



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:58 PM EDT

PDB ID : 3CF3 / pdb\_00003cf3  
Title : Structure of P97/vcp in complex with ADP  
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.  
Deposited on : 2008-03-01  
Resolution : 4.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

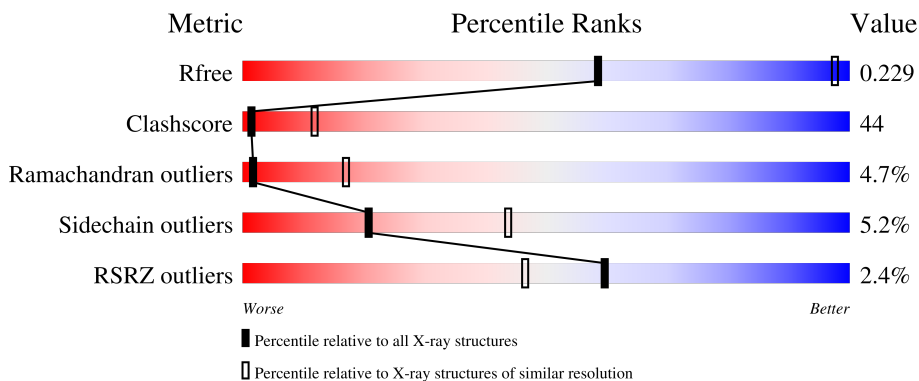
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	806	
1	B	806	
1	C	806	

## 2 Entry composition [i](#)

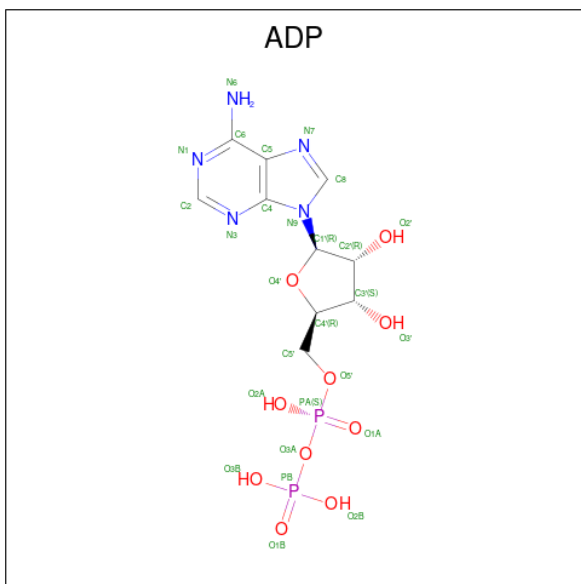
There are 2 unique types of molecules in this entry. The entry contains 17139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	723	Total 5659	C 3561	N 996	O 1072	S 30	0	0	0
1	B	723	Total 5659	C 3561	N 996	O 1072	S 30	0	0	0
1	C	723	Total 5659	C 3561	N 996	O 1072	S 30	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>ZeroOcc</b>	<b>AltConf</b>
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.97Å 178.93Å 320.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 40.00 – 4.25	Depositor EDS
% Data completeness (in resolution range)	86.4 (40.00-4.25) 86.3 (40.00-4.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 4.26Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.226 0.202 , 0.229	Depositor DCC
$R_{free}$ test set	4669 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	143.2	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 242.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.48	1/5751 (0.0%)	1.11	45/7767 (0.6%)
1	B	0.47	0/5751	1.09	40/7767 (0.5%)
1	C	0.48	0/5751	1.09	42/7767 (0.5%)
All	All	0.48	1/17253 (0.0%)	1.10	127/23301 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	ARG	CD-NE	-5.31	1.38	1.46

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ARG	CD-NE-CZ	18.24	149.94	124.40
1	B	287	ARG	CD-NE-CZ	17.86	149.41	124.40
1	A	338	ARG	CD-NE-CZ	17.73	149.23	124.40
1	A	338	ARG	NE-CZ-NH2	16.43	133.99	119.20
1	A	338	ARG	NE-CZ-NH1	-15.76	105.74	121.50
1	C	322	ARG	NE-CZ-NH2	-15.26	105.46	119.20
1	B	287	ARG	NE-CZ-NH2	-14.55	106.11	119.20
1	B	287	ARG	NE-CZ-NH1	12.44	133.94	121.50
1	C	322	ARG	NE-CZ-NH1	12.41	133.91	121.50
1	B	468	VAL	N-CA-C	10.90	123.61	107.80
1	C	435	GLU	N-CA-C	-10.54	100.43	113.18
1	C	287	ARG	CD-NE-CZ	10.11	138.56	124.40
1	B	338	ARG	N-CA-C	-10.06	100.30	111.07
1	C	338	ARG	N-CA-C	-10.02	100.35	111.07
1	A	287	ARG	CD-NE-CZ	10.01	138.41	124.40
1	A	338	ARG	N-CA-C	-9.89	100.48	111.07
1	C	468	VAL	N-CA-C	9.88	123.17	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ARG	CD-NE-CZ	9.57	137.80	124.40
1	A	322	ARG	CD-NE-CZ	9.45	137.63	124.40
1	C	338	ARG	CD-NE-CZ	9.32	137.45	124.40
1	B	338	ARG	CD-NE-CZ	9.25	137.35	124.40
1	A	468	VAL	N-CA-C	8.96	121.94	108.23
1	A	287	ARG	NE-CZ-NH2	8.95	127.25	119.20
1	C	287	ARG	NE-CZ-NH2	8.92	127.23	119.20
1	B	322	ARG	NE-CZ-NH2	8.73	127.05	119.20
1	C	599	ARG	N-CA-C	8.68	120.74	111.28
1	C	287	ARG	NE-CZ-NH1	-8.61	112.89	121.50
1	B	322	ARG	NE-CZ-NH1	-8.58	112.92	121.50
1	A	599	ARG	N-CA-C	8.56	120.61	111.28
1	A	322	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	A	322	ARG	NE-CZ-NH1	-8.34	113.16	121.50
1	B	599	ARG	N-CA-C	8.33	120.36	111.28
1	A	287	ARG	NE-CZ-NH1	-8.22	113.28	121.50
1	A	435	GLU	N-CA-C	-8.11	103.37	113.18
1	A	566	ALA	N-CA-C	-7.63	103.58	113.12
1	B	435	GLU	N-CA-C	-7.52	104.10	113.28
1	A	310	ALA	CA-C-N	-7.21	110.83	119.84
1	A	310	ALA	C-N-CA	-7.21	110.83	119.84
1	B	314	GLU	N-CA-C	-6.88	103.80	111.71
1	A	568	GLN	N-CA-C	-6.87	105.69	112.97
1	C	338	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	B	541	SER	N-CA-C	6.76	120.33	107.75
1	C	541	SER	N-CA-C	6.76	120.33	107.75
1	B	338	ARG	NE-CZ-NH2	-6.76	113.12	119.20
1	A	541	SER	N-CA-C	6.72	120.25	107.75
1	C	761	THR	N-CA-C	-6.71	105.22	113.41
1	B	733	ARG	N-CA-C	6.70	118.24	111.07
1	C	733	ARG	N-CA-C	6.47	118.12	111.14
1	B	645	ILE	CA-C-N	6.44	126.89	120.52
1	B	645	ILE	C-N-CA	6.44	126.89	120.52
1	B	333	ASP	N-CA-C	-6.34	103.89	111.69
1	B	596	ALA	N-CA-C	6.25	117.75	111.07
1	C	314	GLU	N-CA-C	-6.20	104.58	111.71
1	C	333	ASP	N-CA-C	-6.19	104.08	111.69
1	A	333	ASP	N-CA-C	-6.16	104.11	111.69
1	A	664	SER	CA-C-N	6.11	127.48	119.84
1	A	664	SER	C-N-CA	6.11	127.48	119.84
1	B	32	ILE	N-CA-C	-6.11	106.85	112.96
1	A	32	ILE	N-CA-C	-6.10	106.86	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	SER	CA-C-N	6.08	127.44	119.84
1	B	664	SER	C-N-CA	6.08	127.44	119.84
1	C	664	SER	CA-C-N	6.08	127.43	119.84
1	C	664	SER	C-N-CA	6.08	127.43	119.84
1	C	198	LEU	N-CA-C	-6.04	105.89	113.20
1	A	314	GLU	N-CA-C	-6.04	104.82	111.82
1	C	645	ILE	CA-C-N	6.01	126.47	120.52
1	C	645	ILE	C-N-CA	6.01	126.47	120.52
1	A	81	LYS	N-CA-C	5.92	118.18	109.24
1	B	276	SER	N-CA-C	-5.86	106.67	113.88
1	A	645	ILE	CA-C-N	5.83	126.29	120.52
1	A	645	ILE	C-N-CA	5.83	126.29	120.52
1	B	81	LYS	N-CA-C	5.80	118.00	109.24
1	C	276	SER	N-CA-C	-5.74	106.82	113.88
1	C	81	LYS	N-CA-C	5.70	117.85	109.24
1	C	32	ILE	N-CA-C	-5.69	107.27	112.96
1	A	276	SER	N-CA-C	-5.65	106.93	113.88
1	C	533	ASN	N-CA-C	-5.63	105.22	111.36
1	B	533	ASN	N-CA-C	-5.62	105.23	111.36
1	C	338	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	349	ARG	CA-C-N	5.52	124.98	119.24
1	A	349	ARG	C-N-CA	5.52	124.98	119.24
1	B	338	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	198	LEU	N-CA-C	-5.51	106.53	113.20
1	A	533	ASN	N-CA-C	-5.51	105.35	111.36
1	B	198	LEU	N-CA-C	-5.51	106.53	113.20
1	C	349	ARG	CA-C-N	5.50	124.96	119.24
1	C	349	ARG	C-N-CA	5.50	124.96	119.24
1	A	354	ASP	CA-C-N	5.50	125.85	119.47
1	A	354	ASP	C-N-CA	5.50	125.85	119.47
1	B	354	ASP	CA-C-N	5.47	125.82	119.47
1	B	354	ASP	C-N-CA	5.47	125.82	119.47
1	B	349	ARG	CA-C-N	5.42	124.88	119.24
1	B	349	ARG	C-N-CA	5.42	124.88	119.24
1	C	762	LEU	N-CA-C	-5.34	105.86	112.38
1	A	760	GLN	N-CA-C	-5.31	105.61	112.68
1	C	697	LEU	N-CA-C	-5.27	106.91	113.55
1	C	187	GLU	CA-C-N	5.25	126.40	119.84
1	C	187	GLU	C-N-CA	5.25	126.40	119.84
1	C	354	ASP	CA-C-N	5.24	125.55	119.47
1	C	354	ASP	C-N-CA	5.24	125.55	119.47
1	B	697	LEU	N-CA-C	-5.23	106.97	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	CA-C-N	5.21	126.36	119.84
1	A	187	GLU	C-N-CA	5.21	126.36	119.84
1	C	568	GLN	N-CA-C	-5.21	104.41	111.55
1	A	269	ILE	CB-CA-C	-5.20	104.23	110.99
1	A	697	LEU	N-CA-C	-5.20	107.00	113.55
1	A	733	ARG	N-CA-C	5.20	116.76	111.14
1	A	201	VAL	N-CA-C	5.20	116.72	109.55
1	B	624	ASN	N-CA-C	-5.20	106.70	112.57
1	C	201	VAL	N-CA-C	5.19	116.71	109.55
1	C	547	LEU	N-CA-C	-5.18	105.71	111.36
1	C	231	LYS	N-CA-C	-5.18	106.80	113.01
1	A	231	LYS	N-CA-C	-5.14	106.84	113.01
1	C	269	ILE	CB-CA-C	-5.14	104.31	110.99
1	B	269	ILE	CB-CA-C	-5.14	104.31	110.99
1	B	430	ILE	N-CA-C	-5.13	104.68	111.09
1	C	594	GLY	N-CA-C	5.13	120.34	111.98
1	B	231	LYS	N-CA-C	-5.11	106.88	113.01
1	B	385	THR	N-CA-C	-5.07	106.23	114.09
1	A	479	ILE	N-CA-C	5.07	114.04	106.85
1	A	740	MET	N-CA-C	-5.06	107.05	113.18
1	A	133	VAL	N-CA-C	5.06	115.29	110.53
1	B	630	ASP	CA-C-N	5.04	126.14	119.84
1	B	630	ASP	C-N-CA	5.04	126.14	119.84
1	B	479	ILE	N-CA-C	5.02	113.98	106.85
1	C	301	ILE	N-CA-C	-5.02	100.03	107.51
1	A	572	CYS	N-CA-C	5.02	116.14	108.52

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	5659	0	5731	526	0
1	B	5659	0	5731	520	0
1	C	5659	0	5731	502	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	54	0	24	6	0
2	B	54	0	24	4	0
2	C	54	0	24	3	0
All	All	17139	0	17265	1515	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 44.

All (1515) 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:A:206:ILE:CD1	1:A:213:LEU:HD11	1.25	1.64
1:B:206:ILE:CD1	1:B:213:LEU:HD11	1.24	1.61
1:C:206:ILE:CD1	1:C:213:LEU:HD11	1.25	1.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	1.55	1.34
1:C:206:ILE:HD11	1:C:213:LEU:CD1	1.55	1.34
1:B:206:ILE:HD11	1:B:213:LEU:CD1	1.56	1.33
1:B:206:ILE:CD1	1:B:213:LEU:CD1	2.15	1.23
1:A:206:ILE:CD1	1:A:213:LEU:CD1	2.15	1.16
1:B:206:ILE:HD12	1:B:213:LEU:HD11	1.22	1.16
1:C:206:ILE:CD1	1:C:213:LEU:CD1	2.15	1.15
1:C:206:ILE:HD12	1:C:213:LEU:HD11	1.25	1.12
1:A:206:ILE:HD12	1:A:213:LEU:HD11	1.26	1.11
1:C:51:LEU:HD21	1:C:104:PRO:HB3	1.35	1.09
1:B:51:LEU:HD21	1:B:104:PRO:HB3	1.35	1.08
1:A:51:LEU:HD21	1:A:104:PRO:HB3	1.34	1.07
1:B:353:ILE:HG22	1:B:354:ASP:H	1.22	1.04
1:C:353:ILE:HG22	1:C:354:ASP:H	1.21	1.04
1:A:259:ALA:HB2	1:A:300:ILE:HD12	1.38	1.04
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.24	1.03
1:A:353:ILE:HG22	1:A:354:ASP:H	1.22	1.03
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.39	1.02
1:B:158:MET:HE1	1:B:419:ALA:HB1	1.42	1.02
1:A:337:GLN:HE21	1:A:337:GLN:HA	1.24	1.01
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.41	1.01
1:B:337:GLN:HE21	1:B:337:GLN:HA	1.24	1.01
1:C:111:GLY:HA2	1:C:170:PRO:HG2	1.43	1.00
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.42	0.98
1:A:111:GLY:HA2	1:A:170:PRO:HG2	1.39	0.98
1:B:111:GLY:HA2	1:B:170:PRO:HG2	1.45	0.98
1:C:397:GLU:HG2	1:C:401:ASN:HD21	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:MET:HE1	1:C:419:ALA:HB1	1.43	0.97
1:B:397:GLU:HG2	1:B:401:ASN:HD21	1.29	0.97
1:B:466:GLU:HG2	1:B:467:THR:H	1.27	0.96
1:A:397:GLU:HG2	1:A:401:ASN:HD21	1.29	0.96
1:C:313:ARG:O	1:C:316:THR:HG22	1.65	0.95
1:A:133:VAL:HG13	1:A:443:ASN:ND2	1.83	0.94
1:A:164:LYS:HE2	1:A:189:ILE:HD12	1.50	0.94
1:A:126:ILE:HB	1:A:439:ALA:HB2	1.47	0.93
1:B:313:ARG:O	1:B:316:THR:HG22	1.69	0.92
1:C:164:LYS:HE2	1:C:189:ILE:HD12	1.52	0.92
1:C:113:ARG:HG2	1:C:113:ARG:HH11	1.33	0.91
1:B:164:LYS:HE2	1:B:189:ILE:HD12	1.52	0.91
1:A:313:ARG:O	1:A:316:THR:HG22	1.72	0.90
1:C:313:ARG:HG2	1:C:314:GLU:H	1.36	0.88
1:B:113:ARG:HH11	1:B:113:ARG:HG2	1.38	0.87
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.37	0.87
1:A:614:LYS:HD3	1:B:402:GLU:HB2	1.55	0.86
1:B:206:ILE:HD11	1:B:213:LEU:HD11	0.88	0.86
1:A:143:TYR:CE1	1:A:178:PRO:HD2	2.10	0.85
1:A:611:MET:HE1	1:A:619:ILE:HD11	1.59	0.85
1:A:133:VAL:HG13	1:A:443:ASN:HD22	1.38	0.85
1:B:329:LEU:HD22	1:B:362:ARG:NH1	1.92	0.85
1:C:206:ILE:HD11	1:C:213:LEU:HD11	0.86	0.85
1:A:329:LEU:HD22	1:A:362:ARG:NH1	1.92	0.84
1:B:665:PRO:O	1:B:731:ILE:HG22	1.75	0.84
1:A:472:PRO:HG2	1:A:532:ALA:HB3	1.60	0.84
1:A:206:ILE:HD11	1:A:213:LEU:HD11	0.86	0.84
1:A:499:HIS:N	1:A:500:PRO:HD3	1.93	0.84
1:C:329:LEU:HD22	1:C:362:ARG:NH1	1.93	0.84
1:C:499:HIS:N	1:C:500:PRO:HD3	1.93	0.84
1:B:129:ASN:ND2	1:B:132:GLU:HB2	1.94	0.83
1:C:665:PRO:O	1:C:731:ILE:HG22	1.77	0.83
1:A:129:ASN:ND2	1:A:132:GLU:HB2	1.94	0.82
1:A:460:ASN:N	1:A:461:PRO:HD2	1.93	0.82
1:B:499:HIS:N	1:B:500:PRO:HD3	1.94	0.82
1:B:611:MET:HE1	1:B:619:ILE:HD11	1.62	0.81
1:C:143:TYR:CE1	1:C:178:PRO:HD2	2.15	0.81
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.63	0.81
1:C:129:ASN:ND2	1:C:132:GLU:HB2	1.95	0.81
1:B:143:TYR:CE1	1:B:178:PRO:HD2	2.15	0.80
1:B:514:VAL:HG11	1:B:643:ILE:HD12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:HG11	1:A:643:ILE:HD12	1.62	0.80
1:C:514:VAL:HG11	1:C:643:ILE:HD12	1.63	0.80
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.64	0.80
1:C:749:ASP:HA	1:C:752:ILE:HD12	1.63	0.80
1:A:749:ASP:HA	1:A:752:ILE:HD12	1.64	0.80
1:B:749:ASP:HA	1:B:752:ILE:HD12	1.62	0.80
1:C:611:MET:HE1	1:C:619:ILE:HD11	1.64	0.80
1:C:337:GLN:HA	1:C:337:GLN:NE2	1.97	0.79
1:A:158:MET:HE1	1:A:419:ALA:HB1	1.64	0.79
1:B:337:GLN:HA	1:B:337:GLN:NE2	1.98	0.79
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.65	0.79
1:C:336:LYS:C	1:C:338:ARG:H	1.90	0.79
1:B:65:ARG:NH1	1:B:93:ARG:HH12	1.81	0.79
1:C:472:PRO:HG2	1:C:532:ALA:HB3	1.65	0.79
1:A:337:GLN:HA	1:A:337:GLN:NE2	1.98	0.79
1:B:336:LYS:C	1:B:338:ARG:H	1.90	0.79
1:A:267:PHE:HE2	1:A:289:ALA:HB1	1.48	0.78
1:A:336:LYS:C	1:A:338:ARG:H	1.91	0.78
1:A:313:ARG:HG2	1:A:314:GLU:H	1.49	0.78
1:B:206:ILE:HD12	1:B:213:LEU:CD1	1.99	0.78
1:C:216:ILE:HA	1:C:219:MET:HE3	1.65	0.78
1:C:318:GLY:O	1:C:322:ARG:HG3	1.85	0.77
1:A:216:ILE:HA	1:A:219:MET:HE3	1.66	0.77
1:B:500:PRO:O	1:B:504:LEU:HD13	1.83	0.77
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.19	0.77
1:A:500:PRO:O	1:A:504:LEU:HD13	1.83	0.77
1:B:267:PHE:HE2	1:B:289:ALA:HB1	1.49	0.77
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.20	0.77
1:A:62:LYS:O	1:A:64:ARG:N	2.17	0.77
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.67	0.77
1:B:405:GLY:HA3	1:B:465:ARG:HD3	1.67	0.77
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.19	0.77
1:C:267:PHE:HE2	1:C:289:ALA:HB1	1.50	0.77
1:B:329:LEU:HD22	1:B:362:ARG:HH11	1.50	0.77
1:C:658:LYS:O	1:C:662:ARG:HG3	1.86	0.76
1:A:329:LEU:HD22	1:A:362:ARG:HH11	1.51	0.76
1:B:490:GLN:HB3	1:B:494:GLN:HG3	1.68	0.76
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.67	0.76
1:A:506:PHE:CD2	1:B:699:ILE:HG12	2.20	0.76
1:A:512:LYS:HD3	1:A:637:GLY:O	1.86	0.76
1:C:259:ALA:HB2	1:C:300:ILE:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.26	0.76
1:B:216:ILE:HA	1:B:219:MET:HE3	1.67	0.76
1:B:158:MET:HE1	1:B:419:ALA:CB	2.16	0.76
1:B:658:LYS:O	1:B:662:ARG:HG3	1.86	0.76
1:B:233:ILE:HD13	1:C:442:MET:HE2	1.66	0.75
1:C:60:LYS:NZ	1:C:103:GLN:NE2	2.33	0.75
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.68	0.75
1:A:560:ARG:HG3	1:A:560:ARG:HH11	1.51	0.75
1:C:500:PRO:O	1:C:504:LEU:HD13	1.85	0.75
1:C:206:ILE:HD12	1:C:213:LEU:CD1	2.02	0.75
1:C:60:LYS:HZ1	1:C:103:GLN:HE21	1.33	0.75
1:A:133:VAL:CG1	1:A:443:ASN:HD22	1.99	0.75
1:B:313:ARG:HG2	1:B:314:GLU:H	1.52	0.75
1:B:353:ILE:HG22	1:B:354:ASP:N	1.99	0.75
1:A:490:GLN:HB3	1:A:494:GLN:HG3	1.69	0.75
1:A:658:LYS:O	1:A:662:ARG:HG3	1.86	0.75
1:B:323:ARG:HH22	1:C:279:ALA:HB2	1.50	0.75
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.27	0.74
1:C:353:ILE:HG22	1:C:354:ASP:N	1.99	0.74
1:A:328:LEU:HD11	1:A:332:MET:HG2	1.69	0.74
1:B:328:LEU:HD11	1:B:332:MET:HG2	1.69	0.74
1:C:499:HIS:H	1:C:500:PRO:HD3	1.51	0.74
1:C:394:VAL:HA	1:C:449:MET:HB2	1.68	0.74
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.69	0.74
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.69	0.74
1:C:570:ALA:HB1	1:C:616:ASN:HB3	1.68	0.74
1:A:222:LEU:HD21	1:B:424:ARG:HG2	1.70	0.73
1:A:665:PRO:O	1:A:731:ILE:HG22	1.89	0.73
1:C:518:GLY:C	1:C:755:TYR:HE2	1.97	0.73
1:B:560:ARG:HG3	1:B:560:ARG:HH11	1.51	0.73
1:A:394:VAL:HA	1:A:449:MET:HB2	1.68	0.73
1:B:377:ARG:HD2	1:B:403:THR:OG1	1.87	0.73
1:A:377:ARG:HD2	1:A:403:THR:OG1	1.88	0.73
1:A:499:HIS:H	1:A:500:PRO:HD3	1.51	0.73
1:C:490:GLN:HB3	1:C:494:GLN:HG3	1.71	0.73
1:A:353:ILE:HG22	1:A:354:ASP:N	2.00	0.72
1:B:570:ALA:HB1	1:B:616:ASN:HB3	1.69	0.72
1:C:51:LEU:CD2	1:C:104:PRO:HB3	2.16	0.72
1:C:158:MET:HE1	1:C:419:ALA:CB	2.18	0.72
1:C:60:LYS:HZ1	1:C:103:GLN:NE2	1.88	0.72
1:A:110:TYR:CD1	1:A:177:ALA:HB2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LEU:HD22	1:C:362:ARG:HH11	1.51	0.72
1:C:423:ILE:HG12	1:C:445:LEU:HD11	1.72	0.72
1:C:560:ARG:HG3	1:C:560:ARG:HH11	1.52	0.72
1:A:427:MET:HG3	1:A:432:LEU:HG	1.71	0.72
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.29	0.72
1:B:423:ILE:HG12	1:B:445:LEU:HD11	1.71	0.72
1:B:394:VAL:HA	1:B:449:MET:HB2	1.70	0.72
1:A:113:ARG:NH2	1:A:183:HIS:NE2	2.38	0.72
1:A:51:LEU:CD2	1:A:104:PRO:HB3	2.16	0.72
1:B:460:ASN:N	1:B:461:PRO:HD2	2.05	0.72
1:B:51:LEU:CD2	1:B:104:PRO:HB3	2.17	0.71
1:B:170:PRO:HB2	1:B:174:CYS:HB3	1.73	0.71
1:B:259:ALA:HB2	1:B:300:ILE:HD12	1.70	0.71
1:C:110:TYR:CD1	1:C:177:ALA:HB2	2.25	0.71
1:B:499:HIS:H	1:B:500:PRO:HD3	1.52	0.71
1:C:34:GLU:N	1:C:34:GLU:OE1	2.22	0.71
1:B:466:GLU:HG2	1:B:467:THR:N	2.04	0.71
1:C:206:ILE:HD11	1:C:213:LEU:HD13	1.67	0.71
1:A:206:ILE:HD12	1:A:213:LEU:CD1	2.02	0.70
1:A:253:LEU:HD12	2:A:807:ADP:H2'	1.73	0.70
1:A:170:PRO:HB2	1:A:174:CYS:HB3	1.73	0.70
1:B:117:LEU:HD21	1:B:185:GLU:HG2	1.73	0.70
1:B:110:TYR:CD1	1:B:177:ALA:HB2	2.26	0.70
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.72	0.70
1:B:427:MET:HG3	1:B:432:LEU:HG	1.74	0.70
1:A:206:ILE:HD11	1:A:213:LEU:HD13	1.68	0.70
1:B:383:ILE:O	1:B:386:LYS:HG2	1.91	0.70
1:A:398:GLN:HG2	1:A:449:MET:HE1	1.74	0.70
1:C:377:ARG:HD2	1:C:403:THR:OG1	1.91	0.70
1:B:512:LYS:HD3	1:B:637:GLY:O	1.92	0.69
1:C:608:MET:HG3	1:C:619:ILE:CD1	2.22	0.69
1:A:611:MET:CE	1:A:619:ILE:HD11	2.22	0.69
1:A:111:GLY:HA2	1:A:170:PRO:CG	2.20	0.69
1:A:383:ILE:O	1:A:386:LYS:HG2	1.93	0.69
1:C:113:ARG:HH11	1:C:113:ARG:CG	2.05	0.69
1:B:113:ARG:NH2	1:B:183:HIS:NE2	2.41	0.69
1:B:608:MET:HG3	1:B:619:ILE:CD1	2.22	0.69
1:C:328:LEU:HD11	1:C:332:MET:HG2	1.73	0.69
1:C:512:LYS:HD3	1:C:637:GLY:O	1.92	0.69
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.27	0.69
1:B:206:ILE:HD11	1:B:213:LEU:HD13	1.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLN:HG2	1:B:449:MET:HE1	1.75	0.68
1:C:87:VAL:HG22	1:C:198:LEU:HD13	1.74	0.68
1:A:475:THR:HG22	1:A:533:ASN:HD21	1.56	0.68
1:B:270:ASN:HB3	1:B:273:GLU:HB2	1.75	0.68
1:A:95:ARG:HB2	1:A:225:ARG:CZ	2.23	0.68
1:B:87:VAL:HG22	1:B:198:LEU:HD13	1.75	0.68
1:C:398:GLN:HG2	1:C:449:MET:HE1	1.75	0.68
1:C:491:GLU:HG2	1:C:495:TYR:HE2	1.58	0.68
1:C:170:PRO:HB2	1:C:174:CYS:HB3	1.74	0.68
1:C:461:PRO:O	1:C:463:ALA:N	2.26	0.68
1:B:34:GLU:OE1	1:B:34:GLU:N	2.24	0.68
1:C:482:LEU:O	1:C:486:LYS:HG3	1.94	0.68
1:A:151:ILE:HD11	1:A:195:GLU:OE2	1.93	0.67
1:C:514:VAL:HG12	1:C:515:LEU:N	2.09	0.67
1:A:203:TYR:O	1:A:206:ILE:HG12	1.95	0.67
1:A:267:PHE:HE2	1:A:289:ALA:CB	2.07	0.67
1:B:514:VAL:HG12	1:B:515:LEU:N	2.09	0.67
1:C:270:ASN:HB3	1:C:273:GLU:HB2	1.75	0.67
1:C:490:GLN:O	1:C:494:GLN:HB2	1.95	0.67
1:C:612:SER:HB3	1:C:615:LYS:HG2	1.76	0.67
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.21	0.67
1:C:320:VAL:O	1:C:324:ILE:HG13	1.94	0.67
1:A:270:ASN:HB3	1:A:273:GLU:HB2	1.75	0.67
1:A:423:ILE:HG12	1:A:445:LEU:HD11	1.75	0.67
1:B:133:VAL:HG13	1:B:443:ASN:HD22	1.60	0.67
1:B:490:GLN:O	1:B:494:GLN:HB2	1.94	0.67
1:A:117:LEU:HD21	1:A:185:GLU:HG2	1.76	0.67
1:A:251:LYS:HG3	2:A:807:ADP:O2B	1.95	0.67
1:A:608:MET:HG3	1:A:619:ILE:CD1	2.23	0.67
1:C:667:ALA:HB3	1:C:670:VAL:HG23	1.77	0.67
1:A:34:GLU:N	1:A:34:GLU:OE1	2.26	0.67
1:A:437:ILE:HG22	1:A:438:ASP:N	2.09	0.67
1:A:482:LEU:O	1:A:486:LYS:HG3	1.94	0.67
1:A:667:ALA:HB3	1:A:670:VAL:HG23	1.77	0.67
1:A:30:GLU:OE2	1:A:217:LYS:NZ	2.28	0.67
1:A:490:GLN:O	1:A:494:GLN:HB2	1.94	0.67
1:B:612:SER:HB3	1:B:615:LYS:HG2	1.75	0.67
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.22	0.66
1:A:612:SER:HB3	1:A:615:LYS:HG2	1.76	0.66
1:B:253:LEU:C	1:B:253:LEU:HD23	2.20	0.66
1:C:206:ILE:CD1	1:C:213:LEU:HD21	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ILE:O	1:C:386:LYS:HG2	1.95	0.66
1:A:253:LEU:HD23	1:A:253:LEU:C	2.21	0.66
1:C:466:GLU:HG2	1:C:467:THR:H	1.60	0.66
1:B:667:ALA:HB3	1:B:670:VAL:HG23	1.78	0.66
1:A:489:LEU:O	1:A:493:VAL:HG22	1.95	0.66
1:B:267:PHE:HE2	1:B:289:ALA:CB	2.09	0.66
1:B:482:LEU:O	1:B:486:LYS:HG3	1.96	0.66
1:A:259:ALA:CB	1:A:300:ILE:HD12	2.23	0.66
1:C:749:ASP:HA	1:C:752:ILE:CD1	2.27	0.65
1:A:206:ILE:CD1	1:A:213:LEU:HD21	2.26	0.65
1:A:405:GLY:O	1:A:463:ALA:HB3	1.96	0.65
1:A:459:SER:C	1:A:461:PRO:HD2	2.21	0.65
1:B:491:GLU:HG2	1:B:495:TYR:HE2	1.59	0.65
1:A:460:ASN:OD1	1:A:461:PRO:HD3	1.96	0.65
1:C:169:ASP:HB3	1:C:170:PRO:CD	2.22	0.65
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.32	0.65
1:B:611:MET:CE	1:B:619:ILE:HD11	2.26	0.65
1:A:113:ARG:HH11	1:A:113:ARG:CG	2.09	0.65
1:A:567:ARG:NH2	1:A:611:MET:HG3	2.10	0.65
1:A:728:VAL:N	1:A:729:PRO:HD2	2.11	0.65
1:B:518:GLY:C	1:B:755:TYR:HE2	2.04	0.65
1:C:729:PRO:C	1:C:730:GLU:CD	2.64	0.65
1:A:353:ILE:CG2	1:A:354:ASP:H	2.05	0.65
1:A:43:GLN:N	1:A:44:PRO:HD2	2.11	0.65
1:A:201:VAL:HG21	1:A:256:ARG:HD2	1.78	0.65
1:A:335:LEU:C	1:A:337:GLN:H	2.03	0.65
1:A:518:GLY:C	1:A:755:TYR:HE2	2.04	0.65
1:C:611:MET:CE	1:C:619:ILE:HD11	2.27	0.65
1:B:65:ARG:NH1	1:B:93:ARG:NH1	2.45	0.65
1:B:311:PRO:O	1:B:313:ARG:N	2.30	0.65
1:A:87:VAL:HG22	1:A:198:LEU:HD13	1.78	0.65
1:B:749:ASP:HA	1:B:752:ILE:CD1	2.26	0.65
1:C:151:ILE:HD11	1:C:195:GLU:OE2	1.95	0.65
1:A:62:LYS:C	1:A:64:ARG:N	2.51	0.64
1:B:43:GLN:N	1:B:44:PRO:HD2	2.12	0.64
1:C:43:GLN:N	1:C:44:PRO:HD2	2.12	0.64
1:C:460:ASN:N	1:C:461:PRO:HD2	2.11	0.64
1:A:491:GLU:HG2	1:A:495:TYR:HE2	1.59	0.64
1:A:514:VAL:HG12	1:A:515:LEU:N	2.11	0.64
1:A:614:LYS:CD	1:B:402:GLU:HB2	2.27	0.64
1:B:335:LEU:C	1:B:337:GLN:H	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:HB3	1:C:273:GLU:CB	2.28	0.64
1:B:151:ILE:HD11	1:B:195:GLU:OE2	1.96	0.64
1:A:489:LEU:HB3	1:A:531:ILE:HD13	1.80	0.64
1:B:113:ARG:HH11	1:B:113:ARG:CG	2.09	0.64
1:B:177:ALA:O	1:B:179:ASP:N	2.29	0.64
1:C:22:ARG:HB3	1:C:24:ASN:OD1	1.96	0.64
1:C:117:LEU:HD21	1:C:185:GLU:HG2	1.78	0.64
1:C:253:LEU:C	1:C:253:LEU:HD23	2.21	0.64
1:C:335:LEU:C	1:C:337:GLN:H	2.04	0.64
1:B:274:ILE:HG21	1:B:286:LEU:HD21	1.79	0.64
1:B:378:LEU:C	1:B:378:LEU:HD13	2.23	0.64
1:A:311:PRO:O	1:A:313:ARG:N	2.31	0.64
1:B:206:ILE:CD1	1:B:213:LEU:HD21	2.28	0.64
1:B:353:ILE:CG2	1:B:354:ASP:H	2.04	0.64
1:A:432:LEU:HD12	1:A:441:VAL:HG11	1.79	0.64
1:B:489:LEU:O	1:B:493:VAL:HG22	1.97	0.64
1:A:438:ASP:HB3	1:A:441:VAL:HG23	1.80	0.64
1:A:650:GLU:HG2	1:A:677:LYS:HZ3	1.63	0.64
1:B:270:ASN:HB3	1:B:273:GLU:CB	2.28	0.64
1:B:320:VAL:O	1:B:324:ILE:HG13	1.97	0.64
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.80	0.64
1:B:438:ASP:HB3	1:B:441:VAL:HG23	1.80	0.63
1:B:489:LEU:HB3	1:B:531:ILE:HD13	1.80	0.63
1:B:505:LYS:HZ3	1:C:729:PRO:HG3	1.63	0.63
1:C:427:MET:SD	1:C:432:LEU:HD12	2.38	0.63
1:C:489:LEU:O	1:C:493:VAL:HG22	1.98	0.63
1:C:489:LEU:HB3	1:C:531:ILE:HD13	1.79	0.63
1:C:378:LEU:HD13	1:C:378:LEU:C	2.24	0.63
1:A:267:PHE:CE2	1:A:289:ALA:HB1	2.31	0.63
1:A:499:HIS:N	1:A:500:PRO:CD	2.61	0.63
1:A:614:LYS:HE2	1:B:402:GLU:OE1	1.97	0.63
1:C:335:LEU:O	1:C:337:GLN:N	2.32	0.63
1:C:499:HIS:N	1:C:500:PRO:CD	2.61	0.63
1:B:358:ARG:HG3	1:B:358:ARG:HH11	1.64	0.63
1:C:267:PHE:HE2	1:C:289:ALA:CB	2.10	0.63
1:A:328:LEU:CD1	1:A:332:MET:HG2	2.29	0.63
1:A:335:LEU:O	1:A:337:GLN:N	2.32	0.63
1:A:749:ASP:HA	1:A:752:ILE:CD1	2.27	0.63
1:A:378:LEU:HD13	1:A:378:LEU:C	2.23	0.63
1:B:335:LEU:O	1:B:337:GLN:N	2.32	0.63
1:A:177:ALA:O	1:A:179:ASP:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG21	1:A:286:LEU:HD21	1.79	0.63
1:B:153:LEU:HD11	1:B:160:ALA:HB1	1.80	0.63
1:C:111:GLY:HA2	1:C:170:PRO:CG	2.24	0.63
1:C:113:ARG:NH2	1:C:183:HIS:NE2	2.46	0.63
1:B:328:LEU:CD1	1:B:332:MET:HG2	2.29	0.62
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.81	0.62
1:B:499:HIS:N	1:B:500:PRO:CD	2.61	0.62
1:C:177:ALA:O	1:C:179:ASP:N	2.32	0.62
1:C:438:ASP:HB3	1:C:441:VAL:HG23	1.79	0.62
1:A:65:ARG:NH1	1:A:93:ARG:HH12	1.97	0.62
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.34	0.62
1:B:492:LEU:O	1:B:496:PRO:HG3	1.99	0.62
1:B:388:MET:HE3	1:B:447:VAL:HG21	1.80	0.62
1:B:458:GLN:HB3	1:B:460:ASN:OD1	2.00	0.62
1:A:102:ILE:HG12	1:A:103:GLN:N	2.14	0.62
1:B:111:GLY:HA2	1:B:170:PRO:CG	2.26	0.62
1:C:271:GLY:HA2	1:C:309:ILE:HD11	1.82	0.62
1:A:270:ASN:HB3	1:A:273:GLU:CB	2.28	0.62
1:A:458:GLN:HB3	1:A:460:ASN:OD1	1.99	0.62
1:B:119:ILE:HD12	1:B:162:GLU:HB2	1.82	0.62
1:B:267:PHE:CE2	1:B:289:ALA:HB1	2.32	0.62
1:A:91:ASN:N	1:A:91:ASN:HD22	1.97	0.62
1:A:431:ASP:OD1	1:A:433:GLU:HG3	2.00	0.62
1:A:728:VAL:N	1:A:729:PRO:CD	2.63	0.62
1:C:102:ILE:HG12	1:C:103:GLN:N	2.15	0.62
1:C:388:MET:HE3	1:C:447:VAL:HG21	1.82	0.62
1:A:143:TYR:HA	1:A:176:VAL:O	2.00	0.62
1:B:458:GLN:O	1:B:461:PRO:HD2	1.99	0.62
1:C:274:ILE:HG21	1:C:286:LEU:HD21	1.80	0.62
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.81	0.62
1:B:312:LYS:HB3	1:B:354:ASP:CG	2.25	0.62
1:C:567:ARG:HH21	1:C:611:MET:HA	1.64	0.62
1:A:524:LYS:HZ2	1:A:524:LYS:HB2	1.65	0.61
1:A:567:ARG:HH21	1:A:611:MET:CG	2.13	0.61
1:C:267:PHE:CE2	1:C:289:ALA:HB1	2.33	0.61
1:A:129:ASN:CG	1:A:132:GLU:HB2	2.26	0.61
1:A:388:MET:HE3	1:A:447:VAL:HG21	1.82	0.61
1:C:503:PHE:CD1	1:C:510:PRO:HG3	2.35	0.61
1:C:458:GLN:HB3	1:C:460:ASN:OD1	2.00	0.61
1:B:129:ASN:CG	1:B:132:GLU:HB2	2.25	0.61
1:B:503:PHE:CD1	1:B:510:PRO:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:C	1:A:338:ARG:N	2.57	0.61
1:A:347:THR:HB	1:A:353:ILE:HD11	1.82	0.61
1:A:445:LEU:C	1:A:445:LEU:HD23	2.26	0.61
1:B:91:ASN:N	1:B:91:ASN:HD22	1.96	0.61
1:B:232:ALA:HB2	1:C:125:GLY:O	2.01	0.61
1:C:119:ILE:HD12	1:C:162:GLU:HB2	1.83	0.61
1:C:153:LEU:HD11	1:C:160:ALA:HB1	1.82	0.61
1:C:358:ARG:HG3	1:C:358:ARG:HH11	1.65	0.61
1:C:470:GLU:O	1:C:538:ASN:HA	2.00	0.61
1:A:492:LEU:O	1:A:496:PRO:HG3	2.00	0.61
1:A:460:ASN:N	1:A:461:PRO:CD	2.63	0.61
1:B:423:ILE:C	1:B:425:LYS:H	2.09	0.61
1:C:353:ILE:CG2	1:C:354:ASP:H	2.04	0.61
1:B:410:ASP:CG	1:B:463:ALA:HB2	2.25	0.61
1:C:502:LYS:O	1:C:505:LYS:HB2	2.00	0.61
1:C:514:VAL:HG12	1:C:515:LEU:H	1.65	0.61
1:A:358:ARG:HG3	1:A:358:ARG:HH11	1.65	0.61
1:A:503:PHE:CD1	1:A:510:PRO:HG3	2.36	0.61
1:B:251:LYS:HD2	1:B:346:ALA:HB1	1.83	0.61
1:C:492:LEU:O	1:C:496:PRO:HG3	2.01	0.61
1:A:432:LEU:O	1:A:437:ILE:CD1	2.49	0.60
1:A:437:ILE:CG2	1:A:438:ASP:N	2.63	0.60
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.81	0.60
1:B:472:PRO:HB2	1:B:533:ASN:HB2	1.83	0.60
1:B:582:ILE:HD13	1:B:600:VAL:HB	1.83	0.60
1:A:283:GLU:HB3	1:A:327:GLN:HE21	1.66	0.60
1:B:322:ARG:HD3	1:C:321:GLU:OE2	2.02	0.60
1:B:514:VAL:HG12	1:B:515:LEU:H	1.65	0.60
1:B:749:ASP:HA	1:B:752:ILE:CG1	2.31	0.60
1:A:502:LYS:O	1:A:505:LYS:HB2	2.02	0.60
1:C:518:GLY:C	1:C:755:TYR:CE2	2.79	0.60
1:A:271:GLY:HA2	1:A:309:ILE:HD11	1.84	0.60
1:B:573:VAL:HG23	1:B:573:VAL:O	2.00	0.60
1:B:580:ASP:HB2	1:B:628:ILE:HD11	1.83	0.60
1:C:251:LYS:HD2	1:C:346:ALA:HB1	1.82	0.60
1:A:423:ILE:C	1:A:425:LYS:H	2.10	0.60
1:B:313:ARG:HH21	1:B:313:ARG:HG3	1.65	0.60
1:C:143:TYR:HA	1:C:176:VAL:O	2.02	0.60
1:A:65:ARG:NH1	1:A:93:ARG:HH22	2.00	0.60
1:A:407:VAL:HG22	1:A:410:ASP:OD2	2.02	0.60
1:B:502:LYS:O	1:B:505:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG12	1:A:257:ALA:HB2	1.84	0.60
1:A:251:LYS:HD2	1:A:346:ALA:HB1	1.83	0.60
1:B:347:THR:HB	1:B:353:ILE:HD11	1.83	0.60
1:B:445:LEU:HD23	1:B:445:LEU:C	2.27	0.60
1:A:96:LEU:H	1:A:96:LEU:HD22	1.66	0.60
1:B:133:VAL:HG13	1:B:443:ASN:ND2	2.17	0.60
1:B:407:VAL:HG22	1:B:410:ASP:OD2	2.02	0.60
1:A:102:ILE:HG12	1:A:103:GLN:H	1.65	0.60
1:A:153:LEU:HD11	1:A:160:ALA:HB1	1.83	0.60
1:C:312:LYS:HB3	1:C:354:ASP:CG	2.26	0.60
1:C:336:LYS:C	1:C:338:ARG:N	2.57	0.60
1:A:62:LYS:C	1:A:64:ARG:H	2.09	0.59
1:A:496:PRO:O	1:A:500:PRO:HG3	2.02	0.59
1:A:514:VAL:HG12	1:A:515:LEU:H	1.68	0.59
1:C:63:LYS:HD2	1:C:93:ARG:HB3	1.83	0.59
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.84	0.59
1:C:423:ILE:C	1:C:425:LYS:H	2.08	0.59
1:C:466:GLU:O	1:C:468:VAL:HG23	2.02	0.59
1:A:96:LEU:HD22	1:A:96:LEU:N	2.17	0.59
1:A:475:THR:HG22	1:A:533:ASN:ND2	2.18	0.59
1:C:347:THR:HB	1:C:353:ILE:HD11	1.83	0.59
1:C:92:LEU:O	1:C:93:ARG:HB2	2.02	0.59
1:C:524:LYS:HZ2	1:C:524:LYS:HB2	1.67	0.59
1:C:650:GLU:HG2	1:C:677:LYS:HZ3	1.66	0.59
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.67	0.59
1:C:129:ASN:CG	1:C:132:GLU:HB2	2.27	0.59
1:C:515:LEU:HB3	1:C:642:LEU:HD13	1.85	0.59
1:C:749:ASP:HA	1:C:752:ILE:CG1	2.32	0.59
1:A:679:THR:HB	1:A:682:PHE:CD2	2.38	0.59
1:A:749:ASP:HA	1:A:752:ILE:CG1	2.32	0.59
1:B:206:ILE:HD12	1:B:213:LEU:CG	2.33	0.59
1:B:515:LEU:HB3	1:B:642:LEU:HD13	1.85	0.59
1:A:119:ILE:HD12	1:A:162:GLU:HB2	1.85	0.59
1:A:155:ARG:HD3	1:A:386:LYS:O	2.02	0.59
1:B:143:TYR:HA	1:B:176:VAL:O	2.02	0.59
1:C:244:TYR:CZ	1:C:350:PRO:HG3	2.38	0.59
1:C:311:PRO:O	1:C:313:ARG:N	2.35	0.59
1:C:407:VAL:HG22	1:C:410:ASP:OD2	2.03	0.59
1:C:472:PRO:HB2	1:C:533:ASN:HB2	1.84	0.59
1:C:458:GLN:O	1:C:461:PRO:HD2	2.03	0.59
1:A:313:ARG:HH21	1:A:313:ARG:HG3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:N	1:C:91:ASN:HD22	2.00	0.59
1:A:244:TYR:CZ	1:A:350:PRO:HG3	2.38	0.59
1:A:89:ARG:HG2	1:A:94:VAL:O	2.03	0.58
1:B:92:LEU:O	1:B:93:ARG:HB2	2.03	0.58
1:B:472:PRO:HG2	1:B:532:ALA:HB3	1.85	0.58
1:C:283:GLU:HB3	1:C:327:GLN:HE21	1.68	0.58
1:C:445:LEU:C	1:C:445:LEU:HD23	2.27	0.58
1:A:731:ILE:HG23	1:A:731:ILE:O	2.04	0.58
1:B:336:LYS:C	1:B:338:ARG:N	2.57	0.58
1:C:135:LEU:HD22	1:C:135:LEU:H	1.69	0.58
1:C:411:LEU:O	1:C:414:LEU:HB3	2.03	0.58
1:A:206:ILE:HD12	1:A:213:LEU:CG	2.33	0.58
1:A:414:LEU:HD12	1:A:455:ALA:HB1	1.85	0.58
1:A:432:LEU:O	1:A:434:ASP:OD2	2.20	0.58
1:B:244:TYR:CZ	1:B:350:PRO:HG3	2.38	0.58
1:A:514:VAL:HG11	1:A:643:ILE:CD1	2.33	0.58
1:B:184:CYS:C	1:B:186:GLY:H	2.11	0.58
1:A:697:LEU:O	1:A:701:GLU:HG2	2.02	0.58
1:B:667:ALA:HB2	1:B:731:ILE:O	2.03	0.58
1:C:237:PRO:O	1:C:238:PRO:C	2.46	0.58
1:A:233:ILE:HD13	1:B:442:MET:HE2	1.85	0.58
1:B:414:LEU:HD12	1:B:455:ALA:HB1	1.86	0.58
1:C:479:ILE:HD13	1:C:527:LEU:HD23	1.85	0.58
1:B:496:PRO:O	1:B:500:PRO:HG3	2.03	0.58
1:B:650:GLU:HB3	1:B:677:LYS:HZ1	1.69	0.58
1:C:184:CYS:C	1:C:186:GLY:H	2.11	0.58
1:C:337:GLN:HE21	1:C:337:GLN:CA	2.08	0.58
1:B:697:LEU:O	1:B:701:GLU:HG2	2.03	0.58
1:C:697:LEU:O	1:C:701:GLU:HG2	2.02	0.58
1:A:65:ARG:NH1	1:A:93:ARG:NH1	2.52	0.58
1:A:164:LYS:HE2	1:A:189:ILE:CD1	2.29	0.58
1:C:206:ILE:HD12	1:C:213:LEU:CG	2.34	0.58
1:C:414:LEU:HD12	1:C:455:ALA:HB1	1.86	0.58
1:B:679:THR:HB	1:B:682:PHE:CD2	2.39	0.58
1:C:582:ILE:HD13	1:C:600:VAL:HB	1.86	0.58
1:A:237:PRO:O	1:A:238:PRO:C	2.46	0.57
1:B:337:GLN:HE21	1:B:337:GLN:CA	2.08	0.57
1:B:65:ARG:HH11	1:B:93:ARG:NH1	2.02	0.57
1:B:117:LEU:HD21	1:B:185:GLU:CG	2.34	0.57
1:A:249:THR:HG21	1:A:369:ILE:HB	1.85	0.57
1:A:411:LEU:O	1:A:414:LEU:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PRO:O	1:B:238:PRO:C	2.47	0.57
1:C:102:ILE:HG12	1:C:103:GLN:H	1.67	0.57
1:A:95:ARG:HB2	1:A:225:ARG:NH1	2.20	0.57
1:B:96:LEU:H	1:B:96:LEU:HD22	1.69	0.57
1:B:96:LEU:HD22	1:B:96:LEU:N	2.19	0.57
1:C:206:ILE:HG22	1:C:253:LEU:CD2	2.35	0.57
1:C:206:ILE:HG22	1:C:253:LEU:HD22	1.86	0.57
1:C:328:LEU:CD1	1:C:332:MET:HG2	2.34	0.57
1:C:113:ARG:HG2	1:C:113:ARG:NH1	2.12	0.57
1:C:679:THR:HB	1:C:682:PHE:CD2	2.39	0.57
1:A:184:CYS:C	1:A:186:GLY:H	2.13	0.57
1:A:523:GLY:HA2	1:A:526:LEU:HG	1.87	0.57
1:C:313:ARG:HH21	1:C:313:ARG:HG3	1.69	0.57
1:B:249:THR:HG21	1:B:369:ILE:HB	1.86	0.57
1:C:129:ASN:OD1	1:C:132:GLU:N	2.37	0.57
1:C:427:MET:HE1	1:C:437:ILE:HG21	1.86	0.57
1:C:650:GLU:HB3	1:C:677:LYS:HZ1	1.70	0.57
1:A:580:ASP:HB2	1:A:628:ILE:HD11	1.86	0.57
1:C:222:LEU:N	1:C:223:PRO:HD2	2.20	0.57
1:B:102:ILE:HG12	1:B:103:GLN:N	2.20	0.56
1:B:560:ARG:HG3	1:B:560:ARG:NH1	2.20	0.56
1:C:316:THR:HG23	1:C:316:THR:O	2.04	0.56
1:A:275:MET:HG2	1:A:309:ILE:HG12	1.85	0.56
1:A:466:GLU:HG2	1:A:467:THR:H	1.69	0.56
1:B:411:LEU:O	1:B:414:LEU:HB3	2.05	0.56
1:C:253:LEU:HD12	2:C:807:ADP:H2'	1.87	0.56
1:C:577:ASP:O	1:C:578:GLU:C	2.48	0.56
1:A:96:LEU:H	1:A:96:LEU:CD2	2.18	0.56
1:A:129:ASN:OD1	1:A:132:GLU:N	2.37	0.56
1:A:133:VAL:CG1	1:A:443:ASN:ND2	2.62	0.56
1:B:129:ASN:OD1	1:B:132:GLU:N	2.34	0.56
1:C:496:PRO:O	1:C:500:PRO:HG3	2.05	0.56
1:C:96:LEU:N	1:C:96:LEU:HD22	2.20	0.56
1:C:249:THR:HG21	1:C:369:ILE:HB	1.86	0.56
1:A:32:ILE:HG12	1:A:83:ARG:HD3	1.88	0.56
1:A:611:MET:HE1	1:A:619:ILE:CD1	2.34	0.56
1:B:738:GLU:OE2	1:B:741:ARG:HG3	2.05	0.56
1:A:283:GLU:HB3	1:A:327:GLN:NE2	2.21	0.56
1:A:35:ASP:O	1:A:38:VAL:HG12	2.04	0.56
1:B:650:GLU:HG2	1:B:677:LYS:HZ3	1.70	0.56
1:A:427:MET:SD	1:A:432:LEU:HD12	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:LEU:HD12	1:A:647:LEU:H	1.70	0.56
1:B:135:LEU:H	1:B:135:LEU:HD22	1.71	0.56
1:A:65:ARG:NH1	1:A:93:ARG:NH2	2.54	0.56
1:A:515:LEU:HB3	1:A:642:LEU:HD13	1.87	0.56
1:A:582:ILE:HD13	1:A:600:VAL:HB	1.87	0.56
1:C:96:LEU:HD22	1:C:96:LEU:H	1.70	0.56
1:A:92:LEU:O	1:A:93:ARG:HB2	2.06	0.56
1:A:433:GLU:O	1:A:434:ASP:CG	2.49	0.56
1:B:232:ALA:HB2	1:C:125:GLY:C	2.31	0.56
1:B:335:LEU:C	1:B:337:GLN:N	2.64	0.56
1:B:749:ASP:O	1:B:752:ILE:HB	2.06	0.56
1:C:458:GLN:HG3	1:C:459:SER:H	1.71	0.56
1:A:410:ASP:CG	1:A:463:ALA:HB2	2.31	0.55
1:A:515:LEU:HD21	1:A:623:THR:HG22	1.88	0.55
1:B:60:LYS:HB2	1:B:101:SER:OG	2.05	0.55
1:B:201:VAL:HG12	1:B:257:ALA:HB2	1.88	0.55
1:B:96:LEU:H	1:B:96:LEU:CD2	2.19	0.55
1:B:728:VAL:N	1:B:729:PRO:CD	2.69	0.55
1:C:87:VAL:HG22	1:C:198:LEU:CD1	2.36	0.55
1:C:523:GLY:HA2	1:C:526:LEU:HG	1.87	0.55
1:A:206:ILE:CD1	1:A:213:LEU:CD2	2.85	0.55
1:A:458:GLN:HG3	1:A:459:SER:H	1.71	0.55
1:A:738:GLU:OE2	1:A:741:ARG:HG3	2.06	0.55
1:A:28:VAL:HG23	1:A:84:MET:HG2	1.89	0.55
1:A:681:GLY:HA3	1:A:745:ARG:NH2	2.21	0.55
1:B:35:ASP:O	1:B:38:VAL:HG12	2.07	0.55
1:C:28:VAL:HG23	1:C:84:MET:HG2	1.88	0.55
1:C:335:LEU:C	1:C:337:GLN:N	2.65	0.55
1:A:741:ARG:HE	1:A:741:ARG:HA	1.71	0.55
1:B:133:VAL:CG1	1:B:443:ASN:HD22	2.19	0.55
1:B:523:GLY:HA2	1:B:526:LEU:HG	1.89	0.55
1:C:35:ASP:O	1:C:38:VAL:HG12	2.07	0.55
1:C:118:PRO:HG2	1:C:188:PRO:HG3	1.89	0.55
1:A:640:ASP:HB2	1:A:641:GLN:HE21	1.72	0.55
1:C:164:LYS:HE2	1:C:189:ILE:CD1	2.32	0.55
1:C:564:ASP:C	1:C:566:ALA:H	2.14	0.55
1:A:336:LYS:O	1:A:338:ARG:N	2.37	0.55
1:A:438:ASP:OD2	1:A:440:GLU:HB2	2.07	0.55
1:C:206:ILE:CD1	1:C:213:LEU:CD2	2.85	0.55
1:A:335:LEU:C	1:A:337:GLN:N	2.64	0.55
1:B:741:ARG:HE	1:B:741:ARG:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:GLU:OE2	1:C:741:ARG:HG3	2.07	0.55
1:A:117:LEU:HD21	1:A:185:GLU:CG	2.37	0.55
1:A:118:PRO:HG2	1:A:188:PRO:HG3	1.87	0.55
1:B:45:LYS:O	1:B:49:LEU:HD13	2.07	0.55
1:B:640:ASP:HB2	1:B:641:GLN:HE21	1.72	0.55
1:B:283:GLU:HB3	1:B:327:GLN:NE2	2.22	0.54
1:B:438:ASP:OD2	1:B:440:GLU:HB2	2.07	0.54
1:A:45:LYS:O	1:A:49:LEU:HD13	2.07	0.54
1:A:206:ILE:HG22	1:A:253:LEU:HD22	1.88	0.54
1:C:640:ASP:HB2	1:C:641:GLN:HE21	1.72	0.54
1:C:741:ARG:HE	1:C:741:ARG:HA	1.72	0.54
1:A:459:SER:O	1:A:462:SER:OG	2.24	0.54
1:B:624:ASN:H	1:B:624:ASN:ND2	2.06	0.54
1:C:60:LYS:HG2	1:C:66:GLU:HG2	1.90	0.54
1:C:624:ASN:ND2	1:C:624:ASN:H	2.06	0.54
1:B:32:ILE:HG12	1:B:83:ARG:HD3	1.89	0.54
1:B:303:ILE:HD12	1:B:345:ALA:HB2	1.90	0.54
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.89	0.54
1:B:458:GLN:HG3	1:B:459:SER:H	1.72	0.54
1:B:574:LEU:HG	1:B:576:PHE:HE1	1.72	0.54
1:A:600:VAL:O	1:A:604:ILE:HG13	2.07	0.54
1:A:647:LEU:HD21	1:A:747:VAL:HB	1.90	0.54
1:B:694:ALA:HB1	1:B:731:ILE:HD11	1.89	0.54
1:A:57:VAL:CG2	1:A:59:LEU:HD21	2.36	0.54
1:A:206:ILE:HG22	1:A:253:LEU:CD2	2.38	0.54
1:A:570:ALA:HB1	1:A:616:ASN:HB3	1.88	0.54
1:B:89:ARG:HG2	1:B:94:VAL:O	2.08	0.54
1:B:514:VAL:HG11	1:B:643:ILE:CD1	2.35	0.54
1:C:567:ARG:NH2	1:C:611:MET:HA	2.21	0.54
1:A:62:LYS:O	1:A:63:LYS:C	2.49	0.54
1:A:119:ILE:HG13	1:A:162:GLU:O	2.08	0.54
1:B:63:LYS:HD2	1:B:93:ARG:HB3	1.90	0.54
1:B:164:LYS:HE2	1:B:189:ILE:CD1	2.32	0.54
1:B:297:ALA:HA	1:B:298:PRO:C	2.33	0.54
1:B:729:PRO:O	1:B:730:GLU:OE2	2.25	0.54
1:C:96:LEU:H	1:C:96:LEU:CD2	2.21	0.54
1:C:438:ASP:OD2	1:C:440:GLU:HB2	2.08	0.54
1:C:749:ASP:O	1:C:752:ILE:HB	2.07	0.54
1:A:87:VAL:HG22	1:A:198:LEU:CD1	2.37	0.54
1:B:55:ASP:O	1:B:71:VAL:HG12	2.08	0.54
1:B:87:VAL:HG22	1:B:198:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ILE:CD1	1:C:176:VAL:HG22	2.37	0.54
1:C:283:GLU:HB3	1:C:327:GLN:NE2	2.23	0.54
1:A:113:ARG:CG	1:A:113:ARG:NH1	2.70	0.54
1:A:368:ASP:HB2	1:A:568:GLN:CD	2.33	0.54
1:A:502:LYS:HE2	1:B:706:GLU:OE2	2.08	0.54
1:B:206:ILE:HG22	1:B:253:LEU:CD2	2.38	0.54
1:A:55:ASP:O	1:A:71:VAL:HG12	2.08	0.54
1:B:89:ARG:CZ	1:B:96:LEU:HD21	2.38	0.54
1:B:155:ARG:HD3	1:B:386:LYS:O	2.08	0.54
1:B:206:ILE:CD1	1:B:213:LEU:CD2	2.86	0.54
1:B:253:LEU:C	1:B:253:LEU:CD2	2.81	0.54
1:B:254:ILE:O	1:B:258:VAL:HG23	2.08	0.54
1:C:89:ARG:HG2	1:C:94:VAL:O	2.08	0.54
1:C:514:VAL:HG11	1:C:643:ILE:CD1	2.34	0.54
1:A:614:LYS:HE2	1:B:402:GLU:CD	2.32	0.53
1:A:749:ASP:O	1:A:752:ILE:HB	2.08	0.53
1:B:113:ARG:CG	1:B:113:ARG:NH1	2.70	0.53
1:B:206:ILE:HG22	1:B:253:LEU:HD22	1.89	0.53
1:B:647:LEU:HD12	1:B:647:LEU:H	1.73	0.53
1:B:729:PRO:C	1:B:730:GLU:CD	2.76	0.53
1:C:244:TYR:HB2	1:C:368:ASP:HA	1.90	0.53
1:C:437:ILE:HG22	1:C:438:ASP:N	2.22	0.53
1:C:644:TYR:C	1:C:645:ILE:HD12	2.32	0.53
1:C:731:ILE:HG23	1:C:731:ILE:O	2.07	0.53
1:A:489:LEU:HD13	1:A:531:ILE:HB	1.90	0.53
1:B:600:VAL:O	1:B:604:ILE:HG13	2.08	0.53
1:B:647:LEU:HD21	1:B:747:VAL:HB	1.90	0.53
1:C:313:ARG:CG	1:C:314:GLU:H	2.10	0.53
1:A:254:ILE:O	1:A:258:VAL:HG23	2.08	0.53
1:A:347:THR:CB	1:A:353:ILE:HD11	2.38	0.53
1:B:119:ILE:HD12	1:B:162:GLU:CB	2.38	0.53
1:B:201:VAL:HG21	1:B:256:ARG:HD2	1.90	0.53
1:B:222:LEU:N	1:B:223:PRO:HD2	2.23	0.53
1:B:701:GLU:O	1:B:704:GLU:N	2.37	0.53
1:A:252:THR:HA	1:A:302:PHE:CZ	2.44	0.53
1:A:567:ARG:NH2	1:A:611:MET:CG	2.71	0.53
1:B:169:ASP:O	1:B:171:SER:N	2.38	0.53
1:A:89:ARG:CZ	1:A:96:LEU:HD21	2.38	0.53
1:A:297:ALA:HA	1:A:298:PRO:C	2.33	0.53
1:A:490:GLN:CB	1:A:494:GLN:HG3	2.38	0.53
1:A:644:TYR:C	1:A:645:ILE:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HG12	1:B:103:GLN:H	1.72	0.53
1:B:302:PHE:HA	1:B:344:MET:O	2.09	0.53
1:C:89:ARG:CZ	1:C:96:LEU:HD21	2.39	0.53
1:C:647:LEU:HD12	1:C:647:LEU:H	1.73	0.53
1:A:758:PHE:O	1:A:762:LEU:HB2	2.09	0.53
1:B:118:PRO:HG2	1:B:188:PRO:HG3	1.89	0.53
1:B:177:ALA:C	1:B:179:ASP:H	2.16	0.53
1:B:506:PHE:CD2	1:C:699:ILE:HG12	2.43	0.53
1:C:169:ASP:O	1:C:171:SER:N	2.35	0.53
1:C:254:ILE:O	1:C:258:VAL:HG23	2.08	0.53
1:C:532:ALA:HB2	1:C:573:VAL:HG21	1.91	0.53
1:A:157:GLY:O	1:A:159:ARG:HG2	2.08	0.53
1:A:253:LEU:C	1:A:253:LEU:CD2	2.82	0.53
1:A:337:GLN:HE21	1:A:337:GLN:CA	2.09	0.53
1:B:644:TYR:C	1:B:645:ILE:HD12	2.33	0.53
1:C:32:ILE:HG12	1:C:83:ARG:HD3	1.91	0.53
1:C:139:PHE:O	1:C:141:GLU:N	2.42	0.53
1:A:95:ARG:HB2	1:A:225:ARG:NH2	2.23	0.53
1:A:222:LEU:N	1:A:223:PRO:HD2	2.24	0.53
1:A:518:GLY:HA2	1:A:755:TYR:HD2	1.73	0.53
1:B:28:VAL:HG23	1:B:84:MET:HG2	1.89	0.53
1:C:253:LEU:C	1:C:253:LEU:CD2	2.82	0.53
1:A:244:TYR:HB2	1:A:368:ASP:HA	1.90	0.53
1:A:458:GLN:O	1:A:461:PRO:HD2	2.08	0.53
1:C:666:VAL:HG23	1:C:666:VAL:O	2.09	0.53
1:A:466:GLU:HG2	1:A:467:THR:N	2.24	0.52
1:B:269:ILE:HD11	1:B:301:ILE:HG22	1.90	0.52
1:B:728:VAL:N	1:B:729:PRO:HD2	2.24	0.52
1:C:117:LEU:HD21	1:C:185:GLU:CG	2.39	0.52
1:C:518:GLY:HA2	1:C:755:TYR:HD2	1.74	0.52
1:C:560:ARG:HG3	1:C:560:ARG:NH1	2.21	0.52
1:C:568:GLN:O	1:C:568:GLN:HG2	2.08	0.52
1:C:640:ASP:HB2	1:C:641:GLN:NE2	2.24	0.52
1:C:728:VAL:N	1:C:729:PRO:CD	2.72	0.52
1:A:119:ILE:HD12	1:A:162:GLU:CB	2.39	0.52
1:A:650:GLU:HB3	1:A:677:LYS:HZ1	1.73	0.52
1:C:297:ALA:HA	1:C:298:PRO:C	2.34	0.52
1:A:395:ASP:O	1:A:398:GLN:HB3	2.09	0.52
1:A:515:LEU:HA	1:A:621:GLY:O	2.09	0.52
1:B:395:ASP:O	1:B:398:GLN:HB3	2.10	0.52
1:A:135:LEU:HD22	1:A:135:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:THR:CB	1:B:353:ILE:HD11	2.39	0.52
1:B:624:ASN:C	1:B:624:ASN:HD22	2.18	0.52
1:A:269:ILE:HD11	1:A:301:ILE:CG2	2.39	0.52
1:A:614:LYS:HD3	1:B:402:GLU:CB	2.33	0.52
1:A:666:VAL:HG23	1:A:666:VAL:O	2.09	0.52
1:B:656:ILE:HG21	1:B:687:LEU:HD12	1.89	0.52
1:C:312:LYS:HB3	1:C:354:ASP:HB2	1.91	0.52
1:C:336:LYS:O	1:C:338:ARG:N	2.37	0.52
1:C:347:THR:CB	1:C:353:ILE:HD11	2.40	0.52
1:A:540:ILE:HD12	1:A:572:CYS:SG	2.50	0.52
1:C:403:THR:HB	1:C:406:HIS:CG	2.45	0.52
1:A:36:ASN:OD1	1:A:87:VAL:HG21	2.10	0.52
1:A:112:LYS:HB2	1:A:169:ASP:CB	2.39	0.52
1:A:403:THR:HB	1:A:406:HIS:CG	2.44	0.52
1:A:615:LYS:HZ3	1:B:461:PRO:CG	2.23	0.52
1:A:640:ASP:HB2	1:A:641:GLN:NE2	2.24	0.52
1:B:323:ARG:NH1	1:C:278:LEU:HA	2.24	0.52
1:C:313:ARG:O	1:C:316:THR:CG2	2.50	0.52
1:C:729:PRO:O	1:C:730:GLU:CD	2.53	0.52
1:A:318:GLY:O	1:A:322:ARG:HG3	2.10	0.52
1:A:518:GLY:C	1:A:755:TYR:CE2	2.86	0.52
1:B:336:LYS:O	1:B:338:ARG:N	2.37	0.52
1:B:490:GLN:CB	1:B:494:GLN:HG3	2.37	0.52
1:C:65:ARG:NH1	1:C:93:ARG:HH12	2.07	0.52
1:C:299:ALA:HB3	1:C:341:VAL:HG12	1.91	0.52
1:A:299:ALA:HB3	1:A:341:VAL:HG12	1.92	0.52
1:A:624:ASN:H	1:A:624:ASN:ND2	2.06	0.52
1:B:403:THR:HB	1:B:406:HIS:CG	2.44	0.52
1:B:432:LEU:O	1:B:437:ILE:CD1	2.58	0.52
1:B:489:LEU:HD13	1:B:531:ILE:HB	1.91	0.52
1:B:611:MET:HE1	1:B:619:ILE:CD1	2.37	0.52
1:C:108:VAL:HG22	1:C:173:TYR:CD1	2.45	0.52
1:C:269:ILE:HD12	1:C:303:ILE:HG12	1.92	0.52
1:C:728:VAL:N	1:C:729:PRO:HD2	2.25	0.52
1:A:169:ASP:O	1:A:171:SER:N	2.38	0.51
1:B:157:GLY:O	1:B:159:ARG:HG2	2.10	0.51
1:B:410:ASP:CG	1:B:463:ALA:CB	2.83	0.51
1:B:641:GLN:C	1:B:642:LEU:HD22	2.35	0.51
1:C:55:ASP:O	1:C:71:VAL:HG12	2.09	0.51
1:C:648:PRO:HD2	1:C:682:PHE:O	2.10	0.51
1:B:108:VAL:HG22	1:B:173:TYR:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:PHE:CD1	1:B:176:VAL:HG11	2.45	0.51
1:C:395:ASP:O	1:C:398:GLN:HB3	2.10	0.51
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.46	0.51
1:B:299:ALA:HB3	1:B:341:VAL:HG12	1.91	0.51
1:A:63:LYS:HD2	1:A:93:ARG:HB3	1.92	0.51
1:A:479:ILE:HD13	1:A:527:LEU:HD23	1.91	0.51
1:A:614:LYS:CD	1:B:402:GLU:CB	2.88	0.51
1:B:139:PHE:O	1:B:141:GLU:N	2.43	0.51
1:B:410:ASP:OD2	1:B:463:ALA:CB	2.58	0.51
1:B:647:LEU:HB3	1:B:648:PRO:HD2	1.93	0.51
1:A:158:MET:HE1	1:A:419:ALA:CB	2.39	0.51
1:A:495:TYR:N	1:A:496:PRO:HD2	2.25	0.51
1:B:244:TYR:HB2	1:B:368:ASP:HA	1.92	0.51
1:B:437:ILE:HG22	1:B:438:ASP:N	2.24	0.51
1:B:577:ASP:O	1:B:578:GLU:C	2.53	0.51
1:B:640:ASP:HB2	1:B:641:GLN:NE2	2.25	0.51
1:C:201:VAL:HG12	1:C:257:ALA:HB2	1.92	0.51
1:C:269:ILE:HD11	1:C:301:ILE:CG2	2.39	0.51
1:A:624:ASN:C	1:A:624:ASN:HD22	2.18	0.51
1:A:656:ILE:HG21	1:A:687:LEU:HD12	1.92	0.51
1:C:157:GLY:O	1:C:159:ARG:HG2	2.10	0.51
1:A:177:ALA:C	1:A:179:ASP:H	2.18	0.51
1:A:560:ARG:HG3	1:A:560:ARG:NH1	2.20	0.51
1:A:587:GLY:HA3	1:A:591:GLY:HA2	1.93	0.51
1:A:648:PRO:HD2	1:A:682:PHE:O	2.11	0.51
1:A:732:ARG:HD2	1:A:734:ASP:OD1	2.11	0.51
1:B:206:ILE:HG13	1:B:206:ILE:O	2.10	0.51
1:B:648:PRO:HD2	1:B:682:PHE:O	2.11	0.51
1:B:666:VAL:HG23	1:B:666:VAL:O	2.11	0.51
1:C:229:LEU:O	1:C:233:ILE:HG22	2.11	0.51
1:C:624:ASN:C	1:C:624:ASN:HD22	2.18	0.51
1:A:40:SER:HB3	1:A:74:ASP:HB2	1.92	0.51
1:B:431:ASP:O	1:B:432:LEU:HD23	2.11	0.51
1:B:518:GLY:C	1:B:755:TYR:CE2	2.86	0.51
1:C:119:ILE:HD12	1:C:162:GLU:CB	2.40	0.51
1:C:290:PHE:CE2	1:C:331:LEU:HB3	2.46	0.51
1:C:647:LEU:HB3	1:C:648:PRO:HD2	1.93	0.51
1:A:252:THR:HB	2:A:807:ADP:O1A	2.11	0.51
1:B:410:ASP:OD2	1:B:463:ALA:HB1	2.10	0.51
1:C:65:ARG:NH1	1:C:93:ARG:NH1	2.59	0.51
1:C:518:GLY:HA2	1:C:755:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:GLN:C	1:C:642:LEU:HD22	2.36	0.51
1:A:139:PHE:O	1:A:141:GLU:N	2.44	0.50
1:A:290:PHE:CE2	1:A:331:LEU:HB3	2.45	0.50
1:B:495:TYR:N	1:B:496:PRO:HD2	2.25	0.50
1:B:582:ILE:CD1	1:B:600:VAL:HB	2.42	0.50
1:C:732:ARG:HG3	1:C:734:ASP:OD1	2.11	0.50
1:A:641:GLN:C	1:A:642:LEU:HD22	2.35	0.50
1:A:647:LEU:HB3	1:A:648:PRO:HD2	1.93	0.50
1:B:290:PHE:CE2	1:B:331:LEU:HB3	2.47	0.50
1:B:408:GLY:HA3	2:B:807:ADP:N7	2.26	0.50
1:B:489:LEU:HD21	1:B:516:PHE:CZ	2.47	0.50
1:C:656:ILE:HG21	1:C:687:LEU:HD12	1.93	0.50
1:A:65:ARG:HH11	1:A:93:ARG:NH2	2.09	0.50
1:A:95:ARG:HG3	1:A:225:ARG:NH1	2.26	0.50
1:A:437:ILE:CG2	1:A:438:ASP:H	2.25	0.50
1:B:489:LEU:HD21	1:B:516:PHE:HZ	1.76	0.50
1:C:177:ALA:C	1:C:179:ASP:H	2.18	0.50
1:A:89:ARG:HD3	1:A:96:LEU:HD22	1.93	0.50
1:A:489:LEU:HD21	1:A:516:PHE:HZ	1.77	0.50
1:B:113:ARG:HG2	1:B:113:ARG:NH1	2.16	0.50
1:B:575:PHE:HE2	1:B:577:ASP:HB2	1.75	0.50
1:B:681:GLY:HA3	1:B:745:ARG:NH2	2.26	0.50
1:C:302:PHE:HA	1:C:344:MET:O	2.12	0.50
1:B:233:ILE:HD13	1:C:442:MET:CE	2.40	0.50
1:C:40:SER:HB3	1:C:74:ASP:HB2	1.92	0.50
1:C:126:ILE:HG21	1:C:159:ARG:HD2	1.94	0.50
1:C:489:LEU:HD13	1:C:531:ILE:HB	1.91	0.50
1:A:131:PHE:O	1:A:136:LYS:HB2	2.11	0.50
1:B:574:LEU:HG	1:B:576:PHE:CE1	2.47	0.50
1:C:45:LYS:O	1:C:49:LEU:HD13	2.12	0.50
1:B:36:ASN:OD1	1:B:87:VAL:HG21	2.11	0.50
1:B:608:MET:HG3	1:B:619:ILE:HD12	1.94	0.50
1:B:63:LYS:HD2	1:B:93:ARG:CG	2.41	0.50
1:B:460:ASN:N	1:B:461:PRO:CD	2.75	0.50
1:B:463:ALA:O	1:B:464:LEU:C	2.55	0.50
1:C:508:MET:O	1:C:508:MET:HG3	2.09	0.50
1:A:126:ILE:HG21	1:A:159:ARG:HD2	1.94	0.49
1:A:206:ILE:HD13	1:A:213:LEU:HD21	1.93	0.49
1:C:667:ALA:HB2	1:C:731:ILE:O	2.12	0.49
1:A:147:ARG:HB3	1:A:150:ASP:OD2	2.12	0.49
1:A:585:ALA:C	1:A:587:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ALA:HA	1:C:125:GLY:HA3	1.94	0.49
1:C:119:ILE:HG13	1:C:162:GLU:O	2.11	0.49
1:C:681:GLY:HA3	1:C:745:ARG:NH2	2.27	0.49
1:A:206:ILE:HG13	1:A:206:ILE:O	2.11	0.49
1:A:311:PRO:O	1:A:312:LYS:C	2.54	0.49
1:B:183:HIS:HB3	1:B:185:GLU:OE2	2.12	0.49
1:B:408:GLY:HA3	2:B:807:ADP:C8	2.47	0.49
1:C:495:TYR:N	1:C:496:PRO:HD2	2.26	0.49
1:A:57:VAL:HG23	1:A:59:LEU:HD21	1.94	0.49
1:A:540:ILE:CG2	1:A:574:LEU:HD12	2.42	0.49
1:B:112:LYS:HB2	1:B:169:ASP:CB	2.42	0.49
1:B:304:ASP:OD2	1:B:305:GLU:HG3	2.12	0.49
1:B:575:PHE:CE2	1:B:577:ASP:HB2	2.47	0.49
1:B:647:LEU:HD21	1:B:747:VAL:CB	2.43	0.49
1:C:112:LYS:HB2	1:C:169:ASP:CB	2.43	0.49
1:C:184:CYS:O	1:C:186:GLY:N	2.45	0.49
1:C:682:PHE:CE1	1:C:690:ILE:HD11	2.48	0.49
1:A:108:VAL:HG22	1:A:173:TYR:CD1	2.48	0.49
1:A:127:THR:HG22	1:A:438:ASP:HA	1.93	0.49
1:A:248:GLY:O	1:A:249:THR:C	2.55	0.49
1:A:512:LYS:NZ	1:A:608:MET:O	2.25	0.49
1:B:684:GLY:HA3	2:B:900:ADP:C8	2.46	0.49
1:B:694:ALA:CB	1:B:731:ILE:HD11	2.43	0.49
1:C:385:THR:C	1:C:387:ASN:H	2.21	0.49
1:B:147:ARG:HB3	1:B:150:ASP:OD2	2.13	0.49
1:B:385:THR:C	1:B:387:ASN:H	2.21	0.49
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.92	0.49
1:C:611:MET:HE1	1:C:619:ILE:CD1	2.38	0.49
1:A:518:GLY:HA2	1:A:755:TYR:CD2	2.47	0.49
1:C:248:GLY:O	1:C:249:THR:C	2.55	0.49
1:C:542:ILE:HD12	1:C:542:ILE:N	2.27	0.49
1:C:608:MET:HG3	1:C:619:ILE:HD12	1.95	0.49
1:C:647:LEU:HD21	1:C:747:VAL:HB	1.93	0.49
1:C:758:PHE:O	1:C:762:LEU:HB2	2.12	0.49
1:A:281:GLU:O	1:A:284:SER:HB3	2.13	0.49
1:A:489:LEU:HD21	1:A:516:PHE:CZ	2.47	0.49
1:A:633:ILE:HG22	1:A:639:LEU:HD12	1.94	0.49
1:B:229:LEU:O	1:B:233:ILE:HG22	2.12	0.49
1:B:381:LEU:HD21	1:B:411:LEU:HD22	1.95	0.49
1:B:438:ASP:HB3	1:B:441:VAL:CG2	2.42	0.49
1:C:109:LYS:O	1:C:110:TYR:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:HB3	1:A:185:GLU:OE2	2.12	0.49
1:A:265:PHE:CD2	1:A:296:ASN:HB2	2.48	0.49
1:A:542:ILE:N	1:A:542:ILE:HD12	2.27	0.49
1:B:542:ILE:N	1:B:542:ILE:HD12	2.27	0.49
1:B:567:ARG:HB2	1:B:567:ARG:CZ	2.43	0.49
1:C:206:ILE:HG13	1:C:206:ILE:O	2.11	0.49
1:C:755:TYR:HD1	1:C:755:TYR:N	2.11	0.49
1:A:294:GLU:CD	1:A:339:ALA:HB2	2.38	0.49
1:A:729:PRO:C	1:A:730:GLU:CD	2.81	0.49
1:C:60:LYS:NZ	1:C:103:GLN:HE21	1.98	0.49
1:C:206:ILE:CD1	1:C:213:LEU:CG	2.86	0.49
1:C:449:MET:HE3	1:C:453:ARG:HH21	1.78	0.49
1:C:472:PRO:HG2	1:C:532:ALA:CB	2.39	0.49
1:B:43:GLN:N	1:B:44:PRO:CD	2.76	0.48
1:B:427:MET:HE1	1:B:437:ILE:HG21	1.95	0.48
1:B:508:MET:O	1:B:508:MET:HG3	2.12	0.48
1:C:22:ARG:C	1:C:24:ASN:H	2.21	0.48
1:A:385:THR:C	1:A:387:ASN:H	2.22	0.48
1:B:608:MET:HG3	1:B:619:ILE:HD13	1.95	0.48
1:B:665:PRO:C	1:B:731:ILE:HG22	2.37	0.48
1:B:755:TYR:N	1:B:755:TYR:CD1	2.81	0.48
1:C:93:ARG:HG2	1:C:93:ARG:HH11	1.78	0.48
1:C:227:PRO:HA	1:C:340:HIS:CE1	2.48	0.48
1:C:410:ASP:CG	1:C:463:ALA:HB2	2.38	0.48
1:A:348:ASN:O	1:A:349:ARG:HB3	2.14	0.48
1:B:89:ARG:NH1	1:B:96:LEU:HD21	2.28	0.48
1:B:567:ARG:HH21	1:B:611:MET:CG	2.26	0.48
1:B:755:TYR:N	1:B:755:TYR:HD1	2.11	0.48
1:C:431:ASP:OD1	1:C:433:GLU:HG3	2.12	0.48
1:A:503:PHE:HA	1:B:699:ILE:HD13	1.95	0.48
1:B:281:GLU:O	1:B:284:SER:HB3	2.13	0.48
1:B:633:ILE:HG22	1:B:639:LEU:HD12	1.95	0.48
1:A:290:PHE:CD2	1:A:331:LEU:HB3	2.48	0.48
1:A:458:GLN:O	1:A:461:PRO:CD	2.61	0.48
1:A:682:PHE:CE1	1:A:690:ILE:HD11	2.48	0.48
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.79	0.48
1:B:114:ILE:HD13	1:B:146:ILE:HD11	1.95	0.48
1:C:432:LEU:CD1	1:C:441:VAL:HG21	2.44	0.48
1:B:248:GLY:O	1:B:249:THR:C	2.56	0.48
1:B:449:MET:HE3	1:B:453:ARG:HH21	1.79	0.48
1:B:515:LEU:HA	1:B:621:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:HH21	1:B:611:MET:HG3	1.78	0.48
1:C:46:MET:HE3	1:C:71:VAL:HG22	1.96	0.48
1:C:459:SER:O	1:C:462:SER:OG	2.14	0.48
1:C:755:TYR:N	1:C:755:TYR:CD1	2.81	0.48
1:A:44:PRO:HG2	1:A:79:ASP:OD1	2.13	0.48
1:A:89:ARG:HG3	1:A:94:VAL:HG23	1.95	0.48
1:A:123:VAL:O	1:A:124:GLU:C	2.57	0.48
1:A:487:ARG:CZ	1:A:487:ARG:HB3	2.44	0.48
1:B:41:LEU:O	1:B:73:SER:HA	2.14	0.48
1:B:169:ASP:CB	1:B:170:PRO:HD3	2.27	0.48
1:B:540:ILE:HD12	1:B:572:CYS:SG	2.53	0.48
1:B:590:ILE:HG13	1:B:591:GLY:H	1.78	0.48
1:B:758:PHE:O	1:B:762:LEU:HB2	2.13	0.48
1:C:113:ARG:CG	1:C:113:ARG:NH1	2.67	0.48
1:C:133:VAL:HG22	1:C:440:GLU:HA	1.96	0.48
1:C:183:HIS:HB3	1:C:185:GLU:OE2	2.14	0.48
1:C:206:ILE:HD12	1:C:213:LEU:HD21	1.95	0.48
1:A:313:ARG:HG3	1:A:313:ARG:NH2	2.28	0.48
1:B:57:VAL:CG2	1:B:59:LEU:HD21	2.44	0.48
1:B:89:ARG:HD3	1:B:96:LEU:HD22	1.94	0.48
1:B:203:TYR:CE2	1:B:217:LYS:HE2	2.48	0.48
1:B:294:GLU:CD	1:B:339:ALA:HB2	2.38	0.48
1:B:518:GLY:HA2	1:B:755:TYR:HD2	1.79	0.48
1:C:36:ASN:OD1	1:C:87:VAL:HG21	2.13	0.48
1:C:265:PHE:CD2	1:C:296:ASN:HB2	2.49	0.48
1:C:438:ASP:HB3	1:C:441:VAL:CG2	2.42	0.48
1:A:381:LEU:HD21	1:A:411:LEU:HD22	1.95	0.48
1:A:508:MET:O	1:A:508:MET:HG3	2.14	0.48
1:B:25:ARG:HH12	1:B:99:VAL:HG21	1.79	0.48
1:B:427:MET:O	1:B:431:ASP:N	2.46	0.48
1:B:515:LEU:HD13	1:B:634:LEU:HD21	1.95	0.48
1:C:112:LYS:H	1:C:170:PRO:HD3	1.78	0.48
1:C:432:LEU:O	1:C:437:ILE:CD1	2.61	0.48
1:A:26:LEU:HD13	1:A:41:LEU:HD21	1.95	0.48
1:A:647:LEU:HD12	1:A:647:LEU:N	2.28	0.48
1:B:40:SER:HB3	1:B:74:ASP:HB2	1.95	0.48
1:B:44:PRO:HG2	1:B:79:ASP:OD1	2.14	0.48
1:B:227:PRO:HA	1:B:340:HIS:CE1	2.49	0.48
1:B:269:ILE:HD11	1:B:301:ILE:CG2	2.44	0.48
1:B:313:ARG:HG3	1:B:313:ARG:NH2	2.29	0.48
1:B:328:LEU:O	1:B:331:LEU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:VAL:HG21	1:C:72:LEU:HD12	1.96	0.48
1:C:139:PHE:O	1:C:140:LEU:C	2.57	0.48
1:C:147:ARG:HB3	1:C:150:ASP:OD2	2.13	0.48
1:C:294:GLU:CD	1:C:339:ALA:HB2	2.38	0.48
1:C:701:GLU:O	1:C:704:GLU:N	2.42	0.48
1:A:109:LYS:O	1:A:110:TYR:C	2.57	0.47
1:A:112:LYS:H	1:A:170:PRO:HD3	1.78	0.47
1:A:472:PRO:HG2	1:A:532:ALA:CB	2.39	0.47
1:A:608:MET:HG3	1:A:619:ILE:HD13	1.95	0.47
1:B:119:ILE:HG13	1:B:162:GLU:O	2.13	0.47
1:B:206:ILE:HD13	1:B:213:LEU:HD21	1.96	0.47
1:B:515:LEU:HD21	1:B:623:THR:HG22	1.96	0.47
1:C:206:ILE:HD13	1:C:213:LEU:HD21	1.96	0.47
1:A:35:ASP:O	1:A:85:ASN:ND2	2.48	0.47
1:A:438:ASP:HB3	1:A:441:VAL:CG2	2.44	0.47
1:A:532:ALA:HB2	1:A:573:VAL:HG21	1.96	0.47
1:A:608:MET:HG3	1:A:619:ILE:HD12	1.95	0.47
1:A:755:TYR:HD1	1:A:755:TYR:N	2.11	0.47
1:B:388:MET:HE3	1:B:447:VAL:CG2	2.43	0.47
1:C:131:PHE:O	1:C:136:LYS:HB2	2.14	0.47
1:C:281:GLU:O	1:C:284:SER:HB3	2.14	0.47
1:C:490:GLN:CB	1:C:494:GLN:HG3	2.40	0.47
1:A:313:ARG:O	1:A:316:THR:CG2	2.53	0.47
1:A:449:MET:HE3	1:A:453:ARG:HH21	1.79	0.47
1:A:515:LEU:HD13	1:A:634:LEU:HD21	1.95	0.47
1:B:82:ILE:HD13	1:B:84:MET:CE	2.44	0.47
1:C:197:SER:OG	1:C:199:ASN:HB3	2.14	0.47
1:C:269:ILE:HD11	1:C:301:ILE:HG22	1.94	0.47
1:C:489:LEU:HD21	1:C:516:PHE:CZ	2.50	0.47
1:C:515:LEU:C	1:C:515:LEU:HD23	2.40	0.47
1:C:729:PRO:O	1:C:730:GLU:OE2	2.32	0.47
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.80	0.47
1:A:378:LEU:HD22	1:A:378:LEU:O	2.15	0.47
1:B:131:PHE:O	1:B:136:LYS:HB2	2.15	0.47
1:B:503:PHE:HA	1:C:699:ILE:HD13	1.95	0.47
1:A:42:SER:HB2	1:A:44:PRO:HD2	1.96	0.47
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.44	0.47
1:B:193:ASP:O	1:B:195:GLU:N	2.48	0.47
1:B:290:PHE:CD2	1:B:331:LEU:HB3	2.50	0.47
1:B:437:ILE:CG2	1:B:438:ASP:N	2.76	0.47
1:C:410:ASP:OD2	1:C:463:ALA:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:LYS:NZ	1:B:461:PRO:HG2	2.29	0.47
1:B:265:PHE:CD2	1:B:296:ASN:HB2	2.49	0.47
1:B:431:ASP:OD1	1:B:433:GLU:HG3	2.14	0.47
1:C:665:PRO:C	1:C:731:ILE:HG22	2.39	0.47
1:A:43:GLN:N	1:A:44:PRO:CD	2.76	0.47
1:A:89:ARG:NH1	1:A:96:LEU:HD21	2.28	0.47
1:A:191:ARG:NH1	1:A:197:SER:HA	2.29	0.47
1:A:197:SER:OG	1:A:199:ASN:HB3	2.15	0.47
1:B:42:SER:HB2	1:B:44:PRO:HD2	1.96	0.47
1:B:109:LYS:O	1:B:110:TYR:C	2.58	0.47
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.44	0.47
1:B:197:SER:OG	1:B:199:ASN:HB3	2.15	0.47
1:B:206:ILE:CD1	1:B:213:LEU:CG	2.87	0.47
1:B:348:ASN:O	1:B:349:ARG:HB3	2.14	0.47
1:B:544:GLY:O	1:B:547:LEU:HB2	2.14	0.47
1:B:568:GLN:O	1:B:568:GLN:HG2	2.15	0.47
1:C:290:PHE:CD2	1:C:331:LEU:HB3	2.49	0.47
1:C:348:ASN:O	1:C:349:ARG:HB3	2.14	0.47
1:C:751:ASP:O	1:C:752:ILE:C	2.58	0.47
1:A:573:VAL:HG23	1:A:573:VAL:O	2.15	0.47
1:B:184:CYS:O	1:B:186:GLY:N	2.48	0.47
1:C:227:PRO:HA	1:C:340:HIS:HE1	1.78	0.47
1:C:423:ILE:C	1:C:425:LYS:N	2.73	0.47
1:C:556:GLU:OE1	1:C:556:GLU:N	2.46	0.47
1:C:600:VAL:O	1:C:604:ILE:HG13	2.14	0.47
1:C:647:LEU:HD12	1:C:647:LEU:N	2.30	0.47
1:A:206:ILE:CD1	1:A:213:LEU:CG	2.85	0.47
1:A:316:THR:HG23	1:A:316:THR:O	2.15	0.47
1:A:758:PHE:C	1:A:762:LEU:HD12	2.39	0.47
1:B:60:LYS:CE	1:B:103:GLN:HE21	2.28	0.47
1:C:89:ARG:HD3	1:C:96:LEU:HD22	1.96	0.47
1:C:489:LEU:HD21	1:C:516:PHE:HZ	1.79	0.47
1:A:441:VAL:O	1:A:444:SER:OG	2.27	0.47
1:A:544:GLY:O	1:A:547:LEU:HB2	2.13	0.47
1:B:126:ILE:HB	1:B:439:ALA:HB2	1.96	0.47
1:B:323:ARG:HH22	1:C:279:ALA:CB	2.25	0.47
1:C:42:SER:HB2	1:C:44:PRO:HD2	1.96	0.47
1:C:44:PRO:HG2	1:C:79:ASP:OD1	2.14	0.47
1:C:381:LEU:HD21	1:C:411:LEU:HD22	1.96	0.47
1:C:390:LEU:HD22	1:C:394:VAL:HG11	1.96	0.47
1:C:491:GLU:HA	1:C:495:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:GLY:O	1:C:547:LEU:HB2	2.14	0.47
1:A:390:LEU:HD22	1:A:394:VAL:HG11	1.96	0.46
1:A:556:GLU:OE1	1:A:556:GLU:N	2.44	0.46
1:A:703:ILE:O	1:A:707:ILE:HG12	2.15	0.46
1:B:139:PHE:O	1:B:140:LEU:C	2.58	0.46
1:B:427:MET:O	1:B:427:MET:HG2	2.15	0.46
1:B:487:ARG:HB3	1:B:487:ARG:CZ	2.45	0.46
1:B:682:PHE:CE1	1:B:690:ILE:HD11	2.50	0.46
1:C:134:TYR:HB3	1:C:154:VAL:HG11	1.97	0.46
1:A:82:ILE:HD13	1:A:84:MET:CE	2.45	0.46
1:A:388:MET:HE3	1:A:447:VAL:CG2	2.45	0.46
1:B:193:ASP:C	1:B:195:GLU:H	2.23	0.46
1:B:390:LEU:HD22	1:B:394:VAL:HG11	1.96	0.46
1:B:596:ALA:HB1	1:B:630:ASP:HA	1.98	0.46
1:B:610:GLY:O	1:B:611:MET:C	2.58	0.46
1:C:487:ARG:HB3	1:C:487:ARG:CZ	2.45	0.46
1:C:587:GLY:HA3	1:C:591:GLY:HA2	1.97	0.46
1:A:647:LEU:HD21	1:A:747:VAL:CB	2.44	0.46
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.97	0.46
1:C:193:ASP:C	1:C:195:GLU:H	2.24	0.46
1:C:519:PRO:HD2	1:C:645:ILE:O	2.15	0.46
1:C:629:ILE:O	1:C:631:PRO:HD3	2.15	0.46
1:A:634:LEU:HD22	1:A:642:LEU:HD11	1.98	0.46
1:A:755:TYR:N	1:A:755:TYR:CD1	2.81	0.46
1:B:567:ARG:NH2	1:B:611:MET:HG3	2.31	0.46
1:B:629:ILE:O	1:B:631:PRO:HD3	2.16	0.46
1:C:122:THR:O	1:C:161:VAL:HG22	2.16	0.46
1:C:135:LEU:H	1:C:135:LEU:CD2	2.28	0.46
1:C:633:ILE:HG22	1:C:639:LEU:HD12	1.96	0.46
1:A:227:PRO:HA	1:A:340:HIS:CE1	2.50	0.46
1:A:650:GLU:CG	1:A:677:LYS:HZ3	2.27	0.46
1:C:474:VAL:HG22	1:C:475:THR:N	2.31	0.46
1:C:515:LEU:HD13	1:C:634:LEU:HD21	1.97	0.46
1:A:229:LEU:O	1:A:233:ILE:HG22	2.16	0.46
1:A:526:LEU:HD21	2:A:900:ADP:H3'	1.97	0.46
1:B:112:LYS:H	1:B:170:PRO:HD3	1.81	0.46
1:B:203:TYR:O	1:B:206:ILE:HG12	2.16	0.46
1:B:227:PRO:HA	1:B:340:HIS:HE1	1.79	0.46
1:C:43:GLN:N	1:C:44:PRO:CD	2.77	0.46
1:C:706:GLU:O	1:C:707:ILE:O	2.33	0.46
1:A:313:ARG:NE	1:A:351:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MET:HG2	1:A:427:MET:O	2.16	0.46
1:A:611:MET:HE3	1:A:611:MET:HB3	1.80	0.46
1:B:177:ALA:C	1:B:179:ASP:N	2.73	0.46
1:B:441:VAL:O	1:B:444:SER:OG	2.27	0.46
1:B:647:LEU:HD12	1:B:647:LEU:N	2.30	0.46
1:C:63:LYS:HD2	1:C:93:ARG:CB	2.46	0.46
1:C:580:ASP:HB2	1:C:628:ILE:HD11	1.97	0.46
1:A:41:LEU:O	1:A:73:SER:HA	2.15	0.46
1:A:193:ASP:O	1:A:195:GLU:N	2.48	0.46
1:A:197:SER:C	1:A:199:ASN:H	2.24	0.46
1:A:432:LEU:CD1	1:A:441:VAL:HG11	2.44	0.46
1:A:482:LEU:HB3	1:A:485:VAL:CG2	2.46	0.46
1:A:580:ASP:O	1:A:581:SER:C	2.58	0.46
1:B:46:MET:HE3	1:B:71:VAL:HG22	1.97	0.46
1:B:317:HIS:CE1	1:C:317:HIS:NE2	2.83	0.46
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.98	0.46
1:C:327:GLN:O	1:C:331:LEU:HG	2.15	0.46
1:C:437:ILE:CG2	1:C:438:ASP:N	2.78	0.46
1:A:93:ARG:HH21	1:A:194:GLU:HG2	1.81	0.46
1:A:206:ILE:HD12	1:A:213:LEU:HD21	1.97	0.46
1:B:491:GLU:HA	1:B:495:TYR:CD2	2.51	0.46
1:B:592:ASP:OD1	1:B:592:ASP:N	2.49	0.46
1:C:378:LEU:HD22	1:C:378:LEU:O	2.15	0.46
1:C:515:LEU:HA	1:C:621:GLY:O	2.15	0.46
1:A:610:GLY:O	1:A:611:MET:C	2.59	0.46
1:C:388:MET:HE3	1:C:447:VAL:CG2	2.45	0.46
1:C:398:GLN:CG	1:C:449:MET:HE1	2.45	0.46
1:C:410:ASP:OD2	1:C:463:ALA:HB1	2.16	0.46
1:A:470:GLU:O	1:A:538:ASN:HA	2.16	0.45
1:A:485:VAL:HG23	1:A:486:LYS:N	2.31	0.45
1:A:524:LYS:HB2	2:A:900:ADP:O1B	2.16	0.45
1:B:378:LEU:O	1:B:378:LEU:HD22	2.16	0.45
1:B:519:PRO:HD2	1:B:645:ILE:O	2.16	0.45
1:C:123:VAL:O	1:C:124:GLU:C	2.57	0.45
1:C:577:ASP:O	1:C:579:LEU:N	2.49	0.45
1:C:611:MET:HE3	1:C:611:MET:HB3	1.80	0.45
1:C:680:ASN:C	1:C:682:PHE:H	2.24	0.45
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.97	0.45
1:A:491:GLU:HA	1:A:495:TYR:CD2	2.51	0.45
1:A:585:ALA:O	1:A:587:GLY:N	2.49	0.45
1:A:629:ILE:O	1:A:631:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:THR:O	1:B:316:THR:HG23	2.15	0.45
1:B:327:GLN:O	1:B:331:LEU:HG	2.16	0.45
1:B:751:ASP:O	1:B:752:ILE:C	2.59	0.45
1:C:139:PHE:CD1	1:C:176:VAL:HG11	2.51	0.45
1:C:313:ARG:HG3	1:C:313:ARG:NH2	2.31	0.45
1:C:482:LEU:HB3	1:C:485:VAL:CG2	2.46	0.45
1:C:485:VAL:HG23	1:C:486:LYS:N	2.31	0.45
1:C:524:LYS:HB2	2:C:900:ADP:O1B	2.16	0.45
1:A:193:ASP:C	1:A:195:GLU:H	2.25	0.45
1:A:320:VAL:O	1:A:321:GLU:C	2.58	0.45
1:A:377:ARG:O	1:A:381:LEU:HG	2.16	0.45
1:B:126:ILE:HG21	1:B:159:ARG:HD2	1.99	0.45
1:B:322:ARG:HD3	1:C:321:GLU:CD	2.41	0.45
1:C:82:ILE:HD13	1:C:84:MET:CE	2.46	0.45
1:C:89:ARG:NH1	1:C:96:LEU:HD21	2.31	0.45
1:C:640:ASP:O	1:C:642:LEU:CD2	2.65	0.45
1:A:169:ASP:CB	1:A:170:PRO:HD3	2.29	0.45
1:A:38:VAL:HG21	1:A:72:LEU:HD12	1.99	0.45
1:A:46:MET:HE3	1:A:71:VAL:HG22	1.98	0.45
1:A:139:PHE:O	1:A:140:LEU:C	2.60	0.45
1:B:206:ILE:HD12	1:B:213:LEU:HD21	1.97	0.45
1:C:312:LYS:HB3	1:C:354:ASP:CB	2.46	0.45
1:C:564:ASP:C	1:C:566:ALA:N	2.74	0.45
1:A:184:CYS:O	1:A:186:GLY:N	2.49	0.45
1:A:327:GLN:O	1:A:331:LEU:HG	2.17	0.45
1:A:472:PRO:HB2	1:A:533:ASN:HB2	1.98	0.45
1:B:230:PHE:HA	1:B:233:ILE:CG2	2.43	0.45
1:B:354:ASP:OD2	1:B:356:ALA:HB3	2.17	0.45
1:B:377:ARG:O	1:B:381:LEU:HG	2.16	0.45
1:C:610:GLY:O	1:C:611:MET:C	2.58	0.45
1:A:312:LYS:HB3	1:A:354:ASP:CG	2.42	0.45
1:A:328:LEU:O	1:A:331:LEU:N	2.45	0.45
1:A:463:ALA:O	1:A:464:LEU:C	2.59	0.45
1:A:680:ASN:C	1:A:682:PHE:H	2.24	0.45
1:B:123:VAL:O	1:B:124:GLU:C	2.60	0.45
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.17	0.45
1:B:640:ASP:O	1:B:642:LEU:CD2	2.65	0.45
1:C:114:ILE:HD13	1:C:146:ILE:HD11	1.98	0.45
1:C:177:ALA:C	1:C:179:ASP:N	2.75	0.45
1:C:377:ARG:O	1:C:381:LEU:HG	2.16	0.45
1:A:139:PHE:CG	1:A:176:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:C	1:A:179:ASP:N	2.75	0.45
1:A:270:ASN:OD1	1:A:272:PRO:HD2	2.17	0.45
1:B:482:LEU:HB3	1:B:485:VAL:CG2	2.47	0.45
1:B:485:VAL:HG23	1:B:486:LYS:N	2.30	0.45
1:B:586:ARG:NH1	1:B:598:ASP:HB3	2.32	0.45
1:B:682:PHE:CZ	1:B:744:ARG:O	2.70	0.45
1:C:41:LEU:O	1:C:73:SER:HA	2.16	0.45
1:B:680:ASN:C	1:B:682:PHE:H	2.23	0.45
1:C:354:ASP:OD2	1:C:356:ALA:HB3	2.17	0.45
1:A:227:PRO:HA	1:A:340:HIS:HE1	1.80	0.45
1:A:258:VAL:O	1:A:262:THR:HG23	2.16	0.45
1:A:322:ARG:HD3	1:B:321:GLU:OE2	2.17	0.45
1:A:731:ILE:O	1:A:731:ILE:CG2	2.64	0.45
1:B:515:LEU:C	1:B:515:LEU:HD23	2.42	0.45
1:C:496:PRO:HA	1:C:503:PHE:CE2	2.52	0.45
1:A:275:MET:CG	1:A:309:ILE:HG12	2.47	0.44
1:A:306:LEU:HD22	1:A:345:ALA:HB1	1.97	0.44
1:A:398:GLN:CG	1:A:449:MET:HE1	2.45	0.44
1:B:172:PRO:HG2	1:B:173:TYR:CD2	2.52	0.44
1:B:459:SER:C	1:B:461:PRO:HD2	2.42	0.44
1:C:184:CYS:C	1:C:186:GLY:N	2.75	0.44
1:A:519:PRO:HD2	1:A:645:ILE:O	2.18	0.44
1:B:425:LYS:O	1:B:429:LEU:HB2	2.17	0.44
1:B:474:VAL:HG22	1:B:475:THR:N	2.31	0.44
1:B:758:PHE:O	1:B:762:LEU:HG	2.16	0.44
1:C:203:TYR:CE2	1:C:217:LYS:HE2	2.52	0.44
1:C:539:PHE:HD1	1:C:573:VAL:HG23	1.82	0.44
1:C:608:MET:HG3	1:C:619:ILE:HD13	1.96	0.44
1:A:91:ASN:N	1:A:91:ASN:ND2	2.65	0.44
1:A:112:LYS:HB2	1:A:169:ASP:HB3	1.99	0.44
1:A:640:ASP:O	1:A:642:LEU:CD2	2.65	0.44
1:B:423:ILE:C	1:B:425:LYS:N	2.74	0.44
1:B:732:ARG:O	1:B:735:HIS:HB2	2.17	0.44
1:A:172:PRO:HG2	1:A:173:TYR:CD2	2.52	0.44
1:A:423:ILE:C	1:A:425:LYS:N	2.74	0.44
1:A:653:ARG:O	1:A:657:LEU:HG	2.17	0.44
1:B:518:GLY:HA2	1:B:755:TYR:CD2	2.52	0.44
1:B:634:LEU:HD22	1:B:642:LEU:HD11	1.99	0.44
1:C:63:LYS:HD2	1:C:93:ARG:CG	2.47	0.44
1:C:153:LEU:HD12	1:C:161:VAL:O	2.17	0.44
1:C:270:ASN:OD1	1:C:272:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:ASP:OD1	1:C:365:ARG:HG2	2.17	0.44
1:C:427:MET:SD	1:C:441:VAL:HG11	2.57	0.44
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.84	0.44
1:C:648:PRO:HD2	1:C:683:SER:HA	2.00	0.44
1:A:98:ASP:CG	1:A:225:ARG:HH22	2.25	0.44
1:A:395:ASP:CG	1:A:398:GLN:HB2	2.43	0.44
1:A:425:LYS:O	1:A:429:LEU:HB2	2.18	0.44
1:A:707:ILE:HD13	1:A:707:ILE:N	2.31	0.44
1:B:35:ASP:O	1:B:85:ASN:ND2	2.50	0.44
1:B:135:LEU:H	1:B:135:LEU:CD2	2.30	0.44
1:C:540:ILE:HD12	1:C:572:CYS:SG	2.58	0.44
1:A:112:LYS:HB2	1:A:169:ASP:CG	2.43	0.44
1:A:231:LYS:O	1:A:231:LYS:HG2	2.18	0.44
1:A:275:MET:SD	1:A:324:ILE:HD13	2.58	0.44
1:A:614:LYS:CE	1:B:402:GLU:OE1	2.64	0.44
1:A:682:PHE:HE1	1:A:690:ILE:HD11	1.82	0.44
1:A:751:ASP:O	1:A:752:ILE:C	2.60	0.44
1:B:91:ASN:N	1:B:91:ASN:ND2	2.66	0.44
1:B:271:GLY:HA2	1:B:309:ILE:HD11	1.98	0.44
1:B:545:PRO:HD3	1:B:578:GLU:OE1	2.17	0.44
1:C:197:SER:C	1:C:199:ASN:H	2.26	0.44
1:C:313:ARG:CG	1:C:314:GLU:N	2.77	0.44
1:C:397:GLU:O	1:C:398:GLN:C	2.60	0.44
1:C:425:LYS:O	1:C:429:LEU:HB2	2.17	0.44
1:C:448:THR:C	1:C:450:ASP:N	2.74	0.44
1:C:684:GLY:HA3	2:C:900:ADP:C8	2.53	0.44
1:A:82:ILE:HG23	1:A:82:ILE:O	2.18	0.44
1:A:96:LEU:N	1:A:96:LEU:CD2	2.79	0.44
1:A:354:ASP:OD2	1:A:356:ALA:HB3	2.18	0.44
1:A:514:VAL:CG1	1:A:515:LEU:N	2.80	0.44
1:B:65:ARG:HH11	1:B:93:ARG:CZ	2.31	0.44
1:B:605:LEU:HD21	1:B:633:ILE:HG12	2.00	0.44
1:C:311:PRO:O	1:C:312:LYS:C	2.61	0.44
1:C:520:PRO:HG3	1:C:624:ASN:HB2	2.00	0.44
1:C:634:LEU:HD22	1:C:642:LEU:HD11	1.99	0.44
1:C:758:PHE:HB3	1:C:762:LEU:HD12	2.00	0.44
1:A:132:GLU:OE2	1:A:136:LYS:HD3	2.18	0.44
1:B:398:GLN:CG	1:B:449:MET:HE1	2.46	0.44
1:C:84:MET:O	1:C:84:MET:HG3	2.18	0.44
1:C:682:PHE:HE1	1:C:690:ILE:HD11	1.83	0.44
1:B:197:SER:C	1:B:199:ASN:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HB3	1:B:354:ASP:HB2	2.00	0.44
1:B:358:ARG:HG3	1:B:358:ARG:NH1	2.28	0.44
1:B:397:GLU:O	1:B:398:GLN:C	2.60	0.44
1:B:405:GLY:CA	1:B:465:ARG:HD3	2.41	0.44
1:B:496:PRO:HA	1:B:503:PHE:CE2	2.53	0.44
1:C:65:ARG:NH1	1:C:93:ARG:HH22	2.16	0.44
1:A:397:GLU:O	1:A:398:GLN:C	2.60	0.43
1:A:648:PRO:HD2	1:A:683:SER:HA	1.98	0.43
1:C:230:PHE:HA	1:C:233:ILE:CG2	2.44	0.43
1:C:455:ALA:O	1:C:460:ASN:OD1	2.36	0.43
1:C:514:VAL:CG1	1:C:515:LEU:N	2.78	0.43
1:C:515:LEU:HD21	1:C:623:THR:HG22	2.00	0.43
1:A:282:SER:C	1:A:284:SER:N	2.76	0.43
1:A:405:GLY:HA3	1:A:465:ARG:HD3	2.00	0.43
1:A:448:THR:C	1:A:450:ASP:N	2.74	0.43
1:A:515:LEU:HD21	1:A:623:THR:CG2	2.48	0.43
1:B:89:ARG:HG3	1:B:94:VAL:HG23	2.00	0.43
1:B:540:ILE:CG2	1:B:574:LEU:HD12	2.48	0.43
1:C:89:ARG:HG3	1:C:94:VAL:HG23	1.98	0.43
1:C:647:LEU:HD21	1:C:747:VAL:CB	2.48	0.43
1:C:683:SER:O	1:C:684:GLY:C	2.62	0.43
1:A:26:LEU:HD21	1:A:45:LYS:HE2	2.00	0.43
1:B:60:LYS:CE	1:B:103:GLN:NE2	2.81	0.43
1:B:448:THR:C	1:B:450:ASP:N	2.75	0.43
1:B:519:PRO:HG3	1:B:647:LEU:CD1	2.49	0.43
1:C:89:ARG:NH2	1:C:96:LEU:HD11	2.34	0.43
1:C:96:LEU:N	1:C:96:LEU:CD2	2.81	0.43
1:A:45:LYS:HD2	1:A:45:LYS:HA	1.80	0.43
1:A:432:LEU:O	1:A:437:ILE:HD13	2.18	0.43
1:A:496:PRO:HA	1:A:503:PHE:CE2	2.52	0.43
1:A:540:ILE:HG22	1:A:574:LEU:HD12	1.99	0.43
1:B:132:GLU:OE2	1:B:136:LYS:HD3	2.18	0.43
1:B:233:ILE:HG13	1:B:235:VAL:HG23	2.00	0.43
1:B:282:SER:C	1:B:284:SER:N	2.76	0.43
1:B:364:ASP:OD1	1:B:365:ARG:HG2	2.19	0.43
1:B:540:ILE:HG22	1:B:574:LEU:HD12	2.01	0.43
1:A:102:ILE:CG1	1:A:103:GLN:H	2.31	0.43
1:A:615:LYS:NZ	1:B:461:PRO:CG	2.82	0.43
1:B:318:GLY:O	1:B:322:ARG:HG3	2.19	0.43
1:C:193:ASP:O	1:C:195:GLU:N	2.50	0.43
1:C:358:ARG:HG3	1:C:358:ARG:NH1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TYR:CE1	1:A:178:PRO:CD	2.93	0.43
1:A:633:ILE:O	1:A:639:LEU:HB2	2.18	0.43
1:B:89:ARG:NH2	1:B:96:LEU:HD11	2.34	0.43
1:B:229:LEU:O	1:B:229:LEU:HD12	2.19	0.43
1:B:252:THR:HB	2:B:807:ADP:O1A	2.18	0.43
1:A:84:MET:O	1:A:84:MET:HG3	2.19	0.43
1:B:63:LYS:HD2	1:B:93:ARG:CB	2.48	0.43
1:B:139:PHE:CG	1:B:176:VAL:HG11	2.53	0.43
1:B:275:MET:SD	1:B:324:ILE:HD13	2.59	0.43
1:B:358:ARG:O	1:B:359:ARG:C	2.62	0.43
1:B:460:ASN:C	1:B:462:SER:H	2.26	0.43
1:C:258:VAL:O	1:C:262:THR:HG23	2.18	0.43
1:C:285:ASN:N	1:C:285:ASN:HD22	2.16	0.43
1:A:28:VAL:HG23	1:A:84:MET:CG	2.49	0.43
1:A:539:PHE:HD1	1:A:573:VAL:CG2	2.32	0.43
1:B:82:ILE:HG23	1:B:82:ILE:O	2.18	0.43
1:B:272:PRO:O	1:B:276:SER:HB3	2.19	0.43
1:B:405:GLY:O	1:B:463:ALA:HB3	2.19	0.43
1:B:455:ALA:O	1:B:460:ASN:OD1	2.37	0.43
1:B:519:PRO:HA	1:B:520:PRO:HD3	1.78	0.43
1:B:648:PRO:HD2	1:B:683:SER:HA	2.00	0.43
1:B:653:ARG:O	1:B:657:LEU:HG	2.19	0.43
1:C:93:ARG:HH21	1:C:194:GLU:HG2	1.83	0.43
1:C:191:ARG:NH1	1:C:197:SER:HA	2.34	0.43
1:C:272:PRO:O	1:C:276:SER:HB3	2.19	0.43
1:A:65:ARG:HH12	1:A:93:ARG:HH22	1.66	0.43
1:A:89:ARG:NH2	1:A:96:LEU:HD11	2.34	0.43
1:B:120:ASP:OD2	1:B:190:LYS:HA	2.19	0.43
1:B:505:LYS:NZ	1:C:729:PRO:HG3	2.31	0.43
1:C:82:ILE:HG23	1:C:82:ILE:O	2.18	0.43
1:C:172:PRO:HG2	1:C:173:TYR:CD2	2.54	0.43
1:C:459:SER:C	1:C:461:PRO:HD2	2.43	0.43
1:C:585:ALA:C	1:C:587:GLY:H	2.26	0.43
1:A:65:ARG:HH11	1:A:93:ARG:CZ	2.31	0.43
1:A:474:VAL:HG23	1:A:478:ASP:CG	2.44	0.43
1:B:96:LEU:N	1:B:96:LEU:CD2	2.81	0.43
1:B:191:ARG:NH1	1:B:197:SER:HA	2.33	0.43
1:B:231:LYS:O	1:B:231:LYS:HG2	2.19	0.43
1:B:258:VAL:O	1:B:262:THR:HG23	2.18	0.43
1:B:395:ASP:CG	1:B:398:GLN:HB2	2.43	0.43
1:B:683:SER:O	1:B:684:GLY:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:NH1	1:C:93:ARG:NH2	2.66	0.43
1:C:427:MET:O	1:C:427:MET:HG2	2.19	0.43
1:C:650:GLU:CG	1:C:677:LYS:HZ3	2.32	0.43
1:C:653:ARG:O	1:C:657:LEU:HG	2.19	0.43
1:A:114:ILE:HD13	1:A:146:ILE:HD11	2.00	0.42
1:A:364:ASP:OD1	1:A:365:ARG:HG2	2.19	0.42
1:A:648:PRO:CD	1:A:683:SER:HA	2.49	0.42
1:B:514:VAL:CG1	1:B:515:LEU:N	2.77	0.42
1:C:231:LYS:O	1:C:231:LYS:HG2	2.18	0.42
1:C:395:ASP:CG	1:C:398:GLN:HB2	2.44	0.42
1:C:455:ALA:O	1:C:456:LEU:C	2.62	0.42
1:C:659:ALA:HA	1:C:662:ARG:CD	2.49	0.42
1:A:358:ARG:HG3	1:A:358:ARG:NH1	2.29	0.42
1:A:407:VAL:HG23	1:A:408:GLY:N	2.34	0.42
1:A:460:ASN:OD1	1:A:461:PRO:CD	2.65	0.42
1:A:577:ASP:O	1:A:578:GLU:C	2.62	0.42
1:A:759:ALA:HA	1:A:762:LEU:HB2	2.02	0.42
1:B:611:MET:HE3	1:B:611:MET:HB3	1.78	0.42
1:B:759:ALA:HA	1:B:762:LEU:HB2	2.01	0.42
1:C:120:ASP:OD2	1:C:190:LYS:HA	2.19	0.42
1:A:580:ASP:O	1:A:583:ALA:N	2.52	0.42
1:B:433:GLU:O	1:B:434:ASP:OD1	2.37	0.42
1:A:384:HIS:HE1	2:A:807:ADP:N3	2.17	0.42
1:A:515:LEU:HD23	1:A:515:LEU:C	2.43	0.42
1:A:519:PRO:HG3	1:A:647:LEU:HD12	2.00	0.42
1:A:732:ARG:CD	1:A:734:ASP:OD1	2.67	0.42
1:B:437:ILE:HG22	1:B:438:ASP:O	2.20	0.42
1:B:556:GLU:OE1	1:B:556:GLU:N	2.47	0.42
1:B:729:PRO:O	1:B:730:GLU:CD	2.63	0.42
1:C:102:ILE:CG1	1:C:103:GLN:N	2.83	0.42
1:C:575:PHE:CE2	1:C:577:ASP:HB2	2.53	0.42
1:A:233:ILE:HG13	1:A:235:VAL:HG23	2.00	0.42
1:B:26:LEU:CD1	1:B:41:LEU:HD21	2.49	0.42
1:C:169:ASP:CB	1:C:170:PRO:HD3	2.30	0.42
1:C:233:ILE:HG13	1:C:235:VAL:HG23	2.01	0.42
1:C:290:PHE:HE2	1:C:331:LEU:O	2.02	0.42
1:C:694:ALA:O	1:C:697:LEU:HB2	2.19	0.42
1:A:664:SER:HA	1:A:665:PRO:HD3	1.87	0.42
1:B:433:GLU:O	1:B:434:ASP:CG	2.63	0.42
1:B:624:ASN:ND2	1:B:624:ASN:N	2.66	0.42
1:C:129:ASN:OD1	1:C:129:ASN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:PRO:HA	1:C:520:PRO:HD3	1.79	0.42
1:A:228:ALA:O	1:A:229:LEU:C	2.62	0.42
1:A:416:SER:O	1:A:420:LEU:HG	2.19	0.42
1:A:659:ALA:HA	1:A:662:ARG:CD	2.49	0.42
1:B:515:LEU:CD1	1:B:634:LEU:HD21	2.50	0.42
1:C:21:ASN:O	1:C:22:ARG:HB2	2.20	0.42
1:C:112:LYS:HB2	1:C:169:ASP:CG	2.45	0.42
1:C:319:GLU:O	1:C:320:VAL:C	2.62	0.42
1:C:695:CYS:C	1:C:697:LEU:H	2.27	0.42
1:A:431:ASP:O	1:A:432:LEU:HD23	2.19	0.42
1:A:455:ALA:O	1:A:460:ASN:OD1	2.38	0.42
1:B:309:ILE:C	1:B:311:PRO:HD3	2.44	0.42
1:C:328:LEU:O	1:C:331:LEU:N	2.44	0.42
1:C:515:LEU:CD1	1:C:634:LEU:HD21	2.50	0.42
1:C:520:PRO:HG3	1:C:624:ASN:CB	2.50	0.42
1:C:605:LEU:HD21	1:C:633:ILE:HG12	2.02	0.42
1:C:648:PRO:CD	1:C:683:SER:HA	2.50	0.42
1:C:664:SER:HA	1:C:665:PRO:HD3	1.88	0.42
1:A:285:ASN:N	1:A:285:ASN:HD22	2.18	0.42
1:A:461:PRO:O	1:A:463:ALA:N	2.51	0.42
1:A:515:LEU:CD1	1:A:634:LEU:HD21	2.50	0.42
1:C:282:SER:C	1:C:284:SER:N	2.76	0.42
1:C:642:LEU:HD13	1:C:642:LEU:HA	1.88	0.42
1:A:21:ASN:O	1:A:22:ARG:HB2	2.19	0.41
1:A:65:ARG:NH1	1:A:93:ARG:CZ	2.83	0.41
1:A:179:ASP:O	1:A:180:THR:C	2.63	0.41
1:A:269:ILE:HD11	1:A:301:ILE:HG22	2.00	0.41
1:A:292:GLU:O	1:A:292:GLU:HG2	2.20	0.41
1:A:695:CYS:C	1:A:697:LEU:H	2.27	0.41
1:B:232:ALA:CB	1:C:125:GLY:C	2.93	0.41
1:B:479:ILE:HD13	1:B:527:LEU:HD23	2.02	0.41
1:B:731:ILE:O	1:B:731:ILE:HG23	2.20	0.41
1:C:466:GLU:HG2	1:C:467:THR:N	2.32	0.41
1:C:497:VAL:HG13	1:C:498:GLU:HG3	2.02	0.41
1:A:134:TYR:HB3	1:A:154:VAL:HG11	2.01	0.41
1:A:338:ARG:C	1:A:339:ALA:O	2.62	0.41
1:A:427:MET:HE1	1:A:437:ILE:HG21	2.03	0.41
1:B:461:PRO:O	1:B:463:ALA:N	2.46	0.41
1:B:520:PRO:HG3	1:B:624:ASN:HB2	2.03	0.41
1:B:695:CYS:C	1:B:697:LEU:H	2.27	0.41
1:C:416:SER:O	1:C:420:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:O	1:A:273:GLU:HB3	2.21	0.41
1:A:410:ASP:OD2	1:A:463:ALA:HB1	2.20	0.41
1:A:605:LEU:HD21	1:A:633:ILE:HG12	2.01	0.41
1:B:45:LYS:HA	1:B:45:LYS:HD2	1.82	0.41
1:B:585:ALA:C	1:B:587:GLY:H	2.27	0.41
1:B:694:ALA:O	1:B:697:LEU:HB2	2.20	0.41
1:C:460:ASN:N	1:C:461:PRO:CD	2.80	0.41
1:A:421:GLN:C	1:A:423:ILE:H	2.28	0.41
1:A:427:MET:SD	1:A:441:VAL:HG11	2.61	0.41
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.02	0.41
1:B:383:ILE:O	1:B:386:LYS:HE3	2.20	0.41
1:B:427:MET:SD	1:B:441:VAL:HG11	2.61	0.41
1:B:466:GLU:CG	1:B:467:THR:H	2.12	0.41
1:B:642:LEU:HD13	1:B:642:LEU:HA	1.88	0.41
1:C:441:VAL:O	1:C:444:SER:OG	2.28	0.41
1:C:460:ASN:C	1:C:462:SER:N	2.76	0.41
1:C:590:ILE:H	1:C:590:ILE:HG12	1.66	0.41
1:C:701:GLU:C	1:C:703:ILE:N	2.79	0.41
1:A:272:PRO:O	1:A:276:SER:HB3	2.20	0.41
1:B:63:LYS:HD2	1:B:93:ARG:HD2	2.01	0.41
1:B:532:ALA:HB2	1:B:573:VAL:HG21	2.02	0.41
1:B:648:PRO:CD	1:B:683:SER:HA	2.50	0.41
1:C:407:VAL:HG23	1:C:408:GLY:N	2.35	0.41
1:C:421:GLN:C	1:C:423:ILE:H	2.28	0.41
1:C:430:ILE:HD13	1:C:430:ILE:HA	1.92	0.41
1:A:585:ALA:C	1:A:587:GLY:N	2.77	0.41
1:B:112:LYS:HB2	1:B:169:ASP:CG	2.46	0.41
1:B:147:ARG:CG	1:B:148:LYS:N	2.84	0.41
1:B:228:ALA:O	1:B:229:LEU:C	2.64	0.41
1:B:659:ALA:HA	1:B:662:ARG:CD	2.50	0.41
1:C:210:ARG:O	1:C:211:LYS:C	2.63	0.41
1:C:458:GLN:HG3	1:C:459:SER:N	2.36	0.41
1:C:474:VAL:HG23	1:C:478:ASP:CG	2.46	0.41
1:C:624:ASN:ND2	1:C:624:ASN:N	2.66	0.41
1:C:660:ASN:ND2	1:C:688:THR:OG1	2.54	0.41
1:A:135:LEU:H	1:A:135:LEU:CD2	2.33	0.41
1:A:230:PHE:HA	1:A:233:ILE:CG2	2.46	0.41
1:A:455:ALA:O	1:A:456:LEU:C	2.63	0.41
1:B:470:GLU:O	1:B:538:ASN:HA	2.20	0.41
1:B:633:ILE:O	1:B:639:LEU:HB2	2.21	0.41
1:B:667:ALA:HB3	1:B:670:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:VAL:HG22	1:C:173:TYR:CE1	2.55	0.41
1:C:514:VAL:CG1	1:C:515:LEU:H	2.33	0.41
1:C:705:SER:O	1:C:706:GLU:C	2.63	0.41
1:A:221:GLU:HG3	1:A:222:LEU:HD23	2.02	0.41
1:A:519:PRO:HA	1:A:520:PRO:HD3	1.77	0.41
1:B:133:VAL:HG13	1:B:443:ASN:HB2	2.03	0.41
1:B:179:ASP:O	1:B:180:THR:C	2.61	0.41
1:B:338:ARG:O	1:B:339:ALA:C	2.64	0.41
1:B:460:ASN:OD1	1:B:461:PRO:HD3	2.21	0.41
1:C:338:ARG:O	1:C:339:ALA:C	2.63	0.41
1:A:112:LYS:H	1:A:170:PRO:CD	2.34	0.41
1:A:351:ASN:OD1	1:A:351:ASN:N	2.54	0.41
1:A:391:ALA:HB3	1:A:394:VAL:HG23	2.02	0.41
1:A:410:ASP:OD2	1:A:463:ALA:CB	2.69	0.41
1:A:539:PHE:HD1	1:A:573:VAL:HG23	1.85	0.41
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.56	0.41
1:A:660:ASN:ND2	1:A:688:THR:OG1	2.53	0.41
1:A:694:ALA:O	1:A:697:LEU:HB2	2.21	0.41
1:A:751:ASP:O	1:A:754:LYS:HB2	2.20	0.41
1:B:93:ARG:HH21	1:B:194:GLU:HG2	1.86	0.41
1:B:112:LYS:HB2	1:B:169:ASP:HB3	2.01	0.41
1:B:270:ASN:O	1:B:273:GLU:HB3	2.21	0.41
1:B:338:ARG:C	1:B:339:ALA:O	2.62	0.41
1:B:407:VAL:HG23	1:B:408:GLY:N	2.35	0.41
1:B:421:GLN:C	1:B:423:ILE:H	2.29	0.41
1:B:682:PHE:HE1	1:B:690:ILE:HD11	1.85	0.41
1:C:59:LEU:C	1:C:60:LYS:HG3	2.45	0.41
1:C:129:ASN:HD21	1:C:132:GLU:HB2	1.82	0.41
1:C:275:MET:SD	1:C:324:ILE:HD13	2.60	0.41
1:C:292:GLU:O	1:C:292:GLU:HG2	2.21	0.41
1:C:354:ASP:HA	1:C:355:PRO:HD3	1.92	0.41
1:C:645:ILE:HD12	1:C:645:ILE:N	2.36	0.41
1:A:452:PHE:O	1:A:453:ARG:C	2.64	0.41
1:B:108:VAL:HG22	1:B:173:TYR:CE1	2.56	0.41
1:B:285:ASN:N	1:B:285:ASN:HD22	2.17	0.41
1:B:514:VAL:CG1	1:B:515:LEU:H	2.33	0.41
1:B:682:PHE:CE2	1:B:745:ARG:HG2	2.56	0.41
1:C:39:VAL:HG12	1:C:84:MET:HB3	2.03	0.41
1:C:229:LEU:O	1:C:229:LEU:HD12	2.21	0.41
1:C:358:ARG:O	1:C:359:ARG:C	2.63	0.41
1:C:432:LEU:HD12	1:C:441:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:ASP:C	1:C:632:ALA:H	2.29	0.41
1:A:303:ILE:H	1:A:303:ILE:HG13	1.66	0.40
1:A:313:ARG:CG	1:A:314:GLU:H	2.20	0.40
1:A:474:VAL:HG22	1:A:475:THR:N	2.34	0.40
1:B:305:GLU:O	1:B:306:LEU:C	2.63	0.40
1:B:432:LEU:O	1:B:437:ILE:HD11	2.20	0.40
1:B:542:ILE:HG12	1:B:562:ILE:HD13	2.03	0.40
1:C:35:ASP:O	1:C:85:ASN:ND2	2.54	0.40
1:C:262:THR:C	1:C:264:ALA:H	2.29	0.40
1:C:270:ASN:O	1:C:273:GLU:HB3	2.21	0.40
1:C:653:ARG:HD2	1:C:679:THR:OG1	2.21	0.40
1:A:26:LEU:CD1	1:A:41:LEU:HD21	2.52	0.40
1:A:102:ILE:CG1	1:A:103:GLN:N	2.82	0.40
1:A:319:GLU:O	1:A:320:VAL:C	2.62	0.40
1:B:118:PRO:HB2	1:B:123:VAL:HG11	2.02	0.40
1:B:497:VAL:HG13	1:B:498:GLU:HG3	2.03	0.40
1:B:573:VAL:HA	1:B:618:PHE:O	2.21	0.40
1:C:102:ILE:CG1	1:C:103:GLN:H	2.33	0.40
1:C:147:ARG:CG	1:C:148:LYS:N	2.84	0.40
1:C:694:ALA:HB1	1:C:731:ILE:HD11	2.03	0.40
1:C:703:ILE:O	1:C:707:ILE:HG12	2.22	0.40
1:A:95:ARG:HG3	1:A:225:ARG:HH12	1.86	0.40
1:A:122:THR:O	1:A:161:VAL:HG22	2.22	0.40
1:A:334:GLY:O	1:A:336:LYS:N	2.55	0.40
1:A:437:ILE:HG22	1:A:438:ASP:O	2.21	0.40
1:B:38:VAL:HG21	1:B:72:LEU:HD12	2.03	0.40
1:B:290:PHE:HE2	1:B:331:LEU:O	2.05	0.40
1:B:749:ASP:CA	1:B:752:ILE:HD12	2.42	0.40
1:C:26:LEU:HD13	1:C:41:LEU:HD21	2.02	0.40
1:C:206:ILE:CG2	1:C:253:LEU:CD2	3.00	0.40
1:C:397:GLU:O	1:C:401:ASN:ND2	2.54	0.40
1:C:475:THR:HG22	1:C:533:ASN:HD21	1.87	0.40
1:C:514:VAL:HG13	1:C:641:GLN:HB2	2.04	0.40
1:A:147:ARG:CG	1:A:148:LYS:N	2.84	0.40
1:A:497:VAL:HG13	1:A:498:GLU:HG3	2.03	0.40
1:A:506:PHE:CE1	1:B:698:ALA:HB1	2.57	0.40
1:A:568:GLN:O	1:A:568:GLN:HG2	2.21	0.40
1:A:642:LEU:HD13	1:A:642:LEU:HA	1.89	0.40
1:A:653:ARG:HD2	1:A:679:THR:OG1	2.21	0.40
1:B:206:ILE:HD12	1:B:213:LEU:CD2	2.52	0.40
1:B:660:ASN:ND2	1:B:688:THR:OG1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ALA:HB3	1:C:394:VAL:HG23	2.02	0.40
1:C:542:ILE:HG12	1:C:562:ILE:HD13	2.02	0.40
1:A:358:ARG:O	1:A:359:ARG:C	2.63	0.40
1:A:632:ALA:HA	1:A:635:ARG:HG3	2.04	0.40
1:B:22:ARG:C	1:B:24:ASN:H	2.30	0.40
1:C:179:ASP:O	1:C:180:THR:C	2.65	0.40
1:C:228:ALA:O	1:C:229:LEU:C	2.64	0.40
1:C:514:VAL:HG23	1:C:618:PHE:CE2	2.57	0.40
1:C:678:MET:HE2	1:C:678:MET:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/806 (89%)	566 (79%)	119 (17%)	34 (5%)	2	17
1	B	719/806 (89%)	564 (78%)	123 (17%)	32 (4%)	2	17
1	C	719/806 (89%)	561 (78%)	122 (17%)	36 (5%)	1	16
All	All	2157/2418 (89%)	1691 (78%)	364 (17%)	102 (5%)	2	17

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	85	ASN
1	A	140	LEU
1	A	185	GLU
1	A	312	LYS
1	A	426	LYS
1	B	85	ASN
1	B	140	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	185	GLU
1	B	194	GLU
1	B	312	LYS
1	B	426	LYS
1	C	140	LEU
1	C	185	GLU
1	C	304	ASP
1	C	312	LYS
1	C	426	LYS
1	C	462	SER
1	A	62	LYS
1	A	178	PRO
1	A	194	GLU
1	A	221	GLU
1	A	336	LYS
1	A	360	PHE
1	A	431	ASP
1	A	464	LEU
1	A	586	ARG
1	B	62	LYS
1	B	178	PRO
1	B	221	GLU
1	B	336	LYS
1	B	360	PHE
1	B	431	ASP
1	C	62	LYS
1	C	85	ASN
1	C	178	PRO
1	C	194	GLU
1	C	221	GLU
1	C	336	LYS
1	C	360	PHE
1	C	431	ASP
1	C	467	THR
1	C	569	ALA
1	C	578	GLU
1	C	589	ASN
1	A	193	ASP
1	A	335	LEU
1	A	353	ILE
1	A	374	ALA
1	A	424	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	462	SER
1	A	585	ALA
1	A	589	ASN
1	B	30	GLU
1	B	193	ASP
1	B	304	ASP
1	B	335	LEU
1	B	353	ILE
1	B	374	ALA
1	B	424	ARG
1	B	462	SER
1	B	569	ALA
1	C	63	LYS
1	C	353	ILE
1	C	424	ARG
1	C	586	ARG
1	A	22	ARG
1	A	30	GLU
1	A	304	ASP
1	B	22	ARG
1	B	311	PRO
1	B	589	ASN
1	B	729	PRO
1	C	22	ARG
1	C	30	GLU
1	C	193	ASP
1	C	335	LEU
1	C	374	ALA
1	A	611	MET
1	B	120	ASP
1	B	186	GLY
1	B	499	HIS
1	B	611	MET
1	C	120	ASP
1	C	463	ALA
1	C	499	HIS
1	C	611	MET
1	C	729	PRO
1	A	186	GLY
1	A	499	HIS
1	A	631	PRO
1	C	631	PRO

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Mol	Chain	Res	Type
1	A	334	GLY
1	B	334	GLY
1	B	631	PRO
1	C	334	GLY
1	A	729	PRO
1	B	54	GLY
1	C	54	GLY
1	C	186	GLY
1	A	54	GLY
1	A	311	PRO

### 5.3.2 Protein sidechains [i](#)

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	615/678 (91%)	582 (95%)	33 (5%)	20	43
1	B	615/678 (91%)	583 (95%)	32 (5%)	21	44
1	C	615/678 (91%)	584 (95%)	31 (5%)	22	44
All	All	1845/2034 (91%)	1749 (95%)	96 (5%)	21	44

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	64	ARG
1	A	80	GLU
1	A	82	ILE
1	A	91	ASN
1	A	96	LEU
1	A	100	ILE
1	A	113	ARG
1	A	224	LEU
1	A	249	THR
1	A	253	LEU
1	A	314	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	319	GLU
1	A	337	GLN
1	A	340	HIS
1	A	354	ASP
1	A	371	ILE
1	A	378	LEU
1	A	407	VAL
1	A	433	GLU
1	A	436	THR
1	A	440	GLU
1	A	462	SER
1	A	488	GLU
1	A	533	ASN
1	A	556	GLU
1	A	579	LEU
1	A	590	ILE
1	A	611	MET
1	A	613	THR
1	A	624	ASN
1	A	640	ASP
1	A	728	VAL
1	B	64	ARG
1	B	80	GLU
1	B	82	ILE
1	B	91	ASN
1	B	96	LEU
1	B	100	ILE
1	B	113	ARG
1	B	224	LEU
1	B	249	THR
1	B	253	LEU
1	B	287	ARG
1	B	303	ILE
1	B	314	GLU
1	B	319	GLU
1	B	337	GLN
1	B	340	HIS
1	B	354	ASP
1	B	371	ILE
1	B	378	LEU
1	B	407	VAL
1	B	436	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	440	GLU
1	B	488	GLU
1	B	533	ASN
1	B	556	GLU
1	B	579	LEU
1	B	590	ILE
1	B	611	MET
1	B	613	THR
1	B	624	ASN
1	B	640	ASP
1	B	728	VAL
1	C	25	ARG
1	C	80	GLU
1	C	82	ILE
1	C	91	ASN
1	C	96	LEU
1	C	100	ILE
1	C	113	ARG
1	C	224	LEU
1	C	249	THR
1	C	253	LEU
1	C	314	GLU
1	C	319	GLU
1	C	337	GLN
1	C	340	HIS
1	C	354	ASP
1	C	371	ILE
1	C	378	LEU
1	C	407	VAL
1	C	436	THR
1	C	440	GLU
1	C	464	LEU
1	C	488	GLU
1	C	533	ASN
1	C	556	GLU
1	C	579	LEU
1	C	590	ILE
1	C	611	MET
1	C	613	THR
1	C	624	ASN
1	C	640	ASP
1	C	728	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	43	GLN
1	A	91	ASN
1	A	103	GLN
1	A	285	ASN
1	A	317	HIS
1	A	337	GLN
1	A	340	HIS
1	A	348	ASN
1	A	384	HIS
1	A	387	ASN
1	A	401	ASN
1	A	443	ASN
1	A	533	ASN
1	A	589	ASN
1	A	602	ASN
1	A	603	GLN
1	A	616	ASN
1	A	624	ASN
1	A	660	ASN
1	B	43	GLN
1	B	91	ASN
1	B	103	GLN
1	B	285	ASN
1	B	317	HIS
1	B	337	GLN
1	B	340	HIS
1	B	348	ASN
1	B	401	ASN
1	B	406	HIS
1	B	443	ASN
1	B	589	ASN
1	B	602	ASN
1	B	603	GLN
1	B	624	ASN
1	B	641	GLN
1	B	660	ASN
1	B	760	GLN
1	C	43	GLN
1	C	91	ASN
1	C	103	GLN

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	337	GLN
1	C	340	HIS
1	C	348	ASN
1	C	384	HIS
1	C	401	ASN
1	C	406	HIS
1	C	533	ASN
1	C	589	ASN
1	C	624	ASN
1	C	641	GLN
1	C	660	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	C	807	-	28,29,29	1.95	4 (14%)	43,45,45	2.05	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	C	900	-	28,29,29	1.87	8 (28%)	43,45,45	2.03	7 (16%)
2	ADP	A	807	-	28,29,29	2.10	8 (28%)	43,45,45	2.19	11 (25%)
2	ADP	B	900	-	28,29,29	1.58	4 (14%)	43,45,45	1.99	9 (20%)
2	ADP	B	807	-	28,29,29	1.80	6 (21%)	43,45,45	2.11	9 (20%)
2	ADP	A	900	-	28,29,29	1.82	8 (28%)	43,45,45	2.10	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	807	-	-	5/16/32/32	0/3/3/3
2	ADP	C	900	-	-	6/16/32/32	0/3/3/3
2	ADP	A	807	-	-	5/16/32/32	0/3/3/3
2	ADP	B	900	-	-	8/16/32/32	0/3/3/3
2	ADP	B	807	-	-	4/16/32/32	0/3/3/3
2	ADP	A	900	-	-	8/16/32/32	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	ADP	PA-O3A	-6.22	1.52	1.59
2	C	807	ADP	C5-N7	-5.65	1.28	1.39
2	C	900	ADP	C5-N7	-5.20	1.29	1.39
2	C	807	ADP	C4-N9	-4.81	1.27	1.37
2	A	900	ADP	C5-N7	-4.69	1.30	1.39
2	A	807	ADP	C5-N7	-4.56	1.30	1.39
2	B	900	ADP	C5-N7	-4.51	1.30	1.39
2	B	807	ADP	C5-N7	-4.39	1.31	1.39
2	C	900	ADP	C1'-N9	3.83	1.56	1.46
2	C	807	ADP	PA-O3A	-3.73	1.55	1.59
2	A	900	ADP	C1'-N9	3.26	1.55	1.46
2	A	807	ADP	C1'-N9	2.99	1.54	1.46
2	B	807	ADP	PA-O3A	-2.95	1.56	1.59
2	B	807	ADP	C1'-N9	2.82	1.54	1.46
2	B	807	ADP	C2-N3	2.69	1.38	1.33
2	A	900	ADP	PB-O2B	2.63	1.64	1.54
2	B	900	ADP	C4-N9	-2.62	1.32	1.37
2	B	900	ADP	C1'-N9	2.61	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	ADP	C4-N3	2.52	1.39	1.34
2	A	900	ADP	C5'-C4'	2.47	1.59	1.51
2	A	900	ADP	C2-N3	2.40	1.38	1.33
2	A	900	ADP	O4'-C1'	2.37	1.47	1.42
2	C	900	ADP	C4-N9	-2.36	1.32	1.37
2	A	807	ADP	C2-N3	2.32	1.38	1.33
2	C	900	ADP	O4'-C1'	2.31	1.47	1.42
2	A	807	ADP	C2-N1	2.31	1.38	1.33
2	B	807	ADP	C4-N3	2.30	1.38	1.34
2	C	807	ADP	PB-O1B	-2.19	1.43	1.50
2	A	900	ADP	C4-N3	2.15	1.38	1.34
2	C	900	ADP	PA-O3A	-2.13	1.57	1.59
2	A	807	ADP	PB-O2B	2.12	1.62	1.54
2	B	900	ADP	C5-C4	2.10	1.42	1.39
2	B	807	ADP	C2-N1	2.10	1.37	1.33
2	A	900	ADP	C5-C4	2.08	1.42	1.39
2	C	900	ADP	C5-C4	2.06	1.42	1.39
2	C	900	ADP	PB-O2B	2.04	1.62	1.54
2	C	900	ADP	C4-N3	2.03	1.38	1.34
2	A	807	ADP	C6-N1	2.00	1.41	1.35

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	N3-C2-N1	-7.72	116.89	128.58
2	C	900	ADP	N3-C2-N1	-7.50	117.22	128.58
2	A	900	ADP	N3-C2-N1	-7.42	117.35	128.58
2	B	807	ADP	N3-C2-N1	-7.36	117.45	128.58
2	C	807	ADP	N3-C2-N1	-7.35	117.45	128.58
2	B	900	ADP	N3-C2-N1	-6.88	118.16	128.58
2	A	900	ADP	C5-C4-N3	-5.58	119.03	126.72
2	A	807	ADP	C5-C4-N3	-5.42	119.25	126.72
2	B	807	ADP	C5-C4-N3	-5.32	119.39	126.72
2	C	900	ADP	C5-C4-N3	-5.15	119.63	126.72
2	B	900	ADP	C5-C4-N3	-5.02	119.81	126.72
2	A	900	ADP	C2-N3-C4	4.89	123.77	111.83
2	B	807	ADP	C2-N3-C4	4.88	123.74	111.83
2	A	807	ADP	N3-C4-N9	4.85	135.42	127.17
2	A	807	ADP	C2-N3-C4	4.81	123.57	111.83
2	C	807	ADP	C5-C4-N3	-4.74	120.19	126.72
2	C	900	ADP	C2-N3-C4	4.67	123.22	111.83
2	A	900	ADP	N3-C4-N9	4.63	135.04	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	ADP	C2-N3-C4	4.46	122.72	111.83
2	B	807	ADP	N3-C4-N9	4.34	134.54	127.17
2	C	807	ADP	C2-N3-C4	4.33	122.40	111.83
2	C	900	ADP	N3-C4-N9	4.21	134.33	127.17
2	B	900	ADP	N3-C4-N9	3.56	133.23	127.17
2	C	807	ADP	N3-C4-N9	3.42	132.98	127.17
2	B	900	ADP	C5-N7-C8	3.40	108.80	103.45
2	C	807	ADP	N9-C8-N7	-3.21	109.38	113.94
2	A	807	ADP	O5'-C5'-C4'	-3.12	98.36	108.99
2	A	900	ADP	C5-N7-C8	3.11	108.34	103.45
2	C	807	ADP	C2'-C3'-C4'	3.09	108.58	102.61
2	B	807	ADP	C5-N7-C8	2.99	108.16	103.45
2	B	900	ADP	C4-C5-N7	-2.90	107.27	110.58
2	C	807	ADP	C5-N7-C8	2.90	108.00	103.45
2	A	807	ADP	C5-N7-C8	2.77	107.80	103.45
2	B	900	ADP	N9-C8-N7	-2.76	110.02	113.94
2	C	900	ADP	C5-N7-C8	2.69	107.68	103.45
2	B	807	ADP	O5'-C5'-C4'	-2.66	99.94	108.99
2	B	807	ADP	N9-C8-N7	-2.54	110.34	113.94
2	A	900	ADP	N9-C8-N7	-2.45	110.46	113.94
2	A	807	ADP	C2-N1-C6	2.40	122.67	118.73
2	B	807	ADP	C2'-C3'-C4'	2.36	107.18	102.61
2	A	807	ADP	C3'-C2'-C1'	2.31	105.83	101.46
2	C	900	ADP	C2-N1-C6	2.27	122.46	118.73
2	C	807	ADP	C4-C5-N7	-2.27	107.99	110.58
2	A	807	ADP	C2'-C3'-C4'	2.25	106.96	102.61
2	B	900	ADP	C2'-C3'-C4'	2.24	106.93	102.61
2	C	807	ADP	C2-N1-C6	2.23	122.39	118.73
2	C	900	ADP	N9-C8-N7	-2.23	110.78	113.94
2	B	900	ADP	O2'-C2'-C1'	2.19	117.65	110.10
2	B	807	ADP	C4-C5-N7	-2.18	108.08	110.58
2	A	807	ADP	N9-C8-N7	-2.18	110.85	113.94
2	A	807	ADP	O5'-PA-O1A	2.01	116.91	108.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	ADP	C5'-O5'-PA-O1A
2	A	807	ADP	C5'-O5'-PA-O2A
2	A	807	ADP	C5'-O5'-PA-O3A
2	A	900	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	900	ADP	C5'-O5'-PA-O2A
2	A	900	ADP	C5'-O5'-PA-O3A
2	B	807	ADP	C5'-O5'-PA-O1A
2	B	807	ADP	C5'-O5'-PA-O2A
2	B	807	ADP	C5'-O5'-PA-O3A
2	B	900	ADP	C5'-O5'-PA-O1A
2	B	900	ADP	C5'-O5'-PA-O2A
2	B	900	ADP	C5'-O5'-PA-O3A
2	C	807	ADP	C5'-O5'-PA-O1A
2	C	807	ADP	C5'-O5'-PA-O2A
2	C	807	ADP	C5'-O5'-PA-O3A
2	C	900	ADP	C5'-O5'-PA-O1A
2	C	900	ADP	C5'-O5'-PA-O2A
2	C	900	ADP	C5'-O5'-PA-O3A
2	A	900	ADP	O4'-C4'-C5'-O5'
2	B	900	ADP	O4'-C4'-C5'-O5'
2	C	900	ADP	O4'-C4'-C5'-O5'
2	A	807	ADP	O4'-C4'-C5'-O5'
2	A	900	ADP	C3'-C4'-C5'-O5'
2	B	900	ADP	C3'-C4'-C5'-O5'
2	C	807	ADP	O4'-C4'-C5'-O5'
2	B	807	ADP	O4'-C4'-C5'-O5'
2	C	900	ADP	C3'-C4'-C5'-O5'
2	A	900	ADP	PA-O3A-PB-O1B
2	C	807	ADP	C3'-C4'-C5'-O5'
2	A	807	ADP	C3'-C4'-C5'-O5'
2	B	900	ADP	PA-O3A-PB-O1B
2	A	900	ADP	PA-O3A-PB-O2B
2	A	900	ADP	PA-O3A-PB-O3B
2	B	900	ADP	PA-O3A-PB-O2B
2	B	900	ADP	PA-O3A-PB-O3B
2	C	900	ADP	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 13 short contacts:

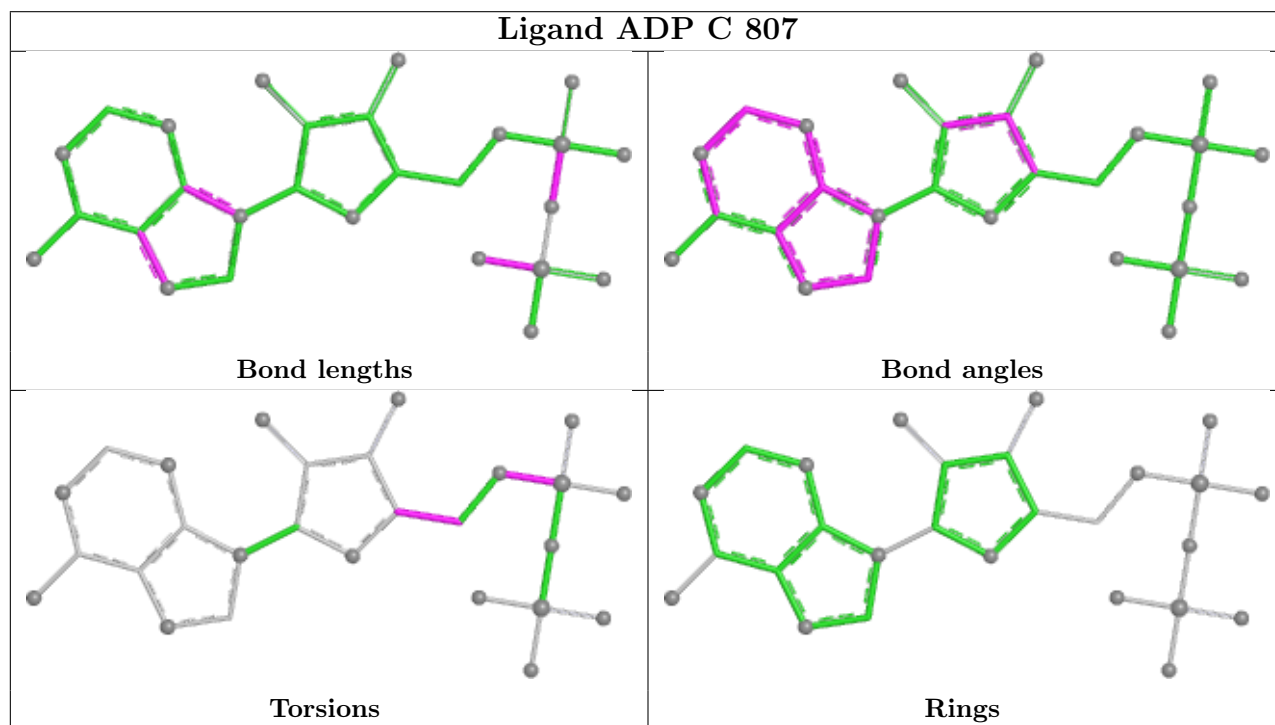
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	807	ADP	1	0
2	C	900	ADP	2	0
2	A	807	ADP	4	0
2	B	900	ADP	1	0
2	B	807	ADP	3	0

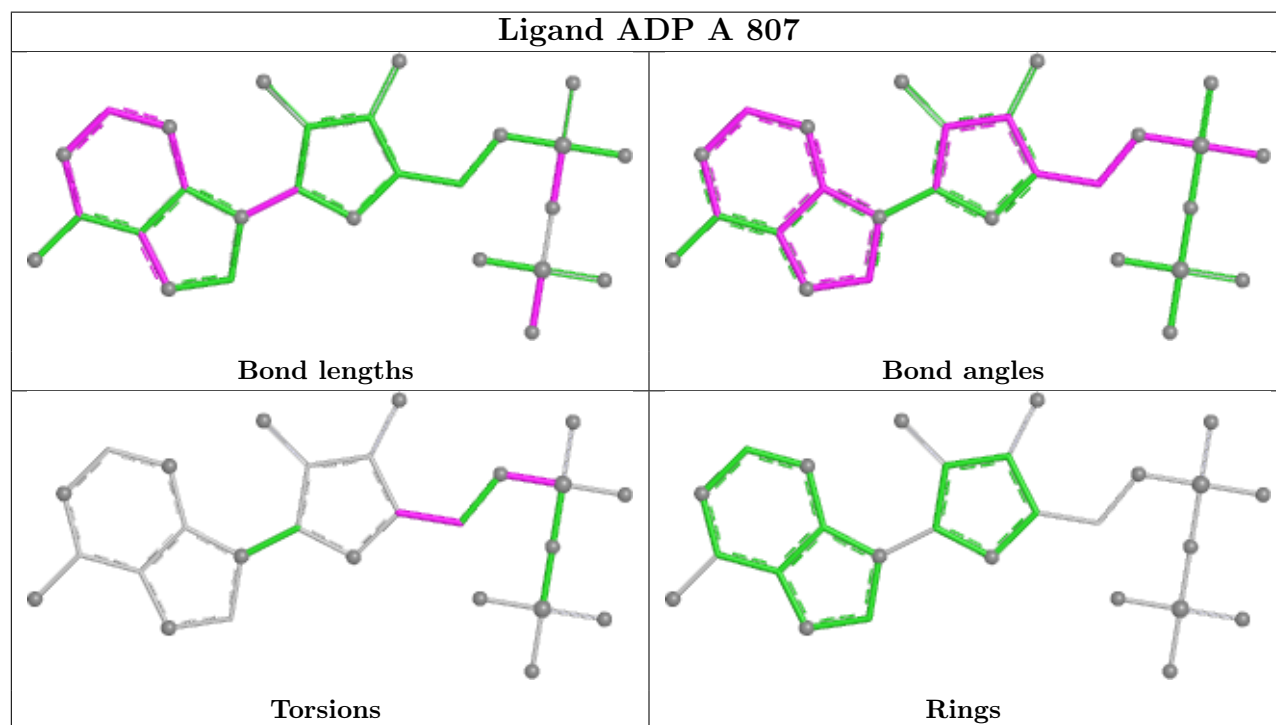
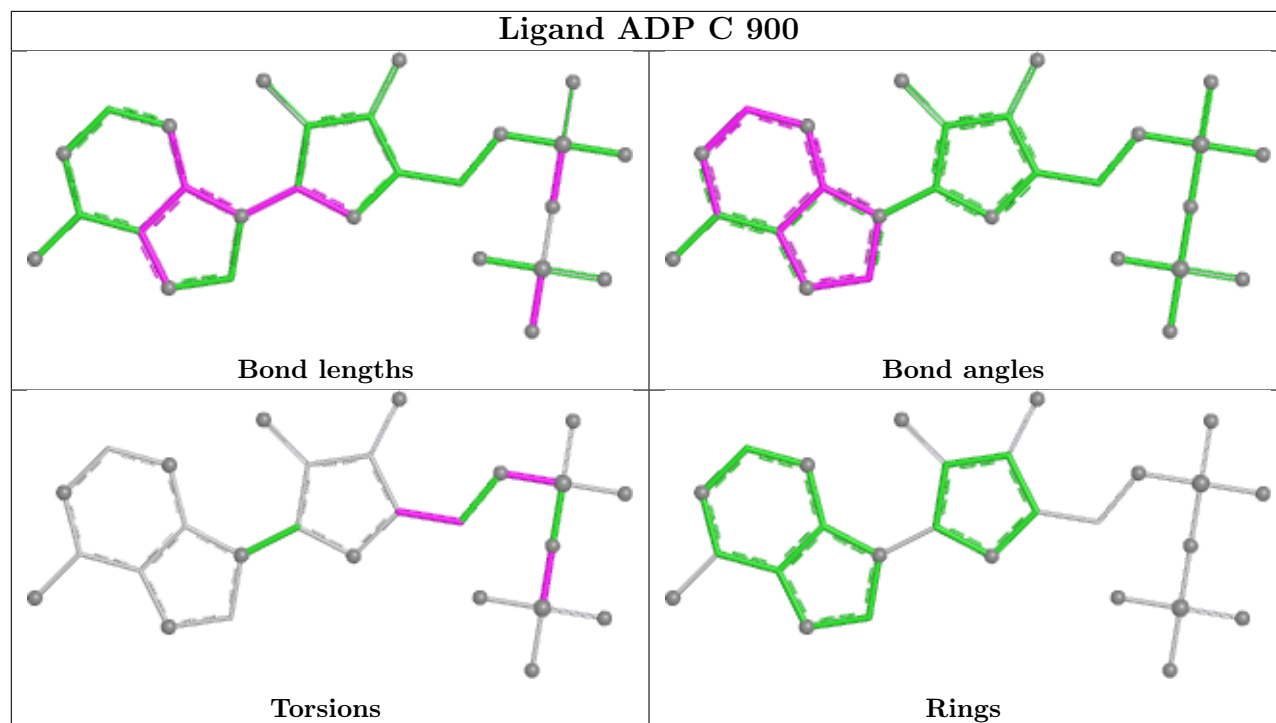
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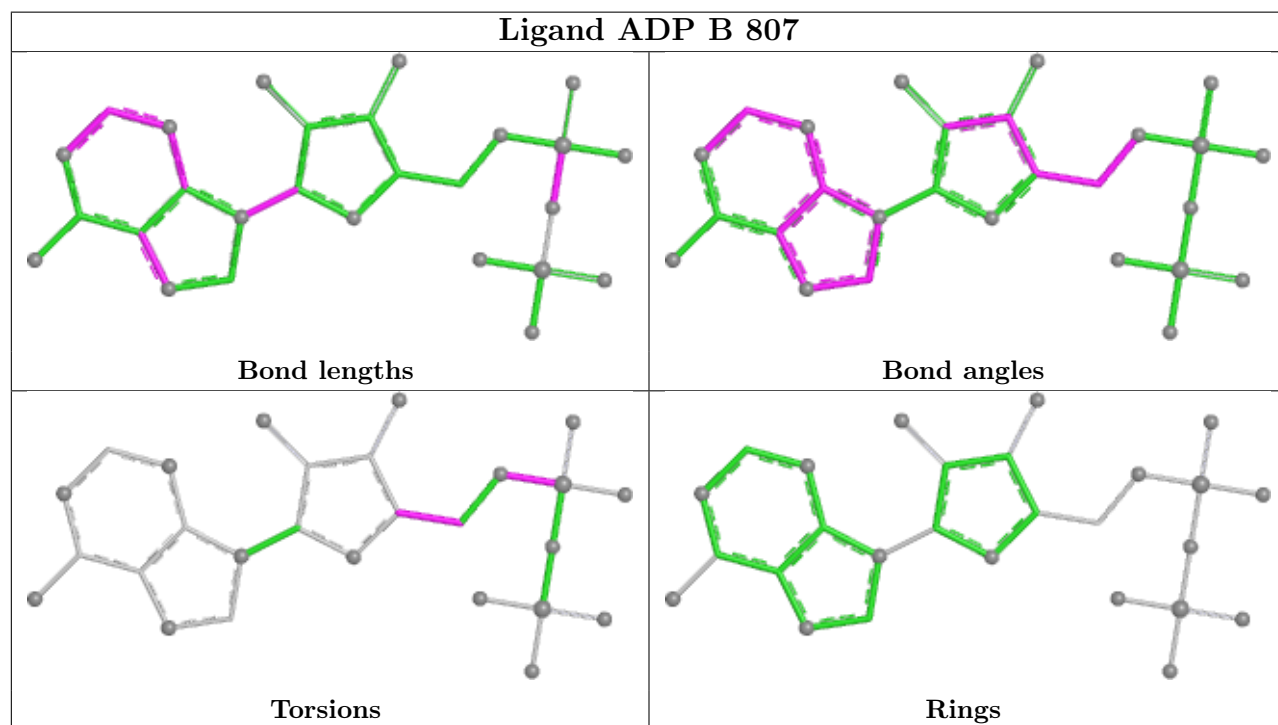
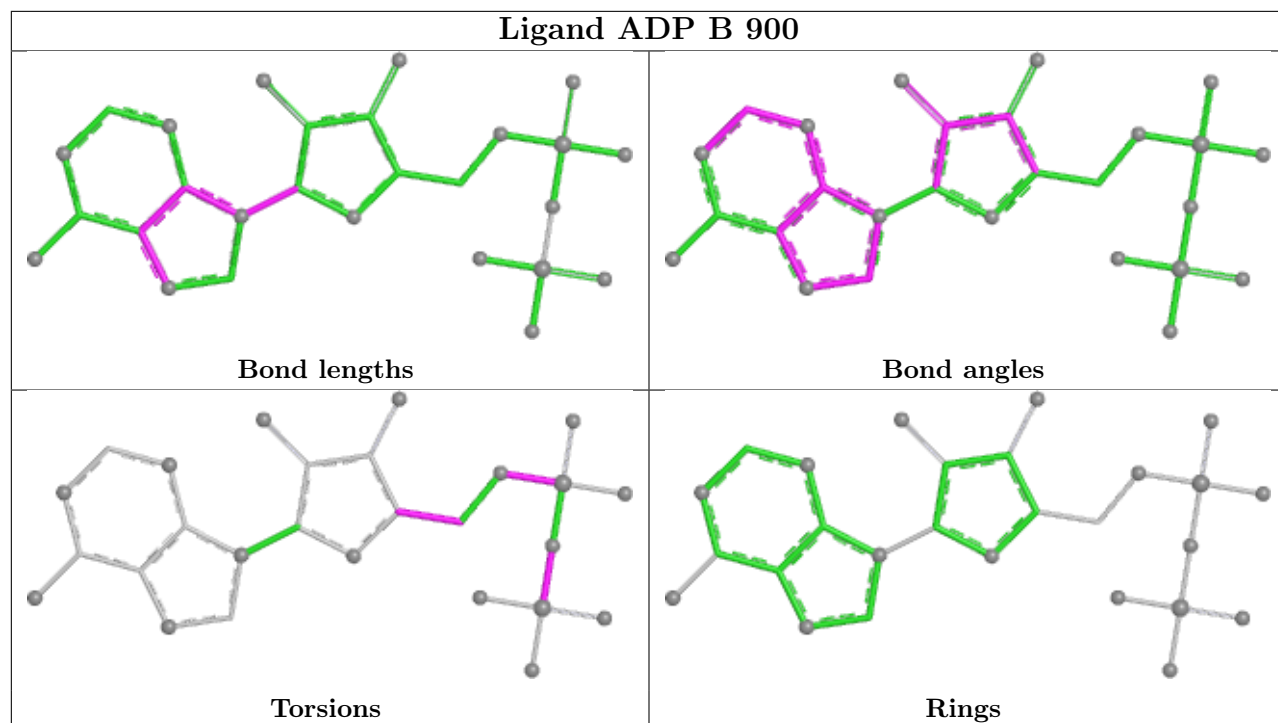
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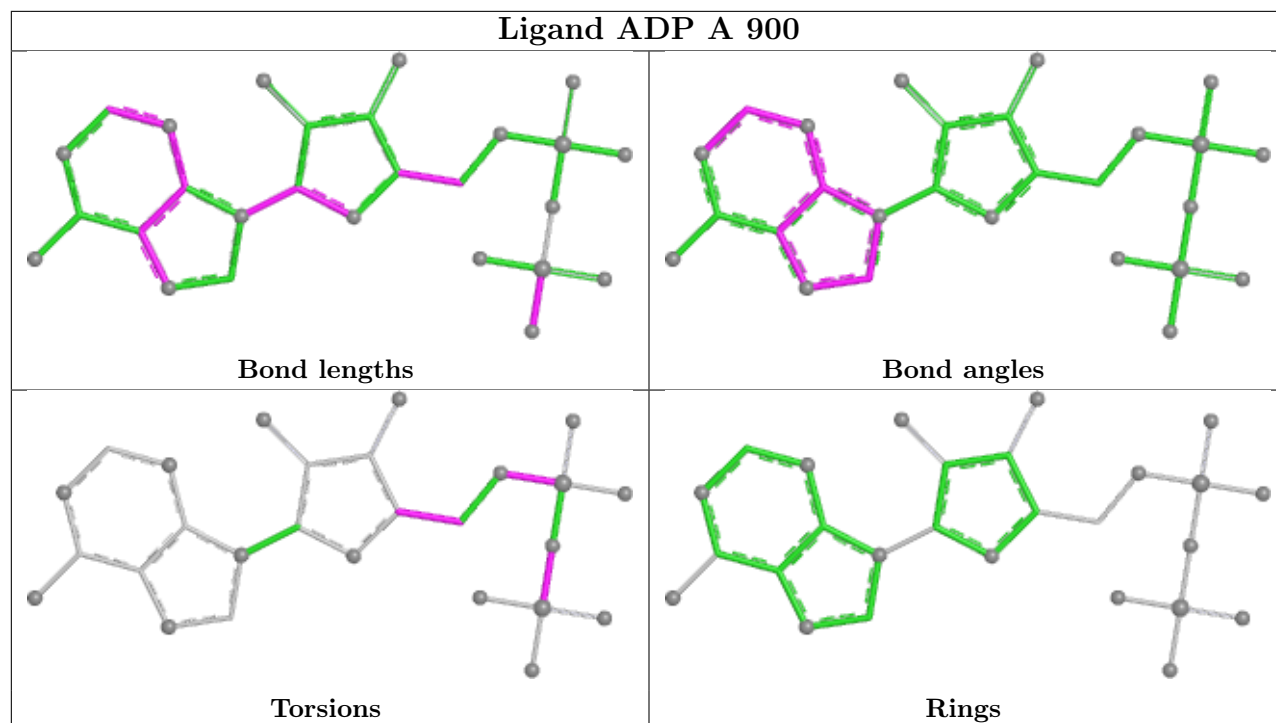
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	ADP	2	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	723/806 (89%)	0.22	19 (2%) 57 44	40, 202, 284, 353	0
1	B	723/806 (89%)	0.17	11 (1%) 72 56	39, 200, 282, 352	0
1	C	723/806 (89%)	0.25	22 (3%) 52 40	38, 202, 283, 352	0
All	All	2169/2418 (89%)	0.21	52 (2%) 59 46	38, 201, 283, 353	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ASN	4.9
1	C	206	ILE	4.7
1	A	206	ILE	4.1
1	C	731	ILE	3.8
1	C	427	MET	3.5
1	B	206	ILE	3.3
1	B	428	ASP	2.9
1	B	224	LEU	2.8
1	C	396	LEU	2.8
1	A	360	PHE	2.8
1	C	736	PHE	2.8
1	C	672	LEU	2.8
1	A	317	HIS	2.7
1	A	728	VAL	2.5
1	A	204	ASP	2.5
1	A	26	LEU	2.5
1	A	736	PHE	2.4
1	A	234	GLY	2.4
1	C	452	PHE	2.4
1	B	606	THR	2.4
1	A	134	TYR	2.4
1	C	390	LEU	2.4
1	C	576	PHE	2.3

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	459	SER	2.3
1	B	317	HIS	2.3
1	A	133	VAL	2.3
1	C	317	HIS	2.3
1	A	131	PHE	2.3
1	A	588	GLY	2.3
1	A	429	LEU	2.2
1	B	153	LEU	2.2
1	C	447	VAL	2.2
1	A	312	LYS	2.2
1	C	337	GLN	2.2
1	B	588	GLY	2.2
1	C	439	ALA	2.2
1	B	426	LYS	2.2
1	C	459	SER	2.2
1	A	390	LEU	2.1
1	C	554	GLU	2.1
1	B	492	LEU	2.1
1	C	371	ILE	2.1
1	C	588	GLY	2.1
1	C	624	ASN	2.1
1	A	135	LEU	2.0
1	C	135	LEU	2.0
1	B	731	ILE	2.0
1	C	234	GLY	2.0
1	A	578	GLU	2.0
1	C	407	VAL	2.0
1	C	445	LEU	2.0
1	B	36	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

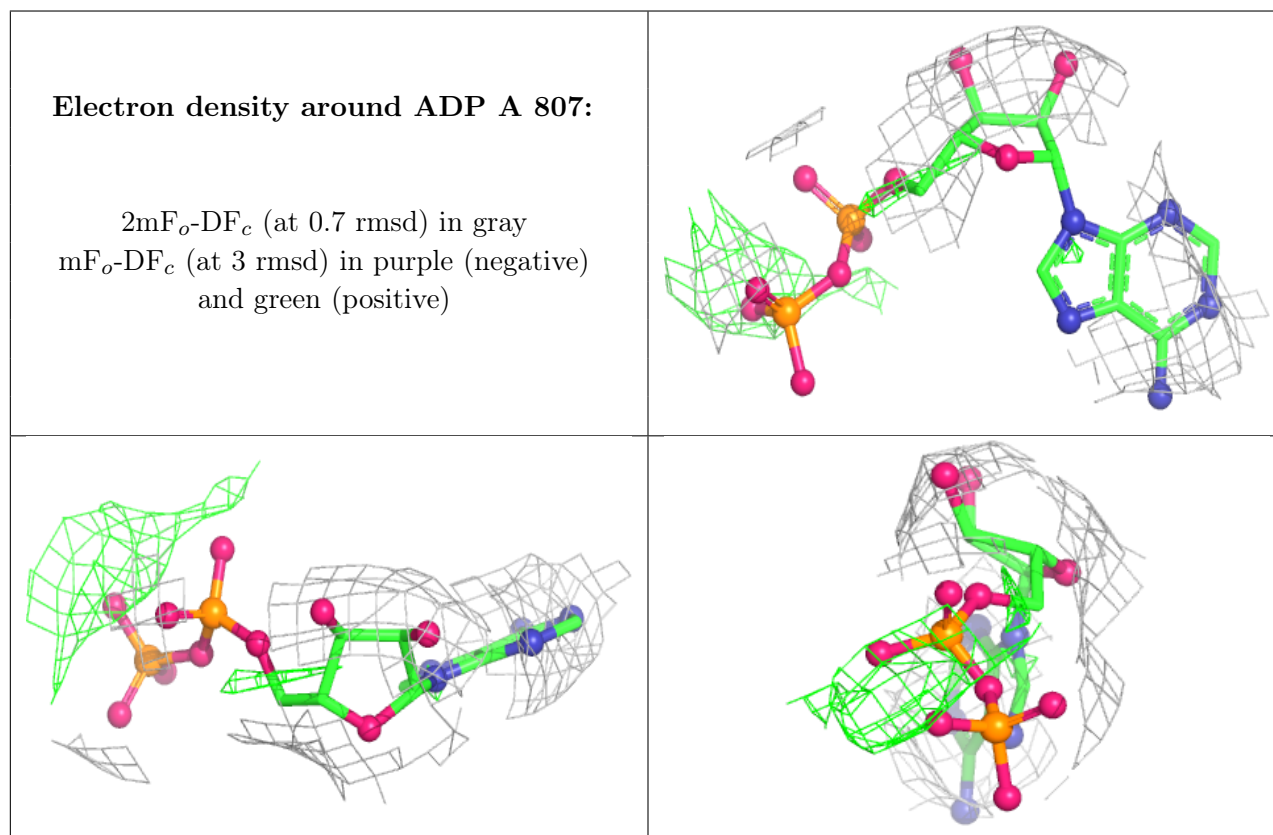
There are no oligosaccharides in this entry.

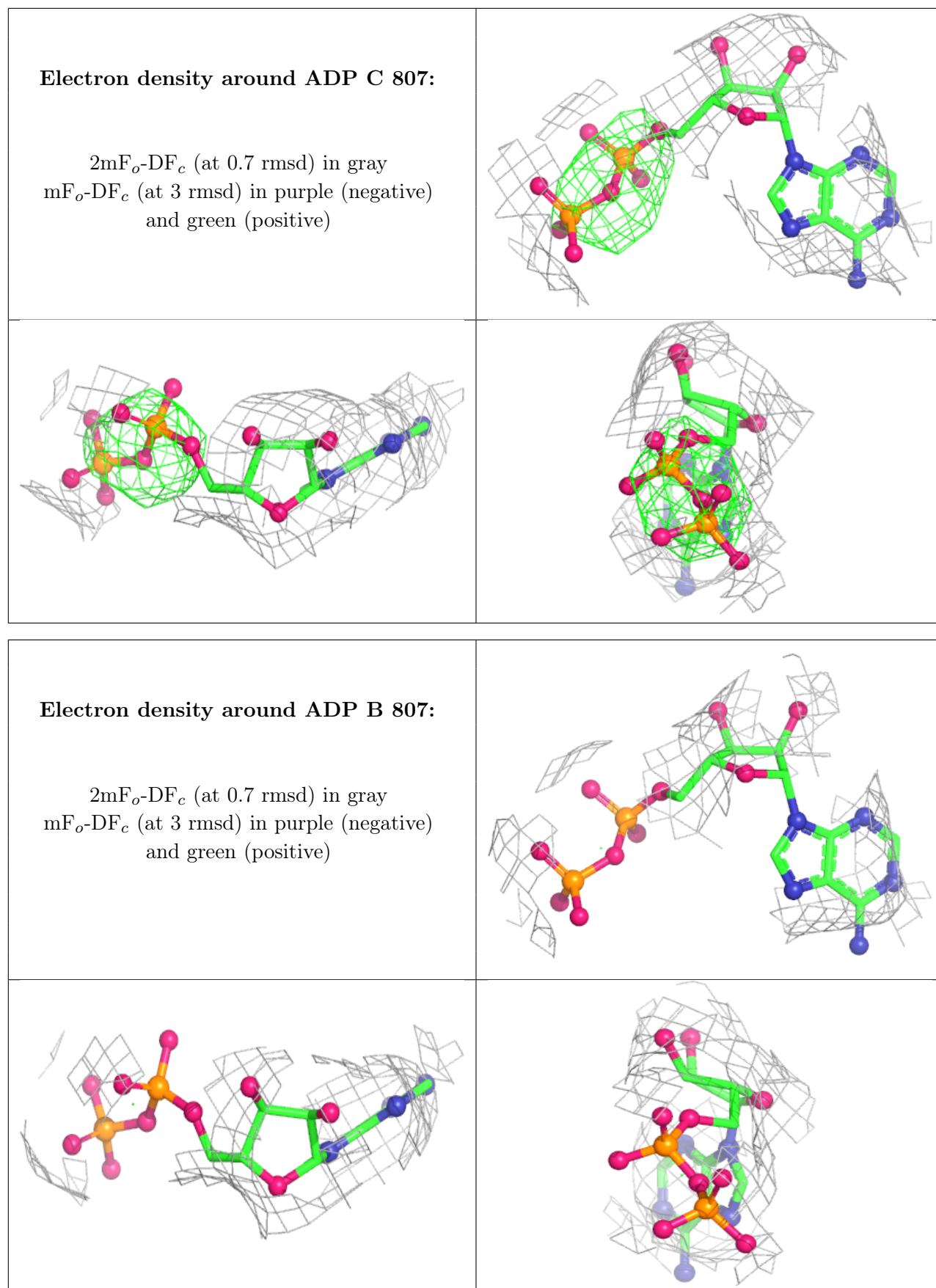
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ADP	A	807	27/27	0.94	0.12	133,149,222,335	0
2	ADP	C	807	27/27	0.95	0.12	144,177,268,273	0
2	ADP	B	807	27/27	0.96	0.10	139,163,218,268	0
2	ADP	B	900	27/27	0.97	0.06	106,157,202,277	0
2	ADP	A	900	27/27	0.97	0.07	122,174,209,218	0
2	ADP	C	900	27/27	0.98	0.08	118,157,187,206	0

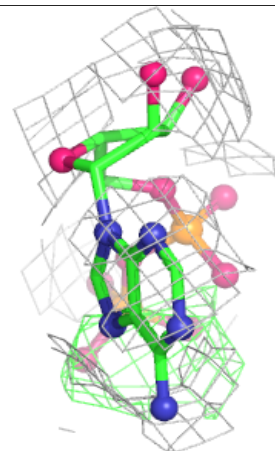
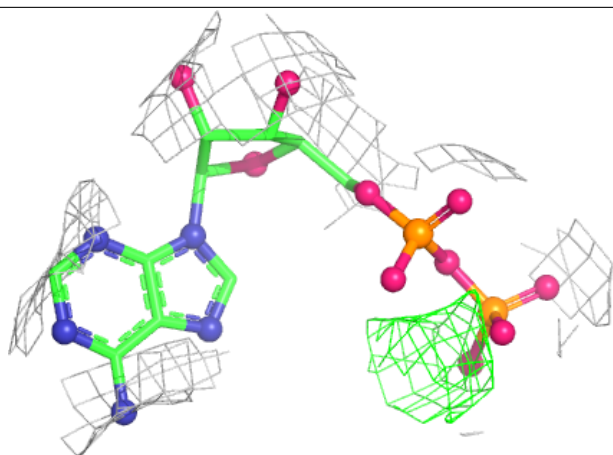
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





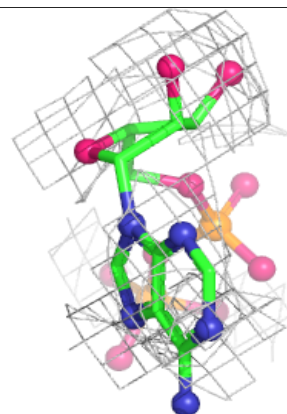
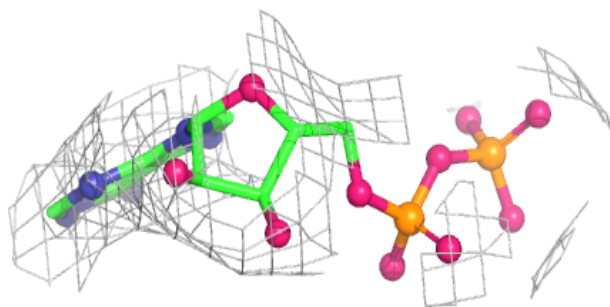
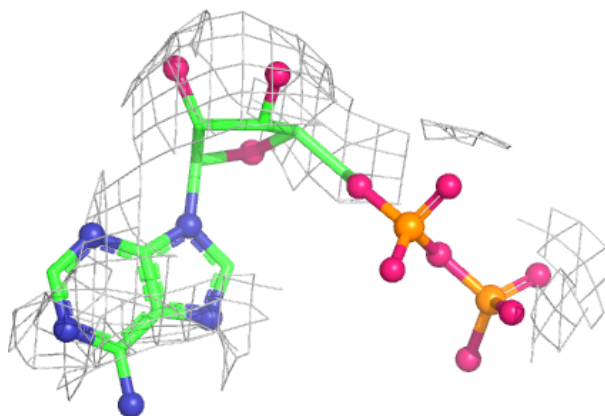
**Electron density around ADP B 900:**

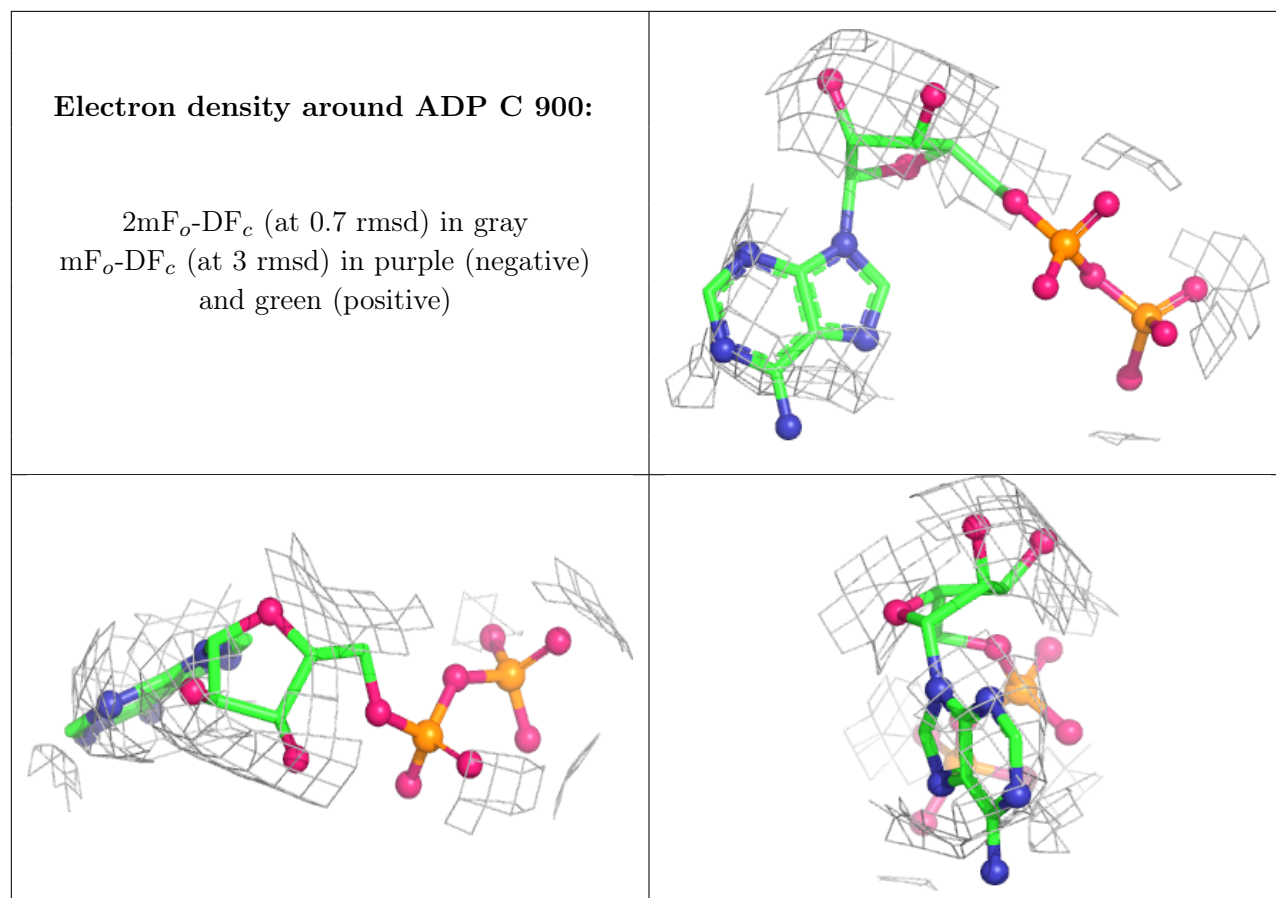
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ADP A 900:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.