



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:43 AM BST

PDB ID : 3M6A
Title : Crystal structure of Bacillus subtilis Lon C-terminal domain
Authors : Duman, R.E.; Lowe, J.Y.
Deposited on : 2010-03-15
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

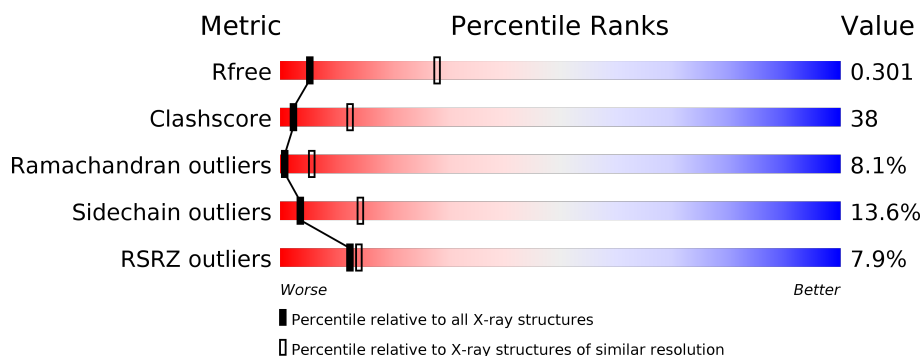
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div>5%</div> <div> <div>39%</div> <div>39%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	543	<div> <div>5%</div> <div> <div>39%</div> <div>38%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	543	<div> <div>7%</div> <div> <div>37%</div> <div>41%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	543	<div> <div>9%</div> <div> <div>37%</div> <div>42%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	543	<div> <div>10%</div> <div> <div>38%</div> <div>40%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	543	<div> <div>7%</div> <div> <div>41%</div> <div>38%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	783	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23196 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 ATP-dependent protease La 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	B	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	C	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	D	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	E	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	F	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			

There are 54 discrepancies between the modelled and reference sequences:

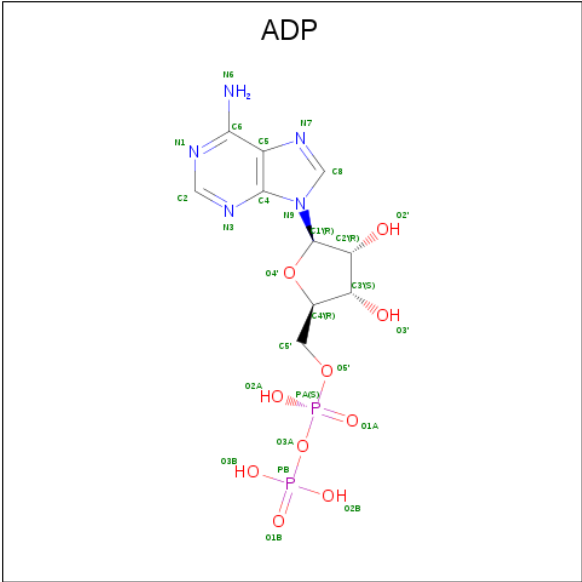
Chain	Residue	Modelled	Actual	Comment	Reference
A	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
A	775	LEU	-	EXPRESSION TAG	UNP P37945
A	776	GLU	-	EXPRESSION TAG	UNP P37945
A	777	HIS	-	EXPRESSION TAG	UNP P37945
A	778	HIS	-	EXPRESSION TAG	UNP P37945
A	779	HIS	-	EXPRESSION TAG	UNP P37945
A	780	HIS	-	EXPRESSION TAG	UNP P37945
A	781	HIS	-	EXPRESSION TAG	UNP P37945
A	782	HIS	-	EXPRESSION TAG	UNP P37945
B	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
B	775	LEU	-	EXPRESSION TAG	UNP P37945
B	776	GLU	-	EXPRESSION TAG	UNP P37945
B	777	HIS	-	EXPRESSION TAG	UNP P37945
B	778	HIS	-	EXPRESSION TAG	UNP P37945
B	779	HIS	-	EXPRESSION TAG	UNP P37945
B	780	HIS	-	EXPRESSION TAG	UNP P37945
B	781	HIS	-	EXPRESSION TAG	UNP P37945

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Chain	Residue	Modelled	Actual	Comment	Reference
B	782	HIS	-	EXPRESSION TAG	UNP P37945
C	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
C	775	LEU	-	EXPRESSION TAG	UNP P37945
C	776	GLU	-	EXPRESSION TAG	UNP P37945
C	777	HIS	-	EXPRESSION TAG	UNP P37945
C	778	HIS	-	EXPRESSION TAG	UNP P37945
C	779	HIS	-	EXPRESSION TAG	UNP P37945
C	780	HIS	-	EXPRESSION TAG	UNP P37945
C	781	HIS	-	EXPRESSION TAG	UNP P37945
C	782	HIS	-	EXPRESSION TAG	UNP P37945
D	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
D	775	LEU	-	EXPRESSION TAG	UNP P37945
D	776	GLU	-	EXPRESSION TAG	UNP P37945
D	777	HIS	-	EXPRESSION TAG	UNP P37945
D	778	HIS	-	EXPRESSION TAG	UNP P37945
D	779	HIS	-	EXPRESSION TAG	UNP P37945
D	780	HIS	-	EXPRESSION TAG	UNP P37945
D	781	HIS	-	EXPRESSION TAG	UNP P37945
D	782	HIS	-	EXPRESSION TAG	UNP P37945
E	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
E	775	LEU	-	EXPRESSION TAG	UNP P37945
E	776	GLU	-	EXPRESSION TAG	UNP P37945
E	777	HIS	-	EXPRESSION TAG	UNP P37945
E	778	HIS	-	EXPRESSION TAG	UNP P37945
E	779	HIS	-	EXPRESSION TAG	UNP P37945
E	780	HIS	-	EXPRESSION TAG	UNP P37945
E	781	HIS	-	EXPRESSION TAG	UNP P37945
E	782	HIS	-	EXPRESSION TAG	UNP P37945
F	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
F	775	LEU	-	EXPRESSION TAG	UNP P37945
F	776	GLU	-	EXPRESSION TAG	UNP P37945
F	777	HIS	-	EXPRESSION TAG	UNP P37945
F	778	HIS	-	EXPRESSION TAG	UNP P37945
F	779	HIS	-	EXPRESSION TAG	UNP P37945
F	780	HIS	-	EXPRESSION TAG	UNP P37945
F	781	HIS	-	EXPRESSION TAG	UNP P37945
F	782	HIS	-	EXPRESSION TAG	UNP P37945

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

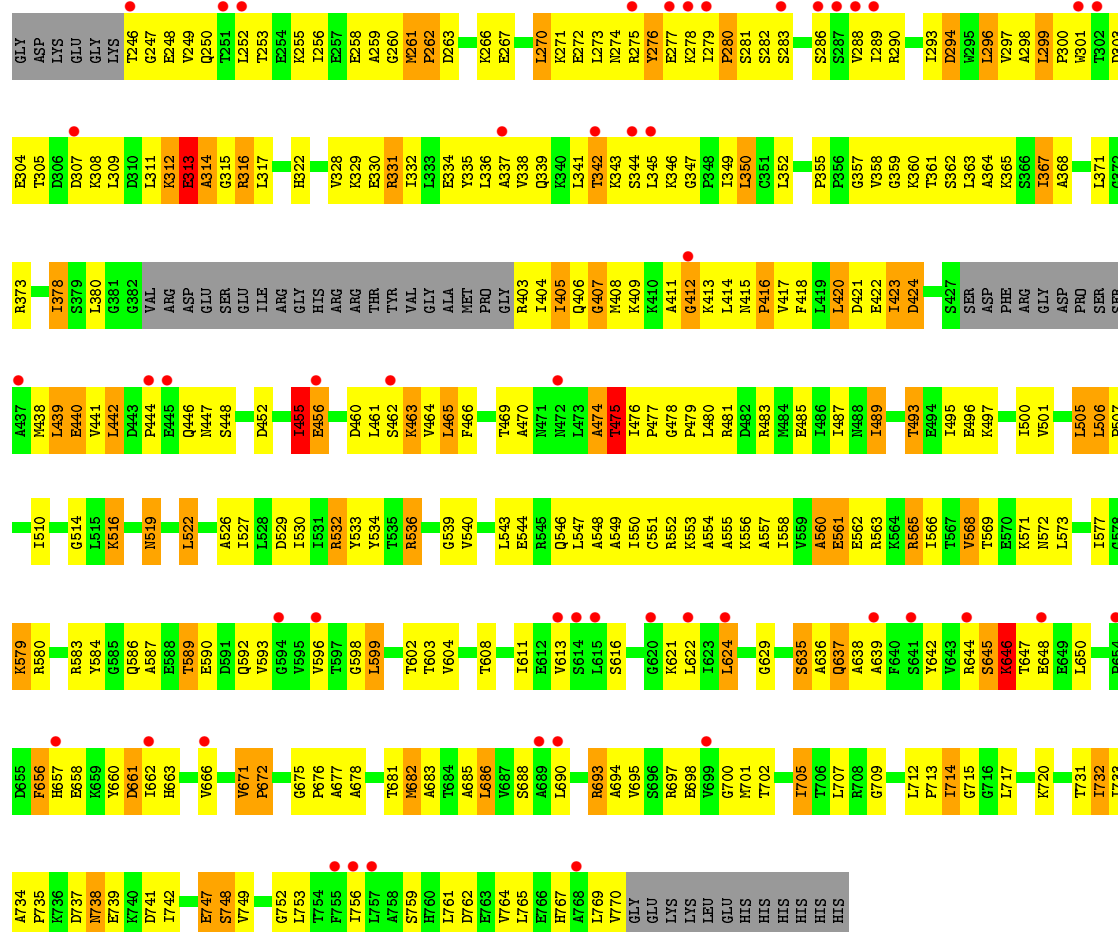


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

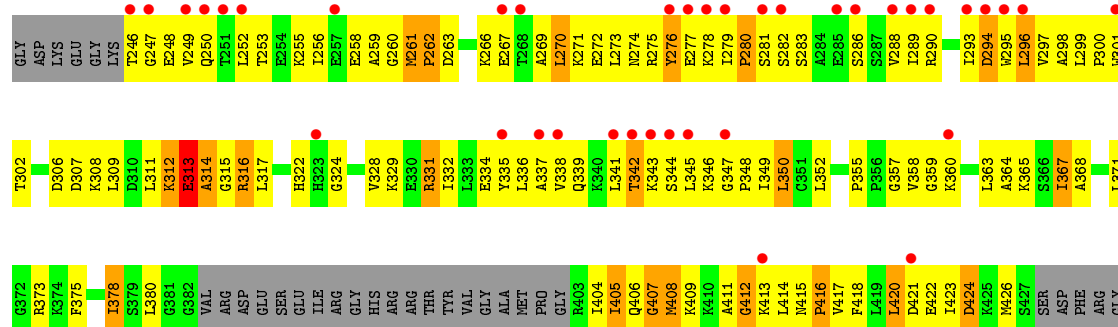


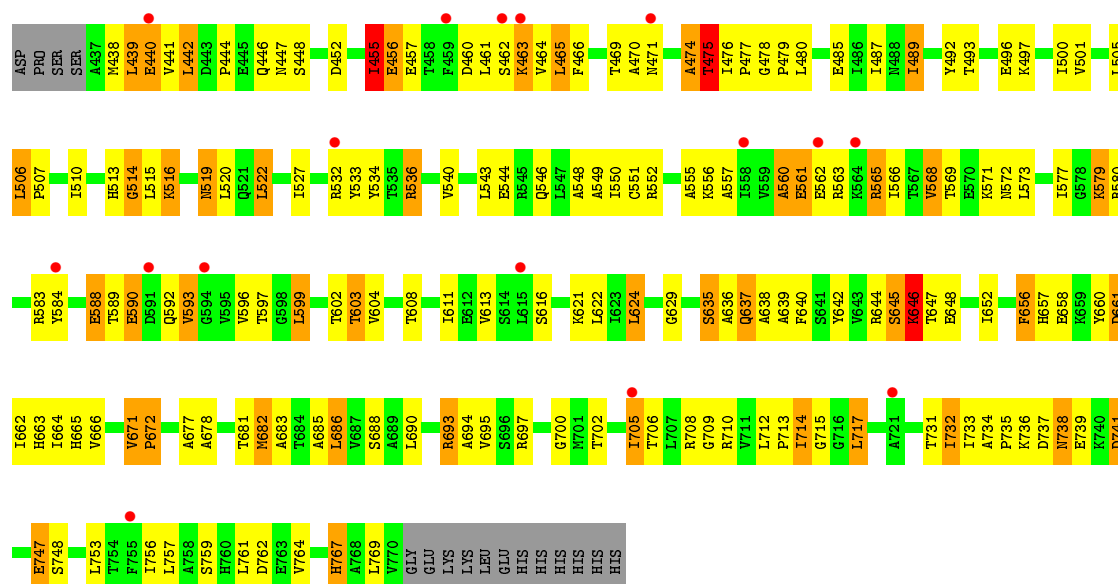


• Molecule 1: ATP-dependent protease La 1

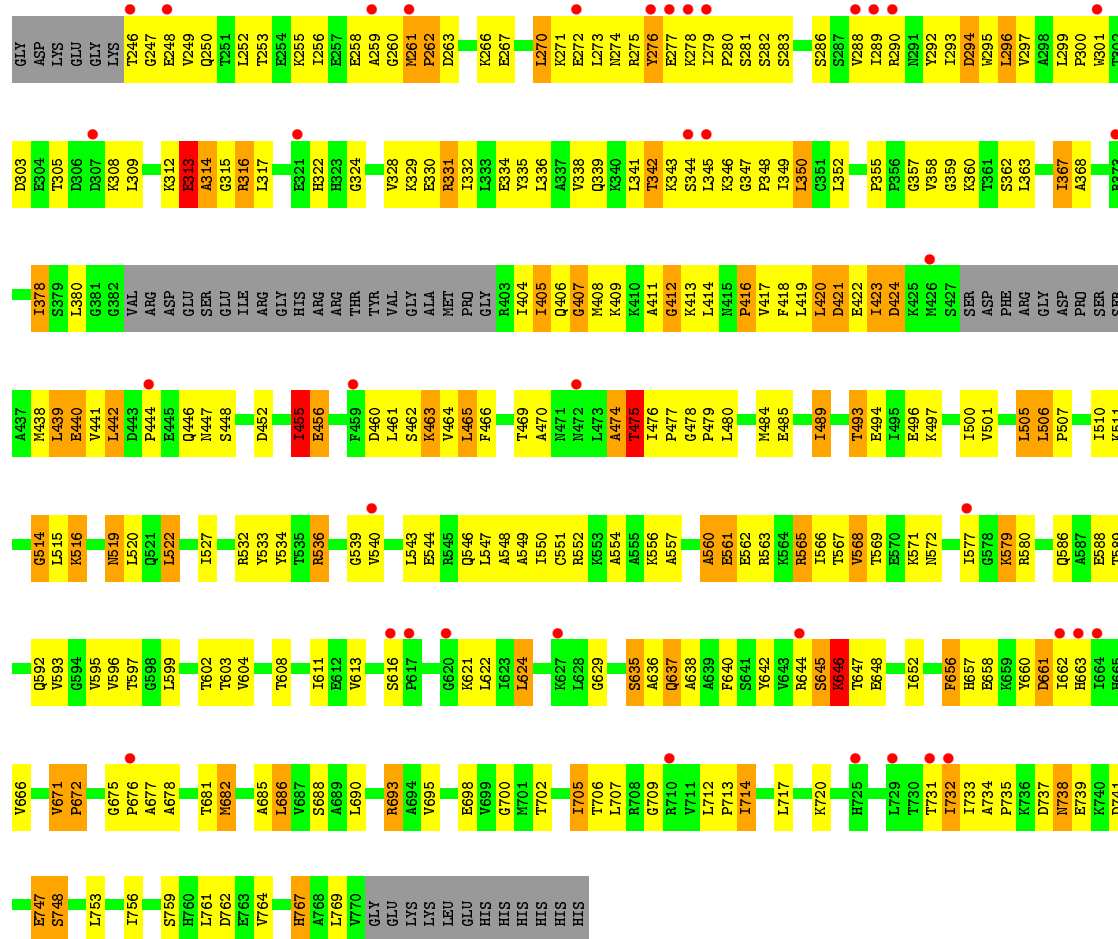


• Molecule 1: ATP-dependent protease La 1





• Molecule 1: ATP-dependent protease La 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.38Å 127.40Å 148.99Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	29.91 – 3.40 58.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.91-3.40) 99.6 (58.42-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_249)	Depositor
R, R_{free}	0.265 , 0.313 0.248 , 0.301	Depositor DCC
R_{free} test set	2607 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	117.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 130.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23196	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.49	0/3892	0.63	0/5246
1	B	0.47	0/3892	0.64	0/5246
1	C	0.45	0/3892	0.62	0/5246
1	D	0.51	0/3892	0.64	1/5246 (0.0%)
1	E	0.46	0/3892	0.63	0/5246
1	F	0.44	0/3892	0.63	1/5246 (0.0%)
All	All	0.47	0/23352	0.63	2/31476 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	505	LEU	CB-CG-CD2	-5.66	101.37	111.00
1	F	505	LEU	CB-CG-CD2	-5.54	101.58	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3839	0	3968	297	0
1	B	3839	0	3968	324	0
1	C	3839	0	3968	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3839	0	3968	300	1
1	E	3839	0	3968	308	0
1	F	3839	0	3968	287	1
2	A	27	0	12	7	0
2	B	27	0	12	7	0
2	C	27	0	12	6	0
2	D	27	0	12	11	0
2	E	27	0	12	6	0
2	F	27	0	12	7	0
All	All	23196	0	23880	1793	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1793) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:ARG:HG3	1:E:338:VAL:HG21	1.31	1.08
1:F:493:THR:HG21	1:F:748:SER:HB2	1.26	1.08
1:C:350:LEU:HD12	1:C:350:LEU:H	1.18	1.02
1:B:337:ALA:CB	1:F:556:LYS:HA	1.89	1.02
1:A:501:VAL:HG11	1:A:527:ILE:HD13	1.39	1.01
1:F:501:VAL:HG11	1:F:527:ILE:HD13	1.42	0.97
1:B:350:LEU:HD12	1:B:350:LEU:H	1.28	0.96
1:B:501:VAL:HG11	1:B:527:ILE:HD13	1.48	0.95
1:D:501:VAL:HG11	1:D:527:ILE:HD13	1.49	0.95
1:F:586:GLN:HG2	1:F:698:GLU:HG2	1.46	0.93
1:C:569:THR:HG23	1:C:571:LYS:H	1.33	0.93
1:A:350:LEU:HD12	1:A:350:LEU:H	1.31	0.93
1:A:378:ILE:O	1:A:378:ILE:HG12	1.69	0.93
1:A:596:VAL:HG22	1:A:695:VAL:HG21	1.48	0.92
1:E:671:VAL:HG22	1:E:672:PRO:HD2	1.51	0.91
1:F:671:VAL:HG22	1:F:672:PRO:HD2	1.49	0.91
1:B:493:THR:HG21	1:B:748:SER:HB2	1.50	0.91
1:B:378:ILE:HG12	1:B:378:ILE:O	1.69	0.91
1:E:501:VAL:HG11	1:E:527:ILE:HD13	1.51	0.91
1:E:350:LEU:HD12	1:E:350:LEU:H	1.32	0.91
1:F:586:GLN:HE21	1:F:698:GLU:HA	1.38	0.89
1:E:536:ARG:HH11	1:E:536:ARG:HG3	1.35	0.89
1:D:350:LEU:H	1:D:350:LEU:HD12	1.36	0.88
1:C:501:VAL:HG11	1:C:527:ILE:HD13	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ILE:HG23	1:D:418:PHE:CE2	2.08	0.88
1:C:536:ARG:HG3	1:C:536:ARG:HH11	1.37	0.88
1:C:671:VAL:HG22	1:C:672:PRO:HD2	1.55	0.88
1:A:569:THR:HG23	1:A:571:LYS:H	1.37	0.88
1:C:337:ALA:CB	1:E:556:LYS:HA	2.03	0.87
1:B:536:ARG:HH11	1:B:536:ARG:HG3	1.40	0.87
1:C:596:VAL:HG22	1:C:695:VAL:HG21	1.56	0.87
1:D:359:GLY:HA2	2:D:783:ADP:C5'	2.04	0.87
1:F:569:THR:HG23	1:F:571:LYS:H	1.37	0.87
1:D:688:SER:HB2	1:D:769:LEU:HD21	1.55	0.87
1:E:569:THR:HG23	1:E:571:LYS:H	1.39	0.87
1:A:536:ARG:HG3	1:A:536:ARG:HH11	1.40	0.86
1:D:671:VAL:HG22	1:D:672:PRO:HD2	1.57	0.86
1:B:569:THR:HG23	1:B:571:LYS:H	1.39	0.86
1:D:378:ILE:HG12	1:D:378:ILE:O	1.74	0.86
1:D:536:ARG:HH11	1:D:536:ARG:HG3	1.39	0.86
1:D:493:THR:HG21	1:D:748:SER:HB2	1.58	0.85
1:E:688:SER:HB2	1:E:769:LEU:HD21	1.56	0.85
1:F:536:ARG:HG3	1:F:536:ARG:HH11	1.42	0.85
1:F:596:VAL:HG22	1:F:695:VAL:HG21	1.58	0.85
1:E:378:ILE:HG12	1:E:378:ILE:O	1.77	0.84
1:B:522:LEU:HD12	1:B:527:ILE:HG12	1.60	0.84
1:D:596:VAL:HG22	1:D:695:VAL:HG21	1.60	0.84
1:A:671:VAL:HG22	1:A:672:PRO:HD2	1.60	0.83
1:D:569:THR:HG23	1:D:571:LYS:H	1.40	0.83
1:C:688:SER:HB2	1:C:769:LEU:HD21	1.59	0.83
1:E:596:VAL:HG22	1:E:695:VAL:HG21	1.60	0.83
1:F:516:LYS:HA	1:F:516:LYS:NZ	1.93	0.83
1:F:360:LYS:HD2	1:F:469:THR:HG23	1.60	0.83
1:B:733:ILE:HG21	1:B:764:VAL:HG13	1.58	0.82
1:A:733:ILE:HG21	1:A:764:VAL:HG13	1.62	0.82
1:D:733:ILE:HG21	1:D:764:VAL:HG13	1.62	0.81
1:F:378:ILE:HG12	1:F:378:ILE:O	1.80	0.81
1:B:516:LYS:O	1:B:519:ASN:HB2	1.80	0.81
1:C:536:ARG:CG	1:C:536:ARG:HH11	1.93	0.81
1:A:411:ALA:O	1:A:413:LYS:N	2.14	0.81
1:F:404:ILE:HG23	1:F:418:PHE:CE2	2.16	0.81
1:F:688:SER:HB2	1:F:769:LEU:HD21	1.63	0.81
1:C:501:VAL:HA	1:C:505:LEU:HB2	1.62	0.81
1:F:516:LYS:O	1:F:519:ASN:HB2	1.81	0.80
1:A:522:LEU:HD12	1:A:527:ILE:HG12	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:LEU:HB3	1:C:568:VAL:HG13	1.62	0.80
1:F:522:LEU:HB3	1:F:568:VAL:HG13	1.64	0.80
1:F:733:ILE:HG21	1:F:764:VAL:HG13	1.63	0.80
1:E:439:LEU:H	1:E:439:LEU:HD22	1.44	0.79
1:F:522:LEU:HD12	1:F:527:ILE:HG12	1.65	0.79
1:D:536:ARG:HH11	1:D:536:ARG:CG	1.96	0.79
1:F:506:LEU:HD21	1:F:522:LEU:HD21	1.65	0.79
1:A:337:ALA:CB	1:C:556:LYS:HA	2.12	0.79
1:C:404:ILE:HG23	1:C:418:PHE:CE2	2.17	0.79
1:C:439:LEU:HD22	1:C:439:LEU:H	1.47	0.79
1:C:506:LEU:HD21	1:C:522:LEU:HD21	1.65	0.79
1:D:522:LEU:HD12	1:D:527:ILE:HG12	1.65	0.79
1:E:536:ARG:HH11	1:E:536:ARG:CG	1.96	0.79
1:F:411:ALA:O	1:F:413:LYS:N	2.17	0.78
1:C:337:ALA:HB1	1:E:556:LYS:HA	1.64	0.78
1:A:338:VAL:HG21	1:C:552:ARG:HG3	1.63	0.78
1:A:536:ARG:CG	1:A:536:ARG:HH11	1.97	0.78
1:B:501:VAL:HA	1:B:505:LEU:HB2	1.65	0.78
1:E:404:ILE:HG23	1:E:418:PHE:CE2	2.19	0.78
1:B:536:ARG:HH11	1:B:536:ARG:CG	1.96	0.78
1:B:688:SER:HB2	1:B:769:LEU:HD21	1.64	0.78
1:E:414:LEU:O	1:E:416:PRO:HD3	1.83	0.78
1:B:337:ALA:HB1	1:F:556:LYS:HA	1.63	0.78
1:F:359:GLY:HA2	2:F:783:ADP:O5'	1.84	0.78
1:E:411:ALA:O	1:E:413:LYS:N	2.18	0.77
1:D:411:ALA:O	1:D:413:LYS:N	2.18	0.77
1:B:282:SER:HB2	1:E:276:TYR:OH	1.82	0.77
1:B:671:VAL:HG22	1:B:672:PRO:HD2	1.66	0.77
1:E:584:TYR:O	1:E:584:TYR:CD1	2.37	0.77
1:B:411:ALA:O	1:B:413:LYS:N	2.17	0.77
1:C:414:LEU:O	1:C:416:PRO:HD3	1.85	0.77
1:D:522:LEU:HB3	1:D:568:VAL:HG13	1.65	0.77
1:A:456:GLU:CD	1:C:291:ASN:HD21	1.88	0.77
1:A:404:ILE:HG23	1:A:418:PHE:CE2	2.20	0.76
1:C:270:LEU:HD21	1:C:296:LEU:HD22	1.66	0.76
1:D:359:GLY:HA2	2:D:783:ADP:O5'	1.85	0.76
1:B:596:VAL:HG22	1:B:695:VAL:HG21	1.66	0.76
1:B:303:ASP:O	1:B:304:GLU:HB2	1.86	0.76
1:A:272:GLU:HB3	1:C:248:GLU:OE1	1.85	0.76
1:B:506:LEU:HB3	1:B:507:PRO:HD3	1.68	0.75
1:C:411:ALA:O	1:C:413:LYS:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD11	1:C:290:ARG:HH12	1.50	0.75
1:B:439:LEU:H	1:B:439:LEU:HD22	1.51	0.75
1:B:506:LEU:HD21	1:B:522:LEU:HD21	1.68	0.75
1:E:516:LYS:O	1:E:519:ASN:HB2	1.86	0.75
1:D:359:GLY:HA2	2:D:783:ADP:H5'2	1.69	0.75
1:E:733:ILE:HG21	1:E:764:VAL:HG13	1.67	0.75
1:D:439:LEU:HD22	1:D:439:LEU:H	1.50	0.75
1:A:439:LEU:H	1:A:439:LEU:HD22	1.51	0.74
1:C:733:ILE:HG21	1:C:764:VAL:HG13	1.68	0.74
1:F:350:LEU:H	1:F:350:LEU:HD12	1.51	0.74
1:F:439:LEU:H	1:F:439:LEU:HD22	1.53	0.74
1:D:505:LEU:HD22	1:D:544:GLU:HG3	1.70	0.74
1:F:536:ARG:CG	1:F:536:ARG:HH11	1.99	0.74
1:C:493:THR:HG21	1:C:748:SER:HB2	1.70	0.74
1:E:270:LEU:HD21	1:E:296:LEU:HD22	1.70	0.74
1:B:359:GLY:HA2	2:B:783:ADP:O5'	1.88	0.74
1:E:738:ASN:O	1:E:741:ASP:HB2	1.88	0.74
1:A:505:LEU:HD22	1:A:544:GLU:HG3	1.68	0.73
1:C:516:LYS:NZ	1:C:516:LYS:HA	2.02	0.73
1:C:522:LEU:HD12	1:C:527:ILE:HG12	1.70	0.73
1:A:688:SER:HB2	1:A:769:LEU:HD21	1.69	0.73
1:E:583:ARG:HD3	1:E:588:GLU:CD	2.08	0.73
1:A:270:LEU:HD21	1:A:296:LEU:HD22	1.70	0.73
1:A:516:LYS:O	1:A:519:ASN:HB2	1.89	0.73
1:D:404:ILE:HG23	1:D:418:PHE:HE2	1.53	0.73
1:E:506:LEU:HD21	1:E:522:LEU:HD21	1.70	0.73
1:C:602:THR:HG22	1:C:604:VAL:H	1.54	0.72
1:D:738:ASN:O	1:D:741:ASP:HB2	1.89	0.72
1:F:501:VAL:CG1	1:F:527:ILE:HD13	2.19	0.72
1:A:501:VAL:CG1	1:A:527:ILE:HD13	2.17	0.72
1:F:516:LYS:HA	1:F:516:LYS:CE	2.19	0.72
1:A:522:LEU:HB3	1:A:568:VAL:HG13	1.72	0.72
1:F:493:THR:HG21	1:F:748:SER:CB	2.15	0.72
1:B:420:LEU:H	1:B:420:LEU:HD22	1.54	0.72
1:B:347:GLY:HA3	1:B:444:PRO:HG3	1.72	0.72
1:B:404:ILE:HG23	1:B:418:PHE:CE2	2.25	0.72
1:C:359:GLY:HA2	2:C:783:ADP:O5'	1.90	0.72
1:C:332:ILE:HD12	1:C:367:ILE:HD11	1.72	0.72
1:D:270:LEU:HD21	1:D:296:LEU:HD22	1.71	0.71
1:E:501:VAL:HA	1:E:505:LEU:HB2	1.72	0.71
1:F:270:LEU:HD21	1:F:296:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ALA:HA	1:A:714:ILE:HD11	1.72	0.71
1:D:677:ALA:HA	1:D:714:ILE:HD11	1.72	0.71
1:B:501:VAL:CG1	1:B:527:ILE:HD13	2.20	0.71
1:C:677:ALA:HA	1:C:714:ILE:HD11	1.72	0.71
1:D:586:GLN:OE1	1:D:586:GLN:HA	1.90	0.71
1:A:559:VAL:HG21	1:D:337:ALA:HB1	1.72	0.71
1:F:347:GLY:HA3	1:F:444:PRO:HG3	1.71	0.71
1:C:506:LEU:HB3	1:C:507:PRO:HD3	1.72	0.71
1:D:347:GLY:HA3	1:D:444:PRO:HG3	1.71	0.71
1:D:501:VAL:HA	1:D:505:LEU:HB2	1.71	0.71
1:E:300:PRO:HB2	1:E:414:LEU:HB3	1.71	0.71
1:F:506:LEU:HB3	1:F:507:PRO:HD3	1.71	0.71
1:B:505:LEU:HD22	1:B:544:GLU:HG3	1.72	0.71
1:C:267:GLU:HA	1:C:270:LEU:HD12	1.73	0.70
1:B:274:ASN:C	1:B:276:TYR:H	1.94	0.70
1:D:506:LEU:HD21	1:D:522:LEU:HD21	1.72	0.70
1:E:506:LEU:HB3	1:E:507:PRO:HD3	1.72	0.70
1:E:352:LEU:HD22	1:E:489:ILE:HD11	1.73	0.70
1:A:271:LYS:HA	1:A:274:ASN:HB3	1.74	0.70
1:E:522:LEU:HD12	1:E:527:ILE:HG12	1.73	0.70
1:B:267:GLU:HA	1:B:270:LEU:HD12	1.72	0.70
1:B:602:THR:HG22	1:B:604:VAL:H	1.56	0.70
1:C:378:ILE:O	1:C:378:ILE:HG12	1.92	0.70
1:E:271:LYS:HA	1:E:274:ASN:HB3	1.72	0.70
1:D:506:LEU:HB3	1:D:507:PRO:HD3	1.74	0.70
1:D:602:THR:HG22	1:D:604:VAL:H	1.56	0.70
1:C:505:LEU:HD22	1:C:544:GLU:HG3	1.74	0.70
1:F:271:LYS:HA	1:F:274:ASN:HB3	1.73	0.70
1:A:347:GLY:HA3	1:A:444:PRO:HG3	1.73	0.70
1:D:271:LYS:HA	1:D:274:ASN:HB3	1.74	0.70
1:D:420:LEU:HD22	1:D:420:LEU:H	1.57	0.70
1:A:337:ALA:HB1	1:C:556:LYS:HA	1.71	0.70
1:D:702:THR:O	1:D:735:PRO:HD3	1.90	0.70
1:B:569:THR:H	1:B:572:ASN:HB2	1.56	0.70
1:C:271:LYS:HA	1:C:274:ASN:HB3	1.74	0.70
1:C:347:GLY:HA3	1:C:444:PRO:HG3	1.73	0.70
1:F:441:VAL:HG13	1:F:442:LEU:HG	1.73	0.70
1:F:671:VAL:CG2	1:F:672:PRO:HD2	2.22	0.70
1:C:350:LEU:N	1:C:350:LEU:HD12	1.98	0.69
1:D:266:LYS:HG3	1:D:267:GLU:N	2.07	0.69
1:C:349:ILE:HD12	1:C:349:ILE:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:LYS:O	1:C:519:ASN:HB2	1.92	0.69
1:C:737:ASP:HB3	1:E:583:ARG:HH12	1.57	0.69
1:F:501:VAL:HA	1:F:505:LEU:HB2	1.73	0.69
1:B:338:VAL:HG21	1:F:552:ARG:HG3	1.74	0.69
1:A:441:VAL:HG13	1:A:442:LEU:HG	1.75	0.69
1:B:271:LYS:HA	1:B:274:ASN:HB3	1.74	0.69
1:B:421:ASP:O	1:B:469:THR:HB	1.92	0.69
1:E:274:ASN:C	1:E:276:TYR:H	1.96	0.69
1:A:506:LEU:HD12	1:A:510:ILE:HG12	1.74	0.69
1:B:677:ALA:HA	1:B:714:ILE:HD11	1.72	0.69
1:F:267:GLU:HA	1:F:270:LEU:HD12	1.75	0.69
1:D:274:ASN:C	1:D:276:TYR:H	1.96	0.69
1:C:266:LYS:HG3	1:C:267:GLU:N	2.08	0.69
1:F:464:VAL:O	1:F:466:PHE:HD1	1.76	0.69
1:B:516:LYS:HA	1:B:516:LYS:NZ	2.08	0.69
1:D:464:VAL:O	1:D:466:PHE:HD1	1.76	0.69
1:D:516:LYS:NZ	1:D:516:LYS:HA	2.07	0.69
1:E:347:GLY:HA3	1:E:444:PRO:HG3	1.73	0.69
1:D:414:LEU:O	1:D:416:PRO:HD3	1.93	0.69
1:D:421:ASP:O	1:D:469:THR:HB	1.92	0.69
1:F:274:ASN:C	1:F:276:TYR:H	1.96	0.69
1:B:464:VAL:O	1:B:466:PHE:HD1	1.76	0.69
1:B:522:LEU:HB3	1:B:568:VAL:HG13	1.73	0.68
1:D:532:ARG:HG2	1:D:584:TYR:CE2	2.28	0.68
1:C:274:ASN:C	1:C:276:TYR:H	1.97	0.68
1:A:501:VAL:HA	1:A:505:LEU:HB2	1.74	0.68
1:C:256:ILE:HD11	1:C:293:ILE:HD11	1.76	0.68
1:B:556:LYS:HA	1:E:337:ALA:HB1	1.75	0.68
1:E:516:LYS:NZ	1:E:516:LYS:HA	2.08	0.68
1:F:424:ASP:HB2	1:F:475:THR:HG23	1.76	0.68
1:F:266:LYS:HG3	1:F:267:GLU:N	2.08	0.68
1:F:295:TRP:CZ3	1:F:405:ILE:HG21	2.28	0.68
1:B:337:ALA:HB3	1:F:556:LYS:HA	1.75	0.68
1:E:335:TYR:HE2	1:E:465:LEU:HD21	1.57	0.68
1:E:420:LEU:H	1:E:420:LEU:HD22	1.58	0.68
1:A:516:LYS:HA	1:A:516:LYS:NZ	2.09	0.68
1:C:506:LEU:HD12	1:C:510:ILE:HG12	1.76	0.68
1:E:505:LEU:HD22	1:E:544:GLU:HG3	1.75	0.68
1:E:421:ASP:O	1:E:469:THR:HB	1.94	0.67
1:E:646:LYS:H	1:E:646:LYS:HD2	1.58	0.67
1:E:702:THR:O	1:E:735:PRO:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:738:ASN:O	1:F:741:ASP:HB2	1.94	0.67
1:A:464:VAL:O	1:A:466:PHE:HD1	1.76	0.67
1:E:266:LYS:HG3	1:E:267:GLU:N	2.09	0.67
1:F:420:LEU:HD22	1:F:420:LEU:H	1.58	0.67
1:F:506:LEU:HD12	1:F:510:ILE:HG12	1.77	0.67
1:A:267:GLU:HA	1:A:270:LEU:HD12	1.75	0.67
1:A:274:ASN:C	1:A:276:TYR:H	1.96	0.67
1:A:420:LEU:HD21	1:A:466:PHE:HD2	1.59	0.67
1:F:505:LEU:HD22	1:F:544:GLU:HG3	1.77	0.67
1:A:266:LYS:HG3	1:A:267:GLU:N	2.09	0.67
1:C:317:LEU:HD23	1:C:317:LEU:O	1.94	0.67
1:B:556:LYS:HA	1:E:337:ALA:CB	2.24	0.67
1:B:270:LEU:HD21	1:B:296:LEU:HD22	1.75	0.67
1:E:464:VAL:O	1:E:466:PHE:HD1	1.77	0.67
1:B:702:THR:O	1:B:735:PRO:HD3	1.94	0.67
1:E:267:GLU:HA	1:E:270:LEU:HD12	1.77	0.67
1:E:671:VAL:CG2	1:E:672:PRO:HD2	2.23	0.67
1:D:441:VAL:HG13	1:D:442:LEU:HG	1.76	0.67
1:D:267:GLU:HA	1:D:270:LEU:HD12	1.76	0.66
1:D:501:VAL:CG1	1:D:527:ILE:HD13	2.24	0.66
1:A:506:LEU:HB3	1:A:507:PRO:HD3	1.75	0.66
1:C:424:ASP:HB2	1:C:475:THR:HG23	1.77	0.66
1:C:702:THR:O	1:C:735:PRO:HD3	1.95	0.66
1:E:441:VAL:HG13	1:E:442:LEU:HG	1.78	0.66
1:A:702:THR:O	1:A:735:PRO:HD3	1.96	0.66
1:F:702:THR:O	1:F:735:PRO:HD3	1.96	0.66
1:B:266:LYS:HG3	1:B:267:GLU:N	2.09	0.66
1:F:421:ASP:O	1:F:469:THR:HB	1.96	0.66
2:C:783:ADP:O1B	2:C:783:ADP:O1A	2.14	0.66
1:D:646:LYS:H	1:D:646:LYS:HD2	1.60	0.66
1:B:414:LEU:O	1:B:416:PRO:HD3	1.96	0.66
1:C:258:GLU:HG2	1:C:260:GLY:H	1.60	0.66
1:C:501:VAL:CG1	1:C:527:ILE:HD13	2.26	0.66
1:D:569:THR:H	1:D:572:ASN:HB2	1.61	0.66
1:F:677:ALA:HA	1:F:714:ILE:HD11	1.78	0.66
1:D:505:LEU:CD2	1:D:544:GLU:HG3	2.25	0.66
1:E:506:LEU:HD12	1:E:510:ILE:HG12	1.76	0.66
1:D:424:ASP:HB2	1:D:475:THR:HG23	1.77	0.65
1:F:474:ALA:O	1:F:476:ILE:N	2.29	0.65
1:A:252:LEU:O	1:A:256:ILE:HG13	1.97	0.65
1:A:258:GLU:HG2	1:A:260:GLY:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ARG:HD2	1:C:616:SER:OG	1.96	0.65
1:B:345:LEU:HD23	1:B:346:LYS:N	2.12	0.65
1:E:345:LEU:HD11	1:E:465:LEU:HD22	1.78	0.65
1:E:474:ALA:O	1:E:476:ILE:N	2.28	0.65
1:E:522:LEU:HB3	1:E:568:VAL:HG13	1.77	0.65
1:E:677:ALA:HA	1:E:714:ILE:HD11	1.77	0.65
1:A:602:THR:HG22	1:A:604:VAL:H	1.61	0.65
1:C:335:TYR:HE2	1:C:465:LEU:HD21	1.61	0.65
1:F:292:TYR:CZ	1:F:455:ILE:HA	2.31	0.65
1:F:646:LYS:HD2	1:F:646:LYS:H	1.61	0.65
1:C:474:ALA:O	1:C:476:ILE:N	2.30	0.65
1:F:300:PRO:HB2	1:F:414:LEU:HB3	1.79	0.65
1:F:579:LYS:O	1:F:579:LYS:HE2	1.96	0.65
1:A:421:ASP:O	1:A:469:THR:HB	1.96	0.65
1:C:420:LEU:HD21	1:C:466:PHE:HD2	1.61	0.65
1:A:579:LYS:HE2	1:A:579:LYS:O	1.96	0.65
1:F:352:LEU:HD22	1:F:489:ILE:HD11	1.77	0.65
1:A:332:ILE:HD12	1:A:367:ILE:HD11	1.79	0.65
1:B:352:LEU:HD22	1:B:489:ILE:HD11	1.79	0.65
1:C:464:VAL:O	1:C:466:PHE:HD1	1.80	0.65
1:E:349:ILE:HD12	1:E:349:ILE:O	1.97	0.65
1:F:252:LEU:O	1:F:256:ILE:HG13	1.97	0.65
1:B:299:LEU:HD12	1:B:301:TRP:HE1	1.62	0.64
1:C:362:SER:HB2	2:C:783:ADP:H5'1	1.78	0.64
1:A:424:ASP:HB2	1:A:475:THR:HG23	1.77	0.64
1:C:646:LYS:HD2	1:C:646:LYS:H	1.61	0.64
1:A:414:LEU:O	1:A:416:PRO:HD3	1.96	0.64
1:C:599:LEU:HD22	1:C:599:LEU:H	1.62	0.64
1:E:252:LEU:O	1:E:256:ILE:HG13	1.98	0.64
1:F:345:LEU:HD11	1:F:465:LEU:HD22	1.79	0.64
1:A:477:PRO:HB2	1:A:480:LEU:HD23	1.79	0.64
1:A:506:LEU:HD21	1:A:522:LEU:HD21	1.78	0.64
1:C:644:ARG:HE	1:C:657:HIS:CG	2.16	0.64
1:D:252:LEU:O	1:D:256:ILE:HG13	1.98	0.64
1:F:569:THR:H	1:F:572:ASN:HB2	1.62	0.64
1:B:258:GLU:HG2	1:B:259:ALA:N	2.13	0.64
1:D:256:ILE:HD11	1:D:293:ILE:HD11	1.79	0.64
1:B:252:LEU:O	1:B:256:ILE:HG13	1.98	0.64
1:B:258:GLU:HG2	1:B:260:GLY:H	1.62	0.64
1:E:644:ARG:HE	1:E:657:HIS:CG	2.16	0.64
1:F:414:LEU:O	1:F:416:PRO:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:644:ARG:HE	1:F:657:HIS:CG	2.15	0.64
1:A:646:LYS:H	1:A:646:LYS:HD2	1.62	0.64
1:B:267:GLU:O	1:B:270:LEU:HB2	1.98	0.64
1:B:424:ASP:HB2	1:B:475:THR:HG23	1.79	0.64
1:E:588:GLU:HG2	1:E:589:THR:N	2.13	0.64
1:E:569:THR:H	1:E:572:ASN:HB2	1.62	0.64
1:F:258:GLU:HG2	1:F:260:GLY:H	1.61	0.64
1:B:493:THR:HG21	1:B:748:SER:CB	2.27	0.64
1:C:267:GLU:O	1:C:270:LEU:HB2	1.97	0.64
1:C:360:LYS:HD2	1:C:469:THR:HG23	1.80	0.64
1:B:644:ARG:HE	1:B:657:HIS:CG	2.16	0.63
1:C:671:VAL:CG2	1:C:672:PRO:HD2	2.26	0.63
1:D:258:GLU:HG2	1:D:260:GLY:H	1.61	0.63
1:D:345:LEU:HD11	1:D:465:LEU:HD22	1.79	0.63
1:D:506:LEU:HD12	1:D:510:ILE:HG12	1.79	0.63
1:E:258:GLU:HG2	1:E:260:GLY:H	1.62	0.63
1:E:253:THR:HA	1:E:256:ILE:HD12	1.79	0.63
1:E:256:ILE:HD11	1:E:293:ILE:HD11	1.80	0.63
1:E:249:VAL:HG12	1:E:278:LYS:HG2	1.81	0.63
1:E:501:VAL:CG1	1:E:527:ILE:HD13	2.26	0.63
1:A:644:ARG:HE	1:A:657:HIS:CG	2.16	0.63
1:B:296:LEU:HA	1:B:299:LEU:HD21	1.79	0.63
1:B:583:ARG:NH1	1:E:737:ASP:OD1	2.31	0.63
1:A:493:THR:HG21	1:A:748:SER:HB2	1.81	0.63
1:E:424:ASP:HB2	1:E:475:THR:HG23	1.81	0.63
1:A:412:GLY:O	1:A:413:LYS:HG2	1.98	0.63
1:B:412:GLY:O	1:B:413:LYS:HG2	1.99	0.63
1:B:444:PRO:HA	1:B:447:ASN:HD21	1.64	0.63
1:C:420:LEU:H	1:C:420:LEU:HD22	1.64	0.63
1:F:253:THR:HA	1:F:256:ILE:HD12	1.81	0.63
1:A:444:PRO:HA	1:A:447:ASN:HD21	1.64	0.63
1:B:493:THR:CG2	1:B:748:SER:HB2	2.25	0.63
1:E:412:GLY:O	1:E:413:LYS:HG2	1.99	0.63
1:C:421:ASP:O	1:C:469:THR:HB	1.98	0.63
1:D:300:PRO:HB3	1:D:412:GLY:C	2.20	0.63
1:F:256:ILE:HD11	1:F:293:ILE:HD11	1.80	0.63
1:F:412:GLY:O	1:F:413:LYS:HG2	1.98	0.63
1:A:256:ILE:HD11	1:A:293:ILE:HD11	1.81	0.62
1:C:258:GLU:HG2	1:C:259:ALA:N	2.14	0.62
1:C:350:LEU:CD1	1:C:350:LEU:H	1.98	0.62
1:A:317:LEU:O	1:A:317:LEU:HD23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HA	1:A:256:ILE:HD12	1.80	0.62
1:A:360:LYS:HD2	1:A:469:THR:HG23	1.80	0.62
1:A:345:LEU:HD11	1:A:465:LEU:HD22	1.82	0.62
1:B:332:ILE:HD12	1:B:367:ILE:HD11	1.80	0.62
1:B:506:LEU:HD12	1:B:506:LEU:C	2.20	0.62
1:D:332:ILE:HD12	1:D:367:ILE:HD11	1.80	0.62
1:F:477:PRO:HB2	1:F:480:LEU:HD23	1.82	0.62
1:A:738:ASN:O	1:A:741:ASP:HB2	2.00	0.62
1:B:315:GLY:C	1:B:316:ARG:HD2	2.20	0.62
1:C:252:LEU:O	1:C:256:ILE:HG13	1.99	0.62
1:C:345:LEU:HD23	1:C:346:LYS:N	2.15	0.62
1:E:477:PRO:HB2	1:E:480:LEU:HD23	1.81	0.62
1:A:352:LEU:HD22	1:A:489:ILE:HD11	1.81	0.62
1:B:277:GLU:HB3	1:B:279:ILE:O	1.99	0.62
1:B:299:LEU:CD1	1:B:301:TRP:HE1	2.12	0.62
1:D:412:GLY:O	1:D:413:LYS:HG2	1.99	0.62
1:D:249:VAL:HG12	1:D:278:LYS:HG2	1.81	0.62
1:D:345:LEU:HD23	1:D:346:LYS:N	2.15	0.62
1:F:613:VAL:HA	1:F:663:HIS:O	2.00	0.62
1:C:253:THR:HA	1:C:256:ILE:HD12	1.82	0.62
1:A:315:GLY:C	1:A:316:ARG:HD2	2.20	0.61
1:A:569:THR:H	1:A:572:ASN:HB2	1.64	0.61
1:A:734:ALA:HB1	1:A:735:PRO:HD2	1.82	0.61
1:B:256:ILE:HD11	1:B:293:ILE:HD11	1.82	0.61
1:D:258:GLU:HG2	1:D:259:ALA:N	2.15	0.61
1:F:602:THR:HG22	1:F:604:VAL:H	1.64	0.61
1:B:474:ALA:O	1:B:476:ILE:N	2.33	0.61
1:C:412:GLY:O	1:C:413:LYS:HG2	1.99	0.61
1:D:671:VAL:CG2	1:D:672:PRO:HD2	2.28	0.61
1:E:734:ALA:HB1	1:E:735:PRO:HD2	1.82	0.61
1:F:444:PRO:HA	1:F:447:ASN:HD21	1.66	0.61
1:B:360:LYS:HD2	1:B:469:THR:HG23	1.82	0.61
1:B:646:LYS:HD2	1:B:646:LYS:H	1.64	0.61
1:D:644:ARG:HE	1:D:657:HIS:CG	2.17	0.61
1:F:368:ALA:HB2	1:F:417:VAL:HG21	1.82	0.61
1:A:258:GLU:HG2	1:A:259:ALA:N	2.14	0.61
1:B:441:VAL:HG13	1:B:442:LEU:HG	1.81	0.61
1:B:253:THR:HA	1:B:256:ILE:HD12	1.80	0.61
1:C:249:VAL:HG12	1:C:278:LYS:HG2	1.81	0.61
1:D:277:GLU:HB3	1:D:279:ILE:O	2.01	0.61
1:F:516:LYS:HZ1	1:F:516:LYS:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:LEU:O	1:C:686:LEU:HD22	2.01	0.61
1:A:474:ALA:O	1:A:476:ILE:N	2.33	0.61
1:D:315:GLY:C	1:D:316:ARG:HD2	2.21	0.61
1:D:565:ARG:HG2	1:D:566:ILE:N	2.14	0.61
1:E:444:PRO:HA	1:E:447:ASN:HD21	1.66	0.61
1:B:506:LEU:HD12	1:B:510:ILE:HG12	1.81	0.61
1:A:249:VAL:HG12	1:A:278:LYS:HG2	1.82	0.61
1:B:565:ARG:HG2	1:B:566:ILE:N	2.14	0.61
1:C:277:GLU:HB3	1:C:279:ILE:O	2.01	0.61
1:E:533:TYR:HB3	1:E:580:ARG:HD2	1.83	0.61
1:B:613:VAL:HA	1:B:663:HIS:O	2.01	0.61
1:C:315:GLY:C	1:C:316:ARG:HD2	2.21	0.61
1:C:345:LEU:HD11	1:C:465:LEU:HD22	1.82	0.61
1:E:602:THR:HG22	1:E:604:VAL:H	1.64	0.61
1:D:253:THR:HA	1:D:256:ILE:HD12	1.81	0.60
1:D:474:ALA:O	1:D:476:ILE:N	2.34	0.60
1:E:258:GLU:HG2	1:E:259:ALA:N	2.15	0.60
1:F:258:GLU:HG2	1:F:259:ALA:N	2.14	0.60
1:F:345:LEU:HD23	1:F:346:LYS:N	2.16	0.60
1:F:540:VAL:HG23	2:F:783:ADP:HI'	1.82	0.60
1:A:300:PRO:HG3	1:A:412:GLY:C	2.22	0.60
1:D:349:ILE:O	1:D:349:ILE:HD12	2.01	0.60
1:F:277:GLU:HB3	1:F:279:ILE:O	2.02	0.60
1:A:560:ALA:O	1:A:562:GLU:HG3	2.01	0.60
1:B:261:MET:H	1:B:262:PRO:HD3	1.66	0.60
1:B:360:LYS:N	2:B:783:ADP:O1B	2.34	0.60
1:C:477:PRO:HB2	1:C:480:LEU:HD23	1.82	0.60
1:C:738:ASN:O	1:C:741:ASP:HB2	2.00	0.60
1:D:560:ALA:O	1:D:562:GLU:HG3	2.01	0.60
1:F:249:VAL:HG12	1:F:278:LYS:HG2	1.82	0.60
1:C:579:LYS:O	1:C:579:LYS:HE2	2.01	0.60
1:D:361:THR:HB	2:D:783:ADP:O1A	2.01	0.60
1:E:315:GLY:C	1:E:316:ARG:HD2	2.22	0.60
1:B:345:LEU:HD11	1:B:465:LEU:HD22	1.82	0.60
1:B:738:ASN:O	1:B:741:ASP:HB2	2.00	0.60
1:D:444:PRO:HA	1:D:447:ASN:HD21	1.67	0.60
1:F:565:ARG:HG2	1:F:566:ILE:N	2.16	0.60
1:F:586:GLN:N	1:F:586:GLN:OE1	2.34	0.60
1:B:359:GLY:HA2	2:B:783:ADP:C5'	2.31	0.60
1:B:560:ALA:O	1:B:562:GLU:HG3	2.02	0.60
1:D:260:GLY:O	1:D:261:MET:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:TYR:HE2	1:D:465:LEU:HD21	1.65	0.60
1:F:261:MET:H	1:F:262:PRO:HD3	1.67	0.60
1:A:345:LEU:HD23	1:A:346:LYS:N	2.16	0.60
1:B:260:GLY:O	1:B:261:MET:HB2	2.02	0.60
1:D:261:MET:N	1:D:262:PRO:HD3	2.17	0.60
1:F:357:GLY:O	1:F:539:GLY:CA	2.49	0.60
1:C:444:PRO:HA	1:C:447:ASN:HD21	1.66	0.60
1:C:469:THR:HG22	1:C:470:ALA:N	2.17	0.60
1:F:380:LEU:HB2	1:F:422:GLU:O	2.02	0.60
1:A:642:TYR:CD2	1:A:761:LEU:HD12	2.37	0.60
1:A:565:ARG:HG2	1:A:566:ILE:N	2.16	0.59
1:D:357:GLY:O	1:D:540:VAL:N	2.33	0.59
1:F:315:GLY:C	1:F:316:ARG:HD2	2.23	0.59
1:A:267:GLU:O	1:A:270:LEU:HB2	2.02	0.59
1:A:420:LEU:H	1:A:420:LEU:HD22	1.66	0.59
1:C:441:VAL:HG13	1:C:442:LEU:HG	1.83	0.59
1:E:345:LEU:HD23	1:E:346:LYS:N	2.17	0.59
1:F:357:GLY:N	2:F:783:ADP:O2B	2.35	0.59
1:A:277:GLU:HB3	1:A:279:ILE:O	2.01	0.59
1:C:380:LEU:HB2	1:C:422:GLU:O	2.02	0.59
1:C:496:GLU:O	1:C:500:ILE:HG13	2.03	0.59
1:C:602:THR:HG21	1:C:604:VAL:HG22	1.83	0.59
1:E:416:PRO:HD2	1:E:464:VAL:HG13	1.84	0.59
1:A:261:MET:N	1:A:262:PRO:HD3	2.17	0.59
1:B:267:GLU:HA	1:B:270:LEU:CG	2.32	0.59
1:E:261:MET:H	1:E:262:PRO:HD3	1.67	0.59
1:F:261:MET:N	1:F:262:PRO:HD3	2.18	0.59
1:F:328:VAL:O	1:F:332:ILE:HG12	2.02	0.59
1:B:249:VAL:HG12	1:B:278:LYS:HG2	1.82	0.59
1:B:380:LEU:HD12	1:B:423:ILE:HG23	1.83	0.59
1:A:341:LEU:HB3	1:C:514:GLY:O	2.03	0.59
1:C:516:LYS:CE	1:C:516:LYS:HA	2.33	0.59
1:E:261:MET:N	1:E:262:PRO:HD3	2.17	0.59
1:F:267:GLU:O	1:F:270:LEU:HB2	2.03	0.59
1:B:267:GLU:HA	1:B:270:LEU:CD1	2.33	0.59
1:D:261:MET:H	1:D:262:PRO:HD3	1.66	0.59
1:D:357:GLY:O	1:D:539:GLY:CA	2.51	0.59
1:F:260:GLY:O	1:F:261:MET:HB2	2.03	0.59
1:A:335:TYR:HE2	1:A:465:LEU:HD21	1.67	0.59
1:B:261:MET:N	1:B:262:PRO:HD3	2.17	0.59
1:C:260:GLY:O	1:C:261:MET:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:GLY:N	2:D:783:ADP:O1B	2.34	0.59
1:E:420:LEU:HD21	1:E:466:PHE:HD2	1.68	0.59
1:A:300:PRO:HB2	1:A:414:LEU:HB3	1.85	0.59
1:C:569:THR:H	1:C:572:ASN:HB2	1.67	0.59
1:C:506:LEU:CD2	1:C:522:LEU:HD21	2.32	0.58
1:C:533:TYR:HB3	1:C:580:ARG:HD2	1.84	0.58
1:E:277:GLU:HB3	1:E:279:ILE:O	2.03	0.58
1:D:352:LEU:HD22	1:D:489:ILE:HD11	1.83	0.58
1:B:276:TYR:CZ	1:F:246:THR:HB	2.38	0.58
1:B:349:ILE:O	1:B:349:ILE:HD12	2.03	0.58
1:C:261:MET:N	1:C:262:PRO:HD3	2.18	0.58
1:C:565:ARG:HG2	1:C:566:ILE:N	2.16	0.58
1:E:380:LEU:HB2	1:E:422:GLU:O	2.03	0.58
1:C:506:LEU:HD12	1:C:506:LEU:C	2.24	0.58
1:D:420:LEU:HD21	1:D:466:PHE:HD2	1.68	0.58
1:E:589:THR:O	1:E:697:ARG:HD2	2.04	0.58
1:F:335:TYR:HE2	1:F:465:LEU:HD21	1.67	0.58
1:F:550:ILE:O	1:F:551:CYS:C	2.42	0.58
1:A:261:MET:H	1:A:262:PRO:HD3	1.66	0.58
1:A:461:LEU:O	1:A:464:VAL:HG23	2.04	0.58
1:B:593:VAL:HB	1:E:708:ARG:NH2	2.18	0.58
1:C:336:LEU:O	1:C:339:GLN:N	2.37	0.58
1:C:602:THR:CG2	1:C:604:VAL:HG22	2.33	0.58
1:E:317:LEU:O	1:E:317:LEU:HD23	2.04	0.58
1:A:671:VAL:CG2	1:A:672:PRO:HD2	2.33	0.58
1:E:590:GLU:HA	1:E:697:ARG:CD	2.33	0.58
1:F:506:LEU:CD2	1:F:522:LEU:HD21	2.33	0.58
1:A:267:GLU:HA	1:A:270:LEU:CG	2.34	0.58
1:C:584:TYR:CD1	1:C:584:TYR:C	2.76	0.58
1:D:477:PRO:HB2	1:D:480:LEU:HD23	1.85	0.58
1:E:613:VAL:HG23	1:E:685:ALA:HB1	1.86	0.58
1:A:260:GLY:O	1:A:261:MET:HB2	2.03	0.58
1:B:316:ARG:HD2	1:B:316:ARG:N	2.19	0.58
1:B:341:LEU:HD13	1:F:514:GLY:O	2.04	0.58
1:B:477:PRO:HB2	1:B:480:LEU:HD23	1.86	0.58
1:C:267:GLU:HA	1:C:270:LEU:CG	2.33	0.58
1:C:261:MET:H	1:C:262:PRO:HD3	1.68	0.58
1:E:260:GLY:O	1:E:261:MET:HB2	2.02	0.58
1:E:700:GLY:O	1:E:732:ILE:HA	2.04	0.58
1:C:705:ILE:HD11	1:C:761:LEU:HD21	1.86	0.57
1:B:336:LEU:O	1:B:339:GLN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:ALA:HB3	1:C:566:ILE:HD11	1.87	0.57
1:D:267:GLU:O	1:D:270:LEU:HB2	2.03	0.57
1:D:368:ALA:HB2	1:D:417:VAL:HG21	1.84	0.57
1:F:294:ASP:HA	1:F:297:VAL:HG23	1.86	0.57
1:B:335:TYR:HE2	1:B:465:LEU:HD21	1.68	0.57
1:B:439:LEU:O	1:B:441:VAL:N	2.37	0.57
1:A:420:LEU:HD21	1:A:466:PHE:CD2	2.40	0.57
1:E:439:LEU:O	1:E:441:VAL:N	2.38	0.57
1:B:536:ARG:NH1	1:B:536:ARG:CG	2.65	0.57
1:F:420:LEU:HD21	1:F:466:PHE:HD2	1.70	0.57
1:F:461:LEU:O	1:F:464:VAL:HG23	2.05	0.57
1:D:250:GLN:HA	1:D:253:THR:OG1	2.05	0.57
1:D:267:GLU:HA	1:D:270:LEU:CG	2.34	0.57
1:E:613:VAL:HA	1:E:663:HIS:O	2.03	0.57
1:A:316:ARG:N	1:A:316:ARG:HD2	2.19	0.57
1:B:250:GLN:HA	1:B:253:THR:OG1	2.05	0.57
1:B:586:GLN:HE22	1:B:729:LEU:HA	1.70	0.57
1:B:734:ALA:HB1	1:B:735:PRO:HD2	1.87	0.57
1:C:516:LYS:HZ1	1:C:516:LYS:HA	1.69	0.57
1:E:497:LYS:HG2	1:E:540:VAL:HG12	1.86	0.57
1:A:506:LEU:HD12	1:A:506:LEU:C	2.24	0.57
1:B:317:LEU:HD23	1:B:317:LEU:O	2.04	0.57
1:C:267:GLU:HA	1:C:270:LEU:CD1	2.34	0.57
1:E:262:PRO:HD2	1:E:301:TRP:CB	2.35	0.57
1:B:276:TYR:OH	1:F:247:GLY:N	2.37	0.57
1:A:439:LEU:O	1:A:441:VAL:N	2.38	0.57
1:C:506:LEU:HD21	1:C:522:LEU:CD2	2.34	0.57
1:C:734:ALA:HB1	1:C:735:PRO:HD2	1.86	0.56
1:E:250:GLN:HA	1:E:253:THR:OG1	2.05	0.56
1:E:350:LEU:N	1:E:350:LEU:HD12	2.07	0.56
1:D:602:THR:HG21	1:D:604:VAL:HG22	1.87	0.56
1:E:565:ARG:HG2	1:E:566:ILE:N	2.20	0.56
1:F:332:ILE:HD12	1:F:367:ILE:HD11	1.86	0.56
1:C:250:GLN:HA	1:C:253:THR:OG1	2.05	0.56
1:B:350:LEU:HD23	1:B:487:ILE:HD11	1.87	0.56
1:B:290:ARG:O	1:B:293:ILE:HG22	2.05	0.56
1:B:294:ASP:HA	1:B:297:VAL:HG23	1.88	0.56
1:C:294:ASP:HA	1:C:297:VAL:HG23	1.87	0.56
1:D:469:THR:O	1:D:470:ALA:HB2	2.05	0.56
1:D:596:VAL:HG23	1:D:685:ALA:HB2	1.87	0.56
1:E:438:MET:O	1:E:439:LEU:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:SER:CB	2:D:783:ADP:H5'1	2.35	0.56
1:E:267:GLU:O	1:E:270:LEU:HB2	2.04	0.56
1:F:586:GLN:HG2	1:F:698:GLU:CG	2.27	0.56
1:A:559:VAL:CG2	1:D:337:ALA:HB1	2.35	0.56
1:F:602:THR:HG21	1:F:604:VAL:HG22	1.86	0.56
1:A:294:ASP:HA	1:A:297:VAL:HG23	1.88	0.56
1:A:557:ALA:HB3	1:A:566:ILE:HD11	1.88	0.56
1:C:352:LEU:HD22	1:C:489:ILE:HD11	1.86	0.56
1:E:294:ASP:HA	1:E:297:VAL:HG23	1.88	0.56
1:F:267:GLU:HA	1:F:270:LEU:CG	2.36	0.56
1:F:602:THR:CG2	1:F:604:VAL:HG22	2.36	0.56
1:B:700:GLY:O	1:B:732:ILE:HA	2.06	0.56
1:C:439:LEU:O	1:C:441:VAL:N	2.39	0.56
1:D:636:ALA:C	1:D:638:ALA:H	2.08	0.56
1:F:250:GLN:HA	1:F:253:THR:OG1	2.04	0.56
1:A:350:LEU:N	1:A:350:LEU:HD12	2.11	0.56
1:D:380:LEU:HB2	1:D:422:GLU:O	2.05	0.56
1:E:316:ARG:N	1:E:316:ARG:HD2	2.21	0.56
1:E:579:LYS:O	1:E:579:LYS:HE2	2.06	0.56
1:F:560:ALA:O	1:F:562:GLU:HG3	2.05	0.56
1:A:250:GLN:HA	1:A:253:THR:OG1	2.05	0.56
1:A:328:VAL:O	1:A:332:ILE:HG12	2.05	0.55
1:A:336:LEU:O	1:A:339:GLN:N	2.39	0.55
1:B:756:ILE:HG13	1:B:767:HIS:CD2	2.41	0.55
1:C:290:ARG:O	1:C:293:ILE:HG22	2.06	0.55
1:D:316:ARG:N	1:D:316:ARG:HD2	2.20	0.55
1:E:267:GLU:HA	1:E:270:LEU:CG	2.37	0.55
1:F:267:GLU:HA	1:F:270:LEU:CD1	2.36	0.55
1:D:328:VAL:O	1:D:332:ILE:HG12	2.05	0.55
1:F:593:VAL:HG13	1:F:693:ARG:O	2.06	0.55
1:A:756:ILE:HG13	1:A:767:HIS:CD2	2.42	0.55
1:B:420:LEU:HD21	1:B:466:PHE:HD2	1.71	0.55
1:D:534:TYR:N	1:D:534:TYR:CD1	2.74	0.55
1:B:579:LYS:O	1:B:579:LYS:HE2	2.05	0.55
2:B:783:ADP:O4'	2:B:783:ADP:O2A	2.24	0.55
1:D:579:LYS:HE2	1:D:579:LYS:O	2.05	0.55
1:D:613:VAL:HA	1:D:663:HIS:O	2.05	0.55
1:A:469:THR:HG22	1:A:470:ALA:N	2.21	0.55
1:C:316:ARG:N	1:C:316:ARG:HD2	2.20	0.55
1:D:350:LEU:N	1:D:350:LEU:HD12	2.14	0.55
1:D:439:LEU:O	1:D:441:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLY:N	2:A:783:ADP:O2B	2.26	0.55
1:B:516:LYS:HA	1:B:516:LYS:CE	2.36	0.55
1:A:267:GLU:HA	1:A:270:LEU:CD1	2.36	0.55
1:D:290:ARG:O	1:D:293:ILE:HG22	2.06	0.55
1:E:290:ARG:O	1:E:293:ILE:HG22	2.06	0.55
1:E:548:ALA:O	1:E:549:ALA:C	2.45	0.55
1:F:317:LEU:HD23	1:F:317:LEU:O	2.07	0.55
1:F:596:VAL:HG23	1:F:685:ALA:HB2	1.87	0.55
1:A:380:LEU:HB2	1:A:422:GLU:O	2.06	0.55
1:B:355:PRO:O	1:B:358:VAL:HG22	2.07	0.55
1:C:613:VAL:HA	1:C:663:HIS:O	2.07	0.55
1:D:336:LEU:O	1:D:339:GLN:N	2.39	0.55
1:D:635:SER:O	1:D:638:ALA:HB3	2.07	0.55
1:E:624:LEU:H	1:E:624:LEU:HD12	1.72	0.55
2:A:783:ADP:O2A	2:A:783:ADP:O4'	2.24	0.55
1:C:378:ILE:HD13	1:C:420:LEU:CD1	2.37	0.55
1:F:316:ARG:N	1:F:316:ARG:HD2	2.21	0.55
1:F:349:ILE:HD12	1:F:349:ILE:O	2.06	0.55
1:F:734:ALA:HB1	1:F:735:PRO:HD2	1.88	0.55
1:B:599:LEU:H	1:B:599:LEU:HD22	1.71	0.54
1:D:461:LEU:O	1:D:464:VAL:HG23	2.07	0.54
1:E:756:ILE:HG13	1:E:767:HIS:CD2	2.42	0.54
1:B:328:VAL:O	1:B:332:ILE:HG12	2.07	0.54
1:C:270:LEU:HD21	1:C:296:LEU:CD2	2.37	0.54
1:D:573:LEU:HG	1:D:577:ILE:HD11	1.88	0.54
1:E:380:LEU:HD12	1:E:423:ILE:HG23	1.89	0.54
1:E:378:ILE:HD13	1:E:420:LEU:CD1	2.37	0.54
1:F:408:MET:HE2	1:F:408:MET:H	1.72	0.54
1:D:602:THR:CG2	1:D:604:VAL:HG22	2.38	0.54
1:D:700:GLY:O	1:D:732:ILE:HA	2.08	0.54
1:F:557:ALA:HB3	1:F:566:ILE:HD11	1.89	0.54
1:F:569:THR:CG2	1:F:572:ASN:H	2.20	0.54
1:C:560:ALA:O	1:C:562:GLU:HG3	2.07	0.54
1:D:362:SER:HB3	2:D:783:ADP:H5'1	1.89	0.54
1:D:516:LYS:O	1:D:519:ASN:HB2	2.07	0.54
1:E:360:LYS:HD2	1:E:469:THR:HG23	1.89	0.54
1:A:273:LEU:HD13	1:A:289:ILE:HD12	1.90	0.54
1:B:282:SER:HA	1:B:286:SER:HB3	1.89	0.54
1:D:267:GLU:HA	1:D:270:LEU:CD1	2.37	0.54
1:D:579:LYS:H	1:D:579:LYS:NZ	2.05	0.54
1:E:282:SER:HA	1:E:286:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:ARG:O	1:F:293:ILE:HG22	2.07	0.54
1:F:522:LEU:HB3	1:F:568:VAL:CG1	2.36	0.54
1:B:708:ARG:HD3	1:F:613:VAL:O	2.07	0.54
1:A:700:GLY:O	1:A:732:ILE:HA	2.07	0.54
1:B:404:ILE:O	1:B:405:ILE:C	2.45	0.54
1:C:420:LEU:HD21	1:C:466:PHE:CD2	2.41	0.54
1:C:536:ARG:CG	1:C:536:ARG:NH1	2.62	0.54
1:D:294:ASP:HA	1:D:297:VAL:HG23	1.90	0.54
1:C:569:THR:CG2	1:C:572:ASN:H	2.21	0.54
1:D:516:LYS:HA	1:D:516:LYS:CE	2.37	0.54
1:A:613:VAL:HA	1:A:663:HIS:O	2.08	0.54
1:B:347:GLY:CA	1:B:444:PRO:HG3	2.38	0.54
1:B:350:LEU:HD12	1:B:350:LEU:N	2.10	0.54
1:A:583:ARG:NH1	1:D:737:ASP:HB3	2.22	0.54
1:E:267:GLU:HA	1:E:270:LEU:CD1	2.38	0.54
1:B:469:THR:HG22	1:B:470:ALA:N	2.23	0.54
1:C:282:SER:HA	1:C:286:SER:HB3	1.90	0.54
1:D:250:GLN:HA	1:D:253:THR:HG1	1.73	0.54
1:E:424:ASP:N	1:E:424:ASP:OD1	2.41	0.54
1:C:250:GLN:HA	1:C:253:THR:HG1	1.74	0.53
1:D:416:PRO:HD2	1:D:464:VAL:HG13	1.89	0.53
1:D:536:ARG:NH1	1:D:536:ARG:HG3	2.16	0.53
1:D:599:LEU:H	1:D:599:LEU:HD22	1.73	0.53
1:E:332:ILE:HD12	1:E:367:ILE:HD11	1.89	0.53
1:E:506:LEU:C	1:E:506:LEU:HD12	2.28	0.53
1:C:338:VAL:HG21	1:E:552:ARG:HG3	1.90	0.53
1:E:560:ALA:O	1:E:562:GLU:HG3	2.08	0.53
1:F:510:ILE:HG22	1:F:515:LEU:O	2.08	0.53
1:A:540:VAL:CG2	2:A:783:ADP:C8	2.90	0.53
1:A:636:ALA:C	1:A:638:ALA:H	2.10	0.53
1:E:506:LEU:CD2	1:E:522:LEU:HD21	2.37	0.53
1:F:516:LYS:HE2	1:F:516:LYS:HA	1.90	0.53
1:A:282:SER:HA	1:A:286:SER:HB3	1.90	0.53
1:C:700:GLY:O	1:C:732:ILE:HA	2.07	0.53
1:D:438:MET:O	1:D:439:LEU:C	2.47	0.53
1:E:492:TYR:OH	2:E:783:ADP:N6	2.41	0.53
1:A:250:GLN:HA	1:A:253:THR:HG1	1.74	0.53
1:B:438:MET:O	1:B:439:LEU:C	2.45	0.53
1:C:368:ALA:HB2	1:C:417:VAL:HG21	1.90	0.53
1:C:599:LEU:HD22	1:C:599:LEU:N	2.23	0.53
1:C:644:ARG:NE	1:C:657:HIS:CG	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:GLU:HA	1:D:697:ARG:CD	2.38	0.53
1:A:705:ILE:HD11	1:A:761:LEU:HD21	1.91	0.53
1:A:747:GLU:H	1:A:747:GLU:CD	2.12	0.53
1:B:300:PRO:HB2	1:B:414:LEU:HB3	1.90	0.53
1:B:305:THR:HB	1:B:415:ASN:HD22	1.74	0.53
1:D:536:ARG:CG	1:D:536:ARG:NH1	2.64	0.53
1:E:461:LEU:O	1:E:464:VAL:HG23	2.09	0.53
1:E:534:TYR:N	1:E:534:TYR:CD1	2.77	0.53
1:F:362:SER:HB2	2:F:783:ADP:H5'1	1.89	0.53
1:A:347:GLY:CA	1:A:444:PRO:HG3	2.39	0.53
1:D:317:LEU:O	1:D:317:LEU:HD23	2.09	0.53
1:F:347:GLY:CA	1:F:444:PRO:HG3	2.37	0.53
1:B:557:ALA:HB3	1:B:566:ILE:HD11	1.90	0.53
1:C:438:MET:O	1:C:439:LEU:C	2.46	0.53
1:E:611:ILE:HD12	1:E:681:THR:CG2	2.39	0.53
1:F:644:ARG:NE	1:F:657:HIS:CG	2.77	0.53
1:A:380:LEU:HD12	1:A:423:ILE:HG23	1.91	0.53
1:B:380:LEU:HB2	1:B:422:GLU:O	2.08	0.53
1:D:533:TYR:HB3	1:D:580:ARG:HD2	1.91	0.53
1:E:307:ASP:HB3	1:E:309:LEU:HD21	1.91	0.53
1:E:569:THR:CG2	1:E:572:ASN:H	2.22	0.53
1:A:408:MET:H	1:A:408:MET:HE2	1.74	0.53
1:B:277:GLU:C	1:B:279:ILE:N	2.62	0.53
1:E:599:LEU:HD22	1:E:599:LEU:H	1.74	0.53
1:F:439:LEU:O	1:F:441:VAL:N	2.41	0.53
1:A:438:MET:O	1:A:439:LEU:C	2.46	0.53
1:A:635:SER:O	1:A:638:ALA:HB3	2.09	0.53
1:B:404:ILE:HG23	1:B:418:PHE:HE2	1.73	0.53
1:E:328:VAL:O	1:E:332:ILE:HG12	2.09	0.53
1:B:276:TYR:CE2	1:F:246:THR:HG21	2.43	0.53
1:F:334:GLU:O	1:F:338:VAL:HB	2.09	0.53
1:B:636:ALA:C	1:B:638:ALA:H	2.12	0.52
1:B:644:ARG:NE	1:B:657:HIS:CG	2.77	0.52
1:B:671:VAL:CG2	1:B:672:PRO:HD2	2.37	0.52
1:E:506:LEU:HD21	1:E:522:LEU:CD2	2.38	0.52
1:E:593:VAL:HG13	1:E:693:ARG:O	2.08	0.52
1:F:506:LEU:HD21	1:F:522:LEU:CD2	2.37	0.52
1:B:747:GLU:H	1:B:747:GLU:CD	2.10	0.52
1:C:313:GLU:O	1:C:315:GLY:N	2.43	0.52
1:D:497:LYS:HG2	1:D:540:VAL:HG12	1.91	0.52
1:D:734:ALA:HB1	1:D:735:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:SER:HA	1:F:286:SER:HB3	1.90	0.52
1:A:313:GLU:O	1:A:315:GLY:N	2.42	0.52
1:E:536:ARG:NH1	1:E:536:ARG:CG	2.64	0.52
1:B:336:LEU:HA	1:B:339:GLN:HB3	1.92	0.52
1:A:644:ARG:HB3	1:C:616:SER:HB2	1.92	0.52
1:E:469:THR:HG22	1:E:470:ALA:N	2.25	0.52
1:E:505:LEU:CD2	1:E:544:GLU:HG3	2.37	0.52
1:F:247:GLY:C	1:F:249:VAL:H	2.13	0.52
1:F:493:THR:O	1:F:494:GLU:C	2.48	0.52
1:A:644:ARG:NE	1:A:657:HIS:CG	2.77	0.52
1:B:461:LEU:O	1:B:464:VAL:HG23	2.10	0.52
1:B:635:SER:O	1:B:638:ALA:HB3	2.10	0.52
1:C:347:GLY:CA	1:C:444:PRO:HG3	2.40	0.52
1:C:636:ALA:C	1:C:638:ALA:H	2.12	0.52
1:E:336:LEU:O	1:E:339:GLN:N	2.43	0.52
1:F:250:GLN:HA	1:F:253:THR:HG1	1.73	0.52
1:A:404:ILE:O	1:A:405:ILE:C	2.47	0.52
1:B:548:ALA:O	1:B:549:ALA:C	2.47	0.52
1:C:406:GLN:O	1:C:407:GLY:C	2.48	0.52
1:F:378:ILE:HD13	1:F:420:LEU:CD1	2.39	0.52
1:F:448:SER:O	1:F:460:ASP:HA	2.08	0.52
1:F:469:THR:HG22	1:F:470:ALA:N	2.24	0.52
1:A:290:ARG:O	1:A:293:ILE:HG22	2.10	0.52
1:A:406:GLN:O	1:A:407:GLY:C	2.48	0.52
1:A:469:THR:O	1:A:470:ALA:HB2	2.09	0.52
1:B:448:SER:O	1:B:460:ASP:HA	2.10	0.52
1:D:378:ILE:HD13	1:D:420:LEU:CD1	2.40	0.52
1:A:274:ASN:C	1:A:276:TYR:N	2.64	0.52
1:C:328:VAL:O	1:C:332:ILE:HG12	2.10	0.52
1:E:516:LYS:CE	1:E:516:LYS:HA	2.40	0.52
1:E:747:GLU:H	1:E:747:GLU:CD	2.13	0.52
1:B:414:LEU:C	1:B:416:PRO:HD3	2.30	0.52
1:D:347:GLY:CA	1:D:444:PRO:HG3	2.38	0.52
1:D:569:THR:CG2	1:D:572:ASN:H	2.22	0.52
1:E:496:GLU:O	1:E:500:ILE:HG13	2.10	0.52
1:F:599:LEU:HD22	1:F:599:LEU:H	1.75	0.52
1:F:611:ILE:HD12	1:F:681:THR:CG2	2.39	0.52
1:F:686:LEU:O	1:F:686:LEU:HD22	2.10	0.52
1:F:714:ILE:HB	1:F:735:PRO:HG2	1.91	0.52
1:B:569:THR:HG22	1:B:572:ASN:OD1	2.10	0.51
1:B:706:THR:OG1	1:B:710:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LEU:HB3	1:C:507:PRO:CD	2.40	0.51
1:C:522:LEU:HB3	1:C:568:VAL:CG1	2.36	0.51
1:D:274:ASN:C	1:D:276:TYR:N	2.63	0.51
1:D:548:ALA:O	1:D:549:ALA:C	2.49	0.51
1:D:557:ALA:HB3	1:D:566:ILE:HD11	1.92	0.51
1:D:613:VAL:HG23	1:D:685:ALA:HB1	1.92	0.51
1:A:414:LEU:C	1:A:416:PRO:HD3	2.31	0.51
1:A:602:THR:HG21	1:A:604:VAL:HG22	1.90	0.51
1:A:624:LEU:HD12	1:A:624:LEU:H	1.74	0.51
1:B:408:MET:H	1:B:408:MET:HE2	1.75	0.51
1:C:656:PHE:C	1:C:658:GLU:H	2.13	0.51
1:D:522:LEU:HB3	1:D:568:VAL:CG1	2.39	0.51
1:F:277:GLU:C	1:F:279:ILE:N	2.63	0.51
1:A:308:LYS:O	1:A:309:LEU:HD23	2.11	0.51
1:A:516:LYS:HA	1:A:516:LYS:CE	2.41	0.51
1:A:714:ILE:HG23	1:A:715:GLY:N	2.24	0.51
1:B:506:LEU:HD12	1:B:506:LEU:O	2.10	0.51
1:E:273:LEU:HD13	1:E:289:ILE:HD12	1.92	0.51
1:E:404:ILE:O	1:E:405:ILE:C	2.49	0.51
1:F:362:SER:HB2	2:F:783:ADP:C5'	2.40	0.51
1:F:438:MET:O	1:F:439:LEU:C	2.48	0.51
1:A:569:THR:CG2	1:A:572:ASN:H	2.22	0.51
1:B:409:LYS:C	1:B:411:ALA:H	2.13	0.51
1:B:624:LEU:H	1:B:624:LEU:HD12	1.75	0.51
1:D:282:SER:HA	1:D:286:SER:HB3	1.91	0.51
1:B:274:ASN:C	1:B:276:TYR:N	2.62	0.51
1:B:380:LEU:HD12	1:B:423:ILE:CG2	2.40	0.51
1:C:334:GLU:O	1:C:338:VAL:HB	2.11	0.51
1:C:624:LEU:H	1:C:624:LEU:HD12	1.76	0.51
1:D:273:LEU:HD13	1:D:289:ILE:HD12	1.92	0.51
1:F:506:LEU:C	1:F:506:LEU:HD12	2.30	0.51
1:F:569:THR:HG22	1:F:572:ASN:OD1	2.11	0.51
1:F:533:TYR:HB3	1:F:580:ARG:HD2	1.92	0.51
1:A:448:SER:O	1:A:460:ASP:HA	2.11	0.51
1:A:462:SER:HB2	1:A:463:LYS:HD2	1.93	0.51
1:A:533:TYR:HB3	1:A:580:ARG:HD2	1.92	0.51
1:B:247:GLY:C	1:B:249:VAL:H	2.14	0.51
1:C:448:SER:O	1:C:460:ASP:HA	2.11	0.51
1:D:308:LYS:O	1:D:309:LEU:HD23	2.11	0.51
1:D:420:LEU:HD21	1:D:466:PHE:CD2	2.46	0.51
1:E:247:GLY:C	1:E:249:VAL:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:PRO:CD	1:E:301:TRP:HB2	2.40	0.51
1:E:274:ASN:C	1:E:276:TYR:N	2.64	0.51
1:F:273:LEU:HD13	1:F:289:ILE:HD12	1.93	0.51
1:A:322:HIS:CE1	1:A:363:LEU:HD23	2.46	0.51
1:A:438:MET:O	1:A:440:GLU:N	2.44	0.51
1:C:747:GLU:H	1:C:747:GLU:CD	2.13	0.51
1:D:404:ILE:O	1:D:405:ILE:C	2.49	0.51
1:E:569:THR:HG22	1:E:572:ASN:OD1	2.11	0.51
1:F:406:GLN:O	1:F:407:GLY:C	2.49	0.51
1:A:286:SER:O	1:A:290:ARG:HB2	2.11	0.51
1:A:350:LEU:HD23	1:A:487:ILE:HD11	1.92	0.51
1:B:305:THR:HB	1:B:415:ASN:ND2	2.25	0.51
1:C:308:LYS:O	1:C:309:LEU:HD23	2.11	0.51
1:C:404:ILE:HG23	1:C:418:PHE:HE2	1.71	0.51
1:D:300:PRO:O	1:D:301:TRP:CD2	2.64	0.51
1:D:438:MET:O	1:D:440:GLU:N	2.44	0.51
2:D:783:ADP:O2A	2:D:783:ADP:C4'	2.59	0.51
1:E:420:LEU:HD21	1:E:466:PHE:CD2	2.45	0.51
1:E:584:TYR:O	1:E:584:TYR:HD1	1.91	0.51
1:A:599:LEU:HD22	1:A:599:LEU:H	1.76	0.51
1:B:368:ALA:HB2	1:B:417:VAL:HG21	1.92	0.51
1:B:506:LEU:HD21	1:B:522:LEU:CD2	2.40	0.51
1:B:516:LYS:HA	1:B:516:LYS:HZ1	1.76	0.51
1:D:644:ARG:NE	1:D:657:HIS:CG	2.78	0.51
1:E:347:GLY:CA	1:E:444:PRO:HG3	2.40	0.51
1:E:602:THR:HG22	1:E:603:THR:N	2.26	0.51
1:F:438:MET:O	1:F:440:GLU:N	2.44	0.51
1:F:497:LYS:HG2	1:F:540:VAL:HG12	1.92	0.51
1:A:334:GLU:O	1:A:338:VAL:HB	2.11	0.51
1:B:250:GLN:HA	1:B:253:THR:HG1	1.74	0.51
1:B:286:SER:O	1:B:290:ARG:HB2	2.11	0.51
1:B:273:LEU:HD13	1:B:289:ILE:HD12	1.93	0.51
1:C:336:LEU:HA	1:C:339:GLN:HB3	1.93	0.51
1:D:611:ILE:HD12	1:D:681:THR:CG2	2.41	0.51
1:C:337:ALA:HB3	1:E:556:LYS:HA	1.92	0.51
1:E:644:ARG:NE	1:E:657:HIS:CG	2.78	0.51
1:F:624:LEU:HD12	1:F:624:LEU:H	1.75	0.51
1:F:586:GLN:NE2	1:F:698:GLU:HA	2.16	0.51
1:F:700:GLY:O	1:F:732:ILE:HA	2.10	0.51
1:F:705:ILE:HD11	1:F:761:LEU:HD21	1.92	0.51
1:B:274:ASN:O	1:B:276:TYR:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LEU:CD2	1:B:522:LEU:HD21	2.38	0.50
1:D:550:ILE:O	1:D:551:CYS:C	2.47	0.50
1:E:557:ALA:HB3	1:E:566:ILE:HD11	1.93	0.50
1:A:277:GLU:C	1:A:279:ILE:N	2.63	0.50
1:B:322:HIS:CE1	1:B:363:LEU:HD23	2.46	0.50
1:B:621:LYS:O	1:B:661:ASP:OD1	2.29	0.50
1:D:277:GLU:C	1:D:279:ILE:N	2.63	0.50
1:D:313:GLU:O	1:D:315:GLY:N	2.44	0.50
1:D:448:SER:O	1:D:460:ASP:HA	2.10	0.50
1:D:536:ARG:HH11	1:D:536:ARG:CB	2.25	0.50
1:D:532:ARG:HG2	1:D:584:TYR:CD2	2.46	0.50
1:E:573:LEU:HG	1:E:577:ILE:HD11	1.93	0.50
1:C:548:ALA:O	1:C:549:ALA:C	2.46	0.50
1:D:714:ILE:HG23	1:D:715:GLY:N	2.25	0.50
1:F:549:ALA:HA	1:F:552:ARG:NH2	2.26	0.50
1:B:317:LEU:HD23	1:B:317:LEU:C	2.32	0.50
1:C:274:ASN:C	1:C:276:TYR:N	2.65	0.50
1:C:329:LYS:C	1:C:331:ARG:N	2.64	0.50
1:C:414:LEU:C	1:C:416:PRO:HD3	2.31	0.50
1:C:536:ARG:CB	1:C:536:ARG:HH11	2.24	0.50
1:D:589:THR:O	1:D:697:ARG:HD2	2.12	0.50
1:D:624:LEU:HD12	1:D:624:LEU:H	1.76	0.50
1:F:286:SER:O	1:F:290:ARG:HB2	2.12	0.50
1:A:247:GLY:C	1:A:249:VAL:H	2.14	0.50
1:B:299:LEU:O	1:B:299:LEU:HD12	2.11	0.50
1:C:300:PRO:HG3	1:C:412:GLY:HA2	1.94	0.50
1:D:406:GLN:O	1:D:407:GLY:C	2.50	0.50
1:D:462:SER:HB2	1:D:463:LYS:HD2	1.94	0.50
1:D:686:LEU:HD22	1:D:686:LEU:O	2.11	0.50
1:E:448:SER:O	1:E:460:ASP:HA	2.12	0.50
1:F:546:GLN:OE1	1:F:577:ILE:HB	2.11	0.50
1:A:329:LYS:O	1:A:331:ARG:N	2.44	0.50
1:A:637:GLN:HG2	1:A:637:GLN:O	2.11	0.50
1:B:438:MET:O	1:B:440:GLU:N	2.45	0.50
1:C:313:GLU:O	1:C:314:ALA:C	2.50	0.50
1:C:439:LEU:CD2	1:C:439:LEU:H	2.20	0.50
1:A:534:TYR:CD1	1:A:534:TYR:N	2.80	0.50
1:D:313:GLU:O	1:D:314:ALA:C	2.50	0.50
1:D:593:VAL:HG13	1:D:693:ARG:O	2.12	0.50
1:E:438:MET:O	1:E:440:GLU:N	2.43	0.50
1:F:404:ILE:O	1:F:405:ILE:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:HB2	1:A:475:THR:CG2	2.42	0.50
1:B:334:GLU:O	1:B:338:VAL:HB	2.11	0.50
1:C:317:LEU:HD23	1:C:317:LEU:C	2.31	0.50
1:C:350:LEU:HD23	1:C:487:ILE:HD11	1.93	0.50
1:D:247:GLY:C	1:D:249:VAL:H	2.15	0.50
1:E:733:ILE:HA	1:E:756:ILE:O	2.12	0.50
1:A:602:THR:CG2	1:A:604:VAL:HG22	2.42	0.50
1:C:277:GLU:C	1:C:279:ILE:N	2.63	0.50
1:C:424:ASP:HB2	1:C:475:THR:CG2	2.42	0.50
1:C:461:LEU:O	1:C:464:VAL:HG23	2.11	0.50
1:E:469:THR:O	1:E:470:ALA:HB2	2.11	0.50
1:F:424:ASP:HB2	1:F:475:THR:CG2	2.42	0.50
1:A:732:ILE:HG21	1:A:753:LEU:HD13	1.94	0.49
1:C:362:SER:CB	2:C:783:ADP:H5'1	2.41	0.49
1:C:438:MET:O	1:C:440:GLU:N	2.45	0.49
1:C:593:VAL:O	1:C:595:VAL:HG23	2.11	0.49
1:E:439:LEU:CD2	1:E:439:LEU:H	2.19	0.49
1:A:313:GLU:O	1:A:314:ALA:C	2.49	0.49
1:A:424:ASP:N	1:A:424:ASP:OD1	2.45	0.49
1:B:596:VAL:HG23	1:B:685:ALA:HB2	1.93	0.49
1:B:687:VAL:O	1:B:691:THR:HG23	2.12	0.49
1:C:408:MET:H	1:C:408:MET:HE2	1.77	0.49
1:C:702:THR:CG2	1:C:702:THR:O	2.60	0.49
1:D:569:THR:HG23	1:D:572:ASN:H	1.78	0.49
1:F:336:LEU:O	1:F:339:GLN:N	2.45	0.49
1:B:462:SER:HB2	1:B:463:LYS:HD2	1.95	0.49
1:D:424:ASP:HB2	1:D:475:THR:CG2	2.41	0.49
1:E:313:GLU:O	1:E:315:GLY:N	2.44	0.49
1:E:359:GLY:HA2	2:E:783:ADP:C5'	2.42	0.49
1:E:407:GLY:HA3	1:E:418:PHE:CZ	2.47	0.49
1:A:520:LEU:HA	1:A:566:ILE:O	2.12	0.49
1:B:299:LEU:HD13	1:B:301:TRP:CZ2	2.47	0.49
1:F:404:ILE:HG23	1:F:418:PHE:HE2	1.70	0.49
1:A:686:LEU:O	1:A:686:LEU:HD22	2.12	0.49
1:B:550:ILE:O	1:B:551:CYS:C	2.49	0.49
1:C:506:LEU:HD12	1:C:506:LEU:O	2.13	0.49
1:D:359:GLY:CA	2:D:783:ADP:O5'	2.58	0.49
1:E:255:LYS:NZ	1:E:255:LYS:HB3	2.28	0.49
1:E:406:GLN:O	1:E:407:GLY:C	2.51	0.49
1:F:455:ILE:O	1:F:456:GLU:C	2.51	0.49
1:A:464:VAL:O	1:A:466:PHE:CD1	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:GLN:HG2	1:D:637:GLN:O	2.11	0.49
1:D:739:GLU:C	1:D:741:ASP:H	2.15	0.49
1:D:742:ILE:O	1:D:742:ILE:HG22	2.13	0.49
1:E:637:GLN:HG2	1:E:637:GLN:O	2.12	0.49
1:A:506:LEU:HD21	1:A:522:LEU:CD2	2.42	0.49
1:B:313:GLU:O	1:B:315:GLY:N	2.46	0.49
1:F:308:LYS:O	1:F:309:LEU:HD23	2.12	0.49
1:F:548:ALA:O	1:F:549:ALA:C	2.51	0.49
1:A:404:ILE:HG23	1:A:418:PHE:HE2	1.72	0.49
1:A:596:VAL:HG23	1:A:685:ALA:HB2	1.94	0.49
1:A:734:ALA:HB1	1:A:735:PRO:CD	2.42	0.49
1:B:378:ILE:HD13	1:B:420:LEU:CD1	2.43	0.49
1:B:533:TYR:HB3	1:B:580:ARG:HD2	1.94	0.49
1:B:602:THR:HG21	1:B:604:VAL:HG22	1.94	0.49
1:D:286:SER:O	1:D:290:ARG:HB2	2.12	0.49
1:E:286:SER:O	1:E:290:ARG:HB2	2.13	0.49
1:E:734:ALA:HB1	1:E:735:PRO:CD	2.42	0.49
1:F:246:THR:HG23	1:F:250:GLN:NE2	2.28	0.49
1:F:255:LYS:NZ	1:F:255:LYS:HB3	2.28	0.49
1:A:407:GLY:HA3	1:A:418:PHE:CZ	2.48	0.49
1:A:708:ARG:NH2	1:C:593:VAL:HB	2.27	0.49
1:C:584:TYR:O	1:C:584:TYR:HD1	1.95	0.49
1:D:705:ILE:HD11	1:D:761:LEU:HD21	1.94	0.49
1:B:573:LEU:HG	1:B:577:ILE:HD11	1.95	0.48
1:D:317:LEU:C	1:D:317:LEU:HD23	2.33	0.48
1:E:313:GLU:O	1:E:314:ALA:C	2.51	0.48
1:A:336:LEU:HA	1:A:339:GLN:HB3	1.95	0.48
1:B:705:ILE:HD11	1:B:761:LEU:HD21	1.95	0.48
1:C:506:LEU:O	1:C:507:PRO:C	2.49	0.48
1:C:756:ILE:HG13	1:C:767:HIS:CD2	2.48	0.48
1:D:255:LYS:HB3	1:D:255:LYS:NZ	2.28	0.48
1:E:455:ILE:O	1:E:456:GLU:C	2.51	0.48
1:F:551:CYS:O	1:F:554:ALA:HB3	2.13	0.48
1:B:444:PRO:HA	1:B:447:ASN:ND2	2.28	0.48
1:B:714:ILE:HB	1:B:735:PRO:HG2	1.94	0.48
1:C:247:GLY:C	1:C:249:VAL:H	2.15	0.48
1:C:501:VAL:HG13	1:C:547:LEU:HD11	1.95	0.48
1:C:635:SER:O	1:C:638:ALA:HB3	2.13	0.48
1:D:329:LYS:C	1:D:331:ARG:N	2.63	0.48
1:D:656:PHE:CE2	1:D:690:LEU:HD11	2.48	0.48
1:E:262:PRO:HG3	1:E:302:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:THR:HG21	1:E:604:VAL:HG22	1.95	0.48
1:C:536:ARG:HG3	1:C:536:ARG:NH1	2.16	0.48
1:C:550:ILE:O	1:C:551:CYS:C	2.51	0.48
1:E:602:THR:C	1:E:604:VAL:H	2.16	0.48
1:F:313:GLU:O	1:F:315:GLY:N	2.47	0.48
1:A:304:GLU:O	1:A:305:THR:C	2.50	0.48
1:A:506:LEU:CD2	1:A:522:LEU:HD21	2.44	0.48
1:A:599:LEU:O	1:A:720:LYS:HE2	2.13	0.48
1:B:642:TYR:CE1	1:B:709:GLY:HA3	2.48	0.48
1:C:642:TYR:CD2	1:C:761:LEU:HD12	2.49	0.48
1:E:686:LEU:O	1:E:686:LEU:HD22	2.14	0.48
1:A:349:ILE:HD12	1:A:349:ILE:O	2.14	0.48
1:A:621:LYS:O	1:A:661:ASP:OD1	2.31	0.48
1:B:350:LEU:H	1:B:350:LEU:CD1	2.10	0.48
1:C:404:ILE:O	1:C:405:ILE:C	2.51	0.48
1:C:705:ILE:HD11	1:C:761:LEU:CD2	2.44	0.48
1:E:424:ASP:HB2	1:E:475:THR:CG2	2.42	0.48
1:F:331:ARG:HH22	1:F:485:GLU:CD	2.17	0.48
1:F:656:PHE:CG	1:F:657:HIS:N	2.80	0.48
1:A:329:LYS:C	1:A:331:ARG:N	2.65	0.48
1:C:462:SER:HB2	1:C:463:LYS:HD2	1.94	0.48
1:E:262:PRO:HD2	1:E:301:TRP:HB3	1.94	0.48
1:E:656:PHE:CG	1:E:657:HIS:N	2.82	0.48
1:F:274:ASN:C	1:F:276:TYR:N	2.64	0.48
1:F:407:GLY:HA3	1:F:418:PHE:CZ	2.49	0.48
1:F:756:ILE:HG13	1:F:767:HIS:CD2	2.49	0.48
1:B:296:LEU:HD23	1:B:299:LEU:HD11	1.95	0.48
1:B:406:GLN:O	1:B:407:GLY:C	2.51	0.48
1:B:536:ARG:HH11	1:B:536:ARG:CB	2.27	0.48
1:C:273:LEU:HD13	1:C:289:ILE:HD12	1.95	0.48
1:C:712:LEU:HB3	1:C:713:PRO:CD	2.43	0.48
1:E:408:MET:H	1:E:408:MET:HE2	1.79	0.48
1:E:462:SER:HB2	1:E:463:LYS:HD2	1.95	0.48
1:E:590:GLU:HA	1:E:697:ARG:HD3	1.96	0.48
1:F:547:LEU:HA	1:F:547:LEU:HD23	1.75	0.48
1:F:642:TYR:CE1	1:F:709:GLY:HA3	2.49	0.48
1:F:739:GLU:C	1:F:741:ASP:H	2.17	0.48
1:D:656:PHE:C	1:D:658:GLU:H	2.16	0.48
1:E:579:LYS:H	1:E:579:LYS:NZ	2.12	0.48
1:E:635:SER:O	1:E:638:ALA:HB3	2.14	0.48
1:F:336:LEU:HA	1:F:339:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ALA:O	1:B:530:ILE:HG13	2.14	0.48
1:C:286:SER:O	1:C:290:ARG:HB2	2.14	0.48
1:E:270:LEU:HD21	1:E:296:LEU:CD2	2.43	0.48
1:E:334:GLU:O	1:E:338:VAL:HB	2.14	0.48
1:E:357:GLY:H	2:E:783:ADP:PB	2.37	0.48
1:F:621:LYS:O	1:F:661:ASP:OD1	2.32	0.48
1:A:350:LEU:CD1	1:A:350:LEU:H	2.07	0.47
1:B:246:THR:HG23	1:B:250:GLN:NE2	2.29	0.47
1:C:656:PHE:CG	1:C:657:HIS:N	2.82	0.47
1:D:678:ALA:O	1:D:682:MET:HG2	2.14	0.47
1:F:536:ARG:HG3	1:F:536:ARG:NH1	2.21	0.47
1:C:255:LYS:NZ	1:C:255:LYS:HB3	2.28	0.47
1:C:329:LYS:O	1:C:331:ARG:N	2.47	0.47
1:D:336:LEU:HA	1:D:339:GLN:HB3	1.96	0.47
1:E:277:GLU:C	1:E:279:ILE:N	2.64	0.47
1:E:416:PRO:HG2	1:E:464:VAL:HG13	1.96	0.47
1:F:420:LEU:HD21	1:F:466:PHE:CD2	2.47	0.47
1:F:642:TYR:CD2	1:F:761:LEU:HD12	2.49	0.47
1:F:362:SER:CB	2:F:783:ADP:H5'2	2.44	0.47
1:B:359:GLY:O	1:B:360:LYS:C	2.52	0.47
1:B:536:ARG:NH1	1:B:536:ARG:HG3	2.18	0.47
1:C:613:VAL:HG23	1:C:685:ALA:HB1	1.95	0.47
1:C:636:ALA:O	1:C:638:ALA:N	2.45	0.47
1:C:734:ALA:HB1	1:C:735:PRO:CD	2.45	0.47
1:C:733:ILE:HA	1:C:756:ILE:O	2.15	0.47
1:D:408:MET:H	1:D:408:MET:HE2	1.79	0.47
1:D:360:LYS:HD2	1:D:469:THR:HG23	1.95	0.47
1:D:529:ASP:O	1:D:530:ILE:C	2.51	0.47
1:E:276:TYR:CD1	1:E:277:GLU:N	2.83	0.47
1:B:424:ASP:HB2	1:B:475:THR:CG2	2.43	0.47
1:C:534:TYR:N	1:C:534:TYR:CD1	2.81	0.47
1:C:569:THR:HG23	1:C:571:LYS:N	2.16	0.47
1:E:317:LEU:HD23	1:E:317:LEU:C	2.34	0.47
1:E:414:LEU:C	1:E:416:PRO:HD3	2.33	0.47
1:E:546:GLN:O	1:E:549:ALA:HB3	2.15	0.47
1:E:717:LEU:O	1:E:717:LEU:HD22	2.14	0.47
1:B:313:GLU:O	1:B:314:ALA:C	2.52	0.47
1:B:656:PHE:C	1:B:658:GLU:H	2.16	0.47
1:B:739:GLU:C	1:B:741:ASP:H	2.17	0.47
1:D:604:VAL:O	1:D:604:VAL:HG23	2.12	0.47
1:E:336:LEU:HA	1:E:339:GLN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:THR:C	1:E:604:VAL:N	2.67	0.47
1:E:656:PHE:C	1:E:658:GLU:H	2.17	0.47
1:F:546:GLN:O	1:F:549:ALA:HB3	2.14	0.47
1:A:478:GLY:N	1:A:479:PRO:HD2	2.30	0.47
1:C:407:GLY:HA3	1:C:418:PHE:CZ	2.49	0.47
1:C:546:GLN:O	1:C:549:ALA:HB3	2.15	0.47
1:C:733:ILE:CD1	1:C:768:ALA:HB2	2.45	0.47
1:D:464:VAL:O	1:D:466:PHE:CD1	2.64	0.47
1:E:364:ALA:O	1:E:365:LYS:C	2.53	0.47
1:F:313:GLU:O	1:F:314:ALA:C	2.53	0.47
1:F:536:ARG:CG	1:F:536:ARG:NH1	2.67	0.47
1:F:599:LEU:HD22	1:F:599:LEU:N	2.29	0.47
1:A:246:THR:HG23	1:A:250:GLN:NE2	2.29	0.47
1:A:270:LEU:HD21	1:A:296:LEU:CD2	2.44	0.47
1:A:452:ASP:O	1:A:455:ILE:HG22	2.15	0.47
1:C:611:ILE:HD12	1:C:681:THR:CG2	2.45	0.47
1:D:334:GLU:O	1:D:338:VAL:HB	2.15	0.47
1:E:308:LYS:O	1:E:309:LEU:HD23	2.14	0.47
1:E:705:ILE:HD11	1:E:761:LEU:HD21	1.96	0.47
1:F:613:VAL:HG23	1:F:685:ALA:HB1	1.97	0.47
1:F:656:PHE:C	1:F:658:GLU:H	2.17	0.47
1:A:647:THR:HG22	1:A:648:GLU:N	2.30	0.47
1:B:255:LYS:HB3	1:B:255:LYS:NZ	2.30	0.47
1:C:469:THR:O	1:C:470:ALA:HB2	2.15	0.47
1:E:705:ILE:HD12	1:E:705:ILE:HA	1.61	0.47
1:F:462:SER:HB2	1:F:463:LYS:HD2	1.95	0.47
1:F:645:SER:O	1:F:647:THR:N	2.47	0.47
1:F:493:THR:CG2	1:F:748:SER:HB2	2.20	0.47
1:B:452:ASP:O	1:B:455:ILE:HG22	2.15	0.47
1:B:331:ARG:HH22	1:B:485:GLU:CD	2.17	0.47
1:B:584:TYR:CE2	1:B:728:GLY:HA3	2.49	0.47
1:B:656:PHE:CG	1:B:657:HIS:N	2.83	0.47
1:C:520:LEU:HA	1:C:566:ILE:O	2.15	0.47
1:D:414:LEU:C	1:D:416:PRO:HD3	2.35	0.47
1:D:455:ILE:O	1:D:456:GLU:C	2.54	0.47
1:D:506:LEU:HD21	1:D:522:LEU:CD2	2.42	0.47
1:E:739:GLU:C	1:E:741:ASP:H	2.17	0.47
1:F:534:TYR:CD2	1:F:577:ILE:HD12	2.50	0.47
1:A:506:LEU:O	1:A:506:LEU:HD12	2.15	0.47
1:A:572:ASN:O	1:A:573:LEU:C	2.53	0.47
1:A:656:PHE:CG	1:A:657:HIS:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ILE:HG22	1:A:705:ILE:HD13	1.97	0.47
1:B:255:LYS:O	1:B:258:GLU:HB3	2.15	0.47
1:B:260:GLY:O	1:B:261:MET:CB	2.63	0.47
1:B:276:TYR:CD1	1:B:277:GLU:N	2.83	0.47
1:B:282:SER:HB2	1:E:276:TYR:HH	1.80	0.47
1:B:455:ILE:O	1:B:456:GLU:C	2.53	0.47
1:B:569:THR:CG2	1:B:572:ASN:H	2.27	0.47
1:B:599:LEU:HD21	1:B:700:GLY:C	2.35	0.47
1:C:712:LEU:HB3	1:C:713:PRO:HD2	1.97	0.47
1:E:274:ASN:O	1:E:276:TYR:N	2.44	0.47
1:F:656:PHE:CE2	1:F:690:LEU:HD11	2.50	0.47
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.29	0.47
1:A:645:SER:O	1:A:647:THR:N	2.48	0.47
1:B:579:LYS:H	1:B:579:LYS:NZ	2.13	0.47
1:B:732:ILE:HD13	1:B:732:ILE:O	2.15	0.47
1:E:329:LYS:C	1:E:331:ARG:N	2.68	0.47
1:E:645:SER:O	1:E:647:THR:N	2.48	0.47
1:E:621:LYS:O	1:E:661:ASP:OD1	2.33	0.47
1:A:255:LYS:O	1:A:258:GLU:HB3	2.16	0.46
1:A:317:LEU:C	1:A:317:LEU:HD23	2.34	0.46
1:A:331:ARG:HH22	1:A:485:GLU:CD	2.18	0.46
2:A:783:ADP:PA	2:A:783:ADP:O4'	2.71	0.46
1:B:636:ALA:O	1:B:638:ALA:N	2.46	0.46
1:C:732:ILE:HG21	1:C:753:LEU:HD13	1.97	0.46
1:D:355:PRO:O	1:D:358:VAL:HG22	2.15	0.46
1:D:444:PRO:HA	1:D:447:ASN:ND2	2.30	0.46
1:D:702:THR:HG23	1:D:702:THR:O	2.16	0.46
1:E:331:ARG:HH22	1:E:485:GLU:CD	2.17	0.46
1:F:593:VAL:O	1:F:595:VAL:HG23	2.15	0.46
1:F:712:LEU:HB3	1:F:713:PRO:HD2	1.97	0.46
1:F:540:VAL:CG2	2:F:783:ADP:H1'	2.45	0.46
1:A:586:GLN:NE2	1:A:728:GLY:O	2.49	0.46
1:B:341:LEU:O	1:B:343:LYS:N	2.48	0.46
1:B:534:TYR:N	1:B:534:TYR:CD1	2.82	0.46
1:C:307:ASP:HB3	1:C:309:LEU:HD21	1.97	0.46
1:C:341:LEU:O	1:C:343:LYS:N	2.48	0.46
1:C:331:ARG:HH22	1:C:485:GLU:CD	2.18	0.46
1:D:246:THR:HG23	1:D:250:GLN:NE2	2.30	0.46
1:E:341:LEU:O	1:E:343:LYS:N	2.48	0.46
1:E:404:ILE:HG23	1:E:418:PHE:HE2	1.72	0.46
1:F:260:GLY:O	1:F:261:MET:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LYS:CD	1:F:469:THR:HG23	2.41	0.46
1:F:496:GLU:O	1:F:500:ILE:HG13	2.14	0.46
1:B:678:ALA:O	1:B:682:MET:HG2	2.15	0.46
1:C:380:LEU:HD12	1:C:423:ILE:CG2	2.46	0.46
1:C:444:PRO:HA	1:C:447:ASN:ND2	2.30	0.46
1:C:714:ILE:HG23	1:C:715:GLY:N	2.29	0.46
1:D:266:LYS:HG3	1:D:267:GLU:H	1.78	0.46
1:E:246:THR:HG23	1:E:250:GLN:NE2	2.30	0.46
1:E:307:ASP:O	1:E:309:LEU:HG	2.16	0.46
1:E:732:ILE:HG21	1:E:753:LEU:HD13	1.96	0.46
1:F:329:LYS:O	1:F:331:ARG:N	2.48	0.46
1:F:329:LYS:C	1:F:331:ARG:N	2.67	0.46
1:A:439:LEU:H	1:A:439:LEU:CD2	2.25	0.46
1:A:444:PRO:HA	1:A:447:ASN:ND2	2.28	0.46
1:A:536:ARG:CB	1:A:536:ARG:HH11	2.28	0.46
1:B:439:LEU:H	1:B:439:LEU:CD2	2.26	0.46
1:C:579:LYS:NZ	1:C:579:LYS:H	2.14	0.46
1:D:569:THR:HG22	1:D:572:ASN:OD1	2.15	0.46
1:D:636:ALA:O	1:D:638:ALA:N	2.40	0.46
1:E:636:ALA:C	1:E:638:ALA:H	2.17	0.46
1:A:409:LYS:C	1:A:411:ALA:H	2.17	0.46
1:A:380:LEU:HD12	1:A:423:ILE:CG2	2.46	0.46
1:A:642:TYR:CE1	1:A:709:GLY:HA3	2.50	0.46
1:B:424:ASP:OD1	1:B:424:ASP:N	2.49	0.46
1:B:637:GLN:O	1:B:637:GLN:HG2	2.15	0.46
1:C:656:PHE:C	1:C:658:GLU:N	2.68	0.46
1:D:478:GLY:N	1:D:479:PRO:HD2	2.31	0.46
1:E:260:GLY:O	1:E:261:MET:CB	2.63	0.46
1:F:352:LEU:HB3	1:F:360:LYS:HG2	1.96	0.46
1:F:637:GLN:HG2	1:F:637:GLN:O	2.16	0.46
1:F:734:ALA:HB1	1:F:735:PRO:CD	2.46	0.46
1:A:274:ASN:O	1:A:276:TYR:N	2.46	0.46
1:C:536:ARG:CB	1:C:536:ARG:NH1	2.79	0.46
1:C:596:VAL:HG23	1:C:685:ALA:HB2	1.97	0.46
1:D:331:ARG:HH22	1:D:485:GLU:CD	2.18	0.46
1:E:368:ALA:HB2	1:E:417:VAL:HG21	1.97	0.46
1:E:478:GLY:N	1:E:479:PRO:HD2	2.30	0.46
1:F:444:PRO:HA	1:F:447:ASN:ND2	2.29	0.46
1:F:569:THR:HG23	1:F:572:ASN:H	1.79	0.46
1:A:311:LEU:O	1:A:312:LYS:C	2.54	0.46
1:A:569:THR:HG22	1:A:572:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ARG:HG2	1:B:710:ARG:HH21	1.81	0.46
1:B:734:ALA:HB1	1:B:735:PRO:CD	2.45	0.46
2:B:783:ADP:H2'	2:B:783:ADP:N3	2.30	0.46
1:C:246:THR:HG23	1:C:250:GLN:NE2	2.30	0.46
1:C:645:SER:O	1:C:647:THR:N	2.49	0.46
1:E:322:HIS:CE1	1:E:363:LEU:HD23	2.51	0.46
1:E:409:LYS:C	1:E:411:ALA:H	2.19	0.46
1:E:444:PRO:HA	1:E:447:ASN:ND2	2.30	0.46
1:F:322:HIS:CE1	1:F:363:LEU:HD23	2.50	0.46
1:F:409:LYS:C	1:F:411:ALA:H	2.18	0.46
1:A:260:GLY:O	1:A:261:MET:CB	2.64	0.46
1:A:505:LEU:CD2	1:A:544:GLU:HG3	2.44	0.46
1:A:604:VAL:HG23	1:A:604:VAL:O	2.16	0.46
1:B:329:LYS:C	1:B:331:ARG:N	2.66	0.46
1:C:266:LYS:HG3	1:C:267:GLU:H	1.80	0.46
1:D:407:GLY:HA3	1:D:418:PHE:CZ	2.50	0.46
1:D:481:ARG:O	1:D:481:ARG:HG2	2.16	0.46
1:D:656:PHE:CG	1:D:657:HIS:N	2.84	0.46
1:E:355:PRO:O	1:E:358:VAL:HG22	2.15	0.46
1:E:506:LEU:HD12	1:E:506:LEU:O	2.15	0.46
1:E:642:TYR:CE1	1:E:709:GLY:HA3	2.51	0.46
1:A:456:GLU:OE2	1:C:291:ASN:ND2	2.49	0.46
1:A:636:ALA:O	1:A:638:ALA:N	2.43	0.46
1:B:290:ARG:HH12	1:E:273:LEU:HD21	1.80	0.46
1:C:260:GLY:O	1:C:261:MET:CB	2.64	0.46
1:C:510:ILE:HG22	1:C:515:LEU:O	2.15	0.46
1:C:569:THR:HG22	1:C:572:ASN:OD1	2.16	0.46
1:D:329:LYS:O	1:D:331:ARG:N	2.48	0.46
1:D:367:ILE:HG22	1:D:368:ALA:N	2.28	0.46
1:D:350:LEU:HD23	1:D:487:ILE:HD11	1.97	0.46
1:E:714:ILE:HG23	1:E:715:GLY:N	2.30	0.46
1:F:534:TYR:N	1:F:534:TYR:CD1	2.84	0.46
1:F:622:LEU:HB2	1:F:662:ILE:HG12	1.98	0.46
1:A:341:LEU:O	1:A:343:LYS:N	2.49	0.46
2:A:783:ADP:O1A	2:A:783:ADP:O1B	2.34	0.46
1:C:546:GLN:OE1	1:C:577:ILE:HB	2.15	0.46
1:C:736:LYS:C	1:C:738:ASN:H	2.17	0.46
1:D:307:ASP:HB3	1:D:309:LEU:HD21	1.98	0.46
1:D:645:SER:O	1:D:647:THR:N	2.48	0.46
1:D:656:PHE:C	1:D:658:GLU:N	2.70	0.46
1:D:733:ILE:HA	1:D:756:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:LEU:HD12	1:F:423:ILE:HG23	1.97	0.46
1:A:378:ILE:HD13	1:A:420:LEU:CD1	2.45	0.45
1:A:496:GLU:O	1:A:500:ILE:HG13	2.16	0.45
1:B:276:TYR:CE2	1:F:246:THR:CG2	3.00	0.45
1:D:341:LEU:O	1:D:343:LYS:N	2.49	0.45
1:D:496:GLU:O	1:D:497:LYS:C	2.55	0.45
1:F:636:ALA:C	1:F:638:ALA:H	2.19	0.45
1:A:656:PHE:C	1:A:658:GLU:H	2.17	0.45
1:A:680:ILE:HG22	1:A:705:ILE:CD1	2.46	0.45
1:B:311:LEU:O	1:B:312:LYS:C	2.54	0.45
1:B:497:LYS:HG2	1:B:540:VAL:HG12	1.99	0.45
1:C:455:ILE:O	1:C:456:GLU:C	2.54	0.45
1:C:469:THR:HG22	1:C:470:ALA:H	1.81	0.45
1:D:260:GLY:O	1:D:261:MET:CB	2.63	0.45
1:D:350:LEU:HA	1:D:485:GLU:O	2.16	0.45
1:D:489:ILE:H	1:D:489:ILE:HG12	1.58	0.45
1:F:255:LYS:O	1:F:258:GLU:HB3	2.16	0.45
1:F:675:GLY:N	1:F:676:PRO:CD	2.79	0.45
1:B:478:GLY:N	1:B:479:PRO:HD2	2.31	0.45
1:B:604:VAL:HG23	1:B:604:VAL:O	2.15	0.45
1:B:656:PHE:C	1:B:658:GLU:N	2.70	0.45
1:B:711:VAL:N	1:B:759:SER:O	2.47	0.45
1:D:452:ASP:O	1:D:455:ILE:HG22	2.17	0.45
1:A:455:ILE:O	1:A:456:GLU:C	2.53	0.45
1:B:645:SER:O	1:B:647:THR:N	2.49	0.45
1:C:380:LEU:HD12	1:C:423:ILE:HG23	1.98	0.45
1:D:357:GLY:H	2:D:783:ADP:PB	2.39	0.45
1:B:276:TYR:OH	1:F:247:GLY:CA	2.64	0.45
1:A:562:GLU:O	1:A:563:ARG:C	2.55	0.45
1:B:308:LYS:O	1:B:309:LEU:HD23	2.17	0.45
1:B:373:ARG:NE	1:B:415:ASN:OD1	2.50	0.45
1:B:505:LEU:CD2	1:B:544:GLU:HG3	2.45	0.45
1:C:714:ILE:HB	1:C:735:PRO:HG2	1.98	0.45
1:D:506:LEU:O	1:D:507:PRO:C	2.55	0.45
1:C:341:LEU:HB3	1:E:514:GLY:O	2.17	0.45
1:E:706:THR:OG1	1:E:710:ARG:HB2	2.15	0.45
1:E:642:TYR:CD2	1:E:761:LEU:HD12	2.52	0.45
1:F:597:THR:O	1:F:700:GLY:HA2	2.16	0.45
1:F:635:SER:O	1:F:638:ALA:HB3	2.16	0.45
1:A:276:TYR:CD1	1:A:277:GLU:N	2.84	0.45
1:A:579:LYS:C	1:A:579:LYS:HE2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:VAL:O	1:B:441:VAL:HG22	2.16	0.45
1:C:274:ASN:O	1:C:276:TYR:N	2.48	0.45
1:C:276:TYR:CD1	1:C:277:GLU:N	2.84	0.45
1:C:424:ASP:OD1	1:C:424:ASP:N	2.50	0.45
1:D:276:TYR:CD1	1:D:277:GLU:N	2.85	0.45
1:E:311:LEU:O	1:E:312:LYS:C	2.55	0.45
1:F:292:TYR:OH	1:F:455:ILE:HA	2.17	0.45
1:F:414:LEU:C	1:F:416:PRO:HD3	2.37	0.45
1:B:560:ALA:O	1:B:562:GLU:N	2.50	0.45
1:C:255:LYS:O	1:C:258:GLU:HB3	2.16	0.45
1:C:714:ILE:HA	1:C:714:ILE:HD12	1.79	0.45
1:D:621:LYS:O	1:D:661:ASP:OD1	2.35	0.45
1:E:452:ASP:O	1:E:455:ILE:HG22	2.17	0.45
1:E:647:THR:HG22	1:E:648:GLU:N	2.32	0.45
1:E:656:PHE:C	1:E:658:GLU:N	2.70	0.45
1:F:276:TYR:CD1	1:F:277:GLU:N	2.84	0.45
1:F:295:TRP:HZ3	1:F:405:ILE:HG21	1.81	0.45
1:A:493:THR:HG21	1:A:748:SER:CB	2.46	0.45
1:B:364:ALA:O	1:B:365:LYS:C	2.55	0.45
1:B:439:LEU:O	1:B:440:GLU:C	2.55	0.45
1:B:464:VAL:O	1:B:466:PHE:CD1	2.63	0.45
1:B:495:ILE:HA	1:B:495:ILE:HD13	1.78	0.45
1:C:373:ARG:NE	1:C:415:ASN:OD1	2.50	0.45
1:C:439:LEU:O	1:C:440:GLU:C	2.55	0.45
1:D:423:ILE:HD13	1:D:423:ILE:HG21	1.62	0.45
1:D:424:ASP:OD1	1:D:424:ASP:N	2.50	0.45
1:D:598:GLY:HA2	1:D:701:MET:O	2.17	0.45
1:D:747:GLU:CD	1:D:747:GLU:H	2.18	0.45
1:A:280:PRO:HB2	1:A:281:SER:H	1.67	0.45
1:B:613:VAL:HG23	1:B:685:ALA:HB1	1.99	0.45
1:D:298:ALA:O	1:D:299:LEU:O	2.35	0.45
1:D:506:LEU:CD2	1:D:522:LEU:HD21	2.44	0.45
1:D:599:LEU:N	1:D:599:LEU:HD22	2.32	0.45
1:F:266:LYS:HG3	1:F:267:GLU:H	1.81	0.45
1:F:412:GLY:C	1:F:413:LYS:HG2	2.37	0.45
1:A:536:ARG:CG	1:A:536:ARG:NH1	2.65	0.45
1:A:569:THR:HG23	1:A:571:LYS:N	2.19	0.45
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.38	0.45
1:B:599:LEU:HD22	1:B:599:LEU:N	2.31	0.45
1:B:714:ILE:HG23	1:B:715:GLY:N	2.31	0.45
1:C:616:SER:O	1:C:661:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:THR:HG22	1:C:648:GLU:N	2.31	0.45
1:F:419:LEU:O	1:F:421:ASP:N	2.50	0.45
1:F:732:ILE:HD13	1:F:732:ILE:O	2.17	0.45
1:B:266:LYS:HG3	1:B:267:GLU:H	1.82	0.44
1:B:414:LEU:HD12	1:B:414:LEU:C	2.37	0.44
1:D:439:LEU:O	1:D:440:GLU:C	2.55	0.44
1:E:712:LEU:HB3	1:E:713:PRO:HD2	1.99	0.44
1:F:478:GLY:N	1:F:479:PRO:HD2	2.31	0.44
1:F:505:LEU:HD23	1:F:505:LEU:HA	1.38	0.44
1:A:493:THR:O	1:A:494:GLU:C	2.54	0.44
1:B:296:LEU:O	1:B:299:LEU:HD11	2.16	0.44
1:B:496:GLU:O	1:B:497:LYS:C	2.54	0.44
1:C:265:VAL:O	1:C:457:GLU:OE1	2.35	0.44
1:C:478:GLY:N	1:C:479:PRO:HD2	2.31	0.44
1:C:322:HIS:HA	2:C:783:ADP:N1	2.32	0.44
1:D:274:ASN:O	1:D:276:TYR:N	2.45	0.44
1:D:602:THR:C	1:D:604:VAL:N	2.71	0.44
1:D:616:SER:O	1:D:661:ASP:N	2.49	0.44
1:D:732:ILE:HG21	1:D:753:LEU:HD13	1.99	0.44
1:E:536:ARG:HH11	1:E:536:ARG:CB	2.30	0.44
1:E:546:GLN:OE1	1:E:577:ILE:HB	2.17	0.44
1:F:380:LEU:HD12	1:F:423:ILE:CG2	2.47	0.44
1:F:732:ILE:HG21	1:F:753:LEU:HD13	1.99	0.44
1:A:550:ILE:O	1:A:551:CYS:C	2.54	0.44
1:A:736:LYS:C	1:A:738:ASN:H	2.20	0.44
1:B:267:GLU:HA	1:B:270:LEU:HG	1.98	0.44
1:B:569:THR:HG23	1:B:571:LYS:N	2.21	0.44
1:C:346:LYS:HG3	1:C:348:PRO:HD2	1.99	0.44
1:C:416:PRO:HD2	1:C:464:VAL:HG13	1.99	0.44
1:D:364:ALA:O	1:D:365:LYS:C	2.56	0.44
1:D:599:LEU:O	1:D:720:LYS:HE2	2.17	0.44
1:D:702:THR:CG2	1:D:702:THR:O	2.65	0.44
1:D:714:ILE:HB	1:D:735:PRO:HG2	2.00	0.44
1:D:362:SER:HB3	2:D:783:ADP:C5'	2.47	0.44
1:E:710:ARG:HH21	1:E:710:ARG:HG2	1.82	0.44
1:F:452:ASP:O	1:F:455:ILE:HG22	2.17	0.44
1:F:520:LEU:HA	1:F:566:ILE:O	2.17	0.44
1:B:280:PRO:HB2	1:B:281:SER:H	1.67	0.44
1:B:350:LEU:HA	1:B:485:GLU:O	2.18	0.44
1:B:407:GLY:HA3	1:B:418:PHE:CZ	2.52	0.44
1:B:420:LEU:HD21	1:B:466:PHE:CD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HA	1:B:566:ILE:O	2.17	0.44
1:C:423:ILE:HG21	1:C:423:ILE:HD13	1.76	0.44
1:C:637:GLN:HA	1:C:640:PHE:HB3	1.99	0.44
1:C:621:LYS:O	1:C:661:ASP:OD1	2.35	0.44
1:D:590:GLU:HA	1:D:697:ARG:HD3	1.99	0.44
1:A:495:ILE:HA	1:A:495:ILE:HD13	1.82	0.44
1:A:497:LYS:HG2	1:A:540:VAL:HG12	2.00	0.44
1:A:546:GLN:O	1:A:549:ALA:HB3	2.17	0.44
1:A:656:PHE:C	1:A:658:GLU:N	2.71	0.44
1:B:299:LEU:O	1:B:301:TRP:CD1	2.70	0.44
1:B:642:TYR:CD2	1:B:761:LEU:HD12	2.53	0.44
1:C:267:GLU:HG3	1:C:270:LEU:HD12	1.99	0.44
1:C:569:THR:HG23	1:C:572:ASN:H	1.82	0.44
1:E:506:LEU:HB3	1:E:507:PRO:CD	2.45	0.44
1:E:569:THR:HG23	1:E:571:LYS:N	2.21	0.44
1:E:736:LYS:C	1:E:738:ASN:H	2.19	0.44
1:F:368:ALA:CB	1:F:417:VAL:HG21	2.47	0.44
1:A:579:LYS:NZ	1:A:579:LYS:H	2.16	0.44
1:B:562:GLU:O	1:B:563:ARG:C	2.56	0.44
1:C:283:SER:N	1:C:286:SER:HB3	2.33	0.44
1:C:298:ALA:O	1:C:299:LEU:C	2.55	0.44
1:C:342:THR:HG22	1:C:344:SER:O	2.18	0.44
1:C:409:LYS:C	1:C:411:ALA:H	2.21	0.44
1:E:562:GLU:O	1:E:563:ARG:C	2.56	0.44
2:E:783:ADP:H5'2	2:E:783:ADP:C8	2.53	0.44
1:F:705:ILE:HD11	1:F:761:LEU:CD2	2.47	0.44
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.45	0.44
1:A:548:ALA:O	1:A:549:ALA:C	2.54	0.44
1:B:262:PRO:HG2	1:B:302:THR:OG1	2.17	0.44
1:B:522:LEU:HB3	1:B:568:VAL:CG1	2.43	0.44
1:E:423:ILE:HG22	1:E:426:MET:HE1	1.99	0.44
1:E:455:ILE:HG23	1:E:455:ILE:O	2.18	0.44
1:E:597:THR:O	1:E:700:GLY:HA2	2.17	0.44
1:E:604:VAL:HG23	1:E:604:VAL:O	2.17	0.44
1:F:317:LEU:HD23	1:F:317:LEU:C	2.38	0.44
1:B:480:LEU:O	1:B:483:ARG:N	2.50	0.44
1:C:602:THR:C	1:C:604:VAL:N	2.70	0.44
1:D:342:THR:HG22	1:D:344:SER:O	2.17	0.44
1:D:586:GLN:HG3	1:D:698:GLU:HG2	2.00	0.44
1:E:255:LYS:O	1:E:258:GLU:HB3	2.18	0.44
1:E:295:TRP:O	1:E:299:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:O	1:A:299:LEU:C	2.54	0.44
1:A:569:THR:HG23	1:A:572:ASN:H	1.82	0.44
1:A:675:GLY:N	1:A:676:PRO:CD	2.81	0.44
1:A:711:VAL:N	1:A:759:SER:O	2.47	0.44
1:B:736:LYS:C	1:B:738:ASN:H	2.20	0.44
1:C:532:ARG:HG2	1:C:584:TYR:CE2	2.53	0.44
1:C:675:GLY:N	1:C:676:PRO:CD	2.81	0.44
1:D:255:LYS:O	1:D:258:GLU:HB3	2.17	0.44
1:D:441:VAL:HG22	1:D:441:VAL:O	2.17	0.44
1:D:506:LEU:HD12	1:D:506:LEU:C	2.38	0.44
1:E:300:PRO:HG3	1:E:413:LYS:N	2.32	0.44
1:F:579:LYS:NZ	1:F:579:LYS:H	2.15	0.44
1:A:267:GLU:HA	1:A:270:LEU:HG	1.99	0.43
1:A:271:LYS:CA	1:A:274:ASN:HB3	2.46	0.43
1:A:439:LEU:O	1:A:440:GLU:C	2.55	0.43
1:A:602:THR:C	1:A:604:VAL:H	2.21	0.43
1:A:493:THR:CG2	1:A:748:SER:HB2	2.47	0.43
1:B:546:GLN:O	1:B:549:ALA:HB3	2.18	0.43
1:C:333:LEU:HD23	1:C:336:LEU:HD12	2.00	0.43
1:D:506:LEU:HD12	1:D:510:ILE:CG1	2.48	0.43
1:D:756:ILE:HG13	1:D:767:HIS:CD2	2.54	0.43
1:E:569:THR:HG23	1:E:572:ASN:H	1.82	0.43
1:F:346:LYS:HG3	1:F:348:PRO:HD2	2.00	0.43
1:A:357:GLY:H	2:A:783:ADP:PB	2.38	0.43
1:A:469:THR:HG22	1:A:470:ALA:H	1.83	0.43
1:B:335:TYR:O	1:B:335:TYR:CD2	2.71	0.43
1:C:557:ALA:CB	1:C:566:ILE:HD11	2.48	0.43
1:D:712:LEU:HB3	1:D:713:PRO:CD	2.47	0.43
1:E:367:ILE:O	1:E:371:LEU:HD13	2.17	0.43
1:E:637:GLN:HA	1:E:640:PHE:HB3	2.00	0.43
1:A:496:GLU:O	1:A:497:LYS:C	2.56	0.43
1:B:514:GLY:O	1:E:341:LEU:HD13	2.17	0.43
1:C:350:LEU:HA	1:C:485:GLU:O	2.18	0.43
1:C:642:TYR:CE1	1:C:709:GLY:HA3	2.52	0.43
1:E:350:LEU:H	1:E:350:LEU:CD1	2.09	0.43
1:A:412:GLY:C	1:A:413:LYS:HG2	2.37	0.43
1:A:536:ARG:CB	1:A:536:ARG:NH1	2.82	0.43
1:C:452:ASP:O	1:C:455:ILE:HG22	2.18	0.43
1:C:562:GLU:O	1:C:563:ARG:C	2.56	0.43
1:C:637:GLN:O	1:C:637:GLN:HG2	2.18	0.43
1:E:602:THR:CG2	1:E:604:VAL:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:616:SER:O	1:E:661:ASP:N	2.52	0.43
1:F:455:ILE:O	1:F:455:ILE:HG23	2.18	0.43
1:A:350:LEU:HA	1:A:485:GLU:O	2.19	0.43
1:C:493:THR:O	1:C:494:GLU:C	2.57	0.43
1:C:589:THR:O	1:C:697:ARG:NE	2.52	0.43
1:D:322:HIS:CE1	1:D:363:LEU:HD23	2.53	0.43
1:D:439:LEU:H	1:D:439:LEU:CD2	2.24	0.43
1:E:342:THR:HG22	1:E:344:SER:O	2.18	0.43
1:E:439:LEU:O	1:E:440:GLU:C	2.57	0.43
1:E:639:ALA:HB1	1:E:683:ALA:HB2	2.00	0.43
1:F:439:LEU:CD2	1:F:439:LEU:H	2.26	0.43
1:A:455:ILE:HG23	1:A:455:ILE:O	2.18	0.43
1:A:714:ILE:HB	1:A:735:PRO:HG2	2.00	0.43
1:A:739:GLU:C	1:A:741:ASP:H	2.21	0.43
1:B:602:THR:HG22	1:B:603:THR:N	2.33	0.43
1:B:613:VAL:O	1:E:708:ARG:HD3	2.17	0.43
1:B:735:PRO:O	1:B:738:ASN:HB2	2.18	0.43
1:C:270:LEU:CD2	1:C:296:LEU:HD22	2.44	0.43
1:C:412:GLY:C	1:C:413:LYS:HG2	2.39	0.43
1:C:693:ARG:O	1:C:694:ALA:HB2	2.19	0.43
1:C:752:GLY:O	1:C:753:LEU:HD23	2.19	0.43
1:D:409:LYS:C	1:D:411:ALA:H	2.20	0.43
1:D:546:GLN:O	1:D:549:ALA:HB3	2.18	0.43
1:E:732:ILE:HD13	1:E:732:ILE:O	2.19	0.43
2:E:783:ADP:C8	2:E:783:ADP:C5'	3.01	0.43
1:A:602:THR:C	1:A:604:VAL:N	2.72	0.43
1:B:267:GLU:HG3	1:B:270:LEU:HD12	2.01	0.43
1:B:299:LEU:CD1	1:B:301:TRP:NE1	2.82	0.43
1:B:493:THR:O	1:B:494:GLU:C	2.57	0.43
1:B:552:ARG:O	1:B:553:LYS:C	2.57	0.43
1:B:362:SER:HB3	2:B:783:ADP:H5'2	2.01	0.43
1:D:311:LEU:O	1:D:312:LYS:C	2.57	0.43
1:E:300:PRO:HB2	1:E:414:LEU:CB	2.46	0.43
1:E:359:GLY:O	1:E:360:LYS:C	2.55	0.43
1:F:357:GLY:O	1:F:539:GLY:HA2	2.18	0.43
1:F:656:PHE:C	1:F:658:GLU:N	2.71	0.43
1:B:416:PRO:HD2	1:B:464:VAL:HG13	2.01	0.43
1:C:338:VAL:HG23	1:E:555:ALA:HB3	2.00	0.43
1:C:732:ILE:O	1:C:732:ILE:HD13	2.18	0.43
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.43
1:E:602:THR:O	1:E:604:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:611:ILE:HG23	1:E:665:HIS:O	2.19	0.43
1:F:579:LYS:C	1:F:579:LYS:HE2	2.38	0.43
1:A:599:LEU:HD22	1:A:599:LEU:N	2.32	0.43
1:B:602:THR:CG2	1:B:604:VAL:HG22	2.48	0.43
1:C:378:ILE:HD13	1:C:420:LEU:HD12	1.99	0.43
1:C:572:ASN:O	1:C:573:LEU:C	2.57	0.43
1:D:332:ILE:CG2	1:D:367:ILE:HD11	2.49	0.43
1:D:647:THR:HG22	1:D:648:GLU:N	2.34	0.43
1:E:416:PRO:CD	1:E:464:VAL:HG13	2.49	0.43
1:F:274:ASN:O	1:F:276:TYR:N	2.46	0.43
1:F:439:LEU:O	1:F:440:GLU:C	2.57	0.43
1:F:350:LEU:HA	1:F:485:GLU:O	2.19	0.43
1:A:283:SER:N	1:A:286:SER:HB3	2.34	0.43
1:A:476:ILE:HG21	1:A:481:ARG:HB2	2.00	0.43
1:E:269:ALA:CB	1:E:457:GLU:OE1	2.67	0.43
1:F:411:ALA:O	1:F:412:GLY:C	2.57	0.43
1:F:712:LEU:HB3	1:F:713:PRO:CD	2.48	0.43
1:F:747:GLU:CD	1:F:747:GLU:H	2.20	0.43
1:A:333:LEU:HD23	1:A:336:LEU:HD12	2.01	0.42
1:A:656:PHE:CD2	1:A:657:HIS:N	2.87	0.42
1:B:273:LEU:O	1:B:276:TYR:HB2	2.19	0.42
1:B:301:TRP:O	1:B:414:LEU:HD21	2.19	0.42
1:B:593:VAL:HG13	1:B:693:ARG:O	2.19	0.42
1:B:622:LEU:HB2	1:B:662:ILE:HG12	2.01	0.42
1:B:637:GLN:HA	1:B:640:PHE:HB3	2.01	0.42
1:B:686:LEU:HD22	1:B:686:LEU:O	2.19	0.42
1:B:733:ILE:HA	1:B:756:ILE:O	2.19	0.42
1:D:267:GLU:HA	1:D:270:LEU:HG	2.00	0.42
1:D:329:LYS:C	1:D:331:ARG:H	2.22	0.42
1:D:411:ALA:O	1:D:412:GLY:C	2.57	0.42
1:D:642:TYR:CE1	1:D:709:GLY:HA3	2.54	0.42
1:E:300:PRO:HG3	1:E:412:GLY:C	2.40	0.42
1:E:373:ARG:NE	1:E:415:ASN:OD1	2.52	0.42
1:E:489:ILE:H	1:E:489:ILE:HG12	1.65	0.42
1:E:682:MET:HE3	1:E:682:MET:HB3	1.68	0.42
1:F:569:THR:HG23	1:F:571:LYS:N	2.19	0.42
1:F:622:LEU:HB2	1:F:662:ILE:CG1	2.49	0.42
1:F:678:ALA:O	1:F:682:MET:HG2	2.19	0.42
1:A:329:LYS:C	1:A:331:ARG:H	2.22	0.42
1:A:546:GLN:OE1	1:A:577:ILE:HB	2.19	0.42
1:B:277:GLU:OE1	1:F:246:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:O	1:B:297:VAL:HG23	2.19	0.42
1:B:546:GLN:OE1	1:B:577:ILE:HB	2.20	0.42
1:B:579:LYS:C	1:B:579:LYS:HE2	2.40	0.42
1:B:647:THR:HG23	1:B:652:ILE:HG23	2.00	0.42
1:C:505:LEU:HD23	1:C:505:LEU:HA	1.43	0.42
1:C:505:LEU:CD2	1:C:544:GLU:HG3	2.47	0.42
1:D:329:LYS:O	1:D:330:GLU:C	2.57	0.42
1:D:403:ARG:O	1:D:403:ARG:CG	2.67	0.42
1:E:516:LYS:HZ1	1:E:516:LYS:HA	1.82	0.42
1:E:550:ILE:O	1:E:551:CYS:C	2.58	0.42
1:E:656:PHE:CD2	1:E:657:HIS:N	2.87	0.42
1:F:464:VAL:CG1	1:F:466:PHE:CE1	3.02	0.42
1:A:342:THR:HG22	1:A:344:SER:O	2.20	0.42
1:B:290:ARG:NH1	1:E:273:LEU:HD21	2.34	0.42
1:B:455:ILE:HG23	1:B:455:ILE:O	2.19	0.42
1:B:712:LEU:HB3	1:B:713:PRO:HD2	2.01	0.42
1:C:464:VAL:O	1:C:466:PHE:CD1	2.68	0.42
1:C:597:THR:O	1:C:700:GLY:HA2	2.19	0.42
1:D:256:ILE:CD1	1:D:293:ILE:HD11	2.48	0.42
1:D:439:LEU:HD13	1:D:480:LEU:HD13	2.00	0.42
1:D:712:LEU:HB3	1:D:713:PRO:HD2	2.01	0.42
1:E:346:LYS:HG3	1:E:348:PRO:HD2	2.01	0.42
1:C:346:LYS:HZ1	1:E:513:HIS:CE1	2.36	0.42
1:F:562:GLU:O	1:F:563:ARG:C	2.58	0.42
1:F:647:THR:HG22	1:F:648:GLU:N	2.34	0.42
1:A:373:ARG:NE	1:A:415:ASN:OD1	2.52	0.42
1:A:456:GLU:O	1:A:457:GLU:HB2	2.20	0.42
1:A:593:VAL:HG13	1:A:693:ARG:O	2.19	0.42
1:B:359:GLY:HA2	2:B:783:ADP:H5'2	2.01	0.42
1:B:569:THR:HG23	1:B:572:ASN:H	1.84	0.42
1:C:455:ILE:O	1:C:455:ILE:HG23	2.18	0.42
1:C:646:LYS:CD	1:C:646:LYS:H	2.32	0.42
1:D:270:LEU:HD21	1:D:296:LEU:CD2	2.45	0.42
1:D:536:ARG:NH1	1:D:536:ARG:CB	2.82	0.42
1:E:298:ALA:O	1:E:299:LEU:C	2.57	0.42
1:B:283:SER:N	1:B:286:SER:HB3	2.34	0.42
1:B:408:MET:N	1:B:408:MET:HE2	2.35	0.42
1:C:305:THR:O	1:C:307:ASP:N	2.52	0.42
1:D:562:GLU:O	1:D:563:ARG:C	2.56	0.42
1:E:299:LEU:O	1:E:301:TRP:CE2	2.73	0.42
1:E:596:VAL:HG23	1:E:685:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:ILE:HD13	1:F:420:LEU:HD12	2.02	0.42
1:F:440:GLU:HG3	1:F:446:GLN:OE1	2.19	0.42
1:A:506:LEU:O	1:A:507:PRO:C	2.58	0.42
1:A:522:LEU:HB3	1:A:568:VAL:CG1	2.45	0.42
1:A:561:GLU:O	1:A:562:GLU:HB2	2.19	0.42
1:A:733:ILE:HA	1:A:756:ILE:O	2.19	0.42
1:B:656:PHE:CD2	1:B:657:HIS:N	2.88	0.42
1:C:279:ILE:HA	1:C:280:PRO:HA	1.86	0.42
1:C:311:LEU:O	1:C:312:LYS:C	2.56	0.42
1:C:536:ARG:NH1	1:C:536:ARG:HB2	2.34	0.42
1:C:627:LYS:O	1:C:627:LYS:HG3	2.20	0.42
1:D:602:THR:C	1:D:604:VAL:H	2.23	0.42
1:E:365:LYS:HG3	1:E:375:PHE:CZ	2.55	0.42
1:E:505:LEU:HD23	1:E:505:LEU:HA	1.38	0.42
1:E:561:GLU:O	1:E:562:GLU:HB2	2.19	0.42
1:E:599:LEU:N	1:E:599:LEU:HD22	2.34	0.42
1:E:714:ILE:HB	1:E:735:PRO:HG2	2.00	0.42
1:F:283:SER:N	1:F:286:SER:HB3	2.35	0.42
1:F:342:THR:HG22	1:F:344:SER:O	2.20	0.42
1:F:599:LEU:O	1:F:720:LYS:HE2	2.20	0.42
1:A:262:PRO:HD2	1:A:301:TRP:HB3	2.01	0.42
1:A:266:LYS:HG3	1:A:267:GLU:H	1.82	0.42
1:B:460:ASP:O	1:B:461:LEU:HD23	2.18	0.42
1:C:271:LYS:CA	1:C:274:ASN:HB3	2.48	0.42
1:D:279:ILE:HA	1:D:280:PRO:HA	1.86	0.42
1:D:283:SER:N	1:D:286:SER:HB3	2.34	0.42
1:E:622:LEU:HB2	1:E:662:ILE:HG12	2.02	0.42
1:F:256:ILE:CD1	1:F:293:ILE:HD11	2.49	0.42
1:F:299:LEU:HA	1:F:300:PRO:HD3	1.69	0.42
1:F:496:GLU:O	1:F:497:LYS:C	2.58	0.42
1:F:705:ILE:HA	1:F:705:ILE:HD12	1.74	0.42
1:A:480:LEU:O	1:A:483:ARG:N	2.53	0.42
1:A:747:GLU:N	1:A:747:GLU:CD	2.72	0.42
1:B:271:LYS:CA	1:B:274:ASN:HB3	2.46	0.42
1:B:329:LYS:O	1:B:331:ARG:N	2.53	0.42
1:C:602:THR:C	1:C:604:VAL:H	2.22	0.42
1:C:706:THR:OG1	1:C:710:ARG:HB2	2.19	0.42
1:D:469:THR:HG22	1:D:470:ALA:N	2.34	0.42
1:A:573:LEU:HA	1:A:573:LEU:HD12	1.93	0.42
1:B:423:ILE:HG22	1:B:426:MET:HE1	2.00	0.42
1:B:561:GLU:O	1:B:562:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:TYR:CD2	1:C:335:TYR:O	2.73	0.42
1:C:593:VAL:HG13	1:C:693:ARG:O	2.19	0.42
1:D:579:LYS:HE2	1:D:579:LYS:C	2.39	0.42
1:D:705:ILE:HD11	1:D:761:LEU:CD2	2.50	0.42
1:E:283:SER:N	1:E:286:SER:HB3	2.34	0.42
1:E:411:ALA:O	1:E:412:GLY:C	2.58	0.42
1:A:441:VAL:HG22	1:A:441:VAL:O	2.19	0.42
1:A:611:ILE:HD12	1:A:681:THR:CG2	2.50	0.42
1:B:342:THR:HG22	1:B:344:SER:O	2.20	0.42
1:B:486:ILE:CG2	1:B:487:ILE:N	2.82	0.42
1:C:293:ILE:O	1:C:297:VAL:HG23	2.18	0.42
1:D:505:LEU:HA	1:D:505:LEU:HD23	1.37	0.42
1:D:739:GLU:C	1:D:741:ASP:N	2.73	0.42
1:E:412:GLY:C	1:E:413:LYS:HG2	2.39	0.42
1:E:589:THR:O	1:E:697:ARG:CD	2.68	0.42
1:F:293:ILE:O	1:F:297:VAL:HG23	2.20	0.42
1:F:682:MET:HE3	1:F:682:MET:HB3	1.77	0.42
1:A:293:ILE:O	1:A:297:VAL:HG23	2.20	0.41
1:A:294:ASP:C	1:A:296:LEU:N	2.72	0.41
1:A:300:PRO:HG3	1:A:412:GLY:HA2	2.02	0.41
1:A:516:LYS:HZ1	1:A:516:LYS:HA	1.82	0.41
1:A:547:LEU:HA	1:A:547:LEU:HD23	1.78	0.41
1:B:732:ILE:HG21	1:B:753:LEU:HD13	2.02	0.41
1:B:747:GLU:N	1:B:747:GLU:CD	2.73	0.41
1:C:329:LYS:O	1:C:332:ILE:N	2.41	0.41
1:C:355:PRO:O	1:C:358:VAL:HG22	2.20	0.41
1:C:680:ILE:HG22	1:C:705:ILE:HD13	2.02	0.41
1:C:747:GLU:N	1:C:747:GLU:CD	2.73	0.41
1:D:368:ALA:CB	1:D:417:VAL:HG21	2.48	0.41
1:D:495:ILE:HA	1:D:495:ILE:HD13	1.87	0.41
1:D:573:LEU:CG	1:D:577:ILE:HD11	2.50	0.41
1:E:423:ILE:C	1:E:424:ASP:OD1	2.58	0.41
1:E:506:LEU:O	1:E:507:PRO:C	2.58	0.41
1:F:267:GLU:HA	1:F:270:LEU:HG	2.02	0.41
1:F:294:ASP:C	1:F:296:LEU:N	2.73	0.41
1:F:329:LYS:O	1:F:330:GLU:C	2.58	0.41
1:F:341:LEU:O	1:F:343:LYS:N	2.53	0.41
1:F:519:ASN:HD22	1:F:519:ASN:HA	1.53	0.41
1:F:536:ARG:CB	1:F:536:ARG:HH11	2.32	0.41
1:F:737:ASP:N	1:F:737:ASP:OD2	2.53	0.41
1:B:705:ILE:HA	1:B:705:ILE:HD12	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:PHE:CD2	1:C:657:HIS:N	2.88	0.41
1:D:496:GLU:O	1:D:500:ILE:HG13	2.18	0.41
1:D:734:ALA:HB1	1:D:735:PRO:CD	2.51	0.41
1:E:579:LYS:HE2	1:E:579:LYS:C	2.41	0.41
1:A:336:LEU:CD2	1:A:371:LEU:HD11	2.51	0.41
1:A:622:LEU:HB2	1:A:662:ILE:HG12	2.03	0.41
1:B:693:ARG:O	1:B:694:ALA:HB2	2.19	0.41
1:B:705:ILE:HD11	1:B:761:LEU:CD2	2.49	0.41
1:C:529:ASP:O	1:C:530:ILE:C	2.58	0.41
1:D:547:LEU:HA	1:D:547:LEU:HD23	1.79	0.41
1:D:558:ILE:H	1:D:558:ILE:HG12	1.65	0.41
1:D:675:GLY:N	1:D:676:PRO:CD	2.83	0.41
1:E:350:LEU:HD23	1:E:487:ILE:HD11	2.02	0.41
1:E:736:LYS:HA	1:E:757:LEU:HB3	2.03	0.41
1:F:423:ILE:HG21	1:F:423:ILE:HD13	1.78	0.41
1:A:355:PRO:O	1:A:358:VAL:HG22	2.20	0.41
1:A:710:ARG:HG2	1:A:710:ARG:HH21	1.85	0.41
1:C:440:GLU:HG3	1:C:446:GLN:OE1	2.20	0.41
1:C:506:LEU:HD12	1:C:510:ILE:CG1	2.49	0.41
1:D:455:ILE:O	1:D:455:ILE:HG23	2.19	0.41
1:D:622:LEU:HB2	1:D:662:ILE:HG12	2.02	0.41
1:D:636:ALA:C	1:D:638:ALA:N	2.73	0.41
1:D:707:LEU:HD23	1:D:707:LEU:HA	1.92	0.41
1:E:329:LYS:O	1:E:331:ARG:N	2.54	0.41
1:F:424:ASP:OD1	1:F:424:ASP:N	2.53	0.41
1:A:359:GLY:O	1:A:360:LYS:C	2.59	0.41
1:A:417:VAL:HG22	1:A:465:LEU:HB3	2.02	0.41
1:B:412:GLY:C	1:B:413:LYS:HG2	2.39	0.41
1:B:419:LEU:O	1:B:421:ASP:N	2.53	0.41
1:B:352:LEU:CD2	1:B:489:ILE:HD11	2.50	0.41
1:C:267:GLU:HA	1:C:270:LEU:HB2	2.02	0.41
1:C:551:CYS:O	1:C:554:ALA:HB3	2.20	0.41
1:C:561:GLU:O	1:C:562:GLU:HB2	2.20	0.41
1:C:579:LYS:HE2	1:C:579:LYS:C	2.40	0.41
1:C:584:TYR:CD1	1:C:584:TYR:O	2.73	0.41
1:D:474:ALA:O	1:D:476:ILE:O	2.38	0.41
1:E:262:PRO:HD2	1:E:301:TRP:HB2	2.03	0.41
1:E:266:LYS:HG3	1:E:267:GLU:H	1.81	0.41
1:A:735:PRO:O	1:A:738:ASN:HB2	2.19	0.41
1:C:267:GLU:HA	1:C:270:LEU:HG	2.01	0.41
1:C:364:ALA:O	1:C:365:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:GLY:C	1:D:413:LYS:HG2	2.39	0.41
1:D:555:ALA:O	1:D:556:LYS:C	2.58	0.41
1:E:464:VAL:O	1:E:466:PHE:CD1	2.64	0.41
1:E:352:LEU:CD2	1:E:489:ILE:HD11	2.47	0.41
1:E:536:ARG:NH1	1:E:536:ARG:HG3	2.14	0.41
1:E:573:LEU:CG	1:E:577:ILE:HD11	2.51	0.41
1:E:717:LEU:HA	1:E:717:LEU:HD23	1.87	0.41
1:A:414:LEU:HD12	1:A:414:LEU:C	2.41	0.41
1:A:712:LEU:HB3	1:A:713:PRO:HD2	2.03	0.41
1:A:736:LYS:HA	1:A:757:LEU:HB3	2.03	0.41
1:B:276:TYR:HD1	1:B:277:GLU:N	2.17	0.41
1:C:476:ILE:HG21	1:C:481:ARG:HB2	2.02	0.41
1:C:569:THR:HG22	1:C:572:ASN:H	1.86	0.41
1:C:599:LEU:O	1:C:720:LYS:HE2	2.21	0.41
1:D:367:ILE:O	1:D:371:LEU:HD13	2.21	0.41
1:D:460:ASP:O	1:D:461:LEU:HD23	2.20	0.41
1:D:639:ALA:HB1	1:D:683:ALA:HA	2.03	0.41
1:E:273:LEU:O	1:E:276:TYR:HB2	2.20	0.41
1:E:678:ALA:O	1:E:682:MET:HG2	2.20	0.41
1:F:637:GLN:HA	1:F:640:PHE:HB3	2.02	0.41
1:F:739:GLU:C	1:F:741:ASP:N	2.74	0.41
1:A:551:CYS:O	1:A:554:ALA:HB3	2.21	0.41
1:B:341:LEU:HB3	1:F:514:GLY:O	2.20	0.41
1:B:506:LEU:CD1	1:B:506:LEU:C	2.88	0.41
1:C:411:ALA:O	1:C:412:GLY:C	2.59	0.41
1:C:678:ALA:O	1:C:682:MET:HG2	2.21	0.41
1:D:506:LEU:HB3	1:D:507:PRO:CD	2.48	0.41
1:F:567:THR:HG22	1:F:567:THR:O	2.21	0.41
1:A:304:GLU:O	1:A:304:GLU:HG2	2.20	0.41
1:A:364:ALA:O	1:A:365:LYS:C	2.56	0.41
1:A:616:SER:O	1:A:661:ASP:N	2.54	0.41
1:B:305:THR:CG2	1:B:306:ASP:N	2.83	0.41
1:B:332:ILE:CG2	1:B:367:ILE:HD11	2.51	0.41
1:B:440:GLU:HG3	1:B:446:GLN:OE1	2.21	0.41
1:B:478:GLY:N	1:B:479:PRO:CD	2.84	0.41
1:B:761:LEU:HA	1:B:761:LEU:HD23	1.95	0.41
1:C:469:THR:CG2	1:C:470:ALA:N	2.82	0.41
1:C:602:THR:HG22	1:C:603:THR:N	2.35	0.41
1:C:711:VAL:N	1:C:759:SER:O	2.51	0.41
1:D:298:ALA:O	1:D:299:LEU:C	2.59	0.41
1:D:572:ASN:O	1:D:573:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:TYR:CD2	1:D:761:LEU:HD12	2.56	0.41
1:E:359:GLY:HA2	2:E:783:ADP:H5'	2.03	0.41
1:E:705:ILE:HD11	1:E:761:LEU:CD2	2.51	0.41
1:F:561:GLU:O	1:F:562:GLU:HB2	2.21	0.41
1:F:707:LEU:HA	1:F:707:LEU:HD23	1.90	0.41
1:A:589:THR:O	1:A:590:GLU:CD	2.59	0.41
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.83	0.41
1:B:489:ILE:H	1:B:489:ILE:HG12	1.49	0.41
1:B:598:GLY:HA2	1:B:701:MET:O	2.21	0.41
1:D:650:LEU:HD11	1:D:765:LEU:HD13	2.03	0.41
1:E:271:LYS:CA	1:E:274:ASN:HB3	2.45	0.41
1:E:520:LEU:HA	1:E:566:ILE:O	2.21	0.41
1:E:693:ARG:HB3	1:E:694:ALA:H	1.73	0.41
1:F:271:LYS:CA	1:F:274:ASN:HB3	2.46	0.41
1:F:656:PHE:CD2	1:F:657:HIS:N	2.89	0.41
1:A:403:ARG:N	1:A:405:ILE:HG13	2.36	0.41
1:A:536:ARG:HG3	1:A:536:ARG:NH1	2.20	0.41
1:A:536:ARG:NH1	1:A:536:ARG:HB2	2.36	0.41
1:B:622:LEU:HB2	1:B:662:ILE:CG1	2.51	0.41
1:C:276:TYR:HD1	1:C:277:GLU:N	2.19	0.41
1:C:710:ARG:HG2	1:C:710:ARG:HH21	1.86	0.41
1:D:403:ARG:HG2	1:D:403:ARG:O	2.21	0.41
1:D:551:CYS:O	1:D:554:ALA:HB3	2.21	0.41
1:D:752:GLY:O	1:D:753:LEU:HD23	2.21	0.41
1:E:267:GLU:HA	1:E:270:LEU:HG	2.01	0.41
1:E:279:ILE:HA	1:E:280:PRO:HA	1.87	0.41
1:F:602:THR:C	1:F:604:VAL:N	2.75	0.41
1:A:557:ALA:CB	1:A:566:ILE:HD11	2.50	0.40
1:B:294:ASP:C	1:B:296:LEU:N	2.72	0.40
1:B:602:THR:C	1:B:604:VAL:N	2.74	0.40
1:B:656:PHE:CE2	1:B:690:LEU:HD11	2.56	0.40
1:C:256:ILE:CD1	1:C:293:ILE:HD11	2.46	0.40
1:C:639:ALA:HB1	1:C:683:ALA:HA	2.04	0.40
1:E:536:ARG:NH2	1:E:583:ARG:O	2.47	0.40
1:F:367:ILE:HG22	1:F:368:ALA:N	2.35	0.40
1:F:557:ALA:CB	1:F:566:ILE:HD11	2.50	0.40
1:A:329:LYS:O	1:A:330:GLU:C	2.59	0.40
1:A:341:LEU:HD13	1:C:514:GLY:O	2.21	0.40
1:A:678:ALA:O	1:A:682:MET:HG2	2.21	0.40
1:A:359:GLY:HA2	2:A:783:ADP:O5'	2.21	0.40
1:B:536:ARG:NH1	1:B:536:ARG:CB	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:C	1:C:331:ARG:H	2.22	0.40
1:C:555:ALA:O	1:C:556:LYS:C	2.57	0.40
1:C:586:GLN:HB3	1:C:697:ARG:HE	1.86	0.40
1:D:373:ARG:NE	1:D:415:ASN:OD1	2.54	0.40
1:D:331:ARG:NH1	1:D:485:GLU:OE1	2.46	0.40
1:D:693:ARG:O	1:D:694:ALA:HB2	2.21	0.40
1:C:708:ARG:NH2	1:E:593:VAL:HB	2.36	0.40
1:F:349:ILE:O	1:F:484:MET:HB2	2.21	0.40
1:A:270:LEU:CD2	1:A:296:LEU:HD22	2.48	0.40
1:A:714:ILE:HD12	1:A:714:ILE:HA	1.79	0.40
1:B:367:ILE:HG22	1:B:368:ALA:N	2.36	0.40
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.76	0.40
1:B:572:ASN:O	1:B:573:LEU:C	2.60	0.40
1:C:537:GLU:HG3	1:C:539:GLY:O	2.22	0.40
1:C:533:TYR:CB	1:C:580:ARG:HD2	2.50	0.40
1:C:687:VAL:O	1:C:691:THR:HG23	2.21	0.40
1:D:267:GLU:HG3	1:D:270:LEU:HD12	2.04	0.40
1:D:307:ASP:O	1:D:309:LEU:HG	2.21	0.40
1:D:440:GLU:HG3	1:D:446:GLN:OE1	2.21	0.40
1:D:534:TYR:CD2	1:D:577:ILE:HD12	2.56	0.40
1:D:646:LYS:H	1:D:646:LYS:CD	2.31	0.40
1:E:656:PHE:CE2	1:E:690:LEU:HD11	2.56	0.40
1:F:355:PRO:O	1:F:358:VAL:HG22	2.21	0.40
1:B:645:SER:HA	1:F:616:SER:HA	2.03	0.40
1:A:262:PRO:HD2	1:A:301:TRP:CB	2.52	0.40
1:A:478:GLY:N	1:A:479:PRO:CD	2.84	0.40
1:B:464:VAL:CG1	1:B:466:PHE:CE1	3.04	0.40
1:B:560:ALA:O	1:B:561:GLU:C	2.59	0.40
1:D:483:ARG:HB3	1:D:483:ARG:NH2	2.37	0.40
1:D:526:ALA:O	1:D:530:ILE:HG13	2.21	0.40
1:E:267:GLU:HG3	1:E:270:LEU:HD12	2.03	0.40
1:E:478:GLY:N	1:E:479:PRO:CD	2.85	0.40
1:F:300:PRO:C	1:F:301:TRP:CG	2.94	0.40
1:A:302:THR:O	1:A:303:ASP:O	2.40	0.40
1:A:408:MET:O	1:A:411:ALA:N	2.50	0.40
1:A:510:ILE:HG22	1:A:515:LEU:O	2.21	0.40
1:B:305:THR:HG22	1:B:306:ASP:N	2.36	0.40
1:B:403:ARG:N	1:B:405:ILE:HG13	2.36	0.40
1:C:362:SER:HB2	2:C:783:ADP:C5'	2.49	0.40
1:C:493:THR:CG2	1:C:748:SER:HB2	2.47	0.40
1:D:552:ARG:O	1:D:553:LYS:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:GLU:O	1:D:562:GLU:HB2	2.21	0.40
1:E:440:GLU:HG3	1:E:446:GLN:OE1	2.20	0.40
1:E:611:ILE:HD12	1:E:681:THR:HG22	2.02	0.40
1:E:622:LEU:HB2	1:E:662:ILE:CG1	2.51	0.40
1:E:613:VAL:HG13	1:E:664:ILE:HG12	2.02	0.40
1:F:276:TYR:HD1	1:F:277:GLU:N	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:ALA:O	1:F:511:LYS:NZ[2_646]	2.14	0.06

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	490/543 (90%)	350 (71%)	97 (20%)	43 (9%)	1	5
1	B	490/543 (90%)	354 (72%)	94 (19%)	42 (9%)	1	5
1	C	490/543 (90%)	347 (71%)	104 (21%)	39 (8%)	1	6
1	D	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	6
1	E	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	6
1	F	490/543 (90%)	352 (72%)	99 (20%)	39 (8%)	1	6
All	All	2940/3258 (90%)	2103 (72%)	598 (20%)	239 (8%)	1	5

All (239) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	TYR
1	A	288	VAL

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Mol	Chain	Res	Type
1	A	303	ASP
1	A	304	GLU
1	A	314	ALA
1	A	407	GLY
1	A	412	GLY
1	A	424	ASP
1	A	439	LEU
1	A	440	GLU
1	A	455	ILE
1	A	475	THR
1	A	560	ALA
1	A	646	LYS
1	A	693	ARG
1	B	276	TYR
1	B	288	VAL
1	B	314	ALA
1	B	405	ILE
1	B	407	GLY
1	B	412	GLY
1	B	424	ASP
1	B	439	LEU
1	B	440	GLU
1	B	455	ILE
1	B	475	THR
1	B	560	ALA
1	B	646	LYS
1	B	693	ARG
1	C	276	TYR
1	C	288	VAL
1	C	306	ASP
1	C	314	ALA
1	C	407	GLY
1	C	412	GLY
1	C	424	ASP
1	C	439	LEU
1	C	440	GLU
1	C	455	ILE
1	C	475	THR
1	C	646	LYS
1	C	693	ARG
1	D	276	TYR
1	D	288	VAL

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Mol	Chain	Res	Type
1	D	314	ALA
1	D	407	GLY
1	D	412	GLY
1	D	424	ASP
1	D	439	LEU
1	D	440	GLU
1	D	455	ILE
1	D	475	THR
1	D	560	ALA
1	D	646	LYS
1	D	693	ARG
1	E	276	TYR
1	E	288	VAL
1	E	314	ALA
1	E	407	GLY
1	E	412	GLY
1	E	424	ASP
1	E	439	LEU
1	E	440	GLU
1	E	455	ILE
1	E	475	THR
1	E	560	ALA
1	E	646	LYS
1	E	693	ARG
1	F	276	TYR
1	F	288	VAL
1	F	314	ALA
1	F	407	GLY
1	F	412	GLY
1	F	424	ASP
1	F	439	LEU
1	F	440	GLU
1	F	455	ILE
1	F	475	THR
1	F	560	ALA
1	F	646	LYS
1	F	693	ARG
1	A	275	ARG
1	A	281	SER
1	A	313	GLU
1	A	405	ILE
1	A	474	ALA

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Mol	Chain	Res	Type
1	A	514	GLY
1	A	603	THR
1	A	629	GLY
1	A	645	SER
1	B	275	ARG
1	B	281	SER
1	B	304	GLU
1	B	313	GLU
1	B	420	LEU
1	B	474	ALA
1	B	514	GLY
1	B	629	GLY
1	B	645	SER
1	C	275	ARG
1	C	281	SER
1	C	313	GLU
1	C	405	ILE
1	C	474	ALA
1	C	514	GLY
1	C	560	ALA
1	C	629	GLY
1	C	645	SER
1	D	275	ARG
1	D	281	SER
1	D	313	GLU
1	D	405	ILE
1	D	474	ALA
1	D	514	GLY
1	D	587	ALA
1	D	629	GLY
1	D	645	SER
1	E	275	ARG
1	E	281	SER
1	E	313	GLU
1	E	405	ILE
1	E	474	ALA
1	E	514	GLY
1	E	629	GLY
1	F	275	ARG
1	F	281	SER
1	F	303	ASP
1	F	313	GLU

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Mol	Chain	Res	Type
1	F	405	ILE
1	F	420	LEU
1	F	514	GLY
1	F	629	GLY
1	F	645	SER
1	A	262	PRO
1	A	342	THR
1	A	416	PRO
1	A	420	LEU
1	A	456	GLU
1	A	637	GLN
1	B	262	PRO
1	B	303	ASP
1	B	342	THR
1	B	456	GLU
1	B	561	GLU
1	B	637	GLN
1	B	672	PRO
1	C	262	PRO
1	C	342	THR
1	C	416	PRO
1	C	456	GLU
1	C	672	PRO
1	D	262	PRO
1	D	299	LEU
1	D	342	THR
1	D	416	PRO
1	D	456	GLU
1	D	561	GLU
1	D	603	THR
1	D	637	GLN
1	D	672	PRO
1	E	262	PRO
1	E	306	ASP
1	E	342	THR
1	E	416	PRO
1	E	456	GLU
1	E	637	GLN
1	E	645	SER
1	E	672	PRO
1	F	262	PRO
1	F	342	THR

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Mol	Chain	Res	Type
1	F	416	PRO
1	F	456	GLU
1	F	474	ALA
1	F	603	THR
1	F	672	PRO
1	A	280	PRO
1	A	305	THR
1	A	330	GLU
1	A	561	GLU
1	A	672	PRO
1	B	280	PRO
1	B	416	PRO
1	B	694	ALA
1	C	280	PRO
1	C	420	LEU
1	C	561	GLU
1	C	637	GLN
1	D	280	PRO
1	E	280	PRO
1	E	420	LEU
1	E	603	THR
1	F	280	PRO
1	F	421	ASP
1	F	637	GLN
1	A	248	GLU
1	A	272	GLU
1	A	591	ASP
1	B	248	GLU
1	B	270	LEU
1	B	272	GLU
1	B	323	HIS
1	B	603	THR
1	C	248	GLU
1	C	270	LEU
1	C	272	GLU
1	C	421	ASP
1	D	248	GLU
1	D	270	LEU
1	D	272	GLU
1	D	304	GLU
1	D	420	LEU
1	E	248	GLU

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Mol	Chain	Res	Type
1	E	270	LEU
1	E	561	GLU
1	F	248	GLU
1	F	270	LEU
1	F	272	GLU
1	F	561	GLU
1	A	261	MET
1	A	270	LEU
1	A	421	ASP
1	B	261	MET
1	B	421	ASP
1	C	261	MET
1	C	330	GLU
1	D	261	MET
1	E	261	MET
1	E	272	GLU
1	F	261	MET
1	C	324	GLY
1	E	324	GLY
1	F	652	ILE
1	B	324	GLY
1	B	652	ILE
1	F	324	GLY
1	C	652	ILE
1	A	324	GLY
1	A	652	ILE
1	E	652	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/454 (91%)	361 (87%)	54 (13%)	4	16
1	B	415/454 (91%)	358 (86%)	57 (14%)	3	14
1	C	415/454 (91%)	357 (86%)	58 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	415/454 (91%)	358 (86%)	57 (14%)	3	14
1	E	415/454 (91%)	357 (86%)	58 (14%)	3	13
1	F	415/454 (91%)	360 (87%)	55 (13%)	4	15
All	All	2490/2724 (91%)	2151 (86%)	339 (14%)	3	14

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	294	ASP
1	A	296	LEU
1	A	312	LYS
1	A	313	GLU
1	A	316	ARG
1	A	331	ARG
1	A	350	LEU
1	A	367	ILE
1	A	378	ILE
1	A	408	MET
1	A	442	LEU
1	A	455	ILE
1	A	463	LYS
1	A	465	LEU
1	A	471	ASN
1	A	475	THR
1	A	489	ILE
1	A	493	THR
1	A	504	HIS
1	A	506	LEU
1	A	516	LYS
1	A	519	ASN
1	A	522	LEU
1	A	532	ARG
1	A	534	TYR
1	A	536	ARG
1	A	543	LEU
1	A	565	ARG
1	A	568	VAL
1	A	579	LYS
1	A	590	GLU
1	A	592	GLN

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Mol	Chain	Res	Type
1	A	608	THR
1	A	624	LEU
1	A	635	SER
1	A	646	LYS
1	A	656	PHE
1	A	660	TYR
1	A	661	ASP
1	A	666	VAL
1	A	671	VAL
1	A	682	MET
1	A	686	LEU
1	A	705	ILE
1	A	714	ILE
1	A	717	LEU
1	A	731	THR
1	A	732	ILE
1	A	738	ASN
1	A	747	GLU
1	A	748	SER
1	A	759	SER
1	A	762	ASP
1	B	263	ASP
1	B	294	ASP
1	B	296	LEU
1	B	299	LEU
1	B	312	LYS
1	B	313	GLU
1	B	316	ARG
1	B	331	ARG
1	B	350	LEU
1	B	367	ILE
1	B	378	ILE
1	B	408	MET
1	B	423	ILE
1	B	442	LEU
1	B	455	ILE
1	B	463	LYS
1	B	465	LEU
1	B	475	THR
1	B	489	ILE
1	B	493	THR
1	B	504	HIS

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Mol	Chain	Res	Type
1	B	506	LEU
1	B	516	LYS
1	B	519	ASN
1	B	522	LEU
1	B	536	ARG
1	B	543	LEU
1	B	565	ARG
1	B	568	VAL
1	B	579	LYS
1	B	589	THR
1	B	590	GLU
1	B	592	GLN
1	B	599	LEU
1	B	608	THR
1	B	624	LEU
1	B	635	SER
1	B	646	LYS
1	B	656	PHE
1	B	660	TYR
1	B	661	ASP
1	B	666	VAL
1	B	671	VAL
1	B	682	MET
1	B	686	LEU
1	B	705	ILE
1	B	714	ILE
1	B	717	LEU
1	B	731	THR
1	B	732	ILE
1	B	738	ASN
1	B	747	GLU
1	B	748	SER
1	B	759	SER
1	B	762	ASP
1	B	767	HIS
1	B	770	VAL
1	C	263	ASP
1	C	294	ASP
1	C	296	LEU
1	C	300	PRO
1	C	303	ASP
1	C	305	THR

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Mol	Chain	Res	Type
1	C	312	LYS
1	C	313	GLU
1	C	316	ARG
1	C	331	ARG
1	C	350	LEU
1	C	367	ILE
1	C	378	ILE
1	C	408	MET
1	C	442	LEU
1	C	455	ILE
1	C	463	LYS
1	C	465	LEU
1	C	475	THR
1	C	489	ILE
1	C	493	THR
1	C	504	HIS
1	C	506	LEU
1	C	516	LYS
1	C	519	ASN
1	C	522	LEU
1	C	532	ARG
1	C	536	ARG
1	C	543	LEU
1	C	565	ARG
1	C	568	VAL
1	C	579	LYS
1	C	583	ARG
1	C	592	GLN
1	C	599	LEU
1	C	608	THR
1	C	624	LEU
1	C	635	SER
1	C	646	LYS
1	C	656	PHE
1	C	660	TYR
1	C	661	ASP
1	C	666	VAL
1	C	671	VAL
1	C	682	MET
1	C	686	LEU
1	C	705	ILE
1	C	714	ILE

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Mol	Chain	Res	Type
1	C	717	LEU
1	C	731	THR
1	C	732	ILE
1	C	738	ASN
1	C	741	ASP
1	C	747	GLU
1	C	748	SER
1	C	759	SER
1	C	762	ASP
1	C	767	HIS
1	D	263	ASP
1	D	294	ASP
1	D	296	LEU
1	D	303	ASP
1	D	305	THR
1	D	312	LYS
1	D	313	GLU
1	D	316	ARG
1	D	331	ARG
1	D	350	LEU
1	D	367	ILE
1	D	378	ILE
1	D	423	ILE
1	D	442	LEU
1	D	455	ILE
1	D	463	LYS
1	D	465	LEU
1	D	475	THR
1	D	489	ILE
1	D	493	THR
1	D	506	LEU
1	D	516	LYS
1	D	519	ASN
1	D	522	LEU
1	D	532	ARG
1	D	536	ARG
1	D	543	LEU
1	D	565	ARG
1	D	568	VAL
1	D	579	LYS
1	D	583	ARG
1	D	589	THR

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Mol	Chain	Res	Type
1	D	592	GLN
1	D	599	LEU
1	D	608	THR
1	D	624	LEU
1	D	635	SER
1	D	646	LYS
1	D	656	PHE
1	D	660	TYR
1	D	661	ASP
1	D	666	VAL
1	D	671	VAL
1	D	682	MET
1	D	686	LEU
1	D	705	ILE
1	D	714	ILE
1	D	717	LEU
1	D	731	THR
1	D	732	ILE
1	D	738	ASN
1	D	747	GLU
1	D	748	SER
1	D	749	VAL
1	D	759	SER
1	D	762	ASP
1	D	770	VAL
1	E	263	ASP
1	E	294	ASP
1	E	296	LEU
1	E	312	LYS
1	E	313	GLU
1	E	316	ARG
1	E	331	ARG
1	E	350	LEU
1	E	367	ILE
1	E	378	ILE
1	E	408	MET
1	E	442	LEU
1	E	455	ILE
1	E	463	LYS
1	E	465	LEU
1	E	471	ASN
1	E	475	THR

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Mol	Chain	Res	Type
1	E	489	ILE
1	E	493	THR
1	E	506	LEU
1	E	515	LEU
1	E	516	LYS
1	E	519	ASN
1	E	522	LEU
1	E	532	ARG
1	E	536	ARG
1	E	543	LEU
1	E	565	ARG
1	E	568	VAL
1	E	579	LYS
1	E	588	GLU
1	E	590	GLU
1	E	592	GLN
1	E	593	VAL
1	E	599	LEU
1	E	608	THR
1	E	624	LEU
1	E	635	SER
1	E	646	LYS
1	E	656	PHE
1	E	660	TYR
1	E	661	ASP
1	E	666	VAL
1	E	671	VAL
1	E	682	MET
1	E	686	LEU
1	E	705	ILE
1	E	714	ILE
1	E	717	LEU
1	E	731	THR
1	E	732	ILE
1	E	738	ASN
1	E	741	ASP
1	E	747	GLU
1	E	748	SER
1	E	759	SER
1	E	762	ASP
1	E	767	HIS
1	F	263	ASP

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Mol	Chain	Res	Type
1	F	294	ASP
1	F	296	LEU
1	F	305	THR
1	F	312	LYS
1	F	313	GLU
1	F	316	ARG
1	F	331	ARG
1	F	350	LEU
1	F	367	ILE
1	F	378	ILE
1	F	423	ILE
1	F	442	LEU
1	F	455	ILE
1	F	463	LYS
1	F	465	LEU
1	F	475	THR
1	F	489	ILE
1	F	493	THR
1	F	506	LEU
1	F	516	LYS
1	F	519	ASN
1	F	522	LEU
1	F	532	ARG
1	F	536	ARG
1	F	543	LEU
1	F	565	ARG
1	F	568	VAL
1	F	579	LYS
1	F	588	GLU
1	F	589	THR
1	F	592	GLN
1	F	608	THR
1	F	624	LEU
1	F	635	SER
1	F	646	LYS
1	F	656	PHE
1	F	660	TYR
1	F	661	ASP
1	F	666	VAL
1	F	671	VAL
1	F	682	MET
1	F	686	LEU

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Mol	Chain	Res	Type
1	F	705	ILE
1	F	706	THR
1	F	714	ILE
1	F	717	LEU
1	F	731	THR
1	F	732	ILE
1	F	738	ASN
1	F	747	GLU
1	F	748	SER
1	F	759	SER
1	F	762	ASP
1	F	767	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	767	HIS
1	B	250	GLN
1	B	446	GLN
1	B	586	GLN
1	B	767	HIS
1	C	250	GLN
1	C	291	ASN
1	C	446	GLN
1	C	586	GLN
1	C	767	HIS
1	D	250	GLN
1	D	767	HIS
1	E	250	GLN
1	E	767	HIS
1	F	250	GLN
1	F	446	GLN
1	F	767	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	783	-	24,29,29	1.25	3 (12%)	29,45,45	2.54	13 (44%)
2	ADP	D	783	-	24,29,29	1.38	4 (16%)	29,45,45	1.99	11 (37%)
2	ADP	A	783	-	24,29,29	1.35	3 (12%)	29,45,45	2.49	12 (41%)
2	ADP	B	783	-	24,29,29	1.17	2 (8%)	29,45,45	1.96	8 (27%)
2	ADP	E	783	-	24,29,29	1.24	4 (16%)	29,45,45	2.19	12 (41%)
2	ADP	F	783	-	24,29,29	1.11	2 (8%)	29,45,45	2.27	11 (37%)

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	783	-	-	5/12/32/32	0/3/3/3
2	ADP	D	783	-	-	4/12/32/32	0/3/3/3
2	ADP	A	783	-	-	3/12/32/32	0/3/3/3
2	ADP	B	783	-	-	3/12/32/32	0/3/3/3
2	ADP	E	783	-	-	6/12/32/32	0/3/3/3
2	ADP	F	783	-	-	5/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	783	ADP	C2'-C1'	-3.52	1.48	1.53
2	A	783	ADP	C5-C4	3.50	1.50	1.40
2	D	783	ADP	C2'-C1'	-3.29	1.48	1.53
2	C	783	ADP	C5-C4	3.19	1.49	1.40
2	A	783	ADP	C2'-C1'	-3.09	1.49	1.53
2	C	783	ADP	C2'-C1'	-3.02	1.49	1.53
2	D	783	ADP	C5-C4	2.88	1.48	1.40
2	F	783	ADP	C2'-C1'	-2.82	1.49	1.53
2	E	783	ADP	C5-C4	2.74	1.48	1.40
2	E	783	ADP	C2'-C1'	-2.67	1.49	1.53
2	E	783	ADP	C2-N3	2.59	1.36	1.32
2	F	783	ADP	C5-C4	2.46	1.47	1.40
2	A	783	ADP	C2-N3	2.31	1.35	1.32
2	B	783	ADP	C5-C4	2.18	1.46	1.40
2	D	783	ADP	PB-O3B	-2.11	1.46	1.54
2	D	783	ADP	C5-N7	-2.02	1.32	1.39
2	C	783	ADP	C2-N3	2.02	1.35	1.32
2	E	783	ADP	C6-C5	2.00	1.50	1.43

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	783	ADP	PA-O3A-PB	-8.71	102.94	132.83
2	C	783	ADP	O4'-C1'-C2'	-5.99	98.17	106.93
2	F	783	ADP	O4'-C1'-C2'	-5.53	98.85	106.93
2	B	783	ADP	PA-O3A-PB	-5.51	113.92	132.83
2	C	783	ADP	PA-O3A-PB	-5.46	114.10	132.83
2	E	783	ADP	C4-C5-N7	-5.33	103.85	109.40
2	E	783	ADP	PA-O3A-PB	-4.79	116.38	132.83
2	F	783	ADP	PA-O3A-PB	-4.70	116.69	132.83
2	A	783	ADP	C4-C5-N7	-4.67	104.53	109.40
2	D	783	ADP	PA-O3A-PB	-4.23	118.32	132.83
2	C	783	ADP	C1'-N9-C4	4.15	133.93	126.64
2	F	783	ADP	O2'-C2'-C1'	-4.00	96.08	110.85
2	A	783	ADP	C1'-N9-C4	3.97	133.62	126.64
2	B	783	ADP	O2'-C2'-C1'	-3.61	97.52	110.85
2	F	783	ADP	C2'-C3'-C4'	-3.60	95.65	102.64
2	C	783	ADP	C4-C5-N7	-3.42	105.83	109.40
2	D	783	ADP	C4-C5-N7	-3.42	105.83	109.40
2	D	783	ADP	C1'-N9-C4	3.39	132.59	126.64
2	B	783	ADP	N3-C2-N1	-3.37	123.42	128.68
2	C	783	ADP	C2'-C3'-C4'	-3.26	96.31	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	783	ADP	O3B-PB-O2B	3.26	120.09	107.64
2	C	783	ADP	O2'-C2'-C1'	-3.23	98.94	110.85
2	D	783	ADP	O3B-PB-O3A	-3.07	94.35	104.64
2	F	783	ADP	N3-C2-N1	-3.02	123.96	128.68
2	C	783	ADP	O2A-PA-O1A	2.95	126.84	112.24
2	D	783	ADP	C5-C6-N6	2.94	124.82	120.35
2	A	783	ADP	C5-C6-N6	2.89	124.74	120.35
2	E	783	ADP	O4'-C1'-C2'	-2.88	102.72	106.93
2	C	783	ADP	O5'-C5'-C4'	-2.81	99.34	108.99
2	E	783	ADP	O5'-C5'-C4'	-2.74	99.57	108.99
2	B	783	ADP	O4'-C1'-C2'	-2.72	102.95	106.93
2	B	783	ADP	C3'-C2'-C1'	2.68	105.02	100.98
2	F	783	ADP	C4-C5-N7	-2.67	106.62	109.40
2	D	783	ADP	N3-C2-N1	-2.63	124.57	128.68
2	B	783	ADP	O2'-C2'-C3'	-2.61	103.37	111.82
2	E	783	ADP	O4'-C4'-C5'	-2.61	100.80	109.37
2	A	783	ADP	O3A-PB-O1B	-2.58	96.90	111.19
2	A	783	ADP	O2'-C2'-C1'	-2.56	101.39	110.85
2	B	783	ADP	C4-C5-N7	-2.55	106.74	109.40
2	F	783	ADP	O3B-PB-O2B	2.50	117.20	107.64
2	D	783	ADP	C2-N1-C6	2.50	123.03	118.75
2	E	783	ADP	O3B-PB-O2B	2.50	117.19	107.64
2	C	783	ADP	N3-C2-N1	-2.48	124.80	128.68
2	E	783	ADP	O2B-PB-O3A	-2.48	96.33	104.64
2	E	783	ADP	O2A-PA-O1A	2.45	124.36	112.24
2	D	783	ADP	O4'-C1'-C2'	-2.44	103.36	106.93
2	F	783	ADP	O2'-C2'-C3'	-2.44	103.93	111.82
2	B	783	ADP	O3A-PB-O1B	-2.44	97.66	111.19
2	E	783	ADP	C5-C6-N6	2.43	124.05	120.35
2	F	783	ADP	O5'-C5'-C4'	-2.36	100.86	108.99
2	D	783	ADP	C5-C6-N1	-2.36	115.00	120.35
2	A	783	ADP	O2B-PB-O3A	2.35	112.51	104.64
2	D	783	ADP	O5'-C5'-C4'	2.23	116.67	108.99
2	E	783	ADP	O5'-PA-O1A	-2.22	100.40	109.07
2	C	783	ADP	C5-C6-N6	2.20	123.70	120.35
2	A	783	ADP	O3B-PB-O1B	2.18	119.21	110.68
2	C	783	ADP	O2'-C2'-C3'	-2.16	104.82	111.82
2	F	783	ADP	O2A-PA-O1A	2.15	122.87	112.24
2	A	783	ADP	O2A-PA-O1A	2.15	122.86	112.24
2	E	783	ADP	PA-O5'-C5'	-2.14	109.11	121.68
2	E	783	ADP	N3-C2-N1	-2.12	125.37	128.68
2	A	783	ADP	O3B-PB-O3A	-2.11	97.56	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	783	ADP	C5-C6-N1	-2.07	115.67	120.35
2	D	783	ADP	O3B-PB-O2B	2.04	115.44	107.64
2	A	783	ADP	C3'-C2'-C1'	2.04	104.05	100.98
2	F	783	ADP	C1'-N9-C4	2.01	130.18	126.64
2	C	783	ADP	C5-C6-N1	-2.01	115.79	120.35

There are no chirality outliers.

All (26) torsion outliers are listed below:

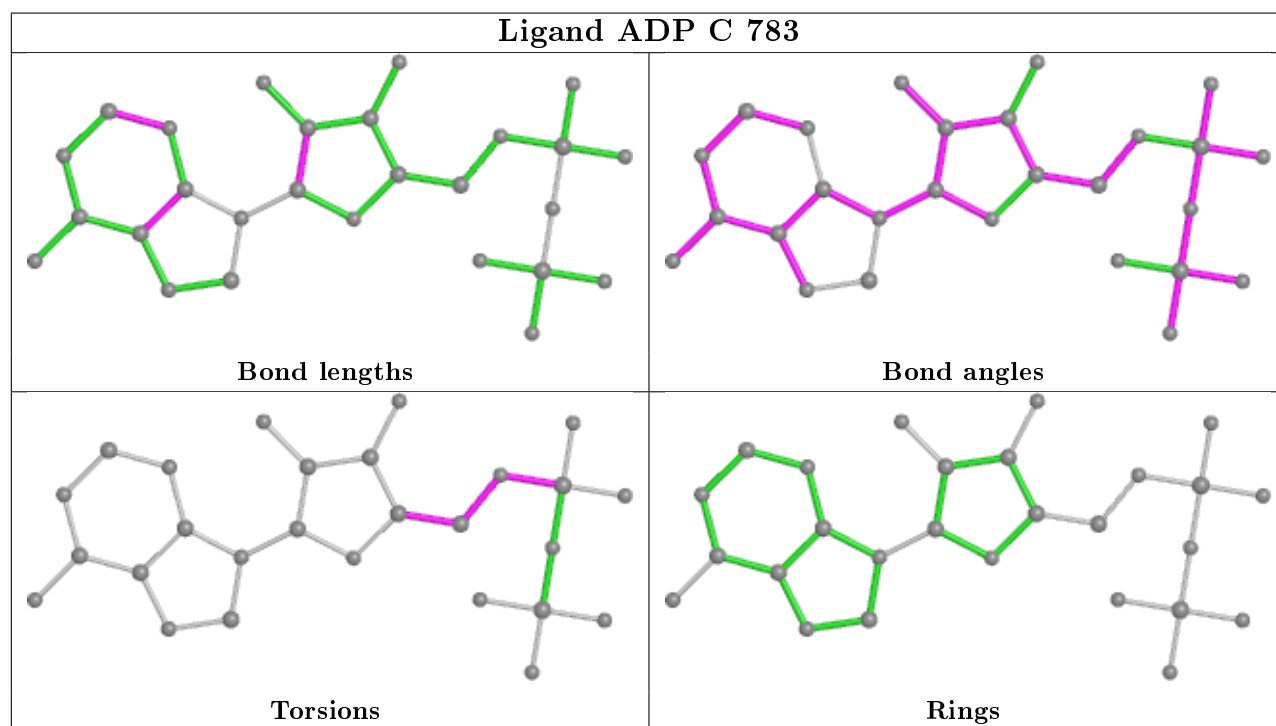
Mol	Chain	Res	Type	Atoms
2	C	783	ADP	O4'-C4'-C5'-O5'
2	C	783	ADP	C3'-C4'-C5'-O5'
2	D	783	ADP	PA-O3A-PB-O3B
2	D	783	ADP	C4'-C5'-O5'-PA
2	A	783	ADP	C4'-C5'-O5'-PA
2	A	783	ADP	O4'-C4'-C5'-O5'
2	A	783	ADP	C3'-C4'-C5'-O5'
2	B	783	ADP	C4'-C5'-O5'-PA
2	B	783	ADP	O4'-C4'-C5'-O5'
2	B	783	ADP	C3'-C4'-C5'-O5'
2	E	783	ADP	C5'-O5'-PA-O1A
2	E	783	ADP	C5'-O5'-PA-O2A
2	F	783	ADP	O4'-C4'-C5'-O5'
2	F	783	ADP	C3'-C4'-C5'-O5'
2	E	783	ADP	C3'-C4'-C5'-O5'
2	E	783	ADP	O4'-C4'-C5'-O5'
2	C	783	ADP	C4'-C5'-O5'-PA
2	E	783	ADP	C4'-C5'-O5'-PA
2	F	783	ADP	C4'-C5'-O5'-PA
2	D	783	ADP	C3'-C4'-C5'-O5'
2	C	783	ADP	C5'-O5'-PA-O2A
2	F	783	ADP	C5'-O5'-PA-O2A
2	D	783	ADP	O4'-C4'-C5'-O5'
2	C	783	ADP	C5'-O5'-PA-O3A
2	E	783	ADP	C5'-O5'-PA-O3A
2	F	783	ADP	C5'-O5'-PA-O3A

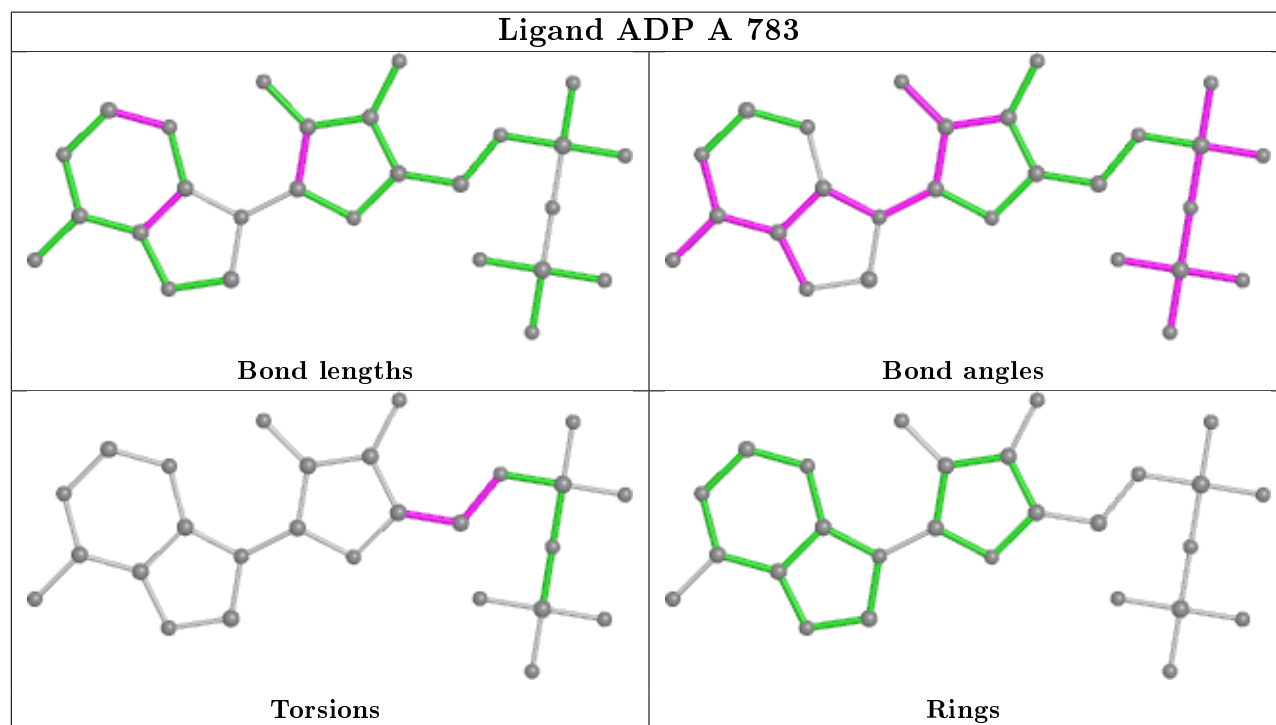
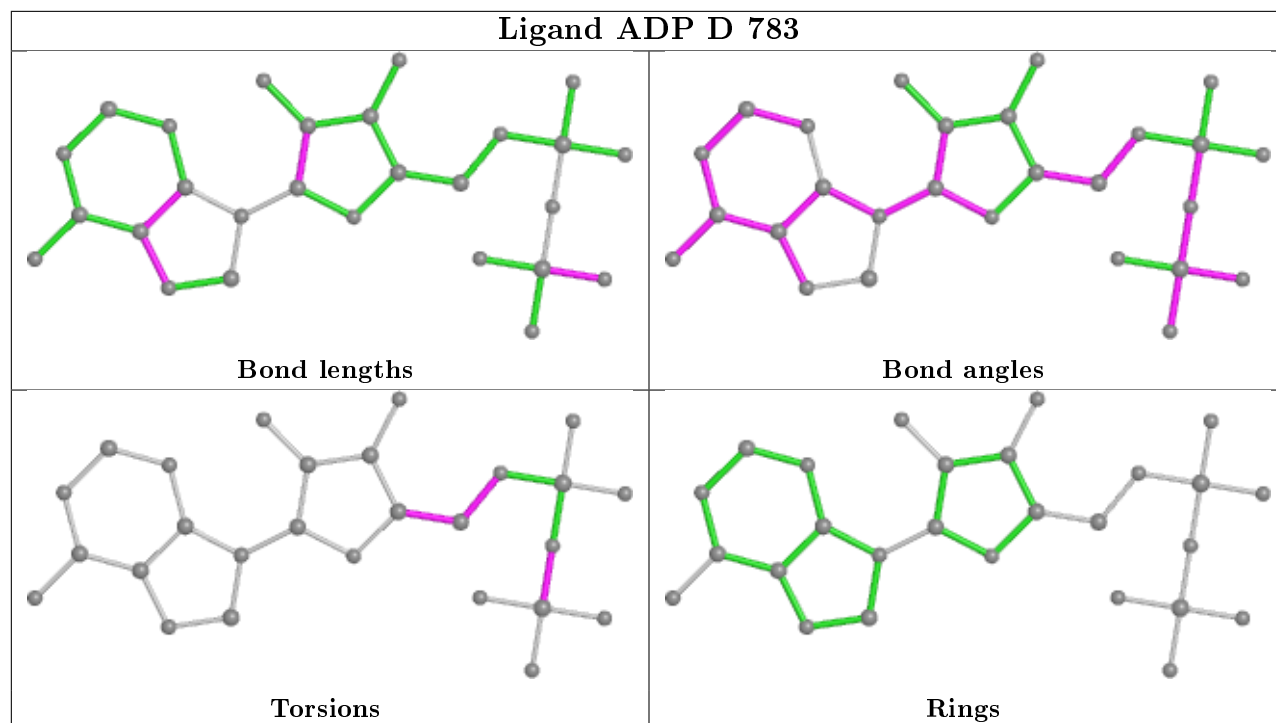
There are no ring outliers.

6 monomers are involved in 44 short contacts:

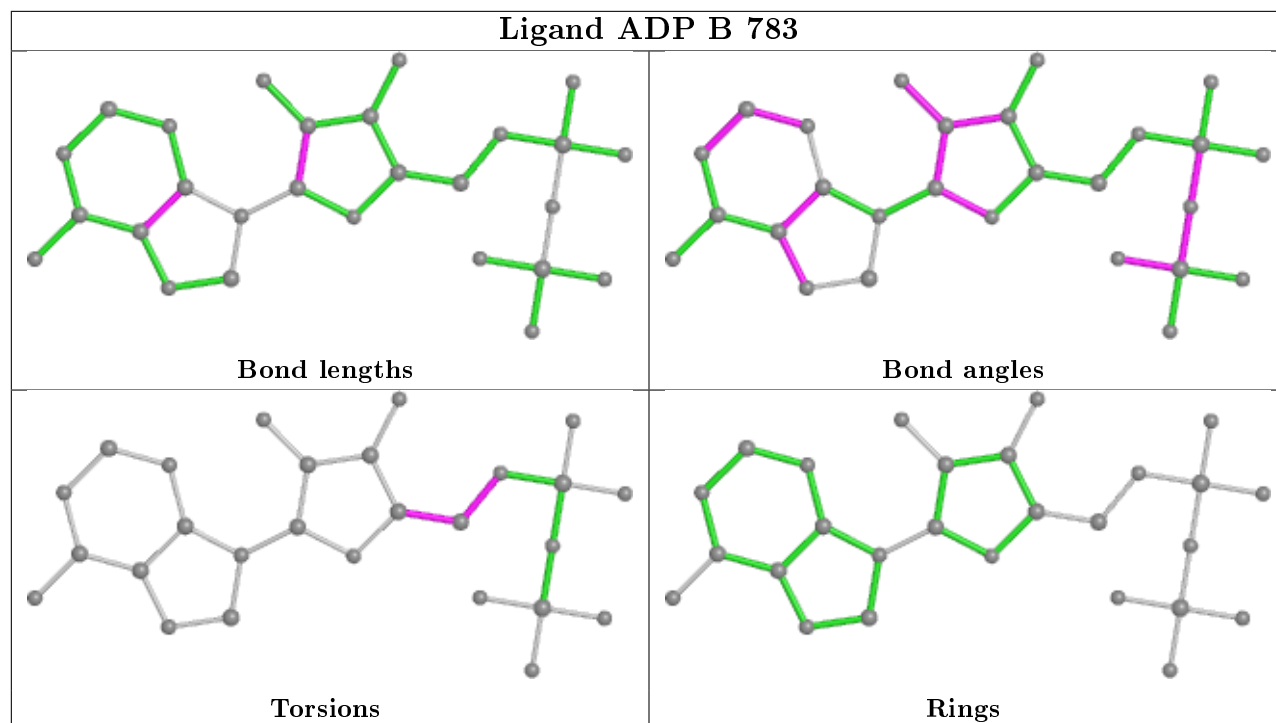
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	783	ADP	6	0
2	D	783	ADP	11	0
2	A	783	ADP	7	0
2	B	783	ADP	7	0
2	E	783	ADP	6	0
2	F	783	ADP	7	0

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

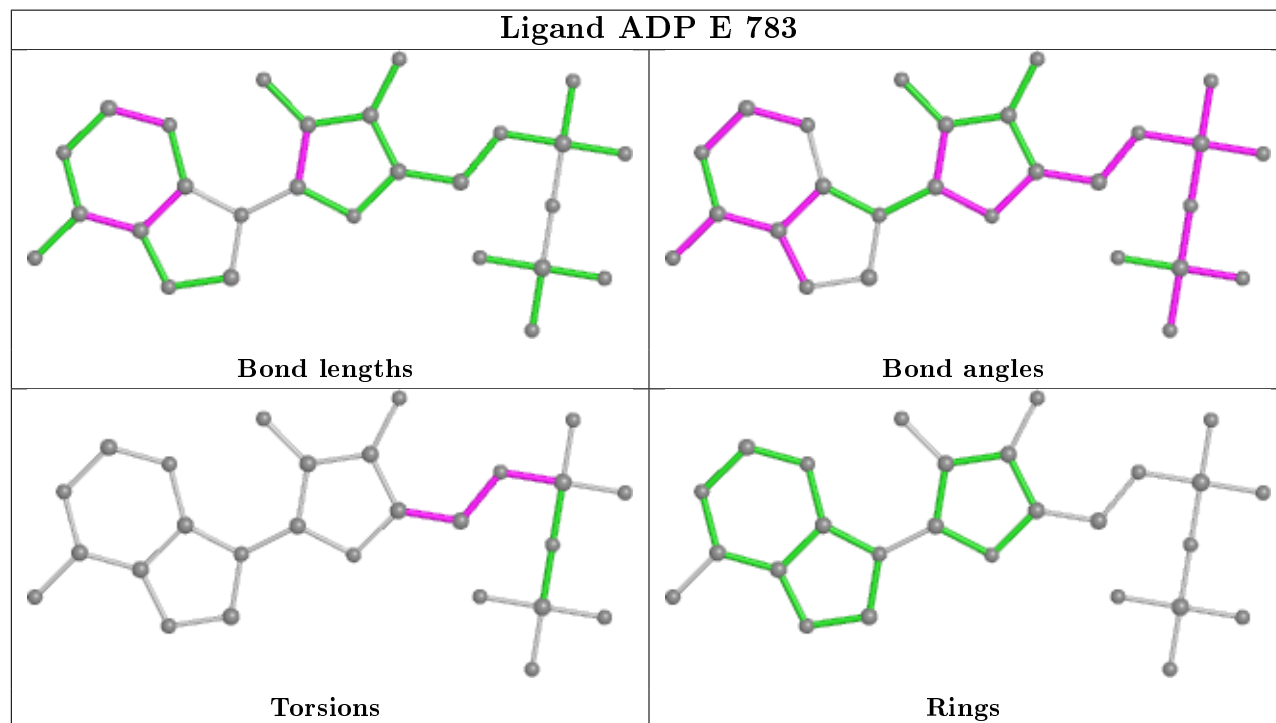


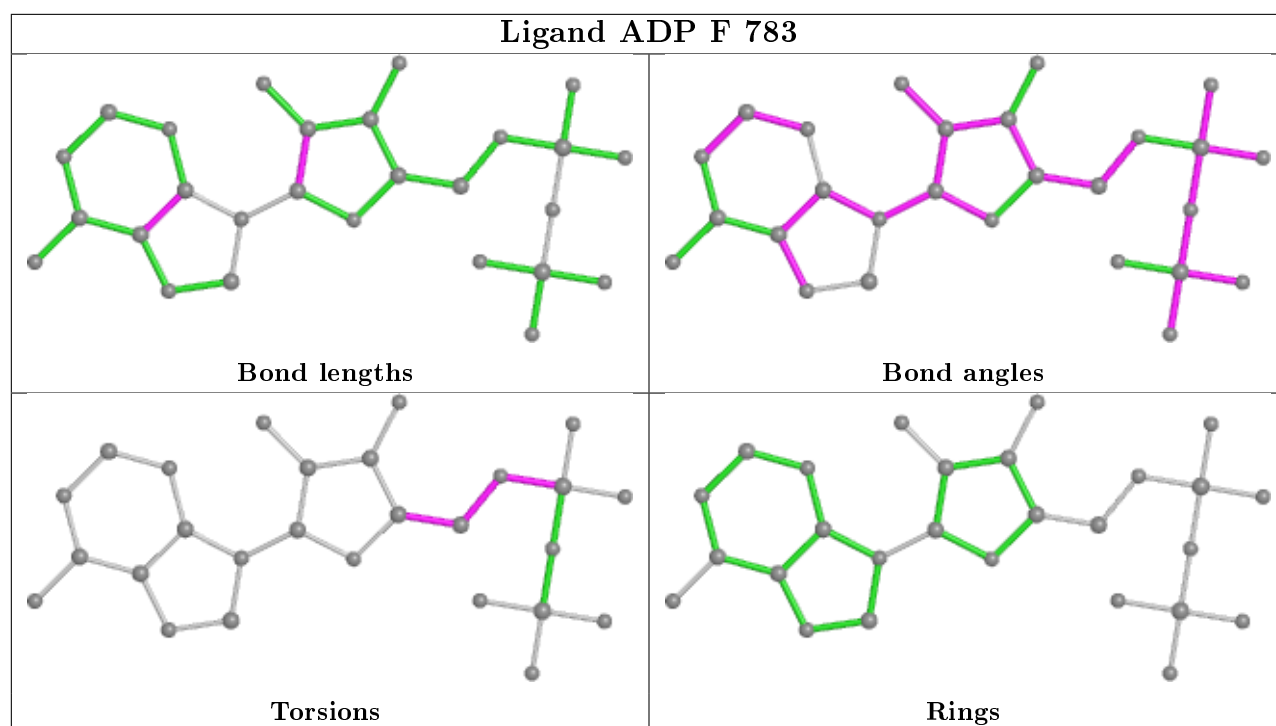


Ligand ADP B 783



Ligand ADP E 783





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	496/543 (91%)	0.16	25 (5%)	28	29	69, 145, 461, 643	0
1	B	496/543 (91%)	0.21	28 (5%)	24	25	75, 143, 456, 637	0
1	C	496/543 (91%)	0.35	40 (8%)	12	13	71, 145, 458, 683	0
1	D	496/543 (91%)	0.42	49 (9%)	7	8	65, 145, 463, 696	0
1	E	496/543 (91%)	0.45	54 (10%)	5	6	75, 146, 466, 682	0
1	F	496/543 (91%)	0.27	38 (7%)	13	15	78, 148, 457, 672	0
All	All	2976/3258 (91%)	0.31	234 (7%)	12	14	65, 145, 464, 696	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	SER	15.2
1	E	246	THR	13.0
1	B	246	THR	11.1
1	F	278	LYS	10.0
1	B	282	SER	9.6
1	C	288	VAL	9.2
1	A	246	THR	8.7
1	C	257	GLU	8.5
1	B	248	GLU	8.2
1	B	251	THR	8.1
1	E	251	THR	6.7
1	C	249	VAL	6.7
1	E	282	SER	6.6
1	D	246	THR	6.3
1	D	278	LYS	5.8
1	E	247	GLY	5.8
1	C	289	ILE	5.6
1	B	254	GLU	5.5
1	A	259	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	307	ASP	5.5
1	C	246	THR	5.4
1	C	286	SER	5.3
1	E	250	GLN	5.2
1	D	615	LEU	5.1
1	D	252	LEU	4.9
1	E	290	ARG	4.9
1	E	281	SER	4.6
1	C	301	TRP	4.6
1	C	337	ALA	4.6
1	B	278	LYS	4.5
1	B	289	ILE	4.5
1	E	293	ILE	4.5
1	E	276	TYR	4.4
1	D	302	THR	4.4
1	C	300	PRO	4.4
1	A	463	LYS	4.4
1	E	347	GLY	4.4
1	D	342	THR	4.4
1	C	427	SER	4.3
1	C	250	GLN	4.3
1	E	459	PHE	4.3
1	C	247	GLY	4.3
1	B	307	ASP	4.2
1	F	277	GLU	4.2
1	B	279	ILE	4.1
1	C	256	ILE	4.1
1	F	644	ARG	4.1
1	E	277	GLU	4.0
1	F	288	VAL	4.0
1	D	620	GLY	4.0
1	D	757	LEU	4.0
1	D	689	ALA	4.0
1	F	627	LYS	3.9
1	C	282	SER	3.9
1	F	472	ASN	3.9
1	D	279	ILE	3.9
1	A	456	GLU	3.9
1	C	290	ARG	3.8
1	B	252	LEU	3.8
1	B	247	GLY	3.8
1	E	285	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	295	TRP	3.8
1	F	279	ILE	3.8
1	D	289	ILE	3.8
1	F	289	ILE	3.7
1	A	251	THR	3.7
1	F	345	LEU	3.7
1	D	614	SER	3.7
1	D	286	SER	3.7
1	E	615	LEU	3.7
1	D	662	ILE	3.6
1	D	456	GLU	3.6
1	F	676	PRO	3.6
1	B	257	GLU	3.6
1	F	272	GLU	3.5
1	B	337	ALA	3.5
1	F	459	PHE	3.4
1	A	337	ALA	3.4
1	F	246	THR	3.4
1	A	338	VAL	3.4
1	E	471	ASN	3.4
1	E	344	SER	3.3
1	E	289	ILE	3.3
1	B	286	SER	3.3
1	C	414	LEU	3.3
1	D	344	SER	3.3
1	F	344	SER	3.2
1	D	624	LEU	3.2
1	B	342	THR	3.2
1	C	283	SER	3.2
1	D	641	SER	3.2
1	C	455	ILE	3.2
1	F	664	ILE	3.2
1	C	662	ILE	3.1
1	A	663	HIS	3.1
1	F	725	HIS	3.0
1	C	338	VAL	3.0
1	E	288	VAL	3.0
1	E	338	VAL	3.0
1	D	594	GLY	3.0
1	D	472	ASN	3.0
1	D	756	ILE	2.9
1	B	276	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	444	PRO	2.9
1	E	278	LYS	2.9
1	E	532	ARG	2.9
1	F	373	ARG	2.9
1	D	657	HIS	2.9
1	A	285	GLU	2.9
1	F	290	ARG	2.9
1	F	663	HIS	2.9
1	B	281	SER	2.8
1	B	341	LEU	2.8
1	D	644	ARG	2.8
1	A	343	LYS	2.8
1	E	343	LYS	2.8
1	E	564	LYS	2.8
1	B	255	LYS	2.8
1	D	301	TRP	2.8
1	E	296	LEU	2.8
1	A	734	ALA	2.8
1	C	284	ALA	2.8
1	C	248	GLU	2.8
1	B	444	PRO	2.8
1	D	288	VAL	2.7
1	E	342	THR	2.7
1	B	295	TRP	2.7
1	C	456	GLU	2.7
1	A	341	LEU	2.7
1	F	617	PRO	2.7
1	E	584	TYR	2.7
1	C	663	HIS	2.7
1	D	613	VAL	2.6
1	D	699	VAL	2.6
1	D	596	VAL	2.6
1	F	731	THR	2.6
1	E	279	ILE	2.6
1	E	591	ASP	2.6
1	B	284	ALA	2.6
1	D	444	PRO	2.6
1	D	639	ALA	2.6
1	B	288	VAL	2.5
1	D	755	PHE	2.5
1	A	462	SER	2.5
1	E	294	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	413	LYS	2.5
1	B	259	ALA	2.5
1	D	337	ALA	2.5
1	F	540	VAL	2.5
1	D	345	LEU	2.5
1	E	360	LYS	2.5
1	E	755	PHE	2.4
1	A	262	PRO	2.4
1	C	558	ILE	2.4
1	C	341	LEU	2.4
1	E	249	VAL	2.4
1	F	259	ALA	2.4
1	F	732	ILE	2.4
1	C	465	LEU	2.4
1	F	261	MET	2.4
1	D	648	GLU	2.4
1	F	248	GLU	2.4
1	A	427	SER	2.4
1	E	558	ILE	2.4
1	F	276	TYR	2.4
1	F	577	ILE	2.4
1	E	257	GLU	2.4
1	E	337	ALA	2.4
1	C	307	ASP	2.4
1	C	566	ILE	2.4
1	C	565	ARG	2.3
1	D	622	LEU	2.3
1	E	440	GLU	2.3
1	E	286	SER	2.3
1	C	278	LYS	2.3
1	E	421	ASP	2.3
1	F	616	SER	2.3
1	F	620	GLY	2.3
1	D	690	LEU	2.3
1	C	342	THR	2.3
1	B	454	TYR	2.3
1	A	445	GLU	2.3
1	C	291	ASN	2.3
1	D	251	THR	2.3
1	D	445	GLU	2.2
1	F	301	TRP	2.2
1	D	283	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	654	PRO	2.2
1	F	662	ILE	2.2
1	C	454	TYR	2.2
1	C	344	SER	2.2
1	A	458	THR	2.2
1	B	301	TRP	2.2
1	E	463	LYS	2.2
1	D	412	GLY	2.2
1	E	705	ILE	2.2
1	E	323	HIS	2.2
1	A	437	ALA	2.2
1	E	335	TYR	2.2
1	E	341	LEU	2.2
1	C	615	LEU	2.2
1	D	462	SER	2.2
1	B	440	GLU	2.2
1	D	277	GLU	2.2
1	F	729	LEU	2.1
1	C	445	GLU	2.1
1	E	462	SER	2.1
1	D	307	ASP	2.1
1	D	437	ALA	2.1
1	E	301	TRP	2.1
1	A	258	GLU	2.1
1	D	666	VAL	2.1
1	D	768	ALA	2.1
1	E	345	LEU	2.1
1	E	252	LEU	2.1
1	E	268	THR	2.1
1	B	462	SER	2.1
1	A	702	THR	2.1
1	F	444	PRO	2.1
1	E	267	GLU	2.1
1	D	275	ARG	2.1
1	C	345	LEU	2.1
1	D	287	SER	2.1
1	C	251	THR	2.0
1	E	721	ALA	2.0
1	E	594	GLY	2.0
1	F	710	ARG	2.0
1	F	321	GLU	2.0
1	F	426	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	614	SER	2.0
1	A	644	ARG	2.0
1	E	562	GLU	2.0
1	A	615	LEU	2.0
1	A	255	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

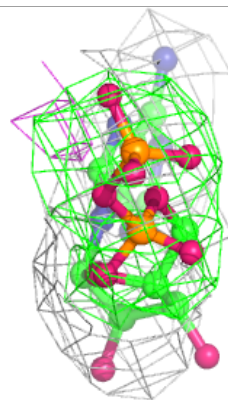
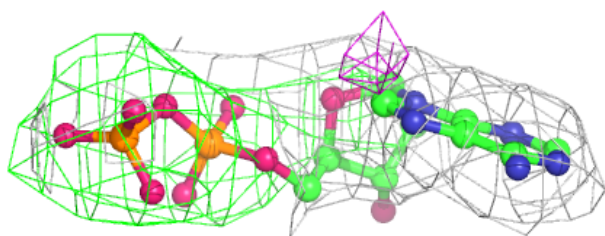
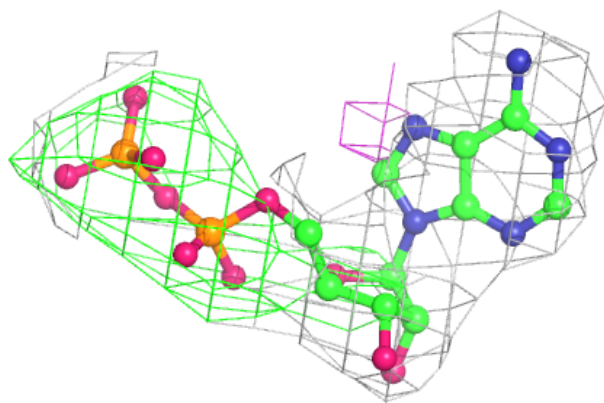
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	D	783	27/27	0.74	0.31	30,142,369,458	0
2	ADP	C	783	27/27	0.89	0.30	57,125,341,462	0
2	ADP	A	783	27/27	0.91	0.22	55,104,341,499	0
2	ADP	B	783	27/27	0.91	0.24	73,123,341,499	0
2	ADP	E	783	27/27	0.93	0.19	53,114,341,491	0
2	ADP	F	783	27/27	0.93	0.21	57,123,341,482	0

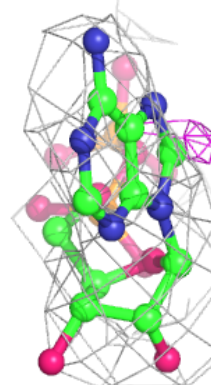
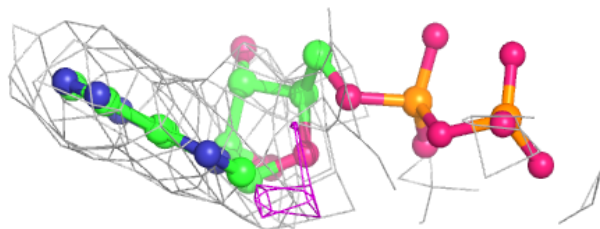
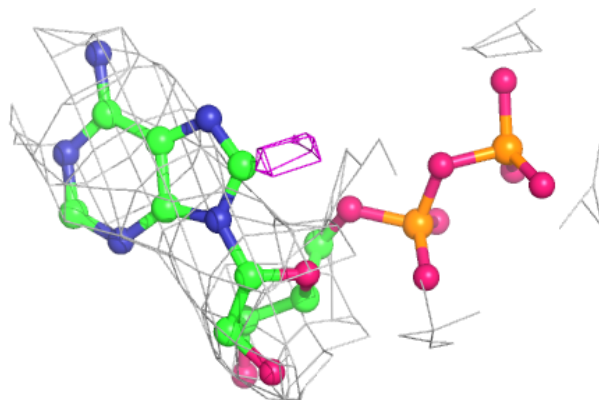
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 783:

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

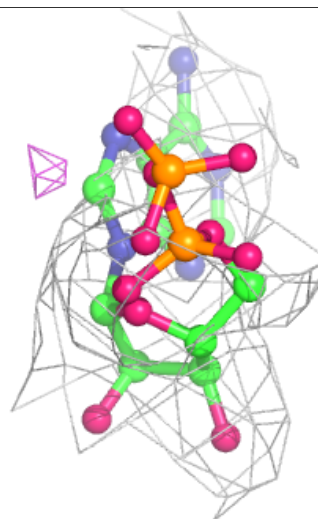
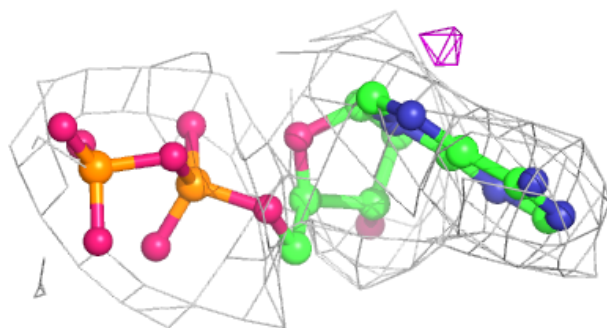
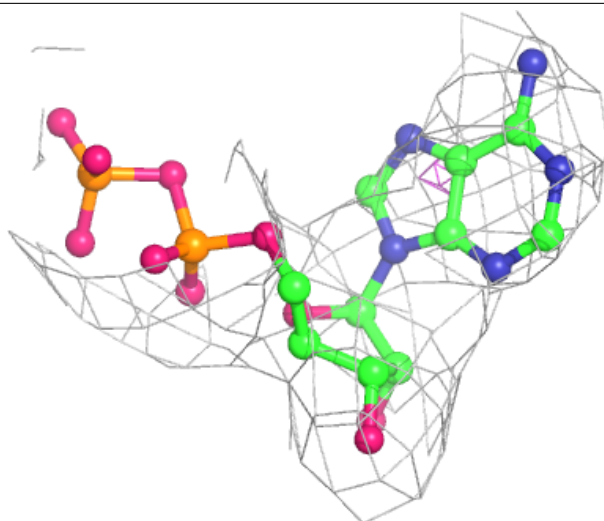
**Electron density around ADP C 783:**

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



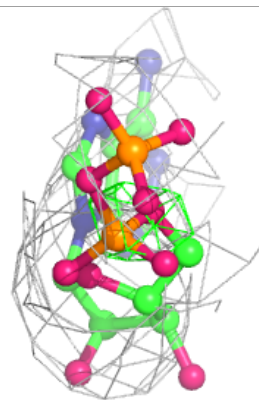
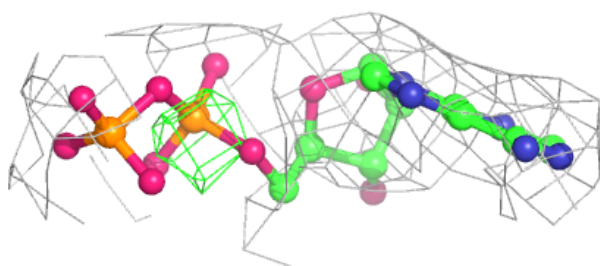
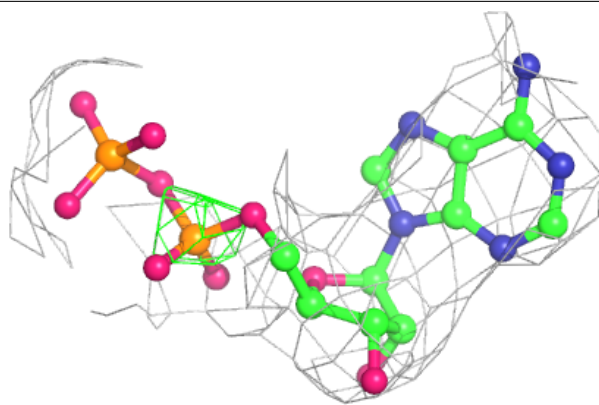
Electron density around ADP A 783:

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



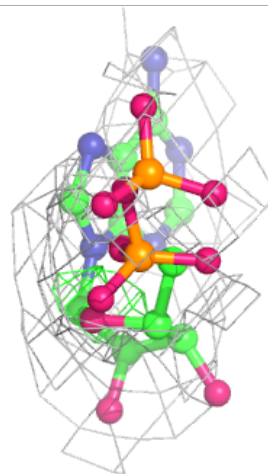
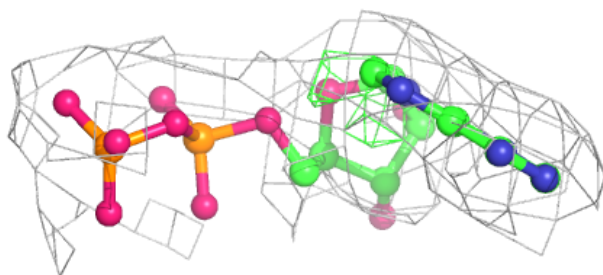
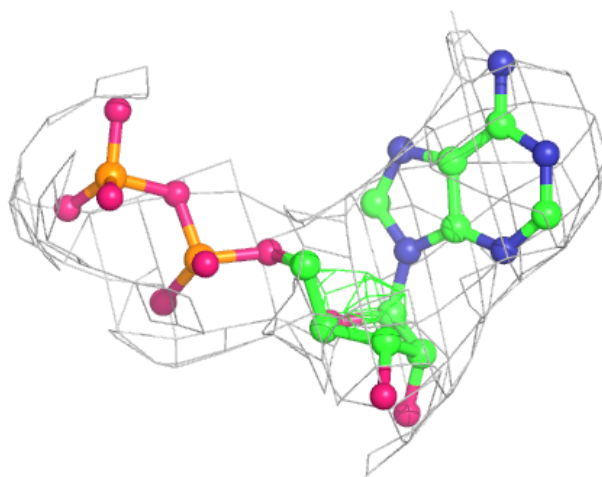
Electron density around ADP B 783:

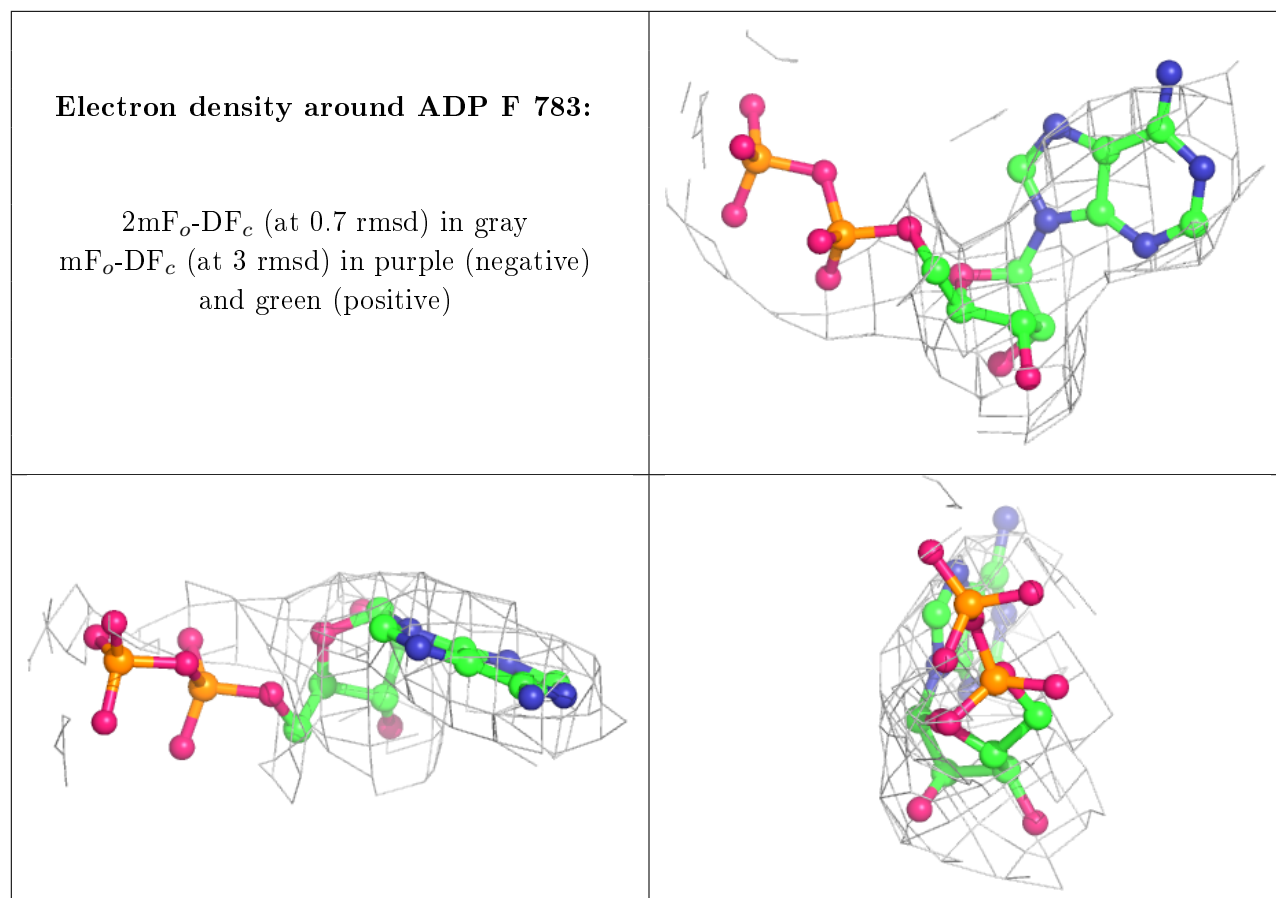
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP E 783:

$2mF_o-DF_c$ (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.