Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 06:18 AM EDT

PDB ID	:	1BR2
Title	:	SMOOTH MUSCLE MYOSIN MOTOR DOMAIN COMPLEXED WITH MGADP.ALF4
Authors	:	Dominguez, R.; Trybus, K.M.; Cohen, C.
Deposited on	:	1998-08-26
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

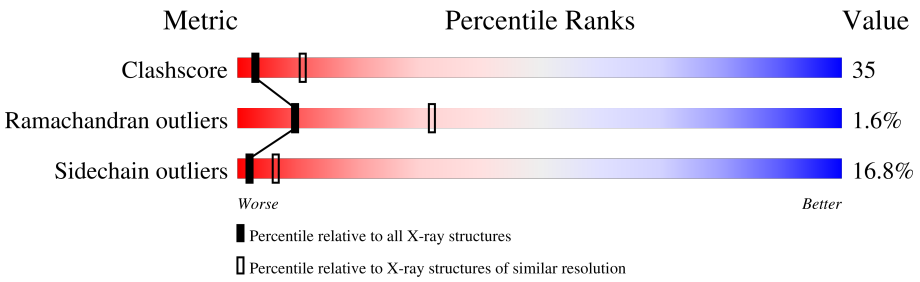
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	791	35% 41% 8% 15%
1	B	791	36% 40% 8% 15%
1	C	791	37% 39% 9% 15%
1	D	791	36% 41% 8% 15%
1	E	791	36% 40% 9% 15%
1	F	791	37% 39% 9% 15%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALF	D	999	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31830 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.

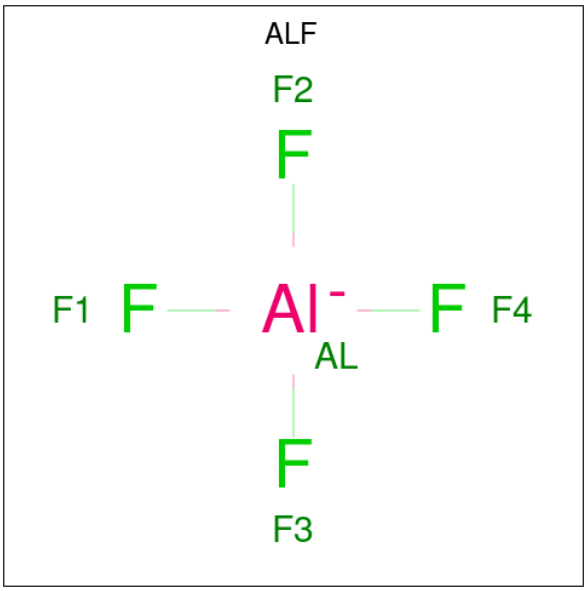
- Molecule 1 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	673	5270	3360	900	982	28	0	0	0
1	B	673	5270	3360	900	982	28	0	0	0
1	C	673	5270	3360	900	982	28	0	0	0
1	D	673	5270	3360	900	982	28	0	0	0
1	E	673	5270	3360	900	982	28	0	0	0
1	F	673	5270	3360	900	982	28	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

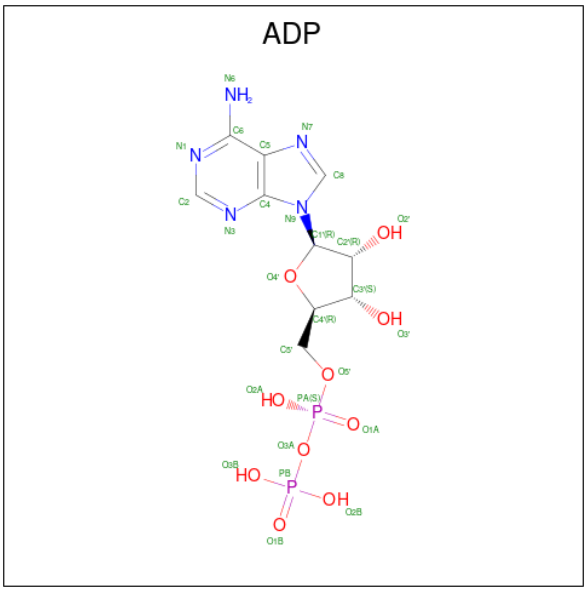
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
3	A	1	5	1	4	0	0
3	B	1	5	1	4	0	0
3	C	1	5	1	4	0	0
3	D	1	5	1	4	0	0
3	E	1	5	1	4	0	0
3	F	1	5	1	4	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	2	2	2	0	0
5	B	2	2	2	0	0
5	C	2	2	2	0	0
5	D	2	2	2	0	0
5	E	2	2	2	0	0
5	F	2	2	2	0	0

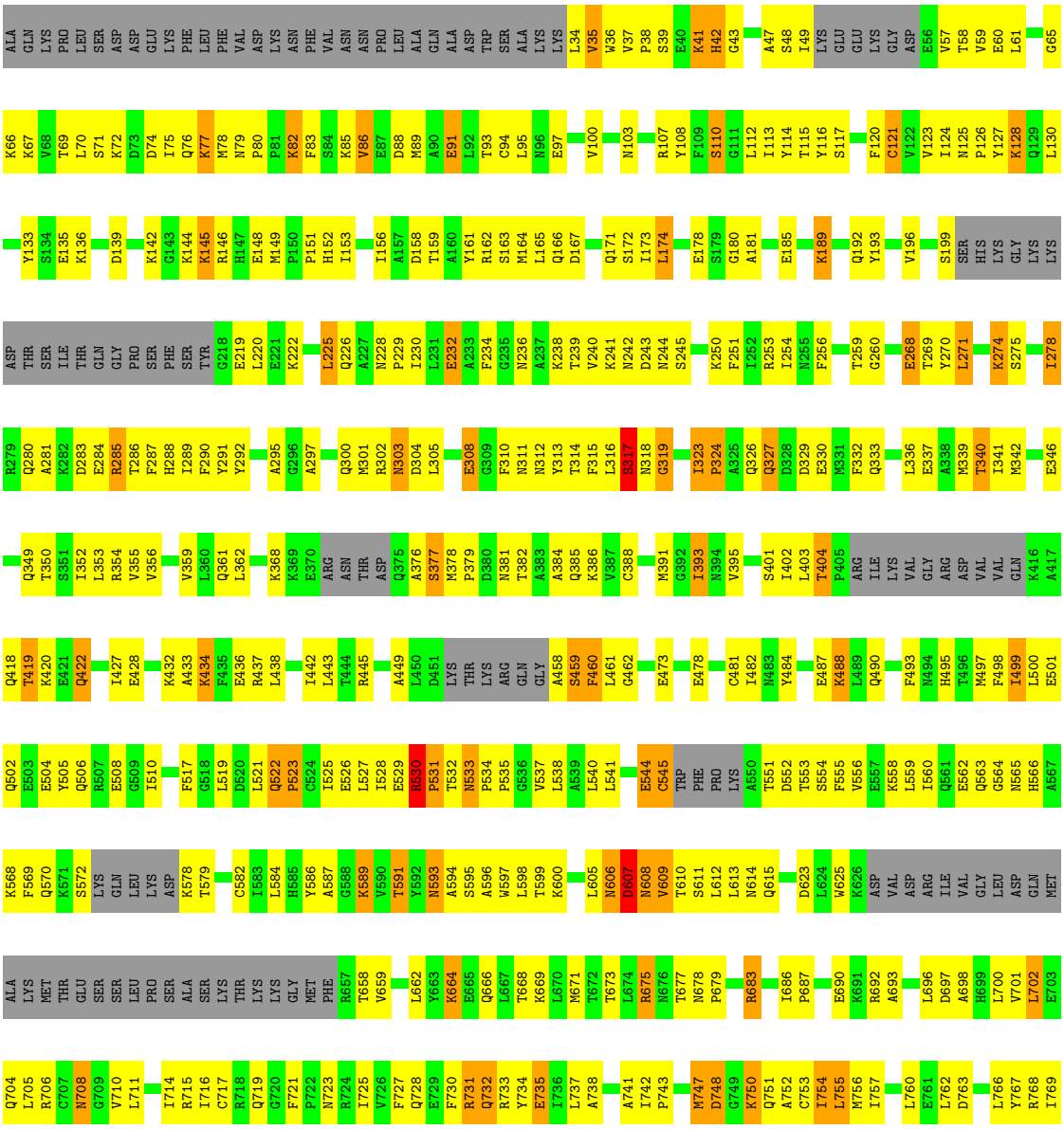
3 Residue-property plots (i)

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

Note EDS was not executed.

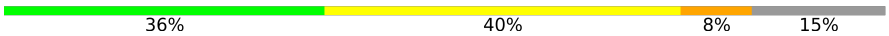
- Molecule 1: MYOSIN

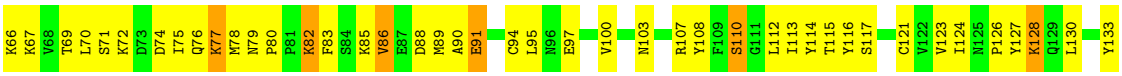
Chain A: 35% 41% 8% 15%

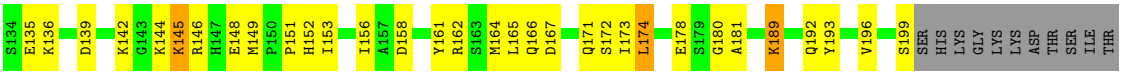


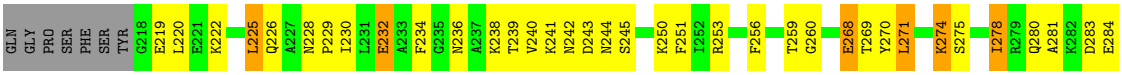
• Molecule 1: MYOSIN

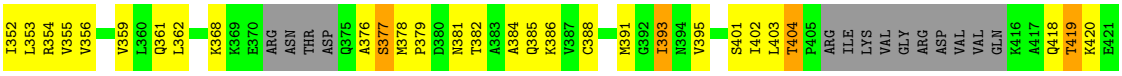
Chain B:

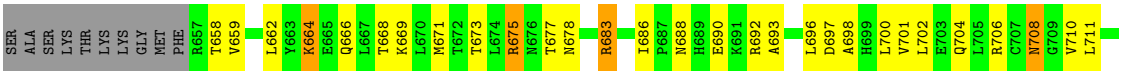


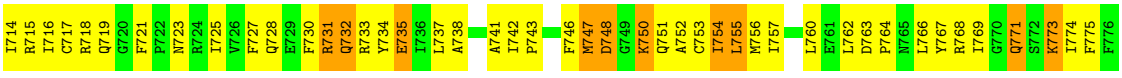


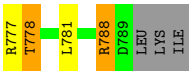






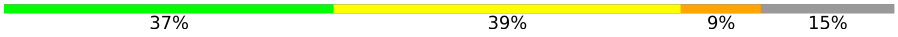


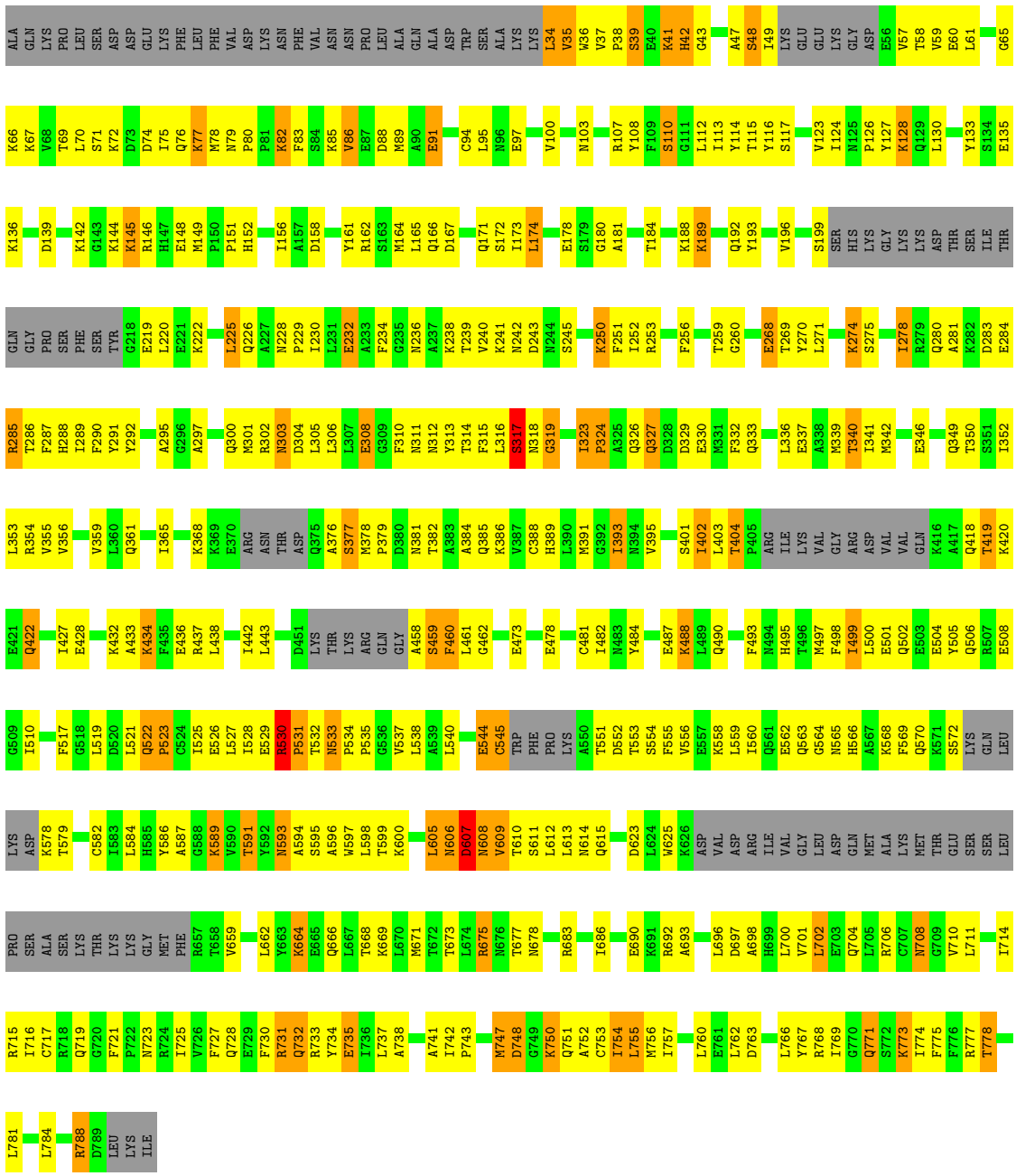




• Molecule 1: MYOSIN

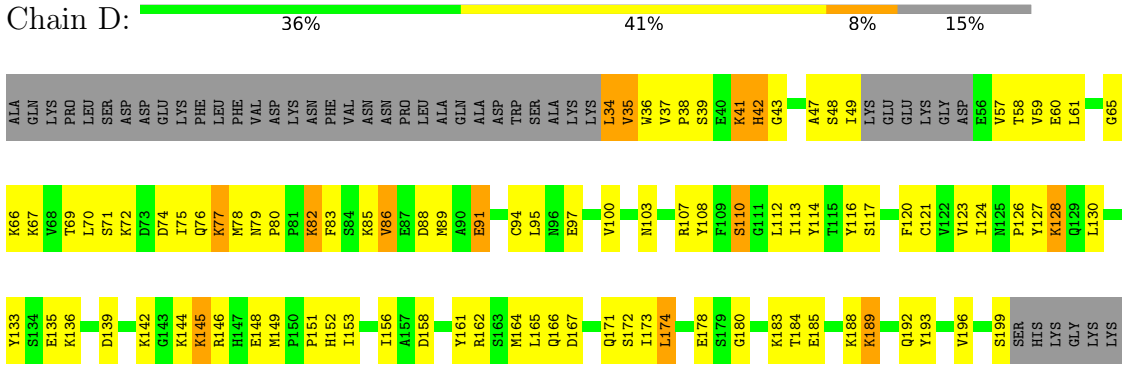
Chain C:

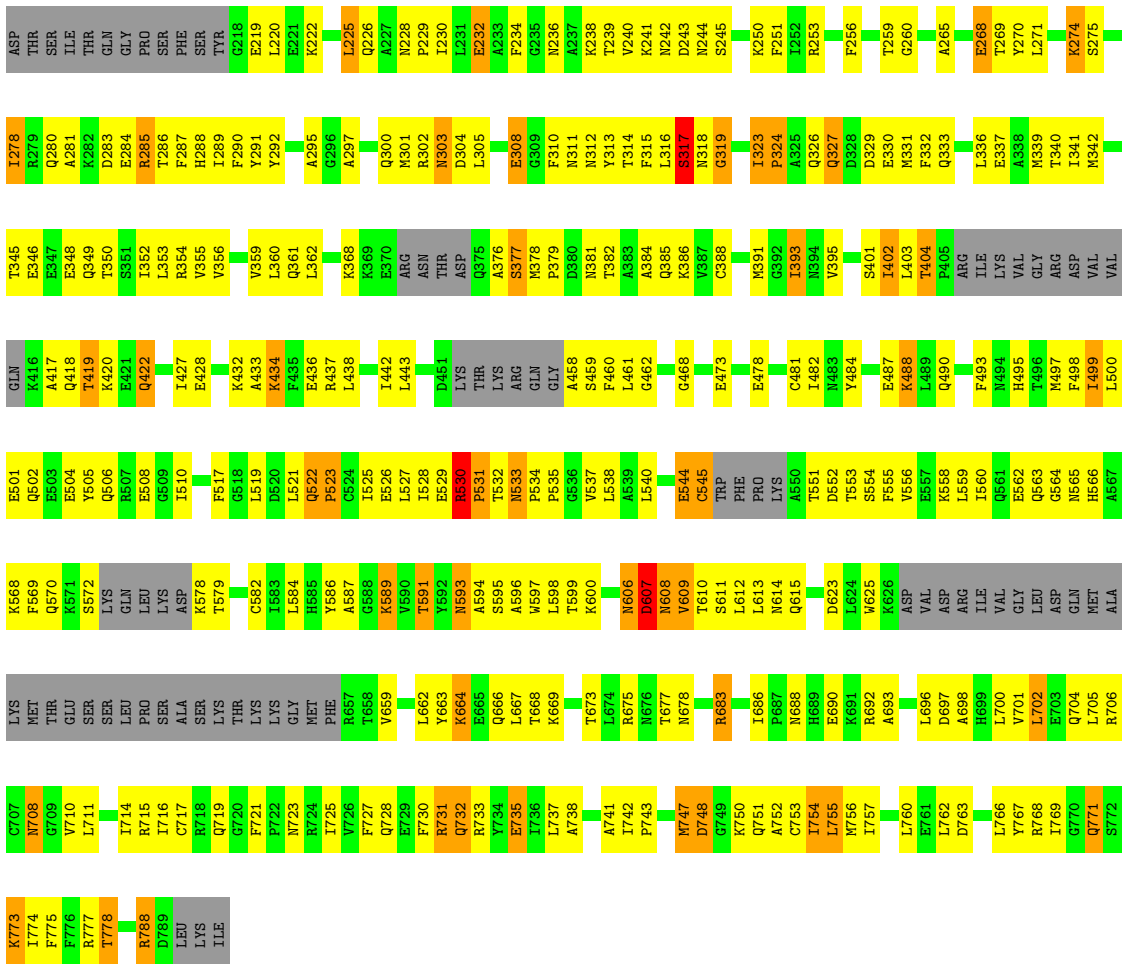




• Molecule 1: MYOSIN

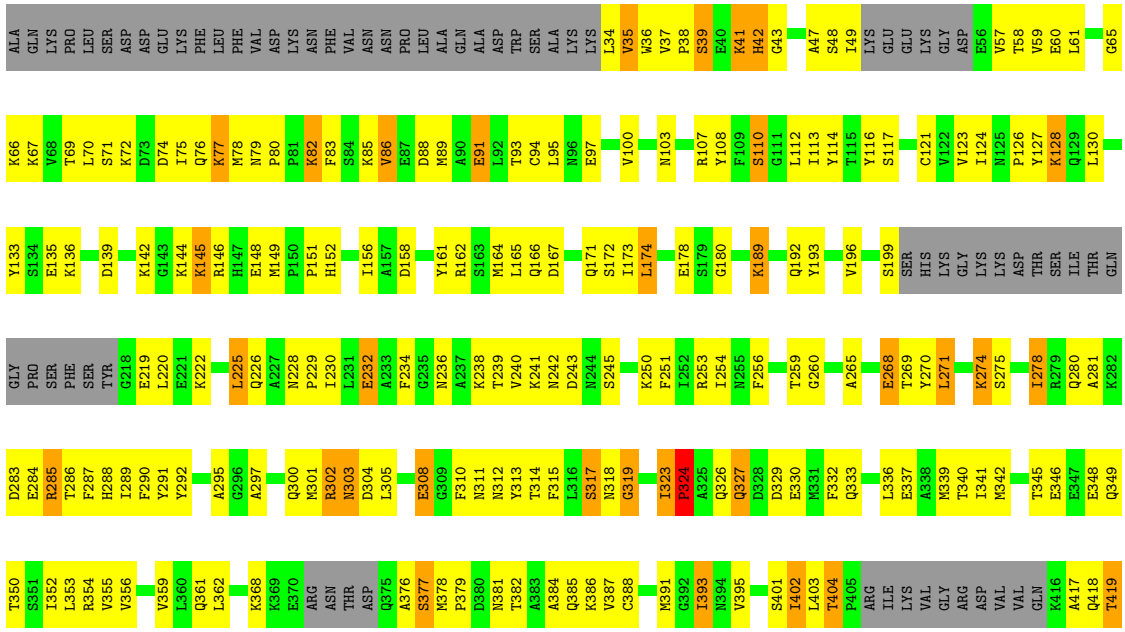
Chain D:

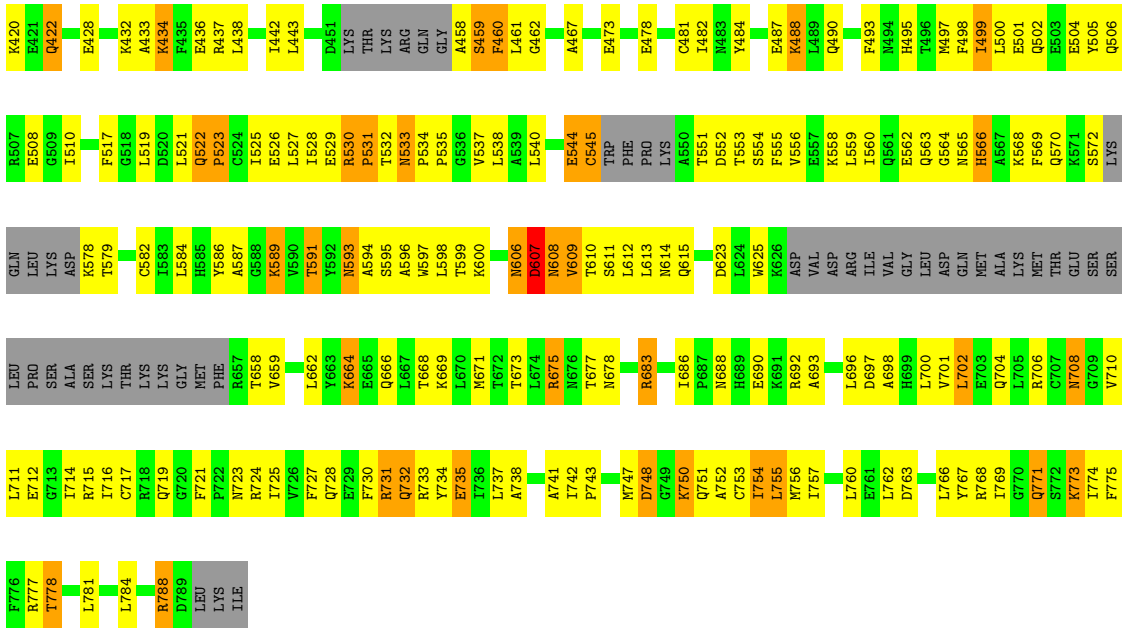




- Molecule 1: MYOSIN

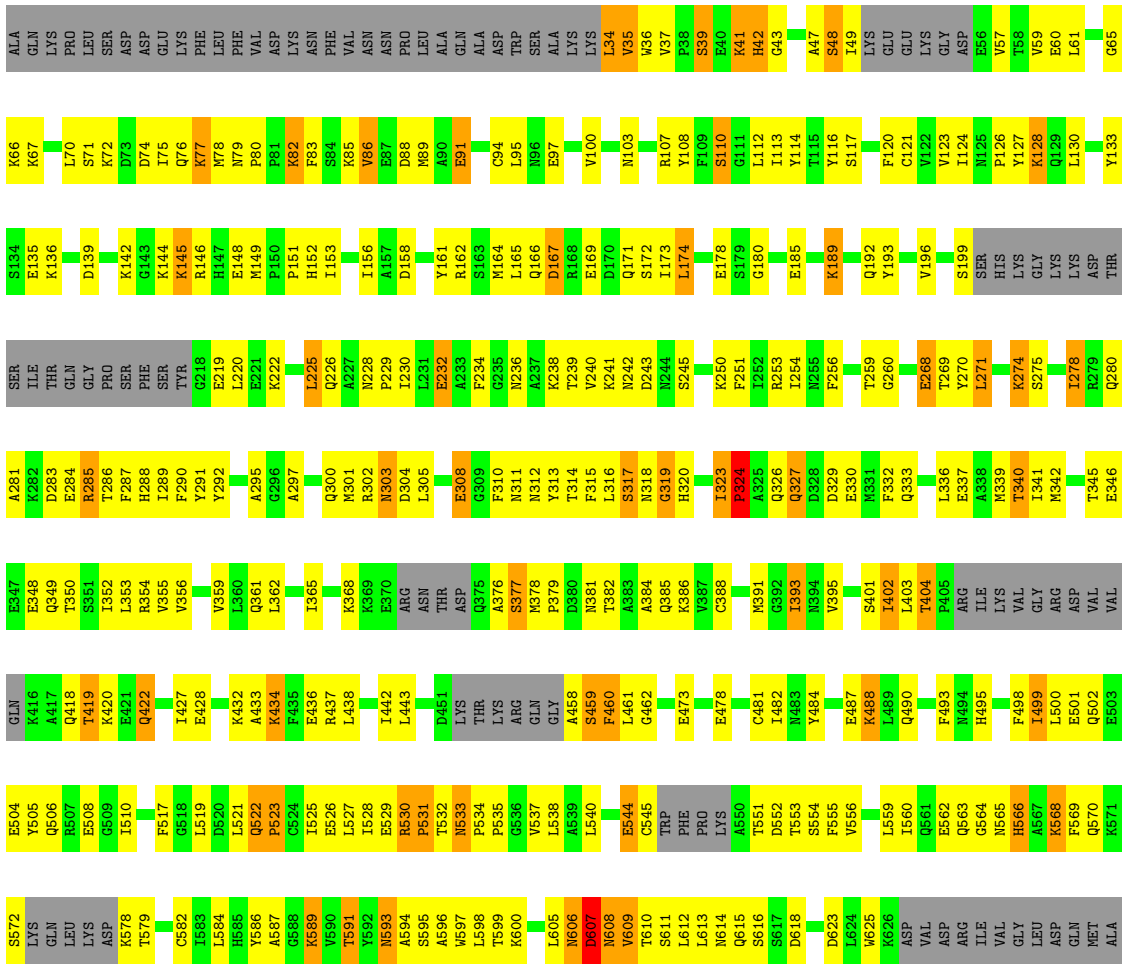
Chain E:

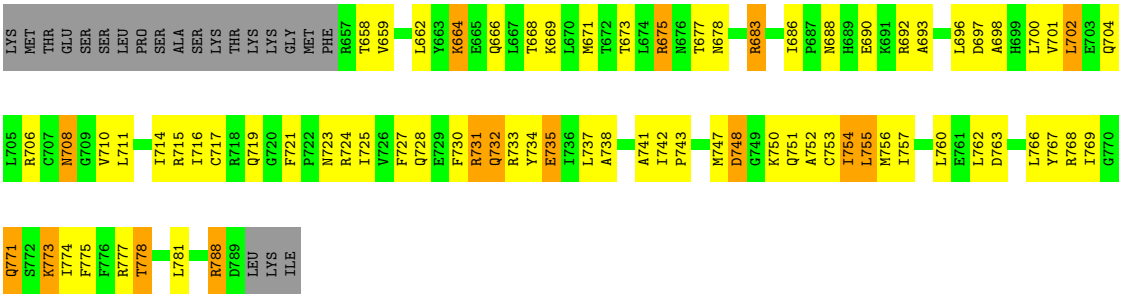




• Molecule 1: MYOSIN

Chain F: 37% 39% 9% 15%




LYS MET THR GLU SER SER LEU PRO SER ALA SER LYS THR LYS LYS GLY MET PHE R657 T658 V659 L662 Y663 K664 E665 Q666 L667 T668 K669 L670 M671 T672 T673 L674 R675 N676 T677 N678 R683 I686 P687 N688 H689 E690 K691 R692 A693 L696 D697 A698 H699 L700 V701 L702 E703 Q704
L705 R706 C707 N708 G709 V710 L711 I714 R715 I716 C717 R718 Q719 G720 F721 P722 N723 R724 I725 V726 F727 Q728 E729 F730 R731 Q732 R733 Y734 E735 I736 L737 A738 A741 I742 P743 M747 D748 G749 K750 Q751 A752 C753 I754 L755 M756 I757 L760 E761 L762 D763 L766 Y767 R768 I769 G770
Q771 S772 K773 I774 F775 F776 R777 T778 L781 R788 D789 LEU LYS ILE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.01Å 107.67Å 188.31Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.232 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31830	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

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: MG, ADP, ALF

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	1/5364 (0.0%)	0.65	2/7253 (0.0%)
1	B	0.48	0/5364	0.65	2/7253 (0.0%)
1	C	0.49	0/5364	0.65	2/7253 (0.0%)
1	D	0.50	0/5364	0.66	2/7253 (0.0%)
1	E	0.46	0/5364	0.61	0/7253
1	F	0.45	0/5364	0.61	0/7253
All	All	0.48	1/32184 (0.0%)	0.64	8/43518 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CYS	CB-SG	-5.00	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	530	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	C	530	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	530	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	D	530	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	747	MET	CG-SD-CE	6.17	110.06	100.20
1	C	747	MET	CG-SD-CE	6.16	110.06	100.20
1	B	747	MET	CG-SD-CE	6.13	110.02	100.20
1	D	747	MET	CG-SD-CE	6.12	109.99	100.20

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	5270	0	5145	373	0
1	B	5270	0	5145	365	0
1	C	5270	0	5145	369	0
1	D	5270	0	5145	354	0
1	E	5270	0	5145	363	0
1	F	5270	0	5145	356	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	2	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
All	All	31830	0	30942	2173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (2173) 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:D:529:GLU:O	1:D:531:PRO:HD3	1.30	1.27
1:A:529:GLU:O	1:A:531:PRO:HD3	1.30	1.24
1:C:529:GLU:O	1:C:531:PRO:HD3	1.30	1.24
1:B:529:GLU:O	1:B:531:PRO:HD3	1.30	1.23
1:D:323:ILE:CG2	1:D:324:PRO:HD2	1.68	1.23
1:B:323:ILE:CG2	1:B:324:PRO:HD2	1.68	1.23
1:C:323:ILE:CG2	1:C:324:PRO:HD2	1.68	1.22
1:A:323:ILE:CG2	1:A:324:PRO:HD2	1.68	1.21
1:D:323:ILE:HG23	1:D:324:PRO:HD2	1.15	1.15
1:D:533:ASN:HB2	1:D:534:PRO:HD2	1.24	1.14
1:B:533:ASN:HB2	1:B:534:PRO:HD2	1.24	1.14
1:F:323:ILE:HG23	1:F:324:PRO:HD2	1.18	1.13
1:A:533:ASN:CB	1:A:534:PRO:CD	2.27	1.12
1:A:533:ASN:HB2	1:A:534:PRO:HD2	1.24	1.12
1:B:533:ASN:CB	1:B:534:PRO:CD	2.27	1.12
1:D:533:ASN:CB	1:D:534:PRO:CD	2.27	1.12
1:F:529:GLU:O	1:F:531:PRO:HD3	1.47	1.12
1:B:323:ILE:HG23	1:B:324:PRO:HD2	1.15	1.12
1:C:323:ILE:HG23	1:C:324:PRO:HD2	1.15	1.11
1:C:533:ASN:CB	1:C:534:PRO:CD	2.27	1.11
1:E:323:ILE:HG23	1:E:324:PRO:HD2	1.19	1.10
1:E:529:GLU:O	1:E:531:PRO:HD3	1.50	1.09
1:C:533:ASN:HB2	1:C:534:PRO:HD2	1.24	1.09
1:A:323:ILE:HG23	1:A:324:PRO:HD2	1.15	1.08
1:E:323:ILE:CG2	1:E:324:PRO:HD2	1.86	1.05
1:E:533:ASN:HB2	1:E:534:PRO:HD2	1.40	1.03
1:F:323:ILE:CG2	1:F:324:PRO:HD2	1.87	1.03
1:F:533:ASN:HB2	1:F:534:PRO:HD2	1.41	1.01
1:D:533:ASN:HB3	1:D:534:PRO:HD3	1.43	1.01
1:C:533:ASN:HB3	1:C:534:PRO:HD3	1.43	1.01
1:B:533:ASN:HB3	1:B:534:PRO:HD3	1.43	1.01
1:B:533:ASN:CB	1:B:534:PRO:HD2	1.89	1.00
1:A:533:ASN:HB3	1:A:534:PRO:HD3	1.43	1.00
1:D:533:ASN:CB	1:D:534:PRO:HD2	1.89	0.98
1:E:533:ASN:CB	1:E:534:PRO:CD	2.41	0.98
1:A:533:ASN:CB	1:A:534:PRO:HD2	1.89	0.97
1:C:533:ASN:CB	1:C:534:PRO:HD2	1.89	0.97
1:A:533:ASN:HB2	1:A:534:PRO:CD	1.94	0.96
1:F:533:ASN:CB	1:F:534:PRO:CD	2.42	0.96
1:C:533:ASN:HB3	1:C:534:PRO:CD	1.94	0.95
1:C:533:ASN:HB2	1:C:534:PRO:CD	1.94	0.95
1:C:544:GLU:HB3	1:C:598:LEU:HD21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:544:GLU:HB3	1:F:598:LEU:HD21	1.49	0.94
1:B:568:LYS:HA	1:B:584:LEU:HD12	1.49	0.93
1:A:533:ASN:HB3	1:A:534:PRO:CD	1.94	0.92
1:E:568:LYS:HA	1:E:584:LEU:HD12	1.51	0.92
1:F:533:ASN:CB	1:F:534:PRO:HD2	1.99	0.92
1:A:568:LYS:HA	1:A:584:LEU:HD12	1.51	0.92
1:A:696:LEU:HD21	1:A:701:VAL:HG21	1.50	0.91
1:D:544:GLU:HB3	1:D:598:LEU:HD21	1.50	0.91
1:A:584:LEU:HD23	1:A:589:LYS:HG3	1.51	0.91
1:E:544:GLU:HB3	1:E:598:LEU:HD21	1.49	0.91
1:A:544:GLU:HB3	1:A:598:LEU:HD21	1.53	0.91
1:B:529:GLU:O	1:B:531:PRO:CD	2.19	0.91
1:C:568:LYS:HA	1:C:584:LEU:HD12	1.53	0.91
1:B:696:LEU:HD21	1:B:701:VAL:HG21	1.54	0.90
1:F:696:LEU:HD21	1:F:701:VAL:HG21	1.52	0.90
1:E:584:LEU:HD23	1:E:589:LYS:HG3	1.51	0.90
1:D:748:ASP:OD1	1:D:751:GLN:N	2.05	0.90
1:B:544:GLU:HB3	1:B:598:LEU:HD21	1.53	0.90
1:C:606:ASN:ND2	1:C:608:ASN:HB2	1.87	0.90
1:C:584:LEU:HD23	1:C:589:LYS:HG3	1.52	0.90
1:A:748:ASP:OD1	1:A:751:GLN:N	2.05	0.89
1:C:529:GLU:O	1:C:531:PRO:CD	2.19	0.89
1:B:748:ASP:OD1	1:B:751:GLN:N	2.05	0.89
1:B:323:ILE:CG2	1:B:324:PRO:CD	2.51	0.89
1:B:533:ASN:HB3	1:B:534:PRO:CD	1.94	0.89
1:A:323:ILE:CG2	1:A:324:PRO:CD	2.51	0.89
1:C:748:ASP:OD1	1:C:751:GLN:N	2.05	0.89
1:D:584:LEU:HD23	1:D:589:LYS:HG3	1.55	0.89
1:A:529:GLU:O	1:A:531:PRO:CD	2.19	0.89
1:D:568:LYS:HA	1:D:584:LEU:HD12	1.55	0.89
1:E:533:ASN:CB	1:E:534:PRO:HD2	1.99	0.89
1:E:696:LEU:HD21	1:E:701:VAL:HG21	1.53	0.89
1:B:584:LEU:HD23	1:B:589:LYS:HG3	1.55	0.88
1:D:323:ILE:CG2	1:D:324:PRO:CD	2.51	0.88
1:F:568:LYS:HA	1:F:584:LEU:HD12	1.52	0.88
1:D:533:ASN:HB3	1:D:534:PRO:CD	1.94	0.88
1:A:606:ASN:ND2	1:A:608:ASN:HB2	1.88	0.88
1:D:696:LEU:HD21	1:D:701:VAL:HG21	1.54	0.87
1:E:533:ASN:HB3	1:E:534:PRO:CD	2.03	0.87
1:F:584:LEU:HD23	1:F:589:LYS:HG3	1.54	0.87
1:F:533:ASN:HB3	1:F:534:PRO:CD	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:HD21	1:C:608:ASN:HB2	1.40	0.87
1:B:323:ILE:HG23	1:B:324:PRO:CD	2.04	0.86
1:D:323:ILE:HG23	1:D:324:PRO:CD	2.04	0.86
1:A:751:GLN:NE2	1:C:692:ARG:HH22	1.73	0.86
1:C:323:ILE:CG2	1:C:324:PRO:CD	2.51	0.86
1:A:742:ILE:HD11	1:A:752:ALA:O	1.75	0.86
1:B:742:ILE:HD11	1:B:752:ALA:O	1.75	0.86
1:B:606:ASN:ND2	1:B:608:ASN:HB2	1.91	0.85
1:F:606:ASN:ND2	1:F:608:ASN:HB2	1.90	0.85
1:D:529:GLU:O	1:D:531:PRO:CD	2.19	0.85
1:F:742:ILE:HD11	1:F:752:ALA:O	1.76	0.85
1:A:323:ILE:HG23	1:A:324:PRO:CD	2.04	0.84
1:D:606:ASN:ND2	1:D:608:ASN:HB2	1.92	0.84
1:B:145:LYS:HB2	1:B:148:GLU:HG3	1.59	0.84
1:C:544:GLU:HG3	1:C:555:PHE:HB2	1.59	0.84
1:A:606:ASN:HD21	1:A:608:ASN:HB2	1.42	0.84
1:A:751:GLN:CD	1:C:692:ARG:HH22	1.81	0.84
1:C:145:LYS:HB2	1:C:148:GLU:HG3	1.58	0.84
1:D:145:LYS:HB2	1:D:148:GLU:HG3	1.60	0.83
1:C:696:LEU:HD21	1:C:701:VAL:HG21	1.57	0.83
1:E:742:ILE:HD11	1:E:752:ALA:O	1.79	0.83
1:F:145:LYS:HB2	1:F:148:GLU:HG3	1.61	0.83
1:A:323:ILE:HG22	1:A:324:PRO:HD2	1.61	0.82
1:F:606:ASN:HD21	1:F:608:ASN:HB2	1.43	0.82
1:A:544:GLU:HG3	1:A:555:PHE:HB2	1.62	0.82
1:A:145:LYS:HB2	1:A:148:GLU:HG3	1.59	0.82
1:E:533:ASN:HB3	1:E:534:PRO:HD3	1.61	0.82
1:B:606:ASN:HD21	1:B:608:ASN:HB2	1.45	0.82
1:E:606:ASN:ND2	1:E:608:ASN:HB2	1.95	0.82
1:C:323:ILE:HG23	1:C:324:PRO:CD	2.04	0.81
1:D:419:THR:H	1:D:422:GLN:HG3	1.45	0.81
1:E:43:GLY:H	1:E:698:ALA:HB1	1.44	0.81
1:A:378:MET:HE2	1:A:381:ASN:HA	1.63	0.81
1:F:544:GLU:HG3	1:F:555:PHE:HB2	1.62	0.81
1:C:742:ILE:HD11	1:C:752:ALA:O	1.79	0.81
1:E:49:ILE:HA	1:E:59:VAL:HG12	1.63	0.81
1:F:49:ILE:HA	1:F:59:VAL:HG12	1.63	0.81
1:D:544:GLU:HG3	1:D:555:PHE:HB2	1.61	0.81
1:D:742:ILE:HD11	1:D:752:ALA:O	1.80	0.81
1:E:419:THR:H	1:E:422:GLN:HG3	1.46	0.81
1:B:156:ILE:HG22	1:B:173:ILE:HD13	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:HG22	1:C:324:PRO:HD2	1.61	0.81
1:C:593:ASN:HD22	1:C:595:SER:H	1.28	0.81
1:E:715:ARG:HH11	1:E:715:ARG:HG3	1.45	0.81
1:B:419:THR:H	1:B:422:GLN:HG3	1.44	0.80
1:E:145:LYS:HB2	1:E:148:GLU:HG3	1.62	0.80
1:E:544:GLU:HG3	1:E:555:PHE:HB2	1.63	0.80
1:B:593:ASN:HD22	1:B:595:SER:H	1.29	0.80
1:A:49:ILE:HA	1:A:59:VAL:HG12	1.64	0.80
1:D:606:ASN:HD21	1:D:608:ASN:HB2	1.46	0.80
1:E:391:MET:HG2	1:E:434:LYS:HZ1	1.47	0.80
1:F:43:GLY:H	1:F:698:ALA:HB1	1.47	0.80
1:B:715:ARG:HH11	1:B:715:ARG:HG3	1.47	0.80
1:B:43:GLY:H	1:B:698:ALA:HB1	1.47	0.80
1:A:128:LYS:HD3	1:A:693:ALA:HB1	1.63	0.80
1:D:323:ILE:HG22	1:D:324:PRO:HD2	1.62	0.80
1:B:323:ILE:HG22	1:B:324:PRO:HD2	1.61	0.79
1:C:49:ILE:HA	1:C:59:VAL:HG12	1.63	0.79
1:A:85:LYS:HB3	1:A:107:ARG:HG2	1.64	0.79
1:B:49:ILE:HA	1:B:59:VAL:HG12	1.63	0.79
1:F:533:ASN:HB3	1:F:534:PRO:HD3	1.64	0.79
1:D:715:ARG:HG3	1:D:715:ARG:HH11	1.47	0.79
1:A:593:ASN:HD22	1:A:595:SER:H	1.29	0.79
1:D:49:ILE:HA	1:D:59:VAL:HG12	1.65	0.79
1:E:593:ASN:HD22	1:E:595:SER:H	1.30	0.79
1:A:751:GLN:HE22	1:C:692:ARG:NH2	1.80	0.79
1:C:715:ARG:HH11	1:C:715:ARG:HG3	1.48	0.79
1:D:43:GLY:H	1:D:698:ALA:HB1	1.46	0.79
1:D:85:LYS:HB3	1:D:107:ARG:HG2	1.64	0.79
1:F:715:ARG:HH11	1:F:715:ARG:HG3	1.47	0.78
1:E:737:LEU:HD21	1:E:788:ARG:HA	1.65	0.78
1:F:85:LYS:HB3	1:F:107:ARG:HG2	1.63	0.78
1:A:743:PRO:HG2	1:A:747:MET:SD	2.24	0.78
1:C:85:LYS:HB3	1:C:107:ARG:HG2	1.64	0.78
1:A:419:THR:H	1:A:422:GLN:HG3	1.48	0.78
1:D:593:ASN:HD22	1:D:595:SER:H	1.27	0.78
1:F:128:LYS:HD3	1:F:693:ALA:HB1	1.66	0.78
1:B:544:GLU:HG3	1:B:555:PHE:HB2	1.64	0.78
1:F:743:PRO:HG2	1:F:747:MET:SD	2.23	0.78
1:B:743:PRO:HG2	1:B:747:MET:SD	2.24	0.78
1:C:498:PHE:O	1:C:502:GLN:HG3	1.84	0.78
1:E:128:LYS:HD3	1:E:693:ALA:HB1	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:748:ASP:OD1	1:E:751:GLN:N	2.16	0.78
1:F:156:ILE:HG22	1:F:173:ILE:HD13	1.65	0.78
1:B:128:LYS:HD3	1:B:693:ALA:HB1	1.65	0.78
1:D:391:MET:HG2	1:D:434:LYS:HZ1	1.48	0.78
1:A:751:GLN:OE1	1:C:692:ARG:NH2	2.16	0.78
1:C:743:PRO:HG2	1:C:747:MET:SD	2.24	0.78
1:A:419:THR:HG23	1:A:422:GLN:NE2	1.99	0.77
1:E:606:ASN:HD21	1:E:608:ASN:HB2	1.49	0.77
1:F:593:ASN:HD22	1:F:595:SER:H	1.32	0.77
1:C:128:LYS:HD3	1:C:693:ALA:HB1	1.66	0.77
1:D:743:PRO:HG2	1:D:747:MET:SD	2.24	0.77
1:B:378:MET:HE1	1:B:384:ALA:HB2	1.67	0.77
1:A:715:ARG:HH11	1:A:715:ARG:HG3	1.48	0.77
1:D:378:MET:HE1	1:D:384:ALA:HB2	1.66	0.77
1:A:43:GLY:H	1:A:698:ALA:HB1	1.49	0.77
1:B:498:PHE:O	1:B:502:GLN:HG3	1.85	0.77
1:F:419:THR:H	1:F:422:GLN:HG3	1.49	0.77
1:E:85:LYS:HB3	1:E:107:ARG:HG2	1.67	0.77
1:D:419:THR:HG23	1:D:422:GLN:NE2	2.00	0.76
1:D:742:ILE:HG13	1:D:747:MET:HG2	1.67	0.76
1:B:742:ILE:HG13	1:B:747:MET:HG2	1.67	0.76
1:D:128:LYS:HD3	1:D:693:ALA:HB1	1.67	0.76
1:B:391:MET:HG2	1:B:434:LYS:HZ1	1.51	0.76
1:E:156:ILE:HG22	1:E:173:ILE:HD13	1.67	0.76
1:C:156:ILE:HG22	1:C:173:ILE:HD13	1.65	0.76
1:F:498:PHE:O	1:F:502:GLN:HG3	1.86	0.76
1:F:378:MET:HE1	1:F:384:ALA:HB2	1.68	0.76
1:C:742:ILE:HG13	1:C:747:MET:HG2	1.67	0.76
1:C:419:THR:HG23	1:C:422:GLN:NE2	2.00	0.76
1:C:43:GLY:H	1:C:698:ALA:HB1	1.48	0.75
1:C:419:THR:H	1:C:422:GLN:HG3	1.48	0.75
1:D:156:ILE:HG22	1:D:173:ILE:HD13	1.68	0.75
1:F:391:MET:HG2	1:F:434:LYS:HZ1	1.51	0.75
1:A:419:THR:H	1:A:422:GLN:HE21	1.34	0.75
1:B:85:LYS:HB3	1:B:107:ARG:HG2	1.67	0.75
1:F:529:GLU:O	1:F:531:PRO:CD	2.32	0.75
1:D:582:CYS:SG	1:D:591:THR:HB	2.27	0.75
1:F:737:LEU:HD21	1:F:788:ARG:HA	1.68	0.75
1:E:743:PRO:HG2	1:E:747:MET:SD	2.27	0.75
1:A:742:ILE:HG13	1:A:747:MET:HG2	1.67	0.74
1:E:527:LEU:O	1:E:527:LEU:HD12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:LEU:HD21	1:B:788:ARG:HA	1.69	0.74
1:F:323:ILE:CG2	1:F:324:PRO:CD	2.66	0.74
1:E:742:ILE:HG13	1:E:747:MET:HG2	1.70	0.74
1:F:748:ASP:OD1	1:F:751:GLN:N	2.20	0.74
1:E:323:ILE:CG2	1:E:324:PRO:CD	2.65	0.74
1:A:156:ILE:HG22	1:A:173:ILE:HD13	1.67	0.74
1:D:737:LEU:HD21	1:D:788:ARG:HA	1.70	0.74
1:E:738:ALA:HB1	1:E:741:ALA:HB2	1.69	0.74
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.68	0.74
1:D:419:THR:H	1:D:422:GLN:HE21	1.36	0.74
1:C:540:LEU:HD13	1:C:559:LEU:HA	1.70	0.73
1:F:743:PRO:CG	1:F:747:MET:SD	2.76	0.73
1:E:498:PHE:O	1:E:502:GLN:HG3	1.89	0.73
1:B:419:THR:HG23	1:B:422:GLN:NE2	2.03	0.73
1:E:529:GLU:O	1:E:531:PRO:CD	2.35	0.73
1:E:419:THR:HG23	1:E:422:GLN:NE2	2.03	0.73
1:B:540:LEU:HD13	1:B:559:LEU:HA	1.69	0.73
1:A:527:LEU:HD12	1:A:527:LEU:O	1.87	0.73
1:A:540:LEU:HD13	1:A:559:LEU:HA	1.70	0.73
1:C:391:MET:HG2	1:C:434:LYS:HZ1	1.54	0.73
1:A:498:PHE:O	1:A:502:GLN:HG3	1.88	0.73
1:C:737:LEU:HD21	1:C:788:ARG:HA	1.69	0.73
1:F:280:GLN:OE1	1:F:317:SER:HB2	1.88	0.73
1:C:419:THR:H	1:C:422:GLN:HE21	1.35	0.73
1:E:508:GLU:HG2	1:E:775:PHE:HE1	1.54	0.73
1:C:401:SER:HB3	1:C:608:ASN:HB3	1.71	0.72
1:E:378:MET:HE1	1:E:384:ALA:HB2	1.70	0.72
1:A:391:MET:HG2	1:A:434:LYS:HZ1	1.53	0.72
1:A:535:PRO:O	1:A:563:GLN:NE2	2.22	0.72
1:C:743:PRO:CG	1:C:747:MET:SD	2.77	0.72
1:C:535:PRO:O	1:C:563:GLN:NE2	2.22	0.72
1:D:743:PRO:CG	1:D:747:MET:SD	2.77	0.72
1:F:419:THR:HG23	1:F:422:GLN:NE2	2.04	0.72
1:D:535:PRO:O	1:D:563:GLN:NE2	2.22	0.72
1:A:743:PRO:CG	1:A:747:MET:SD	2.77	0.72
1:A:738:ALA:HB1	1:A:741:ALA:HB2	1.71	0.72
1:B:508:GLU:HG2	1:B:775:PHE:HE1	1.55	0.72
1:B:535:PRO:O	1:B:563:GLN:NE2	2.22	0.72
1:D:498:PHE:O	1:D:502:GLN:HG3	1.90	0.72
1:D:738:ALA:HB1	1:D:741:ALA:HB2	1.71	0.72
1:B:419:THR:H	1:B:422:GLN:HE21	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:PRO:CG	1:B:747:MET:SD	2.77	0.71
1:F:540:LEU:HD13	1:F:559:LEU:HA	1.71	0.71
1:D:508:GLU:HG2	1:D:775:PHE:HE1	1.54	0.71
1:E:419:THR:H	1:E:422:GLN:HE21	1.37	0.71
1:F:419:THR:H	1:F:422:GLN:HE21	1.36	0.71
1:B:419:THR:N	1:B:422:GLN:HE21	1.89	0.71
1:B:738:ALA:HB1	1:B:741:ALA:HB2	1.71	0.71
1:C:738:ALA:HB1	1:C:741:ALA:HB2	1.71	0.71
1:D:527:LEU:HD12	1:D:527:LEU:O	1.91	0.71
1:A:378:MET:HE1	1:A:384:ALA:HB2	1.72	0.71
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.72	0.71
1:C:378:MET:HE1	1:C:384:ALA:HB2	1.71	0.71
1:C:242:ASN:HB3	1:C:245:SER:HB2	1.72	0.71
1:A:401:SER:HB3	1:A:608:ASN:HB3	1.73	0.71
1:B:527:LEU:O	1:B:527:LEU:HD12	1.91	0.71
1:D:731:ARG:HH21	1:D:742:ILE:HG21	1.55	0.71
1:F:569:PHE:CD1	1:F:570:GLN:N	2.59	0.71
1:E:540:LEU:HD13	1:E:559:LEU:HA	1.71	0.70
1:D:731:ARG:HH11	1:D:731:ARG:HG3	1.57	0.70
1:F:742:ILE:HG13	1:F:747:MET:HG2	1.72	0.70
1:B:526:GLU:O	1:B:530:ARG:HB2	1.92	0.70
1:C:280:GLN:OE1	1:C:317:SER:HB2	1.90	0.70
1:E:569:PHE:CD1	1:E:570:GLN:N	2.60	0.70
1:A:731:ARG:HH11	1:A:731:ARG:HG3	1.57	0.70
1:F:527:LEU:HD12	1:F:527:LEU:O	1.90	0.70
1:A:731:ARG:NH2	1:A:742:ILE:HG21	2.07	0.70
1:C:527:LEU:HD12	1:C:527:LEU:O	1.91	0.70
1:E:378:MET:HE2	1:E:381:ASN:HA	1.74	0.70
1:B:533:ASN:HB2	1:B:534:PRO:CD	1.94	0.70
1:C:731:ARG:HH21	1:C:742:ILE:HG21	1.57	0.70
1:D:731:ARG:NH2	1:D:742:ILE:HG21	2.07	0.70
1:B:401:SER:HB3	1:B:608:ASN:HB3	1.74	0.69
1:E:419:THR:N	1:E:422:GLN:HE21	1.90	0.69
1:F:533:ASN:HB2	1:F:534:PRO:CD	2.13	0.69
1:F:731:ARG:HH21	1:F:742:ILE:HG21	1.55	0.69
1:E:346:GLU:O	1:E:350:THR:HG23	1.93	0.69
1:F:508:GLU:HG2	1:F:775:PHE:HE1	1.56	0.69
1:F:346:GLU:O	1:F:350:THR:HG23	1.92	0.69
1:D:540:LEU:HD13	1:D:559:LEU:HA	1.75	0.69
1:A:419:THR:N	1:A:422:GLN:HE21	1.89	0.69
1:E:743:PRO:CG	1:E:747:MET:SD	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ARG:NH2	1:C:742:ILE:HG21	2.08	0.69
1:D:72:LYS:HA	1:D:75:ILE:HD12	1.73	0.69
1:A:72:LYS:HA	1:A:75:ILE:HD12	1.74	0.69
1:A:569:PHE:CD1	1:A:570:GLN:N	2.61	0.69
1:A:731:ARG:HH21	1:A:742:ILE:HG21	1.57	0.69
1:A:751:GLN:OE1	1:C:692:ARG:NH1	2.26	0.69
1:D:526:GLU:O	1:D:530:ARG:HB2	1.93	0.69
1:A:537:VAL:HG22	1:A:559:LEU:HD11	1.74	0.69
1:C:419:THR:N	1:C:422:GLN:HE21	1.91	0.69
1:C:569:PHE:CD1	1:C:570:GLN:N	2.61	0.69
1:A:274:LYS:HG2	1:A:436:GLU:HB2	1.75	0.69
1:B:280:GLN:OE1	1:B:317:SER:HB2	1.92	0.69
1:E:582:CYS:SG	1:E:591:THR:HB	2.33	0.69
1:F:731:ARG:NH2	1:F:742:ILE:HG21	2.07	0.69
1:C:607:ASP:HA	1:C:610:THR:HB	1.75	0.68
1:D:419:THR:N	1:D:422:GLN:HE21	1.89	0.68
1:E:72:LYS:HA	1:E:75:ILE:HD12	1.74	0.68
1:E:526:GLU:O	1:E:530:ARG:HB2	1.93	0.68
1:F:323:ILE:HG23	1:F:324:PRO:CD	2.11	0.68
1:E:537:VAL:HG22	1:E:559:LEU:HD11	1.75	0.68
1:E:418:GLN:HA	1:E:422:GLN:NE2	2.08	0.68
1:B:708:ASN:HD22	1:B:708:ASN:N	1.91	0.68
1:C:274:LYS:HG2	1:C:436:GLU:HB2	1.75	0.68
1:C:537:VAL:HG22	1:C:559:LEU:HD11	1.74	0.68
1:A:728:GLN:O	1:A:732:GLN:HG2	1.94	0.68
1:D:401:SER:HB3	1:D:608:ASN:HB3	1.76	0.68
1:E:280:GLN:OE1	1:E:317:SER:HB2	1.93	0.68
1:A:582:CYS:SG	1:A:591:THR:HB	2.34	0.68
1:B:537:VAL:HG22	1:B:559:LEU:HD11	1.74	0.68
1:B:731:ARG:HH21	1:B:742:ILE:HG21	1.59	0.68
1:C:72:LYS:HA	1:C:75:ILE:HD12	1.75	0.68
1:D:242:ASN:HB3	1:D:245:SER:HB2	1.74	0.68
1:C:731:ARG:HG3	1:C:731:ARG:HH11	1.59	0.68
1:D:569:PHE:CD1	1:D:570:GLN:N	2.62	0.68
1:B:72:LYS:HA	1:B:75:ILE:HD12	1.74	0.68
1:D:196:VAL:HG12	1:D:196:VAL:O	1.94	0.68
1:F:72:LYS:HA	1:F:75:ILE:HD12	1.75	0.68
1:D:274:LYS:HG2	1:D:436:GLU:HB2	1.75	0.67
1:E:116:TYR:CZ	1:E:151:PRO:HA	2.29	0.67
1:F:401:SER:HB3	1:F:608:ASN:HB3	1.75	0.67
1:A:508:GLU:HG2	1:A:775:PHE:HE1	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:LEU:CD1	1:B:563:GLN:HG3	2.25	0.67
1:F:281:ALA:O	1:F:284:GLU:HB2	1.95	0.67
1:A:596:ALA:O	1:A:600:LYS:HG3	1.94	0.67
1:F:332:PHE:CE2	1:F:336:LEU:HD11	2.29	0.67
1:F:535:PRO:O	1:F:563:GLN:NE2	2.27	0.67
1:F:686:ILE:HG22	1:F:704:GLN:NE2	2.10	0.67
1:A:116:TYR:CZ	1:A:151:PRO:HA	2.29	0.67
1:A:280:GLN:OE1	1:A:317:SER:HB2	1.95	0.67
1:B:232:GLU:O	1:B:236:ASN:HB2	1.95	0.67
1:C:508:GLU:HG2	1:C:775:PHE:HE1	1.57	0.67
1:F:79:ASN:ND2	1:F:94:CYS:HB2	2.10	0.67
1:E:401:SER:HB3	1:E:608:ASN:HB3	1.74	0.67
1:F:274:LYS:HB3	1:F:432:LYS:HB3	1.76	0.67
1:D:332:PHE:CE2	1:D:336:LEU:HD11	2.30	0.67
1:D:418:GLN:HA	1:D:422:GLN:NE2	2.10	0.67
1:E:535:PRO:O	1:E:563:GLN:NE2	2.28	0.67
1:B:274:LYS:HB3	1:B:432:LYS:HB3	1.76	0.67
1:C:526:GLU:O	1:C:530:ARG:HB2	1.94	0.67
1:D:116:TYR:CZ	1:D:151:PRO:HA	2.30	0.67
1:F:419:THR:N	1:F:422:GLN:HE21	1.92	0.67
1:A:332:PHE:CE2	1:A:336:LEU:HD11	2.30	0.67
1:B:274:LYS:HG2	1:B:436:GLU:HB2	1.77	0.67
1:B:731:ARG:NH2	1:B:742:ILE:HG21	2.09	0.67
1:D:725:ILE:HD11	1:D:730:PHE:HD1	1.60	0.67
1:B:116:TYR:CZ	1:B:151:PRO:HA	2.30	0.67
1:B:418:GLN:HA	1:B:422:GLN:NE2	2.09	0.67
1:C:232:GLU:O	1:C:236:ASN:HB2	1.94	0.67
1:D:280:GLN:OE1	1:D:317:SER:HB2	1.94	0.67
1:B:569:PHE:CD1	1:B:570:GLN:N	2.63	0.67
1:C:79:ASN:ND2	1:C:94:CYS:HB2	2.10	0.66
1:F:537:VAL:HG22	1:F:559:LEU:HD11	1.76	0.66
1:B:725:ILE:HD11	1:B:730:PHE:HD1	1.60	0.66
1:D:537:VAL:HG22	1:D:559:LEU:HD11	1.77	0.66
1:E:332:PHE:CE2	1:E:336:LEU:HD11	2.31	0.66
1:E:731:ARG:HH21	1:E:742:ILE:HG21	1.60	0.66
1:B:242:ASN:HB3	1:B:245:SER:HB2	1.76	0.66
1:B:540:LEU:CD1	1:B:559:LEU:HA	2.26	0.66
1:D:281:ALA:O	1:D:284:GLU:HB2	1.95	0.66
1:D:433:ALA:O	1:D:437:ARG:HG3	1.96	0.66
1:A:526:GLU:O	1:A:530:ARG:HB2	1.94	0.66
1:B:103:ASN:O	1:B:107:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ARG:HB3	1:B:112:LEU:HB2	1.78	0.66
1:B:728:GLN:O	1:B:732:GLN:HG2	1.96	0.66
1:C:582:CYS:SG	1:C:591:THR:HB	2.35	0.66
1:C:686:ILE:HG22	1:C:704:GLN:NE2	2.09	0.66
1:E:731:ARG:HH11	1:E:731:ARG:HG3	1.60	0.66
1:E:731:ARG:NH2	1:E:742:ILE:HG21	2.11	0.66
1:F:728:GLN:O	1:F:732:GLN:HG2	1.95	0.66
1:C:274:LYS:HB3	1:C:432:LYS:HB3	1.76	0.66
1:C:596:ALA:O	1:C:600:LYS:HG3	1.96	0.66
1:E:274:LYS:HB3	1:E:432:LYS:HB3	1.77	0.66
1:A:308:GLU:HB3	1:A:312:ASN:HB2	1.77	0.66
1:D:308:GLU:HB3	1:D:312:ASN:HB2	1.77	0.66
1:D:527:LEU:CD1	1:D:563:GLN:HG3	2.26	0.66
1:A:708:ASN:N	1:A:708:ASN:HD22	1.93	0.66
1:B:346:GLU:O	1:B:350:THR:HG23	1.95	0.66
1:C:346:GLU:O	1:C:350:THR:HG23	1.95	0.66
1:C:708:ASN:HD22	1:C:708:ASN:N	1.94	0.66
1:E:433:ALA:O	1:E:437:ARG:HG3	1.95	0.66
1:E:232:GLU:O	1:E:236:ASN:HB2	1.96	0.66
1:B:378:MET:HE2	1:B:381:ASN:HA	1.78	0.66
1:F:607:ASP:HA	1:F:610:THR:HB	1.77	0.66
1:A:79:ASN:ND2	1:A:94:CYS:HB2	2.12	0.65
1:A:607:ASP:HA	1:A:610:THR:HB	1.78	0.65
1:C:418:GLN:HA	1:C:422:GLN:NE2	2.11	0.65
1:C:769:ILE:HD13	1:C:774:ILE:HG23	1.78	0.65
1:E:596:ALA:O	1:E:600:LYS:HG3	1.96	0.65
1:A:725:ILE:HD11	1:A:730:PHE:HD1	1.61	0.65
1:C:728:GLN:O	1:C:732:GLN:HG2	1.96	0.65
1:B:79:ASN:ND2	1:B:94:CYS:HB2	2.11	0.65
1:B:433:ALA:O	1:B:437:ARG:HG3	1.96	0.65
1:B:731:ARG:HH11	1:B:731:ARG:HG3	1.61	0.65
1:D:346:GLU:O	1:D:350:THR:HG23	1.95	0.65
1:C:116:TYR:CZ	1:C:151:PRO:HA	2.31	0.65
1:C:281:ALA:O	1:C:284:GLU:HB2	1.97	0.65
1:E:725:ILE:HD11	1:E:730:PHE:HD1	1.60	0.65
1:F:242:ASN:HB3	1:F:245:SER:HB2	1.76	0.65
1:B:281:ALA:O	1:B:284:GLU:HB2	1.96	0.65
1:C:433:ALA:O	1:C:437:ARG:HG3	1.96	0.65
1:D:686:ILE:HG22	1:D:704:GLN:NE2	2.11	0.65
1:A:77:LYS:H	1:A:77:LYS:CE	2.09	0.65
1:A:433:ALA:O	1:A:437:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:CD1	1:C:559:LEU:HA	2.27	0.65
1:B:332:PHE:CE2	1:B:336:LEU:HD11	2.31	0.65
1:D:596:ALA:O	1:D:600:LYS:HG3	1.97	0.65
1:D:731:ARG:HG3	1:D:731:ARG:NH1	2.11	0.65
1:F:433:ALA:O	1:F:437:ARG:HG3	1.97	0.65
1:A:696:LEU:CD2	1:A:701:VAL:HG21	2.27	0.65
1:B:305:LEU:HD22	1:B:354:ARG:HA	1.79	0.65
1:D:103:ASN:O	1:D:107:ARG:HG3	1.96	0.65
1:E:715:ARG:HG3	1:E:715:ARG:NH1	2.12	0.65
1:F:378:MET:HE2	1:F:381:ASN:HA	1.79	0.65
1:F:582:CYS:SG	1:F:591:THR:HB	2.36	0.65
1:F:731:ARG:HH11	1:F:731:ARG:HG3	1.60	0.65
1:F:769:ILE:HD13	1:F:774:ILE:HG23	1.79	0.65
1:E:607:ASP:HA	1:E:610:THR:HB	1.78	0.65
1:F:596:ALA:O	1:F:600:LYS:HG3	1.97	0.65
1:C:488:LYS:HE2	1:C:529:GLU:OE1	1.97	0.65
1:D:232:GLU:O	1:D:236:ASN:HB2	1.96	0.65
1:D:488:LYS:HE2	1:D:529:GLU:OE1	1.96	0.65
1:E:708:ASN:HD22	1:E:708:ASN:N	1.94	0.65
1:F:526:GLU:O	1:F:530:ARG:HB2	1.96	0.65
1:A:145:LYS:HB2	1:A:148:GLU:CG	2.27	0.64
1:A:540:LEU:CD1	1:A:559:LEU:HA	2.26	0.64
1:D:769:ILE:HD13	1:D:774:ILE:HG23	1.79	0.64
1:E:242:ASN:HB3	1:E:245:SER:HB2	1.80	0.64
1:F:738:ALA:HB1	1:F:741:ALA:HB2	1.78	0.64
1:D:728:GLN:O	1:D:732:GLN:HG2	1.96	0.64
1:E:274:LYS:HG2	1:E:436:GLU:HB2	1.78	0.64
1:F:540:LEU:CD1	1:F:559:LEU:HA	2.27	0.64
1:A:232:GLU:O	1:A:236:ASN:HB2	1.97	0.64
1:B:582:CYS:SG	1:B:591:THR:HB	2.37	0.64
1:B:57:VAL:HB	1:B:75:ILE:HD11	1.80	0.64
1:C:332:PHE:CE2	1:C:336:LEU:HD11	2.32	0.64
1:D:607:ASP:HA	1:D:610:THR:HB	1.79	0.64
1:E:728:GLN:O	1:E:732:GLN:HG2	1.97	0.64
1:A:305:LEU:HD22	1:A:354:ARG:HA	1.80	0.64
1:F:376:ALA:HB2	1:F:420:LYS:N	2.13	0.64
1:A:103:ASN:O	1:A:107:ARG:HG3	1.97	0.64
1:A:281:ALA:O	1:A:284:GLU:HB2	1.96	0.64
1:A:418:GLN:HA	1:A:422:GLN:NE2	2.12	0.64
1:A:527:LEU:CD1	1:A:563:GLN:HG3	2.27	0.64
1:B:596:ALA:O	1:B:600:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HB2	1:C:148:GLU:CG	2.25	0.64
1:E:79:ASN:ND2	1:E:94:CYS:HB2	2.11	0.64
1:E:281:ALA:O	1:E:284:GLU:HB2	1.97	0.64
1:F:274:LYS:HG2	1:F:436:GLU:HB2	1.78	0.64
1:B:715:ARG:HG3	1:B:715:ARG:NH1	2.13	0.64
1:D:79:ASN:ND2	1:D:94:CYS:HB2	2.12	0.64
1:D:274:LYS:HB3	1:D:432:LYS:HB3	1.79	0.64
1:B:607:ASP:HA	1:B:610:THR:HB	1.77	0.64
1:D:593:ASN:ND2	1:D:595:SER:H	1.95	0.64
1:C:527:LEU:CD1	1:C:563:GLN:HG3	2.28	0.64
1:A:196:VAL:O	1:A:196:VAL:HG12	1.98	0.64
1:C:725:ILE:HD11	1:C:730:PHE:HD1	1.63	0.64
1:F:107:ARG:HB3	1:F:112:LEU:HB2	1.80	0.64
1:F:725:ILE:HD11	1:F:730:PHE:HD1	1.63	0.64
1:C:731:ARG:HG2	1:C:756:MET:HE2	1.79	0.63
1:A:346:GLU:O	1:A:350:THR:HG23	1.97	0.63
1:A:673:THR:O	1:A:677:THR:HG23	1.98	0.63
1:F:308:GLU:HB3	1:F:312:ASN:HB2	1.81	0.63
1:A:715:ARG:HG3	1:A:715:ARG:NH1	2.13	0.63
1:F:708:ASN:HD22	1:F:708:ASN:N	1.94	0.63
1:A:488:LYS:HE2	1:A:529:GLU:OE1	1.98	0.63
1:C:103:ASN:O	1:C:107:ARG:HG3	1.99	0.63
1:D:742:ILE:HG23	1:D:743:PRO:HD2	1.81	0.63
1:B:517:PHE:CE2	1:B:716:ILE:HD13	2.34	0.63
1:C:196:VAL:O	1:C:196:VAL:HG12	1.97	0.63
1:D:107:ARG:HB3	1:D:112:LEU:HB2	1.79	0.63
1:E:103:ASN:O	1:E:107:ARG:HG3	1.99	0.63
1:C:305:LEU:HD22	1:C:354:ARG:HA	1.79	0.63
1:E:145:LYS:HB2	1:E:148:GLU:CG	2.27	0.63
1:A:742:ILE:HG23	1:A:743:PRO:HD2	1.81	0.63
1:B:145:LYS:HB2	1:B:148:GLU:CG	2.27	0.63
1:C:57:VAL:HB	1:C:75:ILE:HD11	1.80	0.63
1:C:308:GLU:HB3	1:C:312:ASN:HB2	1.79	0.63
1:D:305:LEU:HD22	1:D:354:ARG:HA	1.81	0.63
1:D:708:ASN:HD22	1:D:708:ASN:N	1.95	0.63
1:E:308:GLU:HB3	1:E:312:ASN:HB2	1.80	0.63
1:F:116:TYR:CZ	1:F:151:PRO:HA	2.34	0.63
1:F:271:LEU:HD23	1:F:482:ILE:HG13	1.81	0.63
1:C:107:ARG:HB3	1:C:112:LEU:HB2	1.79	0.63
1:D:174:LEU:N	1:D:174:LEU:HD23	2.13	0.63
1:F:174:LEU:N	1:F:174:LEU:HD23	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:LEU:HD22	1:F:354:ARG:HA	1.81	0.63
1:C:742:ILE:HG23	1:C:743:PRO:HD2	1.81	0.63
1:D:517:PHE:CE2	1:D:716:ILE:HD13	2.33	0.63
1:F:715:ARG:HG3	1:F:715:ARG:NH1	2.12	0.63
1:B:308:GLU:HB3	1:B:312:ASN:HB2	1.80	0.62
1:D:378:MET:HE2	1:D:381:ASN:HA	1.80	0.62
1:A:748:ASP:OD1	1:A:748:ASP:O	2.18	0.62
1:E:107:ARG:HB3	1:E:112:LEU:HB2	1.80	0.62
1:E:517:PHE:CE2	1:E:716:ILE:HD13	2.34	0.62
1:C:391:MET:HE2	1:C:434:LYS:HE3	1.81	0.62
1:A:107:ARG:HB3	1:A:112:LEU:HB2	1.80	0.62
1:A:274:LYS:HB3	1:A:432:LYS:HB3	1.82	0.62
1:A:686:ILE:HG22	1:A:704:GLN:NE2	2.15	0.62
1:B:488:LYS:HE2	1:B:529:GLU:OE1	1.99	0.62
1:B:673:THR:O	1:B:677:THR:HG23	1.99	0.62
1:B:748:ASP:OD1	1:B:748:ASP:O	2.17	0.62
1:C:715:ARG:HG3	1:C:715:ARG:NH1	2.13	0.62
1:D:748:ASP:OD1	1:D:748:ASP:O	2.18	0.62
1:F:145:LYS:HB2	1:F:148:GLU:CG	2.28	0.62
1:F:418:GLN:HA	1:F:422:GLN:NE2	2.13	0.62
1:A:174:LEU:N	1:A:174:LEU:HD23	2.14	0.62
1:B:174:LEU:N	1:B:174:LEU:HD23	2.15	0.62
1:B:731:ARG:HG3	1:B:731:ARG:NH1	2.15	0.62
1:C:731:ARG:HG3	1:C:731:ARG:NH1	2.13	0.62
1:F:673:THR:O	1:F:677:THR:HG23	1.98	0.62
1:A:377:SER:O	1:A:379:PRO:HD3	2.00	0.62
1:C:419:THR:HG23	1:C:422:GLN:CD	2.20	0.62
1:D:715:ARG:HG3	1:D:715:ARG:NH1	2.13	0.62
1:F:527:LEU:CD1	1:F:563:GLN:HG3	2.30	0.62
1:B:377:SER:O	1:B:379:PRO:HD3	2.00	0.62
1:C:748:ASP:OD1	1:C:748:ASP:O	2.18	0.62
1:E:731:ARG:HG3	1:E:731:ARG:NH1	2.14	0.62
1:C:376:ALA:HB2	1:C:420:LYS:N	2.14	0.61
1:E:540:LEU:CD1	1:E:559:LEU:HA	2.30	0.61
1:A:271:LEU:HD23	1:A:482:ILE:HG13	1.81	0.61
1:B:196:VAL:O	1:B:196:VAL:HG12	1.99	0.61
1:B:271:LEU:HD23	1:B:482:ILE:HG13	1.83	0.61
1:B:552:ASP:O	1:B:555:PHE:HB3	2.00	0.61
1:C:517:PHE:CE2	1:C:716:ILE:HD13	2.35	0.61
1:F:232:GLU:O	1:F:236:ASN:HB2	2.00	0.61
1:A:288:HIS:HB3	1:A:292:TYR:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLU:HG3	1:C:771:GLN:H	1.65	0.61
1:E:488:LYS:HE2	1:E:529:GLU:OE1	2.00	0.61
1:F:225:LEU:N	1:F:225:LEU:HD23	2.15	0.61
1:A:57:VAL:HB	1:A:75:ILE:HD11	1.82	0.61
1:B:742:ILE:HG23	1:B:743:PRO:HD2	1.81	0.61
1:C:271:LEU:HD23	1:C:482:ILE:HG13	1.81	0.61
1:C:673:THR:O	1:C:677:THR:HG23	2.00	0.61
1:F:757:ILE:HA	1:F:760:LEU:HD12	1.82	0.61
1:D:145:LYS:HB2	1:D:148:GLU:CG	2.28	0.61
1:E:552:ASP:O	1:E:555:PHE:HB3	2.01	0.61
1:F:103:ASN:O	1:F:107:ARG:HG3	2.00	0.61
1:A:234:PHE:CE2	1:A:289:ILE:HG12	2.36	0.61
1:F:295:ALA:HB2	1:F:310:PHE:HZ	1.65	0.61
1:E:686:ILE:HG22	1:E:704:GLN:NE2	2.16	0.61
1:F:196:VAL:O	1:F:196:VAL:HG12	2.00	0.61
1:F:731:ARG:HG3	1:F:731:ARG:NH1	2.14	0.61
1:A:133:TYR:CD1	1:A:189:LYS:HD2	2.36	0.61
1:A:769:ILE:HD13	1:A:774:ILE:HG23	1.83	0.61
1:D:673:THR:O	1:D:677:THR:HG23	2.01	0.61
1:A:419:THR:HG23	1:A:422:GLN:CD	2.20	0.61
1:B:593:ASN:ND2	1:B:595:SER:H	1.98	0.61
1:D:77:LYS:H	1:D:77:LYS:CE	2.13	0.61
1:F:57:VAL:HB	1:F:75:ILE:HD11	1.83	0.61
1:A:731:ARG:HG3	1:A:731:ARG:NH1	2.10	0.60
1:C:593:ASN:ND2	1:C:595:SER:H	1.97	0.60
1:D:271:LEU:HD23	1:D:482:ILE:HG13	1.82	0.60
1:B:323:ILE:HG22	1:B:324:PRO:CD	2.26	0.60
1:B:522:GLN:N	1:B:523:PRO:HD2	2.15	0.60
1:C:174:LEU:HD23	1:C:174:LEU:N	2.16	0.60
1:D:388:CYS:SG	1:D:393:ILE:HG22	2.41	0.60
1:D:757:ILE:HA	1:D:760:LEU:HD12	1.84	0.60
1:E:742:ILE:HG23	1:E:743:PRO:HD2	1.83	0.60
1:B:89:MET:CE	1:B:100:VAL:HG13	2.32	0.60
1:C:522:GLN:N	1:C:523:PRO:HD2	2.16	0.60
1:E:174:LEU:N	1:E:174:LEU:HD23	2.16	0.60
1:E:664:LYS:O	1:E:668:THR:HG23	2.00	0.60
1:E:731:ARG:HG2	1:E:756:MET:HE2	1.82	0.60
1:E:769:ILE:HD13	1:E:774:ILE:HG23	1.82	0.60
1:A:323:ILE:HG22	1:A:324:PRO:CD	2.26	0.60
1:A:593:ASN:ND2	1:A:595:SER:H	1.98	0.60
1:B:288:HIS:HB3	1:B:292:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:MET:HG2	1:D:434:LYS:NZ	2.16	0.60
1:E:225:LEU:N	1:E:225:LEU:HD23	2.16	0.60
1:E:673:THR:O	1:E:677:THR:HG23	2.01	0.60
1:A:522:GLN:N	1:A:523:PRO:HD2	2.15	0.60
1:C:664:LYS:O	1:C:668:THR:HG23	2.02	0.60
1:A:376:ALA:HB2	1:A:420:LYS:N	2.16	0.60
1:D:225:LEU:N	1:D:225:LEU:HD23	2.15	0.60
1:A:382:THR:O	1:A:385:GLN:HB2	2.02	0.60
1:B:418:GLN:HA	1:B:422:GLN:HE21	1.66	0.60
1:B:686:ILE:HG22	1:B:704:GLN:NE2	2.16	0.60
1:E:57:VAL:HB	1:E:75:ILE:HD11	1.83	0.60
1:E:288:HIS:HB3	1:E:292:TYR:CZ	2.36	0.60
1:E:305:LEU:HD22	1:E:354:ARG:HA	1.82	0.60
1:E:377:SER:O	1:E:379:PRO:HD3	2.01	0.60
1:E:757:ILE:HA	1:E:760:LEU:HD12	1.84	0.60
1:F:133:TYR:CD1	1:F:189:LYS:HD2	2.36	0.60
1:A:285:ARG:HB2	1:A:291:TYR:CZ	2.37	0.60
1:B:376:ALA:HB2	1:B:420:LYS:N	2.17	0.60
1:B:419:THR:HG23	1:B:422:GLN:CD	2.22	0.60
1:D:664:LYS:O	1:D:668:THR:HG23	2.02	0.60
1:F:696:LEU:CD2	1:F:701:VAL:HG21	2.28	0.60
1:B:77:LYS:CE	1:B:77:LYS:H	2.15	0.60
1:C:77:LYS:CE	1:C:77:LYS:H	2.14	0.60
1:E:593:ASN:ND2	1:E:595:SER:H	1.98	0.60
1:F:664:LYS:O	1:F:668:THR:HG23	2.02	0.60
1:C:288:HIS:HB3	1:C:292:TYR:CZ	2.36	0.60
1:C:391:MET:HG2	1:C:434:LYS:NZ	2.16	0.60
1:D:234:PHE:CE2	1:D:289:ILE:HG12	2.37	0.60
1:D:419:THR:HG23	1:D:422:GLN:CD	2.22	0.60
1:D:593:ASN:HD22	1:D:593:ASN:C	2.04	0.60
1:E:80:PRO:HD2	1:E:83:PHE:CE2	2.37	0.60
1:E:527:LEU:CD1	1:E:563:GLN:HG3	2.31	0.60
1:F:171:GLN:OE1	1:F:678:ASN:HB3	2.02	0.60
1:A:751:GLN:OE1	1:C:692:ARG:CZ	2.50	0.59
1:B:225:LEU:N	1:B:225:LEU:HD23	2.16	0.59
1:E:391:MET:HG2	1:E:434:LYS:NZ	2.17	0.59
1:A:508:GLU:HG3	1:A:771:GLN:H	1.66	0.59
1:B:664:LYS:O	1:B:668:THR:HG23	2.02	0.59
1:F:144:LYS:HG3	1:F:149:MET:HG3	1.83	0.59
1:F:517:PHE:CE1	1:F:716:ILE:HD13	2.37	0.59
1:A:88:ASP:O	1:A:91:GLU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:HG2	1:A:756:MET:HE2	1.83	0.59
1:F:77:LYS:CE	1:F:77:LYS:H	2.14	0.59
1:F:403:LEU:O	1:F:404:THR:HG23	2.02	0.59
1:B:382:THR:O	1:B:385:GLN:HB2	2.02	0.59
1:F:508:GLU:HG3	1:F:771:GLN:H	1.68	0.59
1:D:288:HIS:HB3	1:D:292:TYR:CZ	2.38	0.59
1:A:552:ASP:O	1:A:555:PHE:HB3	2.02	0.59
1:B:234:PHE:CE2	1:B:289:ILE:HG12	2.38	0.59
1:B:696:LEU:CD2	1:B:701:VAL:HG21	2.30	0.59
1:B:767:TYR:O	1:B:768:ARG:NH1	2.35	0.59
1:C:285:ARG:HB2	1:C:291:TYR:CZ	2.37	0.59
1:C:323:ILE:HG22	1:C:324:PRO:CD	2.26	0.59
1:D:696:LEU:CD2	1:D:701:VAL:HG21	2.30	0.59
1:F:488:LYS:HE2	1:F:529:GLU:OE1	2.03	0.59
1:F:767:TYR:O	1:F:768:ARG:NH1	2.36	0.59
1:A:136:LYS:O	1:A:139:ASP:HB2	2.03	0.59
1:A:757:ILE:HG12	1:A:762:LEU:HD12	1.85	0.59
1:C:378:MET:HE2	1:C:381:ASN:HA	1.83	0.59
1:D:171:GLN:OE1	1:D:678:ASN:HB3	2.02	0.59
1:D:377:SER:O	1:D:379:PRO:HD3	2.02	0.59
1:E:271:LEU:HD23	1:E:482:ILE:HG13	1.83	0.59
1:F:552:ASP:O	1:F:555:PHE:HB3	2.02	0.59
1:D:522:GLN:N	1:D:523:PRO:HD2	2.17	0.59
1:E:80:PRO:HD2	1:E:83:PHE:CD2	2.38	0.59
1:E:535:PRO:HB2	1:E:540:LEU:HD21	1.84	0.59
1:C:710:VAL:O	1:C:714:ILE:HG13	2.03	0.59
1:E:376:ALA:HB2	1:E:420:LYS:N	2.18	0.59
1:C:133:TYR:CD1	1:C:189:LYS:HD2	2.37	0.59
1:C:377:SER:O	1:C:379:PRO:HD3	2.02	0.59
1:C:593:ASN:HD22	1:C:593:ASN:C	2.05	0.59
1:E:61:LEU:O	1:E:65:GLY:HA2	2.03	0.59
1:E:77:LYS:CE	1:E:77:LYS:H	2.15	0.59
1:F:593:ASN:ND2	1:F:595:SER:H	2.00	0.59
1:B:80:PRO:HD2	1:B:83:PHE:CD2	2.38	0.58
1:B:419:THR:N	1:B:422:GLN:HG3	2.18	0.58
1:B:606:ASN:HB3	1:B:609:VAL:CG1	2.33	0.58
1:D:535:PRO:HB2	1:D:540:LEU:HD21	1.84	0.58
1:D:540:LEU:CD1	1:D:559:LEU:HA	2.33	0.58
1:E:136:LYS:O	1:E:139:ASP:HB2	2.04	0.58
1:C:225:LEU:N	1:C:225:LEU:HD23	2.17	0.58
1:D:152:HIS:O	1:D:156:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:LYS:O	1:F:376:ALA:HA	2.03	0.58
1:B:757:ILE:HA	1:B:760:LEU:HD12	1.86	0.58
1:C:89:MET:CE	1:C:100:VAL:HG13	2.33	0.58
1:C:544:GLU:HG3	1:C:555:PHE:CB	2.31	0.58
1:E:522:GLN:N	1:E:523:PRO:HD2	2.18	0.58
1:B:757:ILE:HG12	1:B:762:LEU:HD12	1.85	0.58
1:E:144:LYS:HG3	1:E:149:MET:HG3	1.85	0.58
1:A:225:LEU:N	1:A:225:LEU:HD23	2.17	0.58
1:A:606:ASN:HB3	1:A:609:VAL:CG1	2.32	0.58
1:D:349:GLN:O	1:D:353:LEU:HG	2.03	0.58
1:E:696:LEU:CD2	1:E:701:VAL:HG21	2.29	0.58
1:A:391:MET:HG2	1:A:434:LYS:NZ	2.17	0.58
1:A:403:LEU:O	1:A:404:THR:HG23	2.03	0.58
1:D:382:THR:O	1:D:385:GLN:HB2	2.03	0.58
1:A:77:LYS:H	1:A:77:LYS:HZ2	1.52	0.58
1:B:508:GLU:HG3	1:B:771:GLN:H	1.69	0.58
1:B:769:ILE:HD13	1:B:774:ILE:HG23	1.85	0.58
1:C:757:ILE:HA	1:C:760:LEU:HD12	1.85	0.58
1:F:288:HIS:HB3	1:F:292:TYR:CZ	2.39	0.58
1:F:593:ASN:HD22	1:F:593:ASN:C	2.06	0.58
1:A:593:ASN:HD22	1:A:593:ASN:C	2.06	0.58
1:E:133:TYR:CD1	1:E:189:LYS:HD2	2.38	0.58
1:E:285:ARG:HB2	1:E:291:TYR:CZ	2.39	0.58
1:F:61:LEU:O	1:F:65:GLY:HA2	2.04	0.58
1:A:368:LYS:O	1:A:376:ALA:HA	2.04	0.58
1:B:538:LEU:HD12	1:B:664:LYS:HD2	1.85	0.58
1:C:368:LYS:O	1:C:376:ALA:HA	2.04	0.58
1:D:295:ALA:HB2	1:D:310:PHE:HZ	1.69	0.58
1:E:196:VAL:O	1:E:196:VAL:HG12	2.02	0.58
1:F:88:ASP:O	1:F:91:GLU:HB2	2.04	0.58
1:F:544:GLU:HG3	1:F:555:PHE:CB	2.33	0.58
1:A:517:PHE:CE2	1:A:716:ILE:HD13	2.39	0.58
1:B:133:TYR:CD1	1:B:189:LYS:HD2	2.39	0.58
1:D:376:ALA:HB2	1:D:420:LYS:N	2.17	0.58
1:D:418:GLN:HA	1:D:422:GLN:HE21	1.68	0.58
1:E:234:PHE:CE2	1:E:289:ILE:HG12	2.39	0.58
1:E:418:GLN:HA	1:E:422:GLN:HE21	1.68	0.58
1:E:593:ASN:HD22	1:E:593:ASN:C	2.07	0.58
1:A:80:PRO:HD2	1:A:83:PHE:CD2	2.39	0.57
1:C:144:LYS:HG3	1:C:149:MET:HG3	1.86	0.57
1:D:88:ASP:O	1:D:91:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:ASN:HB3	1:E:609:VAL:CG1	2.33	0.57
1:F:391:MET:HG2	1:F:434:LYS:NZ	2.19	0.57
1:A:295:ALA:HB2	1:A:310:PHE:HZ	1.68	0.57
1:A:538:LEU:HD12	1:A:664:LYS:HD2	1.86	0.57
1:A:544:GLU:HG3	1:A:555:PHE:CB	2.32	0.57
1:B:80:PRO:HD2	1:B:83:PHE:CE2	2.39	0.57
1:C:80:PRO:HD2	1:C:83:PHE:CD2	2.39	0.57
1:C:382:THR:O	1:C:385:GLN:HB2	2.04	0.57
1:E:594:ALA:HA	1:E:597:TRP:CD1	2.39	0.57
1:F:606:ASN:HB3	1:F:609:VAL:CG1	2.34	0.57
1:B:171:GLN:OE1	1:B:678:ASN:HB3	2.04	0.57
1:B:288:HIS:HB3	1:B:292:TYR:CE1	2.39	0.57
1:C:418:GLN:HA	1:C:422:GLN:HE21	1.68	0.57
1:D:57:VAL:HB	1:D:75:ILE:HD11	1.83	0.57
1:D:144:LYS:HG3	1:D:149:MET:HG3	1.86	0.57
1:A:144:LYS:HG3	1:A:149:MET:HG3	1.84	0.57
1:B:88:ASP:O	1:B:91:GLU:HB2	2.04	0.57
1:B:725:ILE:HD11	1:B:730:PHE:CD1	2.39	0.57
1:D:391:MET:HE2	1:D:434:LYS:HE3	1.86	0.57
1:D:606:ASN:HB3	1:D:609:VAL:CG1	2.35	0.57
1:E:702:LEU:O	1:E:706:ARG:HG3	2.05	0.57
1:A:80:PRO:HD2	1:A:83:PHE:CE2	2.38	0.57
1:C:295:ALA:HB2	1:C:310:PHE:HZ	1.68	0.57
1:C:552:ASP:O	1:C:555:PHE:HB3	2.04	0.57
1:D:41:LYS:HB2	1:D:42:HIS:CE1	2.39	0.57
1:F:377:SER:O	1:F:379:PRO:HD3	2.04	0.57
1:E:178:GLU:OE2	1:E:686:ILE:HG21	2.05	0.57
1:E:295:ALA:HB2	1:E:310:PHE:HZ	1.70	0.57
1:A:288:HIS:HB3	1:A:292:TYR:CE1	2.40	0.57
1:D:725:ILE:HD11	1:D:730:PHE:CD1	2.40	0.57
1:D:767:TYR:O	1:D:768:ARG:NH1	2.37	0.57
1:F:80:PRO:HD2	1:F:83:PHE:CD2	2.40	0.57
1:B:540:LEU:HD12	1:B:559:LEU:HD12	1.87	0.57
1:B:710:VAL:O	1:B:714:ILE:HG13	2.04	0.57
1:C:61:LEU:O	1:C:65:GLY:HA2	2.05	0.57
1:C:79:ASN:HD21	1:C:94:CYS:HB2	1.70	0.57
1:E:368:LYS:O	1:E:376:ALA:HA	2.05	0.57
1:E:544:GLU:HG3	1:E:555:PHE:CB	2.34	0.57
1:B:61:LEU:O	1:B:65:GLY:HA2	2.04	0.57
1:B:368:LYS:O	1:B:376:ALA:HA	2.05	0.57
1:D:552:ASP:O	1:D:555:PHE:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:ALA:O	1:D:741:ALA:CB	2.53	0.57
1:F:418:GLN:HA	1:F:422:GLN:HE21	1.70	0.57
1:F:522:GLN:N	1:F:523:PRO:HD2	2.19	0.57
1:A:361:GLN:HG2	1:A:386:LYS:HB2	1.87	0.57
1:D:86:VAL:HG23	1:D:103:ASN:ND2	2.20	0.57
1:E:79:ASN:HD21	1:E:94:CYS:HB2	1.70	0.57
1:E:419:THR:HG23	1:E:422:GLN:CD	2.25	0.57
1:E:538:LEU:HD12	1:E:664:LYS:HD2	1.87	0.57
1:F:89:MET:CE	1:F:100:VAL:HG13	2.35	0.57
1:F:382:THR:O	1:F:385:GLN:HB2	2.04	0.57
1:A:171:GLN:OE1	1:A:678:ASN:HB3	2.05	0.56
1:B:391:MET:HG2	1:B:434:LYS:NZ	2.18	0.56
1:C:403:LEU:O	1:C:404:THR:HG23	2.05	0.56
1:E:278:ILE:HD13	1:E:432:LYS:HD3	1.87	0.56
1:E:376:ALA:O	1:E:403:LEU:HD22	2.05	0.56
1:E:743:PRO:HD2	1:E:747:MET:HG2	1.87	0.56
1:E:767:TYR:O	1:E:768:ARG:NH1	2.36	0.56
1:F:742:ILE:HG23	1:F:743:PRO:HD2	1.86	0.56
1:A:767:TYR:O	1:A:768:ARG:NH1	2.36	0.56
1:C:738:ALA:O	1:C:741:ALA:CB	2.53	0.56
1:D:80:PRO:HD2	1:D:83:PHE:CD2	2.40	0.56
1:D:288:HIS:HB3	1:D:292:TYR:CE1	2.40	0.56
1:E:403:LEU:O	1:E:404:THR:HG23	2.05	0.56
1:E:508:GLU:HG3	1:E:771:GLN:H	1.70	0.56
1:E:725:ILE:HD11	1:E:730:PHE:CD1	2.39	0.56
1:F:757:ILE:HG23	1:F:762:LEU:HB2	1.87	0.56
1:A:256:PHE:O	1:A:458:ALA:HB3	2.05	0.56
1:C:77:LYS:H	1:C:77:LYS:HZ2	1.53	0.56
1:C:136:LYS:O	1:C:139:ASP:HB2	2.05	0.56
1:C:686:ILE:HG22	1:C:704:GLN:HE22	1.71	0.56
1:D:133:TYR:CD1	1:D:189:LYS:HD2	2.40	0.56
1:D:323:ILE:HG22	1:D:324:PRO:CD	2.26	0.56
1:D:731:ARG:HG2	1:D:756:MET:HE2	1.87	0.56
1:E:70:LEU:HD12	1:E:71:SER:O	2.06	0.56
1:E:323:ILE:HG23	1:E:324:PRO:CD	2.12	0.56
1:A:738:ALA:O	1:A:741:ALA:CB	2.53	0.56
1:B:41:LYS:HB2	1:B:42:HIS:CE1	2.41	0.56
1:B:144:LYS:HG3	1:B:149:MET:HG3	1.88	0.56
1:B:295:ALA:HB2	1:B:310:PHE:HZ	1.69	0.56
1:B:391:MET:HE2	1:B:434:LYS:HE3	1.87	0.56
1:C:540:LEU:HD12	1:C:559:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LEU:HD21	1:C:562:GLU:HG3	1.87	0.56
1:B:738:ALA:O	1:B:741:ALA:CB	2.53	0.56
1:A:540:LEU:HD21	1:A:562:GLU:HG3	1.87	0.56
1:B:361:GLN:HG2	1:B:386:LYS:HB2	1.87	0.56
1:B:731:ARG:HG2	1:B:756:MET:HE2	1.86	0.56
1:C:88:ASP:O	1:C:91:GLU:HB2	2.05	0.56
1:D:710:VAL:O	1:D:714:ILE:HG13	2.06	0.56
1:E:288:HIS:HB3	1:E:292:TYR:CE1	2.41	0.56
1:F:308:GLU:HB2	1:F:313:TYR:CZ	2.41	0.56
1:A:89:MET:CE	1:A:100:VAL:HG13	2.36	0.56
1:A:108:TYR:CD2	1:A:696:LEU:HD12	2.40	0.56
1:B:278:ILE:HD13	1:B:432:LYS:HD3	1.87	0.56
1:D:256:PHE:O	1:D:458:ALA:HB3	2.04	0.56
1:D:544:GLU:HG3	1:D:555:PHE:CB	2.33	0.56
1:E:88:ASP:O	1:E:91:GLU:HB2	2.06	0.56
1:E:382:THR:O	1:E:385:GLN:HB2	2.04	0.56
1:F:80:PRO:HD2	1:F:83:PHE:CE2	2.40	0.56
1:F:748:ASP:OD1	1:F:748:ASP:O	2.24	0.56
1:A:41:LYS:HB2	1:A:42:HIS:CE1	2.40	0.56
1:B:403:LEU:O	1:B:404:THR:HG23	2.05	0.56
1:D:361:GLN:HG2	1:D:386:LYS:HB2	1.88	0.56
1:F:77:LYS:H	1:F:77:LYS:HZ2	1.54	0.56
1:F:285:ARG:HB2	1:F:291:TYR:CZ	2.41	0.56
1:A:70:LEU:HD12	1:A:71:SER:O	2.06	0.56
1:A:664:LYS:O	1:A:668:THR:HG23	2.05	0.56
1:C:80:PRO:HD2	1:C:83:PHE:CE2	2.40	0.56
1:E:41:LYS:HB2	1:E:42:HIS:CE1	2.41	0.56
1:C:278:ILE:HD13	1:C:432:LYS:HD3	1.88	0.56
1:E:171:GLN:OE1	1:E:678:ASN:HB3	2.05	0.56
1:E:308:GLU:HB2	1:E:313:TYR:CZ	2.41	0.56
1:E:563:GLN:O	1:E:565:ASN:N	2.39	0.56
1:F:41:LYS:HB2	1:F:42:HIS:CE1	2.41	0.56
1:A:308:GLU:HB2	1:A:313:TYR:CZ	2.41	0.55
1:A:710:VAL:O	1:A:714:ILE:HG13	2.05	0.55
1:A:757:ILE:HA	1:A:760:LEU:HD12	1.88	0.55
1:C:725:ILE:HD11	1:C:730:PHE:CD1	2.42	0.55
1:D:80:PRO:HD2	1:D:83:PHE:CE2	2.42	0.55
1:F:419:THR:HG23	1:F:422:GLN:CD	2.26	0.55
1:F:594:ALA:HA	1:F:597:TRP:CD1	2.42	0.55
1:F:743:PRO:CD	1:F:747:MET:SD	2.95	0.55
1:B:301:MET:HA	1:B:304:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:PHE:CZ	1:B:716:ILE:HD13	2.41	0.55
1:E:361:GLN:HG2	1:E:386:LYS:HB2	1.88	0.55
1:E:757:ILE:HG12	1:E:762:LEU:HD12	1.87	0.55
1:A:61:LEU:O	1:A:65:GLY:HA2	2.06	0.55
1:C:41:LYS:HB2	1:C:42:HIS:CE1	2.42	0.55
1:D:61:LEU:O	1:D:65:GLY:HA2	2.07	0.55
1:D:301:MET:HA	1:D:304:ASP:HB3	1.89	0.55
1:E:89:MET:CE	1:E:100:VAL:HG13	2.37	0.55
1:F:540:LEU:HD21	1:F:562:GLU:HG3	1.88	0.55
1:F:690:GLU:HG2	1:F:692:ARG:NH2	2.22	0.55
1:A:349:GLN:O	1:A:353:LEU:HG	2.06	0.55
1:B:79:ASN:HD21	1:B:94:CYS:HB2	1.71	0.55
1:D:97:GLU:HA	1:D:711:LEU:HD11	1.88	0.55
1:E:349:GLN:O	1:E:353:LEU:HG	2.06	0.55
1:B:327:GLN:O	1:B:330:GLU:HB2	2.07	0.55
1:C:152:HIS:O	1:C:156:ILE:HD12	2.07	0.55
1:C:308:GLU:HB2	1:C:313:TYR:CZ	2.42	0.55
1:C:696:LEU:CD2	1:C:701:VAL:HG21	2.33	0.55
1:A:70:LEU:HD13	1:A:74:ASP:HB2	1.88	0.55
1:B:544:GLU:HG3	1:B:555:PHE:CB	2.34	0.55
1:C:757:ILE:HG12	1:C:762:LEU:HD12	1.87	0.55
1:D:419:THR:N	1:D:422:GLN:HG3	2.19	0.55
1:A:86:VAL:HG23	1:A:103:ASN:ND2	2.22	0.55
1:B:95:LEU:HD11	1:B:714:ILE:HG21	1.89	0.55
1:B:285:ARG:HB2	1:B:291:TYR:CZ	2.42	0.55
1:C:234:PHE:CE2	1:C:289:ILE:HG12	2.42	0.55
1:C:594:ALA:HA	1:C:597:TRP:CD1	2.41	0.55
1:D:285:ARG:HB2	1:D:291:TYR:CZ	2.41	0.55
1:F:70:LEU:HD12	1:F:71:SER:O	2.06	0.55
1:F:79:ASN:HD21	1:F:94:CYS:HB2	1.70	0.55
1:B:108:TYR:CD2	1:B:696:LEU:HD12	2.42	0.55
1:D:178:GLU:OE2	1:D:686:ILE:HG21	2.07	0.55
1:D:403:LEU:O	1:D:404:THR:HG23	2.07	0.55
1:A:278:ILE:HD13	1:A:432:LYS:HD3	1.89	0.55
1:B:594:ALA:HA	1:B:597:TRP:CD1	2.42	0.55
1:C:702:LEU:O	1:C:706:ARG:HG3	2.07	0.55
1:F:535:PRO:HB2	1:F:540:LEU:HD21	1.88	0.55
1:F:540:LEU:HD12	1:F:559:LEU:HD12	1.89	0.55
1:A:702:LEU:O	1:A:706:ARG:HG3	2.06	0.55
1:B:376:ALA:O	1:B:403:LEU:HD22	2.07	0.55
1:C:171:GLN:OE1	1:C:678:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:757:ILE:HG23	1:E:762:LEU:HB2	1.88	0.55
1:F:349:GLN:O	1:F:353:LEU:HG	2.08	0.55
1:A:418:GLN:HA	1:A:422:GLN:HE21	1.70	0.54
1:A:725:ILE:HD11	1:A:730:PHE:CD1	2.40	0.54
1:B:77:LYS:H	1:B:77:LYS:HZ2	1.53	0.54
1:B:308:GLU:HB2	1:B:313:TYR:CZ	2.42	0.54
1:B:540:LEU:HD21	1:B:562:GLU:HG3	1.88	0.54
1:B:593:ASN:HD22	1:B:593:ASN:C	2.10	0.54
1:C:538:LEU:HD12	1:C:664:LYS:HD2	1.89	0.54
1:D:243:ASP:OD2	1:D:324:PRO:HG3	2.07	0.54
1:F:136:LYS:O	1:F:139:ASP:HB2	2.07	0.54
1:F:731:ARG:HG2	1:F:756:MET:HE2	1.89	0.54
1:F:757:ILE:HG12	1:F:762:LEU:HD12	1.88	0.54
1:B:136:LYS:O	1:B:139:ASP:HB2	2.07	0.54
1:C:301:MET:HA	1:C:304:ASP:HB3	1.89	0.54
1:E:725:ILE:O	1:E:773:LYS:HB2	2.07	0.54
1:D:368:LYS:O	1:D:376:ALA:HA	2.08	0.54
1:D:757:ILE:HG12	1:D:762:LEU:HD12	1.89	0.54
1:F:710:VAL:O	1:F:714:ILE:HG13	2.06	0.54
1:A:97:GLU:HA	1:A:711:LEU:HD11	1.89	0.54
1:B:349:GLN:O	1:B:353:LEU:HG	2.06	0.54
1:C:97:GLU:HA	1:C:711:LEU:HD11	1.89	0.54
1:C:535:PRO:HB2	1:C:540:LEU:HD21	1.89	0.54
1:D:136:LYS:O	1:D:139:ASP:HB2	2.07	0.54
1:D:508:GLU:HG3	1:D:771:GLN:H	1.71	0.54
1:E:70:LEU:HD13	1:E:74:ASP:HB2	1.90	0.54
1:E:86:VAL:HG23	1:E:103:ASN:ND2	2.22	0.54
1:A:37:VAL:HG11	1:A:59:VAL:HG21	1.90	0.54
1:B:286:THR:OG1	1:B:287:PHE:N	2.40	0.54
1:D:308:GLU:HB2	1:D:313:TYR:CZ	2.42	0.54
1:E:243:ASP:OD2	1:E:324:PRO:HG3	2.08	0.54
1:F:117:SER:HB2	1:F:714:ILE:HD11	1.89	0.54
1:F:391:MET:HE2	1:F:434:LYS:HE3	1.89	0.54
1:B:535:PRO:HB2	1:B:540:LEU:HD21	1.89	0.54
1:B:757:ILE:HG23	1:B:762:LEU:HB2	1.88	0.54
1:C:286:THR:OG1	1:C:287:PHE:N	2.40	0.54
1:C:606:ASN:HB3	1:C:609:VAL:CG1	2.38	0.54
1:D:77:LYS:H	1:D:77:LYS:HZ2	1.54	0.54
1:F:702:LEU:O	1:F:706:ARG:HG3	2.07	0.54
1:A:152:HIS:O	1:A:156:ILE:HD12	2.07	0.54
1:B:70:LEU:HD13	1:B:74:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PHE:O	1:B:458:ALA:HB3	2.08	0.54
1:B:748:ASP:OD1	1:B:748:ASP:C	2.46	0.54
1:C:391:MET:HE2	1:C:434:LYS:CE	2.38	0.54
1:D:89:MET:CE	1:D:100:VAL:HG13	2.37	0.54
1:E:517:PHE:CZ	1:E:716:ILE:HD13	2.43	0.54
1:E:743:PRO:HD2	1:E:747:MET:CG	2.38	0.54
1:F:278:ILE:HD13	1:F:432:LYS:HD3	1.88	0.54
1:F:686:ILE:HG22	1:F:704:GLN:HE22	1.72	0.54
1:B:742:ILE:HD11	1:B:752:ALA:C	2.28	0.54
1:D:79:ASN:HD21	1:D:94:CYS:HB2	1.72	0.54
1:E:499:ILE:HG22	1:E:500:LEU:N	2.22	0.54
1:F:301:MET:HA	1:F:304:ASP:HB3	1.90	0.54
1:A:757:ILE:HG23	1:A:762:LEU:HB2	1.90	0.54
1:C:269:THR:HG23	1:C:443:LEU:HD22	1.90	0.54
1:C:767:TYR:O	1:C:768:ARG:NH1	2.38	0.54
1:D:378:MET:CE	1:D:381:ASN:HA	2.38	0.54
1:E:180:GLY:C	1:E:686:ILE:HD12	2.27	0.54
1:A:594:ALA:HA	1:A:597:TRP:CD1	2.43	0.53
1:A:751:GLN:NE2	1:C:692:ARG:NH2	2.40	0.53
1:D:748:ASP:OD1	1:D:748:ASP:C	2.46	0.53
1:E:540:LEU:HD12	1:E:559:LEU:HD12	1.88	0.53
1:F:85:LYS:HE2	1:F:110:SER:OG	2.07	0.53
1:A:540:LEU:HD12	1:A:559:LEU:HD12	1.90	0.53
1:D:278:ILE:HD13	1:D:432:LYS:HD3	1.89	0.53
1:E:535:PRO:HB2	1:E:540:LEU:CD2	2.39	0.53
1:F:86:VAL:HG23	1:F:103:ASN:ND2	2.23	0.53
1:F:725:ILE:HD11	1:F:730:PHE:CD1	2.42	0.53
1:A:79:ASN:HD21	1:A:94:CYS:HB2	1.71	0.53
1:B:97:GLU:HA	1:B:711:LEU:HD11	1.90	0.53
1:B:743:PRO:HD2	1:B:747:MET:HG2	1.90	0.53
1:C:108:TYR:CD2	1:C:696:LEU:HD12	2.43	0.53
1:C:563:GLN:O	1:C:565:ASN:N	2.41	0.53
1:C:748:ASP:OD1	1:C:748:ASP:C	2.46	0.53
1:D:72:LYS:HA	1:D:75:ILE:CD1	2.38	0.53
1:E:419:THR:N	1:E:422:GLN:HG3	2.20	0.53
1:F:361:GLN:HG2	1:F:386:LYS:HB2	1.90	0.53
1:F:538:LEU:HD12	1:F:664:LYS:HD2	1.90	0.53
1:F:563:GLN:O	1:F:565:ASN:N	2.41	0.53
1:F:748:ASP:OD1	1:F:748:ASP:C	2.47	0.53
1:A:563:GLN:O	1:A:565:ASN:N	2.41	0.53
1:B:70:LEU:HD12	1:B:71:SER:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HG22	1:C:36:TRP:H	1.74	0.53
1:C:70:LEU:HD12	1:C:71:SER:O	2.08	0.53
1:D:173:ILE:C	1:D:174:LEU:HD23	2.28	0.53
1:D:563:GLN:O	1:D:565:ASN:N	2.41	0.53
1:F:97:GLU:HA	1:F:711:LEU:HD11	1.90	0.53
1:F:256:PHE:O	1:F:458:ALA:HB3	2.07	0.53
1:A:77:LYS:H	1:A:77:LYS:NZ	2.06	0.53
1:A:743:PRO:HD2	1:A:747:MET:HG2	1.90	0.53
1:B:37:VAL:HG11	1:B:59:VAL:HG21	1.90	0.53
1:C:86:VAL:HG23	1:C:103:ASN:ND2	2.24	0.53
1:C:349:GLN:O	1:C:353:LEU:HG	2.08	0.53
1:C:419:THR:HG23	1:C:422:GLN:CG	2.39	0.53
1:D:510:ILE:HD12	1:D:768:ARG:HB3	1.89	0.53
1:D:517:PHE:CZ	1:D:716:ILE:HD13	2.43	0.53
1:D:725:ILE:O	1:D:773:LYS:HB2	2.08	0.53
1:E:97:GLU:HA	1:E:711:LEU:HD11	1.90	0.53
1:E:738:ALA:O	1:E:741:ALA:CB	2.57	0.53
1:F:35:VAL:HG22	1:F:36:TRP:H	1.73	0.53
1:F:173:ILE:C	1:F:174:LEU:HD23	2.28	0.53
1:A:72:LYS:HA	1:A:75:ILE:CD1	2.39	0.53
1:E:391:MET:HE2	1:E:434:LYS:HE3	1.89	0.53
1:E:748:ASP:OD1	1:E:748:ASP:O	2.26	0.53
1:F:152:HIS:O	1:F:156:ILE:HD12	2.09	0.53
1:A:180:GLY:C	1:A:686:ILE:HD12	2.28	0.53
1:A:419:THR:N	1:A:422:GLN:HG3	2.21	0.53
1:B:303:ASN:HD22	1:B:304:ASP:N	2.07	0.53
1:C:36:TRP:CE2	1:C:78:MET:HG2	2.44	0.53
1:C:743:PRO:CD	1:C:747:MET:SD	2.97	0.53
1:D:281:ALA:O	1:D:318:ASN:ND2	2.41	0.53
1:D:743:PRO:CD	1:D:747:MET:SD	2.97	0.53
1:E:556:VAL:HG21	1:E:579:THR:CA	2.39	0.53
1:F:376:ALA:O	1:F:403:LEU:HD22	2.09	0.53
1:F:419:THR:N	1:F:422:GLN:HG3	2.23	0.53
1:A:743:PRO:CD	1:A:747:MET:SD	2.97	0.53
1:B:86:VAL:HG23	1:B:103:ASN:ND2	2.24	0.53
1:B:743:PRO:CD	1:B:747:MET:SD	2.97	0.53
1:C:361:GLN:HG2	1:C:386:LYS:HB2	1.91	0.53
1:D:196:VAL:O	1:D:196:VAL:CG1	2.57	0.53
1:F:295:ALA:HB2	1:F:310:PHE:CZ	2.44	0.53
1:F:499:ILE:HG22	1:F:500:LEU:N	2.23	0.53
1:A:243:ASP:OD2	1:A:324:PRO:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ASP:OD1	1:A:748:ASP:C	2.46	0.53
1:B:178:GLU:OE2	1:B:686:ILE:HG21	2.09	0.53
1:C:85:LYS:HE2	1:C:110:SER:OG	2.08	0.53
1:C:180:GLY:C	1:C:686:ILE:HD12	2.30	0.53
1:C:226:GLN:HB2	1:C:342:MET:HE2	1.90	0.53
1:C:288:HIS:HB3	1:C:292:TYR:CE1	2.44	0.53
1:C:303:ASN:HD22	1:C:304:ASP:N	2.07	0.53
1:C:376:ALA:O	1:C:403:LEU:HD22	2.08	0.53
1:C:743:PRO:HD2	1:C:747:MET:HG2	1.90	0.53
1:D:743:PRO:HD2	1:D:747:MET:HG2	1.90	0.53
1:E:152:HIS:O	1:E:156:ILE:HD12	2.09	0.53
1:E:502:GLN:O	1:E:505:TYR:HB2	2.09	0.53
1:E:556:VAL:HG21	1:E:579:THR:HA	1.91	0.53
1:F:725:ILE:O	1:F:773:LYS:HB2	2.09	0.53
1:A:742:ILE:HD11	1:A:752:ALA:C	2.29	0.52
1:D:565:ASN:O	1:D:566:HIS:C	2.48	0.52
1:B:419:THR:H	1:B:422:GLN:NE2	2.06	0.52
1:B:563:GLN:O	1:B:565:ASN:N	2.41	0.52
1:B:702:LEU:O	1:B:706:ARG:HG3	2.10	0.52
1:B:738:ALA:CB	1:B:741:ALA:HB2	2.39	0.52
1:F:742:ILE:HD11	1:F:752:ALA:C	2.29	0.52
1:A:303:ASN:HD22	1:A:304:ASP:N	2.07	0.52
1:A:391:MET:HE2	1:A:434:LYS:HE3	1.91	0.52
1:A:419:THR:HG23	1:A:422:GLN:CG	2.39	0.52
1:D:738:ALA:CB	1:D:741:ALA:HB2	2.39	0.52
1:F:108:TYR:CD2	1:F:696:LEU:HD12	2.44	0.52
1:F:238:LYS:NZ	1:F:283:ASP:O	2.42	0.52
1:F:743:PRO:HD2	1:F:747:MET:CG	2.40	0.52
1:A:161:TYR:O	1:A:164:MET:HB3	2.09	0.52
1:A:499:ILE:HG22	1:A:500:LEU:N	2.25	0.52
1:B:85:LYS:HE2	1:B:110:SER:OG	2.10	0.52
1:B:180:GLY:C	1:B:686:ILE:HD12	2.29	0.52
1:C:243:ASP:OD2	1:C:324:PRO:HG3	2.09	0.52
1:F:288:HIS:HB3	1:F:292:TYR:CE1	2.44	0.52
1:B:565:ASN:O	1:B:566:HIS:C	2.48	0.52
1:D:540:LEU:HD21	1:D:562:GLU:HG3	1.92	0.52
1:F:161:TYR:O	1:F:164:MET:HB3	2.09	0.52
1:A:376:ALA:O	1:A:403:LEU:HD22	2.10	0.52
1:B:746:PHE:HD1	1:C:389:HIS:CD2	2.28	0.52
1:C:565:ASN:O	1:C:566:HIS:C	2.48	0.52
1:D:70:LEU:HD12	1:D:71:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:MET:CE	1:E:381:ASN:HA	2.39	0.52
1:F:517:PHE:CZ	1:F:716:ILE:HD13	2.44	0.52
1:A:327:GLN:O	1:A:330:GLU:HB2	2.10	0.52
1:A:725:ILE:O	1:A:773:LYS:HB2	2.10	0.52
1:C:158:ASP:O	1:C:162:ARG:HG2	2.10	0.52
1:C:256:PHE:O	1:C:458:ALA:HB3	2.09	0.52
1:D:85:LYS:HE2	1:D:110:SER:OG	2.10	0.52
1:A:565:ASN:O	1:A:566:HIS:C	2.48	0.52
1:B:230:ILE:HD11	1:B:342:MET:HB2	1.92	0.52
1:C:690:GLU:HG2	1:C:692:ARG:NH2	2.25	0.52
1:D:540:LEU:HD12	1:D:559:LEU:HD12	1.92	0.52
1:D:594:ALA:HA	1:D:597:TRP:CD1	2.45	0.52
1:F:70:LEU:HD13	1:F:74:ASP:HB2	1.90	0.52
1:A:158:ASP:O	1:A:162:ARG:HG2	2.10	0.52
1:A:508:GLU:HG3	1:A:508:GLU:O	2.10	0.52
1:A:535:PRO:HB2	1:A:540:LEU:HD21	1.90	0.52
1:B:510:ILE:HD12	1:B:768:ARG:HB3	1.90	0.52
1:B:556:VAL:HG21	1:B:579:THR:CA	2.40	0.52
1:C:743:PRO:HD2	1:C:747:MET:CG	2.40	0.52
1:E:540:LEU:HD21	1:E:562:GLU:HG3	1.92	0.52
1:B:318:ASN:O	1:B:319:GLY:C	2.49	0.52
1:C:487:GLU:HG3	1:C:521:LEU:HD13	1.92	0.52
1:C:499:ILE:HG22	1:C:500:LEU:N	2.24	0.52
1:D:43:GLY:H	1:D:698:ALA:CB	2.21	0.52
1:D:535:PRO:HB2	1:D:540:LEU:CD2	2.39	0.52
1:D:686:ILE:HG22	1:D:704:GLN:HE22	1.73	0.52
1:D:702:LEU:O	1:D:706:ARG:HG3	2.10	0.52
1:E:161:TYR:O	1:E:164:MET:HB3	2.09	0.52
1:F:743:PRO:HD2	1:F:747:MET:HG2	1.92	0.52
1:A:510:ILE:HD12	1:A:768:ARG:HB3	1.92	0.51
1:B:243:ASP:OD2	1:B:324:PRO:HG3	2.11	0.51
1:C:742:ILE:HD11	1:C:752:ALA:C	2.30	0.51
1:A:117:SER:HB2	1:A:714:ILE:HD11	1.92	0.51
1:A:173:ILE:C	1:A:174:LEU:HD23	2.31	0.51
1:B:77:LYS:H	1:B:77:LYS:NZ	2.08	0.51
1:B:690:GLU:HG2	1:B:692:ARG:NH2	2.26	0.51
1:D:742:ILE:HD11	1:D:752:ALA:C	2.30	0.51
1:D:743:PRO:HD2	1:D:747:MET:CG	2.40	0.51
1:F:378:MET:HG3	1:F:378:MET:O	2.10	0.51
1:F:535:PRO:HB2	1:F:540:LEU:CD2	2.40	0.51
1:A:690:GLU:HG2	1:A:692:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:THR:HG23	1:B:422:GLN:CG	2.40	0.51
1:D:303:ASN:HD22	1:D:304:ASP:N	2.07	0.51
1:B:161:TYR:O	1:B:164:MET:HB3	2.10	0.51
1:C:556:VAL:HG21	1:C:579:THR:CA	2.41	0.51
1:D:586:TYR:CG	1:D:587:ALA:N	2.78	0.51
1:E:301:MET:HA	1:E:304:ASP:HB3	1.93	0.51
1:B:43:GLY:H	1:B:698:ALA:CB	2.22	0.51
1:B:327:GLN:O	1:B:330:GLU:N	2.44	0.51
1:B:499:ILE:HG22	1:B:500:LEU:N	2.24	0.51
1:C:77:LYS:H	1:C:77:LYS:NZ	2.09	0.51
1:D:70:LEU:HD13	1:D:74:ASP:HB2	1.92	0.51
1:D:286:THR:OG1	1:D:287:PHE:N	2.44	0.51
1:E:419:THR:H	1:E:422:GLN:NE2	2.07	0.51
1:E:586:TYR:CG	1:E:587:ALA:N	2.78	0.51
1:A:301:MET:HA	1:A:304:ASP:HB3	1.91	0.51
1:C:327:GLN:O	1:C:330:GLU:N	2.44	0.51
1:D:37:VAL:HG11	1:D:59:VAL:HG21	1.92	0.51
1:D:161:TYR:O	1:D:164:MET:HB3	2.10	0.51
1:D:238:LYS:NZ	1:D:283:ASP:O	2.44	0.51
1:E:690:GLU:HG2	1:E:692:ARG:NH2	2.26	0.51
1:F:234:PHE:CE2	1:F:289:ILE:HG12	2.45	0.51
1:B:152:HIS:O	1:B:156:ILE:HD12	2.10	0.51
1:B:578:LYS:C	1:B:579:THR:HG23	2.31	0.51
1:B:743:PRO:HD2	1:B:747:MET:CG	2.40	0.51
1:C:527:LEU:HD22	1:C:566:HIS:CD2	2.46	0.51
1:D:36:TRP:CE2	1:D:78:MET:HG2	2.45	0.51
1:D:108:TYR:CD2	1:D:696:LEU:HD12	2.45	0.51
1:D:318:ASN:O	1:D:319:GLY:C	2.49	0.51
1:D:499:ILE:HG22	1:D:500:LEU:N	2.25	0.51
1:F:36:TRP:CE2	1:F:78:MET:HG2	2.46	0.51
1:F:158:ASP:O	1:F:162:ARG:HG2	2.11	0.51
1:F:766:LEU:HA	1:F:777:ARG:HG3	1.93	0.51
1:A:743:PRO:HD2	1:A:747:MET:CG	2.40	0.51
1:C:388:CYS:SG	1:C:393:ILE:HG22	2.51	0.51
1:C:757:ILE:HG23	1:C:762:LEU:HB2	1.92	0.51
1:D:757:ILE:HG23	1:D:762:LEU:HB2	1.92	0.51
1:F:39:SER:HG	1:F:42:HIS:H	1.59	0.51
1:B:35:VAL:HG22	1:B:36:TRP:H	1.76	0.51
1:B:95:LEU:CD1	1:B:714:ILE:HG21	2.40	0.51
1:C:37:VAL:HG11	1:C:59:VAL:HG21	1.93	0.51
1:C:70:LEU:HD13	1:C:74:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:GLY:C	1:D:686:ILE:HD12	2.31	0.51
1:D:327:GLN:O	1:D:330:GLU:N	2.43	0.51
1:E:35:VAL:HG12	1:E:47:ALA:O	2.11	0.51
1:E:37:VAL:HG11	1:E:59:VAL:HG21	1.92	0.51
1:E:72:LYS:HA	1:E:75:ILE:CD1	2.40	0.51
1:E:269:THR:HG23	1:E:443:LEU:HD22	1.92	0.51
1:E:286:THR:OG1	1:E:287:PHE:N	2.43	0.51
1:A:36:TRP:CE2	1:A:78:MET:HG2	2.45	0.51
1:C:318:ASN:O	1:C:319:GLY:C	2.49	0.51
1:D:376:ALA:O	1:D:403:LEU:HD22	2.11	0.51
1:E:578:LYS:C	1:E:579:THR:HG23	2.31	0.51
1:E:743:PRO:CD	1:E:747:MET:SD	2.99	0.51
1:F:158:ASP:O	1:F:161:TYR:HB3	2.11	0.51
1:A:556:VAL:HG21	1:A:579:THR:HA	1.93	0.50
1:A:766:LEU:HA	1:A:777:ARG:HG3	1.92	0.50
1:B:527:LEU:HD22	1:B:566:HIS:CD2	2.46	0.50
1:C:327:GLN:O	1:C:330:GLU:HB2	2.10	0.50
1:D:578:LYS:C	1:D:579:THR:HG23	2.31	0.50
1:E:85:LYS:HE2	1:E:110:SER:OG	2.10	0.50
1:F:419:THR:H	1:F:422:GLN:NE2	2.08	0.50
1:F:490:GLN:O	1:F:493:PHE:HB3	2.11	0.50
1:A:556:VAL:HG21	1:A:579:THR:CA	2.41	0.50
1:C:117:SER:HB2	1:C:714:ILE:HD11	1.93	0.50
1:C:173:ILE:C	1:C:174:LEU:HD23	2.32	0.50
1:E:77:LYS:H	1:E:77:LYS:HZ2	1.58	0.50
1:E:281:ALA:O	1:E:318:ASN:ND2	2.45	0.50
1:E:303:ASN:HD22	1:E:304:ASP:N	2.09	0.50
1:E:710:VAL:O	1:E:714:ILE:HG13	2.11	0.50
1:A:460:PHE:CD1	1:A:460:PHE:C	2.85	0.50
1:C:378:MET:HG3	1:C:378:MET:O	2.12	0.50
1:C:517:PHE:CZ	1:C:716:ILE:HD13	2.46	0.50
1:D:77:LYS:H	1:D:77:LYS:NZ	2.10	0.50
1:D:327:GLN:O	1:D:330:GLU:HB2	2.11	0.50
1:F:243:ASP:OD2	1:F:324:PRO:HG3	2.12	0.50
1:A:527:LEU:HD22	1:A:566:HIS:CD2	2.46	0.50
1:B:72:LYS:HA	1:B:75:ILE:CD1	2.41	0.50
1:B:434:LYS:HG2	1:B:625:TRP:HZ2	1.76	0.50
1:B:725:ILE:O	1:B:773:LYS:HB2	2.11	0.50
1:C:378:MET:CE	1:C:381:ASN:HA	2.41	0.50
1:D:60:GLU:HA	1:D:67:LYS:HA	1.93	0.50
1:F:487:GLU:HG3	1:F:521:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD11	1:A:342:MET:HB2	1.93	0.50
1:A:318:ASN:O	1:A:319:GLY:C	2.49	0.50
1:B:269:THR:HG23	1:B:443:LEU:HD22	1.94	0.50
1:B:586:TYR:CG	1:B:587:ALA:N	2.80	0.50
1:D:35:VAL:HG12	1:D:47:ALA:O	2.11	0.50
1:E:117:SER:HB2	1:E:714:ILE:HD11	1.92	0.50
1:E:510:ILE:HD12	1:E:768:ARG:HB3	1.92	0.50
1:F:72:LYS:HA	1:F:75:ILE:CD1	2.42	0.50
1:B:766:LEU:HA	1:B:777:ARG:HG3	1.93	0.50
1:D:165:LEU:HD21	1:D:260:GLY:HA2	1.94	0.50
1:E:742:ILE:HD11	1:E:752:ALA:C	2.31	0.50
1:F:37:VAL:HG11	1:F:59:VAL:HG21	1.92	0.50
1:A:165:LEU:HD21	1:A:260:GLY:HA2	1.94	0.50
1:A:178:GLU:OE2	1:A:686:ILE:HG21	2.11	0.50
1:B:556:VAL:HG21	1:B:579:THR:HA	1.92	0.50
1:B:611:SER:O	1:B:614:ASN:HB3	2.10	0.50
1:C:43:GLY:H	1:C:698:ALA:CB	2.22	0.50
1:C:438:LEU:O	1:C:442:ILE:HG13	2.12	0.50
1:C:738:ALA:CB	1:C:741:ALA:HB2	2.39	0.50
1:E:388:CYS:SG	1:E:393:ILE:HG22	2.52	0.50
1:E:748:ASP:OD1	1:E:748:ASP:C	2.50	0.50
1:F:556:VAL:HG21	1:F:579:THR:CA	2.41	0.50
1:A:60:GLU:HA	1:A:67:LYS:HA	1.94	0.50
1:A:355:VAL:O	1:A:359:VAL:HG23	2.12	0.50
1:B:158:ASP:O	1:B:161:TYR:HB3	2.12	0.50
1:B:238:LYS:NZ	1:B:283:ASP:O	2.44	0.50
1:B:754:ILE:HD13	1:F:692:ARG:NH2	2.27	0.50
1:C:434:LYS:HG2	1:C:625:TRP:HZ2	1.77	0.50
1:D:690:GLU:HG2	1:D:692:ARG:NH2	2.27	0.50
1:E:230:ILE:HD11	1:E:342:MET:HB2	1.94	0.50
1:F:688:ASN:ND2	1:F:692:ARG:O	2.33	0.50
1:A:526:GLU:HA	1:A:526:GLU:OE1	2.12	0.50
1:B:173:ILE:C	1:B:174:LEU:HD23	2.32	0.50
1:D:36:TRP:NE1	1:D:78:MET:HG2	2.27	0.50
1:E:256:PHE:O	1:E:458:ALA:HB3	2.12	0.50
1:E:337:GLU:O	1:E:341:ILE:HG13	2.12	0.50
1:F:43:GLY:H	1:F:698:ALA:CB	2.21	0.50
1:F:77:LYS:H	1:F:77:LYS:NZ	2.09	0.50
1:A:278:ILE:HD12	1:A:428:GLU:HG2	1.93	0.49
1:B:117:SER:HB2	1:B:714:ILE:HD11	1.92	0.49
1:C:36:TRP:NE1	1:C:78:MET:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ALA:O	1:C:318:ASN:ND2	2.45	0.49
1:C:510:ILE:HD12	1:C:768:ARG:HB3	1.94	0.49
1:C:611:SER:O	1:C:614:ASN:HB3	2.12	0.49
1:D:659:VAL:HA	1:D:662:LEU:HD12	1.95	0.49
1:E:108:TYR:CD2	1:E:696:LEU:HD12	2.47	0.49
1:E:738:ALA:CB	1:E:741:ALA:HB2	2.39	0.49
1:E:754:ILE:HG22	1:E:755:LEU:HD23	1.94	0.49
1:F:60:GLU:HA	1:F:67:LYS:HA	1.94	0.49
1:F:556:VAL:HG21	1:F:579:THR:HA	1.94	0.49
1:A:490:GLN:O	1:A:493:PHE:HB3	2.12	0.49
1:B:498:PHE:CE2	1:B:519:LEU:HD13	2.48	0.49
1:E:165:LEU:HD21	1:E:260:GLY:HA2	1.93	0.49
1:F:303:ASN:HD22	1:F:304:ASP:N	2.09	0.49
1:F:566:HIS:CD2	1:F:568:LYS:H	2.30	0.49
1:A:586:TYR:CG	1:A:587:ALA:N	2.80	0.49
1:B:36:TRP:CE2	1:B:78:MET:HG2	2.47	0.49
1:B:158:ASP:O	1:B:162:ARG:HG2	2.11	0.49
1:B:538:LEU:CD1	1:B:664:LYS:HD2	2.42	0.49
1:C:238:LYS:NZ	1:C:283:ASP:O	2.44	0.49
1:D:230:ILE:HD11	1:D:342:MET:HB2	1.94	0.49
1:F:578:LYS:C	1:F:579:THR:HG23	2.33	0.49
1:A:327:GLN:O	1:A:330:GLU:N	2.45	0.49
1:A:738:ALA:CB	1:A:741:ALA:HB2	2.39	0.49
1:B:35:VAL:HG12	1:B:47:ALA:O	2.12	0.49
1:B:535:PRO:HB2	1:B:540:LEU:CD2	2.43	0.49
1:C:538:LEU:CD1	1:C:664:LYS:HD2	2.43	0.49
1:D:487:GLU:HG3	1:D:521:LEU:HD13	1.93	0.49
1:E:36:TRP:CE2	1:E:78:MET:HG2	2.47	0.49
1:E:419:THR:HG23	1:E:422:GLN:CG	2.43	0.49
1:F:89:MET:HE1	1:F:100:VAL:HG13	1.94	0.49
1:F:565:ASN:O	1:F:566:HIS:C	2.50	0.49
1:B:391:MET:HE2	1:B:434:LYS:CE	2.43	0.49
1:C:161:TYR:O	1:C:164:MET:HB3	2.11	0.49
1:D:117:SER:HB2	1:D:714:ILE:HD11	1.94	0.49
1:D:556:VAL:HG21	1:D:579:THR:CA	2.41	0.49
1:D:606:ASN:HB3	1:D:609:VAL:HG13	1.94	0.49
1:F:290:PHE:CE1	1:F:356:VAL:HG13	2.47	0.49
1:F:586:TYR:CG	1:F:587:ALA:N	2.80	0.49
1:A:35:VAL:HG22	1:A:36:TRP:H	1.76	0.49
1:B:526:GLU:OE1	1:B:526:GLU:HA	2.12	0.49
1:B:767:TYR:O	1:B:768:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:HB1	1:C:301:MET:HG2	1.94	0.49
1:C:725:ILE:O	1:C:773:LYS:HB2	2.12	0.49
1:D:337:GLU:O	1:D:341:ILE:HG13	2.13	0.49
1:D:566:HIS:CD2	1:D:568:LYS:H	2.31	0.49
1:E:60:GLU:HA	1:E:67:LYS:HA	1.93	0.49
1:E:173:ILE:C	1:E:174:LEU:HD23	2.33	0.49
1:F:226:GLN:HB2	1:F:342:MET:HE2	1.95	0.49
1:F:240:VAL:HG23	1:F:241:LYS:HG2	1.95	0.49
1:A:434:LYS:HG2	1:A:625:TRP:HZ2	1.78	0.49
1:A:578:LYS:C	1:A:579:THR:HG23	2.32	0.49
1:A:697:ASP:HB3	1:A:700:LEU:HB3	1.94	0.49
1:C:165:LEU:HD21	1:C:260:GLY:HA2	1.94	0.49
1:C:578:LYS:C	1:C:579:THR:HG23	2.32	0.49
1:D:271:LEU:HG	1:D:271:LEU:O	2.12	0.49
1:D:295:ALA:HB2	1:D:310:PHE:CZ	2.48	0.49
1:D:434:LYS:HG2	1:D:625:TRP:HZ2	1.78	0.49
1:D:611:SER:O	1:D:614:ASN:HB3	2.13	0.49
1:E:763:ASP:HB3	1:E:766:LEU:HG	1.95	0.49
1:F:508:GLU:HG3	1:F:508:GLU:O	2.12	0.49
1:A:226:GLN:HB2	1:A:342:MET:HE2	1.95	0.49
1:A:297:ALA:HB1	1:A:301:MET:HG2	1.95	0.49
1:B:337:GLU:O	1:B:341:ILE:HG13	2.12	0.49
1:B:393:ILE:HG13	1:B:612:LEU:HB3	1.94	0.49
1:C:508:GLU:HG3	1:C:508:GLU:O	2.13	0.49
1:D:419:THR:H	1:D:422:GLN:NE2	2.06	0.49
1:E:39:SER:HG	1:E:42:HIS:H	1.60	0.49
1:E:688:ASN:ND2	1:E:692:ARG:O	2.34	0.49
1:E:727:PHE:HA	1:E:753:CYS:SG	2.53	0.49
1:F:278:ILE:HD12	1:F:428:GLU:HG2	1.93	0.49
1:A:566:HIS:CD2	1:A:568:LYS:H	2.31	0.49
1:B:281:ALA:O	1:B:318:ASN:ND2	2.46	0.49
1:B:478:GLU:OE2	1:B:600:LYS:HE2	2.13	0.49
1:D:89:MET:HE1	1:D:100:VAL:HG13	1.94	0.49
1:D:113:ILE:O	1:D:123:VAL:HA	2.12	0.49
1:D:419:THR:HG23	1:D:422:GLN:CG	2.43	0.49
1:E:565:ASN:O	1:E:566:HIS:C	2.50	0.49
1:F:95:LEU:HD11	1:F:714:ILE:HG21	1.93	0.49
1:F:327:GLN:O	1:F:330:GLU:HB2	2.13	0.49
1:C:158:ASP:O	1:C:161:TYR:HB3	2.12	0.49
1:C:178:GLU:OE2	1:C:686:ILE:HG21	2.12	0.49
1:C:271:LEU:HG	1:C:271:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:TRP:NE1	1:E:78:MET:HG2	2.28	0.49
1:E:434:LYS:HG2	1:E:625:TRP:HZ2	1.78	0.49
1:E:606:ASN:HB3	1:E:609:VAL:HG13	1.94	0.49
1:F:180:GLY:C	1:F:686:ILE:HD12	2.32	0.49
1:F:393:ILE:HD11	1:F:613:LEU:HA	1.95	0.49
1:A:35:VAL:HG12	1:A:47:ALA:O	2.13	0.48
1:A:337:GLU:O	1:A:341:ILE:HG13	2.13	0.48
1:A:419:THR:H	1:A:422:GLN:NE2	2.05	0.48
1:E:290:PHE:CE1	1:E:356:VAL:HG13	2.48	0.48
1:E:327:GLN:O	1:E:330:GLU:HB2	2.13	0.48
1:F:35:VAL:HG22	1:F:76:GLN:O	2.13	0.48
1:F:165:LEU:HD21	1:F:260:GLY:HA2	1.94	0.48
1:F:286:THR:OG1	1:F:287:PHE:N	2.45	0.48
1:A:80:PRO:HB2	1:A:82:LYS:HG2	1.96	0.48
1:A:196:VAL:O	1:A:196:VAL:CG1	2.60	0.48
1:A:295:ALA:HB2	1:A:310:PHE:CZ	2.47	0.48
1:A:606:ASN:HB3	1:A:609:VAL:HG13	1.94	0.48
1:B:196:VAL:O	1:B:196:VAL:CG1	2.61	0.48
1:B:219:GLU:O	1:B:220:LEU:C	2.52	0.48
1:B:508:GLU:HG3	1:B:508:GLU:O	2.14	0.48
1:B:606:ASN:HB3	1:B:609:VAL:HG13	1.94	0.48
1:C:60:GLU:HA	1:C:67:LYS:HA	1.94	0.48
1:C:196:VAL:O	1:C:196:VAL:CG1	2.60	0.48
1:C:278:ILE:HB	1:C:315:PHE:CE1	2.48	0.48
1:C:295:ALA:HB2	1:C:310:PHE:CZ	2.47	0.48
1:D:556:VAL:HG21	1:D:579:THR:HA	1.94	0.48
1:F:460:PHE:CD1	1:F:460:PHE:C	2.86	0.48
1:C:556:VAL:HG21	1:C:579:THR:HA	1.93	0.48
1:E:318:ASN:O	1:E:319:GLY:C	2.51	0.48
1:F:606:ASN:HB3	1:F:609:VAL:HG13	1.94	0.48
1:A:686:ILE:HG22	1:A:704:GLN:HE22	1.77	0.48
1:B:60:GLU:HA	1:B:67:LYS:HA	1.94	0.48
1:C:219:GLU:O	1:C:222:LYS:N	2.46	0.48
1:C:419:THR:H	1:C:422:GLN:NE2	2.07	0.48
1:C:478:GLU:OE2	1:C:600:LYS:HE2	2.14	0.48
1:D:158:ASP:O	1:D:162:ARG:HG2	2.14	0.48
1:E:43:GLY:H	1:E:698:ALA:CB	2.20	0.48
1:E:158:ASP:O	1:E:161:TYR:HB3	2.13	0.48
1:E:540:LEU:HD11	1:E:562:GLU:HB2	1.95	0.48
1:F:337:GLU:O	1:F:341:ILE:HG13	2.13	0.48
1:F:611:SER:O	1:F:614:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:NZ	1:A:283:ASP:O	2.46	0.48
1:B:355:VAL:O	1:B:359:VAL:HG23	2.14	0.48
1:C:95:LEU:HD11	1:C:714:ILE:HG21	1.96	0.48
1:C:766:LEU:HA	1:C:777:ARG:HG3	1.95	0.48
1:D:490:GLN:O	1:D:493:PHE:HB3	2.14	0.48
1:E:526:GLU:OE1	1:E:526:GLU:HA	2.13	0.48
1:F:95:LEU:CD1	1:F:714:ILE:HG21	2.44	0.48
1:F:510:ILE:HD12	1:F:768:ARG:HB3	1.94	0.48
1:F:754:ILE:HG22	1:F:755:LEU:HD23	1.94	0.48
1:A:271:LEU:HG	1:A:271:LEU:O	2.13	0.48
1:A:290:PHE:CE1	1:A:356:VAL:HG13	2.49	0.48
1:B:295:ALA:HB2	1:B:310:PHE:CZ	2.48	0.48
1:B:754:ILE:HG22	1:B:755:LEU:HD23	1.96	0.48
1:C:526:GLU:OE1	1:C:526:GLU:HA	2.14	0.48
1:C:586:TYR:CG	1:C:587:ALA:N	2.82	0.48
1:E:478:GLU:OE2	1:E:600:LYS:HE2	2.14	0.48
1:E:766:LEU:HA	1:E:777:ARG:HG3	1.95	0.48
1:F:178:GLU:OE2	1:F:686:ILE:HG21	2.13	0.48
1:A:487:GLU:HG3	1:A:521:LEU:HD13	1.95	0.48
1:A:535:PRO:HB2	1:A:540:LEU:CD2	2.43	0.48
1:C:107:ARG:NH1	1:C:114:TYR:O	2.46	0.48
1:D:219:GLU:O	1:D:220:LEU:C	2.52	0.48
1:E:731:ARG:HG2	1:E:756:MET:CE	2.44	0.48
1:A:85:LYS:HE2	1:A:110:SER:OG	2.13	0.48
1:C:498:PHE:CE2	1:C:519:LEU:HD13	2.49	0.48
1:F:36:TRP:NE1	1:F:78:MET:HG2	2.28	0.48
1:F:540:LEU:HD11	1:F:562:GLU:HB2	1.96	0.48
1:F:697:ASP:HB3	1:F:700:LEU:HB3	1.96	0.48
1:F:763:ASP:HB3	1:F:766:LEU:HG	1.96	0.48
1:A:77:LYS:HZ2	1:A:77:LYS:N	2.11	0.48
1:C:566:HIS:CD2	1:C:568:LYS:H	2.31	0.48
1:D:508:GLU:HG3	1:D:508:GLU:O	2.13	0.48
1:D:697:ASP:HB3	1:D:700:LEU:HB3	1.96	0.48
1:D:766:LEU:HA	1:D:777:ARG:HG3	1.95	0.48
1:E:487:GLU:HG3	1:E:521:LEU:HD13	1.96	0.48
1:F:742:ILE:HG12	1:F:752:ALA:HB1	1.96	0.48
1:A:517:PHE:CZ	1:A:716:ILE:HD13	2.47	0.48
1:A:538:LEU:CD1	1:A:664:LYS:HD2	2.43	0.48
1:B:35:VAL:HG21	1:B:75:ILE:HG22	1.96	0.48
1:B:226:GLN:HB2	1:B:342:MET:HE2	1.96	0.48
1:B:566:HIS:CD2	1:B:568:LYS:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LYS:H	1:E:77:LYS:NZ	2.11	0.48
1:F:158:ASP:HB2	1:F:193:TYR:CZ	2.49	0.48
1:F:196:VAL:O	1:F:196:VAL:CG1	2.62	0.48
1:F:378:MET:CE	1:F:381:ASN:HA	2.43	0.48
1:A:36:TRP:NE1	1:A:78:MET:HG2	2.29	0.47
1:A:611:SER:O	1:A:614:ASN:HB3	2.14	0.47
1:B:165:LEU:HD21	1:B:260:GLY:HA2	1.95	0.47
1:C:228:ASN:HB2	1:C:229:PRO:HD3	1.96	0.47
1:C:460:PHE:CD1	1:C:460:PHE:C	2.86	0.47
1:C:535:PRO:HB2	1:C:540:LEU:CD2	2.43	0.47
1:D:228:ASN:HB2	1:D:229:PRO:HD3	1.96	0.47
1:D:502:GLN:O	1:D:505:TYR:HB2	2.14	0.47
1:E:327:GLN:O	1:E:330:GLU:N	2.47	0.47
1:E:611:SER:O	1:E:614:ASN:HB3	2.13	0.47
1:A:393:ILE:HG13	1:A:612:LEU:HB3	1.96	0.47
1:A:545:CYS:SG	1:A:598:LEU:HD23	2.53	0.47
1:C:490:GLN:O	1:C:493:PHE:HB3	2.14	0.47
1:F:434:LYS:HG2	1:F:625:TRP:HZ2	1.78	0.47
1:B:378:MET:CE	1:B:381:ASN:HA	2.42	0.47
1:C:89:MET:HE1	1:C:100:VAL:HG13	1.95	0.47
1:D:763:ASP:HB3	1:D:766:LEU:HG	1.96	0.47
1:F:753:CYS:HA	1:F:756:MET:HE3	1.95	0.47
1:A:219:GLU:O	1:A:220:LEU:C	2.53	0.47
1:B:686:ILE:HG22	1:B:704:GLN:HE22	1.78	0.47
1:C:393:ILE:HG13	1:C:612:LEU:HB3	1.95	0.47
1:C:754:ILE:HG22	1:C:755:LEU:HD23	1.97	0.47
1:E:268:GLU:HG2	1:E:270:TYR:OH	2.14	0.47
1:E:538:LEU:CD1	1:E:664:LYS:HD2	2.44	0.47
1:A:158:ASP:HB2	1:A:193:TYR:CZ	2.49	0.47
1:A:540:LEU:HD11	1:A:562:GLU:HB2	1.96	0.47
1:B:35:VAL:HG22	1:B:76:GLN:O	2.14	0.47
1:B:659:VAL:HA	1:B:662:LEU:HD12	1.97	0.47
1:D:727:PHE:HA	1:D:753:CYS:SG	2.55	0.47
1:F:269:THR:HG23	1:F:443:LEU:HD22	1.95	0.47
1:A:158:ASP:O	1:A:161:TYR:HB3	2.14	0.47
1:B:271:LEU:O	1:B:271:LEU:HG	2.14	0.47
1:B:278:ILE:HB	1:B:315:PHE:CE1	2.50	0.47
1:B:666:GLN:HA	1:B:669:LYS:HD3	1.96	0.47
1:B:697:ASP:HB3	1:B:700:LEU:HB3	1.96	0.47
1:C:419:THR:N	1:C:422:GLN:HG3	2.21	0.47
1:D:278:ILE:HB	1:D:315:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:VAL:HG21	1:F:75:ILE:HG22	1.97	0.47
1:F:219:GLU:O	1:F:220:LEU:C	2.53	0.47
1:F:339:MET:CE	1:F:352:ILE:HD13	2.45	0.47
1:A:731:ARG:HG2	1:A:756:MET:CE	2.44	0.47
1:A:754:ILE:HG22	1:A:755:LEU:HD23	1.96	0.47
1:A:767:TYR:O	1:A:768:ARG:HG2	2.15	0.47
1:B:419:THR:H	1:B:422:GLN:CG	2.22	0.47
1:B:487:GLU:HG3	1:B:521:LEU:HD13	1.95	0.47
1:B:742:ILE:HG22	1:B:743:PRO:O	2.15	0.47
1:C:219:GLU:O	1:C:220:LEU:C	2.51	0.47
1:C:337:GLU:O	1:C:341:ILE:HG13	2.15	0.47
1:C:551:THR:CB	1:C:553:THR:HG22	2.45	0.47
1:C:763:ASP:HB3	1:C:766:LEU:HG	1.96	0.47
1:D:35:VAL:HG22	1:D:36:TRP:H	1.80	0.47
1:D:460:PHE:CD1	1:D:460:PHE:C	2.88	0.47
1:E:113:ILE:O	1:E:123:VAL:HA	2.15	0.47
1:E:238:LYS:NZ	1:E:283:ASP:O	2.47	0.47
1:E:278:ILE:HB	1:E:315:PHE:CE1	2.49	0.47
1:E:490:GLN:O	1:E:493:PHE:HB3	2.15	0.47
1:F:116:TYR:CZ	1:F:146:ARG:HG2	2.50	0.47
1:F:164:MET:SD	1:F:459:SER:HB2	2.55	0.47
1:F:230:ILE:HD11	1:F:342:MET:HB2	1.97	0.47
1:F:402:ILE:HG22	1:F:403:LEU:N	2.30	0.47
1:A:734:TYR:OH	1:A:781:LEU:HD22	2.15	0.47
1:B:240:VAL:HG23	1:B:241:LYS:HG2	1.97	0.47
1:B:327:GLN:HB2	1:B:330:GLU:CD	2.35	0.47
1:B:731:ARG:HG2	1:B:756:MET:CE	2.43	0.47
1:D:297:ALA:HB1	1:D:301:MET:HG2	1.96	0.47
1:D:393:ILE:HG13	1:D:612:LEU:HB3	1.97	0.47
1:F:251:PHE:CZ	1:F:462:GLY:HA3	2.50	0.47
1:F:271:LEU:HG	1:F:271:LEU:O	2.15	0.47
1:F:419:THR:HG23	1:F:422:GLN:CG	2.44	0.47
1:A:89:MET:HE1	1:A:100:VAL:HG13	1.97	0.47
1:A:607:ASP:CA	1:A:610:THR:HB	2.45	0.47
1:A:666:GLN:HA	1:A:669:LYS:HD3	1.96	0.47
1:B:734:TYR:OH	1:B:781:LEU:HD22	2.14	0.47
1:E:43:GLY:HA3	1:E:702:LEU:CD1	2.45	0.47
1:E:158:ASP:O	1:E:162:ARG:HG2	2.14	0.47
1:E:228:ASN:HB2	1:E:229:PRO:HD3	1.97	0.47
1:E:271:LEU:HG	1:E:271:LEU:O	2.14	0.47
1:E:566:HIS:CD2	1:E:568:LYS:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:GLY:HA3	1:F:702:LEU:CD1	2.45	0.47
1:A:107:ARG:NH1	1:A:114:TYR:O	2.48	0.47
1:A:278:ILE:HB	1:A:315:PHE:CE1	2.49	0.47
1:A:742:ILE:HG22	1:A:743:PRO:O	2.15	0.47
1:B:460:PHE:CD1	1:B:460:PHE:C	2.88	0.47
1:C:61:LEU:HG	1:C:66:LYS:O	2.15	0.47
1:C:711:LEU:O	1:C:715:ARG:HG2	2.15	0.47
1:D:339:MET:CE	1:D:352:ILE:HD13	2.45	0.47
1:E:297:ALA:HB1	1:E:301:MET:HG2	1.97	0.47
1:E:419:THR:H	1:E:422:GLN:CG	2.24	0.47
1:E:502:GLN:HA	1:E:505:TYR:CD2	2.50	0.47
1:E:658:THR:O	1:E:662:LEU:HD12	2.15	0.47
1:F:253:ARG:HG3	1:F:460:PHE:CD1	2.50	0.47
1:F:281:ALA:O	1:F:318:ASN:ND2	2.48	0.47
1:C:540:LEU:HD11	1:C:562:GLU:HB2	1.97	0.46
1:D:538:LEU:HD12	1:D:664:LYS:HD2	1.96	0.46
1:D:742:ILE:HG22	1:D:743:PRO:O	2.15	0.46
1:E:219:GLU:O	1:E:220:LEU:C	2.52	0.46
1:E:666:GLN:HA	1:E:669:LYS:HD3	1.96	0.46
1:E:686:ILE:HG22	1:E:704:GLN:HE22	1.80	0.46
1:F:527:LEU:HD22	1:F:566:HIS:CD2	2.49	0.46
1:F:731:ARG:O	1:F:735:GLU:HB2	2.15	0.46
1:A:57:VAL:HG12	1:A:59:VAL:HG13	1.98	0.46
1:A:236:ASN:ND2	1:A:244:ASN:O	2.49	0.46
1:A:286:THR:OG1	1:A:287:PHE:N	2.46	0.46
1:A:391:MET:HE2	1:A:434:LYS:CE	2.45	0.46
1:B:228:ASN:HB2	1:B:229:PRO:HD3	1.97	0.46
1:C:158:ASP:HB2	1:C:193:TYR:CZ	2.50	0.46
1:D:393:ILE:HD11	1:D:613:LEU:HA	1.97	0.46
1:D:495:HIS:CD2	1:D:500:LEU:HG	2.50	0.46
1:A:269:THR:HG23	1:A:443:LEU:HD22	1.96	0.46
1:A:551:THR:CB	1:A:553:THR:HG22	2.45	0.46
1:B:57:VAL:HG12	1:B:59:VAL:HG13	1.97	0.46
1:D:278:ILE:HD12	1:D:428:GLU:HG2	1.98	0.46
1:F:731:ARG:HG2	1:F:756:MET:CE	2.45	0.46
1:A:717:CYS:O	1:A:778:THR:HG22	2.15	0.46
1:C:57:VAL:HG12	1:C:59:VAL:HG13	1.98	0.46
1:C:253:ARG:HG3	1:C:460:PHE:CD1	2.50	0.46
1:D:240:VAL:HG23	1:D:241:LYS:HG2	1.96	0.46
1:D:566:HIS:HD2	1:D:568:LYS:H	1.64	0.46
1:D:754:ILE:HG22	1:D:755:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:ASP:CA	1:E:610:THR:HB	2.46	0.46
1:E:697:ASP:HB3	1:E:700:LEU:HB3	1.97	0.46
1:F:532:THR:OG1	1:F:533:ASN:ND2	2.48	0.46
1:C:607:ASP:CA	1:C:610:THR:HB	2.43	0.46
1:E:323:ILE:HG22	1:E:324:PRO:CD	2.45	0.46
1:E:498:PHE:CE2	1:E:519:LEU:HD13	2.50	0.46
1:F:297:ALA:HB1	1:F:301:MET:HG2	1.97	0.46
1:B:36:TRP:NE1	1:B:78:MET:HG2	2.31	0.46
1:B:77:LYS:HZ2	1:B:77:LYS:N	2.14	0.46
1:B:427:ILE:HD13	1:B:427:ILE:HA	1.78	0.46
1:C:72:LYS:HA	1:C:75:ILE:CD1	2.43	0.46
1:C:172:SER:HA	1:C:462:GLY:O	2.15	0.46
1:C:290:PHE:CE1	1:C:356:VAL:HG13	2.49	0.46
1:C:731:ARG:O	1:C:735:GLU:HB2	2.16	0.46
1:C:742:ILE:HG22	1:C:743:PRO:O	2.15	0.46
1:D:540:LEU:HD11	1:D:562:GLU:HB2	1.98	0.46
1:E:251:PHE:CZ	1:E:462:GLY:HA3	2.51	0.46
1:E:508:GLU:HG3	1:E:508:GLU:O	2.16	0.46
1:F:659:VAL:HA	1:F:662:LEU:HD12	1.98	0.46
1:A:738:ALA:O	1:A:741:ALA:HB2	2.16	0.46
1:B:43:GLY:HA3	1:B:702:LEU:CD1	2.46	0.46
1:B:121:CYS:O	1:B:683:ARG:HG2	2.16	0.46
1:B:727:PHE:HA	1:B:753:CYS:SG	2.55	0.46
1:C:659:VAL:HA	1:C:662:LEU:HD12	1.97	0.46
1:D:36:TRP:HB2	1:D:76:GLN:O	2.16	0.46
1:E:527:LEU:HD22	1:E:566:HIS:CD2	2.50	0.46
1:E:532:THR:OG1	1:E:533:ASN:ND2	2.49	0.46
1:E:584:LEU:HD23	1:E:589:LYS:CG	2.36	0.46
1:E:712:GLU:OE1	1:E:712:GLU:N	2.43	0.46
1:F:607:ASP:CA	1:F:610:THR:HB	2.45	0.46
1:A:532:THR:OG1	1:A:533:ASN:ND2	2.49	0.46
1:B:226:GLN:C	1:B:229:PRO:HD2	2.35	0.46
1:B:278:ILE:HD12	1:B:428:GLU:HG2	1.97	0.46
1:C:39:SER:HG	1:C:42:HIS:H	1.62	0.46
1:C:77:LYS:HZ2	1:C:77:LYS:N	2.14	0.46
1:C:606:ASN:HB3	1:C:609:VAL:HG13	1.98	0.46
1:D:77:LYS:HZ2	1:D:77:LYS:N	2.13	0.46
1:D:378:MET:HE1	1:D:384:ALA:CB	2.42	0.46
1:D:666:GLN:HA	1:D:669:LYS:HD3	1.98	0.46
1:E:295:ALA:HB2	1:E:310:PHE:CZ	2.49	0.46
1:E:495:HIS:CD2	1:E:500:LEU:HG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:727:PHE:HA	1:F:753:CYS:SG	2.56	0.46
1:F:738:ALA:O	1:F:741:ALA:CB	2.64	0.46
1:B:339:MET:CE	1:B:352:ILE:HD13	2.45	0.46
1:B:607:ASP:CA	1:B:610:THR:HB	2.46	0.46
1:C:697:ASP:HB3	1:C:700:LEU:HB3	1.98	0.46
1:D:34:LEU:HD12	1:D:34:LEU:HA	1.74	0.46
1:E:57:VAL:HG12	1:E:59:VAL:HG13	1.97	0.46
1:F:381:ASN:O	1:F:382:THR:C	2.54	0.46
1:F:478:GLU:OE2	1:F:600:LYS:HE2	2.15	0.46
1:A:35:VAL:HG22	1:A:76:GLN:O	2.16	0.46
1:B:251:PHE:CZ	1:B:462:GLY:HA3	2.51	0.46
1:B:738:ALA:O	1:B:741:ALA:HB2	2.16	0.46
1:C:35:VAL:HG22	1:C:76:GLN:O	2.15	0.46
1:C:35:VAL:HG21	1:C:75:ILE:HG22	1.98	0.46
1:C:508:GLU:HG3	1:C:771:GLN:N	2.29	0.46
1:D:419:THR:H	1:D:422:GLN:CG	2.23	0.46
1:D:502:GLN:HA	1:D:505:TYR:CD2	2.51	0.46
1:D:532:THR:OG1	1:D:533:ASN:ND2	2.49	0.46
1:E:460:PHE:C	1:E:460:PHE:CD1	2.89	0.46
1:E:563:GLN:OE1	1:E:563:GLN:HA	2.16	0.46
1:F:239:THR:HG23	1:F:245:SER:HB3	1.98	0.46
1:A:173:ILE:HG13	1:A:461:LEU:HD21	1.99	0.45
1:A:300:GLN:O	1:A:304:ASP:HB2	2.17	0.45
1:B:290:PHE:CE1	1:B:356:VAL:HG13	2.51	0.45
1:B:508:GLU:HG3	1:B:771:GLN:N	2.31	0.45
1:B:532:THR:OG1	1:B:533:ASN:ND2	2.49	0.45
1:B:540:LEU:HD11	1:B:562:GLU:HB2	1.97	0.45
1:B:566:HIS:HD2	1:B:568:LYS:H	1.64	0.45
1:D:268:GLU:HG2	1:D:270:TYR:OH	2.16	0.45
1:D:526:GLU:OE1	1:D:526:GLU:HA	2.16	0.45
1:E:226:GLN:HB2	1:E:342:MET:HE2	1.98	0.45
1:E:659:VAL:HA	1:E:662:LEU:HD12	1.97	0.45
1:F:327:GLN:O	1:F:330:GLU:N	2.48	0.45
1:F:393:ILE:HG13	1:F:612:LEU:HB3	1.99	0.45
1:F:502:GLN:HA	1:F:505:TYR:CD2	2.51	0.45
1:F:743:PRO:HD2	1:F:747:MET:SD	2.56	0.45
1:A:393:ILE:HD11	1:A:613:LEU:HA	1.98	0.45
1:A:478:GLU:OE2	1:A:600:LYS:HE2	2.17	0.45
1:A:498:PHE:CE2	1:A:519:LEU:HD13	2.51	0.45
1:A:563:GLN:HA	1:A:563:GLN:OE1	2.17	0.45
1:B:508:GLU:HG2	1:B:775:PHE:CE1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:999:ALF:F4	4:B:998:ADP:PB	2.65	0.45
1:C:271:LEU:HD22	1:C:481:CYS:HB2	1.98	0.45
1:D:41:LYS:H	1:D:41:LYS:HG2	1.44	0.45
1:D:607:ASP:CA	1:D:610:THR:HB	2.45	0.45
1:E:35:VAL:HG22	1:E:76:GLN:O	2.16	0.45
1:E:35:VAL:HG22	1:E:36:TRP:H	1.82	0.45
1:E:196:VAL:O	1:E:196:VAL:CG1	2.64	0.45
1:C:126:PRO:HB3	1:C:130:LEU:HD11	1.98	0.45
1:F:35:VAL:HG13	1:F:36:TRP:N	2.30	0.45
1:F:228:ASN:HB2	1:F:229:PRO:HD3	1.98	0.45
1:F:498:PHE:CE2	1:F:519:LEU:HD13	2.51	0.45
1:F:711:LEU:O	1:F:715:ARG:HG2	2.16	0.45
1:A:43:GLY:HA3	1:A:702:LEU:CD1	2.46	0.45
1:A:97:GLU:HG2	1:A:711:LEU:CD1	2.47	0.45
1:A:251:PHE:CZ	1:A:462:GLY:HA3	2.51	0.45
1:A:659:VAL:HA	1:A:662:LEU:HD12	1.96	0.45
1:C:95:LEU:CD1	1:C:714:ILE:HG21	2.45	0.45
1:C:173:ILE:HG13	1:C:461:LEU:HD21	1.99	0.45
1:D:551:THR:CB	1:D:553:THR:HG22	2.47	0.45
1:E:253:ARG:HG3	1:E:460:PHE:CD1	2.52	0.45
1:F:318:ASN:O	1:F:319:GLY:C	2.54	0.45
1:A:228:ASN:HB2	1:A:229:PRO:HD3	1.99	0.45
1:A:281:ALA:O	1:A:318:ASN:ND2	2.47	0.45
1:C:532:THR:OG1	1:C:533:ASN:ND2	2.49	0.45
1:E:738:ALA:O	1:E:741:ALA:HB3	2.16	0.45
1:F:538:LEU:CD1	1:F:664:LYS:HD2	2.46	0.45
1:A:43:GLY:H	1:A:698:ALA:CB	2.24	0.45
1:A:316:LEU:O	1:A:317:SER:C	2.55	0.45
1:B:35:VAL:HG11	1:B:75:ILE:CG2	2.47	0.45
1:C:35:VAL:HG11	1:C:75:ILE:CG2	2.46	0.45
1:C:240:VAL:HG23	1:C:241:LYS:HG2	1.97	0.45
1:C:545:CYS:SG	1:C:598:LEU:HD23	2.56	0.45
1:C:731:ARG:HG2	1:C:756:MET:CE	2.45	0.45
1:D:391:MET:HE2	1:D:434:LYS:CE	2.47	0.45
1:D:738:ALA:O	1:D:741:ALA:HB2	2.16	0.45
1:E:80:PRO:HB2	1:E:82:LYS:HG2	1.99	0.45
1:E:393:ILE:HG13	1:E:612:LEU:HB3	1.97	0.45
1:E:731:ARG:O	1:E:735:GLU:HB2	2.17	0.45
1:F:438:LEU:O	1:F:442:ILE:HG13	2.15	0.45
1:A:271:LEU:HD22	1:A:481:CYS:HB2	1.97	0.45
1:A:711:LEU:O	1:A:715:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:999:ALF:F4	4:A:998:ADP:PB	2.65	0.45
1:B:381:ASN:O	1:B:382:THR:C	2.55	0.45
1:B:552:ASP:HA	1:B:598:LEU:HD12	1.99	0.45
1:C:502:GLN:HA	1:C:505:TYR:CD2	2.51	0.45
1:D:478:GLU:OE2	1:D:600:LYS:HE2	2.17	0.45
1:D:717:CYS:O	1:D:778:THR:HG22	2.17	0.45
1:F:323:ILE:HG22	1:F:324:PRO:CD	2.47	0.45
1:F:566:HIS:HD2	1:F:568:LYS:H	1.64	0.45
1:F:666:GLN:HA	1:F:669:LYS:HD3	1.98	0.45
1:A:268:GLU:HG2	1:A:270:TYR:OH	2.17	0.45
1:A:525:ILE:O	1:A:529:GLU:HG2	2.17	0.45
1:A:658:THR:O	1:A:662:LEU:HD12	2.17	0.45
1:B:80:PRO:HB2	1:B:82:LYS:HG2	1.98	0.45
1:B:238:LYS:HB3	1:B:285:ARG:HG2	1.98	0.45
1:B:525:ILE:O	1:B:529:GLU:HG2	2.17	0.45
1:C:34:LEU:HD12	1:C:34:LEU:HA	1.74	0.45
1:C:35:VAL:HG12	1:C:47:ALA:O	2.17	0.45
1:C:381:ASN:O	1:C:382:THR:C	2.55	0.45
1:C:566:HIS:HD2	1:C:568:LYS:H	1.63	0.45
1:D:239:THR:HG23	1:D:245:SER:HB3	1.99	0.45
1:D:242:ASN:OD1	1:D:243:ASP:N	2.49	0.45
1:D:711:LEU:O	1:D:715:ARG:HG2	2.17	0.45
1:A:95:LEU:HD11	1:A:714:ILE:HG21	1.98	0.45
1:A:219:GLU:O	1:A:222:LYS:N	2.50	0.45
1:A:566:HIS:HD2	1:A:568:LYS:H	1.64	0.45
1:B:490:GLN:O	1:B:493:PHE:HB3	2.16	0.45
1:B:731:ARG:HH11	1:B:731:ARG:CG	2.30	0.45
1:C:268:GLU:HG2	1:C:270:TYR:OH	2.16	0.45
1:D:158:ASP:O	1:D:161:TYR:HB3	2.15	0.45
1:D:538:LEU:CD1	1:D:664:LYS:HD2	2.47	0.45
1:E:242:ASN:OD1	1:E:243:ASP:N	2.50	0.45
1:E:551:THR:CB	1:E:553:THR:HG22	2.47	0.45
1:F:35:VAL:HG11	1:F:75:ILE:CG2	2.46	0.45
1:F:327:GLN:HB2	1:F:330:GLU:CD	2.38	0.45
1:F:502:GLN:O	1:F:505:TYR:HB2	2.16	0.45
1:A:114:TYR:CE1	1:A:153:ILE:HB	2.52	0.45
1:A:226:GLN:C	1:A:229:PRO:HD2	2.37	0.45
1:A:508:GLU:HG3	1:A:771:GLN:N	2.31	0.45
1:B:438:LEU:O	1:B:442:ILE:HG13	2.16	0.45
1:D:95:LEU:CD1	1:D:714:ILE:HG21	2.47	0.45
1:D:427:ILE:HA	1:D:427:ILE:HD13	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:LEU:HD22	1:D:566:HIS:CD2	2.52	0.45
1:A:95:LEU:CD1	1:A:714:ILE:HG21	2.47	0.44
1:A:508:GLU:HG2	1:A:775:PHE:CE1	2.46	0.44
1:A:721:PHE:HB2	1:A:775:PHE:HB3	1.98	0.44
1:B:116:TYR:CZ	1:B:146:ARG:HG2	2.52	0.44
1:C:230:ILE:HD11	1:C:342:MET:HB2	1.99	0.44
1:D:355:VAL:O	1:D:359:VAL:HG23	2.17	0.44
3:D:999:ALF:F4	4:D:998:ADP:PB	2.65	0.44
1:E:271:LEU:HD22	1:E:481:CYS:HB2	1.99	0.44
1:E:734:TYR:OH	1:E:781:LEU:HD22	2.17	0.44
1:F:219:GLU:O	1:F:222:LYS:N	2.50	0.44
1:F:271:LEU:HD22	1:F:481:CYS:HB2	1.99	0.44
1:A:41:LYS:H	1:A:41:LYS:HG2	1.46	0.44
1:A:738:ALA:O	1:A:741:ALA:HB3	2.17	0.44
1:B:297:ALA:HB1	1:B:301:MET:HG2	1.98	0.44
1:B:378:MET:O	1:B:378:MET:HG3	2.16	0.44
1:C:738:ALA:O	1:C:741:ALA:HB3	2.17	0.44
1:C:756:MET:HB2	1:C:756:MET:HE3	1.55	0.44
1:E:742:ILE:HG12	1:E:752:ALA:HB1	1.99	0.44
1:A:388:CYS:SG	1:A:393:ILE:HG22	2.57	0.44
1:A:502:GLN:HA	1:A:505:TYR:CD2	2.52	0.44
1:B:746:PHE:CG	1:C:306:LEU:HD11	2.52	0.44
1:C:239:THR:HG23	1:C:245:SER:HB3	1.99	0.44
1:C:402:ILE:HG22	1:C:403:LEU:N	2.33	0.44
1:C:563:GLN:OE1	1:C:563:GLN:HA	2.16	0.44
1:D:114:TYR:CE1	1:D:153:ILE:HB	2.53	0.44
1:D:269:THR:HG23	1:D:443:LEU:HD22	2.00	0.44
1:E:355:VAL:O	1:E:359:VAL:HG23	2.17	0.44
1:E:711:LEU:O	1:E:715:ARG:HG2	2.18	0.44
1:F:61:LEU:HG	1:F:66:LYS:O	2.18	0.44
1:F:80:PRO:HB2	1:F:82:LYS:HG2	1.99	0.44
1:F:551:THR:CB	1:F:553:THR:HG22	2.48	0.44
1:A:164:MET:SD	1:A:459:SER:HB2	2.57	0.44
1:B:219:GLU:O	1:B:222:LYS:N	2.51	0.44
1:C:316:LEU:O	1:C:317:SER:C	2.55	0.44
1:C:666:GLN:HA	1:C:669:LYS:HD3	1.98	0.44
1:C:767:TYR:CD1	1:C:767:TYR:C	2.90	0.44
1:D:393:ILE:HD11	1:D:612:LEU:O	2.17	0.44
1:D:526:GLU:OE1	1:D:530:ARG:HD3	2.17	0.44
1:D:552:ASP:HA	1:D:598:LEU:HD12	1.99	0.44
1:D:731:ARG:HG2	1:D:756:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:VAL:HG12	1:F:47:ALA:O	2.17	0.44
1:F:584:LEU:HD23	1:F:589:LYS:CG	2.37	0.44
1:B:97:GLU:HG2	1:B:711:LEU:CD1	2.48	0.44
1:B:158:ASP:HB2	1:B:193:TYR:CZ	2.53	0.44
1:D:42:HIS:O	1:D:43:GLY:C	2.55	0.44
1:D:97:GLU:HG2	1:D:711:LEU:CD1	2.48	0.44
1:D:107:ARG:NH1	1:D:114:TYR:O	2.50	0.44
1:D:300:GLN:O	1:D:304:ASP:HB2	2.17	0.44
1:D:327:GLN:HB2	1:D:330:GLU:CD	2.38	0.44
1:D:438:LEU:O	1:D:442:ILE:HG13	2.18	0.44
1:E:238:LYS:HB3	1:E:285:ARG:HG2	2.00	0.44
1:E:566:HIS:HD2	1:E:568:LYS:H	1.65	0.44
1:F:385:GLN:HA	1:F:395:VAL:HG22	2.00	0.44
1:F:388:CYS:SG	1:F:393:ILE:HG22	2.57	0.44
1:F:508:GLU:HG3	1:F:771:GLN:N	2.30	0.44
1:B:268:GLU:HG2	1:B:270:TYR:OH	2.18	0.44
1:B:747:MET:CE	1:B:751:GLN:HB3	2.47	0.44
1:C:327:GLN:HB2	1:C:330:GLU:CD	2.38	0.44
1:C:393:ILE:HD11	1:C:613:LEU:HA	1.98	0.44
1:C:434:LYS:HG2	1:C:625:TRP:CZ2	2.53	0.44
1:D:116:TYR:CZ	1:D:146:ARG:HG2	2.53	0.44
1:D:563:GLN:HA	1:D:563:GLN:OE1	2.17	0.44
1:E:756:MET:HB2	1:E:756:MET:HE3	1.56	0.44
1:A:584:LEU:HD23	1:A:589:LYS:CG	2.35	0.44
1:B:242:ASN:OD1	1:B:243:ASP:N	2.51	0.44
1:B:551:THR:CB	1:B:553:THR:HG22	2.47	0.44
1:C:278:ILE:HD12	1:C:428:GLU:HG2	1.99	0.44
3:C:999:ALF:F4	4:C:998:ADP:PB	2.65	0.44
1:D:493:PHE:CZ	1:D:497:MET:HG3	2.52	0.44
1:D:688:ASN:ND2	1:D:692:ARG:O	2.35	0.44
1:E:158:ASP:HB2	1:E:193:TYR:CZ	2.52	0.44
1:E:240:VAL:HG23	1:E:241:LYS:HG2	1.99	0.44
1:E:742:ILE:HG23	1:E:743:PRO:CD	2.47	0.44
1:F:173:ILE:HG13	1:F:461:LEU:HD21	1.99	0.44
1:F:340:THR:HG22	1:F:341:ILE:N	2.33	0.44
1:A:222:LYS:O	1:A:226:GLN:HG2	2.18	0.44
1:A:240:VAL:HG23	1:A:241:LYS:HG2	1.99	0.44
1:B:42:HIS:O	1:B:43:GLY:C	2.56	0.44
1:B:393:ILE:HD11	1:B:613:LEU:HA	1.99	0.44
1:D:251:PHE:CZ	1:D:462:GLY:HA3	2.53	0.44
1:D:545:CYS:SG	1:D:598:LEU:HD23	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:HD11	1:E:714:ILE:HG21	2.00	0.44
1:E:508:GLU:HG3	1:E:771:GLN:N	2.32	0.44
1:E:751:GLN:O	1:E:755:LEU:HG	2.18	0.44
1:F:36:TRP:HB2	1:F:76:GLN:O	2.18	0.44
1:F:77:LYS:HZ2	1:F:77:LYS:N	2.14	0.44
1:F:427:ILE:HD13	1:F:427:ILE:HA	1.80	0.44
1:C:97:GLU:HG2	1:C:711:LEU:CD1	2.48	0.44
1:C:164:MET:SD	1:C:459:SER:HB2	2.58	0.44
1:C:251:PHE:CZ	1:C:462:GLY:HA3	2.53	0.44
1:C:738:ALA:O	1:C:741:ALA:HB2	2.16	0.44
1:D:225:LEU:N	1:D:225:LEU:CD2	2.81	0.44
1:D:738:ALA:O	1:D:741:ALA:HB3	2.17	0.44
1:D:751:GLN:O	1:D:755:LEU:HG	2.18	0.44
1:E:89:MET:HE1	1:E:100:VAL:HG13	1.98	0.44
1:E:558:LYS:O	1:E:562:GLU:HG2	2.18	0.44
1:F:113:ILE:O	1:F:123:VAL:HA	2.18	0.44
1:F:126:PRO:HB3	1:F:130:LEU:HD11	1.99	0.44
1:A:378:MET:HG3	1:A:378:MET:O	2.18	0.43
1:B:495:HIS:CD2	1:B:500:LEU:HG	2.53	0.43
1:C:751:GLN:O	1:C:755:LEU:HG	2.18	0.43
1:E:41:LYS:H	1:E:41:LYS:HG2	1.47	0.43
1:E:508:GLU:HG2	1:E:775:PHE:CE1	2.43	0.43
1:F:116:TYR:CE2	1:F:146:ARG:HG2	2.53	0.43
1:F:355:VAL:O	1:F:359:VAL:HG23	2.17	0.43
1:A:116:TYR:CZ	1:A:146:ARG:HG2	2.53	0.43
1:A:323:ILE:HG22	1:A:324:PRO:N	2.34	0.43
1:A:495:HIS:CD2	1:A:500:LEU:HG	2.54	0.43
1:A:742:ILE:HG23	1:A:743:PRO:CD	2.47	0.43
1:B:289:ILE:HD12	1:B:289:ILE:HA	1.85	0.43
1:B:558:LYS:O	1:B:562:GLU:HG2	2.18	0.43
1:C:35:VAL:HG13	1:C:36:TRP:N	2.32	0.43
1:C:734:TYR:OH	1:C:781:LEU:HD22	2.18	0.43
1:D:508:GLU:HG3	1:D:771:GLN:N	2.33	0.43
1:D:558:LYS:O	1:D:562:GLU:HG2	2.18	0.43
1:D:742:ILE:HG23	1:D:743:PRO:CD	2.47	0.43
1:D:747:MET:CE	1:D:751:GLN:HB3	2.48	0.43
1:E:95:LEU:CD1	1:E:714:ILE:HG21	2.48	0.43
1:F:121:CYS:O	1:F:683:ARG:HG2	2.18	0.43
1:F:717:CYS:O	1:F:778:THR:HG22	2.17	0.43
1:A:35:VAL:HG11	1:A:75:ILE:CG2	2.49	0.43
1:A:727:PHE:HA	1:A:753:CYS:SG	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:MET:HE3	1:A:756:MET:HB2	1.57	0.43
1:B:253:ARG:HG3	1:B:460:PHE:CD1	2.54	0.43
1:B:316:LEU:O	1:B:317:SER:C	2.55	0.43
1:B:563:GLN:OE1	1:B:563:GLN:HA	2.16	0.43
1:B:717:CYS:O	1:B:778:THR:HG22	2.18	0.43
1:B:731:ARG:O	1:B:735:GLU:HB2	2.18	0.43
1:C:43:GLY:HA3	1:C:702:LEU:CD1	2.47	0.43
1:D:158:ASP:HB2	1:D:193:TYR:CZ	2.53	0.43
1:D:316:LEU:O	1:D:317:SER:C	2.55	0.43
1:D:381:ASN:O	1:D:382:THR:C	2.57	0.43
1:D:498:PHE:CE2	1:D:519:LEU:HD13	2.52	0.43
1:E:42:HIS:O	1:E:43:GLY:C	2.56	0.43
1:E:323:ILE:HG22	1:E:324:PRO:HD2	1.90	0.43
1:F:42:HIS:O	1:F:43:GLY:C	2.56	0.43
1:F:721:PHE:HB2	1:F:775:PHE:HB3	2.00	0.43
1:A:327:GLN:HB2	1:A:330:GLU:CD	2.39	0.43
1:B:721:PHE:HB2	1:B:775:PHE:HB3	1.99	0.43
1:C:323:ILE:HG22	1:C:324:PRO:N	2.33	0.43
1:D:35:VAL:N	1:D:47:ALA:O	2.51	0.43
1:E:393:ILE:HD11	1:E:613:LEU:HA	1.98	0.43
1:F:391:MET:HE2	1:F:434:LYS:CE	2.48	0.43
1:F:751:GLN:O	1:F:755:LEU:HG	2.19	0.43
1:A:239:THR:HG23	1:A:245:SER:HB3	1.99	0.43
1:A:242:ASN:OD1	1:A:243:ASP:N	2.51	0.43
1:B:181:ALA:N	1:B:686:ILE:HD12	2.32	0.43
1:C:48:SER:O	1:C:59:VAL:HB	2.19	0.43
1:C:225:LEU:N	1:C:225:LEU:CD2	2.82	0.43
1:D:95:LEU:HD11	1:D:714:ILE:HG21	2.00	0.43
1:E:107:ARG:NH1	1:E:114:TYR:O	2.51	0.43
1:E:126:PRO:HB3	1:E:130:LEU:HD11	2.00	0.43
1:E:345:THR:HG23	1:E:348:GLU:OE1	2.19	0.43
1:E:767:TYR:O	1:E:768:ARG:HG2	2.18	0.43
1:F:35:VAL:HG21	1:F:75:ILE:CG2	2.48	0.43
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.88	0.43
1:C:116:TYR:CZ	1:C:146:ARG:HG2	2.54	0.43
1:C:181:ALA:N	1:C:686:ILE:HD12	2.33	0.43
1:C:242:ASN:OD1	1:C:243:ASP:N	2.51	0.43
1:C:250:LYS:HD2	1:C:252:ILE:HD11	2.01	0.43
1:D:35:VAL:HG21	1:D:75:ILE:HG22	2.01	0.43
1:E:228:ASN:O	1:E:229:PRO:C	2.56	0.43
1:E:526:GLU:OE1	1:E:530:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:717:CYS:O	1:E:778:THR:HG22	2.19	0.43
1:F:242:ASN:OD1	1:F:243:ASP:N	2.51	0.43
1:F:268:GLU:HG2	1:F:270:TYR:OH	2.19	0.43
1:F:278:ILE:HB	1:F:315:PHE:CE1	2.54	0.43
1:A:35:VAL:HG21	1:A:75:ILE:HG22	1.99	0.43
1:A:528:ILE:HG23	1:A:538:LEU:HG	2.00	0.43
1:B:658:THR:O	1:B:662:LEU:HD12	2.19	0.43
1:C:238:LYS:HB3	1:C:285:ARG:HG2	2.01	0.43
1:D:57:VAL:HG12	1:D:59:VAL:HG13	1.99	0.43
1:D:468:GLY:N	3:D:999:ALF:F1	2.40	0.43
1:D:767:TYR:C	1:D:767:TYR:CD1	2.92	0.43
1:E:525:ILE:O	1:E:529:GLU:HG2	2.19	0.43
1:F:225:LEU:N	1:F:225:LEU:CD2	2.80	0.43
1:F:526:GLU:OE1	1:F:530:ARG:HD3	2.19	0.43
1:A:126:PRO:HB3	1:A:130:LEU:HD11	2.01	0.43
1:A:333:GLN:O	1:A:337:GLU:HB2	2.19	0.43
1:A:381:ASN:O	1:A:382:THR:C	2.55	0.43
1:A:493:PHE:CZ	1:A:497:MET:HG3	2.54	0.43
1:A:747:MET:CE	1:A:751:GLN:HB3	2.48	0.43
1:B:271:LEU:HD22	1:B:481:CYS:HB2	2.00	0.43
1:B:300:GLN:O	1:B:304:ASP:HB2	2.18	0.43
1:C:300:GLN:O	1:C:304:ASP:HB2	2.18	0.43
1:C:526:GLU:OE1	1:C:530:ARG:HD3	2.19	0.43
1:D:378:MET:HG3	1:D:378:MET:O	2.19	0.43
1:D:721:PHE:HB2	1:D:775:PHE:HB3	2.00	0.43
1:E:192:GLN:O	1:E:196:VAL:HG23	2.19	0.43
1:E:219:GLU:O	1:E:222:LYS:N	2.52	0.43
1:E:333:GLN:O	1:E:337:GLU:HB2	2.18	0.43
1:F:365:ILE:HG23	1:F:378:MET:HE3	2.01	0.43
1:F:747:MET:CE	1:F:751:GLN:HB3	2.49	0.43
1:A:327:GLN:HE21	1:A:327:GLN:HB3	1.73	0.43
1:B:35:VAL:HG13	1:B:36:TRP:N	2.34	0.43
1:B:61:LEU:HG	1:B:66:LYS:O	2.18	0.43
1:B:493:PHE:CZ	1:B:497:MET:HG3	2.54	0.43
1:B:763:ASP:HB3	1:B:766:LEU:HG	2.01	0.43
1:E:79:ASN:OD1	1:E:93:THR:HB	2.19	0.43
1:E:528:ILE:HG23	1:E:538:LEU:HG	2.01	0.43
1:E:708:ASN:N	1:E:708:ASN:ND2	2.65	0.43
1:E:750:LYS:HE3	1:E:769:ILE:HG22	2.01	0.43
1:F:48:SER:O	1:F:59:VAL:HB	2.19	0.43
1:F:57:VAL:HG12	1:F:59:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:GLN:O	1:F:304:ASP:HB2	2.19	0.43
1:F:528:ILE:HG23	1:F:538:LEU:HG	2.01	0.43
1:B:172:SER:HA	1:B:462:GLY:O	2.18	0.43
1:B:688:ASN:ND2	1:B:692:ARG:O	2.36	0.43
1:C:493:PHE:CZ	1:C:497:MET:HG3	2.54	0.43
1:C:605:LEU:HD12	1:C:605:LEU:HA	1.85	0.43
1:D:323:ILE:HG22	1:D:324:PRO:N	2.34	0.43
1:F:767:TYR:O	1:F:768:ARG:HG2	2.18	0.43
1:A:113:ILE:O	1:A:123:VAL:HA	2.19	0.42
1:A:274:LYS:CG	1:A:436:GLU:HB2	2.46	0.42
1:A:419:THR:H	1:A:422:GLN:CG	2.26	0.42
1:A:767:TYR:C	1:A:767:TYR:CD1	2.91	0.42
1:B:339:MET:HE2	1:B:352:ILE:HD13	2.01	0.42
1:C:528:ILE:HG23	1:C:538:LEU:HG	2.01	0.42
1:E:747:MET:HE3	1:E:751:GLN:HB3	2.01	0.42
1:F:172:SER:HA	1:F:462:GLY:O	2.19	0.42
1:F:495:HIS:CD2	1:F:500:LEU:HG	2.54	0.42
1:F:731:ARG:HH11	1:F:731:ARG:CG	2.30	0.42
1:A:172:SER:HA	1:A:462:GLY:O	2.19	0.42
1:B:48:SER:O	1:B:59:VAL:HB	2.19	0.42
1:B:323:ILE:HG22	1:B:324:PRO:N	2.33	0.42
1:C:355:VAL:O	1:C:359:VAL:HG23	2.19	0.42
1:E:544:GLU:OE1	1:E:544:GLU:HA	2.20	0.42
1:E:721:PHE:HB2	1:E:775:PHE:HB3	2.01	0.42
1:F:526:GLU:OE1	1:F:526:GLU:HA	2.18	0.42
1:A:731:ARG:O	1:A:735:GLU:HB2	2.20	0.42
1:B:126:PRO:HB3	1:B:130:LEU:HD11	2.01	0.42
1:B:164:MET:SD	1:B:459:SER:HB2	2.59	0.42
1:B:225:LEU:N	1:B:225:LEU:CD2	2.82	0.42
1:B:746:PHE:CD1	1:C:306:LEU:HD11	2.54	0.42
1:C:58:THR:HA	1:C:69:THR:HA	2.01	0.42
1:C:291:TYR:HA	1:C:310:PHE:HE1	1.84	0.42
1:C:747:MET:CE	1:C:751:GLN:HB3	2.49	0.42
1:D:80:PRO:HB2	1:D:82:LYS:HG2	2.01	0.42
1:D:271:LEU:HD22	1:D:481:CYS:HB2	2.02	0.42
1:D:345:THR:HG23	1:D:348:GLU:OE1	2.19	0.42
1:D:731:ARG:O	1:D:735:GLU:HB2	2.19	0.42
1:E:36:TRP:HB2	1:E:76:GLN:O	2.19	0.42
1:E:116:TYR:CZ	1:E:146:ARG:HG2	2.55	0.42
1:E:756:MET:O	1:E:760:LEU:HG	2.19	0.42
1:F:192:GLN:O	1:F:196:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:GLU:HG2	1:F:775:PHE:CE1	2.45	0.42
1:F:527:LEU:HB2	1:F:566:HIS:CE1	2.55	0.42
1:F:563:GLN:OE1	1:F:563:GLN:HA	2.19	0.42
1:A:537:VAL:HG22	1:A:559:LEU:CD1	2.47	0.42
1:A:750:LYS:HE3	1:A:769:ILE:HG22	2.01	0.42
1:B:173:ILE:HG13	1:B:461:LEU:HD21	2.00	0.42
1:B:239:THR:HG23	1:B:245:SER:HB3	2.00	0.42
1:B:525:ILE:O	1:B:529:GLU:CG	2.67	0.42
1:C:525:ILE:O	1:C:529:GLU:HG2	2.19	0.42
1:D:61:LEU:HG	1:D:66:LYS:O	2.19	0.42
1:D:162:ARG:HG2	1:D:162:ARG:H	1.68	0.42
1:D:290:PHE:CE1	1:D:356:VAL:HG13	2.54	0.42
1:D:401:SER:HB3	1:D:608:ASN:CB	2.48	0.42
1:E:381:ASN:O	1:E:382:THR:C	2.56	0.42
1:A:117:SER:OG	1:A:120:PHE:CE2	2.73	0.42
1:A:339:MET:CE	1:A:352:ILE:HD13	2.49	0.42
1:A:605:LEU:HD12	1:A:605:LEU:HA	1.88	0.42
1:B:35:VAL:HG21	1:B:75:ILE:CG2	2.49	0.42
1:C:271:LEU:HD22	1:C:481:CYS:CB	2.49	0.42
1:C:495:HIS:CD2	1:C:500:LEU:HG	2.55	0.42
1:E:724:ARG:HG3	1:E:724:ARG:O	2.20	0.42
1:E:747:MET:CE	1:E:751:GLN:HB3	2.48	0.42
1:F:525:ILE:O	1:F:529:GLU:HG2	2.20	0.42
1:F:738:ALA:CB	1:F:741:ALA:HB2	2.47	0.42
1:A:253:ARG:HG3	1:A:460:PHE:CD1	2.54	0.42
1:B:292:TYR:CE2	1:B:331:MET:HB3	2.54	0.42
1:B:528:ILE:HG23	1:B:538:LEU:HG	2.01	0.42
1:B:690:GLU:C	1:B:692:ARG:N	2.70	0.42
1:B:711:LEU:O	1:B:715:ARG:HG2	2.20	0.42
1:C:36:TRP:HB2	1:C:76:GLN:O	2.20	0.42
1:C:333:GLN:O	1:C:337:GLU:HB2	2.19	0.42
1:C:385:GLN:HA	1:C:395:VAL:HG22	2.00	0.42
1:C:558:LYS:O	1:C:562:GLU:HG2	2.19	0.42
1:C:750:LYS:HE3	1:C:769:ILE:HG22	2.01	0.42
1:D:172:SER:HA	1:D:462:GLY:O	2.20	0.42
1:D:219:GLU:O	1:D:222:LYS:N	2.52	0.42
1:D:236:ASN:ND2	1:D:244:ASN:O	2.52	0.42
1:E:173:ILE:HG13	1:E:461:LEU:HD21	2.00	0.42
1:E:225:LEU:N	1:E:225:LEU:CD2	2.82	0.42
1:E:327:GLN:HB2	1:E:330:GLU:CD	2.40	0.42
1:E:339:MET:CE	1:E:352:ILE:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:MET:HE2	1:E:434:LYS:CE	2.48	0.42
1:E:545:CYS:SG	1:E:598:LEU:HD23	2.60	0.42
1:F:97:GLU:HG2	1:F:711:LEU:CD1	2.49	0.42
1:F:254:ILE:O	1:F:460:PHE:HA	2.20	0.42
1:F:724:ARG:O	1:F:724:ARG:HG3	2.20	0.42
1:F:767:TYR:CD1	1:F:767:TYR:C	2.92	0.42
1:A:61:LEU:HG	1:A:66:LYS:O	2.20	0.42
1:A:192:GLN:O	1:A:196:VAL:HG23	2.19	0.42
1:A:763:ASP:HB3	1:A:766:LEU:HG	2.01	0.42
1:B:41:LYS:H	1:B:41:LYS:HG2	1.44	0.42
1:B:333:GLN:O	1:B:337:GLU:HB2	2.19	0.42
1:B:393:ILE:HD11	1:B:612:LEU:O	2.19	0.42
1:B:502:GLN:HA	1:B:505:TYR:CD2	2.54	0.42
1:B:750:LYS:HE3	1:B:769:ILE:HG22	2.02	0.42
1:C:427:ILE:HA	1:C:427:ILE:HD13	1.75	0.42
1:C:742:ILE:HG12	1:C:752:ALA:HB1	2.00	0.42
1:D:253:ARG:HG3	1:D:460:PHE:CD1	2.54	0.42
1:D:291:TYR:HA	1:D:310:PHE:HE1	1.84	0.42
1:D:743:PRO:HD2	1:D:747:MET:SD	2.60	0.42
1:E:278:ILE:HD12	1:E:428:GLU:HG2	2.00	0.42
1:F:34:LEU:HD12	1:F:34:LEU:HA	1.75	0.42
1:F:434:LYS:HG2	1:F:625:TRP:CZ2	2.55	0.42
1:F:756:MET:HE3	1:F:756:MET:HB2	1.57	0.42
1:A:308:GLU:HB3	1:A:312:ASN:CB	2.48	0.42
1:A:393:ILE:HD11	1:A:612:LEU:O	2.20	0.42
1:A:401:SER:HB3	1:A:608:ASN:CB	2.47	0.42
1:A:671:MET:O	1:A:675:ARG:HD2	2.20	0.42
1:A:743:PRO:HD2	1:A:747:MET:SD	2.60	0.42
1:B:340:THR:HG22	1:B:341:ILE:N	2.35	0.42
1:B:388:CYS:SG	1:B:393:ILE:HG22	2.60	0.42
1:B:526:GLU:OE1	1:B:530:ARG:HD3	2.19	0.42
1:B:545:CYS:SG	1:B:598:LEU:HD23	2.59	0.42
1:B:742:ILE:HG12	1:B:752:ALA:HB1	2.02	0.42
1:C:80:PRO:HB2	1:C:82:LYS:HG2	2.01	0.42
1:C:540:LEU:HD12	1:C:559:LEU:CD1	2.50	0.42
1:C:717:CYS:O	1:C:778:THR:HG22	2.19	0.42
1:D:117:SER:OG	1:D:120:PHE:CE2	2.72	0.42
1:E:671:MET:O	1:E:675:ARG:HD2	2.20	0.42
1:E:690:GLU:C	1:E:692:ARG:N	2.73	0.42
1:A:107:ARG:HD3	1:A:115:THR:OG1	2.20	0.42
1:A:271:LEU:HD22	1:A:481:CYS:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:GLU:C	1:A:692:ARG:N	2.72	0.42
1:B:58:THR:OG1	1:B:69:THR:HG23	2.20	0.42
1:B:385:GLN:HA	1:B:395:VAL:HG22	2.02	0.42
1:C:222:LYS:O	1:C:226:GLN:HG2	2.19	0.42
1:C:274:LYS:CG	1:C:436:GLU:HB2	2.47	0.42
1:D:385:GLN:HA	1:D:395:VAL:HG22	2.02	0.42
1:D:402:ILE:HG22	1:D:403:LEU:N	2.33	0.42
1:E:97:GLU:HG2	1:E:711:LEU:CD1	2.49	0.42
1:E:162:ARG:HG2	1:E:162:ARG:H	1.64	0.42
1:E:401:SER:HB3	1:E:608:ASN:CB	2.45	0.42
1:E:417:ALA:C	1:E:418:GLN:HE21	2.22	0.42
1:E:747:MET:HE3	1:E:751:GLN:CB	2.50	0.42
1:F:226:GLN:C	1:F:229:PRO:HD2	2.40	0.42
1:F:228:ASN:O	1:F:229:PRO:C	2.56	0.42
1:A:42:HIS:O	1:A:43:GLY:C	2.58	0.42
1:B:274:LYS:CG	1:B:436:GLU:HB2	2.48	0.42
1:B:671:MET:O	1:B:675:ARG:HD2	2.19	0.42
1:D:121:CYS:O	1:D:683:ARG:HG2	2.20	0.42
1:D:290:PHE:HD1	1:D:360:LEU:HD11	1.85	0.42
1:E:61:LEU:O	1:E:65:GLY:CA	2.68	0.42
1:E:385:GLN:HA	1:E:395:VAL:HG22	2.01	0.42
1:E:402:ILE:HD13	1:E:402:ILE:HA	1.93	0.42
1:A:527:LEU:HB2	1:A:566:HIS:CE1	2.54	0.41
1:B:58:THR:HA	1:B:69:THR:HA	2.02	0.41
1:B:113:ILE:O	1:B:123:VAL:HA	2.20	0.41
1:B:742:ILE:HG23	1:B:743:PRO:CD	2.47	0.41
1:B:753:CYS:HA	1:B:756:MET:HE3	2.01	0.41
1:C:593:ASN:ND2	1:C:593:ASN:C	2.73	0.41
1:C:743:PRO:HD2	1:C:747:MET:SD	2.60	0.41
1:D:43:GLY:HA3	1:D:702:LEU:CD1	2.49	0.41
1:D:72:LYS:O	1:D:75:ILE:HD12	2.20	0.41
1:D:173:ILE:HG13	1:D:461:LEU:HD21	2.02	0.41
1:E:38:PRO:HD3	1:E:74:ASP:O	2.20	0.41
1:E:271:LEU:HD22	1:E:481:CYS:CB	2.50	0.41
1:A:185:GLU:O	1:A:189:LYS:HG2	2.20	0.41
1:A:438:LEU:O	1:A:442:ILE:HG13	2.20	0.41
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.50	0.41
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.89	0.41
1:B:107:ARG:NH1	1:B:114:TYR:O	2.54	0.41
1:B:291:TYR:HA	1:B:310:PHE:HE1	1.85	0.41
1:D:58:THR:OG1	1:D:69:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLN:HB2	1:D:342:MET:HE2	2.01	0.41
1:D:525:ILE:O	1:D:529:GLU:HG2	2.20	0.41
1:E:77:LYS:HZ2	1:E:77:LYS:N	2.18	0.41
1:E:323:ILE:HG22	1:E:324:PRO:N	2.34	0.41
1:E:362:LEU:HD23	1:E:387:VAL:HG21	2.01	0.41
1:E:606:ASN:O	1:E:609:VAL:HG13	2.21	0.41
1:F:362:LEU:HD23	1:F:362:LEU:HA	1.90	0.41
1:F:609:VAL:O	1:F:612:LEU:HB2	2.19	0.41
1:F:742:ILE:HG23	1:F:743:PRO:CD	2.51	0.41
1:A:38:PRO:HD3	1:A:74:ASP:O	2.21	0.41
1:A:77:LYS:H	1:A:77:LYS:CD	2.32	0.41
1:A:181:ALA:N	1:A:686:ILE:HD12	2.34	0.41
1:A:385:GLN:HA	1:A:395:VAL:HG22	2.02	0.41
1:A:525:ILE:O	1:A:529:GLU:CG	2.68	0.41
1:A:558:LYS:O	1:A:562:GLU:HG2	2.20	0.41
1:B:35:VAL:CG2	1:B:75:ILE:HG22	2.51	0.41
1:B:192:GLN:O	1:B:196:VAL:HG23	2.20	0.41
1:B:605:LEU:HD12	1:B:605:LEU:HA	1.85	0.41
1:C:340:THR:HG22	1:C:341:ILE:N	2.36	0.41
1:C:727:PHE:HA	1:C:753:CYS:SG	2.59	0.41
1:D:333:GLN:O	1:D:337:GLU:HB2	2.20	0.41
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.87	0.41
1:D:690:GLU:C	1:D:692:ARG:N	2.72	0.41
1:E:172:SER:HA	1:E:462:GLY:O	2.20	0.41
1:E:434:LYS:HG2	1:E:625:TRP:CZ2	2.54	0.41
1:E:467:ALA:HB3	1:E:482:ILE:HG12	2.02	0.41
1:F:715:ARG:NH1	1:F:715:ARG:CG	2.81	0.41
1:B:738:ALA:O	1:B:741:ALA:HB3	2.17	0.41
1:D:183:LYS:HZ1	1:D:468:GLY:HA3	1.86	0.41
1:D:300:GLN:O	1:D:303:ASN:ND2	2.53	0.41
1:D:508:GLU:HG2	1:D:775:PHE:CE1	2.43	0.41
1:E:88:ASP:HA	1:E:116:TYR:O	2.20	0.41
1:F:303:ASN:HD22	1:F:303:ASN:C	2.24	0.41
1:F:671:MET:O	1:F:675:ARG:HD2	2.20	0.41
1:F:721:PHE:CB	1:F:775:PHE:HB3	2.51	0.41
1:B:345:THR:HG23	1:B:348:GLU:OE1	2.21	0.41
1:B:721:PHE:CB	1:B:775:PHE:HB3	2.51	0.41
1:C:393:ILE:HD11	1:C:612:LEU:O	2.20	0.41
1:C:527:LEU:HB2	1:C:566:HIS:CE1	2.55	0.41
1:E:527:LEU:HB2	1:E:566:HIS:CE1	2.55	0.41
1:F:616:SER:C	1:F:618:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HA	1:A:69:THR:HA	2.02	0.41
1:B:114:TYR:CE1	1:B:153:ILE:HB	2.55	0.41
1:B:238:LYS:HB3	1:B:285:ARG:HD3	2.03	0.41
1:B:271:LEU:HD22	1:B:481:CYS:CB	2.50	0.41
1:B:756:MET:HE3	1:B:756:MET:HB2	1.55	0.41
1:C:192:GLN:O	1:C:196:VAL:HG23	2.20	0.41
1:D:35:VAL:HG22	1:D:76:GLN:O	2.19	0.41
1:D:116:TYR:CE2	1:D:146:ARG:HG2	2.55	0.41
1:D:192:GLN:O	1:D:196:VAL:HG23	2.20	0.41
1:D:327:GLN:HE21	1:D:327:GLN:HB3	1.73	0.41
1:E:300:GLN:O	1:E:304:ASP:HB2	2.20	0.41
1:E:340:THR:HG22	1:E:341:ILE:N	2.35	0.41
1:E:438:LEU:O	1:E:442:ILE:HG13	2.20	0.41
1:E:743:PRO:HD2	1:E:747:MET:SD	2.61	0.41
1:E:781:LEU:HD23	1:E:784:LEU:HD12	2.01	0.41
1:F:289:ILE:HD12	1:F:289:ILE:HA	1.81	0.41
1:F:658:THR:O	1:F:662:LEU:HD12	2.21	0.41
1:A:254:ILE:O	1:A:460:PHE:HA	2.21	0.41
1:C:82:LYS:HE2	1:C:82:LYS:HB3	1.90	0.41
1:D:226:GLN:C	1:D:229:PRO:HD2	2.40	0.41
1:D:292:TYR:CE2	1:D:331:MET:HB3	2.56	0.41
1:D:417:ALA:C	1:D:418:GLN:HE21	2.24	0.41
1:D:528:ILE:HG23	1:D:538:LEU:HG	2.02	0.41
1:D:701:VAL:O	1:D:705:LEU:HG	2.19	0.41
1:E:61:LEU:HG	1:E:66:LYS:O	2.20	0.41
1:E:121:CYS:O	1:E:683:ARG:HG2	2.21	0.41
1:E:254:ILE:O	1:E:460:PHE:HA	2.20	0.41
1:B:362:LEU:HA	1:B:362:LEU:HD23	1.86	0.41
1:B:566:HIS:O	1:B:569:PHE:N	2.53	0.41
1:D:434:LYS:HG2	1:D:625:TRP:CZ2	2.56	0.41
1:E:222:LYS:O	1:E:226:GLN:HG2	2.21	0.41
1:E:540:LEU:HD12	1:E:559:LEU:CD1	2.51	0.41
1:A:35:VAL:HG21	1:A:75:ILE:CG2	2.51	0.41
1:A:159:THR:O	1:A:163:SER:HB2	2.21	0.41
1:A:419:THR:O	1:A:420:LYS:C	2.59	0.41
1:A:427:ILE:HD13	1:A:427:ILE:HA	1.75	0.41
1:A:677:THR:O	1:A:679:PRO:HD3	2.21	0.41
1:A:742:ILE:HG12	1:A:752:ALA:HB1	2.03	0.41
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.74	0.41
1:B:107:ARG:HD3	1:B:115:THR:OG1	2.21	0.41
1:B:527:LEU:HB2	1:B:566:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:H	1:C:41:LYS:HG2	1.46	0.41
1:C:113:ILE:O	1:C:123:VAL:HA	2.21	0.41
1:C:671:MET:O	1:C:675:ARG:HD2	2.21	0.41
1:D:419:THR:O	1:D:420:LYS:C	2.58	0.41
1:D:663:TYR:CE2	1:D:667:LEU:HD22	2.56	0.41
1:E:291:TYR:HA	1:E:310:PHE:HE1	1.86	0.41
1:E:297:ALA:HB3	1:E:302:ARG:HD2	2.03	0.41
1:E:731:ARG:HH11	1:E:731:ARG:CG	2.29	0.41
1:F:107:ARG:NH1	1:F:114:TYR:O	2.54	0.41
1:F:114:TYR:CE1	1:F:153:ILE:HB	2.56	0.41
1:F:117:SER:OG	1:F:120:PHE:CE2	2.72	0.41
1:F:310:PHE:CE1	1:F:320:HIS:HD2	2.39	0.41
1:F:731:ARG:HA	1:F:756:MET:HE1	2.03	0.41
1:A:121:CYS:O	1:A:683:ARG:HG2	2.21	0.41
1:A:225:LEU:N	1:A:225:LEU:CD2	2.82	0.41
1:A:552:ASP:HA	1:A:598:LEU:HD12	2.03	0.41
1:B:36:TRP:HB2	1:B:76:GLN:O	2.21	0.41
1:B:90:ALA:O	1:B:718:ARG:NH1	2.53	0.41
1:B:434:LYS:HG2	1:B:625:TRP:CZ2	2.53	0.41
1:B:743:PRO:HD2	1:B:747:MET:SD	2.60	0.41
1:C:38:PRO:HD3	1:C:74:ASP:O	2.21	0.41
1:C:184:THR:HG22	1:C:188:LYS:HE3	2.02	0.41
1:C:365:ILE:HG23	1:C:378:MET:HE3	2.03	0.41
1:C:403:LEU:HD23	1:C:403:LEU:HA	1.94	0.41
1:C:781:LEU:HD23	1:C:784:LEU:HD12	2.02	0.41
1:E:35:VAL:HG21	1:E:75:ILE:HG22	2.02	0.41
1:E:164:MET:SD	1:E:459:SER:HB2	2.61	0.41
1:E:239:THR:HG23	1:E:245:SER:HB3	2.03	0.41
1:F:393:ILE:HD11	1:F:612:LEU:O	2.21	0.41
1:A:79:ASN:OD1	1:A:93:THR:HB	2.21	0.40
1:A:721:PHE:CD1	1:A:721:PHE:N	2.89	0.40
1:B:763:ASP:OD1	1:B:764:PRO:HD2	2.21	0.40
1:C:226:GLN:C	1:C:229:PRO:HD2	2.41	0.40
1:C:419:THR:H	1:C:422:GLN:CG	2.26	0.40
1:D:58:THR:HA	1:D:69:THR:HA	2.02	0.40
1:D:145:LYS:CB	1:D:148:GLU:HG3	2.43	0.40
1:F:291:TYR:HA	1:F:310:PHE:HE1	1.85	0.40
1:F:690:GLU:C	1:F:692:ARG:N	2.72	0.40
1:A:125:ASN:O	1:A:687:PRO:HG3	2.21	0.40
1:A:340:THR:HG22	1:A:341:ILE:N	2.36	0.40
1:A:606:ASN:O	1:A:609:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:MET:CE	1:A:751:GLN:CB	3.00	0.40
1:C:35:VAL:HG21	1:C:75:ILE:CG2	2.51	0.40
1:C:690:GLU:C	1:C:692:ARG:N	2.73	0.40
1:C:721:PHE:HB2	1:C:775:PHE:HB3	2.02	0.40
1:C:747:MET:HG3	1:C:752:ALA:HB2	2.03	0.40
1:D:184:THR:HG22	1:D:188:LYS:HE3	2.03	0.40
1:E:35:VAL:N	1:E:47:ALA:O	2.51	0.40
1:E:402:ILE:HG22	1:E:403:LEU:N	2.36	0.40
1:F:167:ASP:HB2	1:F:169:GLU:HG2	2.03	0.40
1:F:323:ILE:HG22	1:F:324:PRO:N	2.35	0.40
1:F:345:THR:HG23	1:F:348:GLU:OE1	2.21	0.40
1:F:734:TYR:OH	1:F:781:LEU:HD22	2.21	0.40
1:A:445:ARG:HH12	1:A:449:ALA:HB2	1.86	0.40
1:A:541:LEU:O	1:A:544:GLU:N	2.54	0.40
1:C:35:VAL:N	1:C:47:ALA:O	2.55	0.40
1:C:61:LEU:O	1:C:65:GLY:CA	2.70	0.40
1:C:107:ARG:HD3	1:C:115:THR:OG1	2.21	0.40
1:C:228:ASN:O	1:C:229:PRO:C	2.59	0.40
1:C:742:ILE:HG23	1:C:743:PRO:CD	2.47	0.40
1:D:38:PRO:HD3	1:D:74:ASP:O	2.22	0.40
1:D:126:PRO:HB3	1:D:130:LEU:HD11	2.03	0.40
1:D:185:GLU:O	1:D:189:LYS:HG2	2.22	0.40
1:E:493:PHE:CZ	1:E:497:MET:HG3	2.56	0.40
1:E:721:PHE:CB	1:E:775:PHE:HB3	2.50	0.40
1:F:185:GLU:O	1:F:189:LYS:HG2	2.21	0.40
1:F:333:GLN:O	1:F:337:GLU:HB2	2.20	0.40
1:A:228:ASN:O	1:A:229:PRO:C	2.60	0.40
1:C:285:ARG:HB2	1:C:291:TYR:CE2	2.56	0.40
1:C:525:ILE:O	1:C:529:GLU:CG	2.70	0.40
1:E:35:VAL:HG11	1:E:75:ILE:CG2	2.51	0.40
1:E:378:MET:HG3	1:E:378:MET:O	2.22	0.40
1:A:526:GLU:OE1	1:A:530:ARG:HD3	2.22	0.40
1:A:701:VAL:O	1:A:705:LEU:HG	2.21	0.40
1:B:236:ASN:ND2	1:B:244:ASN:O	2.55	0.40
1:C:339:MET:CE	1:C:352:ILE:HD13	2.52	0.40
1:C:378:MET:HE1	1:C:384:ALA:CB	2.48	0.40
1:E:58:THR:HA	1:E:69:THR:HA	2.04	0.40
1:E:278:ILE:CD1	1:E:432:LYS:HD3	2.52	0.40
1:F:316:LEU:O	1:F:317:SER:C	2.60	0.40
1:F:544:GLU:OE1	1:F:544:GLU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/791 (83%)	582 (89%)	63 (10%)	10 (2%)	10	34
1	B	655/791 (83%)	586 (90%)	59 (9%)	10 (2%)	10	34
1	C	655/791 (83%)	583 (89%)	63 (10%)	9 (1%)	11	36
1	D	655/791 (83%)	583 (89%)	62 (10%)	10 (2%)	10	34
1	E	655/791 (83%)	581 (89%)	62 (10%)	12 (2%)	8	29
1	F	655/791 (83%)	585 (89%)	59 (9%)	11 (2%)	9	31
All	All	3930/4746 (83%)	3500 (89%)	368 (9%)	62 (2%)	9	32

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	324	PRO
1	A	533	ASN
1	A	564	GLY
1	B	317	SER
1	B	324	PRO
1	B	533	ASN
1	B	564	GLY
1	C	317	SER
1	C	324	PRO
1	C	533	ASN
1	C	564	GLY
1	D	317	SER
1	D	324	PRO
1	D	533	ASN
1	D	564	GLY
1	E	317	SER
1	E	533	ASN
1	E	564	GLY
1	F	317	SER

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Mol	Chain	Res	Type
1	F	324	PRO
1	F	533	ASN
1	F	564	GLY
1	A	319	GLY
1	A	530	ARG
1	A	607	ASP
1	B	319	GLY
1	B	530	ARG
1	B	607	ASP
1	C	319	GLY
1	C	530	ARG
1	C	607	ASP
1	D	319	GLY
1	D	530	ARG
1	E	319	GLY
1	E	324	PRO
1	E	607	ASP
1	F	319	GLY
1	F	607	ASP
1	D	607	ASP
1	E	531	PRO
1	F	531	PRO
1	A	531	PRO
1	B	531	PRO
1	C	531	PRO
1	D	531	PRO
1	E	530	ARG
1	F	530	ARG
1	A	523	PRO
1	B	523	PRO
1	C	523	PRO
1	D	265	ALA
1	D	523	PRO
1	E	265	ALA
1	E	523	PRO
1	F	271	LEU
1	F	523	PRO
1	A	271	LEU
1	B	271	LEU
1	E	271	LEU
1	E	566	HIS
1	F	566	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	555/696 (80%)	462 (83%)	93 (17%)	2 6
1	B	555/696 (80%)	463 (83%)	92 (17%)	2 7
1	C	555/696 (80%)	461 (83%)	94 (17%)	2 6
1	D	555/696 (80%)	463 (83%)	92 (17%)	2 7
1	E	555/696 (80%)	463 (83%)	92 (17%)	2 7
1	F	555/696 (80%)	460 (83%)	95 (17%)	2 6
All	All	3330/4176 (80%)	2772 (83%)	558 (17%)	2 6

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	VAL
1	A	39	SER
1	A	41	LYS
1	A	42	HIS
1	A	48	SER
1	A	77	LYS
1	A	82	LYS
1	A	86	VAL
1	A	91	GLU
1	A	110	SER
1	A	124	ILE
1	A	127	TYR
1	A	128	LYS
1	A	135	GLU
1	A	142	LYS
1	A	145	LYS
1	A	166	GLN
1	A	167	ASP
1	A	174	LEU
1	A	189	LYS
1	A	199	SER

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Mol	Chain	Res	Type
1	A	225	LEU
1	A	232	GLU
1	A	250	LYS
1	A	259	THR
1	A	268	GLU
1	A	274	LYS
1	A	275	SER
1	A	278	ILE
1	A	285	ARG
1	A	302	ARG
1	A	303	ASN
1	A	308	GLU
1	A	311	ASN
1	A	314	THR
1	A	317	SER
1	A	323	ILE
1	A	326	GLN
1	A	327	GLN
1	A	329	ASP
1	A	340	THR
1	A	377	SER
1	A	393	ILE
1	A	402	ILE
1	A	404	THR
1	A	419	THR
1	A	422	GLN
1	A	434	LYS
1	A	459	SER
1	A	460	PHE
1	A	473	GLU
1	A	484	TYR
1	A	488	LYS
1	A	499	ILE
1	A	501	GLU
1	A	504	GLU
1	A	506	GLN
1	A	522	GLN
1	A	544	GLU
1	A	545	CYS
1	A	554	SER
1	A	560	ILE
1	A	572	SER

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Mol	Chain	Res	Type
1	A	589	LYS
1	A	591	THR
1	A	593	ASN
1	A	599	THR
1	A	606	ASN
1	A	607	ASP
1	A	608	ASN
1	A	609	VAL
1	A	615	GLN
1	A	623	ASP
1	A	664	LYS
1	A	675	ARG
1	A	683	ARG
1	A	702	LEU
1	A	708	ASN
1	A	719	GLN
1	A	723	ASN
1	A	731	ARG
1	A	732	GLN
1	A	733	ARG
1	A	735	GLU
1	A	748	ASP
1	A	750	LYS
1	A	754	ILE
1	A	755	LEU
1	A	771	GLN
1	A	773	LYS
1	A	778	THR
1	A	788	ARG
1	B	34	LEU
1	B	35	VAL
1	B	39	SER
1	B	41	LYS
1	B	42	HIS
1	B	48	SER
1	B	77	LYS
1	B	82	LYS
1	B	86	VAL
1	B	91	GLU
1	B	110	SER
1	B	124	ILE
1	B	127	TYR

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Mol	Chain	Res	Type
1	B	128	LYS
1	B	135	GLU
1	B	142	LYS
1	B	145	LYS
1	B	166	GLN
1	B	167	ASP
1	B	174	LEU
1	B	189	LYS
1	B	199	SER
1	B	225	LEU
1	B	232	GLU
1	B	250	LYS
1	B	259	THR
1	B	268	GLU
1	B	274	LYS
1	B	275	SER
1	B	278	ILE
1	B	285	ARG
1	B	302	ARG
1	B	303	ASN
1	B	308	GLU
1	B	311	ASN
1	B	314	THR
1	B	317	SER
1	B	323	ILE
1	B	326	GLN
1	B	327	GLN
1	B	329	ASP
1	B	340	THR
1	B	377	SER
1	B	393	ILE
1	B	402	ILE
1	B	404	THR
1	B	419	THR
1	B	422	GLN
1	B	434	LYS
1	B	459	SER
1	B	473	GLU
1	B	484	TYR
1	B	488	LYS
1	B	499	ILE
1	B	501	GLU

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Mol	Chain	Res	Type
1	B	504	GLU
1	B	506	GLN
1	B	522	GLN
1	B	544	GLU
1	B	545	CYS
1	B	554	SER
1	B	560	ILE
1	B	572	SER
1	B	589	LYS
1	B	591	THR
1	B	593	ASN
1	B	599	THR
1	B	605	LEU
1	B	606	ASN
1	B	607	ASP
1	B	608	ASN
1	B	609	VAL
1	B	615	GLN
1	B	623	ASP
1	B	664	LYS
1	B	675	ARG
1	B	683	ARG
1	B	708	ASN
1	B	719	GLN
1	B	723	ASN
1	B	731	ARG
1	B	732	GLN
1	B	733	ARG
1	B	735	GLU
1	B	748	ASP
1	B	750	LYS
1	B	754	ILE
1	B	755	LEU
1	B	771	GLN
1	B	773	LYS
1	B	778	THR
1	B	788	ARG
1	C	34	LEU
1	C	35	VAL
1	C	39	SER
1	C	41	LYS
1	C	42	HIS

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Mol	Chain	Res	Type
1	C	48	SER
1	C	77	LYS
1	C	82	LYS
1	C	86	VAL
1	C	91	GLU
1	C	110	SER
1	C	124	ILE
1	C	127	TYR
1	C	128	LYS
1	C	135	GLU
1	C	142	LYS
1	C	145	LYS
1	C	166	GLN
1	C	167	ASP
1	C	174	LEU
1	C	189	LYS
1	C	199	SER
1	C	225	LEU
1	C	232	GLU
1	C	250	LYS
1	C	259	THR
1	C	268	GLU
1	C	274	LYS
1	C	275	SER
1	C	278	ILE
1	C	285	ARG
1	C	302	ARG
1	C	303	ASN
1	C	308	GLU
1	C	311	ASN
1	C	314	THR
1	C	317	SER
1	C	323	ILE
1	C	326	GLN
1	C	327	GLN
1	C	329	ASP
1	C	340	THR
1	C	377	SER
1	C	393	ILE
1	C	402	ILE
1	C	404	THR
1	C	419	THR

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Mol	Chain	Res	Type
1	C	422	GLN
1	C	434	LYS
1	C	459	SER
1	C	460	PHE
1	C	473	GLU
1	C	484	TYR
1	C	488	LYS
1	C	499	ILE
1	C	501	GLU
1	C	504	GLU
1	C	506	GLN
1	C	522	GLN
1	C	544	GLU
1	C	545	CYS
1	C	554	SER
1	C	560	ILE
1	C	572	SER
1	C	589	LYS
1	C	591	THR
1	C	593	ASN
1	C	599	THR
1	C	605	LEU
1	C	606	ASN
1	C	607	ASP
1	C	608	ASN
1	C	609	VAL
1	C	615	GLN
1	C	623	ASP
1	C	664	LYS
1	C	675	ARG
1	C	683	ARG
1	C	702	LEU
1	C	708	ASN
1	C	719	GLN
1	C	723	ASN
1	C	731	ARG
1	C	732	GLN
1	C	733	ARG
1	C	735	GLU
1	C	748	ASP
1	C	750	LYS
1	C	754	ILE

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Mol	Chain	Res	Type
1	C	755	LEU
1	C	771	GLN
1	C	773	LYS
1	C	778	THR
1	C	788	ARG
1	D	34	LEU
1	D	35	VAL
1	D	39	SER
1	D	41	LYS
1	D	42	HIS
1	D	48	SER
1	D	77	LYS
1	D	82	LYS
1	D	86	VAL
1	D	91	GLU
1	D	110	SER
1	D	124	ILE
1	D	127	TYR
1	D	128	LYS
1	D	135	GLU
1	D	142	LYS
1	D	145	LYS
1	D	166	GLN
1	D	167	ASP
1	D	174	LEU
1	D	189	LYS
1	D	199	SER
1	D	225	LEU
1	D	232	GLU
1	D	250	LYS
1	D	259	THR
1	D	268	GLU
1	D	274	LYS
1	D	275	SER
1	D	278	ILE
1	D	285	ARG
1	D	302	ARG
1	D	303	ASN
1	D	308	GLU
1	D	311	ASN
1	D	314	THR
1	D	317	SER

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Mol	Chain	Res	Type
1	D	323	ILE
1	D	326	GLN
1	D	327	GLN
1	D	329	ASP
1	D	340	THR
1	D	377	SER
1	D	393	ILE
1	D	402	ILE
1	D	404	THR
1	D	419	THR
1	D	422	GLN
1	D	434	LYS
1	D	459	SER
1	D	473	GLU
1	D	484	TYR
1	D	488	LYS
1	D	499	ILE
1	D	501	GLU
1	D	504	GLU
1	D	506	GLN
1	D	522	GLN
1	D	544	GLU
1	D	545	CYS
1	D	554	SER
1	D	560	ILE
1	D	572	SER
1	D	589	LYS
1	D	591	THR
1	D	593	ASN
1	D	599	THR
1	D	606	ASN
1	D	607	ASP
1	D	608	ASN
1	D	609	VAL
1	D	615	GLN
1	D	623	ASP
1	D	664	LYS
1	D	675	ARG
1	D	683	ARG
1	D	702	LEU
1	D	708	ASN
1	D	719	GLN

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Mol	Chain	Res	Type
1	D	723	ASN
1	D	731	ARG
1	D	732	GLN
1	D	733	ARG
1	D	735	GLU
1	D	748	ASP
1	D	750	LYS
1	D	754	ILE
1	D	755	LEU
1	D	771	GLN
1	D	773	LYS
1	D	778	THR
1	D	788	ARG
1	E	34	LEU
1	E	35	VAL
1	E	39	SER
1	E	41	LYS
1	E	42	HIS
1	E	48	SER
1	E	77	LYS
1	E	82	LYS
1	E	86	VAL
1	E	91	GLU
1	E	110	SER
1	E	124	ILE
1	E	127	TYR
1	E	128	LYS
1	E	135	GLU
1	E	142	LYS
1	E	145	LYS
1	E	166	GLN
1	E	167	ASP
1	E	174	LEU
1	E	189	LYS
1	E	199	SER
1	E	225	LEU
1	E	232	GLU
1	E	250	LYS
1	E	259	THR
1	E	268	GLU
1	E	274	LYS
1	E	275	SER

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Mol	Chain	Res	Type
1	E	278	ILE
1	E	285	ARG
1	E	302	ARG
1	E	303	ASN
1	E	308	GLU
1	E	311	ASN
1	E	314	THR
1	E	323	ILE
1	E	324	PRO
1	E	326	GLN
1	E	327	GLN
1	E	329	ASP
1	E	377	SER
1	E	393	ILE
1	E	402	ILE
1	E	404	THR
1	E	419	THR
1	E	422	GLN
1	E	434	LYS
1	E	459	SER
1	E	460	PHE
1	E	473	GLU
1	E	484	TYR
1	E	488	LYS
1	E	499	ILE
1	E	501	GLU
1	E	504	GLU
1	E	506	GLN
1	E	522	GLN
1	E	544	GLU
1	E	545	CYS
1	E	554	SER
1	E	560	ILE
1	E	572	SER
1	E	589	LYS
1	E	591	THR
1	E	593	ASN
1	E	599	THR
1	E	606	ASN
1	E	607	ASP
1	E	608	ASN
1	E	609	VAL

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Mol	Chain	Res	Type
1	E	615	GLN
1	E	623	ASP
1	E	664	LYS
1	E	675	ARG
1	E	683	ARG
1	E	702	LEU
1	E	708	ASN
1	E	719	GLN
1	E	723	ASN
1	E	731	ARG
1	E	732	GLN
1	E	733	ARG
1	E	735	GLU
1	E	748	ASP
1	E	750	LYS
1	E	754	ILE
1	E	755	LEU
1	E	771	GLN
1	E	773	LYS
1	E	778	THR
1	E	788	ARG
1	F	34	LEU
1	F	35	VAL
1	F	39	SER
1	F	41	LYS
1	F	42	HIS
1	F	48	SER
1	F	77	LYS
1	F	82	LYS
1	F	86	VAL
1	F	91	GLU
1	F	110	SER
1	F	124	ILE
1	F	127	TYR
1	F	128	LYS
1	F	135	GLU
1	F	142	LYS
1	F	145	LYS
1	F	166	GLN
1	F	167	ASP
1	F	174	LEU
1	F	189	LYS

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Mol	Chain	Res	Type
1	F	199	SER
1	F	225	LEU
1	F	232	GLU
1	F	250	LYS
1	F	259	THR
1	F	268	GLU
1	F	274	LYS
1	F	275	SER
1	F	278	ILE
1	F	285	ARG
1	F	302	ARG
1	F	303	ASN
1	F	308	GLU
1	F	311	ASN
1	F	314	THR
1	F	323	ILE
1	F	324	PRO
1	F	326	GLN
1	F	327	GLN
1	F	329	ASP
1	F	340	THR
1	F	377	SER
1	F	393	ILE
1	F	402	ILE
1	F	404	THR
1	F	419	THR
1	F	422	GLN
1	F	434	LYS
1	F	459	SER
1	F	460	PHE
1	F	473	GLU
1	F	484	TYR
1	F	488	LYS
1	F	499	ILE
1	F	501	GLU
1	F	504	GLU
1	F	506	GLN
1	F	522	GLN
1	F	544	GLU
1	F	545	CYS
1	F	554	SER
1	F	560	ILE

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Mol	Chain	Res	Type
1	F	568	LYS
1	F	572	SER
1	F	589	LYS
1	F	591	THR
1	F	593	ASN
1	F	599	THR
1	F	605	LEU
1	F	606	ASN
1	F	607	ASP
1	F	608	ASN
1	F	609	VAL
1	F	615	GLN
1	F	623	ASP
1	F	664	LYS
1	F	675	ARG
1	F	683	ARG
1	F	702	LEU
1	F	708	ASN
1	F	719	GLN
1	F	723	ASN
1	F	731	ARG
1	F	732	GLN
1	F	733	ARG
1	F	735	GLU
1	F	748	ASP
1	F	750	LYS
1	F	754	ILE
1	F	755	LEU
1	F	771	GLN
1	F	773	LYS
1	F	778	THR
1	F	788	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	303	ASN
1	A	327	GLN
1	A	333	GLN
1	A	418	GLN
1	A	422	GLN

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Mol	Chain	Res	Type
1	A	533	ASN
1	A	566	HIS
1	A	593	ASN
1	A	606	ASN
1	A	614	ASN
1	A	666	GLN
1	A	699	HIS
1	A	708	ASN
1	A	719	GLN
1	B	236	ASN
1	B	303	ASN
1	B	327	GLN
1	B	333	GLN
1	B	418	GLN
1	B	422	GLN
1	B	533	ASN
1	B	566	HIS
1	B	593	ASN
1	B	606	ASN
1	B	614	ASN
1	B	666	GLN
1	B	699	HIS
1	B	708	ASN
1	B	719	GLN
1	C	303	ASN
1	C	327	GLN
1	C	333	GLN
1	C	418	GLN
1	C	422	GLN
1	C	533	ASN
1	C	566	HIS
1	C	593	ASN
1	C	606	ASN
1	C	614	ASN
1	C	666	GLN
1	C	699	HIS
1	C	708	ASN
1	C	719	GLN
1	C	751	GLN
1	D	236	ASN
1	D	303	ASN
1	D	327	GLN

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Mol	Chain	Res	Type
1	D	333	GLN
1	D	418	GLN
1	D	422	GLN
1	D	533	ASN
1	D	566	HIS
1	D	593	ASN
1	D	606	ASN
1	D	614	ASN
1	D	666	GLN
1	D	699	HIS
1	D	708	ASN
1	D	719	GLN
1	D	751	GLN
1	E	236	ASN
1	E	303	ASN
1	E	327	GLN
1	E	333	GLN
1	E	418	GLN
1	E	422	GLN
1	E	533	ASN
1	E	566	HIS
1	E	593	ASN
1	E	606	ASN
1	E	614	ASN
1	E	666	GLN
1	E	699	HIS
1	E	708	ASN
1	E	719	GLN
1	E	751	GLN
1	F	303	ASN
1	F	327	GLN
1	F	333	GLN
1	F	418	GLN
1	F	422	GLN
1	F	533	ASN
1	F	566	HIS
1	F	593	ASN
1	F	606	ASN
1	F	614	ASN
1	F	666	GLN
1	F	699	HIS
1	F	708	ASN

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Mol	Chain	Res	Type
1	F	719	GLN
1	F	751	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ALF	C	999	2,4,5	0,4,4	-	-	-		
3	ALF	F	999	2,1,4	0,4,4	-	-	-		
3	ALF	D	999	2,1,4,5	0,4,4	-	-	-		
4	ADP	E	998	2,3	24,29,29	0.94	1 (4%)	29,45,45	1.08	1 (3%)
4	ADP	D	998	2,3	24,29,29	0.77	0	29,45,45	1.25	3 (10%)
4	ADP	B	998	2,3	24,29,29	0.78	0	29,45,45	1.24	3 (10%)
3	ALF	B	999	2,1,4,5	0,4,4	-	-	-		
4	ADP	F	998	2,3	24,29,29	1.06	2 (8%)	29,45,45	1.12	3 (10%)
3	ALF	A	999	2,4,5	0,4,4	-	-	-		
3	ALF	E	999	2,4	0,4,4	-	-	-		
4	ADP	A	998	2,3	24,29,29	0.77	0	29,45,45	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	C	998	2,3	24,29,29	0.78	0	29,45,45	1.24	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	E	998	2,3	-	5/12/32/32	0/3/3/3
4	ADP	D	998	2,3	-	5/12/32/32	0/3/3/3
4	ADP	B	998	2,3	-	5/12/32/32	0/3/3/3
4	ADP	F	998	2,3	-	5/12/32/32	0/3/3/3
4	ADP	A	998	2,3	-	5/12/32/32	0/3/3/3
4	ADP	C	998	2,3	-	5/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	998	ADP	PB-O3B	-2.23	1.46	1.54
4	E	998	ADP	O4'-C1'	-2.22	1.38	1.41
4	F	998	ADP	C2-N3	2.08	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	998	ADP	C5-C6-N6	2.90	124.77	120.35
4	C	998	ADP	C5-C6-N6	2.86	124.69	120.35
4	B	998	ADP	C5-C6-N6	2.84	124.67	120.35
4	A	998	ADP	C5-C6-N6	2.84	124.66	120.35
4	F	998	ADP	C5-C6-N6	2.46	124.08	120.35
4	A	998	ADP	O3'-C3'-C2'	2.44	119.72	111.82
4	D	998	ADP	O3'-C3'-C2'	2.43	119.69	111.82
4	B	998	ADP	O3'-C3'-C2'	2.42	119.66	111.82
4	C	998	ADP	O3'-C3'-C2'	2.41	119.63	111.82
4	F	998	ADP	O3'-C3'-C2'	2.30	119.27	111.82
4	C	998	ADP	O2B-PB-O3A	2.26	112.23	104.64
4	B	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	D	998	ADP	O2B-PB-O3A	2.26	112.20	104.64
4	A	998	ADP	O2B-PB-O3A	2.25	112.17	104.64
4	E	998	ADP	C5-C6-N6	2.19	123.68	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	998	ADP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	998	ADP	C5'-O5'-PA-O1A
4	A	998	ADP	C5'-O5'-PA-O2A
4	B	998	ADP	C5'-O5'-PA-O1A
4	B	998	ADP	C5'-O5'-PA-O2A
4	C	998	ADP	C5'-O5'-PA-O1A
4	C	998	ADP	C5'-O5'-PA-O2A
4	D	998	ADP	C5'-O5'-PA-O1A
4	D	998	ADP	C5'-O5'-PA-O2A
4	E	998	ADP	C5'-O5'-PA-O1A
4	E	998	ADP	C5'-O5'-PA-O2A
4	F	998	ADP	C5'-O5'-PA-O1A
4	F	998	ADP	C5'-O5'-PA-O2A
4	A	998	ADP	O4'-C4'-C5'-O5'
4	A	998	ADP	C3'-C4'-C5'-O5'
4	B	998	ADP	O4'-C4'-C5'-O5'
4	B	998	ADP	C3'-C4'-C5'-O5'
4	C	998	ADP	O4'-C4'-C5'-O5'
4	C	998	ADP	C3'-C4'-C5'-O5'
4	D	998	ADP	O4'-C4'-C5'-O5'
4	D	998	ADP	C3'-C4'-C5'-O5'
4	E	998	ADP	C3'-C4'-C5'-O5'
4	F	998	ADP	C3'-C4'-C5'-O5'
4	E	998	ADP	O4'-C4'-C5'-O5'
4	F	998	ADP	O4'-C4'-C5'-O5'
4	A	998	ADP	C5'-O5'-PA-O3A
4	B	998	ADP	C5'-O5'-PA-O3A
4	C	998	ADP	C5'-O5'-PA-O3A
4	D	998	ADP	C5'-O5'-PA-O3A
4	E	998	ADP	C5'-O5'-PA-O3A
4	F	998	ADP	C5'-O5'-PA-O3A

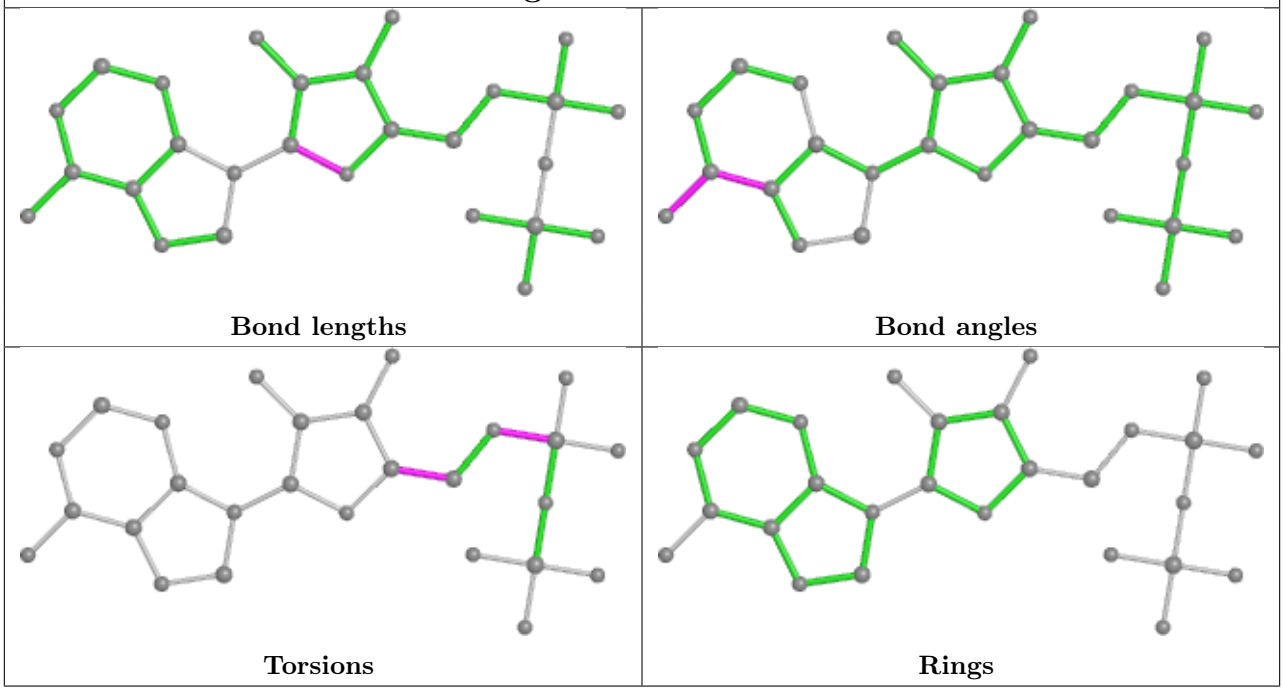
There are no ring outliers.

8 monomers are involved in 5 short contacts:

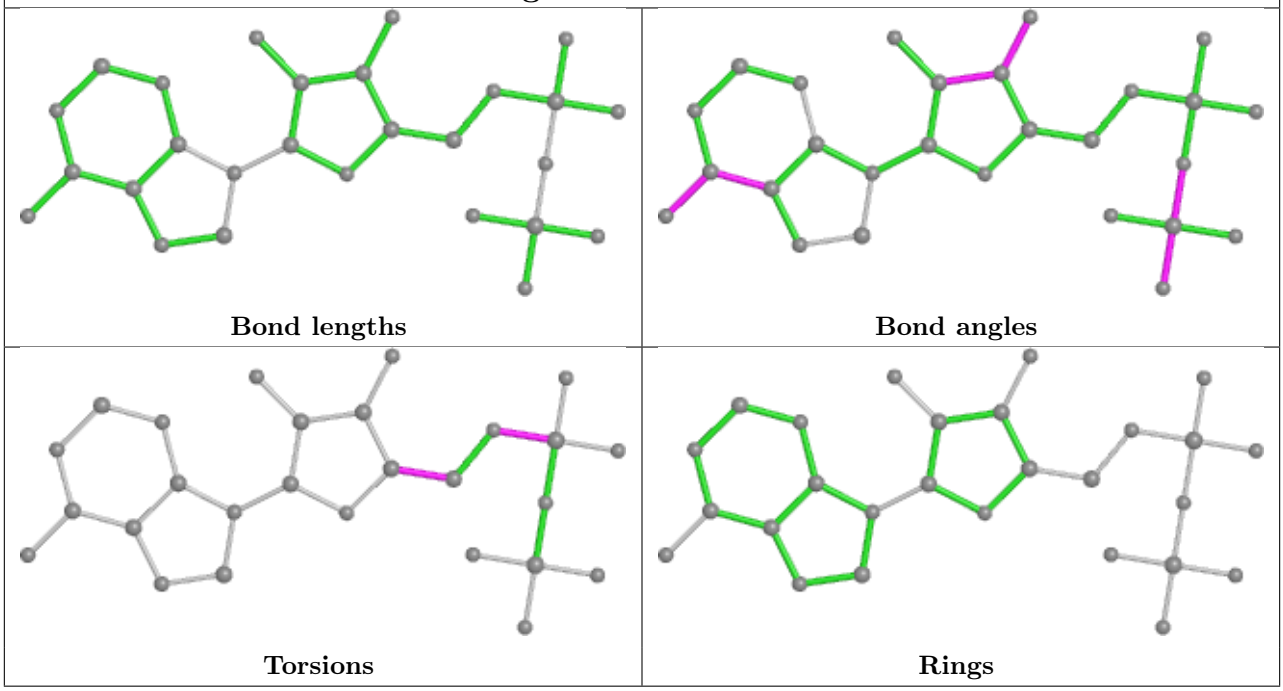
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	ALF	1	0
3	D	999	ALF	2	0
4	D	998	ADP	1	0
4	B	998	ADP	1	0
3	B	999	ALF	1	0
3	A	999	ALF	1	0
4	A	998	ADP	1	0
4	C	998	ADP	1	0

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

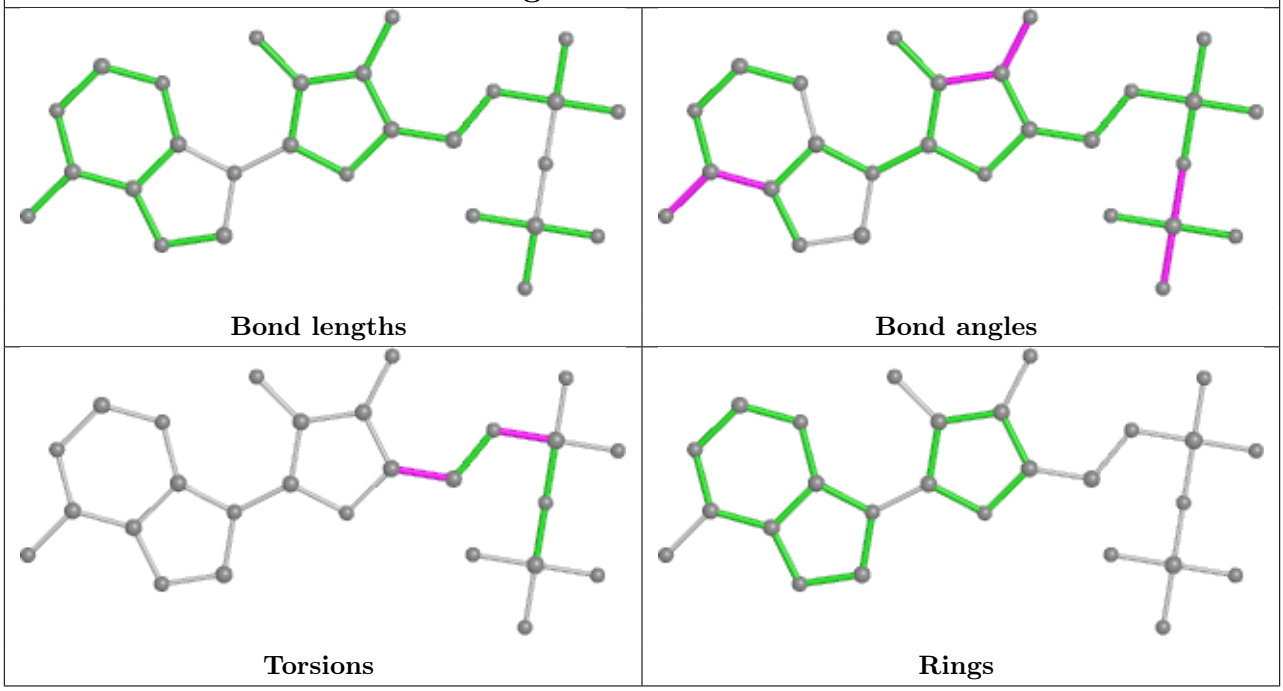
Ligand ADP E 998



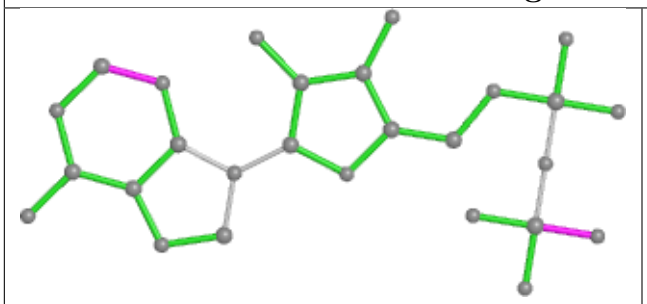
Ligand ADP D 998



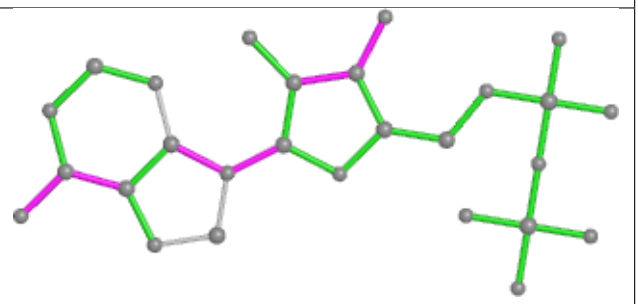
Ligand ADP B 998



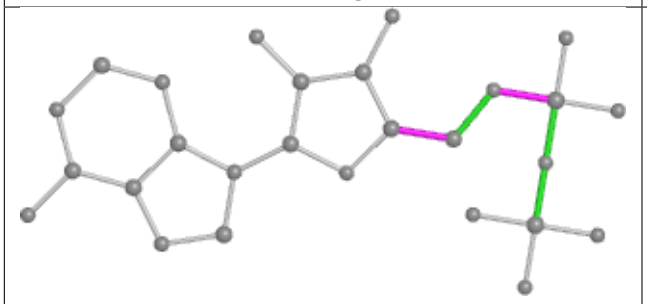
Ligand ADP F 998



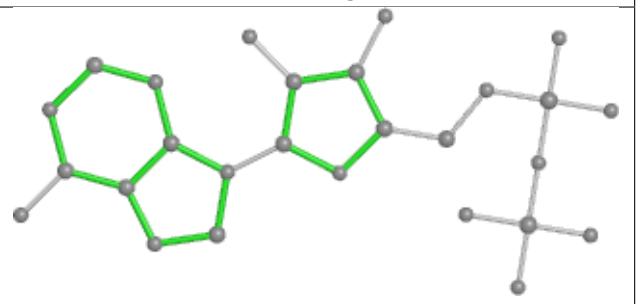
Bond lengths



Bond angles

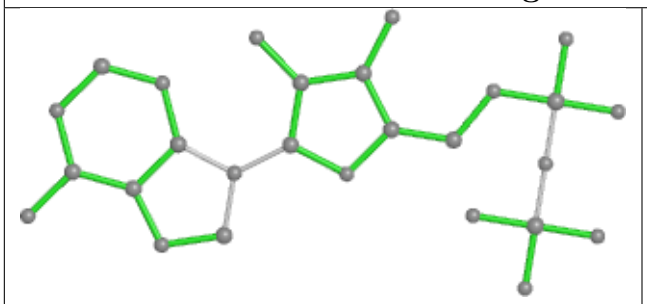


Torsions

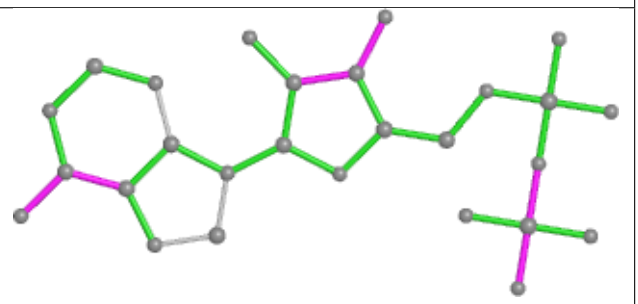


Rings

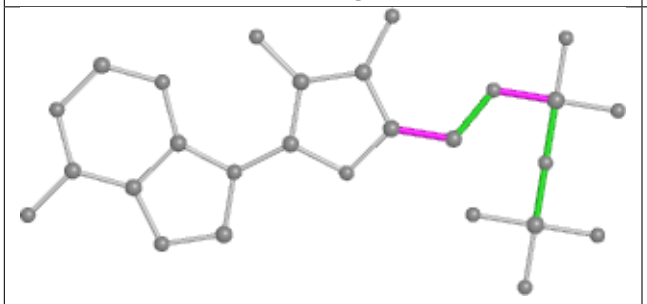
Ligand ADP A 998



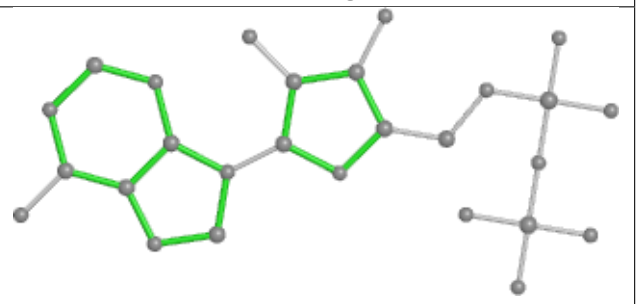
Bond lengths



Bond angles

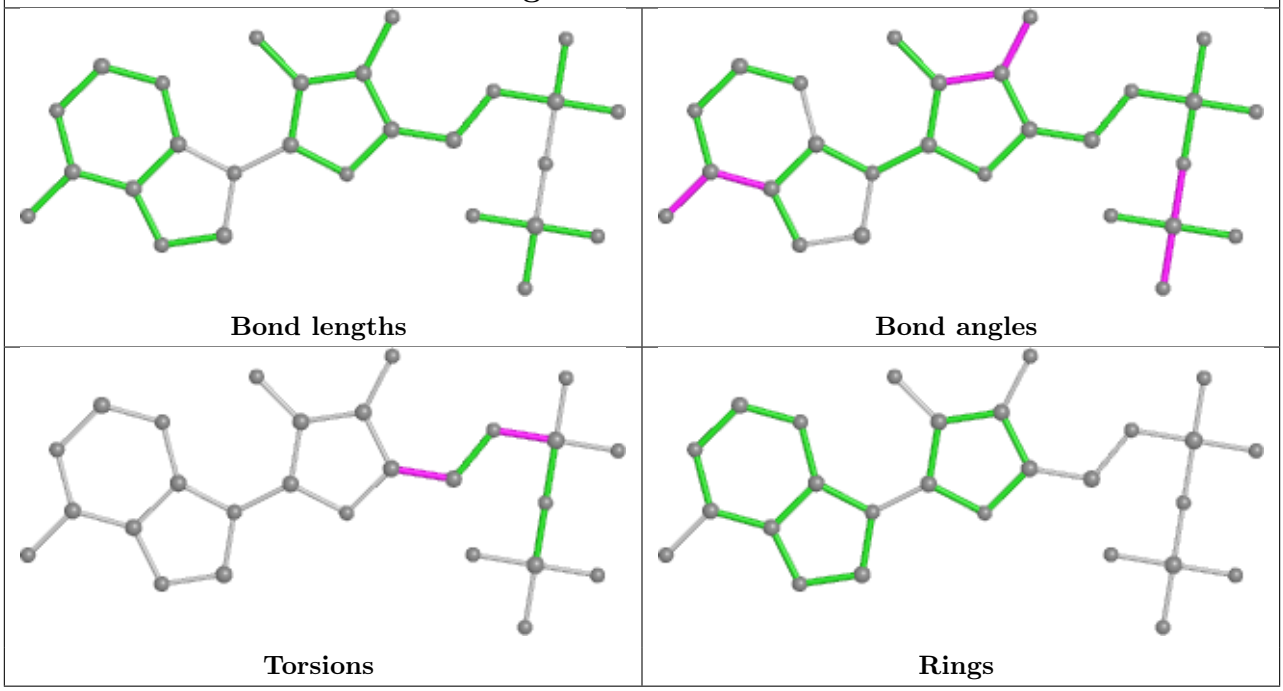


Torsions



Rings

Ligand ADP C 998



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.