



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:04 AM UTC

PDB ID : 8K3Y / pdb_00008k3y
EMDB ID : EMD-36867
Title : The "5+1" heteromeric structure of Lon protease consisting of a spiral pentamer with Y224S mutation and an N-terminal-truncated monomeric E613K mutant
Authors : Li, S.; Hsieh, K.Y.; Kuo, C.I.; Zhang, K.; Chang, C.I.
Deposited on : 2023-07-17
Resolution : 4.42 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

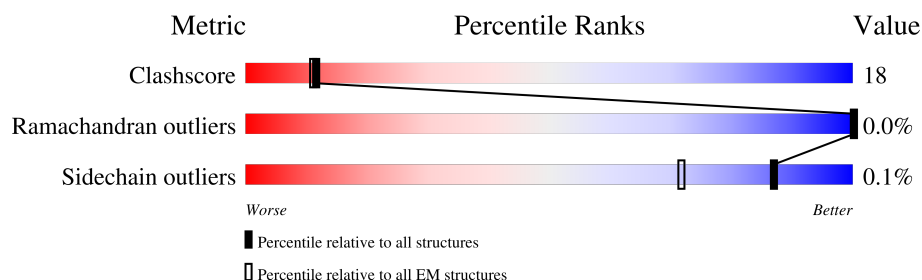
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.42 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	799	60% 37% .
1	B	799	62% 35% .
1	C	799	60% 36% .
1	D	799	63% 34% .
1	E	799	55% 42% . .
2	F	570	56% 37% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34589 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	773	Total	C	N	O	S	0	0
			6069	3832	1067	1149	21		
1	B	773	Total	C	N	O	S	0	0
			6069	3832	1067	1149	21		
1	C	773	Total	C	N	O	S	0	0
			6069	3832	1067	1149	21		
1	D	773	Total	C	N	O	S	0	0
			6069	3832	1067	1149	21		
1	E	773	Total	C	N	O	S	0	0
			6069	3832	1067	1149	21		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	SER	TYR	engineered mutation	UNP A0A059VAZ3
A	794	HIS	-	expression tag	UNP A0A059VAZ3
A	795	HIS	-	expression tag	UNP A0A059VAZ3
A	796	HIS	-	expression tag	UNP A0A059VAZ3
A	797	HIS	-	expression tag	UNP A0A059VAZ3
A	798	HIS	-	expression tag	UNP A0A059VAZ3
A	799	HIS	-	expression tag	UNP A0A059VAZ3
B	224	SER	TYR	engineered mutation	UNP A0A059VAZ3
B	794	HIS	-	expression tag	UNP A0A059VAZ3
B	795	HIS	-	expression tag	UNP A0A059VAZ3
B	796	HIS	-	expression tag	UNP A0A059VAZ3
B	797	HIS	-	expression tag	UNP A0A059VAZ3
B	798	HIS	-	expression tag	UNP A0A059VAZ3
B	799	HIS	-	expression tag	UNP A0A059VAZ3
C	224	SER	TYR	engineered mutation	UNP A0A059VAZ3
C	794	HIS	-	expression tag	UNP A0A059VAZ3
C	795	HIS	-	expression tag	UNP A0A059VAZ3
C	796	HIS	-	expression tag	UNP A0A059VAZ3
C	797	HIS	-	expression tag	UNP A0A059VAZ3
C	798	HIS	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	799	HIS	-	expression tag	UNP A0A059VAZ3
D	224	SER	TYR	engineered mutation	UNP A0A059VAZ3
D	794	HIS	-	expression tag	UNP A0A059VAZ3
D	795	HIS	-	expression tag	UNP A0A059VAZ3
D	796	HIS	-	expression tag	UNP A0A059VAZ3
D	797	HIS	-	expression tag	UNP A0A059VAZ3
D	798	HIS	-	expression tag	UNP A0A059VAZ3
D	799	HIS	-	expression tag	UNP A0A059VAZ3
E	224	SER	TYR	engineered mutation	UNP A0A059VAZ3
E	794	HIS	-	expression tag	UNP A0A059VAZ3
E	795	HIS	-	expression tag	UNP A0A059VAZ3
E	796	HIS	-	expression tag	UNP A0A059VAZ3
E	797	HIS	-	expression tag	UNP A0A059VAZ3
E	798	HIS	-	expression tag	UNP A0A059VAZ3
E	799	HIS	-	expression tag	UNP A0A059VAZ3

- Molecule 2 is a protein called Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	531	Total	C	N	O	S	0	0
			4136	2615	726	780	15		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	224	HIS	-	expression tag	UNP A0A059VAZ3
F	225	HIS	-	expression tag	UNP A0A059VAZ3
F	226	HIS	-	expression tag	UNP A0A059VAZ3
F	227	HIS	-	expression tag	UNP A0A059VAZ3
F	228	HIS	-	expression tag	UNP A0A059VAZ3
F	229	HIS	-	expression tag	UNP A0A059VAZ3
F	230	SER	-	expression tag	UNP A0A059VAZ3
F	231	SER	-	expression tag	UNP A0A059VAZ3
F	232	GLY	-	expression tag	UNP A0A059VAZ3
F	233	GLU	-	expression tag	UNP A0A059VAZ3
F	234	ASN	-	expression tag	UNP A0A059VAZ3
F	235	LEU	-	expression tag	UNP A0A059VAZ3
F	236	TYR	-	expression tag	UNP A0A059VAZ3
F	237	PHE	-	expression tag	UNP A0A059VAZ3
F	238	GLN	-	expression tag	UNP A0A059VAZ3
F	239	GLY	-	expression tag	UNP A0A059VAZ3
F	240	HIS	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	241	MET	-	expression tag	UNP A0A059VAZ3
F	613	LYS	GLU	engineered mutation	UNP A0A059VAZ3

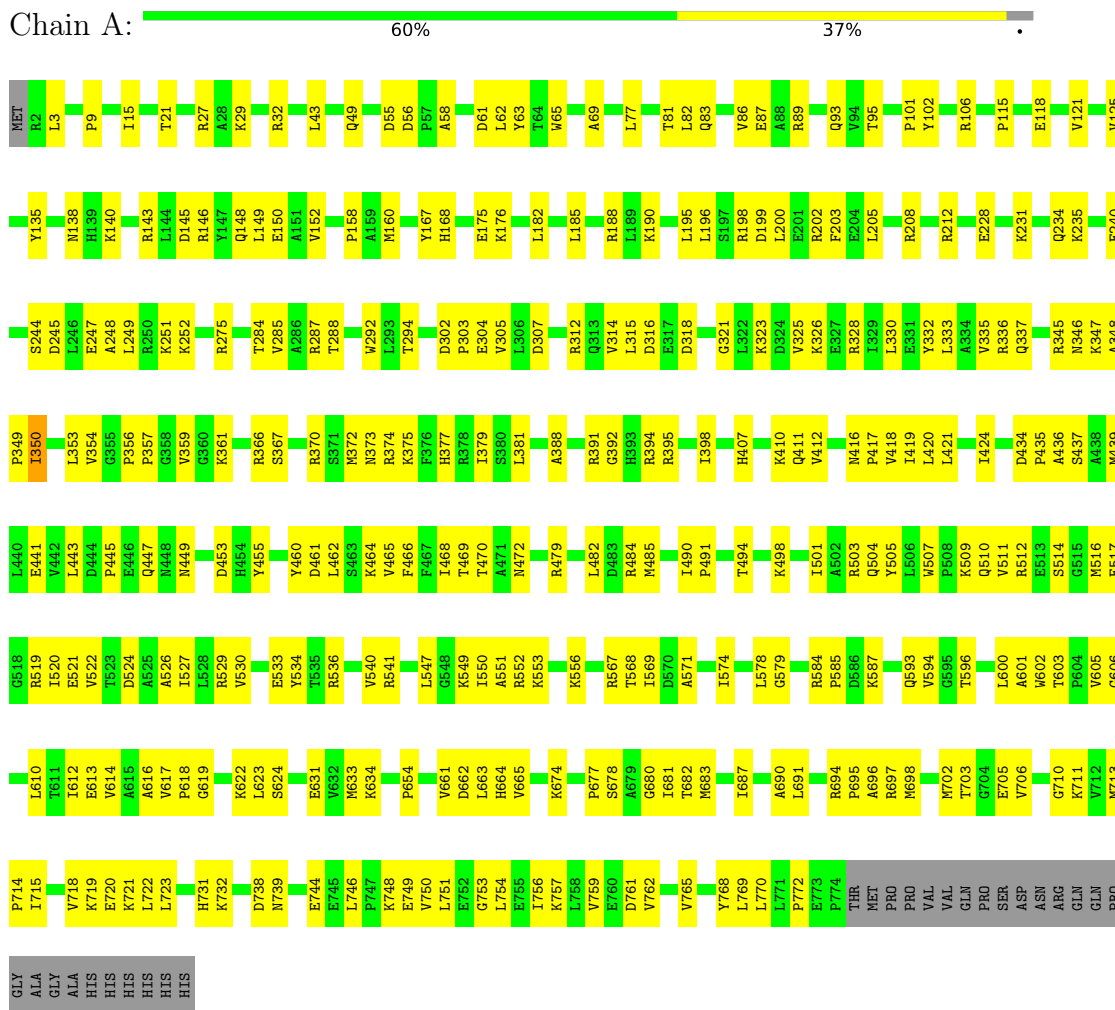
- # ADP

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

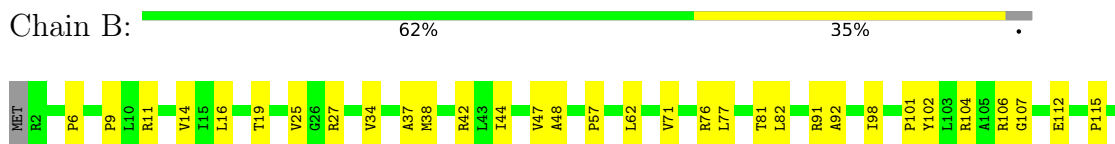
3 Residue-property plots

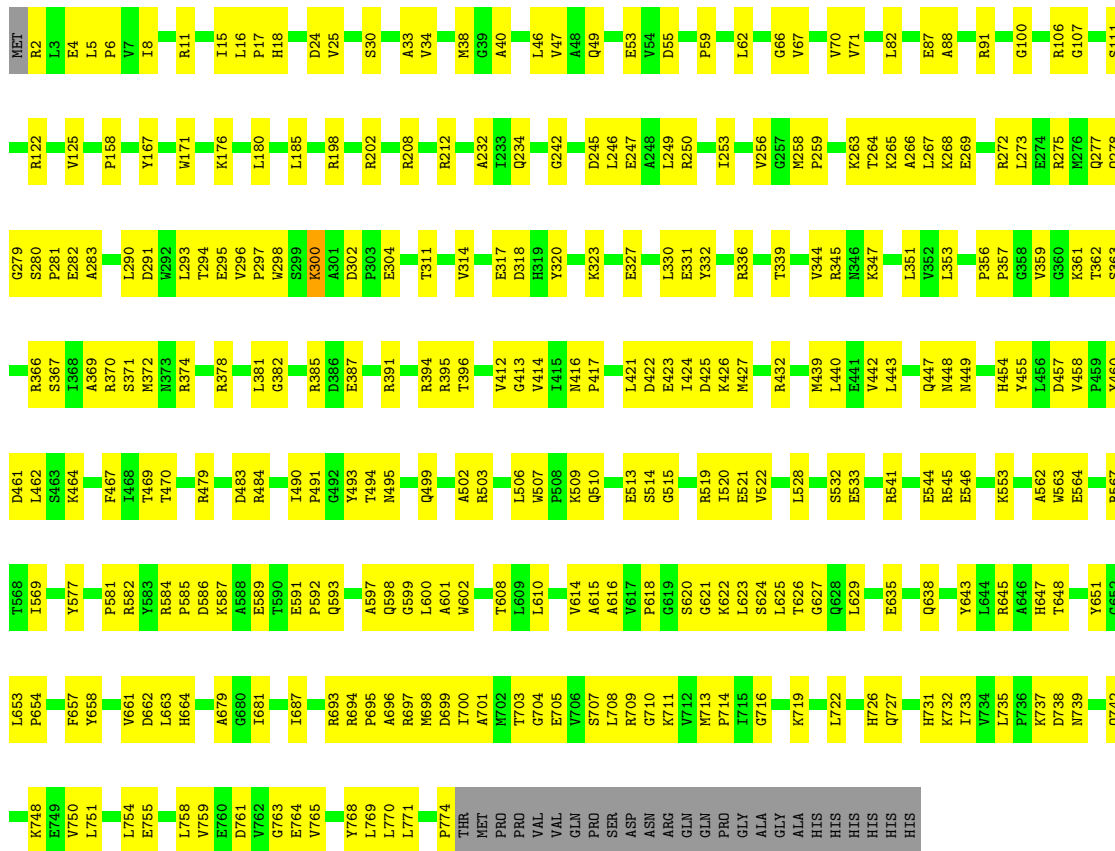
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: Lon protease



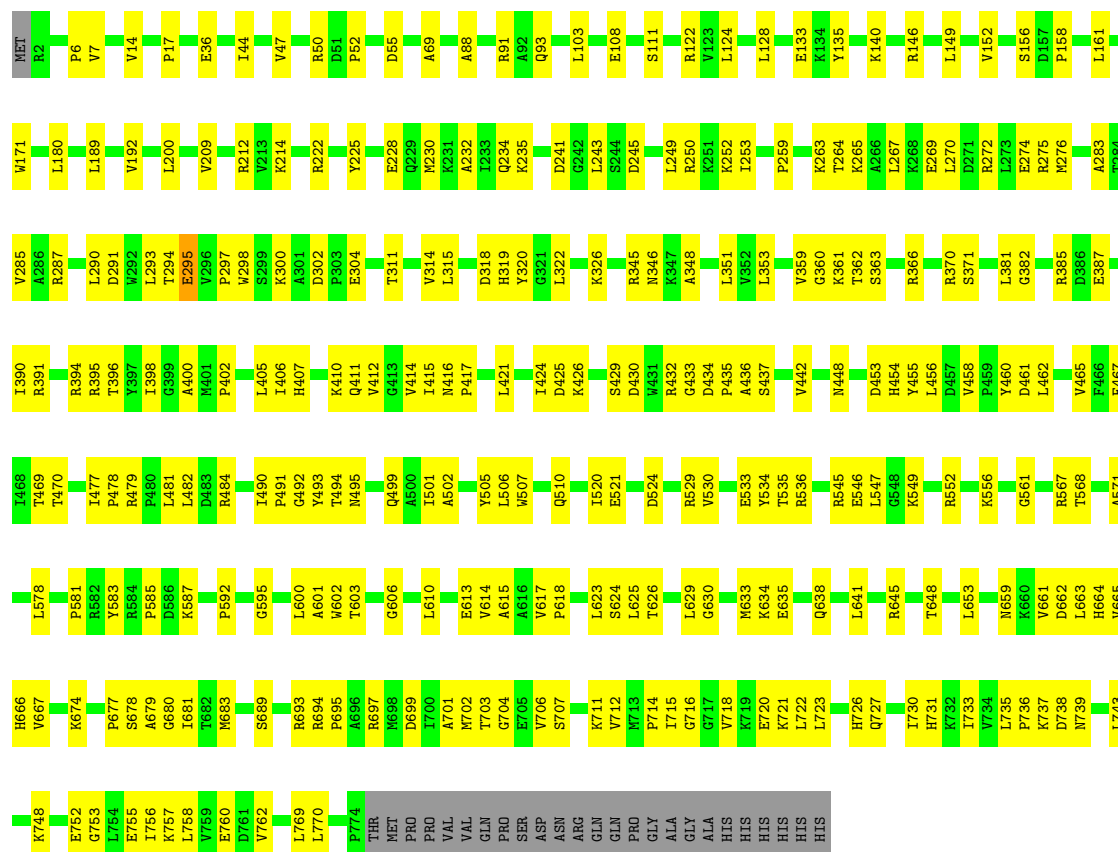
• Molecule 1: Lon protease





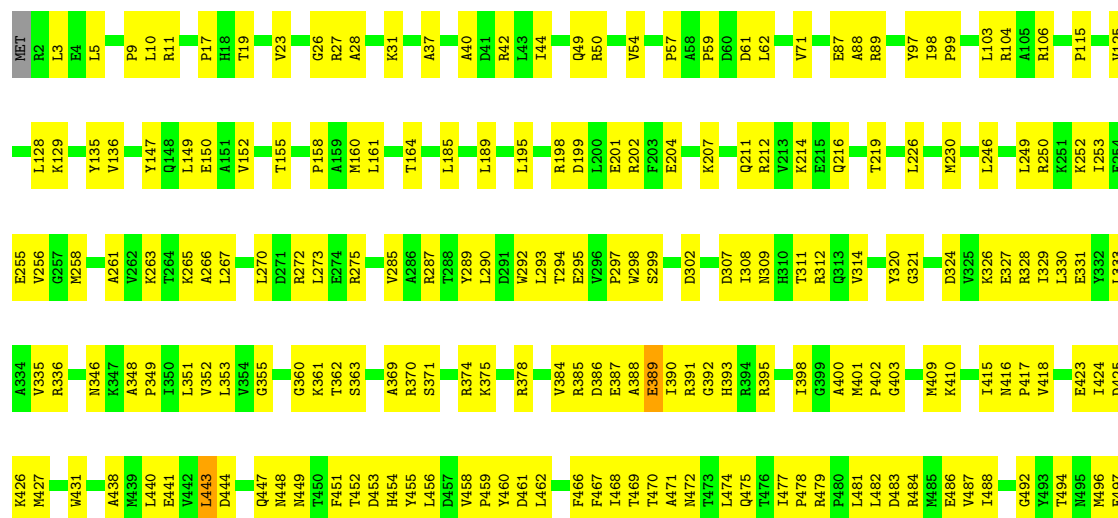
- Molecule 1: Lon protease

Chain D:  63% 34%



- Molecule 1: Lon protease

Chain E:  55% 42%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70828	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/6177	0.62	1/8370 (0.0%)
1	B	0.30	0/6177	0.66	5/8370 (0.1%)
1	C	0.30	0/6177	0.65	2/8370 (0.0%)
1	D	0.30	0/6177	0.65	2/8370 (0.0%)
1	E	0.31	0/6177	0.67	3/8370 (0.0%)
2	F	0.28	0/4213	0.65	0/5709
All	All	0.30	0/35098	0.65	13/47559 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	760	GLU	N-CA-C	-7.67	105.08	114.75
1	C	296	VAL	N-CA-C	-6.40	102.68	108.95
1	C	300	LYS	N-CA-C	-5.87	101.84	110.52
1	E	443	LEU	N-CA-C	5.56	117.03	110.97
1	D	295	GLU	N-CA-C	-5.53	104.64	111.33
1	B	478	PRO	CA-C-N	5.21	126.25	120.06
1	B	478	PRO	C-N-CA	5.21	126.25	120.06
1	A	350	ILE	N-CA-C	-5.20	107.76	113.43
1	E	389	GLU	N-CA-C	-5.20	107.00	113.55
1	D	228	GLU	N-CA-CB	5.15	119.06	110.41
1	B	576	THR	N-CA-C	-5.14	107.17	113.50
1	B	243	LEU	CA-C-N	5.02	129.17	121.19
1	B	243	LEU	C-N-CA	5.02	129.17	121.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6069	0	6184	235	0
1	B	6069	0	6184	209	0
1	C	6069	0	6184	213	0
1	D	6069	0	6184	212	0
1	E	6069	0	6184	265	0
2	F	4136	0	4222	156	0
3	B	27	0	12	1	0
3	C	27	0	12	3	0
3	D	27	0	12	3	0
3	E	27	0	12	4	0
All	All	34589	0	35190	1238	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 18.

All (1238) 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:E:392:GLY:HA3	1:E:455:TYR:HB2	1.44	0.97
1:A:398:ILE:HG21	1:C:432:ARG:HD3	1.47	0.96
1:D:253:ILE:HG23	1:D:294:THR:HG21	1.47	0.96
1:E:516:MET:HE2	1:E:520:ILE:HG13	1.46	0.95
1:D:293:LEU:HD13	1:D:458:VAL:HG11	1.55	0.88
1:B:424:ILE:HA	1:B:427:MET:HE3	1.54	0.88
2:F:549:LYS:HE2	2:F:578:LEU:HD21	1.52	0.88
1:A:374:ARG:HB2	1:A:418:VAL:HG23	1.59	0.85
1:B:578:LEU:HD23	1:B:579:GLY:H	1.43	0.83
1:D:530:VAL:O	1:D:534:TYR:HB2	1.78	0.83
1:C:291:ASP:O	1:C:295:GLU:HB2	1.82	0.79
2:F:772:PRO:HB2	2:F:774:PRO:HD2	1.64	0.79
1:E:363:SER:HB2	3:E:801:ADP:H8	1.50	0.76
1:C:624:SER:HG	1:C:664:HIS:HD1	1.33	0.74
1:D:245:ASP:O	1:D:249:LEU:HB2	1.88	0.74
1:C:367:SER:O	1:C:371:SER:HB3	1.88	0.74
1:E:389:GLU:O	1:E:403:GLY:HA2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:700:ILE:HD12	1:E:769:LEU:HG	1.69	0.74
1:B:501:ILE:O	1:B:505:TYR:HB2	1.88	0.73
1:C:562:ALA:HA	1:C:567:ARG:HD2	1.71	0.73
1:D:533:GLU:HB3	1:D:581:PRO:HB3	1.71	0.71
1:A:718:VAL:O	1:A:722:LEU:HB2	1.90	0.71
1:C:300:LYS:HG2	1:C:413:GLY:O	1.91	0.71
1:D:602:TRP:HB2	1:D:674:LYS:HD3	1.73	0.70
2:F:549:LYS:HE2	2:F:578:LEU:CD2	2.20	0.70
1:D:625:LEU:HG	1:D:634:LYS:HG2	1.74	0.69
2:F:378:ARG:HA	2:F:420:LEU:HB3	1.75	0.69
1:C:246:LEU:HA	1:C:249:LEU:HD12	1.76	0.68
1:B:424:ILE:O	1:B:427:MET:HG2	1.94	0.68
2:F:600:LEU:HB2	2:F:703:THR:HB	1.76	0.68
1:C:601:ALA:HB3	1:C:608:THR:H	1.58	0.68
1:D:297:PRO:HG3	1:D:412:VAL:HG23	1.75	0.68
1:C:592:PRO:HB2	1:C:695:PRO:HB2	1.74	0.67
1:E:613:GLU:HB2	1:E:666:HIS:HB3	1.76	0.67
1:C:509:LYS:O	1:C:513:GLU:HB2	1.95	0.67
1:A:353:LEU:HB2	1:A:470:THR:HG23	1.77	0.67
1:A:550:ILE:HG13	1:A:578:LEU:HD21	1.77	0.67
1:E:516:MET:CE	1:E:520:ILE:HG13	2.22	0.67
1:E:667:VAL:HG11	1:E:671:ALA:HA	1.77	0.67
1:A:624:SER:HB3	1:A:664:HIS:HA	1.77	0.66
1:C:423:GLU:HB3	1:C:426:LYS:HB2	1.77	0.66
1:C:584:ARG:HB2	1:C:585:PRO:HD2	1.77	0.66
1:E:761:ASP:HB3	1:E:764:GLU:HG3	1.77	0.66
1:A:377:HIS:NE2	1:A:412:VAL:HG12	2.11	0.66
1:A:503:ARG:NH1	1:A:522:VAL:O	2.28	0.66
1:D:311:THR:HG22	1:D:371:SER:HB3	1.76	0.66
1:B:307:ASP:OD2	1:B:310:HIS:ND1	2.29	0.66
1:C:300:LYS:HB3	1:C:414:VAL:HG12	1.77	0.65
1:E:530:VAL:O	1:E:534:TYR:HB2	1.96	0.65
1:E:441:GLU:HG3	1:E:451:PHE:HD1	1.60	0.65
1:A:140:LYS:HA	1:A:143:ARG:HB2	1.78	0.65
1:A:49:GLN:HB3	1:A:62:LEU:HD23	1.77	0.65
1:C:394:ARG:NH1	1:C:454:HIS:O	2.30	0.65
1:A:521:GLU:HB3	1:A:568:THR:HA	1.77	0.65
1:E:706:VAL:HG23	1:E:762:VAL:HG21	1.79	0.65
1:E:104:ARG:HD2	1:E:106:ARG:HH22	1.62	0.65
2:F:289:TYR:HE1	2:F:456:LEU:HG	1.62	0.64
1:B:334:ALA:O	1:B:338:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ARG:HE	1:D:482:LEU:HD12	1.61	0.64
1:E:329:ILE:HG23	1:E:351:LEU:HD21	1.79	0.64
1:E:625:LEU:HD12	1:E:629:LEU:HB2	1.80	0.64
1:D:230:MET:SD	1:D:234:GLN:NE2	2.70	0.64
1:E:252:LYS:HD3	1:E:295:GLU:HA	1.78	0.64
1:D:135:TYR:HA	1:D:200:LEU:HD21	1.80	0.64
1:B:221:GLN:HB2	1:E:202:ARG:HE	1.63	0.64
1:A:622:LYS:HD2	1:A:623:LEU:H	1.61	0.64
1:C:495:ASN:ND2	1:C:726:HIS:O	2.31	0.63
2:F:391:ARG:HD2	2:F:453:ASP:HA	1.80	0.63
1:A:152:VAL:HB	1:A:160:MET:HE1	1.81	0.63
1:B:308:ILE:HG23	1:B:312:ARG:HH21	1.63	0.63
1:B:598:GLN:HG2	1:B:611:THR:HG22	1.79	0.63
1:E:751:LEU:HA	1:E:754:LEU:HD12	1.80	0.63
2:F:350:ILE:HG23	2:F:484:ARG:HH22	1.63	0.63
2:F:694:ARG:HE	2:F:772:PRO:HG3	1.63	0.63
1:B:662:ASP:HB2	1:C:645:ARG:HH22	1.62	0.63
2:F:453:ASP:HB3	2:F:456:LEU:HB2	1.80	0.63
1:E:349:PRO:HB2	1:E:486:GLU:HB2	1.81	0.63
1:E:643:TYR:O	1:E:647:HIS:ND1	2.31	0.63
1:A:350:ILE:O	1:A:468:ILE:HD12	1.99	0.63
1:D:390:ILE:HG21	1:D:435:PRO:HA	1.81	0.63
2:F:449:ASN:HA	2:F:461:ASP:HA	1.80	0.63
2:F:625:LEU:HB3	2:F:629:LEU:HD12	1.80	0.63
2:F:315:LEU:HD13	2:F:322:LEU:HD12	1.81	0.62
2:F:479:ARG:HA	2:F:482:LEU:HB2	1.80	0.62
1:A:375:LYS:HG3	1:A:417:PRO:HB3	1.81	0.62
1:C:541:ARG:HA	1:C:544:GLU:HB2	1.81	0.62
1:D:253:ILE:CG2	1:D:294:THR:HG21	2.26	0.62
1:C:532:SER:HB2	1:C:585:PRO:O	2.00	0.62
1:B:356:PRO:O	1:B:361:LYS:NZ	2.31	0.62
1:E:59:PRO:HB2	1:E:97:TYR:HB3	1.81	0.62
1:E:739:ASN:ND2	1:E:742:GLN:OE1	2.32	0.62
2:F:681:ILE:HB	2:F:765:VAL:HG21	1.80	0.62
1:D:362:THR:HB	1:D:366:ARG:HH21	1.64	0.62
1:A:574:ILE:HG23	1:A:578:LEU:HD12	1.81	0.62
1:B:38:MET:HE1	1:B:76:ARG:HH22	1.63	0.62
1:B:354:VAL:HG22	1:B:471:ALA:HB3	1.82	0.62
1:B:385:ARG:HA	1:B:428:SER:O	2.00	0.62
1:D:613:GLU:HB2	1:D:666:HIS:HB3	1.80	0.62
1:A:526:ALA:HB1	1:A:574:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:VAL:HG21	1:C:417:PRO:HB3	1.81	0.62
1:D:495:ASN:HB2	1:D:727:GLN:HA	1.82	0.62
1:E:618:PRO:HA	1:E:661:VAL:HA	1.81	0.62
1:E:516:MET:CE	1:E:551:ALA:HA	2.30	0.61
1:E:613:GLU:HB3	2:F:708:LEU:HB2	1.82	0.61
1:E:615:ALA:HB3	1:E:664:HIS:HB3	1.80	0.61
1:E:201:GLU:O	1:E:204:GLU:HG2	1.99	0.61
1:E:502:ALA:HA	1:E:506:LEU:HB2	1.81	0.61
2:F:403:GLY:O	2:F:407:HIS:ND1	2.33	0.61
2:F:529:ARG:HH12	2:F:575:PRO:HD3	1.65	0.61
1:E:351:LEU:HA	1:E:486:GLU:HB3	1.82	0.61
1:D:402:PRO:HB2	1:D:406:ILE:HD12	1.83	0.61
1:A:622:LYS:HD2	1:A:623:LEU:N	2.15	0.61
1:B:694:ARG:HB3	1:B:772:PRO:HG2	1.81	0.61
1:E:623:LEU:HA	1:E:663:LEU:HB3	1.83	0.61
1:E:628:GLN:HB2	1:E:670:GLY:HA2	1.83	0.61
2:F:495:ASN:ND2	2:F:726:HIS:O	2.34	0.61
1:E:623:LEU:HD11	1:E:634:LYS:HB3	1.82	0.61
1:E:690:ALA:O	1:E:693:ARG:NH1	2.34	0.61
1:B:444:ASP:HB3	1:B:447:GLN:HB3	1.83	0.61
1:D:520:ILE:HG22	1:D:567:ARG:HB2	1.83	0.61
2:F:361:LYS:H	2:F:541:ARG:HH21	1.48	0.61
1:A:434:ASP:HB3	1:A:436:ALA:H	1.65	0.61
1:C:256:VAL:HG11	1:C:294:THR:HG22	1.82	0.61
1:A:702:MET:HE1	1:A:765:VAL:HB	1.83	0.60
1:B:622:LYS:HE3	1:B:662:ASP:HB3	1.82	0.60
1:E:587:LYS:HB2	1:E:728:ALA:HB1	1.84	0.60
2:F:265:LYS:NZ	2:F:456:LEU:HD23	2.17	0.60
1:B:115:PRO:HG3	1:B:185:LEU:HD11	1.82	0.60
1:B:578:LEU:HD23	1:B:579:GLY:N	2.14	0.60
1:D:694:ARG:HD2	1:D:695:PRO:HD2	1.83	0.60
1:E:285:VAL:HG21	1:E:400:ALA:HB3	1.81	0.60
1:C:49:GLN:HB2	1:C:53:GLU:HG3	1.84	0.60
1:C:300:LYS:HB2	1:C:414:VAL:HA	1.83	0.60
1:D:387:GLU:HB2	1:D:433:GLY:HA3	1.83	0.60
1:E:136:VAL:HG11	1:E:149:LEU:HB2	1.84	0.60
1:E:362:THR:OG1	1:E:378:ARG:NH1	2.34	0.60
1:E:712:VAL:HG12	1:E:736:PRO:HG3	1.83	0.60
1:B:403:GLY:O	1:B:407:HIS:ND1	2.33	0.60
1:E:462:LEU:HD22	1:E:467:PHE:HZ	1.66	0.60
2:F:592:PRO:HB2	2:F:695:PRO:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:GLU:O	1:B:567:ARG:NH1	2.34	0.60
1:D:253:ILE:HG23	1:D:294:THR:CG2	2.28	0.60
1:E:423:GLU:HA	1:E:471:ALA:HA	1.82	0.60
1:E:625:LEU:HB2	1:E:629:LEU:HD12	1.83	0.60
1:C:449:ASN:HA	1:C:461:ASP:HA	1.83	0.60
1:D:699:ASP:HA	1:D:730:ILE:HD12	1.84	0.60
1:D:359:VAL:O	1:D:361:LYS:NZ	2.32	0.59
1:E:125:VAL:HG13	1:E:161:LEU:HD22	1.85	0.59
1:E:521:GLU:HB3	1:E:568:THR:HA	1.83	0.59
1:A:275:ARG:HB3	1:E:431:TRP:HE1	1.66	0.59
1:B:594:VAL:HG12	1:C:709:ARG:HH21	1.67	0.59
1:E:583:TYR:HB3	1:E:587:LYS:HZ1	1.66	0.59
2:F:296:VAL:HG23	2:F:409:MET:HG3	1.84	0.59
2:F:345:ARG:HH12	2:F:448:ASN:HD21	1.50	0.59
2:F:773:GLU:HG3	2:F:774:PRO:HD3	1.82	0.59
1:A:182:LEU:O	1:A:188:ARG:NH1	2.36	0.59
1:B:250:ARG:HD3	1:B:270:LEU:HD22	1.84	0.59
1:C:293:LEU:O	1:C:298:TRP:NE1	2.35	0.59
1:B:493:TYR:O	1:B:727:GLN:NE2	2.34	0.59
1:D:385:ARG:NH2	1:D:430:ASP:OD2	2.35	0.59
1:E:520:ILE:HD13	1:E:567:ARG:HB2	1.85	0.59
2:F:597:ALA:HB3	2:F:612:ILE:H	1.68	0.59
1:C:291:ASP:O	1:C:295:GLU:CB	2.50	0.59
1:C:424:ILE:HA	1:C:427:MET:HE2	1.83	0.59
1:C:278:GLN:NE2	1:D:395:ARG:O	2.35	0.58
1:E:540:VAL:O	1:E:544:GLU:N	2.35	0.58
1:C:357:PRO:O	1:C:361:LYS:NZ	2.36	0.58
1:E:538:ALA:HB2	1:E:607:GLY:H	1.68	0.58
2:F:549:LYS:HD2	2:F:578:LEU:HD11	1.84	0.58
1:A:441:GLU:HG2	1:A:447:GLN:HB3	1.84	0.58
1:B:351:LEU:HB2	1:B:468:ILE:HA	1.86	0.58
1:D:265:LYS:HD3	1:D:458:VAL:HA	1.85	0.58
1:C:412:VAL:HG11	1:C:417:PRO:HG3	1.85	0.58
1:E:388:ALA:HB1	1:E:393:HIS:CE1	2.38	0.58
1:C:546:GLU:OE2	1:C:582:ARG:NH2	2.36	0.58
1:E:494:THR:O	1:E:498:LYS:N	2.35	0.58
1:E:722:LEU:HD12	1:E:754:LEU:HD13	1.85	0.58
1:B:737:LYS:HB3	1:B:760:GLU:HB3	1.85	0.58
1:C:47:VAL:HG22	1:C:66:GLY:HA3	1.85	0.58
1:C:591:GLU:O	1:C:593:GLN:NE2	2.35	0.58
1:D:561:GLY:O	1:D:567:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:GLU:HG2	1:C:708:LEU:HD22	1.85	0.58
1:D:243:LEU:HD21	1:D:276:MET:HG2	1.86	0.58
1:E:289:TYR:HE1	1:E:456:LEU:HA	1.67	0.58
1:E:614:VAL:HG22	1:E:665:VAL:HG23	1.85	0.58
2:F:306:LEU:HB3	2:F:337:GLN:HB3	1.86	0.58
1:B:449:ASN:HA	1:B:461:ASP:HA	1.85	0.58
1:B:562:ALA:HA	1:B:567:ARG:HH22	1.69	0.58
1:C:387:GLU:O	1:C:391:ARG:N	2.37	0.58
1:E:98:ILE:HD12	1:E:106:ARG:HH11	1.69	0.58
1:B:427:MET:HA	1:B:427:MET:HE2	1.85	0.57
1:C:25:VAL:HB	1:C:82:LEU:HB3	1.86	0.57
1:C:716:GLY:HA2	1:C:742:GLN:HE22	1.69	0.57
1:B:309:ASN:OD1	1:B:312:ARG:NH2	2.37	0.57
1:C:553:LYS:HE2	1:C:577:TYR:HA	1.85	0.57
1:C:624:SER:O	1:C:664:HIS:ND1	2.37	0.57
1:E:115:PRO:HD3	1:E:185:LEU:HB3	1.86	0.57
1:E:448:ASN:HB2	1:E:462:LEU:HB2	1.85	0.57
1:E:207:LYS:O	1:E:211:GLN:NE2	2.36	0.57
1:B:552:ARG:HB3	1:C:331:GLU:HB3	1.86	0.57
1:B:645:ARG:NH2	1:B:655:GLU:O	2.38	0.57
1:D:615:ALA:HB3	1:D:664:HIS:HB2	1.86	0.57
1:A:292:TRP:HZ2	1:B:454:HIS:HB3	1.69	0.57
1:B:389:GLU:OE2	1:B:432:ARG:NH1	2.37	0.57
1:E:449:ASN:HA	1:E:461:ASP:HA	1.86	0.57
2:F:530:VAL:O	2:F:534:TYR:HB2	2.05	0.57
1:D:679:ALA:HA	1:D:704:GLY:H	1.68	0.57
1:E:355:GLY:O	1:E:472:ASN:ND2	2.32	0.57
1:A:619:GLY:HA3	1:A:662:ASP:HB3	1.86	0.57
1:C:268:LYS:HG2	1:C:272:ARG:HH21	1.70	0.57
1:C:440:LEU:O	1:C:447:GLN:NE2	2.37	0.57
1:A:357:PRO:O	1:A:541:ARG:NH1	2.37	0.57
1:B:380:SER:HA	1:B:422:ASP:HB2	1.87	0.57
1:B:649:GLN:NE2	1:B:650:ASP:OD1	2.38	0.57
1:E:460:TYR:CD2	1:E:462:LEU:HD23	2.39	0.57
1:A:501:ILE:HA	1:A:504:GLN:HB2	1.85	0.57
1:B:501:ILE:HA	1:B:505:TYR:HD2	1.70	0.57
1:C:91:ARG:HG3	1:C:111:SER:HB2	1.85	0.57
1:E:384:VAL:HG11	1:E:390:ILE:HG13	1.87	0.57
1:A:366:ARG:HG3	1:A:370:ARG:NH1	2.20	0.56
1:A:696:ALA:HB1	1:A:769:LEU:O	2.04	0.56
1:B:748:LYS:HA	1:B:751:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:PRO:HB2	1:C:185:LEU:HD21	1.87	0.56
1:C:625:LEU:HB2	1:C:629:LEU:HD13	1.86	0.56
1:E:545:ARG:NH1	1:E:546:GLU:OE2	2.37	0.56
1:E:536:ARG:NH1	1:E:727:GLN:O	2.38	0.56
2:F:375:LYS:HG3	2:F:414:VAL:HG13	1.87	0.56
1:A:249:LEU:HD12	1:A:252:LYS:HE3	1.87	0.56
1:B:510:GLN:O	1:B:514:SER:HB3	2.05	0.56
1:B:593:GLN:HB3	1:B:596:THR:HB	1.86	0.56
1:D:122:ARG:NH1	1:D:156:SER:O	2.38	0.56
1:D:298:TRP:O	1:D:300:LYS:NZ	2.38	0.56
1:D:300:LYS:HB2	1:D:414:VAL:HA	1.87	0.56
1:E:211:GLN:HA	1:E:214:LYS:HG2	1.86	0.56
1:E:392:GLY:HA3	1:E:455:TYR:CB	2.26	0.56
2:F:379:ILE:HD13	2:F:408:ALA:HB2	1.87	0.56
1:A:336:ARG:HH21	1:A:348:ALA:HB1	1.71	0.56
1:A:517:GLU:O	1:A:519:ARG:NH1	2.39	0.56
1:A:618:PRO:O	1:A:661:VAL:HA	2.04	0.56
1:D:407:HIS:HA	1:D:410:LYS:HE3	1.87	0.56
1:E:42:ARG:HB3	1:E:71:VAL:HB	1.85	0.56
1:E:644:LEU:HA	1:E:647:HIS:HB2	1.85	0.56
1:A:731:HIS:ND1	1:A:753:GLY:O	2.38	0.56
2:F:425:ASP:HB3	2:F:471:ALA:HB1	1.88	0.56
1:A:702:MET:HG2	1:A:769:LEU:HD22	1.88	0.56
1:C:369:ALA:O	1:C:374:ARG:N	2.38	0.56
1:E:270:LEU:HA	1:E:273:LEU:HB2	1.87	0.56
1:E:614:VAL:O	2:F:709:ARG:NH1	2.38	0.56
2:F:269:GLU:HA	2:F:272:ARG:HB3	1.88	0.56
1:B:592:PRO:HB2	1:B:695:PRO:HB2	1.87	0.56
1:B:269:GLU:HG3	1:B:272:ARG:HD2	1.86	0.56
1:C:298:TRP:H	1:C:300:LYS:NZ	2.03	0.56
1:D:618:PRO:HA	1:D:661:VAL:HA	1.88	0.56
1:E:302:ASP:H	1:E:416:ASN:HD21	1.54	0.56
2:F:448:ASN:ND2	2:F:462:LEU:O	2.39	0.56
1:A:115:PRO:HG3	1:A:158:PRO:HG2	1.88	0.56
1:A:345:ARG:HA	1:A:445:PRO:HG2	1.87	0.56
1:A:377:HIS:HB2	1:A:419:ILE:HG12	1.88	0.56
1:B:395:ARG:NH2	1:B:400:ALA:O	2.39	0.56
1:C:304:GLU:HB3	1:C:372:MET:HE3	1.87	0.56
1:A:367:SER:HA	1:A:370:ARG:NE	2.21	0.56
1:A:505:TYR:O	1:A:509:LYS:N	2.37	0.56
1:B:436:ALA:HB1	1:B:480:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:THR:HG23	1:E:164:THR:HG23	1.87	0.56
1:E:252:LYS:HA	1:E:255:GLU:HG3	1.88	0.56
1:E:314:VAL:O	1:E:370:ARG:NH2	2.38	0.56
1:E:674:LYS:HD3	1:E:678:SER:HB3	1.88	0.56
1:E:712:VAL:N	1:E:760:GLU:O	2.36	0.56
1:A:379:ILE:HD12	1:A:419:ILE:HG21	1.88	0.55
1:B:532:SER:O	1:B:536:ARG:NH2	2.39	0.55
1:C:282:GLU:HG2	1:C:396:THR:HA	1.87	0.55
1:E:462:LEU:HD22	1:E:467:PHE:CZ	2.41	0.55
2:F:448:ASN:HB2	2:F:462:LEU:HB2	1.87	0.55
1:E:516:MET:HE1	1:E:551:ALA:HA	1.88	0.55
2:F:496:MET:HE1	2:F:752:GLU:HB3	1.88	0.55
1:A:248:ALA:HA	1:A:251:LYS:HG2	1.87	0.55
1:A:744:GLU:HG3	1:A:748:LYS:HZ2	1.71	0.55
1:D:693:ARG:HH22	1:E:709:ARG:HH12	1.53	0.55
1:A:302:ASP:H	1:A:416:ASN:HD21	1.52	0.55
1:D:629:LEU:HD21	1:D:667:VAL:H	1.72	0.55
1:D:304:GLU:OE2	1:D:416:ASN:ND2	2.39	0.55
1:D:421:LEU:HB3	1:D:424:ILE:HD11	1.89	0.55
1:A:619:GLY:HA3	1:A:662:ASP:CB	2.37	0.55
1:C:259:PRO:O	1:C:263:LYS:N	2.36	0.55
1:D:405:LEU:HG	1:D:406:ILE:HG13	1.86	0.55
1:E:441:GLU:HA	1:E:447:GLN:HE22	1.70	0.55
1:B:696:ALA:HB1	1:B:769:LEU:HG	1.89	0.55
1:D:448:ASN:HB2	1:D:462:LEU:HD12	1.87	0.55
1:D:592:PRO:HB3	1:D:697:ARG:HA	1.88	0.55
1:E:216:GLN:HA	1:E:219:THR:HG22	1.88	0.55
1:E:393:HIS:HD2	1:E:401:MET:O	1.90	0.55
1:B:293:LEU:O	1:B:293:LEU:HD23	2.07	0.55
1:B:502:ALA:HA	1:B:506:LEU:HB2	1.88	0.55
2:F:249:LEU:HA	2:F:252:LYS:HG2	1.87	0.55
1:D:614:VAL:HG12	1:D:665:VAL:HG12	1.87	0.55
1:E:551:ALA:O	1:E:555:ALA:HB2	2.06	0.55
2:F:285:VAL:HG21	2:F:400:ALA:HB3	1.89	0.55
1:A:443:LEU:O	1:A:484:ARG:NH1	2.40	0.54
1:A:618:PRO:HD2	1:B:645:ARG:HG3	1.89	0.54
1:C:739:ASN:ND2	1:C:742:GLN:OE1	2.40	0.54
1:D:701:ALA:HB2	1:D:730:ILE:HG22	1.90	0.54
1:E:128:LEU:HD13	1:E:189:LEU:HD23	1.87	0.54
2:F:510:GLN:NE2	2:F:544:GLU:OE1	2.39	0.54
1:D:499:GLN:NE2	1:D:524:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:TYR:O	1:E:582:ARG:NH2	2.41	0.54
1:B:159:ALA:HB2	1:B:185:LEU:HD22	1.90	0.54
1:D:124:LEU:HB3	1:D:189:LEU:HD13	1.89	0.54
1:E:311:THR:HG23	1:E:371:SER:HB2	1.89	0.54
1:A:288:THR:HG23	1:B:394:ARG:HB3	1.89	0.54
1:A:314:VAL:HG11	1:A:370:ARG:HE	1.72	0.54
1:B:697:ARG:N	1:B:769:LEU:O	2.38	0.54
1:A:491:PRO:HB2	1:A:723:LEU:HD12	1.89	0.54
1:A:536:ARG:NH2	1:A:584:ARG:O	2.38	0.54
1:B:395:ARG:HB3	1:B:400:ALA:HB3	1.89	0.54
1:E:230:MET:SD	2:F:272:ARG:NH2	2.80	0.54
1:E:425:ASP:OD2	1:E:426:LYS:NZ	2.38	0.54
1:D:249:LEU:HD21	1:D:291:ASP:OD2	2.08	0.54
1:E:353:LEU:N	1:E:469:THR:O	2.37	0.54
2:F:309:ASN:OD1	2:F:312:ARG:NH2	2.40	0.54
1:C:448:ASN:HB2	1:C:462:LEU:HB2	1.89	0.54
1:D:595:GLY:H	1:D:689:SER:HB3	1.73	0.54
1:D:731:HIS:ND1	1:D:753:GLY:O	2.41	0.54
2:F:362:THR:OG1	2:F:509:LYS:NZ	2.40	0.54
1:D:536:ARG:HH21	1:D:587:LYS:HG2	1.73	0.54
1:D:735:LEU:HB3	1:D:758:LEU:HD23	1.89	0.54
1:E:694:ARG:HG3	1:E:773:GLU:HA	1.90	0.54
2:F:345:ARG:NH2	2:F:448:ASN:OD1	2.40	0.54
1:A:357:PRO:HD3	1:A:605:VAL:HA	1.90	0.54
1:B:417:PRO:HD2	1:B:465:VAL:HA	1.90	0.54
1:B:719:LYS:HA	1:B:746:LEU:HD11	1.89	0.54
1:D:733:ILE:N	1:D:755:GLU:O	2.40	0.54
1:D:737:LYS:HA	1:D:758:LEU:HB3	1.90	0.54
1:E:369:ALA:HA	1:E:374:ARG:HB2	1.89	0.54
1:E:385:ARG:NH1	1:E:386:ASP:OD1	2.41	0.54
1:E:610:LEU:HD22	1:E:668:PRO:HB2	1.90	0.54
1:A:407:HIS:HA	1:A:410:LYS:HD3	1.89	0.54
1:B:499:GLN:HG2	1:B:503:ARG:HE	1.73	0.54
1:D:715:ILE:HD12	1:D:721:LYS:HD2	1.90	0.54
1:E:641:LEU:O	1:E:645:ARG:N	2.38	0.54
1:A:596:THR:HG23	1:A:613:GLU:HB3	1.90	0.53
1:A:751:LEU:HB3	1:A:756:ILE:HD11	1.90	0.53
1:B:701:ALA:H	1:B:730:ILE:HG21	1.72	0.53
1:C:327:GLU:HA	1:C:330:LEU:HD12	1.89	0.53
1:A:381:LEU:HD23	1:A:421:LEU:HG	1.90	0.53
1:C:234:GLN:OE1	1:D:275:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:O	1:C:469:THR:OG1	2.25	0.53
1:E:510:GLN:O	1:E:514:SER:OG	2.25	0.53
1:E:718:VAL:HG21	1:E:739:ASN:HB3	1.91	0.53
2:F:735:LEU:HD13	2:F:739:ASN:HB3	1.91	0.53
1:A:244:SER:OG	1:B:268:LYS:O	2.26	0.53
1:B:14:VAL:HA	1:B:48:ALA:HB1	1.90	0.53
1:C:5:LEU:HD13	1:C:40:ALA:HB1	1.91	0.53
1:E:418:VAL:HG13	1:E:468:ILE:HD13	1.90	0.53
1:A:69:ALA:HB1	1:A:86:VAL:HB	1.89	0.53
1:C:246:LEU:HD22	1:C:273:LEU:HD22	1.90	0.53
1:D:362:THR:OG1	3:D:801:ADP:O3B	2.26	0.53
1:D:625:LEU:HD13	1:D:665:VAL:HG23	1.91	0.53
1:E:682:THR:OG1	1:E:702:MET:O	2.27	0.53
2:F:536:ARG:NH1	2:F:607:GLY:O	2.41	0.53
2:F:734:VAL:HG12	2:F:757:LYS:HB2	1.90	0.53
1:A:361:LYS:HG2	1:A:490:ILE:HB	1.90	0.53
1:D:394:ARG:NH1	1:D:454:HIS:O	2.42	0.53
1:D:493:TYR:O	1:D:727:GLN:NE2	2.34	0.53
1:E:246:LEU:HD23	1:E:249:LEU:HD21	1.89	0.53
1:E:387:GLU:CD	1:E:391:ARG:HH11	2.16	0.53
2:F:534:TYR:HB3	2:F:582:ARG:HH21	1.74	0.53
1:B:381:LEU:O	1:B:427:MET:HE1	2.09	0.53
1:C:275:ARG:HB2	1:C:283:ALA:HB2	1.91	0.53
1:C:714:PRO:HG3	1:C:738:ASP:HB2	1.90	0.53
1:D:361:LYS:NZ	3:D:801:ADP:O1B	2.35	0.53
1:D:733:ILE:HB	1:D:756:ILE:HA	1.90	0.53
1:A:138:ASN:HB3	1:A:203:PHE:HB3	1.90	0.53
1:B:92:ALA:HB1	1:B:107:GLY:HA3	1.90	0.53
1:D:249:LEU:HA	1:D:252:LYS:HD2	1.91	0.53
1:D:387:GLU:N	1:D:432:ARG:O	2.38	0.53
1:D:630:GLY:H	1:D:633:MET:HE2	1.74	0.53
1:E:734:VAL:HG11	1:E:765:VAL:HB	1.90	0.53
1:A:199:ASP:OD1	1:A:200:LEU:N	2.40	0.53
1:A:601:ALA:HB3	1:A:610:LEU:HD12	1.90	0.53
1:C:311:THR:HA	1:C:371:SER:HB2	1.90	0.53
1:D:492:GLY:N	1:D:720:GLU:OE2	2.40	0.53
1:D:300:LYS:H	1:D:415:ILE:HG23	1.74	0.53
1:D:410:LYS:NZ	1:D:411:GLN:OE1	2.39	0.53
2:F:422:ASP:OD1	2:F:470:THR:OG1	2.24	0.53
1:A:449:ASN:ND2	1:A:460:TYR:O	2.42	0.53
1:C:748:LYS:HA	1:C:751:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:LYS:HB2	1:E:417:PRO:HB3	1.91	0.53
1:A:392:GLY:N	1:A:453:ASP:OD1	2.41	0.52
1:A:744:GLU:HA	1:A:748:LYS:HZ1	1.73	0.52
1:D:417:PRO:HD2	1:D:465:VAL:HG13	1.90	0.52
1:D:615:ALA:HB1	1:E:642:THR:HG21	1.91	0.52
1:E:265:LYS:CG	1:E:458:VAL:HG23	2.39	0.52
1:E:600:LEU:HB2	1:E:701:ALA:HB1	1.90	0.52
1:A:32:ARG:HH22	1:A:101:PRO:HG3	1.73	0.52
2:F:712:VAL:HG12	2:F:736:PRO:HG3	1.89	0.52
2:F:742:GLN:HA	2:F:745:GLU:HB2	1.91	0.52
1:A:135:TYR:CZ	1:A:199:ASP:HB2	2.44	0.52
1:A:507:TRP:HA	1:A:510:GLN:HG2	1.91	0.52
1:A:617:VAL:HG11	1:B:642:THR:HB	1.92	0.52
1:C:18:HIS:HA	1:C:87:GLU:HG3	1.91	0.52
1:C:614:VAL:HG11	1:C:687:ILE:HG22	1.91	0.52
1:D:319:HIS:HA	3:D:801:ADP:HN61	1.72	0.52
1:D:694:ARG:NH1	1:D:695:PRO:O	2.41	0.52
1:E:391:ARG:HG3	1:E:453:ASP:HA	1.91	0.52
1:A:312:ARG:HD3	1:A:330:LEU:HD22	1.91	0.52
1:C:298:TRP:O	1:C:300:LYS:HD2	2.10	0.52
1:C:394:ARG:NH2	1:C:455:TYR:O	2.43	0.52
1:E:392:GLY:HA2	1:E:402:PRO:HA	1.91	0.52
1:A:196:LEU:HA	1:A:199:ASP:OD2	2.10	0.52
1:C:751:LEU:HA	1:C:754:LEU:HD12	1.91	0.52
1:D:694:ARG:HG3	1:D:770:LEU:HD11	1.91	0.52
1:E:667:VAL:CG1	1:E:671:ALA:HA	2.40	0.52
1:E:701:ALA:HB2	1:E:730:ILE:HD13	1.92	0.52
2:F:498:LYS:HE3	2:F:540:VAL:HG12	1.92	0.52
1:A:202:ARG:HA	1:D:222:ARG:NH2	2.24	0.52
1:B:237:LEU:HD22	1:B:274:GLU:HA	1.92	0.52
2:F:385:ARG:NH1	2:F:426:LYS:HD3	2.25	0.52
1:A:681:ILE:HA	1:A:706:VAL:HG23	1.92	0.52
1:A:697:ARG:HB2	1:A:769:LEU:HD12	1.92	0.52
1:B:298:TRP:O	1:B:300:LYS:NZ	2.36	0.52
1:E:444:ASP:HB2	1:E:447:GLN:HG3	1.92	0.52
1:E:588:ALA:O	1:E:598:GLN:NE2	2.43	0.52
1:A:388:ALA:HA	1:A:391:ARG:HB2	1.91	0.52
1:C:15:ILE:HG13	1:C:46:LEU:HD13	1.92	0.52
1:C:425:ASP:N	1:C:425:ASP:OD1	2.38	0.52
1:C:709:ARG:HB2	1:C:711:LYS:HE2	1.92	0.52
1:E:505:TYR:HB2	1:E:506:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:O	1:A:83:GLN:NE2	2.43	0.52
1:A:305:VAL:O	1:A:337:GLN:NE2	2.43	0.52
1:C:493:TYR:O	1:C:727:GLN:NE2	2.43	0.52
1:C:722:LEU:HD21	1:C:735:LEU:HD11	1.91	0.52
1:D:7:VAL:HB	1:D:103:LEU:HB2	1.92	0.52
1:D:429:SER:OG	1:D:434:ASP:OD1	2.28	0.52
2:F:322:LEU:HB3	2:F:325:VAL:HB	1.91	0.52
1:A:244:SER:HA	1:A:247:GLU:HB3	1.91	0.52
1:B:282:GLU:HA	1:B:285:VAL:HG12	1.92	0.52
1:B:290:LEU:O	1:B:294:THR:OG1	2.27	0.52
1:B:529:ARG:HH11	1:B:571:ALA:HB1	1.75	0.52
1:E:387:GLU:O	1:E:391:ARG:HB2	2.10	0.52
2:F:584:ARG:HD2	2:F:585:PRO:HD2	1.90	0.52
1:A:719:LYS:HB3	1:A:746:LEU:HD21	1.92	0.51
1:C:624:SER:N	1:C:663:LEU:O	2.43	0.51
2:F:533:GLU:HA	2:F:583:TYR:HB2	1.92	0.51
1:A:87:GLU:OE2	1:A:89:ARG:NH1	2.43	0.51
1:C:381:LEU:H	1:C:422:ASP:HB2	1.74	0.51
1:D:209:VAL:HG13	1:D:212:ARG:HH21	1.75	0.51
1:E:595:GLY:HA3	2:F:709:ARG:HH21	1.75	0.51
1:E:697:ARG:NH1	1:E:768:TYR:O	2.42	0.51
1:A:27:ARG:HD2	1:A:55:ASP:HA	1.91	0.51
1:A:411:GLN:HG2	1:A:412:VAL:HG13	1.92	0.51
1:B:520:ILE:HA	1:B:567:ARG:HB2	1.93	0.51
1:C:38:MET:HE1	1:C:71:VAL:HG11	1.92	0.51
1:C:208:ARG:O	1:C:212:ARG:NH1	2.44	0.51
1:C:624:SER:OG	1:C:664:HIS:ND1	2.35	0.51
1:D:158:PRO:HA	1:D:161:LEU:HB2	1.92	0.51
1:D:421:LEU:HD22	1:D:469:THR:HG22	1.92	0.51
2:F:300:LYS:H	2:F:415:ILE:HG13	1.75	0.51
1:A:316:ASP:OD1	1:A:326:LYS:NZ	2.43	0.51
1:B:361:LYS:NZ	3:B:801:ADP:O1B	2.39	0.51
1:D:529:ARG:NH1	1:D:571:ALA:O	2.43	0.51
2:F:740:GLU:HG3	2:F:758:LEU:HD13	1.91	0.51
1:A:587:LYS:HB2	1:A:698:MET:HB3	1.92	0.51
1:A:731:HIS:HA	1:A:754:LEU:HD23	1.91	0.51
1:B:391:ARG:HB3	1:B:454:HIS:H	1.76	0.51
1:C:584:ARG:HG2	1:C:587:LYS:HD2	1.93	0.51
1:D:91:ARG:HG3	1:D:111:SER:HB2	1.91	0.51
1:D:629:LEU:O	1:D:634:LYS:NZ	2.43	0.51
1:D:648:THR:HA	1:D:653:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:GLY:N	1:D:704:GLY:O	2.43	0.51
1:D:748:LYS:O	1:D:752:GLU:N	2.43	0.51
1:A:332:TYR:OH	1:A:349:PRO:O	2.28	0.51
1:A:603:THR:OG1	1:A:606:GLY:O	2.28	0.51
1:A:682:THR:OG1	1:A:702:MET:O	2.28	0.51
1:C:339:THR:HG21	1:C:345:ARG:H	1.75	0.51
1:D:250:ARG:HB2	1:D:270:LEU:HD11	1.92	0.51
1:D:715:ILE:HD11	1:D:718:VAL:HG23	1.93	0.51
2:F:272:ARG:HH12	2:F:278:GLN:HG2	1.74	0.51
1:A:353:LEU:H	1:A:470:THR:HA	1.75	0.51
1:B:253:ILE:HG12	1:B:266:ALA:HB1	1.93	0.51
1:B:448:ASN:HB2	1:B:462:LEU:HB2	1.91	0.51
1:C:584:ARG:NH1	1:C:589:GLU:HB2	2.26	0.51
1:E:49:GLN:HA	1:E:62:LEU:HA	1.92	0.51
1:E:266:ALA:O	1:E:270:LEU:HB2	2.11	0.51
1:E:516:MET:HE3	1:E:551:ALA:O	2.11	0.51
2:F:511:VAL:HG12	2:F:520:ILE:HD12	1.93	0.51
1:A:77:LEU:HB2	1:A:82:LEU:HG	1.92	0.51
1:A:714:PRO:HB3	1:A:738:ASP:HB3	1.93	0.51
1:C:648:THR:HA	1:C:653:LEU:HD12	1.93	0.51
1:B:613:GLU:OE2	1:B:666:HIS:ND1	2.36	0.51
1:C:2:ARG:N	1:C:107:GLY:O	2.44	0.51
1:C:394:ARG:NH1	1:C:457:ASP:OD1	2.42	0.51
2:F:697:ARG:HB2	2:F:769:LEU:HA	1.91	0.51
2:F:731:HIS:ND1	2:F:753:GLY:O	2.44	0.51
1:A:498:LYS:HE2	1:A:540:VAL:HG12	1.93	0.51
1:A:682:THR:HG23	1:A:702:MET:HB2	1.93	0.51
1:B:25:VAL:HB	1:B:82:LEU:HB2	1.92	0.51
1:B:697:ARG:NH1	1:B:698:MET:O	2.44	0.51
1:B:743:LEU:HA	1:B:746:LEU:HD23	1.93	0.51
1:D:702:MET:SD	1:D:769:LEU:HD21	2.51	0.51
1:E:265:LYS:HG2	1:E:458:VAL:HG23	1.92	0.51
2:F:305:VAL:HG11	2:F:310:HIS:HB3	1.93	0.51
1:A:612:ILE:HD12	1:A:682:THR:HB	1.93	0.50
1:A:680:GLY:HA2	1:A:683:MET:HE1	1.92	0.50
1:C:592:PRO:HA	1:C:698:MET:HG2	1.93	0.50
1:D:269:GLU:HG2	1:D:272:ARG:HH12	1.75	0.50
1:D:291:ASP:O	1:D:295:GLU:HB2	2.10	0.50
1:E:739:ASN:O	1:E:743:LEU:N	2.44	0.50
1:A:510:GLN:HB3	1:A:551:ALA:HB2	1.94	0.50
1:A:584:ARG:HD3	1:A:585:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD13	1:B:326:LYS:HD2	1.92	0.50
1:B:682:THR:O	1:B:685:THR:OG1	2.26	0.50
1:D:348:ALA:H	1:D:484:ARG:HH21	1.58	0.50
1:E:500:ALA:O	1:E:504:GLN:HB2	2.11	0.50
1:A:304:GLU:HA	1:A:373:ASN:HB2	1.93	0.50
1:A:460:TYR:HB3	1:A:462:LEU:HG	1.92	0.50
1:C:253:ILE:HG12	1:C:290:LEU:HD11	1.94	0.50
1:C:599:GLY:HA3	1:C:610:LEU:HB2	1.93	0.50
1:D:171:TRP:HZ2	1:D:192:VAL:HG13	1.76	0.50
1:D:425:ASP:OD1	1:D:425:ASP:N	2.42	0.50
1:E:87:GLU:O	1:E:89:ARG:NH1	2.44	0.50
2:F:374:ARG:HB3	2:F:414:VAL:HG21	1.93	0.50
1:A:115:PRO:HB3	1:A:185:LEU:HD22	1.94	0.50
1:A:145:ASP:OD1	1:A:145:ASP:N	2.45	0.50
1:A:567:ARG:HE	1:A:569:ILE:HD11	1.76	0.50
1:C:269:GLU:OE2	1:C:395:ARG:NH1	2.44	0.50
1:C:597:ALA:HA	1:C:698:MET:HE1	1.92	0.50
1:E:375:LYS:O	1:E:418:VAL:N	2.35	0.50
1:E:384:VAL:HG13	1:E:389:GLU:HB2	1.93	0.50
1:B:374:ARG:HH22	1:B:466:PHE:HB2	1.76	0.50
1:B:763:GLY:HA2	1:B:766:LEU:HD12	1.94	0.50
1:C:584:ARG:HB2	1:C:585:PRO:CD	2.41	0.50
1:D:624:SER:N	1:D:663:LEU:O	2.44	0.50
1:E:26:GLY:O	1:E:31:LYS:NZ	2.42	0.50
2:F:286:ALA:HA	2:F:289:TYR:HB3	1.93	0.50
1:A:9:PRO:HB2	1:A:27:ARG:HH12	1.77	0.50
1:A:56:ASP:HB3	1:A:101:PRO:HD3	1.92	0.50
1:A:375:LYS:HD2	1:A:412:VAL:HB	1.93	0.50
1:B:448:ASN:HD22	1:B:467:PHE:HE2	1.59	0.50
1:B:600:LEU:HD21	1:B:701:ALA:HB1	1.93	0.50
1:C:258:MET:O	1:C:263:LYS:NZ	2.44	0.50
1:D:351:LEU:O	1:D:469:THR:OG1	2.27	0.50
1:E:226:LEU:HB3	2:F:280:SER:HA	1.93	0.50
1:E:746:LEU:O	1:E:748:LYS:NZ	2.39	0.50
1:A:346:ASN:OD1	1:A:347:LYS:N	2.45	0.50
1:A:529:ARG:NH1	1:A:571:ALA:O	2.44	0.50
1:A:624:SER:H	1:A:663:LEU:HD12	1.76	0.50
1:B:392:GLY:HA3	1:B:455:TYR:HB2	1.94	0.50
1:B:598:GLN:HB3	1:B:609:LEU:HD22	1.94	0.50
1:C:30:SER:OG	1:C:55:ASP:O	2.30	0.50
1:C:297:PRO:HB2	1:C:300:LYS:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:SER:HA	1:D:366:ARG:HB2	1.94	0.50
1:D:535:THR:OG1	1:D:545:ARG:NH2	2.45	0.50
1:D:714:PRO:HB3	1:D:738:ASP:HB3	1.93	0.50
1:A:602:TRP:O	1:A:674:LYS:NZ	2.45	0.50
1:B:302:ASP:HB3	1:B:374:ARG:HG2	1.93	0.50
1:C:16:LEU:HD23	1:C:180:LEU:HD13	1.93	0.50
1:C:499:GLN:HE21	1:C:528:LEU:HB3	1.75	0.50
1:E:253:ILE:HG23	1:E:258:MET:HG2	1.92	0.50
1:E:391:ARG:HG3	1:E:453:ASP:CA	2.42	0.50
2:F:703:THR:OG1	2:F:721:LYS:NZ	2.38	0.50
1:A:350:ILE:HG21	1:A:469:THR:HG23	1.94	0.50
1:C:584:ARG:HG3	1:C:586:ASP:H	1.76	0.50
1:E:346:ASN:HB3	1:E:348:ALA:HB3	1.92	0.50
1:A:622:LYS:O	1:A:662:ASP:HA	2.12	0.49
1:D:552:ARG:HH22	1:E:335:VAL:HB	1.76	0.49
1:E:9:PRO:HG3	1:E:103:LEU:HD11	1.93	0.49
1:E:374:ARG:HH22	1:E:466:PHE:H	1.59	0.49
1:E:477:ILE:O	1:E:479:ARG:NH2	2.45	0.49
1:E:530:VAL:HG21	1:E:550:ILE:HD11	1.94	0.49
2:F:361:LYS:HB3	2:F:420:LEU:HD11	1.94	0.49
1:A:421:LEU:HD21	1:A:424:ILE:HG23	1.93	0.49
1:A:461:ASP:OD2	1:A:464:LYS:NZ	2.45	0.49
1:B:322:LEU:HD22	1:B:326:LYS:HB3	1.94	0.49
1:C:483:ASP:OD1	1:C:483:ASP:N	2.44	0.49
1:D:712:VAL:HG12	1:D:736:PRO:HG3	1.94	0.49
1:D:722:LEU:HD22	1:D:733:ILE:HD12	1.94	0.49
1:E:369:ALA:O	1:E:374:ARG:N	2.44	0.49
2:F:685:THR:HG21	2:F:702:MET:HE2	1.93	0.49
1:A:516:MET:HB3	1:B:338:LEU:HD21	1.94	0.49
1:A:759:VAL:HB	1:A:768:TYR:HE2	1.77	0.49
1:B:374:ARG:HB2	1:B:418:VAL:HG23	1.94	0.49
1:C:412:VAL:HG22	1:C:414:VAL:H	1.78	0.49
1:D:625:LEU:HD12	1:D:629:LEU:HB3	1.94	0.49
1:E:533:GLU:HB3	1:E:581:PRO:HA	1.94	0.49
1:A:437:SER:OG	2:F:664:HIS:ND1	2.37	0.49
1:C:6:PRO:HB2	1:C:33:ALA:HA	1.94	0.49
1:C:234:GLN:NE2	1:D:274:GLU:O	2.46	0.49
1:D:122:ARG:HD3	1:D:158:PRO:HG3	1.94	0.49
1:E:129:LYS:HB2	1:E:161:LEU:HD11	1.93	0.49
2:F:674:LYS:HB3	2:F:678:SER:HA	1.94	0.49
1:A:284:THR:HG23	1:B:396:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ILE:HB	1:C:46:LEU:HD21	1.93	0.49
1:E:320:TYR:O	1:E:505:TYR:OH	2.29	0.49
1:E:700:ILE:HG21	1:E:769:LEU:HD11	1.94	0.49
1:A:167:TYR:HA	1:A:176:LYS:HD3	1.94	0.49
1:A:190:LYS:HB2	1:D:214:LYS:HG3	1.94	0.49
1:A:303:PRO:O	1:A:373:ASN:HB2	2.12	0.49
1:A:434:ASP:O	2:F:624:SER:OG	2.30	0.49
1:C:503:ARG:NH1	1:C:522:VAL:O	2.46	0.49
1:C:616:ALA:HB3	1:C:693:ARG:HH12	1.78	0.49
2:F:600:LEU:HD21	2:F:725:ALA:HB2	1.95	0.49
2:F:631:GLU:HA	2:F:634:LYS:HE2	1.94	0.49
1:A:199:ASP:O	1:A:202:ARG:HG2	2.12	0.49
1:A:366:ARG:HG3	1:A:370:ARG:HH12	1.78	0.49
1:A:494:THR:HG22	1:A:750:VAL:HG22	1.95	0.49
1:B:601:ALA:HB2	1:B:610:LEU:HD11	1.93	0.49
1:C:520:ILE:HG22	1:C:567:ARG:HB2	1.95	0.49
1:D:222:ARG:NH1	1:D:225:TYR:HD2	2.11	0.49
1:D:346:ASN:O	1:D:484:ARG:NE	2.43	0.49
1:E:478:PRO:HB2	1:E:481:LEU:HG	1.95	0.49
1:E:507:TRP:HD1	1:E:547:LEU:HD11	1.77	0.49
2:F:253:ILE:HD13	2:F:270:LEU:HB2	1.94	0.49
1:B:279:GLY:H	1:C:280:SER:HB3	1.77	0.49
1:B:662:ASP:OD2	1:C:658:TYR:OH	2.31	0.49
1:B:707:SER:OG	1:B:711:LYS:N	2.39	0.49
1:C:11:ARG:HA	1:C:53:GLU:HB3	1.94	0.49
1:D:360:GLY:N	1:D:493:TYR:OH	2.44	0.49
1:D:615:ALA:N	1:D:664:HIS:O	2.45	0.49
1:A:623:LEU:HA	1:A:663:LEU:HG	1.94	0.49
1:B:570:ASP:OD1	1:B:570:ASP:N	2.41	0.49
1:C:732:LYS:HA	1:C:755:GLU:HG3	1.94	0.49
1:D:478:PRO:HD2	1:D:481:LEU:HD12	1.95	0.49
1:E:250:ARG:HH21	1:E:270:LEU:HD22	1.75	0.49
2:F:312:ARG:HA	2:F:330:LEU:HD11	1.93	0.49
2:F:440:LEU:HB2	2:F:480:PRO:HB2	1.93	0.49
1:A:234:GLN:NE2	1:A:240:GLU:OE1	2.46	0.48
1:A:678:SER:O	1:A:703:THR:OG1	2.31	0.48
1:B:9:PRO:O	1:B:27:ARG:NH2	2.46	0.48
1:C:247:GLU:HG2	1:C:250:ARG:HH21	1.78	0.48
1:D:737:LYS:HB2	1:D:760:GLU:HG2	1.95	0.48
1:E:147:TYR:HA	1:E:150:GLU:HG3	1.95	0.48
2:F:404:LYS:O	2:F:408:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:577:TYR:O	2:F:578:LEU:HB2	2.12	0.48
1:A:58:ALA:HB3	1:A:61:ASP:HB2	1.95	0.48
1:B:34:VAL:HG12	1:B:38:MET:HE3	1.95	0.48
1:C:67:VAL:HG12	1:C:91:ARG:HA	1.94	0.48
1:C:300:LYS:CB	1:C:414:VAL:HA	2.44	0.48
1:C:600:LEU:HD11	1:C:701:ALA:HB1	1.94	0.48
1:D:387:GLU:HA	1:D:390:ILE:HB	1.95	0.48
1:E:253:ILE:HA	1:E:258:MET:HE3	1.94	0.48
1:A:614:VAL:HG21	1:A:687:ILE:HG13	1.95	0.48
1:C:242:GLY:HA2	1:C:245:ASP:OD2	2.13	0.48
1:E:353:LEU:HD23	1:E:488:ILE:HB	1.95	0.48
1:E:500:ALA:O	1:E:504:GLN:CB	2.61	0.48
2:F:348:ALA:O	2:F:484:ARG:NH2	2.46	0.48
1:A:244:SER:N	1:B:271:ASP:O	2.40	0.48
1:A:312:ARG:HB2	1:A:330:LEU:HD13	1.96	0.48
1:C:171:TRP:O	1:C:176:LYS:NZ	2.46	0.48
1:C:618:PRO:O	1:D:645:ARG:NH2	2.47	0.48
1:D:250:ARG:HA	1:D:253:ILE:HB	1.95	0.48
1:D:298:TRP:CZ2	1:D:460:TYR:CD1	3.01	0.48
1:D:353:LEU:HB3	1:D:490:ILE:HD11	1.96	0.48
1:D:477:ILE:O	1:D:479:ARG:NH2	2.46	0.48
1:E:324:ASP:OD1	1:E:324:ASP:N	2.46	0.48
2:F:612:ILE:HD12	2:F:667:VAL:HG22	1.95	0.48
1:A:15:ILE:HA	1:A:21:THR:HG21	1.96	0.48
1:A:349:PRO:HA	1:A:485:MET:HA	1.96	0.48
1:A:421:LEU:HB3	1:A:469:THR:HA	1.95	0.48
1:B:681:ILE:HD12	1:B:765:VAL:HG11	1.96	0.48
1:C:681:ILE:HG23	1:C:704:GLY:HA3	1.95	0.48
1:E:362:THR:HG23	1:E:378:ARG:HD2	1.94	0.48
1:E:737:LYS:N	1:E:759:VAL:O	2.46	0.48
1:A:435:PRO:HB2	1:A:439:MET:HE1	1.96	0.48
1:A:533:GLU:HG2	1:A:585:PRO:HD3	1.94	0.48
1:B:452:THR:HB	1:B:459:PRO:HG3	1.95	0.48
1:D:6:PRO:HG3	1:D:36:GLU:HB3	1.96	0.48
1:D:314:VAL:O	1:D:370:ARG:NH2	2.46	0.48
1:E:308:ILE:HG23	1:E:330:LEU:HD22	1.93	0.48
1:E:516:MET:O	1:E:516:MET:HG2	2.11	0.48
1:E:574:ILE:HD12	1:E:577:TYR:HB2	1.94	0.48
2:F:304:GLU:OE2	2:F:416:ASN:ND2	2.36	0.48
1:B:593:GLN:NE2	1:B:598:GLN:HE21	2.11	0.48
1:B:597:ALA:O	1:B:612:ILE:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:GLY:O	1:B:721:LYS:N	2.43	0.48
1:A:696:ALA:HA	1:A:770:LEU:HA	1.95	0.48
1:C:510:GLN:O	1:C:514:SER:OG	2.32	0.48
1:C:696:ALA:HB1	1:C:769:LEU:HG	1.95	0.48
1:E:460:TYR:HD2	1:E:462:LEU:HD23	1.78	0.48
1:A:202:ARG:HA	1:D:222:ARG:CZ	2.44	0.48
1:B:526:ALA:HB1	1:B:574:ILE:HD11	1.95	0.48
1:E:352:VAL:HG12	1:E:469:THR:HB	1.96	0.48
1:E:483:ASP:OD1	1:E:483:ASP:N	2.47	0.48
1:A:616:ALA:HA	1:A:663:LEU:HA	1.95	0.47
1:B:310:HIS:HA	1:B:313:GLN:HG2	1.95	0.47
1:C:47:VAL:HB	1:C:62:LEU:HD22	1.96	0.47
1:C:731:HIS:O	1:C:755:GLU:N	2.47	0.47
1:D:133:GLU:O	1:D:146:ARG:NH2	2.47	0.47
1:D:545:ARG:NH1	1:D:546:GLU:OE2	2.47	0.47
1:E:27:ARG:NH1	1:E:54:VAL:O	2.47	0.47
2:F:335:VAL:HG12	2:F:339:THR:HG23	1.96	0.47
1:A:600:LEU:HD13	1:A:721:LYS:HB3	1.94	0.47
1:B:102:TYR:OH	1:B:104:ARG:NH1	2.47	0.47
1:B:218:ASP:OD1	1:B:221:GLN:NE2	2.46	0.47
1:B:420:LEU:HA	1:B:468:ILE:HB	1.96	0.47
1:B:500:ALA:HA	1:B:503:ARG:HD2	1.96	0.47
1:C:443:LEU:HD21	1:C:484:ARG:HB2	1.95	0.47
1:D:232:ALA:HA	1:D:235:LYS:HE2	1.95	0.47
1:E:212:ARG:NH1	1:E:216:GLN:OE1	2.47	0.47
1:E:451:PHE:CD2	1:E:462:LEU:HD11	2.49	0.47
1:A:711:LYS:NZ	1:A:761:ASP:OD1	2.46	0.47
1:B:590:THR:HB	1:B:698:MET:HE3	1.96	0.47
1:C:320:TYR:O	1:C:323:LYS:NZ	2.40	0.47
1:C:592:PRO:HG3	1:C:771:LEU:HD13	1.95	0.47
1:C:654:PRO:HG2	1:C:657:PHE:HB3	1.95	0.47
2:F:250:ARG:NH2	2:F:274:GLU:OE2	2.47	0.47
1:D:617:VAL:O	1:D:662:ASP:N	2.48	0.47
1:E:603:THR:HG22	1:E:673:PRO:HG2	1.95	0.47
1:A:195:LEU:HA	1:A:198:ARG:HG2	1.96	0.47
1:A:231:LYS:HA	1:A:235:LYS:HE3	1.96	0.47
1:B:529:ARG:NH1	1:B:571:ALA:O	2.48	0.47
1:C:707:SER:OG	1:C:711:LYS:N	2.45	0.47
1:D:678:SER:O	1:D:703:THR:OG1	2.32	0.47
2:F:386:ASP:OD1	2:F:386:ASP:N	2.47	0.47
1:A:9:PRO:O	1:A:27:ARG:NH2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:NE	1:D:180:LEU:O	2.47	0.47
1:D:635:GLU:HA	1:D:638:GLN:HG2	1.97	0.47
1:D:716:GLY:O	1:D:721:LYS:NZ	2.41	0.47
1:E:452:THR:HB	1:E:459:PRO:HG3	1.96	0.47
1:A:321:GLY:H	1:A:323:LYS:HD3	1.80	0.47
1:A:732:LYS:HD2	1:A:757:LYS:HE3	1.97	0.47
1:B:295:GLU:HG2	1:B:410:LYS:HD2	1.96	0.47
1:B:448:ASN:ND2	1:B:462:LEU:O	2.48	0.47
1:B:618:PRO:O	1:C:645:ARG:NH2	2.48	0.47
1:C:345:ARG:HD3	1:C:347:LYS:HE2	1.95	0.47
1:C:439:MET:HA	1:C:442:VAL:HG22	1.97	0.47
1:E:443:LEU:HD22	1:E:484:ARG:HB2	1.95	0.47
2:F:362:THR:HG1	2:F:509:LYS:HZ1	1.61	0.47
2:F:421:LEU:HB3	2:F:424:ILE:HD11	1.97	0.47
2:F:531:ILE:HG12	2:F:543:LEU:HD11	1.96	0.47
1:A:146:ARG:HG3	1:A:149:LEU:HD23	1.96	0.47
1:B:440:LEU:HD22	1:B:480:PRO:HB3	1.95	0.47
1:C:279:GLY:HA3	1:D:396:THR:HA	1.96	0.47
1:E:28:ALA:HA	1:E:31:LYS:HB2	1.97	0.47
1:E:50:ARG:NH2	1:E:61:ASP:OD1	2.48	0.47
2:F:387:GLU:HG3	2:F:435:PRO:HB3	1.95	0.47
2:F:392:GLY:HA3	2:F:455:TYR:HB2	1.96	0.47
1:C:277:GLN:HG2	1:C:283:ALA:HB3	1.97	0.47
2:F:719:LYS:HE3	2:F:746:LEU:HD22	1.97	0.47
1:B:129:LYS:HE3	1:B:161:LEU:HD11	1.96	0.47
1:E:250:ARG:HA	1:E:253:ILE:HD12	1.96	0.47
1:E:440:LEU:HD23	1:E:443:LEU:HD12	1.96	0.47
1:E:731:HIS:ND1	1:E:753:GLY:O	2.48	0.47
1:B:423:GLU:HG2	1:B:426:LYS:HE3	1.95	0.46
1:E:496:MET:O	1:E:499:GLN:NE2	2.48	0.46
2:F:429:SER:HB2	2:F:434:ASP:HA	1.97	0.46
2:F:633:MET:HE3	2:F:672:THR:H	1.80	0.46
1:B:98:ILE:HD11	1:B:106:ARG:HE	1.80	0.46
1:B:278:GLN:HG2	1:C:281:PRO:HA	1.97	0.46
1:B:293:LEU:HD12	1:B:456:LEU:HA	1.96	0.46
1:C:265:LYS:HD2	1:C:458:VAL:H	1.80	0.46
1:C:339:THR:HG21	1:C:344:VAL:HA	1.97	0.46
1:C:382:GLY:O	1:C:385:ARG:NH2	2.37	0.46
1:C:733:ILE:N	1:C:755:GLU:O	2.39	0.46
1:C:759:VAL:HG21	1:C:765:VAL:HB	1.96	0.46
1:E:290:LEU:O	1:E:294:THR:OG1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:GLU:OE2	1:E:391:ARG:HD3	2.15	0.46
2:F:350:ILE:HG21	2:F:467:PHE:HB2	1.96	0.46
1:A:55:ASP:OD1	1:A:55:ASP:N	2.47	0.46
1:B:599:GLY:N	1:B:610:LEU:O	2.34	0.46
1:B:726:HIS:HB2	1:B:754:LEU:HD21	1.96	0.46
1:C:563:TRP:CD1	1:C:564:GLU:HG3	2.51	0.46
1:D:44:ILE:HG23	1:D:69:ALA:HB3	1.97	0.46
1:D:387:GLU:OE2	1:D:437:SER:OG	2.32	0.46
1:E:391:ARG:HD3	1:E:438:ALA:HB2	1.98	0.46
1:E:614:VAL:HG11	1:E:687:ILE:HA	1.97	0.46
1:A:549:LYS:HA	1:A:552:ARG:HB2	1.97	0.46
1:D:285:VAL:HG21	1:D:400:ALA:HB3	1.96	0.46
1:D:507:TRP:HD1	1:D:547:LEU:HD11	1.81	0.46
1:E:10:LEU:HD11	1:E:23:VAL:HG22	1.97	0.46
1:E:129:LYS:HE2	1:E:152:VAL:HG23	1.97	0.46
1:E:384:VAL:HG13	1:E:389:GLU:OE1	2.15	0.46
1:B:37:ALA:HB1	1:B:44:ILE:HG12	1.97	0.46
1:B:522:VAL:HA	1:B:569:ILE:HB	1.98	0.46
1:C:359:VAL:O	1:C:361:LYS:NZ	2.40	0.46
1:C:494:THR:HG21	1:C:750:VAL:HA	1.97	0.46
1:C:620:SER:OG	1:C:622:LYS:NZ	2.47	0.46
1:D:739:ASN:O	1:D:743:LEU:N	2.49	0.46
1:E:510:GLN:HA	1:E:513:GLU:HG3	1.97	0.46
1:E:697:ARG:HD2	1:E:771:LEU:HB2	1.98	0.46
1:A:316:ASP:HA	1:A:323:LYS:HZ1	1.81	0.46
1:A:350:ILE:N	1:A:350:ILE:HD12	2.31	0.46
1:B:416:ASN:HB3	1:B:464:LYS:HB3	1.96	0.46
1:C:541:ARG:NH2	3:C:801:ADP:O3B	2.48	0.46
1:E:543:LEU:HA	1:E:546:GLU:HB2	1.96	0.46
1:E:700:ILE:HD13	1:E:768:TYR:CE2	2.50	0.46
2:F:249:LEU:HD23	2:F:252:LYS:HD3	1.98	0.46
1:A:212:ARG:HH11	1:C:232:ALA:HB1	1.81	0.46
1:A:547:LEU:HD23	1:A:550:ILE:HD12	1.98	0.46
1:B:442:VAL:HG13	1:B:462:LEU:HD13	1.97	0.46
1:C:302:ASP:HB3	1:C:416:ASN:HD21	1.80	0.46
1:C:439:MET:O	1:C:443:LEU:N	2.48	0.46
1:C:623:LEU:HA	1:C:663:LEU:HB2	1.97	0.46
1:E:256:VAL:HG21	1:E:297:PRO:HA	1.97	0.46
1:E:360:GLY:HA2	3:E:801:ADP:H5'1	1.98	0.46
1:E:714:PRO:HB3	1:E:738:ASP:HB3	1.98	0.46
1:A:3:LEU:HD21	1:A:43:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:O	1:A:373:ASN:ND2	2.49	0.46
1:D:302:ASP:H	1:D:416:ASN:HD21	1.62	0.46
1:A:29:LYS:HB2	1:A:55:ASP:HB2	1.97	0.46
1:A:494:THR:HG21	1:A:749:GLU:HB3	1.98	0.46
1:B:329:ILE:HD11	1:B:488:ILE:HG13	1.97	0.46
1:C:24:ASP:OD1	1:C:24:ASP:N	2.43	0.46
1:D:55:ASP:OD1	1:D:55:ASP:N	2.47	0.46
1:D:506:LEU:O	1:D:510:GLN:N	2.43	0.46
1:D:680:GLY:HA2	1:D:683:MET:HE2	1.97	0.46
2:F:265:LYS:HB3	2:F:458:VAL:HB	1.98	0.46
2:F:395:ARG:NH1	2:F:455:TYR:O	2.48	0.46
2:F:536:ARG:NH1	2:F:537:GLU:OE2	2.48	0.46
1:A:354:VAL:HA	1:A:472:ASN:HA	1.97	0.46
1:A:511:VAL:O	1:A:516:MET:N	2.49	0.46
1:B:125:VAL:HG13	1:B:161:LEU:HD22	1.96	0.46
1:B:304:GLU:HG2	1:B:374:ARG:HD2	1.97	0.46
1:B:385:ARG:HB2	1:B:428:SER:OG	2.16	0.46
1:B:688:ALA:HA	1:B:691:LEU:HB2	1.98	0.46
1:C:4:GLU:HB3	1:C:106:ARG:HH21	1.81	0.46
2:F:262:VAL:HG13	2:F:265:LYS:HE3	1.98	0.46
2:F:298:TRP:O	2:F:300:LYS:NZ	2.36	0.46
1:A:118:GLU:HA	1:A:121:VAL:HB	1.99	0.45
1:A:552:ARG:HH11	1:B:331:GLU:HG3	1.82	0.45
1:B:455:TYR:HD1	1:B:456:LEU:HD23	1.80	0.45
1:C:362:THR:OG1	1:C:378:ARG:NH2	2.49	0.45
1:D:69:ALA:HA	1:D:88:ALA:HA	1.98	0.45
2:F:439:MET:SD	2:F:439:MET:N	2.88	0.45
2:F:523:THR:O	2:F:527:ILE:N	2.44	0.45
1:B:77:LEU:HD12	1:B:81:THR:HB	1.97	0.45
1:B:314:VAL:HA	1:B:317:GLU:HG2	1.98	0.45
1:C:318:ASP:OD2	1:C:370:ARG:NH1	2.49	0.45
1:D:293:LEU:HD11	1:D:458:VAL:HG21	1.97	0.45
1:D:320:TYR:O	1:D:326:LYS:NZ	2.37	0.45
1:E:694:ARG:NE	1:E:772:PRO:O	2.44	0.45
2:F:619:GLY:N	2:F:660:LYS:O	2.50	0.45
1:A:205:LEU:HD23	1:D:222:ARG:NH2	2.31	0.45
1:B:575:PRO:HG3	1:B:581:PRO:HD3	1.98	0.45
1:B:629:LEU:HA	1:B:670:GLY:HA3	1.97	0.45
1:D:706:VAL:HG23	1:D:762:VAL:HG21	1.97	0.45
1:A:307:ASP:OD1	1:A:307:ASP:N	2.48	0.45
1:B:16:LEU:O	1:B:19:THR:OG1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:GLU:HB3	1:C:581:PRO:HB3	1.98	0.45
1:C:598:GLN:HE22	1:C:699:ASP:H	1.64	0.45
1:C:618:PRO:HA	1:C:661:VAL:HG23	1.97	0.45
1:D:623:LEU:HD22	1:D:638:GLN:HE22	1.81	0.45
1:D:707:SER:HB2	1:D:711:LYS:H	1.81	0.45
1:E:718:VAL:HG23	1:E:735:LEU:HD11	1.98	0.45
1:A:312:ARG:HA	1:A:315:LEU:HD12	1.98	0.45
1:A:694:ARG:HB3	1:A:772:PRO:HD2	1.98	0.45
1:C:378:ARG:NH2	3:C:801:ADP:O2B	2.50	0.45
1:E:27:ARG:HH11	1:E:57:PRO:HG3	1.81	0.45
2:F:587:LYS:HA	2:F:590:THR:HB	1.97	0.45
1:A:325:VAL:HG12	1:A:328:ARG:HG3	1.98	0.45
1:C:490:ILE:HD12	1:C:491:PRO:HD2	1.99	0.45
1:C:737:LYS:HA	1:C:758:LEU:HD22	1.97	0.45
1:D:345:ARG:O	1:D:484:ARG:NH2	2.50	0.45
2:F:326:LYS:O	2:F:330:LEU:HB2	2.17	0.45
1:C:621:GLY:N	1:C:662:ASP:OD1	2.43	0.45
1:D:264:THR:HA	1:D:267:LEU:HD12	1.98	0.45
1:E:263:LYS:HE3	1:E:267:LEU:HD11	1.99	0.45
2:F:249:LEU:HD22	2:F:290:LEU:HG	1.99	0.45
1:B:351:LEU:O	1:B:469:THR:OG1	2.30	0.45
1:C:421:LEU:HD23	1:C:467:PHE:HB3	1.98	0.45
1:D:387:GLU:HA	1:D:391:ARG:H	1.82	0.45
1:E:307:ASP:OD1	1:E:309:ASN:ND2	2.49	0.45
1:A:63:TYR:HB3	1:A:65:TRP:H	1.82	0.45
1:A:335:VAL:HB	1:A:336:ARG:HH11	1.81	0.45
1:B:696:ALA:HA	1:B:770:LEU:HA	1.99	0.45
1:E:386:ASP:HB2	1:E:389:GLU:HG3	1.99	0.45
1:E:395:ARG:NH1	1:E:455:TYR:O	2.50	0.45
1:E:648:THR:OG1	1:E:649:GLN:N	2.50	0.45
1:A:374:ARG:NH1	1:A:464:LYS:O	2.50	0.45
1:A:534:TYR:OH	1:A:579:GLY:O	2.33	0.45
1:B:648:THR:OG1	1:B:649:GLN:OE1	2.34	0.45
1:C:394:ARG:HH21	1:C:395:ARG:HG2	1.80	0.45
1:C:697:ARG:HE	1:C:700:ILE:HG13	1.82	0.45
1:D:600:LEU:HB2	1:D:703:THR:HB	1.98	0.45
1:E:391:ARG:CD	1:E:438:ALA:HB2	2.46	0.45
1:E:424:ILE:HD13	1:E:427:MET:HE3	1.99	0.45
1:E:713:MET:SD	1:E:713:MET:N	2.90	0.45
1:A:516:MET:HE1	1:A:519:ARG:H	1.82	0.44
1:E:556:LYS:NZ	1:E:560:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HG2	1:A:150:GLU:HG3	1.99	0.44
1:A:356:PRO:HG2	1:A:359:VAL:HG11	1.98	0.44
1:C:332:TYR:CZ	1:C:336:ARG:HD3	2.51	0.44
1:D:50:ARG:HD2	1:D:52:PRO:HD2	1.99	0.44
1:E:330:LEU:HD23	1:E:333:LEU:HD12	2.00	0.44
1:E:541:ARG:NH2	3:E:801:ADP:O5'	2.51	0.44
1:E:581:PRO:HB3	1:E:585:PRO:HD3	1.98	0.44
2:F:350:ILE:HG13	2:F:352:VAL:HG13	1.99	0.44
2:F:456:LEU:HD12	2:F:456:LEU:N	2.32	0.44
1:B:91:ARG:NH1	1:B:112:GLU:OE2	2.50	0.44
1:B:598:GLN:HA	1:B:611:THR:HA	2.00	0.44
1:B:651:TYR:OH	1:B:763:GLY:O	2.35	0.44
1:E:17:PRO:HA	1:E:88:ALA:HB3	1.99	0.44
1:E:298:TRP:CZ3	1:E:460:TYR:HA	2.53	0.44
1:E:451:PHE:O	1:E:460:TYR:N	2.47	0.44
2:F:379:ILE:HB	2:F:404:LYS:HE3	1.99	0.44
2:F:385:ARG:HH11	2:F:426:LYS:HD3	1.82	0.44
2:F:618:PRO:HB3	2:F:660:LYS:HZ3	1.83	0.44
1:A:353:LEU:HB3	1:A:361:LYS:HB3	1.99	0.44
1:B:258:MET:HG2	1:B:262:VAL:HG11	1.98	0.44
1:B:718:VAL:HA	1:B:721:LYS:HB2	1.98	0.44
1:D:291:ASP:HB3	1:D:295:GLU:CD	2.41	0.44
1:A:614:VAL:HG22	1:A:665:VAL:HG22	1.99	0.44
1:B:701:ALA:N	1:B:730:ILE:HG21	2.32	0.44
1:D:290:LEU:HD22	1:D:293:LEU:HD23	1.99	0.44
1:D:494:THR:HB	1:D:726:HIS:HD2	1.82	0.44
1:D:618:PRO:O	1:E:645:ARG:NH2	2.36	0.44
1:E:155:THR:HG22	1:E:160:MET:HG3	1.99	0.44
1:E:273:LEU:HD21	1:E:287:ARG:HG3	2.00	0.44
2:F:501:ILE:HG23	2:F:505:TYR:HB2	1.98	0.44
1:A:318:ASP:OD2	1:A:367:SER:OG	2.31	0.44
1:B:98:ILE:HB	1:B:104:ARG:HB2	2.00	0.44
1:B:230:MET:HE3	1:B:270:LEU:HD23	1.98	0.44
1:B:347:LYS:HA	1:B:347:LYS:HD3	1.71	0.44
1:C:569:ILE:HG23	1:C:577:TYR:HE2	1.83	0.44
1:D:241:ASP:OD1	1:D:241:ASP:N	2.51	0.44
2:F:336:ARG:NH1	2:F:343:ASP:O	2.50	0.44
1:A:417:PRO:HD2	1:A:465:VAL:HG13	2.00	0.44
1:A:715:ILE:O	1:A:739:ASN:ND2	2.51	0.44
1:B:452:THR:OG1	1:B:453:ASP:N	2.51	0.44
1:C:381:LEU:HG	1:C:421:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:GLY:O	1:C:519:ARG:NE	2.40	0.44
1:D:533:GLU:HA	1:D:583:TYR:HB2	1.99	0.44
1:E:59:PRO:HG3	1:E:99:PRO:HA	1.99	0.44
1:E:474:LEU:HD11	1:E:487:VAL:HG21	1.98	0.44
2:F:508:PRO:HA	2:F:511:VAL:HG22	2.00	0.44
2:F:587:LYS:HE3	2:F:699:ASP:HA	2.00	0.44
2:F:695:PRO:HG2	2:F:771:LEU:HB3	1.99	0.44
1:A:366:ARG:O	1:A:370:ARG:HG2	2.18	0.44
1:A:394:ARG:HA	1:A:394:ARG:HD3	1.84	0.44
1:A:594:VAL:HA	1:A:695:PRO:HA	1.99	0.44
1:B:391:ARG:HH22	1:B:452:THR:HG23	1.82	0.44
1:B:658:TYR:HA	1:B:661:VAL:HG12	2.00	0.44
1:C:626:THR:OG1	1:C:627:GLY:N	2.51	0.44
1:C:651:TYR:OH	1:C:763:GLY:O	2.36	0.44
1:B:473:THR:HA	1:B:674:LYS:HE3	2.00	0.44
1:E:261:ALA:HB1	1:E:458:VAL:HG21	1.98	0.44
2:F:384:VAL:HG13	2:F:389:GLU:HB2	2.00	0.44
1:C:507:TRP:HZ2	1:C:521:GLU:HB2	1.83	0.43
1:D:629:LEU:HD12	1:D:633:MET:HG2	2.00	0.43
1:D:720:GLU:HA	1:D:723:LEU:HD12	2.00	0.43
1:E:292:TRP:HZ3	1:E:410:LYS:HE2	1.82	0.43
2:F:473:THR:OG1	2:F:476:THR:OG1	2.35	0.43
2:F:588:ALA:HA	2:F:591:GLU:HG2	1.98	0.43
2:F:680:GLY:H	2:F:705:GLU:HA	1.82	0.43
1:A:125:VAL:HG21	1:A:158:PRO:HB3	2.00	0.43
1:A:148:GLN:HB2	1:A:168:HIS:CE1	2.52	0.43
1:A:375:LYS:O	1:A:377:HIS:HD2	2.01	0.43
1:B:47:VAL:HG11	1:B:62:LEU:HB3	2.00	0.43
1:B:387:GLU:HG3	1:B:435:PRO:HA	1.99	0.43
1:B:439:MET:HE1	1:B:481:LEU:HG	2.00	0.43
1:C:16:LEU:HD12	1:C:167:TYR:HB2	1.99	0.43
1:D:128:LEU:HD11	1:D:192:VAL:HG12	1.98	0.43
1:E:391:ARG:HG3	1:E:454:HIS:H	1.83	0.43
1:E:623:LEU:HG	1:E:663:LEU:HD23	2.00	0.43
2:F:361:LYS:H	2:F:541:ARG:NH2	2.16	0.43
1:A:420:LEU:HA	1:A:468:ILE:HG23	2.00	0.43
1:B:427:MET:HA	1:B:427:MET:CE	2.46	0.43
1:B:498:LYS:HB2	1:B:498:LYS:HE2	1.86	0.43
1:D:290:LEU:HA	1:D:293:LEU:HB3	2.00	0.43
1:D:315:LEU:HG	1:D:326:LYS:HD2	2.00	0.43
2:F:706:VAL:HG23	2:F:762:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HB3	1:C:290:LEU:HD23	1.99	0.43
1:C:353:LEU:HB3	1:C:470:THR:HG23	2.00	0.43
1:C:635:GLU:HA	1:C:638:GLN:HB2	2.00	0.43
1:D:402:PRO:HB3	1:D:455:TYR:CG	2.53	0.43
1:D:546:GLU:HA	1:D:549:LYS:HE2	1.99	0.43
1:D:578:LEU:HD12	1:D:578:LEU:HA	1.79	0.43
1:E:57:PRO:HB2	1:E:103:LEU:HD13	2.00	0.43
1:E:392:GLY:CA	1:E:455:TYR:HB2	2.33	0.43
1:E:622:LYS:N	1:E:662:ASP:OD1	2.45	0.43
1:E:626:THR:OG1	1:E:665:VAL:O	2.31	0.43
2:F:439:MET:HB3	2:F:481:LEU:HD21	2.00	0.43
1:A:304:GLU:HB2	1:A:372:MET:HA	1.99	0.43
1:A:654:PRO:HD2	1:A:691:LEU:HB3	2.00	0.43
1:A:718:VAL:HA	1:A:721:LYS:HE2	2.00	0.43
1:C:202:ARG:NE	2:F:276:MET:SD	2.91	0.43
1:D:91:ARG:HH21	1:D:180:LEU:HA	1.83	0.43
1:D:442:VAL:HG13	1:D:462:LEU:HD13	2.01	0.43
1:D:556:LYS:HB2	1:E:331:GLU:HG3	2.00	0.43
1:D:633:MET:HG3	1:D:677:PRO:HB3	2.00	0.43
1:E:353:LEU:HD12	1:E:470:THR:HG22	2.01	0.43
1:E:453:ASP:OD1	1:E:456:LEU:N	2.46	0.43
1:A:512:ARG:O	1:B:340:GLN:NE2	2.37	0.43
1:A:571:ALA:HA	1:A:574:ILE:HG12	2.01	0.43
1:A:614:VAL:O	1:A:690:ALA:HB2	2.18	0.43
1:B:388:ALA:HB3	1:B:432:ARG:HB3	1.99	0.43
1:B:412:VAL:HG21	1:B:417:PRO:HG3	1.99	0.43
1:C:696:ALA:HA	1:C:770:LEU:HA	2.00	0.43
1:D:353:LEU:HB2	1:D:470:THR:HG22	2.00	0.43
1:D:601:ALA:HB3	1:D:610:LEU:HB2	2.01	0.43
1:D:623:LEU:HD21	1:D:641:LEU:HD22	2.00	0.43
1:D:648:THR:HG23	1:D:653:LEU:HB2	1.99	0.43
1:E:353:LEU:HB2	1:E:470:THR:HA	1.99	0.43
1:E:757:LYS:HE3	1:E:768:TYR:CE2	2.54	0.43
1:B:379:ILE:HD12	1:B:381:LEU:HD21	2.00	0.43
1:C:320:TYR:H	3:C:801:ADP:HN61	1.67	0.43
1:C:615:ALA:N	1:C:664:HIS:O	2.49	0.43
1:E:135:TYR:HE1	1:E:199:ASP:HB2	1.83	0.43
1:E:556:LYS:HB3	2:F:331:GLU:HG3	2.01	0.43
2:F:371:SER:OG	2:F:372:MET:N	2.50	0.43
1:A:633:MET:HE1	1:A:674:LYS:HG2	2.00	0.43
1:A:705:GLU:HB3	1:A:713:MET:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HG2	1:B:27:ARG:HH12	1.84	0.43
1:C:491:PRO:HD3	1:C:719:LYS:HD3	2.01	0.43
2:F:289:TYR:CE1	2:F:456:LEU:HG	2.48	0.43
2:F:453:ASP:OD1	2:F:455:TYR:N	2.46	0.43
1:A:287:ARG:HG2	1:B:396:THR:HB	2.00	0.43
1:B:483:ASP:OD1	1:B:483:ASP:N	2.52	0.43
1:D:7:VAL:HG13	1:D:47:VAL:H	1.82	0.43
1:D:757:LYS:HE3	1:D:757:LYS:HB3	1.89	0.43
1:E:416:ASN:OD1	1:E:416:ASN:N	2.52	0.43
1:B:57:PRO:HG2	1:B:101:PRO:HB3	2.00	0.43
1:B:473:THR:OG1	1:B:474:LEU:N	2.52	0.43
1:D:432:ARG:HD2	1:D:432:ARG:HA	1.85	0.43
1:E:677:PRO:HB2	1:E:705:GLU:HB3	2.01	0.43
1:A:333:LEU:HD12	1:A:337:GLN:HB2	2.01	0.42
1:A:418:VAL:HG13	1:A:466:PHE:HD2	1.84	0.42
1:A:722:LEU:HG	1:A:754:LEU:CD1	2.48	0.42
1:B:385:ARG:HD3	1:B:431:TRP:H	1.84	0.42
1:B:732:LYS:HA	1:B:732:LYS:HD3	1.84	0.42
1:C:332:TYR:HB2	1:C:351:LEU:HD21	2.00	0.42
1:D:697:ARG:HE	1:D:769:LEU:HA	1.84	0.42
2:F:700:ILE:HD13	2:F:768:TYR:HB3	2.01	0.42
1:A:622:LYS:HE3	1:A:662:ASP:OD1	2.18	0.42
1:C:198:ARG:HH12	1:C:202:ARG:HD2	1.85	0.42
1:C:314:VAL:HA	1:C:317:GLU:HG2	2.01	0.42
1:C:502:ALA:HA	1:C:506:LEU:HB2	2.00	0.42
1:C:705:GLU:HG2	1:C:713:MET:HE2	2.00	0.42
1:E:37:ALA:HB1	1:E:44:ILE:HG12	2.01	0.42
1:A:252:LYS:O	1:A:294:THR:OG1	2.33	0.42
1:A:367:SER:HA	1:A:370:ARG:CZ	2.49	0.42
1:B:227:ARG:HA	1:B:230:MET:HB3	2.01	0.42
1:B:678:SER:HA	1:B:705:GLU:HB2	2.01	0.42
1:B:707:SER:OG	1:B:710:GLY:N	2.52	0.42
1:C:479:ARG:O	1:C:479:ARG:NE	2.52	0.42
1:D:297:PRO:CG	1:D:412:VAL:HG23	2.47	0.42
1:D:603:THR:OG1	1:D:606:GLY:N	2.50	0.42
1:E:293:LEU:O	1:E:298:TRP:NE1	2.43	0.42
1:E:516:MET:SD	1:E:520:ILE:HB	2.59	0.42
1:E:681:ILE:HG13	1:E:702:MET:HB3	2.00	0.42
2:F:644:LEU:O	2:F:648:THR:OG1	2.29	0.42
1:A:374:ARG:CB	1:A:418:VAL:HG23	2.40	0.42
1:A:553:LYS:HG2	1:A:556:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:TYR:CZ	1:B:578:LEU:HD22	2.55	0.42
1:C:679:ALA:HA	1:C:703:THR:HA	2.01	0.42
1:D:222:ARG:HH12	1:D:225:TYR:HD2	1.67	0.42
1:E:475:GLN:NE2	1:E:673:PRO:O	2.52	0.42
1:E:612:ILE:CD1	1:E:667:VAL:HG13	2.49	0.42
1:E:642:THR:HA	1:E:645:ARG:HB2	2.00	0.42
1:A:372:MET:HE2	1:A:372:MET:HB3	1.83	0.42
1:A:498:LYS:HA	1:A:501:ILE:HG12	2.01	0.42
1:B:185:LEU:HA	1:B:188:ARG:HG2	2.02	0.42
1:B:333:LEU:HD12	1:B:336:ARG:HB3	2.02	0.42
1:C:332:TYR:OH	1:C:336:ARG:NH1	2.52	0.42
1:E:312:ARG:NH1	1:E:327:GLU:OE2	2.52	0.42
1:E:361:LYS:NZ	1:E:471:ALA:O	2.52	0.42
1:E:541:ARG:NH2	3:E:801:ADP:O3'	2.52	0.42
1:E:633:MET:HE3	1:E:672:THR:OG1	2.18	0.42
1:A:521:GLU:N	1:A:567:ARG:O	2.53	0.42
1:B:602:TRP:HA	1:B:607:GLY:HA2	2.02	0.42
1:C:253:ILE:HD13	1:C:266:ALA:HB1	2.02	0.42
1:D:382:GLY:HA2	1:D:426:LYS:HB2	2.00	0.42
1:D:587:LYS:HA	1:D:587:LYS:HD3	1.78	0.42
1:E:510:GLN:HG3	1:E:547:LEU:HG	2.01	0.42
1:E:643:TYR:CD1	1:E:710:GLY:HA3	2.55	0.42
2:F:603:THR:OG1	2:F:606:GLY:O	2.28	0.42
2:F:773:GLU:N	2:F:774:PRO:CD	2.82	0.42
1:C:707:SER:OG	1:C:710:GLY:N	2.52	0.42
1:D:603:THR:N	1:D:606:GLY:O	2.51	0.42
1:E:158:PRO:HB2	1:E:185:LEU:HD21	2.00	0.42
1:E:246:LEU:HA	1:E:249:LEU:HG	2.02	0.42
1:E:574:ILE:HD11	1:E:578:LEU:HD13	2.00	0.42
2:F:358:GLY:O	2:F:541:ARG:N	2.41	0.42
2:F:439:MET:HB2	2:F:439:MET:HE2	1.82	0.42
1:A:65:TRP:HA	1:A:93:GLN:HA	2.02	0.42
1:A:520:ILE:HG13	1:A:567:ARG:HB2	2.01	0.42
1:A:677:PRO:HG2	1:A:705:GLU:HG3	2.02	0.42
1:B:441:GLU:HG3	1:B:447:GLN:HG3	2.02	0.42
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.86	0.42
1:B:615:ALA:N	1:C:708:LEU:HD23	2.35	0.42
1:B:742:GLN:OE1	1:B:742:GLN:N	2.50	0.42
1:C:264:THR:HA	1:C:267:LEU:HD12	2.01	0.42
1:D:250:ARG:HA	1:D:253:ILE:HD12	2.01	0.42
1:D:453:ASP:N	1:D:456:LEU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:VAL:O	2:F:329:ILE:HG12	2.20	0.42
2:F:498:LYS:HE2	2:F:543:LEU:HD13	2.01	0.42
1:C:17:PRO:HA	1:C:88:ALA:HB3	2.01	0.42
1:D:381:LEU:HD12	1:D:424:ILE:HG12	2.02	0.42
1:E:726:HIS:HB2	1:E:754:LEU:HD21	2.00	0.42
2:F:748:LYS:HD3	2:F:751:LEU:HD12	2.02	0.42
2:F:770:LEU:HG	2:F:772:PRO:HD2	2.02	0.42
1:B:42:ARG:HB2	1:B:71:VAL:HB	2.01	0.42
1:B:715:ILE:HD12	1:B:721:LYS:HE3	2.01	0.42
1:E:297:PRO:HD2	1:E:409:MET:HE3	2.02	0.42
1:B:327:GLU:HA	1:B:330:LEU:HB2	2.02	0.41
1:C:91:ARG:HH21	1:C:180:LEU:HD12	1.85	0.41
1:C:356:PRO:HG3	1:C:602:TRP:HH2	1.85	0.41
1:D:421:LEU:O	1:D:470:THR:N	2.48	0.41
2:F:516:MET:HG3	2:F:520:ILE:HG13	2.02	0.41
1:A:205:LEU:HA	1:A:208:ARG:HG2	2.01	0.41
1:A:245:ASP:HA	1:B:272:ARG:HG2	2.01	0.41
1:A:631:GLU:HA	1:A:634:LYS:HB3	2.02	0.41
1:B:386:ASP:OD1	1:B:386:ASP:N	2.53	0.41
1:B:697:ARG:HH11	1:B:700:ILE:HG13	1.84	0.41
1:C:374:ARG:NH2	1:C:464:LYS:O	2.53	0.41
1:C:697:ARG:NH1	1:C:768:TYR:O	2.54	0.41
1:C:697:ARG:HB3	1:C:771:LEU:HB2	2.02	0.41
1:D:14:VAL:HG11	1:D:180:LEU:HD22	2.02	0.41
1:D:501:ILE:HG23	1:D:505:TYR:HD2	1.84	0.41
1:D:694:ARG:HD2	1:D:694:ARG:HA	1.82	0.41
1:E:299:SER:HA	1:E:415:ILE:HD13	2.03	0.41
2:F:570:ASP:OD1	2:F:570:ASP:N	2.49	0.41
1:A:95:THR:OG1	1:A:106:ARG:NH2	2.53	0.41
1:A:101:PRO:HA	1:A:102:TYR:HA	1.86	0.41
1:A:228:GLU:O	1:E:216:GLN:NE2	2.54	0.41
1:A:479:ARG:HA	1:A:482:LEU:HB2	2.03	0.41
1:A:732:LYS:HA	1:A:732:LYS:HD3	1.91	0.41
1:B:91:ARG:HH22	1:B:188:ARG:HD3	1.85	0.41
1:B:705:GLU:HB3	1:B:713:MET:HB2	2.02	0.41
1:B:757:LYS:HD2	1:B:768:TYR:CG	2.55	0.41
1:C:297:PRO:O	1:C:460:TYR:OH	2.29	0.41
1:D:93:GLN:H	1:D:108:GLU:HB2	1.85	0.41
1:E:336:ARG:HD2	1:E:336:ARG:HA	1.81	0.41
1:B:304:GLU:HA	1:B:374:ARG:HD2	2.01	0.41
1:B:374:ARG:HH11	1:B:374:ARG:HD3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HA	1:D:152:VAL:HG22	2.02	0.41
1:D:681:ILE:HD12	1:D:702:MET:HE2	2.02	0.41
1:E:11:ARG:HA	1:E:11:ARG:HD3	1.91	0.41
1:E:443:LEU:HD23	1:E:443:LEU:HA	1.86	0.41
1:B:612:ILE:HG12	1:B:668:PRO:HD2	2.02	0.41
1:C:59:PRO:HA	1:C:100:GLY:H	1.85	0.41
2:F:250:ARG:HG3	2:F:270:LEU:HD11	2.03	0.41
2:F:417:PRO:HD2	2:F:465:VAL:HG13	2.02	0.41
1:B:593:GLN:O	1:B:696:ALA:N	2.45	0.41
1:C:70:VAL:N	1:C:87:GLU:O	2.47	0.41
1:C:250:ARG:HA	1:C:253:ILE:HD12	2.01	0.41
1:C:336:ARG:HE	1:C:344:VAL:HG22	1.85	0.41
1:C:722:LEU:HD11	1:C:733:ILE:HG21	2.02	0.41
1:D:17:PRO:HA	1:D:88:ALA:HB3	2.02	0.41
1:D:322:LEU:HD13	1:D:491:PRO:HG2	2.01	0.41
1:D:613:GLU:O	1:D:666:HIS:N	2.45	0.41
1:E:5:LEU:HD22	1:E:40:ALA:HB1	2.03	0.41
2:F:390:ILE:HG22	2:F:405:LEU:HD11	2.01	0.41
1:A:377:HIS:CD2	1:A:412:VAL:HG12	2.56	0.41
1:B:277:GLN:HE21	1:B:283:ALA:HB1	1.85	0.41
1:B:384:VAL:HG11	1:B:390:ILE:HD11	2.02	0.41
1:B:387:GLU:HG2	1:B:391:ARG:HB2	2.03	0.41
1:D:140:LYS:HD2	1:D:146:ARG:HD3	2.02	0.41
1:D:259:PRO:O	1:D:263:LYS:N	2.45	0.41
1:E:393:HIS:CD2	1:E:401:MET:H	2.39	0.41
1:E:556:LYS:HD2	2:F:327:GLU:HG3	2.02	0.41
1:A:696:ALA:CB	1:A:769:LEU:O	2.68	0.41
1:B:731:HIS:O	1:B:732:LYS:NZ	2.43	0.41
1:C:643:TYR:O	1:C:647:HIS:N	2.54	0.41
1:C:697:ARG:HG2	1:C:769:LEU:O	2.21	0.41
1:D:128:LEU:HD23	1:D:189:LEU:HD23	2.02	0.41
1:D:737:LYS:NZ	1:D:758:LEU:O	2.34	0.41
1:E:386:ASP:HB2	1:E:389:GLU:CG	2.51	0.41
1:E:497:GLU:O	1:E:501:ILE:HG12	2.21	0.41
1:E:621:GLY:N	1:E:662:ASP:OD1	2.54	0.41
2:F:385:ARG:HG2	2:F:428:SER:H	1.86	0.41
2:F:681:ILE:HA	2:F:684:ALA:HB3	2.01	0.41
1:A:377:HIS:N	1:A:418:VAL:O	2.49	0.41
1:A:491:PRO:HG3	1:A:719:LYS:HD3	2.03	0.41
1:A:530:VAL:HG13	1:A:534:TYR:HD2	1.85	0.41
1:A:674:LYS:NZ	1:A:678:SER:OG	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LEU:HA	1:B:531:ILE:HD12	2.03	0.41
1:C:363:SER:HA	1:C:366:ARG:HE	1.85	0.41
1:C:592:PRO:HB3	1:C:697:ARG:HA	2.02	0.41
1:C:600:LEU:HA	1:C:600:LEU:HD23	1.84	0.41
1:D:283:ALA:O	1:D:287:ARG:HG3	2.21	0.41
1:D:462:LEU:HD22	1:D:467:PHE:HZ	1.86	0.41
1:D:659:ASN:OD1	1:D:659:ASN:N	2.46	0.41
1:E:272:ARG:O	1:E:275:ARG:NH2	2.51	0.41
1:A:510:GLN:O	1:A:514:SER:OG	2.27	0.41
1:B:630:GLY:H	1:B:633:MET:HE2	1.86	0.41
1:C:25:VAL:HG21	1:C:34:VAL:HG21	2.03	0.41
1:C:122:ARG:HA	1:C:125:VAL:HG12	2.03	0.41
1:C:302:ASP:HB3	1:C:416:ASN:ND2	2.35	0.41
1:D:293:LEU:HD12	1:D:293:LEU:O	2.21	0.41
1:D:502:ALA:HA	1:D:506:LEU:HB2	2.02	0.41
1:E:3:LEU:HA	1:E:106:ARG:HE	1.85	0.41
1:E:553:LYS:NZ	1:E:577:TYR:O	2.38	0.41
1:E:733:ILE:HD11	1:E:754:LEU:HD22	2.02	0.41
2:F:455:TYR:HB3	2:F:456:LEU:HD12	2.02	0.41
2:F:674:LYS:NZ	2:F:716:GLY:O	2.49	0.41
1:A:175:GLU:OE1	1:A:198:ARG:NH2	2.54	0.40
1:A:350:ILE:CG2	1:A:469:THR:HG23	2.51	0.40
1:A:356:PRO:HD3	1:A:720:GLU:OE1	2.20	0.40
1:A:377:HIS:CE1	1:A:412:VAL:HG12	2.56	0.40
1:A:395:ARG:HG2	1:A:455:TYR:CD1	2.56	0.40
1:B:278:GLN:HE22	1:C:277:GLN:HA	1.87	0.40
1:C:245:ASP:OD1	1:C:246:LEU:N	2.55	0.40
1:C:545:ARG:HH12	1:C:582:ARG:HH22	1.69	0.40
1:C:761:ASP:HB2	1:C:764:GLU:HG3	2.03	0.40
1:D:626:THR:O	1:D:666:HIS:ND1	2.44	0.40
1:E:492:GLY:O	1:E:727:GLN:NE2	2.53	0.40
2:F:346:ASN:HD21	2:F:467:PHE:HE2	1.68	0.40
2:F:462:LEU:HB3	2:F:467:PHE:HZ	1.86	0.40
1:A:710:GLY:HA2	1:A:762:VAL:HB	2.03	0.40
1:B:397:TYR:OH	1:C:432:ARG:NE	2.54	0.40
1:B:421:LEU:N	1:B:468:ILE:O	2.51	0.40
1:C:694:ARG:HG3	1:C:774:PRO:HD2	2.02	0.40
1:C:748:LYS:HD2	1:C:751:LEU:HB2	2.03	0.40
1:D:285:VAL:HB	1:D:398:ILE:HA	2.03	0.40
1:E:321:GLY:H	1:E:326:LYS:HD3	1.86	0.40
1:E:391:ARG:HG3	1:E:454:HIS:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:ILE:HD12	1:E:398:ILE:HA	1.92	0.40
1:E:479:ARG:HH11	1:E:482:LEU:HD11	1.87	0.40
2:F:735:LEU:HD23	2:F:735:LEU:HA	1.92	0.40
1:A:196:LEU:HA	1:A:199:ASP:CG	2.46	0.40
1:A:252:LYS:HZ2	1:A:252:LYS:HG3	1.46	0.40
1:B:404:LYS:HB2	1:B:404:LYS:HE2	1.89	0.40
1:D:461:ASP:OD1	1:D:461:ASP:N	2.54	0.40
1:D:521:GLU:HG3	1:D:568:THR:HA	2.03	0.40
1:D:536:ARG:NH2	1:D:585:PRO:O	2.54	0.40
1:E:324:ASP:HB2	1:E:328:ARG:NH2	2.37	0.40
1:A:285:VAL:HG22	1:A:398:ILE:HA	2.04	0.40
1:A:524:ASP:HA	1:A:527:ILE:HD12	2.03	0.40
1:B:359:VAL:HG12	1:B:539:GLY:HA2	2.04	0.40
1:B:423:GLU:CG	1:B:426:LYS:HE3	2.50	0.40
1:D:259:PRO:CD	1:D:298:TRP:CE3	3.05	0.40
1:D:318:ASP:OD1	1:D:318:ASP:N	2.45	0.40
1:D:436:ALA:HA	1:D:481:LEU:HD21	2.03	0.40
1:E:530:VAL:HG11	1:E:550:ILE:HD11	2.02	0.40
1:E:590:THR:HG21	1:E:598:GLN:HG2	2.04	0.40
2:F:536:ARG:HG2	2:F:727:GLN:HB3	2.03	0.40
1:A:350:ILE:HG22	1:A:468:ILE:HA	2.03	0.40
1:A:593:GLN:HB3	1:A:696:ALA:HB3	2.03	0.40
1:B:6:PRO:HB2	1:B:37:ALA:HB2	2.04	0.40
1:B:25:VAL:HG21	1:B:34:VAL:HG21	2.04	0.40
1:B:425:ASP:HB3	1:B:471:ALA:HB1	2.03	0.40
1:C:648:THR:O	1:C:653:LEU:N	2.46	0.40
1:E:195:LEU:HB3	1:E:198:ARG:HH21	1.86	0.40
1:E:392:GLY:C	1:E:454:HIS:HB3	2.47	0.40
1:E:425:ASP:OD1	1:E:425:ASP:N	2.54	0.40
2:F:253:ILE:HG12	2:F:266:ALA:HB1	2.04	0.40
2:F:265:LYS:HD3	2:F:458:VAL:HB	2.04	0.40
2:F:623:LEU:HD13	2:F:663:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	771/799 (96%)	716 (93%)	55 (7%)	0	100	100
1	B	771/799 (96%)	716 (93%)	55 (7%)	0	100	100
1	C	771/799 (96%)	726 (94%)	45 (6%)	0	100	100
1	D	771/799 (96%)	722 (94%)	49 (6%)	0	100	100
1	E	771/799 (96%)	715 (93%)	56 (7%)	0	100	100
2	F	529/570 (93%)	486 (92%)	42 (8%)	1 (0%)	43	77
All	All	4384/4565 (96%)	4081 (93%)	302 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	339	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	649/671 (97%)	649 (100%)	0	100	100
1	B	649/671 (97%)	648 (100%)	1 (0%)	87	85
1	C	649/671 (97%)	649 (100%)	0	100	100
1	D	649/671 (97%)	649 (100%)	0	100	100
1	E	649/671 (97%)	648 (100%)	1 (0%)	87	85
2	F	442/474 (93%)	442 (100%)	0	100	100
All	All	3687/3829 (96%)	3685 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	578	LEU
1	E	700	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	68	GLN
1	A	177	GLN
1	A	220	ASN
1	A	229	GLN
1	A	277	GLN
1	A	319	HIS
1	A	340	GLN
1	A	373	ASN
1	A	475	GLN
1	A	649	GLN
1	A	659	ASN
1	B	510	GLN
1	B	598	GLN
1	C	49	GLN
1	C	313	GLN
1	C	393	HIS
1	C	495	ASN
1	C	666	HIS
1	C	739	ASN
1	C	742	GLN
1	D	68	GLN
1	D	139	HIS
1	D	216	GLN
1	D	229	GLN
1	D	337	GLN
1	D	340	GLN
1	D	649	GLN
1	D	726	HIS
1	E	49	GLN
1	E	138	ASN
1	E	313	GLN
1	E	337	GLN
1	E	346	ASN
1	E	449	ASN
1	E	598	GLN
1	E	649	GLN

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Mol	Chain	Res	Type
2	F	310	HIS
2	F	628	GLN
2	F	638	GLN
2	F	649	GLN
2	F	742	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	801	-	28,29,29	1.39	4 (14%)	43,45,45	1.95	8 (18%)
3	ADP	D	801	-	28,29,29	1.44	4 (14%)	43,45,45	1.84	8 (18%)
3	ADP	C	801	-	28,29,29	1.43	5 (17%)	43,45,45	1.78	12 (27%)
3	ADP	E	801	-	28,29,29	1.43	5 (17%)	43,45,45	1.75	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	801	-	-	4/16/32/32	0/3/3/3
3	ADP	D	801	-	-	7/16/32/32	0/3/3/3
3	ADP	C	801	-	-	8/16/32/32	0/3/3/3
3	ADP	E	801	-	-	8/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	ADP	C5-C4	4.82	1.47	1.39
3	E	801	ADP	C5-C4	4.76	1.47	1.39
3	B	801	ADP	C5-C4	4.74	1.47	1.39
3	C	801	ADP	C5-C4	4.61	1.47	1.39
3	E	801	ADP	C5-N7	-2.72	1.34	1.39
3	B	801	ADP	C5-N7	-2.67	1.34	1.39
3	D	801	ADP	C5-C6	2.62	1.48	1.41
3	D	801	ADP	C5-N7	-2.60	1.34	1.39
3	C	801	ADP	C5-N7	-2.59	1.34	1.39
3	E	801	ADP	C5-C6	2.54	1.48	1.41
3	B	801	ADP	C5-C6	2.48	1.47	1.41
3	C	801	ADP	C5-C6	2.47	1.47	1.41
3	D	801	ADP	C8-N7	2.31	1.36	1.31
3	C	801	ADP	C8-N7	2.29	1.36	1.31
3	C	801	ADP	C4-N9	-2.26	1.33	1.37
3	E	801	ADP	C4-N9	-2.15	1.33	1.37
3	B	801	ADP	C8-N7	2.12	1.35	1.31
3	E	801	ADP	C8-N9	-2.00	1.34	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	ADP	C5-C4-N3	-6.19	118.20	126.72
3	D	801	ADP	C5-C4-N3	-5.92	118.56	126.72
3	E	801	ADP	C5-C4-N3	-5.55	119.08	126.72
3	C	801	ADP	C5-C4-N3	-5.15	119.62	126.72
3	B	801	ADP	N3-C4-N9	4.90	135.50	127.17
3	D	801	ADP	N3-C4-N9	4.45	134.74	127.17
3	E	801	ADP	N3-C4-N9	4.17	134.26	127.17
3	B	801	ADP	O4'-C1'-N9	4.17	116.09	108.09
3	C	801	ADP	N3-C4-N9	4.10	134.14	127.17
3	D	801	ADP	O4'-C1'-N9	3.74	115.27	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	801	ADP	C4-C5-N7	-3.68	106.38	110.58
3	B	801	ADP	C2-N3-C4	3.62	120.68	111.83
3	D	801	ADP	C2-N3-C4	3.56	120.52	111.83
3	D	801	ADP	C4-C5-N7	-3.48	106.60	110.58
3	C	801	ADP	C2-N3-C4	3.40	120.15	111.83
3	B	801	ADP	C4-C5-N7	-3.37	106.72	110.58
3	C	801	ADP	C4-C5-N7	-3.33	106.78	110.58
3	C	801	ADP	N3-C2-N1	-3.24	123.67	128.58
3	E	801	ADP	C2-N3-C4	3.21	119.68	111.83
3	B	801	ADP	N3-C2-N1	-2.79	124.36	128.58
3	C	801	ADP	C4-N9-C8	2.78	108.66	105.74
3	D	801	ADP	N3-C2-N1	-2.77	124.39	128.58
3	B	801	ADP	C5-N7-C8	2.44	107.29	103.45
3	E	801	ADP	N3-C2-N1	-2.41	124.93	128.58
3	C	801	ADP	C5-N7-C8	2.41	107.23	103.45
3	D	801	ADP	C5-N7-C8	2.38	107.19	103.45
3	E	801	ADP	C5-N7-C8	2.33	107.11	103.45
3	C	801	ADP	C2'-C1'-N9	-2.32	107.53	113.30
3	E	801	ADP	O2A-PA-O3A	2.28	113.43	107.27
3	D	801	ADP	C3'-C2'-C1'	2.26	105.73	101.46
3	C	801	ADP	C2-N1-C6	2.22	122.38	118.73
3	C	801	ADP	C6-C5-N7	2.21	136.35	132.09
3	B	801	ADP	C4-N9-C8	2.20	108.05	105.74
3	C	801	ADP	C3'-C2'-C1'	2.12	105.47	101.46
3	E	801	ADP	O3B-PB-O2B	2.04	115.46	107.80
3	C	801	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	ADP	C5'-O5'-PA-O1A
3	C	801	ADP	PA-O3A-PB-O2B
3	D	801	ADP	C5'-O5'-PA-O1A
3	D	801	ADP	C5'-O5'-PA-O2A
3	D	801	ADP	C5'-O5'-PA-O3A
3	D	801	ADP	O4'-C1'-N9-C8
3	D	801	ADP	O4'-C1'-N9-C4
3	E	801	ADP	PA-O3A-PB-O3B
3	D	801	ADP	C3'-C4'-C5'-O5'
3	C	801	ADP	O4'-C4'-C5'-O5'
3	D	801	ADP	O4'-C4'-C5'-O5'

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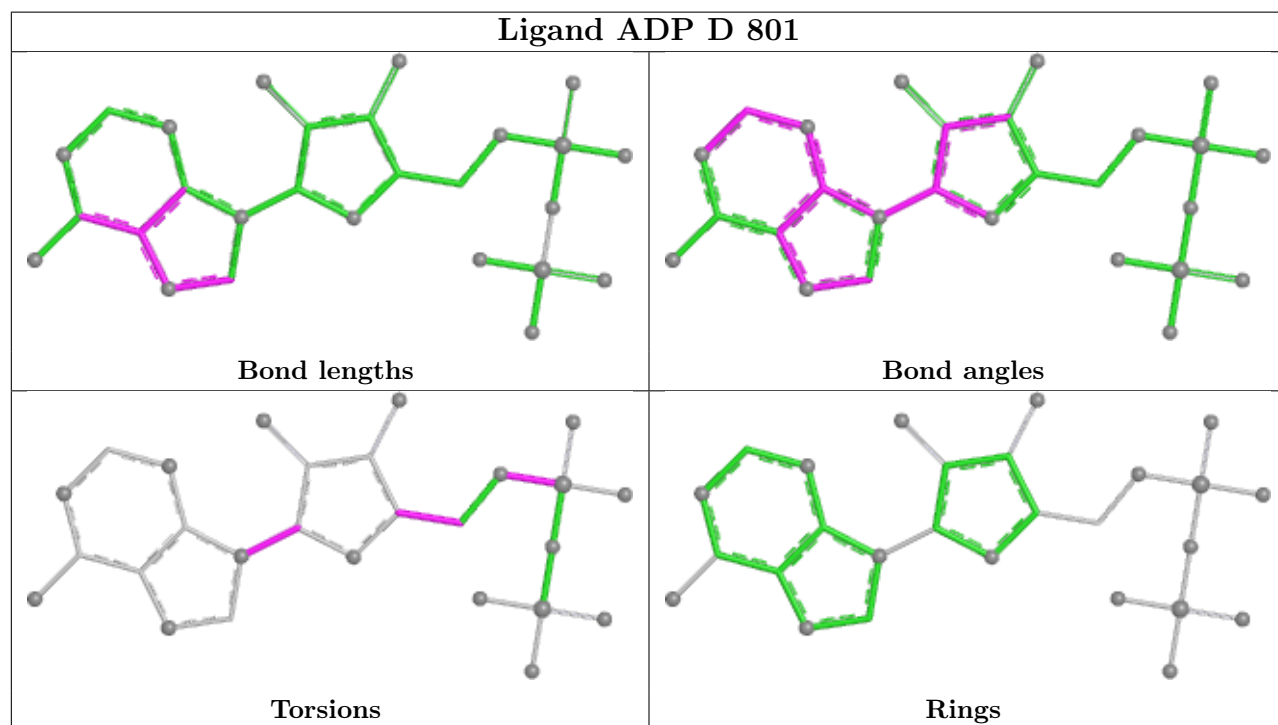
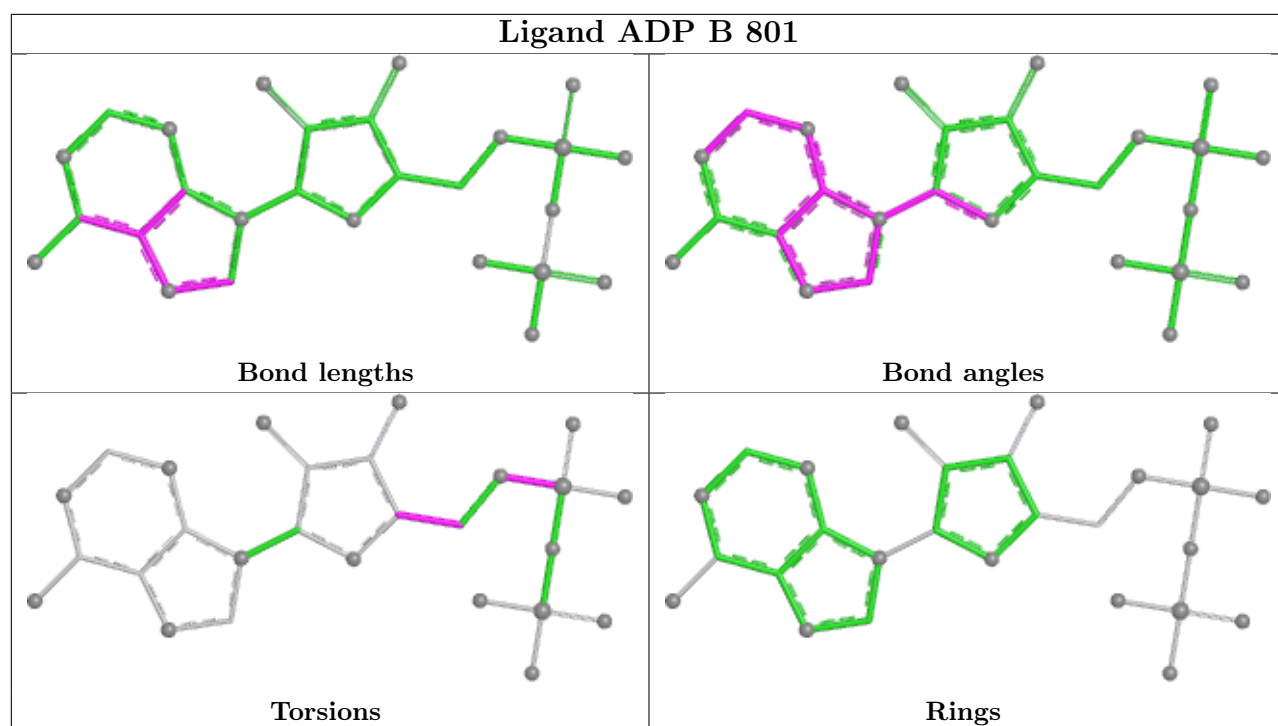
Mol	Chain	Res	Type	Atoms
3	C	801	ADP	C3'-C4'-C5'-O5'
3	E	801	ADP	PA-O3A-PB-O2B
3	E	801	ADP	C2'-C1'-N9-C8
3	C	801	ADP	C4'-C5'-O5'-PA
3	B	801	ADP	C5'-O5'-PA-O2A
3	B	801	ADP	C5'-O5'-PA-O3A
3	C	801	ADP	C5'-O5'-PA-O1A
3	E	801	ADP	C2'-C1'-N9-C4
3	B	801	ADP	O4'-C4'-C5'-O5'
3	E	801	ADP	O4'-C4'-C5'-O5'
3	C	801	ADP	O4'-C1'-N9-C4
3	C	801	ADP	O4'-C1'-N9-C8
3	E	801	ADP	PA-O3A-PB-O1B
3	C	801	ADP	PA-O3A-PB-O3B
3	E	801	ADP	O4'-C1'-N9-C8
3	E	801	ADP	O4'-C1'-N9-C4

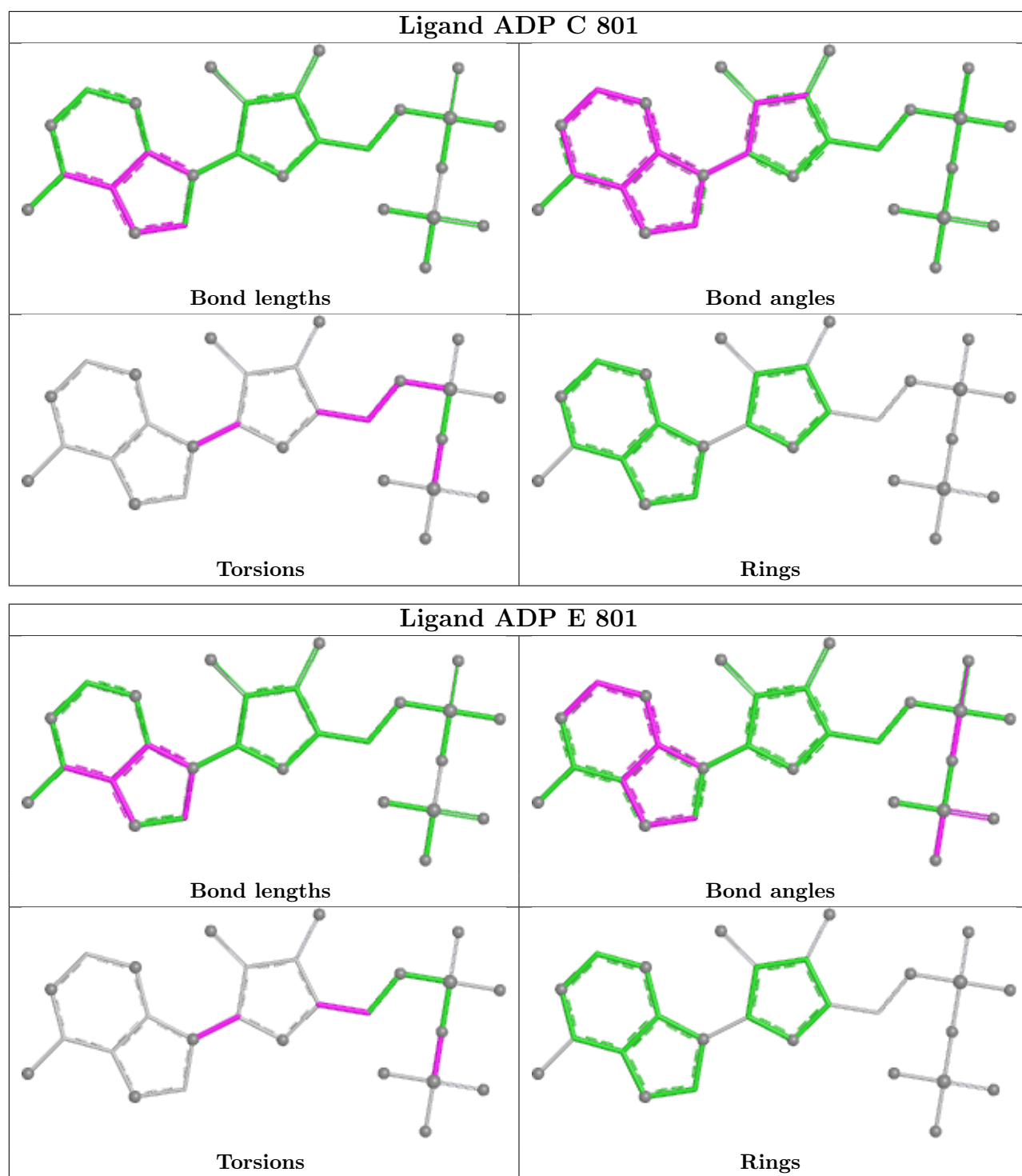
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	ADP	1	0
3	D	801	ADP	3	0
3	C	801	ADP	3	0
3	E	801	ADP	4	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36867. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.