	TYR	4.6
1	C	145	HIS	4.6
1	C	6	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	247	PHE	4.4
1	C	49	LEU	4.4
1	C	103	ASP	4.3
1	A	419	ALA	4.3
1	C	97	LEU	4.3
1	C	496	GLU	4.2
1	C	428	SER	4.2
1	C	483	GLN	4.1
1	B	427	ASP	4.0
1	B	494	TYR	4.0
1	C	132	LEU	4.0
1	C	146	ALA	4.0
1	C	160	LEU	4.0
1	C	106	VAL	3.9
1	C	114	ALA	3.9
1	A	323	ARG	3.9
1	C	431	ARG	3.9
1	C	104	ARG	3.8
1	C	518	ARG	3.8
1	C	111	LEU	3.8
1	A	426	PRO	3.8
1	C	317	ASP	3.8
1	C	73	LYS	3.8
1	C	115	LEU	3.8
1	A	247	PHE	3.8
1	C	484	TYR	3.7
1	A	435	ILE	3.7
1	C	463	LEU	3.7
1	C	113	LEU	3.7
1	C	93	ARG	3.6
1	C	131	ALA	3.6
1	A	433	LYS	3.5
1	C	68	LEU	3.5
1	C	22	GLN	3.4
1	C	9	ALA	3.4
1	A	190	THR	3.4
1	A	139	ARG	3.4
1	B	428	SER	3.4
1	C	57	PRO	3.3
1	A	797	ARG	3.3
1	A	184	GLN	3.3
1	C	10	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	324	PHE	3.3
1	C	17	ALA	3.3
1	A	413	LEU	3.3
1	C	23	ARG	3.3
1	C	422	LYS	3.2
1	C	482	ARG	3.2
1	C	117	GLU	3.2
1	C	423	GLU	3.2
1	C	53	ALA	3.1
1	C	479	LEU	3.1
1	C	490	ALA	3.1
1	C	495	GLY	3.0
1	B	631	HIS	3.0
1	C	119	THR	3.0
1	C	80	GLY	3.0
1	A	429	GLN	3.0
1	B	489	ALA	3.0
1	C	121	GLY	3.0
1	C	40	LYS	3.0
1	C	7	THR	2.9
1	C	100	GLU	2.9
1	A	424	LYS	2.9
1	C	128	LEU	2.9
1	B	103	ASP	2.8
1	A	631	HIS	2.8
1	C	21	ALA	2.8
1	A	420	LEU	2.8
1	C	122	LEU	2.8
1	C	133	LYS	2.7
1	C	316	LYS	2.7
1	A	147	GLU	2.7
1	C	116	ALA	2.7
1	C	156	TYR	2.7
1	B	102	LYS	2.7
1	B	141	VAL	2.6
1	B	435	ILE	2.6
1	A	425	ASP	2.6
1	B	190	THR	2.6
1	C	488	ARG	2.6
1	C	480	ALA	2.6
1	C	834	ARG	2.6
1	A	423	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	95	GLU	2.6
1	C	149	THR	2.6
1	C	43	ARG	2.6
1	C	98	MET	2.6
1	A	635	ARG	2.6
1	A	66	ARG	2.5
1	A	325	GLN	2.5
1	B	723	TRP	2.5
1	C	78	GLU	2.5
1	C	297	ARG	2.5
1	C	293	PRO	2.5
1	A	256	GLN	2.5
1	C	28	ALA	2.5
1	C	127	ALA	2.5
1	C	199	GLU	2.5
1	C	464	ARG	2.5
1	C	70	ARG	2.4
1	C	120	PRO	2.4
1	A	512	ARG	2.4
1	C	20	LEU	2.4
1	B	438	GLU	2.4
1	A	293	PRO	2.4
1	C	143	THR	2.4
1	C	8	GLN	2.3
1	A	430	GLU	2.3
1	B	321	GLU	2.3
1	C	485	ASP	2.3
1	C	16	GLN	2.3
1	C	81	GLN	2.3
1	A	471	ASP	2.3
1	A	305	ALA	2.3
1	C	101	LEU	2.3
1	A	451	ALA	2.3
1	A	348	TYR	2.3
1	A	148	SER	2.3
1	A	422	LYS	2.3
1	B	145	HIS	2.2
1	C	52	LYS	2.2
1	C	493	ARG	2.2
1	C	471	ASP	2.2
1	C	92	ASN	2.2
1	C	494	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	314	ILE	2.2
1	C	419	ALA	2.2
1	C	65	GLU	2.2
1	C	147	GLU	2.2
1	C	516	PHE	2.2
1	C	435	ILE	2.2
1	C	254	VAL	2.2
1	A	421	LYS	2.1
1	C	90	ALA	2.1
1	A	195	VAL	2.1
1	C	198	GLY	2.1
1	C	31	LEU	2.1
1	B	142	GLN	2.1
1	C	169	LEU	2.1
1	A	320	LEU	2.1
1	A	202	VAL	2.0
1	C	34	LEU	2.0
1	C	56	ASP	2.0
1	C	36	ALA	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 carbohydrates 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(Å ²)	Q<0.9
2	PT	A	861	1/1	0.79	0.18	45,45,45,45	1
3	ANP	C	903	31/31	0.85	0.30	114,149,172,173	0
2	PT	B	860	1/1	0.85	0.74	34,34,34,34	1
2	PT	C	859	1/1	0.86	0.25	51,51,51,51	1

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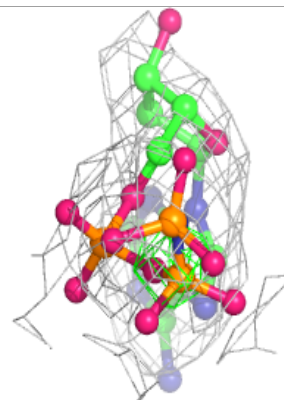
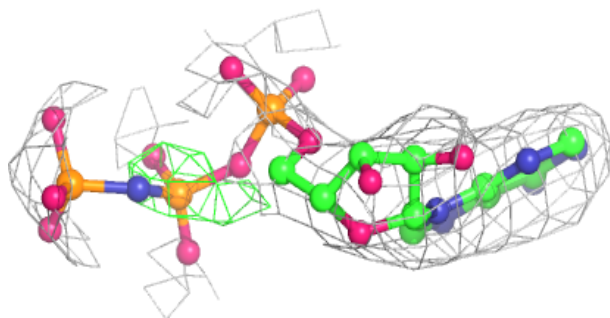
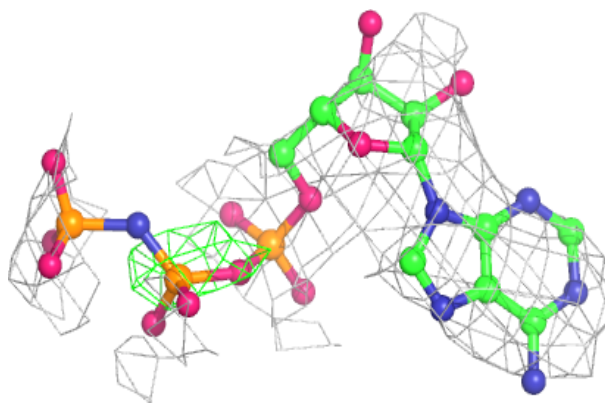
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PT	A	860	1/1	0.86	0.45	66,66,66,66	1
2	PT	B	862	1/1	0.87	0.48	52,52,52,52	1
2	PT	A	857	1/1	0.89	0.58	44,44,44,44	1
2	PT	C	858	1/1	0.89	0.12	80,80,80,80	1
2	PT	C	856	1/1	0.89	0.15	19,19,19,19	1
2	PT	C	860	1/1	0.91	0.20	90,90,90,90	1
2	PT	A	859	1/1	0.91	0.32	59,59,59,59	1
2	PT	C	861	1/1	0.91	0.29	42,42,42,42	1
3	ANP	A	911	31/31	0.92	0.24	55,79,110,119	0
3	ANP	A	901	31/31	0.92	0.20	75,108,124,130	0
2	PT	B	858	1/1	0.92	0.60	31,31,31,31	1
2	PT	B	859	1/1	0.92	0.24	50,50,50,50	1
3	ANP	C	913	31/31	0.92	0.27	31,66,117,121	0
3	ANP	B	912	31/31	0.93	0.23	42,71,130,136	0
3	ANP	B	902	31/31	0.93	0.27	64,80,143,146	0
2	PT	C	855	1/1	0.93	0.37	46,46,46,46	1
2	PT	B	861	1/1	0.95	0.14	47,47,47,47	1
2	PT	A	855	1/1	0.95	0.42	52,52,52,52	1
2	PT	A	858	1/1	0.95	0.29	49,49,49,49	1
2	PT	B	857	1/1	0.96	0.50	16,16,16,16	1
2	PT	C	857	1/1	0.96	0.27	41,41,41,41	1
2	PT	A	856	1/1	0.96	0.33	69,69,69,69	1
2	PT	A	862	1/1	0.97	0.13	53,53,53,53	1
2	PT	B	855	1/1	0.98	0.47	54,54,54,54	1
2	PT	B	856	1/1	0.98	0.35	39,39,39,39	1

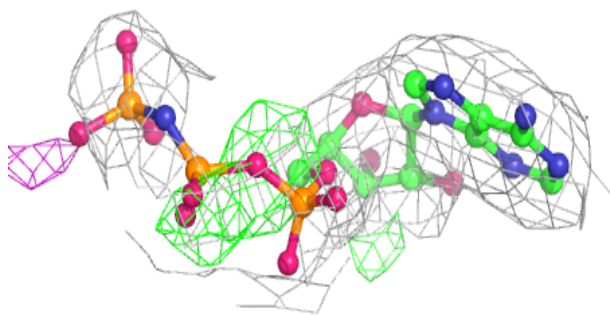
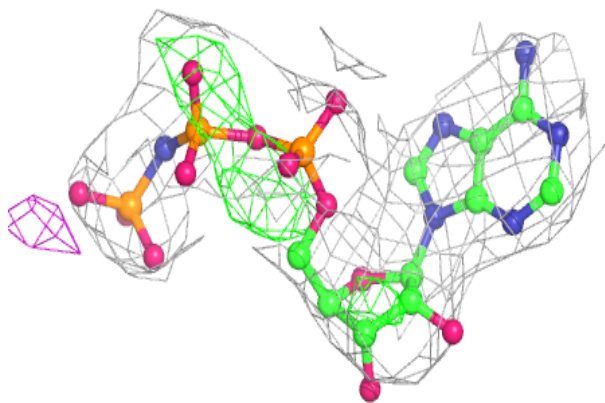
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 903:

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

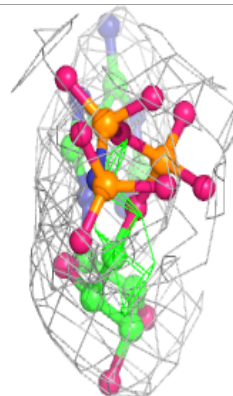
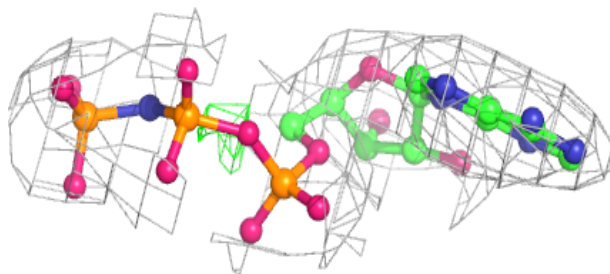
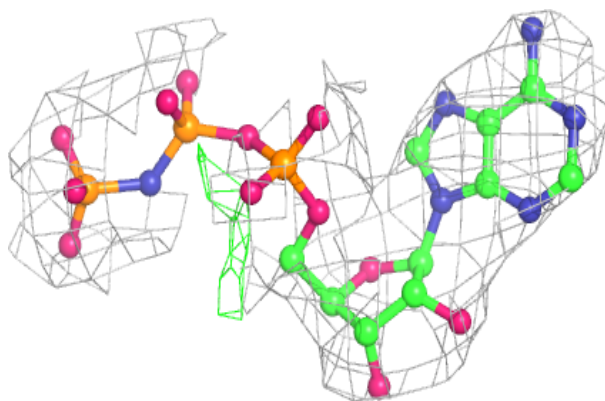
**Electron density around ANP A 911:**

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

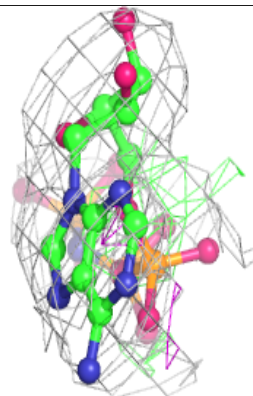
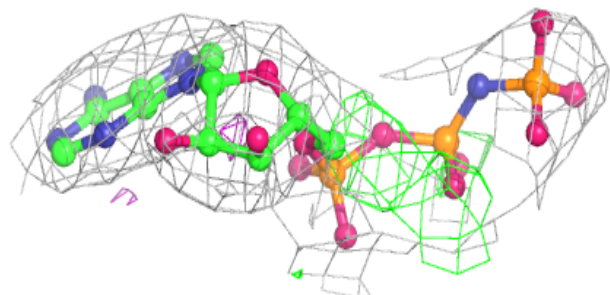
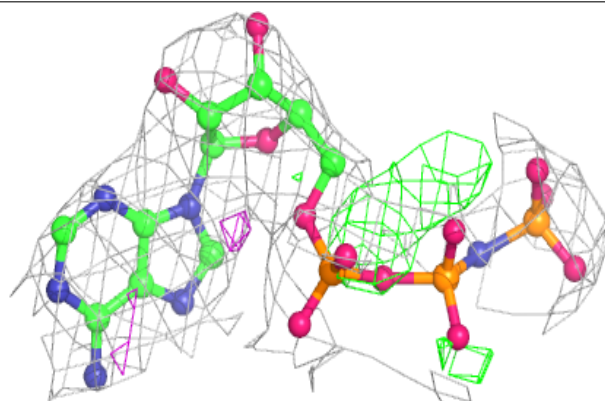


Electron density around ANP A 901:

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

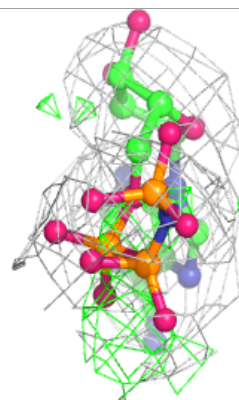
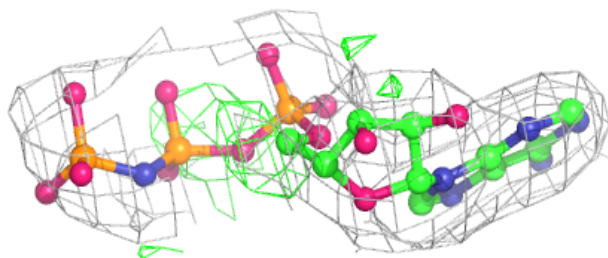
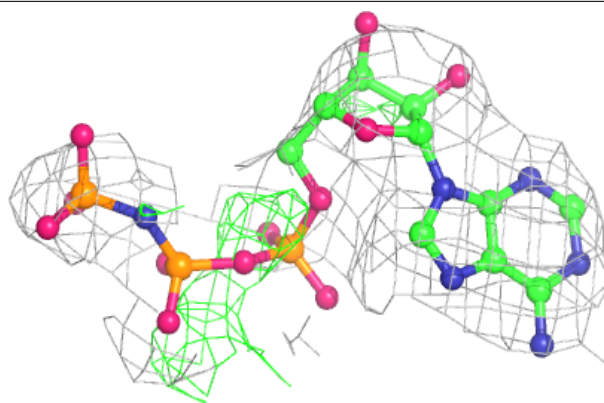
**Electron density around ANP C 913:**

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

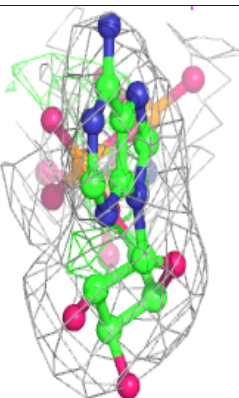
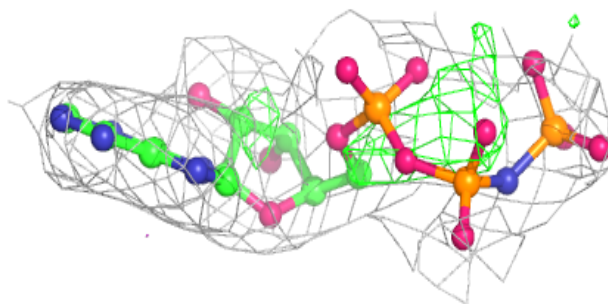
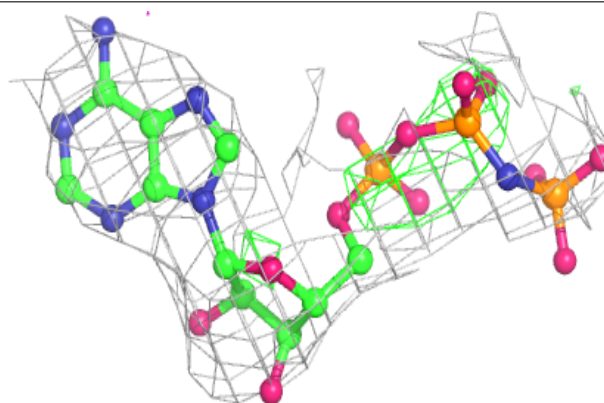


Electron density around ANP B 912:

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

**Electron density around ANP B 902:**

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



6.5 Other polymers

There are no such residues in this entry.