Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 07:45 PM JST

PDB ID	:	4YPL
Title	:	Crystal structure of a hexameric LonA protease bound to three ADPs
Authors	:	Lin, C.-C.; Chang, C.-I.
Deposited on	:	2015-03-13
Resolution	:	3.45 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 (i)) were used in the production of this report:

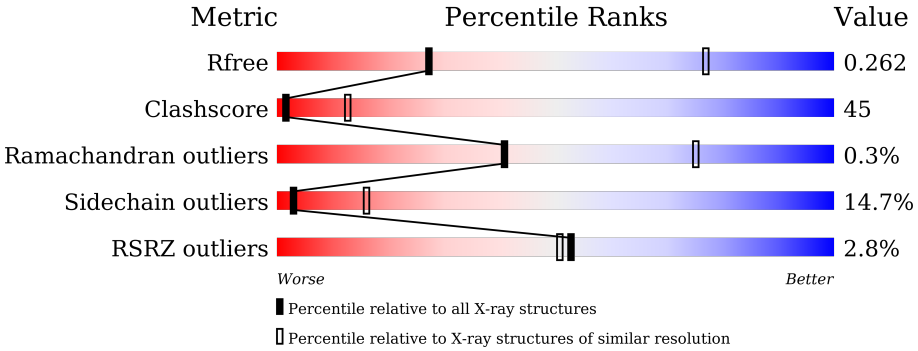
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	% 43% 46% 7% •
1	B	555	% 48% 42% 7% •
1	C	555	5% 39% 46% 12% •
1	D	555	2% 43% 47% 7% •
1	E	555	5% 36% 49% 12% •
1	F	555	2% 46% 43% 7% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25358 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 Lon protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4179	2643	732	788	16	0	0	0
1	B	537	4179	2643	732	788	16	0	0	0
1	C	538	4187	2649	733	789	16	0	0	0
1	F	538	4188	2648	734	790	16	0	0	0
1	D	537	4179	2643	732	788	16	0	0	0
1	E	537	4179	2643	732	788	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	expression tag	UNP A0A059VAZ3
A	240	HIS	-	expression tag	UNP A0A059VAZ3
A	241	MET	-	expression tag	UNP A0A059VAZ3
A	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3
B	239	GLY	-	expression tag	UNP A0A059VAZ3
B	240	HIS	-	expression tag	UNP A0A059VAZ3
B	241	MET	-	expression tag	UNP A0A059VAZ3
B	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3
C	239	GLY	-	expression tag	UNP A0A059VAZ3
C	240	HIS	-	expression tag	UNP A0A059VAZ3
C	241	MET	-	expression tag	UNP A0A059VAZ3
C	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3
F	239	GLY	-	expression tag	UNP A0A059VAZ3
F	240	HIS	-	expression tag	UNP A0A059VAZ3
F	241	MET	-	expression tag	UNP A0A059VAZ3
F	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3
D	239	GLY	-	expression tag	UNP A0A059VAZ3

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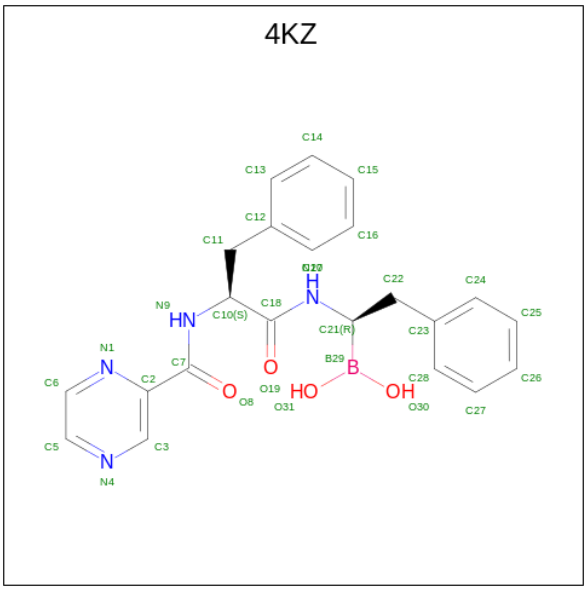
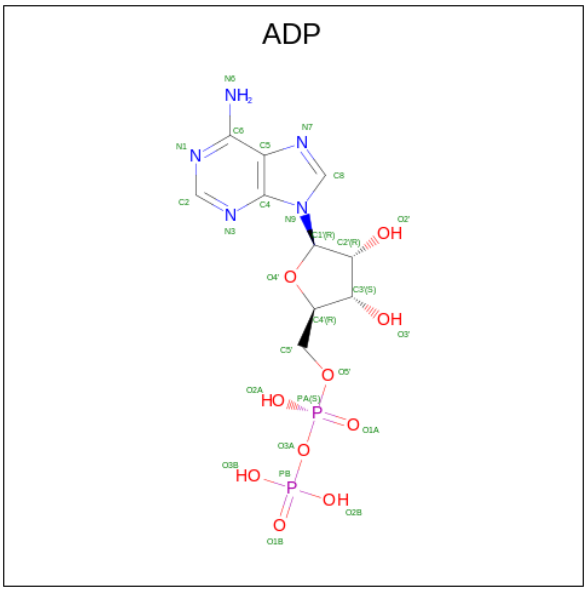
Chain	Residue	Modelled	Actual	Comment	Reference
D	240	HIS	-	expression tag	UNP A0A059VAZ3
D	241	MET	-	expression tag	UNP A0A059VAZ3
D	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3
E	239	GLY	-	expression tag	UNP A0A059VAZ3
E	240	HIS	-	expression tag	UNP A0A059VAZ3
E	241	MET	-	expression tag	UNP A0A059VAZ3
E	423	GLN	GLU	engineered mutation	UNP A0A059VAZ3

- Molecule 2 is N-[(1R)-1-(dihydroxyboranyl)-2-phenylethyl]-Nalpha-(pyrazin-2-ylcarbonyl)-L-phenylalaninamide (three-letter code: 4KZ) (formula: $C_{22}H_{23}BN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
2	A	1	31	1	22	4	4	0	0
2	B	1	31	1	22	4	4	0	0
2	C	1	31	1	22	4	4	0	0
2	F	1	31	1	22	4	4	0	0
2	D	1	31	1	22	4	4	0	0
2	E	1	31	1	22	4	4	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



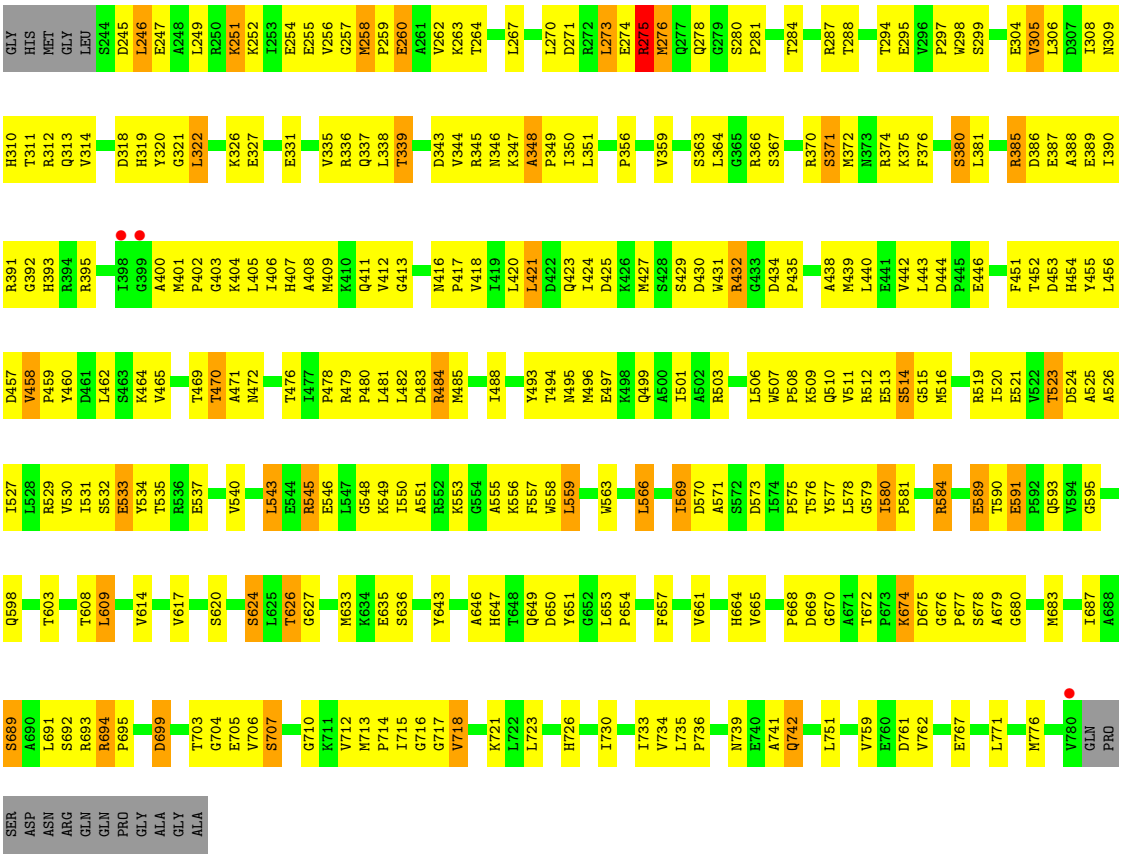
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	F	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	D	1	27	10	5	10	2	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

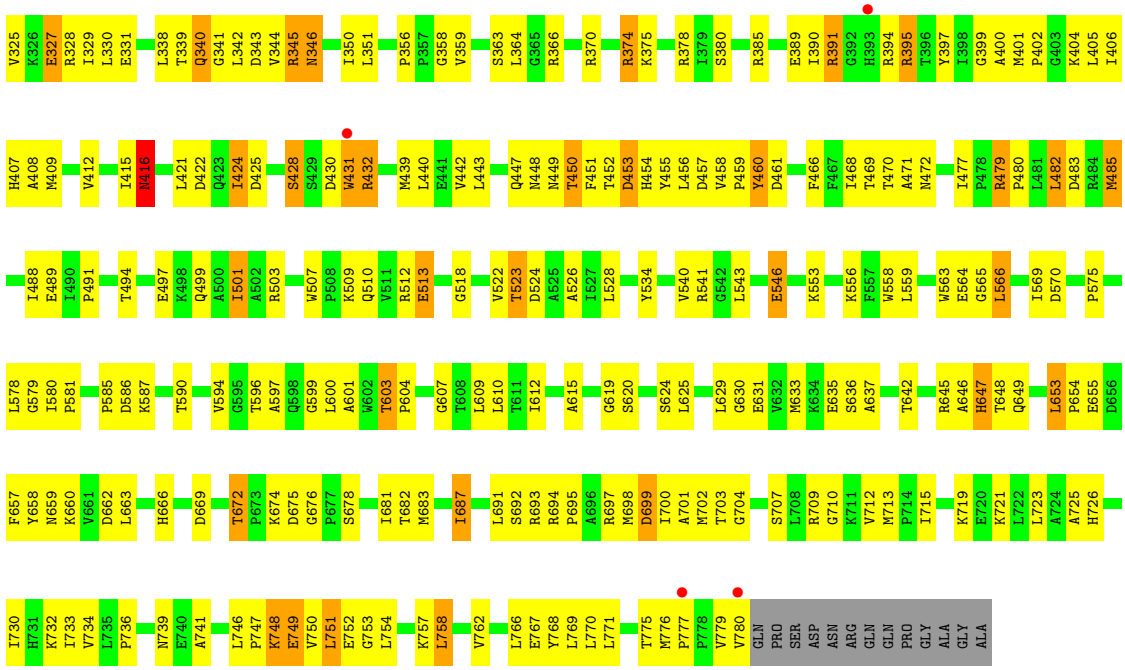
• Molecule 1: Lon protease

Chain A:



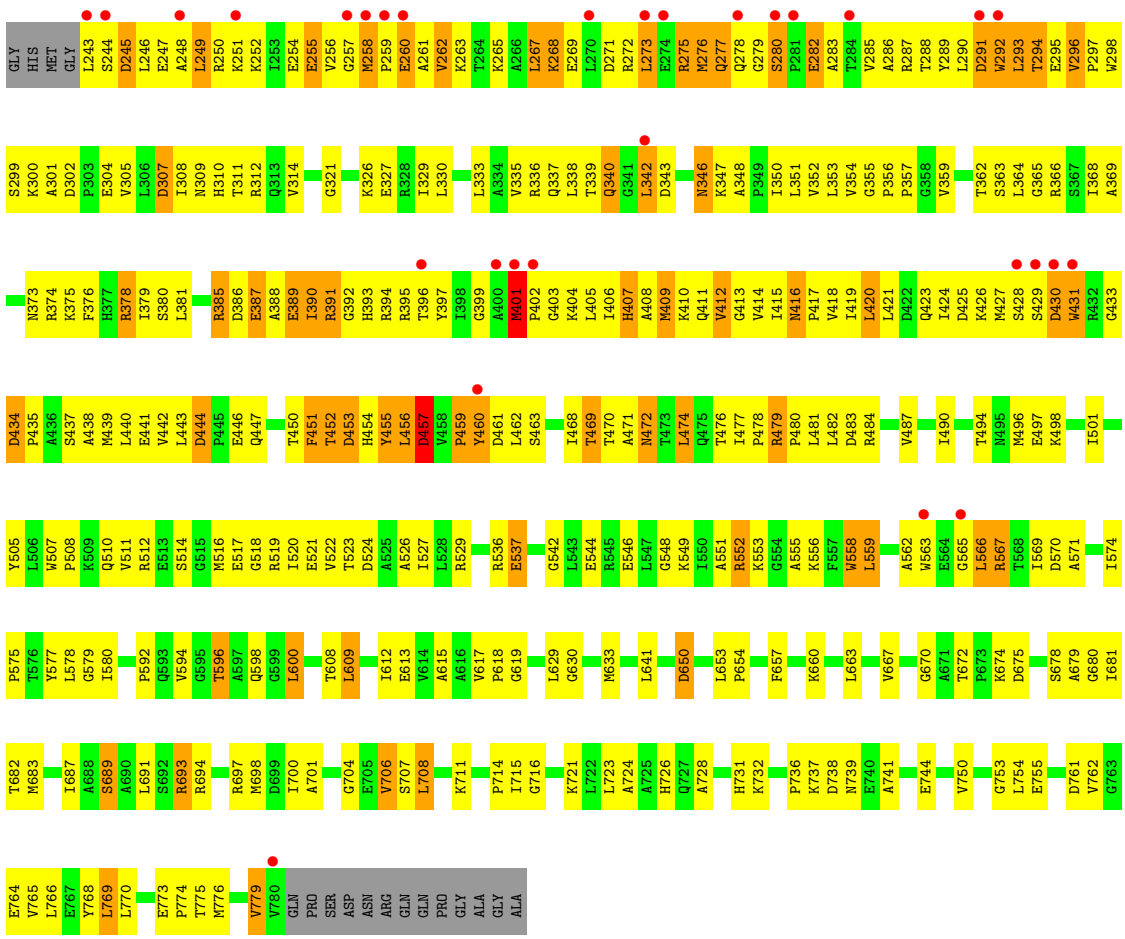
• Molecule 1: Lon protease

Chain B:



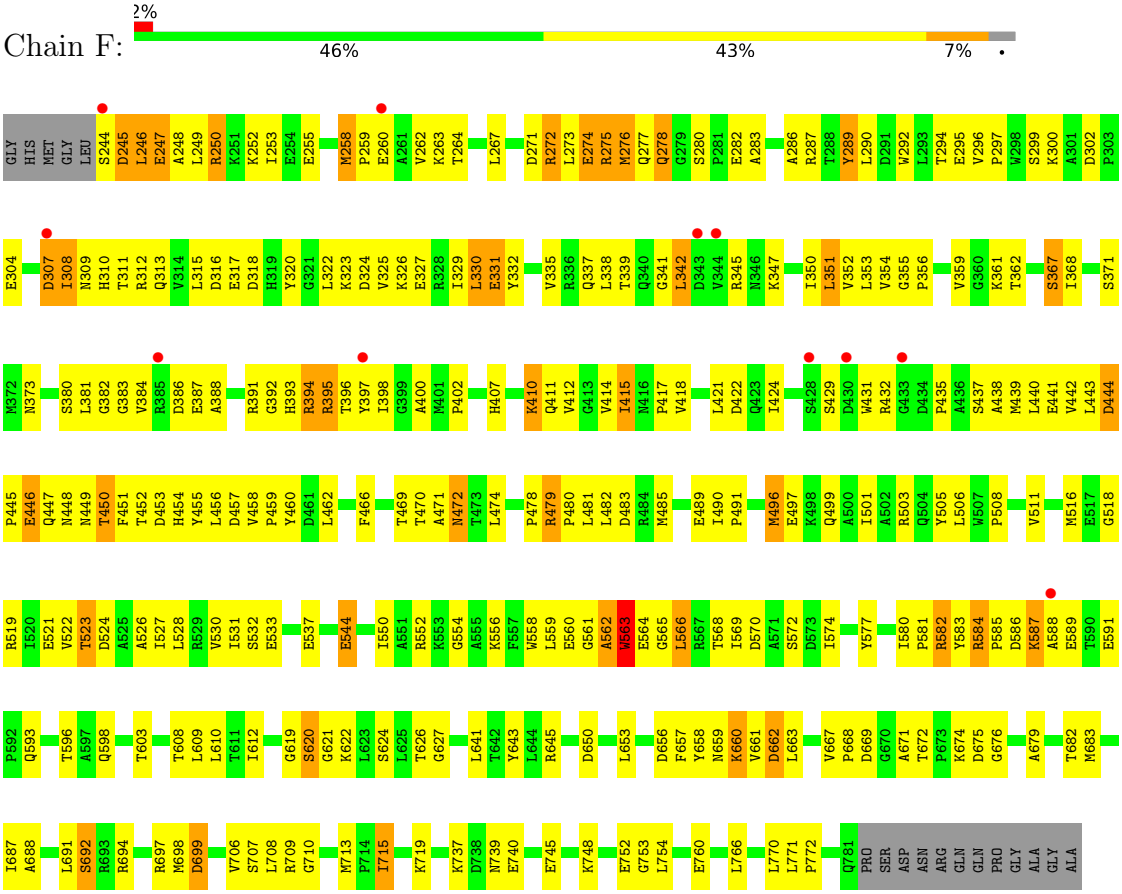
- Molecule 1: Lon protease

Chain C:



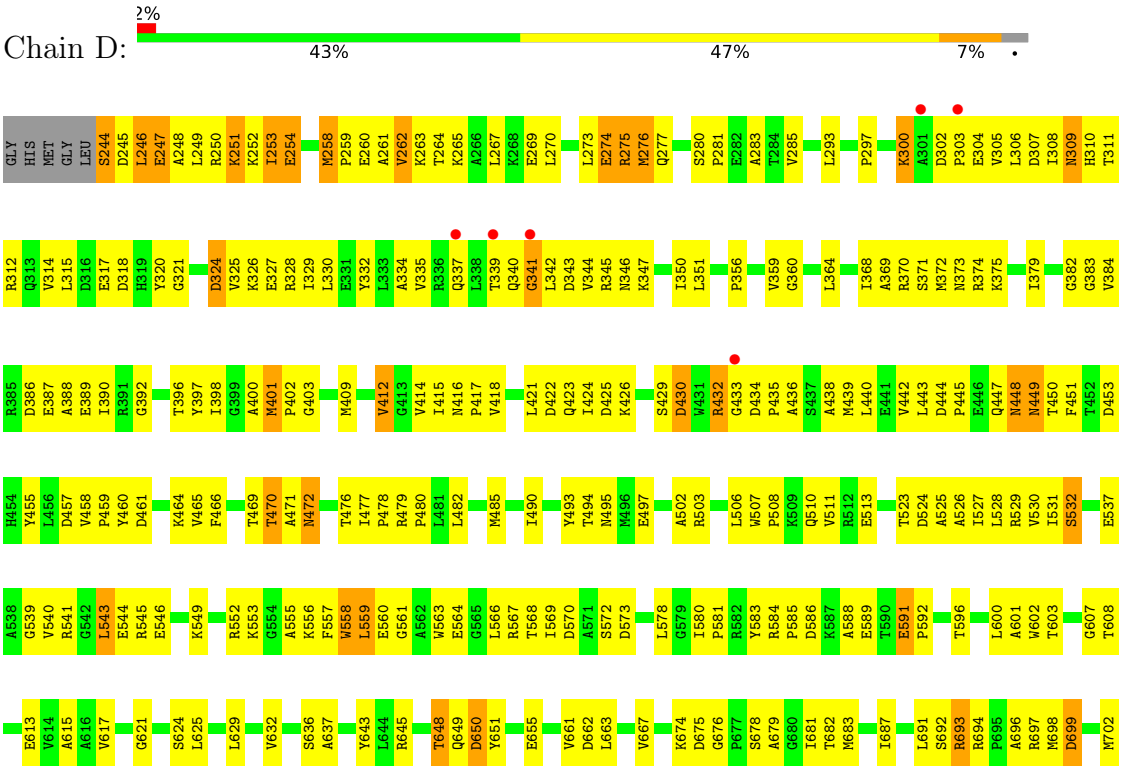
• Molecule 1: Lon protease

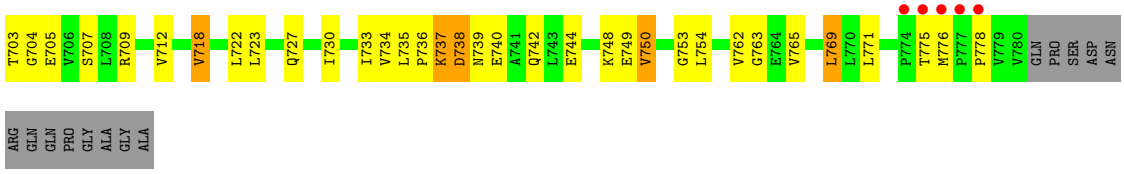
Chain F:



• Molecule 1: Lon protease

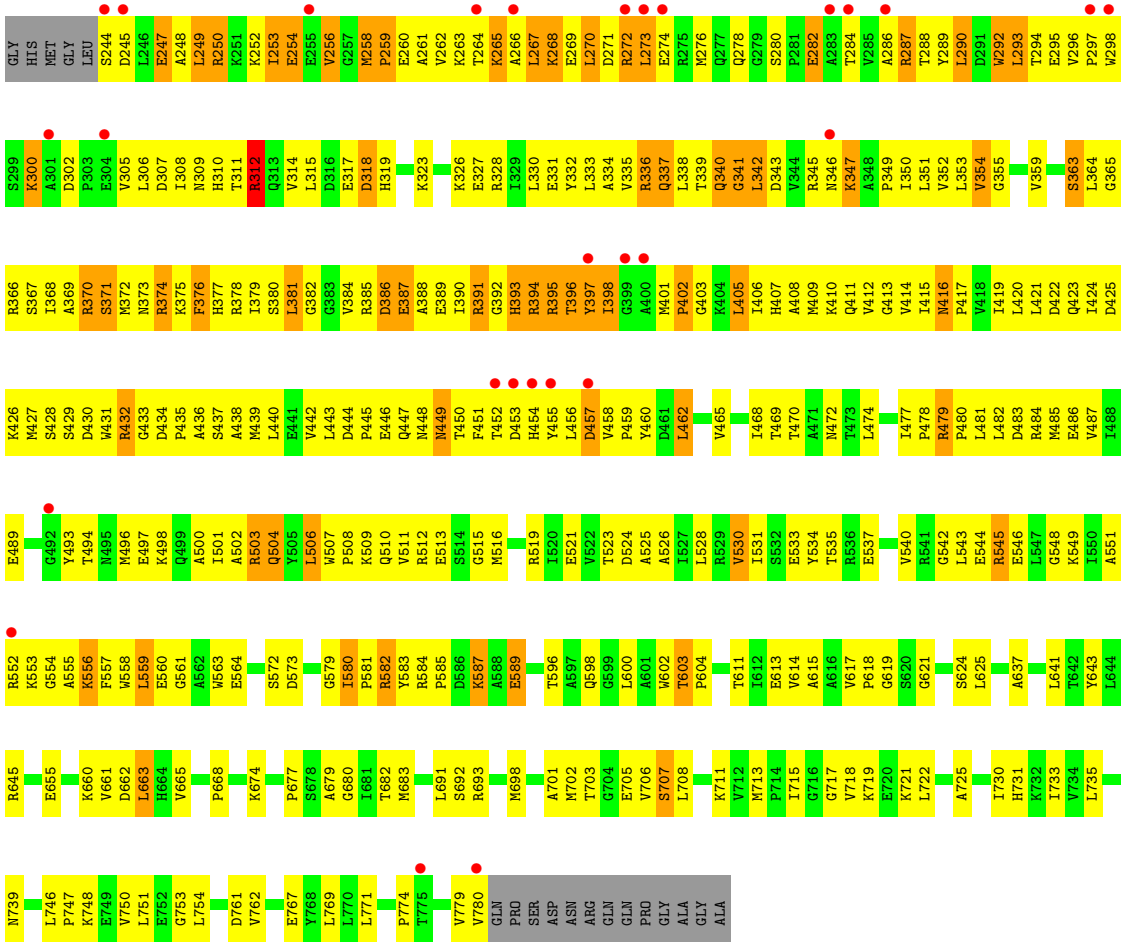
Chain D:





- Molecule 1: Lon protease

Chain E: 5% 36% 49% 12%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.04Å 169.13Å 135.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.45 46.90 – 3.44	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-3.45) 93.0 (46.90-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.265 0.237 , 0.262	Depositor DCC
R_{free} test set	2459 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	25358	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4KZ, 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	0.42	0/4258	0.72	4/5774 (0.1%)
1	B	0.41	0/4258	0.71	3/5774 (0.1%)
1	C	0.42	0/4266	0.75	1/5785 (0.0%)
1	D	0.41	0/4258	0.68	0/5774
1	E	0.42	0/4258	0.74	4/5774 (0.1%)
1	F	0.42	0/4267	0.72	2/5786 (0.0%)
All	All	0.42	0/25565	0.72	14/34667 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	4
1	D	0	2
1	E	0	5
1	F	0	1
All	All	0	15

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	391	ARG	N-CA-C	-8.40	88.33	111.00
1	E	312	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	F	563	TRP	N-CA-C	-7.10	91.84	111.00
1	E	312	ARG	NE-CZ-NH1	-5.93	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	312	ARG	CG-CD-NE	5.78	123.94	111.80
1	A	280	SER	N-CA-C	-5.53	96.06	111.00
1	A	275	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	374	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	607	GLY	N-CA-C	-5.30	99.84	113.10
1	F	660	LYS	CB-CA-C	-5.26	99.88	110.40
1	E	258	MET	C-N-CD	-5.13	109.32	120.60
1	A	374	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	374	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	565	GLY	N-CA-C	-5.03	100.54	113.10

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	457	ASP	Peptide
1	B	431	TRP	Peptide
1	B	564	GLU	Peptide
1	C	451	PHE	Peptide
1	C	453	ASP	Peptide
1	C	457	ASP	Peptide
1	C	459	PRO	Peptide
1	D	341	GLY	Peptide
1	D	566	LEU	Peptide
1	E	259	PRO	Peptide
1	E	280	SER	Peptide
1	E	341	GLY	Peptide
1	E	396	THR	Peptide
1	E	397	TYR	Peptide
1	F	562	ALA	Peptide

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	4179	0	4264	298	0
1	B	4179	0	4264	297	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4187	0	4275	583	0
1	D	4179	0	4264	306	0
1	E	4179	0	4262	524	0
1	F	4188	0	4272	334	0
2	A	31	0	0	4	0
2	B	31	0	0	2	0
2	C	31	0	0	0	0
2	D	31	0	0	4	0
2	E	31	0	0	0	0
2	F	31	0	0	1	0
3	B	27	0	12	0	0
3	D	27	0	12	0	0
3	F	27	0	12	3	0
All	All	25358	0	25637	2297	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 45.

All (2297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:HIS:CB	1:C:402:PRO:HD3	1.35	1.54
1:C:393:HIS:HB2	1:C:402:PRO:CD	1.41	1.45
1:E:402:PRO:HD3	1:E:455:TYR:CD2	1.59	1.36
1:C:393:HIS:N	1:C:454:HIS:HB2	1.40	1.32
1:E:381:LEU:HD23	1:E:424:ILE:CG2	1.60	1.31
1:C:289:TYR:CD2	1:C:456:LEU:HG	1.67	1.30
1:C:289:TYR:CE2	1:C:456:LEU:HG	1.66	1.28
1:C:392:GLY:HA3	1:C:454:HIS:N	1.53	1.22
1:E:287:ARG:HA	1:E:290:LEU:CD1	1.69	1.21
1:E:292:TRP:CH2	1:E:407:HIS:HB3	1.75	1.20
1:C:300:LYS:O	1:C:414:VAL:HG13	1.43	1.17
1:C:556:LYS:O	1:C:559:LEU:HD22	1.40	1.16
1:C:389:GLU:HA	1:C:404:LYS:H	1.11	1.14
1:E:267:LEU:HA	1:E:270:LEU:HB3	1.26	1.14
1:C:392:GLY:C	1:C:454:HIS:HB2	1.69	1.14
1:B:344:VAL:HG13	1:B:346:ASN:O	1.44	1.13
1:D:258:MET:SD	1:D:262:VAL:HG23	1.88	1.13
1:C:388:ALA:CB	1:C:402:PRO:HG3	1.78	1.13
1:C:454:HIS:HB3	1:C:455:TYR:HA	1.19	1.12
1:B:273:LEU:HA	1:B:276:MET:HE2	1.24	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:ALA:HB1	1:C:402:PRO:CG	1.79	1.12
1:C:402:PRO:HG2	1:C:403:GLY:CA	1.79	1.12
1:C:402:PRO:CG	1:C:403:GLY:HA3	1.78	1.11
1:E:381:LEU:HD23	1:E:424:ILE:HG23	1.31	1.11
1:B:703:THR:HG23	1:B:715:ILE:CD1	1.79	1.11
1:B:703:THR:HG23	1:B:715:ILE:HD11	1.26	1.10
1:C:354:VAL:O	1:C:490:ILE:HG22	1.48	1.10
1:E:287:ARG:CA	1:E:290:LEU:HD12	1.80	1.10
1:F:596:THR:HG23	1:F:698:MET:HE2	1.34	1.10
1:E:296:VAL:HG13	1:E:297:PRO:HD2	1.21	1.10
1:B:586:ASP:HA	1:B:587:LYS:HB2	1.34	1.09
1:F:250:ARG:HA	1:F:253:ILE:HD12	1.19	1.09
1:A:425:ASP:CG	1:A:471:ALA:HB1	1.74	1.09
1:C:440:LEU:HB2	1:C:481:LEU:HD21	1.23	1.08
1:D:258:MET:SD	1:D:262:VAL:CG2	2.42	1.07
1:C:350:ILE:HG12	1:C:443:LEU:HD12	1.34	1.07
1:E:292:TRP:NE1	1:E:402:PRO:HD2	1.70	1.07
1:E:381:LEU:HD23	1:E:424:ILE:HG22	1.33	1.07
1:B:507:TRP:CE2	1:B:522:VAL:HG23	1.89	1.06
1:E:392:GLY:HA3	1:E:455:TYR:CB	1.85	1.06
1:E:451:PHE:O	1:E:459:PRO:HA	1.56	1.06
1:C:273:LEU:HD11	1:C:286:ALA:HB1	1.24	1.06
1:E:296:VAL:CG1	1:E:297:PRO:HD2	1.84	1.06
1:C:404:LYS:HG2	1:C:454:HIS:O	1.53	1.06
1:E:510:GLN:HE21	1:E:551:ALA:HB3	0.93	1.06
1:B:749:GLU:HA	1:B:752:GLU:HB2	1.13	1.05
1:C:389:GLU:O	1:C:404:LYS:HD3	1.55	1.05
1:E:292:TRP:HH2	1:E:407:HIS:CB	1.69	1.04
1:F:596:THR:HG23	1:F:698:MET:CE	1.86	1.04
1:E:384:VAL:O	1:E:428:SER:HB3	1.55	1.04
1:C:390:ILE:O	1:C:404:LYS:NZ	1.90	1.04
1:E:258:MET:O	1:E:263:LYS:HD2	1.57	1.04
1:E:259:PRO:HD3	1:E:298:TRP:CD1	1.93	1.03
1:C:292:TRP:HE3	1:C:455:TYR:CE1	1.77	1.03
1:C:402:PRO:HG2	1:C:403:GLY:HA3	1.05	1.03
1:E:510:GLN:NE2	1:E:551:ALA:HB3	1.74	1.02
1:C:289:TYR:CD2	1:C:456:LEU:CG	2.42	1.02
1:C:440:LEU:HB2	1:C:481:LEU:CD2	1.90	1.02
1:B:507:TRP:CZ2	1:B:522:VAL:HG23	1.94	1.02
1:C:392:GLY:H	1:C:453:ASP:HB3	1.21	1.01
1:E:510:GLN:HE21	1:E:551:ALA:CB	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:HIS:HB3	1:A:400:ALA:HB1	1.42	1.01
1:F:657:PHE:HB2	1:F:661:VAL:HG11	1.43	1.01
1:E:292:TRP:CH2	1:E:407:HIS:CB	2.43	1.00
1:C:450:THR:HG22	1:C:451:PHE:H	1.22	1.00
1:E:287:ARG:HA	1:E:290:LEU:HD12	1.00	1.00
1:E:342:LEU:HB2	1:E:346:ASN:HB2	1.42	0.99
1:C:450:THR:HB	1:C:460:TYR:HB2	1.45	0.99
1:B:297:PRO:O	1:B:415:ILE:HG23	1.63	0.99
1:C:272:ARG:HA	1:C:275:ARG:CZ	1.94	0.98
1:F:260:GLU:HA	1:F:263:LYS:HG3	1.45	0.98
1:E:402:PRO:HD3	1:E:455:TYR:HD2	1.22	0.97
1:C:388:ALA:HB1	1:C:402:PRO:HG3	1.00	0.97
1:F:619:GLY:HA3	1:F:662:ASP:OD1	1.65	0.96
1:C:450:THR:CB	1:C:460:TYR:HB2	1.95	0.96
1:E:386:ASP:O	1:E:389:GLU:HB3	1.64	0.96
1:C:450:THR:CG2	1:C:451:PHE:H	1.79	0.96
1:B:523:THR:HB	1:B:569:ILE:O	1.63	0.96
1:C:450:THR:HG21	1:C:461:ASP:N	1.81	0.95
1:C:295:GLU:OE1	1:C:295:GLU:N	1.97	0.95
1:C:393:HIS:N	1:C:454:HIS:CB	2.29	0.95
1:C:259:PRO:HG2	1:C:298:TRP:CZ2	2.01	0.95
1:C:386:ASP:OD1	1:C:387:GLU:N	2.00	0.95
1:C:392:GLY:N	1:C:453:ASP:HB3	1.80	0.95
1:D:637:ALA:HB2	1:D:683:MET:HE1	1.48	0.94
1:A:297:PRO:HD2	1:A:460:TYR:OH	1.67	0.94
1:F:297:PRO:O	1:F:415:ILE:HD11	1.66	0.94
1:B:276:MET:SD	1:B:283:ALA:HA	2.08	0.94
1:C:526:ALA:HB1	1:C:571:ALA:HA	1.48	0.94
1:D:337:GLN:O	1:D:340:GLN:HG2	1.68	0.94
1:F:289:TYR:HA	1:F:455:TYR:OH	1.68	0.93
1:C:289:TYR:CE2	1:C:456:LEU:CG	2.52	0.93
1:F:422:ASP:OD1	1:F:470:THR:HG21	1.67	0.93
1:E:402:PRO:CD	1:E:455:TYR:CD2	2.51	0.93
1:F:621:GLY:HA3	1:F:658:TYR:O	1.67	0.92
1:D:339:THR:HG23	1:D:343:ASP:HB2	1.48	0.92
1:D:592:PRO:HB3	1:D:696:ALA:O	1.68	0.92
1:F:258:MET:HB3	1:F:262:VAL:HB	1.52	0.92
1:E:392:GLY:O	1:E:454:HIS:HB2	1.69	0.92
1:E:392:GLY:HA3	1:E:455:TYR:HB2	1.50	0.92
1:D:694:ARG:HD2	1:D:771:LEU:O	1.70	0.92
1:E:408:ALA:HA	1:E:411:GLN:HG2	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:VAL:O	1:E:339:THR:HG22	1.71	0.91
1:A:321:GLY:O	1:A:326:LYS:HE3	1.71	0.91
1:E:267:LEU:CA	1:E:270:LEU:HB3	1.99	0.91
1:E:297:PRO:HB3	1:E:413:GLY:O	1.71	0.91
1:D:555:ALA:O	1:D:559:LEU:HD12	1.71	0.90
1:E:267:LEU:CD2	1:E:270:LEU:HD12	2.00	0.90
1:C:259:PRO:CG	1:C:298:TRP:CZ2	2.54	0.90
1:C:289:TYR:CE1	1:C:293:LEU:HD13	2.05	0.90
1:C:450:THR:HG21	1:C:461:ASP:CA	2.01	0.90
1:E:292:TRP:O	1:E:296:VAL:HG23	1.71	0.90
1:C:450:THR:HG22	1:C:451:PHE:N	1.83	0.90
1:D:637:ALA:HA	1:D:683:MET:HE2	1.53	0.89
1:D:651:TYR:OH	1:D:763:GLY:HA2	1.73	0.89
1:D:424:ILE:HG22	1:D:470:THR:O	1.71	0.89
1:B:273:LEU:HD13	1:B:276:MET:HE3	1.54	0.89
1:F:297:PRO:HD3	1:F:410:LYS:HA	1.52	0.89
1:A:262:VAL:HG12	1:A:458:VAL:HG11	1.55	0.89
1:A:350:ILE:CD1	1:A:443:LEU:HD23	2.01	0.89
1:A:462:LEU:O	1:A:465:VAL:HG12	1.73	0.89
1:E:558:TRP:HE3	1:E:563:TRP:CH2	1.90	0.88
1:B:675:ASP:OD1	1:B:676:GLY:N	2.06	0.88
1:D:445:PRO:HA	1:D:448:ASN:OD1	1.73	0.88
1:C:392:GLY:HA3	1:C:454:HIS:H	1.36	0.88
1:F:683:MET:O	1:F:687:ILE:HD12	1.74	0.88
1:E:267:LEU:CD1	1:E:268:LYS:HD2	2.04	0.88
1:A:345:ARG:HA	1:A:348:ALA:HB2	1.55	0.87
1:D:356:PRO:O	1:D:359:VAL:HG23	1.74	0.87
1:F:250:ARG:CA	1:F:253:ILE:HD12	2.04	0.87
1:C:630:GLY:HA3	1:C:675:ASP:OD1	1.75	0.87
1:F:715:ILE:HG22	1:F:739:ASN:HD21	1.39	0.87
1:D:372:MET:HE3	1:D:374:ARG:HD3	1.57	0.87
1:C:292:TRP:CE3	1:C:455:TYR:CE1	2.63	0.87
1:C:393:HIS:CD2	1:C:402:PRO:HB3	2.10	0.87
1:D:258:MET:HB2	1:D:262:VAL:HG21	1.55	0.87
1:C:454:HIS:HB3	1:C:455:TYR:CA	2.05	0.87
1:F:246:LEU:HA	1:F:249:LEU:CD2	2.05	0.87
1:E:703:THR:OG1	1:E:715:ILE:HD13	1.75	0.87
1:C:273:LEU:HD11	1:C:286:ALA:CB	2.05	0.86
1:E:293:LEU:O	1:E:298:TRP:CH2	2.28	0.86
1:B:749:GLU:HA	1:B:752:GLU:CB	2.04	0.86
1:E:267:LEU:HD13	1:E:268:LYS:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:LEU:CD2	1:E:424:ILE:HG23	2.06	0.86
1:C:596:THR:HB	1:C:698:MET:CE	2.04	0.86
1:F:249:LEU:HD12	1:F:250:ARG:N	1.90	0.86
1:D:304:GLU:N	1:D:304:GLU:OE1	2.08	0.86
1:C:455:TYR:CE1	1:C:456:LEU:HD22	2.11	0.86
1:C:258:MET:SD	1:C:262:VAL:HG13	2.16	0.86
1:E:444:ASP:O	1:E:448:ASN:HB2	1.74	0.86
1:F:452:THR:OG1	1:F:459:PRO:HA	1.76	0.85
1:A:287:ARG:NH1	1:A:287:ARG:O	2.08	0.85
1:C:389:GLU:OE1	1:C:389:GLU:N	2.09	0.85
1:E:270:LEU:HD13	1:E:271:ASP:N	1.91	0.85
1:E:385:ARG:HD3	1:E:428:SER:CB	2.06	0.85
1:C:394:ARG:O	1:C:395:ARG:HG2	1.76	0.85
1:F:596:THR:CG2	1:F:698:MET:CE	2.55	0.85
1:C:362:THR:HG21	1:C:378:ARG:HH22	1.42	0.85
1:F:620:SER:HA	1:F:659:ASN:O	1.76	0.85
1:A:675:ASP:OD1	1:A:676:GLY:N	2.10	0.85
1:C:404:LYS:CG	1:C:454:HIS:O	2.25	0.85
1:F:587:LYS:HG3	1:F:588:ALA:O	1.76	0.85
1:F:275:ARG:HB3	1:F:275:ARG:HH11	1.40	0.85
1:D:339:THR:HG22	1:D:341:GLY:O	1.75	0.84
1:C:259:PRO:CG	1:C:298:TRP:HZ2	1.90	0.84
1:E:450:THR:O	1:E:450:THR:HG22	1.77	0.84
1:A:347:LYS:O	1:A:349:PRO:HD3	1.78	0.84
1:E:558:TRP:CD1	1:E:558:TRP:O	2.29	0.84
1:C:526:ALA:HB1	1:C:571:ALA:CA	2.06	0.84
1:A:425:ASP:OD2	1:A:471:ALA:HB1	1.78	0.84
1:E:296:VAL:CG1	1:E:297:PRO:CD	2.56	0.84
1:E:494:THR:HG22	1:E:497:GLU:OE2	1.78	0.84
1:A:387:GLU:OE1	1:A:438:ALA:HB2	1.77	0.83
1:F:441:GLU:OE1	1:F:451:PHE:HB3	1.78	0.83
1:F:453:ASP:OD1	1:F:454:HIS:N	2.10	0.83
1:D:621:GLY:HA2	1:D:661:VAL:O	1.77	0.83
1:A:281:PRO:O	1:A:284:THR:HG22	1.78	0.83
1:A:531:ILE:HA	1:A:535:THR:CG2	2.08	0.83
1:C:392:GLY:HA3	1:C:454:HIS:CA	2.07	0.83
1:A:545:ARG:NH1	1:B:483:ASP:OD1	2.10	0.83
1:C:289:TYR:CD2	1:C:456:LEU:CD2	2.61	0.83
1:D:343:ASP:N	1:D:344:VAL:HA	1.93	0.83
1:E:311:THR:HG23	1:E:371:SER:OG	1.77	0.83
1:D:311:THR:O	1:D:315:LEU:HD12	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:ARG:N	1:E:376:PHE:HE2	1.77	0.83
1:E:506:LEU:HD21	1:E:544:GLU:HG3	1.60	0.83
1:C:393:HIS:CA	1:C:402:PRO:HD3	2.07	0.83
1:E:385:ARG:CD	1:E:428:SER:CB	2.57	0.83
1:C:388:ALA:CB	1:C:402:PRO:CG	2.48	0.83
1:D:617:VAL:O	1:D:661:VAL:HG13	1.78	0.83
1:B:654:PRO:HB2	1:B:657:PHE:HB3	1.59	0.83
1:C:350:ILE:CG1	1:C:443:LEU:HD12	2.08	0.83
1:C:262:VAL:HG21	1:C:298:TRP:CH2	2.13	0.83
1:C:700:ILE:HD13	1:C:768:TYR:CE2	2.13	0.83
1:F:412:VAL:HG11	1:F:417:PRO:HG3	1.58	0.83
1:E:345:ARG:O	1:E:345:ARG:NE	2.10	0.83
1:C:386:ASP:O	1:C:435:PRO:HG3	1.78	0.82
1:C:389:GLU:HA	1:C:404:LYS:N	1.92	0.82
1:F:258:MET:O	1:F:263:LYS:HD3	1.79	0.82
1:B:703:THR:CG2	1:B:715:ILE:HD11	2.09	0.82
1:B:341:GLY:HA3	1:B:343:ASP:O	1.79	0.82
1:C:450:THR:HG21	1:C:461:ASP:C	2.00	0.82
1:C:389:GLU:CA	1:C:404:LYS:H	1.92	0.82
1:B:278:GLN:HG3	1:C:396:THR:OG1	1.80	0.82
1:C:441:GLU:HA	1:C:444:ASP:OD1	1.79	0.82
1:C:683:MET:O	1:C:687:ILE:HG13	1.79	0.82
1:C:413:GLY:O	1:C:414:VAL:HG23	1.79	0.82
1:E:267:LEU:HD23	1:E:270:LEU:HD12	1.62	0.81
1:E:296:VAL:HG13	1:E:297:PRO:CD	2.07	0.81
1:F:582:ARG:O	1:F:583:TYR:CD1	2.33	0.81
1:D:449:ASN:HD22	1:D:450:THR:H	1.28	0.81
1:C:390:ILE:CD1	1:C:438:ALA:C	2.49	0.81
1:E:637:ALA:HB2	1:E:683:MET:CE	2.11	0.81
1:B:344:VAL:CG1	1:B:346:ASN:O	2.28	0.81
1:C:439:MET:O	1:C:442:VAL:HG22	1.80	0.81
1:A:350:ILE:HD13	1:A:443:LEU:HD23	1.62	0.81
1:D:258:MET:SD	1:D:262:VAL:HG21	2.19	0.81
1:C:393:HIS:HE1	1:C:395:ARG:O	1.62	0.81
1:C:425:ASP:HA	1:C:477:ILE:HG22	1.63	0.81
1:A:580:ILE:HD11	1:B:741:ALA:O	1.80	0.81
1:E:402:PRO:HD3	1:E:455:TYR:CE2	2.16	0.81
1:B:273:LEU:CD1	1:B:276:MET:HE3	2.11	0.80
1:C:262:VAL:HG21	1:C:298:TRP:CZ3	2.15	0.80
1:E:600:LEU:HD21	1:E:725:ALA:HB2	1.63	0.80
1:B:489:GLU:OE1	1:B:489:GLU:N	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:ALA:CB	1:C:571:ALA:CA	2.60	0.80
1:D:251:LYS:HG3	1:D:252:LYS:HD2	1.64	0.80
1:E:263:LYS:O	1:E:266:ALA:HB3	1.81	0.80
1:B:273:LEU:CA	1:B:276:MET:HE2	2.10	0.80
1:B:749:GLU:CA	1:B:752:GLU:HB2	2.05	0.80
1:C:526:ALA:CB	1:C:571:ALA:N	2.44	0.80
1:E:292:TRP:HH2	1:E:407:HIS:HB3	1.23	0.80
1:A:523:THR:OG1	1:A:570:ASP:HA	1.82	0.80
1:C:293:LEU:HD23	1:C:294:THR:HA	1.64	0.80
1:D:643:TYR:CE2	1:D:762:VAL:HG11	2.17	0.80
1:C:455:TYR:CE1	1:C:456:LEU:CD2	2.64	0.80
1:C:512:ARG:HH11	1:C:517:GLU:HB3	1.47	0.80
1:D:675:ASP:OD1	1:D:676:GLY:N	2.12	0.80
1:E:385:ARG:HD2	1:E:431:TRP:CD1	2.17	0.80
1:B:600:LEU:HD22	1:B:721:LYS:HB3	1.63	0.79
1:F:277:GLN:HB2	1:F:280:SER:HB3	1.63	0.79
1:E:273:LEU:O	1:E:276:MET:HB2	1.82	0.79
1:F:506:LEU:HD22	1:F:544:GLU:HG3	1.64	0.79
1:C:408:ALA:O	1:C:411:GLN:HG2	1.83	0.79
1:D:273:LEU:O	1:D:274:GLU:C	2.19	0.79
1:C:289:TYR:HE2	1:C:456:LEU:HG	1.47	0.79
1:E:385:ARG:HD2	1:E:431:TRP:HD1	1.45	0.79
1:F:386:ASP:OD2	1:F:388:ALA:HB3	1.83	0.78
1:A:537:GLU:N	1:A:537:GLU:OE1	2.16	0.78
1:C:395:ARG:HB3	1:C:396:THR:HA	1.64	0.78
1:E:256:VAL:HG23	1:E:263:LYS:HE2	1.64	0.78
1:C:249:LEU:HA	1:C:252:LYS:HE3	1.64	0.78
1:C:596:THR:HB	1:C:698:MET:HE1	1.65	0.78
1:C:629:LEU:HD22	1:C:633:MET:HE3	1.63	0.78
1:D:555:ALA:O	1:D:559:LEU:CD1	2.31	0.78
1:C:258:MET:HB3	1:C:262:VAL:CG1	2.12	0.78
1:F:294:THR:HG23	1:F:295:GLU:HG3	1.63	0.78
1:E:351:LEU:O	1:E:469:THR:HB	1.82	0.78
1:B:585:PRO:O	1:B:587:LYS:HD2	1.82	0.78
1:C:526:ALA:HB2	1:C:571:ALA:N	1.99	0.78
1:E:247:GLU:HA	1:E:250:ARG:HB2	1.64	0.78
1:C:259:PRO:CD	1:C:298:TRP:CZ2	2.67	0.78
1:B:374:ARG:HH21	1:B:416:ASN:HD21	1.30	0.77
1:F:657:PHE:O	1:F:661:VAL:HG12	1.83	0.77
1:E:312:ARG:NH2	1:E:330:LEU:CD1	2.47	0.77
1:E:598:GLN:HG2	1:E:698:MET:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ASN:HD22	1:D:450:THR:N	1.83	0.77
1:E:290:LEU:HA	1:E:293:LEU:HD12	1.65	0.77
1:E:292:TRP:HE1	1:E:402:PRO:HD2	1.50	0.77
1:C:450:THR:HG21	1:C:462:LEU:N	1.99	0.77
1:F:412:VAL:HG13	1:F:414:VAL:HG22	1.65	0.77
1:E:381:LEU:CD2	1:E:424:ILE:CG2	2.53	0.77
1:E:385:ARG:CD	1:E:428:SER:HB2	2.14	0.77
1:E:392:GLY:HA3	1:E:455:TYR:HB3	1.66	0.77
1:C:520:ILE:HD11	1:C:569:ILE:HD11	1.66	0.77
1:D:259:PRO:O	1:D:262:VAL:HG22	1.84	0.77
1:F:444:ASP:O	1:F:448:ASN:HB2	1.84	0.77
1:D:531:ILE:HG12	1:D:543:LEU:HD11	1.65	0.77
1:E:307:ASP:HB3	1:E:310:HIS:HB3	1.67	0.77
1:A:305:VAL:HG22	1:A:372:MET:HA	1.67	0.76
1:A:654:PRO:O	1:A:657:PHE:HD1	1.68	0.76
1:B:408:ALA:O	1:B:412:VAL:HG12	1.85	0.76
1:A:555:ALA:O	1:A:558:TRP:HB3	1.86	0.76
1:C:517:GLU:N	1:C:517:GLU:OE2	2.18	0.76
1:D:549:LYS:O	1:D:553:LYS:HG2	1.84	0.76
1:E:267:LEU:HA	1:E:270:LEU:CB	2.11	0.76
1:C:298:TRP:O	1:C:415:ILE:HG23	1.86	0.76
1:C:437:SER:O	1:C:440:LEU:HB3	1.85	0.76
1:B:649:GLN:NE2	1:B:655:GLU:HG2	2.00	0.76
1:C:248:ALA:HA	1:C:251:LYS:HG3	1.65	0.76
1:C:450:THR:CG2	1:C:461:ASP:N	2.48	0.76
1:C:519:ARG:HD2	1:C:558:TRP:HH2	1.50	0.76
1:E:292:TRP:HH2	1:E:407:HIS:HB2	1.50	0.76
1:E:384:VAL:O	1:E:428:SER:CB	2.34	0.76
1:B:292:TRP:O	1:B:296:VAL:HG13	1.84	0.76
1:B:406:ILE:HD13	1:B:453:ASP:OD2	1.85	0.76
1:C:529:ARG:HD3	1:C:574:ILE:HD12	1.66	0.76
1:C:393:HIS:CE1	1:C:395:ARG:O	2.39	0.76
1:C:715:ILE:H	1:C:739:ASN:ND2	1.83	0.76
1:E:385:ARG:HD3	1:E:428:SER:HB2	1.67	0.76
1:B:289:TYR:CD2	1:B:395:ARG:HD3	2.21	0.75
1:C:389:GLU:O	1:C:404:LYS:HA	1.84	0.75
1:C:259:PRO:O	1:C:262:VAL:HG12	1.86	0.75
1:F:245:ASP:HA	1:F:248:ALA:HB3	1.67	0.75
1:E:388:ALA:HB1	1:E:393:HIS:HA	1.68	0.75
1:A:534:TYR:CE1	1:A:581:PRO:HA	2.21	0.75
1:C:507:TRP:CE2	1:C:522:VAL:HG23	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:GLY:O	1:C:566:LEU:CD1	2.34	0.75
1:F:263:LYS:O	1:F:267:LEU:HG	1.87	0.75
1:A:453:ASP:OD1	1:A:454:HIS:N	2.19	0.75
1:C:401:MET:O	1:C:455:TYR:HB3	1.86	0.75
1:A:687:ILE:O	1:A:691:LEU:HD12	1.87	0.75
1:C:295:GLU:HB2	1:C:297:PRO:HD3	1.67	0.75
1:F:245:ASP:HA	1:F:248:ALA:CB	2.16	0.75
1:E:439:MET:HA	1:E:442:VAL:CG2	2.17	0.75
1:E:408:ALA:HA	1:E:411:GLN:CG	2.16	0.75
1:B:351:LEU:HD11	1:B:488:ILE:HD11	1.67	0.75
1:C:273:LEU:HD21	1:C:286:ALA:HB3	1.67	0.75
1:C:410:LYS:HG3	1:C:411:GLN:N	2.02	0.75
1:A:458:VAL:HG12	1:A:459:PRO:HD2	1.68	0.75
1:A:595:GLY:HA2	1:A:689:SER:OG	1.87	0.74
1:B:269:GLU:O	1:B:272:ARG:HG3	1.87	0.74
1:C:296:VAL:O	1:C:297:PRO:C	2.23	0.74
1:E:391:ARG:HB2	1:E:453:ASP:HA	1.69	0.74
1:C:304:GLU:CD	1:C:374:ARG:HH21	1.90	0.74
1:D:523:THR:HB	1:D:570:ASP:OD1	1.87	0.74
1:C:570:ASP:CG	1:C:571:ALA:H	1.90	0.74
1:D:374:ARG:HH21	1:D:416:ASN:C	1.90	0.74
1:A:412:VAL:HG21	1:A:417:PRO:HG3	1.67	0.74
1:C:395:ARG:HH11	1:C:395:ARG:HG3	1.52	0.74
1:C:425:ASP:HA	1:C:477:ILE:CG2	2.16	0.74
1:F:596:THR:CG2	1:F:698:MET:HE3	2.16	0.74
1:F:292:TRP:O	1:F:296:VAL:HG23	1.88	0.74
1:F:523:THR:HG22	1:F:526:ALA:N	2.01	0.74
1:E:267:LEU:HD22	1:E:270:LEU:HD12	1.69	0.74
1:C:289:TYR:HD2	1:C:456:LEU:HG	1.47	0.74
1:F:297:PRO:O	1:F:415:ILE:CD1	2.36	0.74
1:C:394:ARG:HG3	1:C:395:ARG:HG2	1.68	0.74
1:C:715:ILE:H	1:C:739:ASN:HD21	1.34	0.74
1:C:450:THR:CG2	1:C:462:LEU:N	2.51	0.74
1:E:258:MET:O	1:E:263:LYS:CD	2.35	0.74
1:E:270:LEU:O	1:E:273:LEU:HD23	1.87	0.74
1:D:246:LEU:HD23	1:D:246:LEU:H	1.52	0.73
1:C:291:ASP:OD1	1:C:292:TRP:N	2.21	0.73
1:C:558:TRP:HE3	1:C:563:TRP:CZ3	2.07	0.73
1:F:619:GLY:O	1:F:660:LYS:HA	1.87	0.73
1:F:246:LEU:HD12	1:F:287:ARG:NH2	2.04	0.73
1:D:648:THR:HG21	1:D:655:GLU:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:LEU:O	1:C:440:LEU:HD12	1.88	0.73
1:F:448:ASN:ND2	1:F:462:LEU:HB2	2.04	0.73
1:F:657:PHE:HB2	1:F:661:VAL:CG1	2.16	0.73
1:F:620:SER:CA	1:F:659:ASN:O	2.37	0.73
1:E:296:VAL:HA	1:E:410:LYS:HG2	1.70	0.73
1:B:507:TRP:CZ2	1:B:522:VAL:CG2	2.70	0.73
1:E:585:PRO:CG	1:E:587:LYS:HD3	2.19	0.73
1:E:643:TYR:CE2	1:E:762:VAL:HG11	2.23	0.73
1:A:508:PRO:O	1:A:512:ARG:HG3	1.89	0.73
1:B:649:GLN:HE21	1:B:655:GLU:HG2	1.54	0.73
1:C:450:THR:C	1:C:460:TYR:HB2	2.09	0.73
1:F:297:PRO:CD	1:F:410:LYS:HA	2.18	0.73
1:D:558:TRP:O	1:D:561:GLY:HA3	1.88	0.73
1:A:530:VAL:O	1:A:535:THR:HG22	1.89	0.73
1:B:318:ASP:O	1:B:319:HIS:ND1	2.21	0.73
1:E:451:PHE:CD1	1:E:452:THR:N	2.56	0.73
1:C:680:GLY:HA3	1:C:706:VAL:HG12	1.71	0.72
1:B:746:LEU:HD12	1:B:751:LEU:HD22	1.69	0.72
1:B:289:TYR:HD2	1:B:395:ARG:HD3	1.55	0.72
1:D:643:TYR:CZ	1:D:762:VAL:HG11	2.25	0.72
1:E:385:ARG:HD2	1:E:428:SER:OG	1.89	0.72
1:E:392:GLY:CA	1:E:455:TYR:HB2	2.18	0.72
1:E:558:TRP:HA	1:E:561:GLY:O	1.89	0.72
1:B:507:TRP:CE2	1:B:522:VAL:CG2	2.72	0.72
1:B:703:THR:O	1:B:736:PRO:HD3	1.89	0.72
1:D:693:ARG:NH1	1:D:776:MET:SD	2.62	0.72
1:E:331:GLU:O	1:E:335:VAL:HG12	1.89	0.72
1:E:555:ALA:O	1:E:559:LEU:N	2.22	0.72
1:C:455:TYR:HE1	1:C:456:LEU:HD22	1.55	0.72
1:A:393:HIS:CB	1:A:400:ALA:HB1	2.19	0.72
1:B:600:LEU:CD2	1:B:721:LYS:O	2.38	0.72
1:F:273:LEU:O	1:F:276:MET:HG3	1.89	0.72
1:F:322:LEU:O	1:F:326:LYS:HG3	1.90	0.72
1:F:394:ARG:H	1:F:394:ARG:HD2	1.55	0.72
1:D:679:ALA:HB1	1:D:682:THR:CG2	2.19	0.72
1:B:703:THR:CG2	1:B:715:ILE:CD1	2.64	0.71
1:C:413:GLY:O	1:C:414:VAL:CG2	2.37	0.71
1:D:390:ILE:O	1:D:403:GLY:HA3	1.90	0.71
1:E:319:HIS:CE1	1:E:363:SER:HB2	2.24	0.71
1:A:311:THR:HG23	1:A:371:SER:CB	2.19	0.71
1:E:290:LEU:HA	1:E:293:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:637:ALA:HB2	1:E:683:MET:HE1	1.72	0.71
1:B:297:PRO:HG2	1:B:460:TYR:OH	1.90	0.71
1:C:354:VAL:C	1:C:490:ILE:HG22	2.10	0.71
1:F:271:ASP:O	1:F:274:GLU:HG3	1.91	0.71
1:F:715:ILE:HG22	1:F:739:ASN:ND2	2.06	0.71
1:E:305:VAL:C	1:E:306:LEU:HD12	2.10	0.71
1:D:637:ALA:HB2	1:D:683:MET:CE	2.21	0.71
1:C:259:PRO:HG2	1:C:298:TRP:HZ2	1.49	0.71
1:C:399:GLY:O	1:C:455:TYR:CD2	2.43	0.71
1:E:438:ALA:O	1:E:442:VAL:HG23	1.91	0.71
1:E:506:LEU:CD2	1:E:544:GLU:HG3	2.20	0.71
1:C:406:ILE:HA	1:C:409:MET:HB3	1.71	0.71
1:C:440:LEU:CB	1:C:481:LEU:HD21	2.13	0.71
1:F:621:GLY:CA	1:F:658:TYR:O	2.38	0.71
1:E:359:VAL:HG23	1:E:359:VAL:O	1.91	0.71
1:A:627:GLY:O	1:A:674:LYS:NZ	2.24	0.70
1:A:351:LEU:HD11	1:A:488:ILE:CD1	2.21	0.70
1:C:451:PHE:CD2	1:C:462:LEU:HB3	2.27	0.70
1:C:507:TRP:CZ2	1:C:522:VAL:HG23	2.26	0.70
1:D:585:PRO:HA	1:D:586:ASP:HB3	1.73	0.70
1:E:319:HIS:CD2	1:E:367:SER:OG	2.44	0.70
1:A:521:GLU:O	1:A:569:ILE:HG13	1.91	0.70
1:C:392:GLY:CA	1:C:454:HIS:HB2	2.21	0.70
1:E:274:GLU:OE1	1:E:274:GLU:HA	1.91	0.70
1:A:385:ARG:HD3	1:A:386:ASP:H	1.56	0.70
1:B:394:ARG:HG2	1:B:454:HIS:HB3	1.72	0.70
1:E:311:THR:O	1:E:315:LEU:HD12	1.92	0.70
1:C:518:GLY:O	1:C:566:LEU:HD12	1.91	0.70
1:A:439:MET:O	1:A:442:VAL:HG12	1.91	0.70
1:F:264:THR:HA	1:F:267:LEU:CD1	2.22	0.70
1:F:422:ASP:HA	1:F:470:THR:HB	1.74	0.70
1:B:694:ARG:HD2	1:B:771:LEU:O	1.92	0.69
1:D:523:THR:CB	1:D:570:ASP:OD1	2.39	0.69
1:F:317:GLU:O	1:F:505:TYR:HE1	1.75	0.69
1:A:319:HIS:CE1	1:A:364:LEU:HD23	2.27	0.69
1:C:392:GLY:CA	1:C:454:HIS:N	2.46	0.69
1:C:405:LEU:O	1:C:408:ALA:N	2.25	0.69
1:F:250:ARG:HA	1:F:253:ILE:CD1	2.09	0.69
1:C:340:GLN:HA	1:C:340:GLN:HE21	1.57	0.69
1:F:688:ALA:O	1:F:692:SER:HB2	1.91	0.69
1:C:447:GLN:HG2	1:C:451:PHE:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:TRP:O	1:E:511:VAL:HG23	1.93	0.69
1:A:350:ILE:HD13	1:A:443:LEU:CD2	2.22	0.69
1:C:401:MET:CE	1:C:407:HIS:HE1	2.05	0.69
1:C:558:TRP:CE3	1:C:563:TRP:CZ3	2.80	0.69
1:E:405:LEU:O	1:E:409:MET:N	2.24	0.69
1:E:501:ILE:HD12	1:E:502:ALA:N	2.08	0.69
1:A:507:TRP:O	1:A:511:VAL:HG23	1.92	0.69
1:B:307:ASP:O	1:B:310:HIS:N	2.26	0.69
1:D:507:TRP:O	1:D:511:VAL:HG23	1.93	0.69
1:A:343:ASP:O	1:A:346:ASN:HB3	1.92	0.69
1:B:448:ASN:OD1	1:B:449:ASN:N	2.26	0.69
1:C:393:HIS:O	1:C:454:HIS:CG	2.45	0.69
1:E:385:ARG:HH21	1:E:428:SER:CB	2.06	0.69
1:A:514:SER:OG	1:A:551:ALA:HB1	1.94	0.68
1:C:268:LYS:HD3	1:C:271:ASP:OD2	1.93	0.68
1:C:293:LEU:O	1:C:296:VAL:N	2.26	0.68
1:B:749:GLU:O	1:B:753:GLY:N	2.27	0.68
1:B:750:VAL:O	1:B:754:LEU:HD12	1.92	0.68
1:F:289:TYR:CA	1:F:455:TYR:OH	2.38	0.68
1:E:585:PRO:HG2	1:E:587:LYS:HD3	1.74	0.68
1:A:318:ASP:OD2	1:A:367:SER:HB2	1.94	0.68
1:B:586:ASP:HA	1:B:587:LYS:CB	2.11	0.68
1:C:629:LEU:HD22	1:C:633:MET:CE	2.23	0.68
1:F:563:TRP:HB2	1:F:565:GLY:CA	2.23	0.68
1:B:619:GLY:HA3	1:B:662:ASP:OD1	1.93	0.68
1:D:503:ARG:NE	1:D:524:ASP:OD1	2.25	0.68
1:C:390:ILE:HD11	1:C:438:ALA:C	2.13	0.68
1:C:505:TYR:O	1:C:508:PRO:HD2	1.94	0.68
1:F:264:THR:HA	1:F:267:LEU:HD12	1.75	0.68
1:F:593:GLN:HB2	1:F:596:THR:CG2	2.24	0.68
1:E:365:GLY:C	1:E:376:PHE:HE2	1.97	0.68
1:B:601:ALA:HB2	2:B:802:4KZ:C27	2.24	0.68
1:D:552:ARG:HG2	1:E:331:GLU:HB3	1.76	0.68
1:F:317:GLU:O	1:F:505:TYR:CE1	2.46	0.68
1:C:425:ASP:CG	1:C:471:ALA:HB1	2.13	0.68
1:C:356:PRO:O	1:C:359:VAL:HG12	1.94	0.67
1:F:608:THR:HG22	1:F:609:LEU:O	1.93	0.67
1:D:280:SER:O	1:D:283:ALA:N	2.26	0.67
1:B:374:ARG:NH1	1:B:466:PHE:HB2	2.09	0.67
1:C:390:ILE:C	1:C:391:ARG:O	2.24	0.67
1:C:442:VAL:HG23	1:C:443:LEU:CD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ILE:O	1:D:371:SER:HB3	1.93	0.67
1:E:359:VAL:HB	1:E:493:TYR:CE2	2.29	0.67
1:E:395:ARG:NH1	1:E:457:ASP:OD1	2.27	0.67
1:A:260:GLU:O	1:A:264:THR:HG23	1.95	0.67
1:A:405:LEU:HD22	1:A:442:VAL:HG21	1.76	0.67
1:A:496:MET:O	1:A:499:GLN:HB3	1.94	0.67
1:E:265:LYS:CE	1:E:269:GLU:HG3	2.24	0.67
1:A:312:ARG:NH1	1:A:327:GLU:OE2	2.26	0.67
1:C:387:GLU:HG3	1:C:433:GLY:HA3	1.76	0.67
1:F:244:SER:O	1:F:247:GLU:HB3	1.92	0.67
1:E:319:HIS:HE1	1:E:363:SER:HB2	1.58	0.67
1:A:443:LEU:O	1:A:484:ARG:NH1	2.27	0.67
1:C:619:GLY:N	1:C:660:LYS:O	2.27	0.67
1:D:372:MET:CE	1:D:374:ARG:HD3	2.25	0.67
1:C:300:LYS:O	1:C:414:VAL:CG1	2.35	0.67
1:D:244:SER:OG	1:D:245:ASP:N	2.28	0.67
1:D:585:PRO:HA	1:D:586:ASP:CB	2.24	0.67
1:E:363:SER:O	1:E:366:ARG:N	2.27	0.67
1:A:526:ALA:HB2	1:A:570:ASP:OD1	1.95	0.67
1:C:289:TYR:HE1	1:C:293:LEU:HD13	1.57	0.67
1:F:441:GLU:OE1	1:F:451:PHE:CB	2.42	0.67
1:E:311:THR:HG23	1:E:371:SER:CB	2.25	0.67
1:C:394:ARG:C	1:C:395:ARG:HG2	2.13	0.67
1:D:244:SER:N	1:D:247:GLU:OE1	2.28	0.66
1:C:388:ALA:CB	1:C:402:PRO:CB	2.73	0.66
1:D:325:VAL:O	1:D:329:ILE:HG13	1.95	0.66
1:D:386:ASP:OD1	1:D:387:GLU:N	2.28	0.66
1:D:412:VAL:HG13	1:D:414:VAL:H	1.59	0.66
1:E:293:LEU:O	1:E:298:TRP:HH2	1.76	0.66
1:E:500:ALA:O	1:E:503:ARG:HB3	1.95	0.66
1:A:405:LEU:CD2	1:A:442:VAL:HG21	2.26	0.66
1:A:439:MET:O	1:A:443:LEU:HD12	1.95	0.66
1:D:718:VAL:O	1:D:722:LEU:HD13	1.94	0.66
1:E:333:LEU:O	1:E:336:ARG:HB3	1.95	0.66
1:B:409:MET:HA	1:B:412:VAL:HG12	1.77	0.66
1:A:312:ARG:NH2	1:F:560:GLU:OE2	2.28	0.66
1:C:450:THR:CA	1:C:460:TYR:HB2	2.24	0.66
1:D:356:PRO:O	1:D:359:VAL:CG2	2.43	0.66
1:A:309:ASN:O	1:A:313:GLN:NE2	2.28	0.66
1:B:700:ILE:HD13	1:B:768:TYR:CE1	2.31	0.66
1:C:406:ILE:HA	1:C:409:MET:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ASN:O	1:F:312:ARG:HB3	1.96	0.66
1:E:359:VAL:O	1:E:359:VAL:CG2	2.43	0.66
1:C:404:LYS:CB	1:C:454:HIS:O	2.43	0.66
1:F:246:LEU:HA	1:F:249:LEU:HD23	1.77	0.66
1:F:355:GLY:HA3	1:F:490:ILE:O	1.96	0.66
1:D:324:ASP:O	1:D:328:ARG:HG2	1.95	0.66
1:D:762:VAL:HG13	1:D:763:GLY:N	2.10	0.66
1:C:440:LEU:HD22	1:C:481:LEU:CD2	2.25	0.66
1:F:277:GLN:HB2	1:F:280:SER:CB	2.25	0.66
1:D:307:ASP:O	1:D:311:THR:HG22	1.96	0.66
1:E:267:LEU:HD13	1:E:268:LYS:HD2	1.78	0.66
1:B:327:GLU:O	1:B:331:GLU:HG3	1.96	0.66
1:A:350:ILE:CD1	1:A:443:LEU:CD2	2.72	0.66
1:A:624:SER:CB	1:A:664:HIS:ND1	2.59	0.66
1:C:529:ARG:CD	1:C:574:ILE:HD12	2.25	0.66
1:E:384:VAL:HG13	1:E:389:GLU:HG2	1.76	0.66
1:E:479:ARG:HA	1:E:482:LEU:HB3	1.78	0.66
1:E:665:VAL:HG11	1:E:683:MET:HE3	1.77	0.66
1:C:399:GLY:O	1:C:455:TYR:HD2	1.76	0.65
1:A:271:ASP:HA	1:A:274:GLU:OE1	1.95	0.65
1:C:401:MET:HE1	1:C:407:HIS:HE1	1.60	0.65
1:D:332:TYR:CZ	1:D:351:LEU:CD1	2.80	0.65
1:E:311:THR:HA	1:E:371:SER:OG	1.95	0.65
1:E:715:ILE:HG13	1:E:739:ASN:ND2	2.11	0.65
1:A:595:GLY:N	1:A:689:SER:OG	2.30	0.65
1:B:276:MET:SD	1:B:283:ALA:CA	2.83	0.65
1:C:295:GLU:HB2	1:C:297:PRO:CD	2.27	0.65
1:C:524:ASP:O	1:C:527:ILE:HG22	1.97	0.65
1:F:452:THR:HG21	1:F:458:VAL:O	1.96	0.65
1:D:343:ASP:HB3	1:D:345:ARG:O	1.95	0.65
1:B:244:SER:O	1:B:247:GLU:HG2	1.97	0.65
1:A:703:THR:OG1	1:A:721:LYS:NZ	2.29	0.65
1:C:510:GLN:O	1:C:514:SER:N	2.28	0.65
1:F:273:LEU:O	1:F:276:MET:CG	2.44	0.65
1:D:637:ALA:CA	1:D:683:MET:HE2	2.25	0.65
1:A:523:THR:OG1	1:A:570:ASP:CA	2.44	0.65
1:A:761:ASP:OD1	1:A:762:VAL:N	2.29	0.65
1:C:295:GLU:CB	1:C:297:PRO:HG3	2.26	0.65
1:E:388:ALA:HA	1:E:391:ARG:O	1.96	0.65
1:C:402:PRO:CD	1:C:403:GLY:HA3	2.27	0.65
1:C:519:ARG:HA	1:C:566:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:HIS:O	1:A:411:GLN:HG2	1.97	0.65
1:A:595:GLY:H	1:A:689:SER:HG	1.45	0.65
1:C:265:LYS:O	1:C:267:LEU:N	2.26	0.65
1:F:282:GLU:HA	1:F:282:GLU:OE2	1.97	0.65
1:D:503:ARG:NH2	1:D:524:ASP:OD1	2.30	0.65
1:A:297:PRO:HB3	1:A:413:GLY:O	1.96	0.65
1:F:394:ARG:H	1:F:394:ARG:CD	2.09	0.65
1:C:613:GLU:OE1	1:D:707:SER:HB2	1.96	0.65
1:C:272:ARG:HE	1:C:273:LEU:HD12	1.61	0.64
1:C:425:ASP:OD1	1:C:426:LYS:N	2.31	0.64
1:C:450:THR:HB	1:C:460:TYR:CB	2.24	0.64
1:C:549:LYS:HA	1:C:552:ARG:HD2	1.78	0.64
1:D:321:GLY:O	1:D:326:LYS:HD2	1.97	0.64
1:E:296:VAL:HA	1:E:410:LYS:CG	2.26	0.64
1:E:556:LYS:O	1:E:560:GLU:HB2	1.97	0.64
1:A:389:GLU:O	1:A:391:ARG:N	2.27	0.64
1:A:534:TYR:HE1	1:A:580:ILE:O	1.80	0.64
1:C:292:TRP:CE3	1:C:455:TYR:CD1	2.85	0.64
1:C:350:ILE:HD13	1:C:443:LEU:HD11	1.78	0.64
1:F:259:PRO:O	1:F:263:LYS:HG2	1.97	0.64
1:C:390:ILE:HD11	1:C:438:ALA:HB1	1.79	0.64
1:C:450:THR:CG2	1:C:451:PHE:N	2.47	0.64
1:C:512:ARG:HA	1:C:517:GLU:HG3	1.78	0.64
1:F:275:ARG:HB3	1:F:275:ARG:NH1	2.13	0.64
1:F:452:THR:HG22	1:F:453:ASP:N	2.13	0.64
1:D:250:ARG:O	1:D:253:ILE:HG22	1.98	0.64
1:E:405:LEU:O	1:E:409:MET:HB2	1.97	0.64
1:A:318:ASP:HB3	1:A:319:HIS:CD2	2.33	0.64
1:E:247:GLU:HA	1:E:250:ARG:CB	2.28	0.64
1:E:296:VAL:HG12	1:E:297:PRO:N	2.13	0.64
1:E:308:ILE:O	1:E:312:ARG:HB2	1.97	0.64
1:A:262:VAL:CG1	1:A:458:VAL:HG11	2.28	0.64
1:C:293:LEU:HD23	1:C:294:THR:CA	2.28	0.64
1:C:393:HIS:HD2	1:C:402:PRO:CA	2.11	0.64
1:A:529:ARG:HD2	1:A:571:ALA:HB1	1.80	0.64
1:B:297:PRO:O	1:B:415:ILE:CG2	2.43	0.64
1:B:391:ARG:HA	1:B:453:ASP:HB2	1.80	0.64
1:E:265:LYS:O	1:E:265:LYS:HE3	1.97	0.64
1:E:388:ALA:CB	1:E:393:HIS:HA	2.27	0.64
1:A:351:LEU:HD11	1:A:488:ILE:HD12	1.80	0.64
1:B:374:ARG:HH21	1:B:416:ASN:ND2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:THR:OG1	1:F:371:SER:HB3	1.98	0.64
1:F:429:SER:HA	1:F:435:PRO:HD2	1.80	0.64
1:D:332:TYR:CE1	1:D:351:LEU:HD11	2.33	0.64
1:D:422:ASP:HB2	1:D:470:THR:OG1	1.97	0.64
1:E:267:LEU:HD22	1:E:267:LEU:O	1.98	0.64
1:E:558:TRP:HE3	1:E:563:TRP:CZ2	2.16	0.64
1:E:637:ALA:HB2	1:E:683:MET:HE2	1.78	0.64
1:C:385:ARG:HB3	1:C:429:SER:OG	1.97	0.64
1:C:393:HIS:O	1:C:454:HIS:CD2	2.50	0.64
1:C:404:LYS:HE2	1:C:453:ASP:O	1.98	0.64
1:C:519:ARG:HD2	1:C:558:TRP:CH2	2.30	0.64
1:F:392:GLY:HA3	1:F:402:PRO:O	1.98	0.64
1:E:444:ASP:OD2	1:E:446:GLU:HB3	1.97	0.64
1:E:508:PRO:O	1:E:511:VAL:N	2.29	0.64
1:A:385:ARG:H	1:A:385:ARG:CD	2.08	0.64
1:B:259:PRO:O	1:B:262:VAL:HG22	1.98	0.64
1:C:414:VAL:HG12	1:C:416:ASN:H	1.62	0.64
1:F:332:TYR:O	1:F:335:VAL:HG22	1.98	0.64
1:D:750:VAL:HG23	1:D:754:LEU:HD12	1.80	0.64
1:A:318:ASP:OD2	1:A:367:SER:CB	2.46	0.63
1:F:483:ASP:O	1:E:545:ARG:HD3	1.98	0.63
1:D:360:GLY:O	1:D:364:LEU:HD12	1.97	0.63
1:E:424:ILE:HD11	1:E:469:THR:HG21	1.79	0.63
1:A:672:THR:O	1:A:674:LYS:HE3	1.98	0.63
1:E:540:VAL:O	1:E:543:LEU:N	2.31	0.63
1:B:311:THR:HG22	1:B:330:LEU:HD21	1.80	0.63
1:C:411:GLN:O	1:C:412:VAL:C	2.36	0.63
1:F:444:ASP:OD1	1:F:446:GLU:N	2.31	0.63
1:D:430:ASP:HA	1:D:433:GLY:C	2.19	0.63
1:E:533:GLU:OE2	1:E:581:PRO:HB3	1.99	0.63
1:B:259:PRO:HB2	1:B:262:VAL:HG13	1.81	0.63
1:F:521:GLU:HB3	1:F:568:THR:HG22	1.81	0.63
1:D:263:LYS:O	1:D:267:LEU:HG	1.98	0.63
1:A:263:LYS:O	1:A:267:LEU:HD12	1.98	0.63
1:E:374:ARG:CZ	1:E:416:ASN:O	2.46	0.63
1:A:425:ASP:HB2	1:A:476:THR:OG1	1.99	0.63
1:B:700:ILE:CD1	1:B:768:TYR:CE1	2.81	0.63
1:F:407:HIS:O	1:F:410:LYS:HG3	1.98	0.63
1:D:383:GLY:N	1:D:426:LYS:O	2.31	0.63
1:E:259:PRO:HD3	1:E:298:TRP:NE1	2.13	0.63
1:E:266:ALA:O	1:E:270:LEU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:LEU:O	1:E:484:ARG:N	2.32	0.63
1:E:558:TRP:HE3	1:E:563:TRP:CZ3	2.16	0.63
1:C:246:LEU:O	1:C:249:LEU:HB3	1.99	0.63
1:C:291:ASP:O	1:C:294:THR:HG22	1.98	0.63
1:A:386:ASP:HB2	1:A:432:ARG:HB3	1.80	0.63
1:A:735:LEU:O	1:A:759:VAL:HG22	1.98	0.63
1:B:278:GLN:CG	1:C:396:THR:OG1	2.45	0.63
1:B:298:TRP:CD1	1:B:298:TRP:N	2.66	0.63
1:B:646:ALA:C	1:B:647:HIS:HD1	2.02	0.63
1:C:254:GLU:C	1:C:255:GLU:OE2	2.37	0.63
1:C:414:VAL:HG12	1:C:415:ILE:N	2.13	0.63
1:C:523:THR:O	1:C:527:ILE:N	2.32	0.63
1:F:249:LEU:O	1:F:253:ILE:HG13	1.99	0.63
1:F:503:ARG:CZ	1:F:524:ASP:OD1	2.46	0.63
1:D:384:VAL:HG22	1:D:389:GLU:HG3	1.81	0.63
1:E:319:HIS:O	1:E:326:LYS:NZ	2.31	0.63
1:A:345:ARG:O	1:A:348:ALA:N	2.31	0.63
1:E:314:VAL:O	1:E:317:GLU:N	2.32	0.63
1:B:431:TRP:N	1:B:432:ARG:HA	2.14	0.62
1:C:388:ALA:HB1	1:C:402:PRO:CB	2.28	0.62
1:C:680:GLY:CA	1:C:706:VAL:HG12	2.27	0.62
1:A:339:THR:CG2	1:A:344:VAL:HB	2.29	0.62
1:F:393:HIS:HB2	1:F:400:ALA:HB1	1.81	0.62
1:A:247:GLU:O	1:A:251:LYS:HG3	1.98	0.62
1:A:595:GLY:CA	1:A:689:SER:OG	2.46	0.62
1:C:293:LEU:HD23	1:C:293:LEU:C	2.20	0.62
1:E:424:ILE:O	1:E:427:MET:HG2	1.99	0.62
1:C:425:ASP:HB3	1:C:471:ALA:HB1	1.81	0.62
1:C:529:ARG:HB3	1:C:574:ILE:CD1	2.28	0.62
1:F:562:ALA:HB1	1:F:563:TRP:O	2.00	0.62
1:B:406:ILE:CD1	1:B:453:ASP:OD2	2.46	0.62
1:C:390:ILE:CD1	1:C:438:ALA:O	2.47	0.62
1:C:558:TRP:HB3	1:C:559:LEU:HD13	1.82	0.62
1:D:621:GLY:N	1:D:662:ASP:OD1	2.32	0.62
1:A:514:SER:CB	1:A:551:ALA:HB1	2.29	0.62
1:A:271:ASP:HA	1:A:274:GLU:HB2	1.81	0.62
1:C:259:PRO:HD2	1:C:298:TRP:CZ2	2.34	0.62
1:C:393:HIS:H	1:C:454:HIS:HB2	1.52	0.62
1:B:273:LEU:CD1	1:B:276:MET:CE	2.78	0.62
1:C:278:GLN:HA	1:C:280:SER:HB2	1.80	0.62
1:C:456:LEU:HD13	1:C:456:LEU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:TRP:CZ3	1:E:563:TRP:CE2	2.87	0.62
1:F:523:THR:HG22	1:F:526:ALA:H	1.64	0.62
1:E:494:THR:HG22	1:E:497:GLU:CD	2.19	0.62
1:A:549:LYS:O	1:A:553:LYS:HG2	1.99	0.62
1:B:374:ARG:HH12	1:B:466:PHE:HB2	1.65	0.61
1:B:733:ILE:HG13	1:B:754:LEU:HD22	1.83	0.61
1:C:379:ILE:HD11	1:C:419:ILE:HG21	1.83	0.61
1:C:433:GLY:O	1:C:435:PRO:HD3	2.01	0.61
1:C:526:ALA:O	1:C:574:ILE:HD11	2.00	0.61
1:D:648:THR:CG2	1:D:655:GLU:HA	2.31	0.61
1:A:259:PRO:O	1:A:262:VAL:HG22	2.00	0.61
1:C:736:PRO:HG2	1:C:739:ASN:HD22	1.64	0.61
1:F:450:THR:OG1	1:F:451:PHE:N	2.32	0.61
1:F:645:ARG:NH2	1:E:618:PRO:O	2.33	0.61
1:D:592:PRO:CB	1:D:696:ALA:O	2.46	0.61
1:D:705:GLU:O	1:D:712:VAL:HA	2.00	0.61
1:E:403:GLY:HA2	1:E:407:HIS:CD2	2.35	0.61
1:E:424:ILE:HD11	1:E:469:THR:CG2	2.30	0.61
1:A:380:SER:O	1:A:404:LYS:NZ	2.33	0.61
1:A:392:GLY:N	1:A:453:ASP:OD1	2.31	0.61
1:C:262:VAL:CG2	1:C:298:TRP:CH2	2.84	0.61
1:F:497:GLU:O	1:F:501:ILE:HD12	2.01	0.61
1:D:588:ALA:HB3	1:D:589:GLU:O	2.01	0.61
1:E:289:TYR:CE1	1:E:456:LEU:HG	2.35	0.61
1:E:387:GLU:O	1:E:391:ARG:CD	2.48	0.61
1:E:406:ILE:O	1:E:409:MET:HB3	1.99	0.61
1:B:603:THR:HG22	1:B:604:PRO:HD2	1.82	0.61
1:F:278:GLN:HG2	1:F:278:GLN:O	2.01	0.61
1:F:694:ARG:NH1	1:F:771:LEU:O	2.33	0.61
1:D:556:LYS:O	1:D:560:GLU:HG3	2.00	0.61
1:E:439:MET:O	1:E:442:VAL:N	2.33	0.61
1:A:385:ARG:HD3	1:A:386:ASP:N	2.15	0.61
1:A:573:ASP:O	1:A:576:THR:HB	2.00	0.61
1:C:415:ILE:C	1:C:417:PRO:HD3	2.21	0.61
1:D:563:TRP:CZ3	1:D:567:ARG:HD3	2.36	0.61
1:E:366:ARG:HA	1:E:376:PHE:CD2	2.35	0.61
1:E:390:ILE:HD12	1:E:435:PRO:HB2	1.82	0.61
1:E:509:LYS:O	1:E:513:GLU:HG3	2.01	0.61
1:C:273:LEU:HA	1:C:276:MET:HB2	1.82	0.61
1:C:392:GLY:H	1:C:453:ASP:CB	2.06	0.61
1:E:263:LYS:O	1:E:266:ALA:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:GLN:OE1	1:E:552:ARG:NH1	2.33	0.61
1:C:553:LYS:O	1:C:556:LYS:HB3	2.01	0.61
1:D:375:LYS:HB2	1:D:417:PRO:HB3	1.82	0.61
1:E:340:GLN:NE2	1:E:340:GLN:H	1.99	0.61
1:C:409:MET:O	1:C:412:VAL:N	2.30	0.61
1:C:450:THR:C	1:C:460:TYR:CB	2.70	0.61
1:D:332:TYR:O	1:D:335:VAL:HG22	2.00	0.61
1:E:352:VAL:CG1	1:E:487:VAL:HA	2.30	0.61
1:A:359:VAL:HG23	1:A:493:TYR:CZ	2.36	0.60
1:C:308:ILE:O	1:C:311:THR:N	2.33	0.60
1:F:707:SER:HB3	1:F:713:MET:SD	2.41	0.60
1:E:394:ARG:O	1:E:455:TYR:HD1	1.83	0.60
1:E:546:GLU:HA	1:E:546:GLU:OE2	2.01	0.60
1:A:699:ASP:N	1:A:699:ASP:OD1	2.35	0.60
1:B:351:LEU:HD11	1:B:488:ILE:CD1	2.31	0.60
1:B:758:LEU:N	1:B:758:LEU:HD23	2.16	0.60
1:C:526:ALA:CB	1:C:571:ALA:HA	2.26	0.60
1:F:245:ASP:CA	1:F:248:ALA:HB3	2.31	0.60
1:F:246:LEU:HD23	1:F:246:LEU:C	2.20	0.60
1:B:325:VAL:O	1:B:329:ILE:HG13	2.01	0.60
1:D:424:ILE:HB	1:D:469:THR:HG23	1.83	0.60
1:E:419:ILE:HG22	1:E:421:LEU:HD12	1.83	0.60
1:E:267:LEU:O	1:E:270:LEU:N	2.34	0.60
1:E:405:LEU:HD23	1:E:405:LEU:C	2.20	0.60
1:E:479:ARG:O	1:E:483:ASP:N	2.31	0.60
1:E:558:TRP:CE3	1:E:563:TRP:CZ3	2.88	0.60
1:C:247:GLU:O	1:C:250:ARG:HB3	2.00	0.60
1:F:286:ALA:O	1:F:290:LEU:HD23	2.02	0.60
1:E:286:ALA:O	1:E:290:LEU:CD1	2.50	0.60
1:B:314:VAL:HG13	1:B:370:ARG:CZ	2.31	0.60
1:C:392:GLY:CA	1:C:454:HIS:H	2.10	0.60
1:D:438:ALA:O	1:D:442:VAL:HG23	2.01	0.60
1:D:679:ALA:HB1	1:D:682:THR:HG21	1.83	0.60
1:E:270:LEU:HD13	1:E:270:LEU:C	2.21	0.60
1:A:430:ASP:OD1	1:A:431:TRP:N	2.34	0.60
1:E:338:LEU:C	1:E:340:GLN:NE2	2.55	0.60
1:C:394:ARG:HG3	1:C:395:ARG:CG	2.31	0.60
1:C:420:LEU:HA	1:C:468:ILE:O	2.02	0.60
1:C:442:VAL:HG23	1:C:443:LEU:HD23	1.82	0.60
1:F:564:GLU:N	1:F:565:GLY:HA3	2.17	0.60
1:F:570:ASP:OD1	1:F:570:ASP:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:715:ILE:CG2	1:F:739:ASN:HD21	2.14	0.60
1:D:477:ILE:HG22	1:D:478:PRO:O	2.01	0.60
1:E:319:HIS:HE1	1:E:363:SER:CB	2.15	0.60
1:E:422:ASP:HB3	1:E:470:THR:HB	1.83	0.60
1:C:280:SER:CB	1:C:283:ALA:HB3	2.31	0.60
1:C:378:ARG:CB	1:C:378:ARG:HH21	2.14	0.60
1:C:732:LYS:NZ	1:C:755:GLU:OE1	2.34	0.60
1:D:265:LYS:O	1:D:269:GLU:HG2	2.01	0.60
1:D:424:ILE:CG2	1:D:471:ALA:HB2	2.31	0.60
1:D:557:PHE:O	1:D:561:GLY:HA2	2.02	0.60
1:E:261:ALA:O	1:E:264:THR:HB	2.02	0.60
1:C:388:ALA:HB3	1:C:389:GLU:OE1	2.00	0.60
1:C:526:ALA:HB2	1:C:571:ALA:HB2	1.84	0.60
1:A:643:TYR:CE1	1:A:647:HIS:CD2	2.90	0.59
1:B:494:THR:O	1:B:497:GLU:N	2.36	0.59
1:F:407:HIS:NE2	1:F:411:GLN:OE1	2.35	0.59
1:D:416:ASN:HB3	1:D:464:LYS:HG2	1.82	0.59
1:C:258:MET:CB	1:C:262:VAL:HG11	2.32	0.59
1:F:412:VAL:HG12	1:F:414:VAL:H	1.67	0.59
1:B:374:ARG:NH2	1:B:416:ASN:ND2	2.51	0.59
1:D:537:GLU:HG3	1:D:539:GLY:O	2.02	0.59
1:E:558:TRP:CE3	1:E:563:TRP:CH2	2.82	0.59
1:A:497:GLU:O	1:A:501:ILE:HG22	2.02	0.59
1:B:245:ASP:HB2	1:C:395:ARG:NH2	2.17	0.59
1:B:642:THR:O	1:B:645:ARG:HB2	2.02	0.59
1:D:350:ILE:O	1:D:485:MET:HA	2.01	0.59
1:B:600:LEU:HD23	1:B:721:LYS:O	2.02	0.59
1:C:295:GLU:O	1:C:296:VAL:HG13	2.02	0.59
1:C:396:THR:HG22	1:C:397:TYR:O	2.02	0.59
1:C:416:ASN:N	1:C:417:PRO:HD3	2.18	0.59
1:C:425:ASP:CB	1:C:471:ALA:HB1	2.32	0.59
1:D:386:ASP:OD2	1:D:388:ALA:HB3	2.02	0.59
1:B:378:ARG:NH1	1:B:380:SER:OG	2.34	0.59
1:E:267:LEU:HD13	1:E:268:LYS:CA	2.31	0.59
1:E:345:ARG:HH12	1:E:347:LYS:HD3	1.66	0.59
1:E:537:GLU:OE2	1:E:542:GLY:N	2.30	0.59
1:E:558:TRP:HZ3	1:E:563:TRP:CE2	2.21	0.59
1:E:717:GLY:O	1:E:721:LYS:HG3	2.03	0.59
1:A:252:LYS:O	1:A:255:GLU:HG2	2.02	0.59
1:C:364:LEU:O	1:C:368:ILE:HD12	2.02	0.59
1:D:637:ALA:CB	1:D:683:MET:HE1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:SER:HB3	1:A:664:HIS:ND1	2.18	0.59
1:C:254:GLU:OE1	1:C:263:LYS:NZ	2.36	0.59
1:C:258:MET:CB	1:C:262:VAL:CG1	2.79	0.59
1:C:298:TRP:O	1:C:415:ILE:CG2	2.51	0.59
1:F:422:ASP:OD1	1:F:470:THR:CG2	2.46	0.59
1:F:563:TRP:HB2	1:F:565:GLY:HA3	1.85	0.59
1:E:296:VAL:HG12	1:E:297:PRO:CD	2.31	0.59
1:A:297:PRO:CD	1:A:460:TYR:OH	2.47	0.59
1:B:276:MET:SD	1:B:283:ALA:CB	2.90	0.59
1:C:304:GLU:OE1	1:C:374:ARG:NH2	2.36	0.59
1:C:390:ILE:HD13	1:C:439:MET:N	2.18	0.59
1:C:440:LEU:HD13	1:C:481:LEU:HD22	1.83	0.59
1:C:455:TYR:HE1	1:C:456:LEU:CD2	2.13	0.59
1:C:510:GLN:HA	1:C:510:GLN:NE2	2.18	0.59
1:F:518:GLY:O	1:F:566:LEU:HD23	2.02	0.59
1:D:430:ASP:N	1:D:430:ASP:OD1	2.36	0.59
1:E:429:SER:OG	1:E:430:ASP:N	2.30	0.59
1:A:626:THR:OG1	1:A:664:HIS:NE2	2.35	0.58
1:A:654:PRO:O	1:A:657:PHE:CD1	2.53	0.58
1:E:364:LEU:O	1:E:368:ILE:HG13	2.02	0.58
1:E:385:ARG:HG3	1:E:431:TRP:HE1	1.68	0.58
1:C:295:GLU:HB3	1:C:297:PRO:HG3	1.84	0.58
1:F:706:VAL:O	1:F:706:VAL:HG13	2.04	0.58
1:D:318:ASP:CG	1:D:370:ARG:NH2	2.56	0.58
1:E:287:ARG:CA	1:E:290:LEU:CD1	2.59	0.58
1:C:427:MET:HB2	1:C:428:SER:HA	1.84	0.58
1:E:244:SER:HB2	1:E:247:GLU:HB3	1.85	0.58
1:B:292:TRP:HH2	1:B:407:HIS:CE1	2.20	0.58
1:B:314:VAL:HG13	1:B:370:ARG:NH2	2.19	0.58
1:B:707:SER:O	1:B:710:GLY:N	2.36	0.58
1:C:259:PRO:HG2	1:C:298:TRP:CH2	2.39	0.58
1:C:301:ALA:CB	1:C:415:ILE:HD11	2.32	0.58
1:C:353:LEU:HB2	1:C:470:THR:HG22	1.86	0.58
1:C:518:GLY:O	1:C:566:LEU:HD11	2.04	0.58
1:F:258:MET:HB2	1:F:263:LYS:CD	2.33	0.58
1:F:450:THR:O	1:F:459:PRO:CB	2.51	0.58
1:E:498:LYS:O	1:E:501:ILE:HG13	2.04	0.58
1:E:558:TRP:CE3	1:E:563:TRP:CZ2	2.92	0.58
1:A:262:VAL:HG12	1:A:458:VAL:CG1	2.31	0.58
1:A:511:VAL:O	1:A:515:GLY:N	2.37	0.58
1:B:269:GLU:HA	1:B:272:ARG:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:HIS:CG	1:C:402:PRO:HD3	2.29	0.58
1:C:559:LEU:HD13	1:C:559:LEU:N	2.19	0.58
1:E:249:LEU:O	1:E:253:ILE:HG23	2.03	0.58
1:E:385:ARG:HD2	1:E:428:SER:CB	2.32	0.58
1:C:374:ARG:HD3	1:C:416:ASN:O	2.03	0.58
1:C:393:HIS:CD2	1:C:402:PRO:CB	2.85	0.58
1:C:575:PRO:O	1:C:579:GLY:N	2.31	0.58
1:F:388:ALA:O	1:F:392:GLY:N	2.34	0.58
1:D:589:GLU:HB3	1:D:591:GLU:HG3	1.85	0.58
1:E:312:ARG:NH2	1:E:330:LEU:HD11	2.19	0.58
1:E:345:ARG:NH1	1:E:347:LYS:HD3	2.18	0.58
1:E:393:HIS:CD2	1:E:393:HIS:H	2.20	0.58
1:E:747:PRO:HG2	1:E:750:VAL:HG23	1.85	0.58
1:F:247:GLU:O	1:F:250:ARG:HG2	2.03	0.58
1:F:431:TRP:HA	1:F:432:ARG:C	2.24	0.58
1:E:270:LEU:O	1:E:270:LEU:HD22	2.04	0.58
1:E:420:LEU:C	1:E:421:LEU:HD12	2.23	0.58
1:E:332:TYR:O	1:E:335:VAL:CG1	2.52	0.58
1:E:405:LEU:HD23	1:E:406:ILE:N	2.18	0.58
1:B:534:TYR:CZ	1:B:581:PRO:HA	2.39	0.58
1:E:366:ARG:HA	1:E:376:PHE:CE2	2.39	0.58
1:C:700:ILE:CD1	1:C:768:TYR:CE2	2.86	0.58
1:F:397:TYR:N	1:F:398:ILE:HA	2.18	0.58
1:E:396:THR:OG1	1:E:397:TYR:N	2.37	0.58
1:B:748:LYS:O	1:B:752:GLU:N	2.37	0.57
1:D:430:ASP:HA	1:D:433:GLY:O	2.03	0.57
1:D:449:ASN:HA	1:D:461:ASP:OD1	2.02	0.57
1:E:297:PRO:CB	1:E:413:GLY:O	2.49	0.57
1:E:617:VAL:O	1:E:661:VAL:HG13	2.04	0.57
1:A:710:GLY:O	1:A:762:VAL:HG23	2.04	0.57
1:C:689:SER:HB3	1:C:694:ARG:O	2.04	0.57
1:D:246:LEU:HA	1:D:249:LEU:HB3	1.85	0.57
1:D:342:LEU:HG	1:D:342:LEU:O	2.04	0.57
1:E:449:ASN:HD22	1:E:449:ASN:H	1.52	0.57
1:A:556:LYS:HG3	1:A:557:PHE:N	2.19	0.57
1:C:450:THR:HG21	1:C:461:ASP:H	1.67	0.57
1:E:439:MET:HA	1:E:442:VAL:HG23	1.86	0.57
1:A:318:ASP:CB	1:A:319:HIS:CD2	2.88	0.57
1:A:339:THR:HB	1:A:344:VAL:CG2	2.34	0.57
1:B:279:GLY:O	1:B:280:SER:C	2.43	0.57
1:D:552:ARG:CG	1:E:331:GLU:HB3	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:ALA:CB	1:D:683:MET:CE	2.81	0.57
1:B:341:GLY:N	1:B:342:LEU:HA	2.19	0.57
1:C:392:GLY:HA3	1:C:454:HIS:CB	2.34	0.57
1:C:693:ARG:CD	1:C:776:MET:HB2	2.33	0.57
1:F:667:VAL:HB	1:F:674:LYS:HE3	1.86	0.57
1:E:315:LEU:O	1:E:326:LYS:NZ	2.36	0.57
1:E:531:ILE:O	1:E:535:THR:HB	2.05	0.57
1:E:637:ALA:CB	1:E:683:MET:HE2	2.35	0.57
1:C:393:HIS:HE1	1:C:395:ARG:C	2.07	0.57
1:F:533:GLU:HB3	1:F:581:PRO:HB3	1.86	0.57
1:E:352:VAL:HG13	1:E:487:VAL:HA	1.85	0.57
1:E:385:ARG:HD3	1:E:428:SER:HB3	1.85	0.57
1:E:385:ARG:NH2	1:E:428:SER:HB2	2.20	0.57
1:B:499:GLN:OE1	1:B:528:LEU:HB2	2.04	0.57
1:C:287:ARG:O	1:C:290:LEU:HB2	2.04	0.57
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.17	0.57
1:F:667:VAL:O	1:F:674:LYS:HE3	2.05	0.57
1:E:432:ARG:HG2	1:E:433:GLY:N	2.19	0.57
1:A:356:PRO:O	1:A:359:VAL:HG12	2.05	0.57
1:A:543:LEU:HD12	1:A:543:LEU:O	2.05	0.57
1:C:285:VAL:O	1:C:288:THR:HB	2.04	0.57
1:C:249:LEU:CA	1:C:252:LYS:HE3	2.33	0.57
1:D:588:ALA:HB3	1:D:589:GLU:C	2.25	0.57
1:E:311:THR:O	1:E:315:LEU:CD1	2.51	0.57
1:E:369:ALA:O	1:E:373:ASN:N	2.37	0.57
1:C:260:GLU:OE2	1:C:261:ALA:N	2.37	0.57
1:C:321:GLY:O	1:C:326:LYS:NZ	2.34	0.57
1:D:588:ALA:N	1:D:589:GLU:HA	2.19	0.57
1:E:682:THR:HG22	1:E:702:MET:HB2	1.86	0.57
1:B:425:ASP:OD1	1:B:471:ALA:HB1	2.05	0.56
1:E:414:VAL:HG22	1:E:416:ASN:H	1.70	0.56
1:B:258:MET:SD	1:B:262:VAL:HG23	2.45	0.56
1:B:669:ASP:CG	1:B:672:THR:HG22	2.25	0.56
1:C:243:LEU:HA	1:C:246:LEU:HD13	1.87	0.56
1:C:549:LYS:HA	1:C:552:ARG:CD	2.34	0.56
1:C:617:VAL:HG11	1:D:645:ARG:HB3	1.86	0.56
1:F:381:LEU:HD11	1:F:421:LEU:HB3	1.88	0.56
1:D:402:PRO:HG3	1:D:455:TYR:CD1	2.39	0.56
1:D:733:ILE:HG22	1:D:734:VAL:N	2.19	0.56
1:E:432:ARG:HG2	1:E:433:GLY:H	1.69	0.56
1:B:288:THR:O	1:B:291:ASP:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:MET:HA	1:B:412:VAL:CG1	2.35	0.56
1:C:507:TRP:CE2	1:C:522:VAL:CG2	2.89	0.56
1:F:708:LEU:HD21	1:E:615:ALA:HB2	1.88	0.56
1:D:245:ASP:OD1	1:D:246:LEU:N	2.37	0.56
1:D:300:LYS:O	1:D:415:ILE:HG22	2.05	0.56
1:E:339:THR:OG1	1:E:346:ASN:ND2	2.32	0.56
1:E:392:GLY:O	1:E:454:HIS:CB	2.47	0.56
1:E:392:GLY:CA	1:E:455:TYR:H	2.19	0.56
1:C:265:LYS:C	1:C:267:LEU:H	2.07	0.56
1:E:292:TRP:NE1	1:E:402:PRO:CD	2.58	0.56
1:E:405:LEU:HD23	1:E:406:ILE:HA	1.87	0.56
1:E:458:VAL:HG22	1:E:459:PRO:O	2.05	0.56
1:E:503:ARG:CZ	1:E:524:ASP:OD1	2.54	0.56
1:C:248:ALA:HA	1:C:251:LYS:CG	2.36	0.56
1:C:689:SER:O	1:C:693:ARG:N	2.38	0.56
1:F:311:THR:HG23	1:F:371:SER:OG	2.05	0.56
1:D:332:TYR:CZ	1:D:351:LEU:HD11	2.40	0.56
1:A:689:SER:O	1:A:693:ARG:N	2.31	0.56
1:C:301:ALA:HB2	1:C:415:ILE:HD11	1.87	0.56
1:F:410:LYS:HG3	1:F:411:GLN:N	2.20	0.56
1:D:592:PRO:HB3	1:D:696:ALA:C	2.25	0.56
1:E:366:ARG:CA	1:E:376:PHE:CE2	2.88	0.56
1:A:523:THR:OG1	1:A:570:ASP:CB	2.54	0.56
1:B:273:LEU:HA	1:B:276:MET:HG2	1.88	0.56
1:C:514:SER:HB2	1:C:551:ALA:HB1	1.88	0.56
1:C:526:ALA:HB2	1:C:571:ALA:CA	2.33	0.56
1:F:656:ASP:O	1:F:660:LYS:HD2	2.06	0.56
1:D:318:ASP:OD1	1:D:370:ARG:NH2	2.39	0.56
1:D:434:ASP:OD1	1:D:436:ALA:N	2.39	0.56
1:E:296:VAL:HA	1:E:410:LYS:HD3	1.86	0.56
1:A:306:LEU:O	1:A:337:GLN:CD	2.44	0.56
1:B:590:THR:CG2	1:B:699:ASP:HB3	2.35	0.56
1:D:274:GLU:O	1:D:275:ARG:C	2.42	0.56
1:E:391:ARG:HA	1:E:453:ASP:OD1	2.05	0.56
1:E:478:PRO:C	1:E:480:PRO:HD2	2.26	0.56
1:A:295:GLU:OE1	1:A:295:GLU:HA	2.05	0.56
1:A:392:GLY:O	1:A:454:HIS:HB2	2.06	0.56
1:B:270:LEU:O	1:B:273:LEU:HB3	2.06	0.56
1:B:391:ARG:HD3	1:B:454:HIS:CE1	2.40	0.56
1:C:435:PRO:O	1:C:439:MET:N	2.34	0.56
1:C:507:TRP:CZ2	1:C:522:VAL:CG2	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:PRO:HB3	1:C:697:ARG:HA	1.88	0.56
1:E:284:THR:O	1:E:288:THR:HG23	2.06	0.56
1:A:246:LEU:O	1:A:249:LEU:HB3	2.06	0.56
1:B:289:TYR:CD2	1:B:395:ARG:CD	2.89	0.56
1:B:375:LYS:NZ	1:B:412:VAL:O	2.29	0.56
1:C:258:MET:SD	1:C:262:VAL:CG1	2.91	0.56
1:C:272:ARG:O	1:C:275:ARG:HG2	2.05	0.56
1:F:244:SER:OG	1:F:246:LEU:HB3	2.06	0.56
1:D:765:VAL:HG12	1:D:769:LEU:HD23	1.86	0.56
1:E:447:GLN:HG3	1:E:450:THR:HB	1.87	0.56
1:B:401:MET:O	1:B:455:TYR:CD2	2.58	0.55
1:C:340:GLN:O	1:C:340:GLN:NE2	2.38	0.55
1:C:570:ASP:CG	1:C:571:ALA:N	2.58	0.55
1:F:246:LEU:HD12	1:F:287:ARG:HH22	1.71	0.55
1:F:337:GLN:O	1:F:341:GLY:N	2.38	0.55
1:F:412:VAL:CG1	1:F:414:VAL:HG22	2.34	0.55
1:E:265:LYS:NZ	1:E:268:LYS:HB3	2.20	0.55
1:E:318:ASP:OD1	1:E:318:ASP:N	2.36	0.55
1:E:387:GLU:O	1:E:391:ARG:HD3	2.06	0.55
1:E:405:LEU:O	1:E:409:MET:CB	2.53	0.55
1:E:453:ASP:O	1:E:456:LEU:O	2.23	0.55
1:E:474:LEU:HA	1:E:477:ILE:CD1	2.36	0.55
1:E:558:TRP:O	1:E:558:TRP:HD1	1.85	0.55
1:F:245:ASP:O	1:F:249:LEU:N	2.31	0.55
1:F:325:VAL:O	1:F:329:ILE:HG12	2.06	0.55
1:E:267:LEU:C	1:E:270:LEU:HB3	2.26	0.55
1:E:292:TRP:CE2	1:E:402:PRO:HD2	2.41	0.55
1:E:296:VAL:CG1	1:E:297:PRO:N	2.69	0.55
1:B:273:LEU:HD12	1:B:276:MET:CE	2.36	0.55
1:C:296:VAL:O	1:C:298:TRP:HB2	2.06	0.55
1:F:276:MET:O	1:F:278:GLN:HB3	2.05	0.55
1:F:308:ILE:HG23	1:F:310:HIS:HB3	1.89	0.55
1:F:626:THR:HG22	1:F:627:GLY:N	2.20	0.55
1:D:359:VAL:HG12	1:D:490:ILE:HG22	1.87	0.55
1:E:339:THR:O	1:E:342:LEU:HB3	2.06	0.55
1:B:278:GLN:NE2	1:C:396:THR:HG23	2.22	0.55
1:C:269:GLU:OE2	1:C:272:ARG:NH1	2.39	0.55
1:C:275:ARG:CB	1:C:275:ARG:HH21	2.19	0.55
1:C:414:VAL:CG1	1:C:415:ILE:N	2.69	0.55
1:C:482:LEU:HD12	1:C:482:LEU:O	2.06	0.55
1:D:699:ASP:O	1:D:730:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HD2	1:A:255:GLU:CD	2.27	0.55
1:A:531:ILE:HA	1:A:535:THR:HG21	1.89	0.55
1:A:694:ARG:NH1	1:A:767:GLU:OE1	2.40	0.55
1:C:249:LEU:C	1:C:249:LEU:HD23	2.27	0.55
1:F:246:LEU:HA	1:F:249:LEU:CG	2.36	0.55
1:F:563:TRP:HB2	1:F:565:GLY:C	2.27	0.55
1:E:267:LEU:HD13	1:E:267:LEU:C	2.26	0.55
1:B:669:ASP:OD1	1:B:672:THR:CG2	2.54	0.55
1:F:442:VAL:HB	1:F:443:LEU:HD13	1.89	0.55
1:D:373:ASN:O	1:D:373:ASN:ND2	2.40	0.55
1:E:263:LYS:O	1:E:266:ALA:N	2.39	0.55
1:E:366:ARG:CA	1:E:376:PHE:HE2	2.19	0.55
1:D:318:ASP:OD2	1:D:370:ARG:NH2	2.39	0.55
1:D:540:VAL:HG22	1:D:543:LEU:HB2	1.87	0.55
1:E:385:ARG:NH2	1:E:428:SER:CB	2.69	0.55
1:B:766:LEU:H	1:B:766:LEU:HD12	1.72	0.55
1:C:272:ARG:NE	1:C:273:LEU:HD12	2.22	0.55
1:C:693:ARG:HG3	1:C:776:MET:HB2	1.89	0.55
1:A:389:GLU:HA	1:A:403:GLY:HA2	1.89	0.55
1:A:442:VAL:CG1	1:A:443:LEU:HD12	2.37	0.55
1:C:693:ARG:CG	1:C:776:MET:HB2	2.37	0.55
1:F:437:SER:HA	1:F:440:LEU:HD13	1.89	0.55
1:E:290:LEU:CA	1:E:293:LEU:HD12	2.35	0.55
1:E:440:LEU:HD11	1:E:480:PRO:HB2	1.89	0.55
1:E:474:LEU:O	1:E:477:ILE:HD12	2.07	0.55
1:A:549:LYS:O	1:A:553:LYS:CG	2.54	0.55
1:C:275:ARG:NH2	1:C:275:ARG:HB3	2.22	0.55
1:C:766:LEU:HD23	1:C:770:LEU:HD11	1.89	0.55
1:B:400:ALA:O	1:B:401:MET:HG2	2.07	0.54
1:C:289:TYR:CZ	1:C:293:LEU:HD13	2.42	0.54
1:F:246:LEU:HA	1:F:249:LEU:HG	1.89	0.54
1:F:609:LEU:O	1:F:610:LEU:HG	2.07	0.54
1:E:259:PRO:CD	1:E:298:TRP:CD1	2.81	0.54
1:A:255:GLU:CG	1:A:256:VAL:N	2.70	0.54
1:B:245:ASP:CG	1:C:395:ARG:HH22	2.10	0.54
1:B:546:GLU:HG3	1:B:578:LEU:HD13	1.89	0.54
1:C:272:ARG:HA	1:C:275:ARG:NH1	2.22	0.54
1:C:455:TYR:CD1	1:C:456:LEU:HD13	2.41	0.54
1:F:246:LEU:O	1:F:249:LEU:HG	2.07	0.54
1:D:453:ASP:OD1	1:D:455:TYR:N	2.40	0.54
1:E:450:THR:O	1:E:450:THR:CG2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:LEU:O	1:E:645:ARG:HG3	2.07	0.54
1:B:374:ARG:NH2	1:B:416:ASN:HD21	2.01	0.54
1:C:451:PHE:HD2	1:C:462:LEU:HB3	1.68	0.54
1:F:445:PRO:O	1:F:448:ASN:N	2.40	0.54
1:E:500:ALA:O	1:E:504:GLN:HG2	2.08	0.54
1:B:245:ASP:CB	1:C:395:ARG:HH22	2.21	0.54
1:B:269:GLU:HA	1:B:272:ARG:CG	2.37	0.54
1:B:681:ILE:HG22	1:B:762:VAL:HG23	1.90	0.54
1:C:258:MET:CG	1:C:262:VAL:HG11	2.37	0.54
1:C:293:LEU:HD23	1:C:294:THR:N	2.22	0.54
1:C:407:HIS:CD2	1:C:408:ALA:N	2.75	0.54
1:C:630:GLY:CA	1:C:675:ASP:OD1	2.51	0.54
1:C:680:GLY:C	1:C:706:VAL:HG12	2.28	0.54
1:F:453:ASP:OD1	1:F:455:TYR:N	2.37	0.54
1:E:596:THR:OG1	1:E:698:MET:SD	2.60	0.54
1:A:635:GLU:HB3	1:F:626:THR:HG23	1.89	0.54
1:C:494:THR:HB	1:C:497:GLU:HG3	1.89	0.54
1:C:514:SER:OG	1:C:516:MET:HB2	2.06	0.54
1:A:405:LEU:HD22	1:A:442:VAL:CG2	2.37	0.54
1:A:423:GLN:N	1:A:470:THR:O	2.40	0.54
1:B:637:ALA:HB2	1:B:683:MET:CE	2.38	0.54
1:C:425:ASP:OD2	1:C:471:ALA:HB1	2.07	0.54
1:C:512:ARG:NH1	1:C:517:GLU:HB3	2.21	0.54
1:F:353:LEU:O	1:F:361:LYS:HD2	2.07	0.54
1:D:494:THR:O	1:D:497:GLU:N	2.40	0.54
1:D:580:ILE:HG23	1:D:581:PRO:HD2	1.90	0.54
1:A:440:LEU:HG	1:A:481:LEU:HD23	1.90	0.54
1:A:633:MET:HE2	1:A:683:MET:CE	2.38	0.54
1:B:695:PRO:HD3	1:B:775:THR:CG2	2.37	0.54
1:C:447:GLN:HG2	1:C:451:PHE:HE1	1.70	0.54
1:F:663:LEU:HD21	1:F:691:LEU:HD21	1.88	0.54
1:E:262:VAL:CG1	1:E:458:VAL:HG23	2.37	0.54
1:B:600:LEU:CD2	1:B:721:LYS:HB3	2.35	0.54
1:C:401:MET:CE	1:C:407:HIS:CE1	2.88	0.54
1:C:526:ALA:CB	1:C:571:ALA:HB2	2.38	0.54
1:D:699:ASP:OD1	1:D:699:ASP:N	2.41	0.54
1:C:615:ALA:O	1:C:663:LEU:HD23	2.08	0.54
1:F:527:ILE:O	1:F:530:VAL:HB	2.08	0.54
1:E:391:ARG:HB3	1:E:391:ARG:HH11	1.72	0.54
1:E:449:ASN:HD22	1:E:449:ASN:N	2.06	0.54
1:A:590:THR:O	1:A:591:GLU:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:ALA:HB2	1:B:683:MET:HE1	1.88	0.54
1:D:359:VAL:CG1	1:D:490:ILE:HG22	2.38	0.54
1:D:667:VAL:O	1:D:674:LYS:HE3	2.08	0.54
1:E:394:ARG:O	1:E:455:TYR:CD1	2.61	0.54
1:C:290:LEU:O	1:C:294:THR:N	2.41	0.53
1:F:351:LEU:O	1:F:469:THR:HB	2.08	0.53
1:D:258:MET:CB	1:D:262:VAL:HG21	2.34	0.53
1:E:402:PRO:HB2	1:E:406:ILE:HG21	1.89	0.53
1:A:540:VAL:O	1:A:543:LEU:N	2.40	0.53
1:C:478:PRO:C	1:C:480:PRO:HD2	2.29	0.53
1:C:511:VAL:O	1:C:514:SER:HB3	2.07	0.53
1:C:762:VAL:HG22	1:C:762:VAL:O	2.09	0.53
1:F:315:LEU:HD23	1:F:326:LYS:HD3	1.90	0.53
1:F:697:ARG:NH2	1:F:699:ASP:OD2	2.31	0.53
1:E:247:GLU:O	1:E:250:ARG:HB3	2.08	0.53
1:E:262:VAL:CG1	1:E:458:VAL:CG2	2.86	0.53
1:E:267:LEU:HD22	1:E:267:LEU:C	2.28	0.53
1:E:392:GLY:HA3	1:E:455:TYR:H	1.73	0.53
1:B:669:ASP:OD1	1:B:669:ASP:N	2.36	0.53
1:F:386:ASP:OD2	1:F:388:ALA:CB	2.54	0.53
1:D:601:ALA:HB1	2:D:802:4KZ:O19	2.08	0.53
1:D:750:VAL:O	1:D:753:GLY:N	2.41	0.53
1:E:265:LYS:HE2	1:E:269:GLU:HG3	1.89	0.53
1:E:319:HIS:CD2	1:E:367:SER:HG	2.26	0.53
1:B:245:ASP:CB	1:C:395:ARG:NH2	2.71	0.53
1:C:275:ARG:HH21	1:C:275:ARG:HB3	1.74	0.53
1:C:294:THR:HG23	1:C:295:GLU:OE1	2.08	0.53
1:F:657:PHE:C	1:F:661:VAL:HG12	2.28	0.53
1:E:295:GLU:O	1:E:410:LYS:HE2	2.08	0.53
1:E:388:ALA:HB1	1:E:393:HIS:CA	2.38	0.53
1:E:422:ASP:CB	1:E:470:THR:HB	2.38	0.53
1:E:706:VAL:HG22	1:E:707:SER:O	2.09	0.53
1:C:245:ASP:O	1:C:248:ALA:HB3	2.08	0.53
1:C:305:VAL:HG12	1:C:373:ASN:HB2	1.90	0.53
1:F:309:ASN:OD1	1:F:312:ARG:HD2	2.09	0.53
1:F:589:GLU:HA	1:F:589:GLU:OE2	2.09	0.53
1:E:378:ARG:HG2	1:E:379:ILE:N	2.24	0.53
1:A:311:THR:HG23	1:A:371:SER:HB2	1.88	0.53
1:A:458:VAL:HG12	1:A:459:PRO:CD	2.37	0.53
1:B:767:GLU:OE1	1:B:767:GLU:HA	2.08	0.53
1:C:362:THR:O	1:C:365:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ILE:HD12	1:C:406:ILE:N	2.23	0.53
1:F:516:MET:HE1	1:F:554:GLY:O	2.09	0.53
1:D:244:SER:HB3	1:D:246:LEU:HD21	1.89	0.53
1:D:602:TRP:HA	1:D:607:GLY:HA2	1.90	0.53
1:D:737:LYS:O	1:D:740:GLU:N	2.38	0.53
1:E:267:LEU:O	1:E:270:LEU:HB3	2.08	0.53
1:A:514:SER:OG	1:A:551:ALA:CB	2.56	0.53
1:B:319:HIS:HE1	1:B:363:SER:OG	1.91	0.53
1:B:776:MET:HG3	1:B:777:PRO:HD2	1.89	0.53
1:C:278:GLN:HA	1:C:283:ALA:HB3	1.90	0.53
1:C:289:TYR:CD2	1:C:456:LEU:HD21	2.41	0.53
1:C:362:THR:HG21	1:C:378:ARG:NH2	2.16	0.53
1:C:390:ILE:HD11	1:C:438:ALA:CB	2.38	0.53
1:C:558:TRP:CE3	1:C:563:TRP:CE3	2.96	0.53
1:F:503:ARG:NH2	1:F:522:VAL:O	2.42	0.53
1:F:612:ILE:HD12	1:F:682:THR:HG21	1.91	0.53
1:D:482:LEU:O	1:D:482:LEU:HD23	2.09	0.53
1:D:615:ALA:HB2	1:E:708:LEU:HD21	1.91	0.53
1:E:434:ASP:OD2	1:E:437:SER:N	2.31	0.53
1:E:494:THR:HG23	1:E:497:GLU:HG2	1.91	0.53
1:E:705:GLU:HB3	1:E:713:MET:HB2	1.90	0.53
1:A:678:SER:CB	2:A:801:4KZ:O31	2.56	0.53
1:C:476:THR:O	1:C:476:THR:HG22	2.09	0.53
1:E:253:ILE:O	1:E:256:VAL:HG23	2.09	0.53
1:B:633:MET:O	1:B:636:SER:HB3	2.08	0.53
1:C:307:ASP:OD1	1:C:308:ILE:N	2.42	0.53
1:C:447:GLN:CG	1:C:451:PHE:HE1	2.21	0.53
1:F:326:LYS:O	1:F:330:LEU:HD22	2.09	0.53
1:F:679:ALA:HB2	2:F:802:4KZ:C24	2.39	0.53
1:D:458:VAL:HG12	1:D:459:PRO:O	2.08	0.53
1:D:502:ALA:HA	1:D:506:LEU:HB2	1.91	0.53
1:D:681:ILE:HG13	1:D:682:THR:N	2.24	0.53
1:A:435:PRO:O	1:A:438:ALA:N	2.41	0.53
1:A:633:MET:CE	1:A:683:MET:CE	2.87	0.53
1:A:668:PRO:HA	1:A:669:ASP:C	2.28	0.53
1:B:585:PRO:O	1:B:587:LYS:CD	2.54	0.53
1:B:631:GLU:O	1:B:635:GLU:HG3	2.09	0.53
1:C:262:VAL:CG2	1:C:298:TRP:CZ3	2.89	0.53
1:C:630:GLY:HA3	1:C:675:ASP:CG	2.29	0.53
1:F:745:GLU:OE1	1:E:580:ILE:HD12	2.09	0.53
1:D:369:ALA:O	1:D:374:ARG:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:TYR:OH	1:E:456:LEU:HG	2.09	0.53
1:E:451:PHE:O	1:E:452:THR:HB	2.09	0.53
1:B:697:ARG:NH2	1:B:732:LYS:HE2	2.24	0.52
1:C:355:GLY:HA3	1:C:490:ILE:HG23	1.91	0.52
1:F:503:ARG:NH1	1:F:524:ASP:OD1	2.42	0.52
1:D:472:ASN:N	1:D:472:ASN:OD1	2.42	0.52
1:E:387:GLU:O	1:E:391:ARG:HD2	2.08	0.52
1:E:388:ALA:CA	1:E:391:ARG:O	2.57	0.52
1:A:275:ARG:HD3	1:A:276:MET:N	2.25	0.52
1:C:390:ILE:HG13	1:C:391:ARG:N	2.24	0.52
1:D:351:LEU:O	1:D:469:THR:HB	2.08	0.52
1:D:383:GLY:HA2	1:D:426:LYS:O	2.09	0.52
1:D:663:LEU:HD12	1:D:663:LEU:N	2.25	0.52
1:E:365:GLY:C	1:E:376:PHE:CE2	2.81	0.52
1:C:479:ARG:N	1:C:480:PRO:CD	2.72	0.52
1:C:715:ILE:N	1:C:739:ASN:HD21	2.03	0.52
1:F:258:MET:N	1:F:258:MET:SD	2.82	0.52
1:F:526:ALA:HB2	1:F:570:ASP:HA	1.92	0.52
1:D:250:ARG:O	1:D:254:GLU:HG2	2.09	0.52
1:A:524:ASP:OD1	1:A:525:ALA:N	2.42	0.52
1:C:307:ASP:OD1	1:C:309:ASN:N	2.42	0.52
1:C:454:HIS:CB	1:C:455:TYR:HA	2.11	0.52
1:D:247:GLU:HG2	1:D:248:ALA:N	2.24	0.52
1:E:427:MET:CE	1:E:435:PRO:HG2	2.39	0.52
1:E:582:ARG:O	1:E:583:TYR:CD1	2.63	0.52
1:B:341:GLY:CA	1:B:343:ASP:O	2.53	0.52
1:F:447:GLN:NE2	1:F:451:PHE:CE2	2.77	0.52
1:D:308:ILE:HA	1:D:311:THR:CG2	2.39	0.52
1:E:253:ILE:HG13	1:E:254:GLU:N	2.24	0.52
1:E:332:TYR:O	1:E:335:VAL:HG12	2.09	0.52
1:B:596:THR:OG1	1:B:698:MET:SD	2.59	0.52
1:B:619:GLY:CA	1:B:662:ASP:OD1	2.58	0.52
1:F:396:THR:C	1:F:398:ILE:HA	2.30	0.52
1:E:403:GLY:CA	1:E:407:HIS:CD2	2.93	0.52
1:E:427:MET:HE2	1:E:435:PRO:HG2	1.91	0.52
1:E:439:MET:O	1:E:442:VAL:HB	2.10	0.52
1:A:434:ASP:OD1	1:A:434:ASP:O	2.28	0.52
1:C:246:LEU:HA	1:C:249:LEU:HB3	1.90	0.52
1:C:393:HIS:HD2	1:C:402:PRO:CB	2.23	0.52
1:D:476:THR:HG22	1:D:476:THR:O	2.09	0.52
1:D:479:ARG:N	1:D:480:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:LEU:O	1:E:294:THR:N	2.42	0.52
1:E:342:LEU:C	1:E:342:LEU:HD12	2.30	0.52
1:E:419:ILE:HG22	1:E:421:LEU:CD1	2.40	0.52
1:C:393:HIS:CB	1:C:402:PRO:CD	2.31	0.52
1:F:402:PRO:CA	1:F:453:ASP:OD2	2.57	0.52
1:E:750:VAL:HG12	1:E:754:LEU:HD11	1.92	0.52
1:A:322:LEU:O	1:A:326:LYS:HG3	2.10	0.52
1:E:415:ILE:C	1:E:417:PRO:HD3	2.31	0.52
1:A:519:ARG:O	1:A:563:TRP:HZ2	1.93	0.52
1:A:549:LYS:HB2	1:A:578:LEU:HD23	1.92	0.52
1:B:264:THR:HG22	1:B:265:LYS:N	2.24	0.52
1:B:409:MET:CA	1:B:412:VAL:HG12	2.39	0.52
1:B:683:MET:O	1:B:687:ILE:HG13	2.10	0.52
1:F:393:HIS:O	1:F:454:HIS:C	2.48	0.52
1:F:737:LYS:O	1:F:740:GLU:N	2.42	0.52
1:B:612:ILE:HD12	1:B:682:THR:HG22	1.91	0.51
1:C:243:LEU:O	1:C:246:LEU:N	2.38	0.51
1:C:352:VAL:HG13	1:C:487:VAL:HA	1.92	0.51
1:F:272:ARG:O	1:F:275:ARG:HB2	2.09	0.51
1:F:393:HIS:HB2	1:F:400:ALA:CB	2.40	0.51
1:F:556:LYS:O	1:F:560:GLU:HG3	2.10	0.51
1:E:267:LEU:C	1:E:270:LEU:H	2.14	0.51
1:B:297:PRO:CG	1:B:460:TYR:OH	2.56	0.51
1:C:350:ILE:CG1	1:C:443:LEU:CD1	2.86	0.51
1:C:714:PRO:HB3	1:C:738:ASP:HB2	1.91	0.51
1:A:506:LEU:O	1:A:510:GLN:HG2	2.10	0.51
1:B:277:GLN:HB3	1:B:280:SER:OG	2.09	0.51
1:B:340:GLN:OE1	1:B:340:GLN:HA	2.09	0.51
1:B:344:VAL:O	1:B:344:VAL:HG12	2.10	0.51
1:B:534:TYR:CE1	1:B:581:PRO:HA	2.45	0.51
1:C:289:TYR:HD2	1:C:456:LEU:CG	2.09	0.51
1:C:765:VAL:O	1:C:769:LEU:HB2	2.10	0.51
1:F:596:THR:HG21	1:F:698:MET:HE3	1.92	0.51
1:D:738:ASP:OD1	1:D:738:ASP:N	2.43	0.51
1:E:388:ALA:O	1:E:391:ARG:O	2.29	0.51
1:E:534:TYR:CE2	1:E:580:ILE:O	2.62	0.51
1:A:284:THR:O	1:A:288:THR:HG23	2.09	0.51
1:A:440:LEU:HG	1:A:481:LEU:CD2	2.41	0.51
1:B:600:LEU:HD22	1:B:721:LYS:CB	2.36	0.51
1:C:295:GLU:HB2	1:C:297:PRO:HG3	1.93	0.51
1:F:442:VAL:O	1:F:448:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ARG:N	1:F:480:PRO:CD	2.74	0.51
1:F:619:GLY:CA	1:F:662:ASP:OD1	2.49	0.51
1:D:592:PRO:HG3	1:D:697:ARG:HA	1.91	0.51
1:E:312:ARG:HH21	1:E:330:LEU:HD11	1.74	0.51
1:A:442:VAL:HG12	1:A:443:LEU:HD12	1.92	0.51
1:C:715:ILE:O	1:C:739:ASN:ND2	2.41	0.51
1:F:289:TYR:CE2	1:F:395:ARG:HG3	2.45	0.51
1:D:308:ILE:HA	1:D:311:THR:HG22	1.92	0.51
1:D:569:ILE:HG23	1:D:573:ASP:HB3	1.93	0.51
1:E:391:ARG:HB2	1:E:453:ASP:CA	2.39	0.51
1:E:512:ARG:O	1:E:515:GLY:N	2.40	0.51
1:E:600:LEU:HB3	1:E:721:LYS:HB3	1.92	0.51
1:A:390:ILE:HG21	1:A:438:ALA:HB3	1.91	0.51
1:A:715:ILE:HD12	1:A:715:ILE:C	2.31	0.51
1:C:336:ARG:HA	1:C:339:THR:HG22	1.92	0.51
1:C:405:LEU:O	1:C:408:ALA:HB3	2.11	0.51
1:F:435:PRO:O	1:F:438:ALA:N	2.44	0.51
1:D:369:ALA:HB2	1:D:418:VAL:HB	1.93	0.51
1:E:262:VAL:HG13	1:E:458:VAL:HG23	1.93	0.51
1:E:270:LEU:HD13	1:E:271:ASP:CA	2.40	0.51
1:E:385:ARG:HG3	1:E:431:TRP:NE1	2.25	0.51
1:E:750:VAL:HG12	1:E:754:LEU:CD1	2.40	0.51
1:A:338:LEU:HD21	1:F:516:MET:SD	2.50	0.51
1:C:348:ALA:O	1:C:484:ARG:NH2	2.44	0.51
1:F:574:ILE:O	1:F:577:TYR:N	2.44	0.51
1:D:569:ILE:HG23	1:D:573:ASP:CB	2.41	0.51
1:D:585:PRO:CA	1:D:586:ASP:HB3	2.40	0.51
1:E:384:VAL:C	1:E:385:ARG:HD3	2.31	0.51
1:E:693:ARG:HB2	1:E:774:PRO:HB3	1.93	0.51
1:A:320:TYR:CD1	1:A:321:GLY:N	2.79	0.51
1:A:689:SER:HB2	1:A:694:ARG:O	2.09	0.51
1:C:455:TYR:CE1	1:C:456:LEU:HD21	2.44	0.51
1:C:697:ARG:HG2	1:C:769:LEU:HD13	1.93	0.51
1:E:340:GLN:O	1:E:342:LEU:HD23	2.10	0.51
1:A:390:ILE:HG21	1:A:438:ALA:CB	2.41	0.51
1:A:624:SER:HB3	1:A:664:HIS:CE1	2.45	0.51
1:F:271:ASP:HA	1:F:274:GLU:HG3	1.92	0.51
1:F:523:THR:HB	1:F:569:ILE:O	2.11	0.51
1:A:395:ARG:HD3	1:A:455:TYR:O	2.10	0.51
1:B:654:PRO:O	1:B:657:PHE:HD1	1.93	0.51
1:B:736:PRO:HB2	1:B:739:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ALA:O	1:C:287:ARG:C	2.48	0.51
1:C:653:LEU:CD2	1:C:691:LEU:HB2	2.41	0.51
1:C:654:PRO:O	1:C:657:PHE:HD1	1.95	0.51
1:F:380:SER:HA	1:F:422:ASP:HB3	1.93	0.51
1:F:387:GLU:HA	1:F:435:PRO:HA	1.92	0.51
1:F:387:GLU:HG3	1:F:435:PRO:HA	1.93	0.51
1:F:445:PRO:HA	1:F:448:ASN:HB3	1.92	0.51
1:F:656:ASP:HB2	1:F:660:LYS:NZ	2.25	0.51
1:E:308:ILE:O	1:E:312:ARG:N	2.43	0.51
1:E:525:ALA:O	1:E:528:LEU:HB3	2.11	0.51
1:A:510:GLN:HA	1:A:510:GLN:HE21	1.76	0.50
1:A:553:LYS:HE3	1:A:577:TYR:O	2.10	0.50
1:B:452:THR:HG22	1:B:458:VAL:C	2.31	0.50
1:B:580:ILE:HG23	1:B:581:PRO:HD2	1.93	0.50
1:C:302:ASP:HB2	1:C:414:VAL:HG21	1.92	0.50
1:C:304:GLU:CD	1:C:374:ARG:NH2	2.61	0.50
1:C:404:LYS:O	1:C:407:HIS:N	2.27	0.50
1:C:440:LEU:CB	1:C:481:LEU:CD2	2.77	0.50
1:F:315:LEU:HB3	1:F:326:LYS:HD3	1.94	0.50
1:F:355:GLY:CA	1:F:490:ILE:O	2.59	0.50
1:E:516:MET:HA	1:E:519:ARG:NE	2.26	0.50
1:A:482:LEU:O	1:A:482:LEU:HD23	2.11	0.50
1:A:510:GLN:HA	1:A:510:GLN:NE2	2.27	0.50
1:A:516:MET:HE3	1:A:519:ARG:HB2	1.93	0.50
1:B:421:LEU:N	1:B:468:ILE:O	2.38	0.50
1:C:407:HIS:CD2	1:C:407:HIS:C	2.84	0.50
1:C:424:ILE:HG21	1:C:469:THR:CG2	2.41	0.50
1:F:496:MET:HA	1:F:496:MET:HE2	1.93	0.50
1:D:311:THR:O	1:D:315:LEU:CD1	2.54	0.50
1:D:506:LEU:HD22	1:D:544:GLU:HB2	1.93	0.50
1:E:434:ASP:OD1	1:E:436:ALA:HB3	2.11	0.50
1:E:462:LEU:HD23	1:E:462:LEU:O	2.11	0.50
1:E:544:GLU:O	1:E:548:GLY:N	2.38	0.50
1:A:452:THR:HG22	1:A:459:PRO:CA	2.41	0.50
1:C:388:ALA:HB3	1:C:402:PRO:CG	2.38	0.50
1:F:354:VAL:HA	1:F:471:ALA:O	2.11	0.50
1:F:474:LEU:HD22	1:F:482:LEU:HD11	1.92	0.50
1:D:702:MET:HB2	1:D:734:VAL:HB	1.92	0.50
1:E:381:LEU:O	1:E:384:VAL:HB	2.11	0.50
1:A:402:PRO:HB3	1:A:453:ASP:OD2	2.10	0.50
1:A:534:TYR:CE1	1:A:580:ILE:O	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLU:HB2	1:C:297:PRO:CG	2.42	0.50
1:C:641:LEU:O	1:C:641:LEU:HD12	2.12	0.50
1:E:319:HIS:NE2	1:E:367:SER:OG	2.36	0.50
1:E:462:LEU:CD2	1:E:465:VAL:HG21	2.41	0.50
1:E:385:ARG:CD	1:E:431:TRP:CD1	2.92	0.50
1:E:580:ILE:HG12	1:E:581:PRO:HD2	1.93	0.50
1:E:719:LYS:HA	1:E:746:LEU:HD11	1.93	0.50
1:A:452:THR:HG22	1:A:459:PRO:HA	1.94	0.50
1:C:441:GLU:O	1:C:444:ASP:HB2	2.11	0.50
1:C:598:GLN:OE1	1:C:609:LEU:CD2	2.60	0.50
1:F:361:LYS:N	3:F:801:ADP:O3B	2.45	0.50
1:F:452:THR:CG2	1:F:453:ASP:N	2.74	0.50
1:F:519:ARG:O	1:F:563:TRP:NE1	2.45	0.50
1:E:292:TRP:CZ3	1:E:407:HIS:HA	2.46	0.50
1:E:462:LEU:HG	1:E:465:VAL:HG21	1.93	0.50
1:A:453:ASP:O	1:A:456:LEU:O	2.29	0.50
1:C:249:LEU:O	1:C:252:LYS:HB2	2.11	0.50
1:C:289:TYR:CD1	1:C:289:TYR:C	2.84	0.50
1:F:297:PRO:HG2	1:F:460:TYR:OH	2.12	0.50
1:F:342:LEU:HD23	1:F:342:LEU:O	2.12	0.50
1:F:407:HIS:CD2	1:F:411:GLN:OE1	2.65	0.50
1:F:593:GLN:CB	1:F:596:THR:CG2	2.89	0.50
1:E:621:GLY:N	1:E:661:VAL:O	2.42	0.50
1:E:701:ALA:HB2	1:E:730:ILE:CD1	2.42	0.50
1:A:484:ARG:HG3	1:A:484:ARG:O	2.11	0.50
1:A:712:VAL:HG11	1:A:759:VAL:HG23	1.94	0.50
1:B:307:ASP:HB3	1:B:310:HIS:HB3	1.93	0.50
1:B:397:TYR:O	1:B:399:GLY:N	2.44	0.50
1:C:447:GLN:HG2	1:C:451:PHE:CD1	2.45	0.50
1:C:526:ALA:HB2	1:C:571:ALA:H	1.77	0.50
1:D:687:ILE:O	1:D:691:LEU:HD12	2.12	0.50
1:E:253:ILE:HA	1:E:256:VAL:CG2	2.40	0.50
1:E:295:GLU:O	1:E:410:LYS:CE	2.59	0.50
1:E:350:ILE:O	1:E:485:MET:HB2	2.11	0.50
1:E:530:VAL:CG1	1:E:543:LEU:HD21	2.41	0.50
1:B:350:ILE:HD13	1:B:443:LEU:HD23	1.93	0.50
1:C:693:ARG:HD2	1:C:776:MET:HB2	1.94	0.50
1:F:307:ASP:N	1:F:307:ASP:OD1	2.45	0.50
1:F:323:LYS:O	1:F:327:GLU:HG2	2.12	0.50
1:A:580:ILE:HD11	1:B:741:ALA:C	2.33	0.49
1:B:509:LYS:O	1:B:513:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:TYR:CE1	1:B:659:ASN:HB3	2.46	0.49
1:C:394:ARG:O	1:C:395:ARG:CG	2.56	0.49
1:F:521:GLU:HG3	1:F:522:VAL:N	2.27	0.49
1:F:619:GLY:H	1:F:660:LYS:C	2.14	0.49
1:E:296:VAL:HA	1:E:410:LYS:CD	2.42	0.49
1:A:444:ASP:OD1	1:A:446:GLU:N	2.45	0.49
1:C:386:ASP:OD1	1:C:388:ALA:N	2.41	0.49
1:C:497:GLU:O	1:C:501:ILE:HG22	2.11	0.49
1:C:681:ILE:HG12	1:C:704:GLY:O	2.11	0.49
1:D:308:ILE:O	1:D:311:THR:CG2	2.60	0.49
1:D:314:VAL:O	1:D:317:GLU:N	2.45	0.49
1:E:327:GLU:O	1:E:330:LEU:HB2	2.12	0.49
1:A:275:ARG:HH11	1:A:276:MET:HA	1.77	0.49
1:A:366:ARG:HG3	1:A:376:PHE:CD2	2.47	0.49
1:A:386:ASP:O	1:A:389:GLU:OE2	2.30	0.49
1:A:540:VAL:O	1:A:543:LEU:HB3	2.13	0.49
1:B:620:SER:N	1:B:662:ASP:OD1	2.45	0.49
1:C:401:MET:HE3	1:C:407:HIS:CE1	2.47	0.49
1:C:526:ALA:HB2	1:C:571:ALA:CB	2.41	0.49
1:D:246:LEU:H	1:D:246:LEU:CD2	2.22	0.49
1:D:326:LYS:O	1:D:330:LEU:HD12	2.12	0.49
1:D:649:GLN:OE1	1:D:649:GLN:N	2.46	0.49
1:E:244:SER:HB2	1:E:247:GLU:H	1.77	0.49
1:E:456:LEU:HD23	1:E:458:VAL:CG1	2.43	0.49
1:E:502:ALA:HA	1:E:506:LEU:CB	2.42	0.49
1:E:509:LYS:NZ	1:E:544:GLU:OE2	2.36	0.49
1:A:256:VAL:O	1:A:258:MET:HB2	2.13	0.49
1:B:374:ARG:HE	1:B:416:ASN:ND2	2.10	0.49
1:C:441:GLU:CA	1:C:444:ASP:OD1	2.57	0.49
1:F:518:GLY:O	1:F:566:LEU:CD2	2.60	0.49
1:E:311:THR:CG2	1:E:371:SER:OG	2.57	0.49
1:B:297:PRO:C	1:B:460:TYR:HH	2.15	0.49
1:F:362:THR:N	3:F:801:ADP:O3B	2.40	0.49
1:E:338:LEU:O	1:E:340:GLN:NE2	2.45	0.49
1:E:341:GLY:O	1:E:342:LEU:HG	2.12	0.49
1:A:678:SER:O	1:A:704:GLY:N	2.39	0.49
1:C:296:VAL:O	1:C:296:VAL:HG22	2.13	0.49
1:C:392:GLY:CA	1:C:454:HIS:CB	2.91	0.49
1:C:490:ILE:HG23	1:C:490:ILE:O	2.12	0.49
1:D:650:ASP:OD1	1:D:650:ASP:N	2.42	0.49
1:D:762:VAL:CG1	1:D:763:GLY:N	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:O	1:E:336:ARG:CB	2.61	0.49
1:E:554:GLY:O	1:E:557:PHE:HB2	2.12	0.49
1:A:386:ASP:CB	1:A:432:ARG:HB3	2.41	0.49
1:A:559:LEU:HD21	1:B:338:LEU:HD22	1.94	0.49
1:B:491:PRO:HB3	1:B:719:LYS:HD2	1.95	0.49
1:B:747:PRO:O	1:B:750:VAL:HB	2.13	0.49
1:E:250:ARG:HA	1:E:253:ILE:HG12	1.93	0.49
1:E:374:ARG:NH1	1:E:416:ASN:O	2.46	0.49
1:E:554:GLY:O	1:E:558:TRP:N	2.43	0.49
1:E:555:ALA:O	1:E:559:LEU:HB2	2.13	0.49
1:E:558:TRP:CH2	1:E:563:TRP:O	2.65	0.49
1:A:331:GLU:HB3	1:F:552:ARG:HB3	1.94	0.49
1:A:350:ILE:HD11	1:A:443:LEU:HD23	1.89	0.49
1:A:529:ARG:CD	1:A:571:ALA:HB1	2.42	0.49
1:A:695:PRO:HG2	1:A:771:LEU:HD22	1.95	0.49
1:C:409:MET:O	1:C:410:LYS:C	2.51	0.49
1:C:577:TYR:HB2	1:C:578:LEU:HD13	1.95	0.49
1:C:650:ASP:N	1:C:650:ASP:OD1	2.45	0.49
1:E:402:PRO:CD	1:E:455:TYR:HD2	2.07	0.49
1:E:556:LYS:O	1:E:560:GLU:CB	2.61	0.49
1:A:570:ASP:OD1	1:A:571:ALA:N	2.41	0.49
1:B:658:TYR:CE1	1:B:659:ASN:ND2	2.81	0.49
1:B:678:SER:O	1:B:704:GLY:N	2.45	0.49
1:C:268:LYS:O	1:C:271:ASP:N	2.44	0.49
1:C:374:ARG:HD2	1:C:418:VAL:HG23	1.95	0.49
1:C:442:VAL:HG23	1:C:443:LEU:HD22	1.94	0.49
1:F:418:VAL:HG22	1:F:466:PHE:HD2	1.78	0.49
1:D:244:SER:O	1:D:247:GLU:N	2.43	0.49
1:D:580:ILE:H	1:D:580:ILE:HD12	1.77	0.49
1:D:681:ILE:CG2	1:D:712:VAL:HG22	2.42	0.49
1:E:245:ASP:O	1:E:248:ALA:HB3	2.12	0.49
1:E:302:ASP:C	1:E:302:ASP:OD1	2.51	0.49
1:E:366:ARG:HG3	1:E:376:PHE:CD2	2.48	0.49
1:E:420:LEU:O	1:E:421:LEU:HD12	2.12	0.49
1:A:381:LEU:HD13	1:A:427:MET:CE	2.43	0.49
1:C:390:ILE:HD13	1:C:438:ALA:C	2.29	0.49
1:C:679:ALA:O	1:C:680:GLY:C	2.51	0.49
1:F:563:TRP:N	1:F:563:TRP:CE3	2.80	0.49
1:D:589:GLU:HA	1:D:589:GLU:OE1	2.12	0.49
1:E:534:TYR:HE2	1:E:580:ILE:H	1.60	0.49
1:E:558:TRP:CZ3	1:E:563:TRP:CD2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ASP:HA	1:B:432:ARG:HG2	1.95	0.48
1:B:430:ASP:C	1:B:432:ARG:HA	2.33	0.48
1:C:472:ASN:OD1	1:C:472:ASN:N	2.45	0.48
1:C:526:ALA:HB1	1:C:571:ALA:N	2.19	0.48
1:C:726:HIS:CD2	1:C:731:HIS:CE1	3.00	0.48
1:A:345:ARG:CA	1:A:348:ALA:HB2	2.33	0.48
1:A:350:ILE:O	1:A:485:MET:HA	2.13	0.48
1:A:598:GLN:CG	1:A:609:LEU:HD13	2.43	0.48
1:C:406:ILE:CD1	1:C:406:ILE:H	2.26	0.48
1:C:558:TRP:HE3	1:C:563:TRP:CE3	2.31	0.48
1:F:315:LEU:HD23	1:F:326:LYS:CD	2.42	0.48
1:F:318:ASP:OD2	1:F:367:SER:HB2	2.12	0.48
1:D:531:ILE:CG1	1:D:543:LEU:HD11	2.38	0.48
1:E:312:ARG:HH21	1:E:312:ARG:HG3	1.78	0.48
1:B:451:PHE:O	1:B:459:PRO:HA	2.13	0.48
1:C:272:ARG:HE	1:C:273:LEU:CD1	2.26	0.48
1:F:246:LEU:C	1:F:249:LEU:HG	2.32	0.48
1:F:258:MET:HB2	1:F:263:LYS:HD2	1.94	0.48
1:F:292:TRP:O	1:F:296:VAL:CG2	2.60	0.48
1:F:522:VAL:HG22	1:F:526:ALA:HB3	1.95	0.48
1:A:531:ILE:O	1:A:535:THR:HG23	2.13	0.48
1:E:405:LEU:HD23	1:E:406:ILE:CA	2.43	0.48
1:E:425:ASP:OD1	1:E:426:LYS:N	2.46	0.48
1:E:506:LEU:HD11	1:E:540:VAL:HG13	1.94	0.48
1:A:451:PHE:O	1:A:460:TYR:N	2.40	0.48
1:A:715:ILE:HD12	1:A:716:GLY:N	2.29	0.48
1:B:456:LEU:O	1:B:458:VAL:HG23	2.13	0.48
1:B:553:LYS:O	1:B:556:LYS:HB3	2.14	0.48
1:C:292:TRP:CZ3	1:C:455:TYR:CD1	3.02	0.48
1:C:378:ARG:HH21	1:C:378:ARG:CG	2.26	0.48
1:C:452:THR:O	1:C:453:ASP:OD1	2.32	0.48
1:C:511:VAL:CG1	1:C:517:GLU:HA	2.43	0.48
1:C:750:VAL:O	1:C:753:GLY:N	2.47	0.48
1:F:412:VAL:HG11	1:F:417:PRO:CG	2.35	0.48
1:D:444:ASP:HB3	1:D:447:GLN:HB3	1.95	0.48
1:E:516:MET:C	1:E:519:ARG:HG3	2.34	0.48
1:B:442:VAL:HG23	1:B:443:LEU:CD1	2.43	0.48
1:B:479:ARG:N	1:B:480:PRO:CD	2.75	0.48
1:C:272:ARG:NH1	1:C:286:ALA:HB1	2.27	0.48
1:C:401:MET:HB2	1:C:402:PRO:HA	1.95	0.48
1:C:479:ARG:N	1:C:480:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLU:O	1:E:410:LYS:CD	2.61	0.48
1:C:259:PRO:HD2	1:C:262:VAL:HG11	1.94	0.48
1:F:300:LYS:HG3	1:F:300:LYS:O	2.13	0.48
1:F:581:PRO:O	1:F:582:ARG:HD3	2.13	0.48
1:E:386:ASP:HB3	1:E:389:GLU:H	1.78	0.48
1:A:386:ASP:O	1:A:388:ALA:N	2.47	0.48
1:A:595:GLY:N	1:A:689:SER:HG	2.10	0.48
1:B:356:PRO:O	1:B:359:VAL:HG22	2.14	0.48
1:B:430:ASP:CG	1:B:432:ARG:HG3	2.34	0.48
1:B:510:GLN:O	1:B:513:GLU:N	2.46	0.48
1:C:392:GLY:C	1:C:454:HIS:CB	2.62	0.48
1:F:386:ASP:CG	1:F:388:ALA:HB3	2.34	0.48
1:F:394:ARG:HD3	1:F:397:TYR:CG	2.49	0.48
1:F:669:ASP:OD2	1:F:672:THR:OG1	2.22	0.48
1:D:253:ILE:O	1:D:253:ILE:HD13	2.14	0.48
1:E:494:THR:O	1:E:497:GLU:HG2	2.13	0.48
1:E:748:LYS:O	1:E:751:LEU:N	2.46	0.48
1:A:336:ARG:O	1:A:337:GLN:C	2.52	0.48
1:A:386:ASP:C	1:A:388:ALA:H	2.16	0.48
1:C:290:LEU:O	1:C:294:THR:HG22	2.14	0.48
1:C:409:MET:O	1:C:412:VAL:HB	2.14	0.48
1:D:332:TYR:CE1	1:D:351:LEU:CD1	2.97	0.48
1:D:383:GLY:CA	1:D:426:LYS:O	2.62	0.48
1:E:319:HIS:CE1	1:E:364:LEU:HD23	2.49	0.48
1:B:642:THR:O	1:B:645:ARG:N	2.46	0.48
1:B:681:ILE:HD13	1:B:704:GLY:HA3	1.95	0.48
1:C:390:ILE:HD11	1:C:438:ALA:O	2.13	0.48
1:C:450:THR:HG23	1:C:462:LEU:HB3	1.95	0.48
1:D:436:ALA:O	1:D:439:MET:HB2	2.14	0.48
1:E:256:VAL:CG2	1:E:263:LYS:HE2	2.38	0.48
1:E:300:LYS:O	1:E:414:VAL:HG23	2.13	0.48
1:E:319:HIS:C	1:E:326:LYS:HZ1	2.14	0.48
1:E:352:VAL:O	1:E:353:LEU:HD23	2.14	0.48
1:D:324:ASP:O	1:D:327:GLU:HG2	2.14	0.47
1:D:382:GLY:HA2	1:D:426:LYS:HB2	1.96	0.47
1:D:559:LEU:HD11	1:E:334:ALA:HB1	1.96	0.47
1:E:643:TYR:CE2	1:E:762:VAL:CG1	2.94	0.47
1:A:479:ARG:N	1:A:480:PRO:CD	2.77	0.47
1:D:253:ILE:HG12	1:D:258:MET:HE1	1.96	0.47
1:D:400:ALA:O	1:D:401:MET:SD	2.72	0.47
1:A:516:MET:CE	1:A:519:ARG:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLU:OE1	1:A:589:GLU:HA	2.13	0.47
1:C:412:VAL:HG11	1:C:417:PRO:CG	2.45	0.47
1:C:516:MET:N	1:C:517:GLU:OE2	2.48	0.47
1:F:450:THR:O	1:F:459:PRO:CA	2.62	0.47
1:F:587:LYS:CG	1:F:588:ALA:O	2.58	0.47
1:F:748:LYS:O	1:F:752:GLU:HG2	2.14	0.47
1:D:297:PRO:HD3	1:D:409:MET:O	2.14	0.47
1:D:416:ASN:HB3	1:D:464:LYS:CG	2.44	0.47
1:D:678:SER:O	1:D:704:GLY:O	2.32	0.47
1:E:333:LEU:O	1:E:336:ARG:N	2.47	0.47
1:A:545:ARG:O	1:A:546:GLU:C	2.51	0.47
1:C:350:ILE:HD13	1:C:443:LEU:CD1	2.44	0.47
1:C:393:HIS:HD2	1:C:402:PRO:HA	1.79	0.47
1:F:452:THR:OG1	1:F:459:PRO:CA	2.57	0.47
1:D:424:ILE:CG2	1:D:470:THR:O	2.54	0.47
1:E:349:PRO:C	1:E:350:ILE:HD12	2.35	0.47
1:A:273:LEU:HD12	1:A:273:LEU:O	2.14	0.47
1:B:273:LEU:HD12	1:B:276:MET:SD	2.55	0.47
1:C:259:PRO:HB2	1:C:262:VAL:HB	1.96	0.47
1:C:431:TRP:CE3	1:C:431:TRP:HA	2.50	0.47
1:F:368:ILE:O	1:F:371:SER:HB2	2.14	0.47
1:D:339:THR:O	1:D:342:LEU:HB3	2.15	0.47
1:A:523:THR:HB	1:A:526:ALA:CB	2.44	0.47
1:A:717:GLY:O	1:A:721:LYS:HG3	2.15	0.47
1:D:601:ALA:HB2	2:D:802:4KZ:C25	2.45	0.47
1:E:643:TYR:HE2	1:E:762:VAL:HG11	1.74	0.47
1:A:310:HIS:O	1:A:314:VAL:HG23	2.15	0.47
1:A:406:ILE:HD12	1:A:406:ILE:N	2.30	0.47
1:A:718:VAL:HG11	1:A:742:GLN:HB2	1.97	0.47
1:B:590:THR:HG21	1:B:699:ASP:HB3	1.95	0.47
1:B:701:ALA:HB2	1:B:730:ILE:HG21	1.97	0.47
1:C:305:VAL:O	1:C:305:VAL:HG13	2.15	0.47
1:C:379:ILE:HB	1:C:421:LEU:HD23	1.96	0.47
1:C:395:ARG:HD3	1:C:397:TYR:CD1	2.50	0.47
1:C:401:MET:CB	1:C:402:PRO:HA	2.45	0.47
1:C:406:ILE:N	1:C:406:ILE:CD1	2.77	0.47
1:F:309:ASN:O	1:F:312:ARG:N	2.45	0.47
1:F:641:LEU:O	1:F:645:ARG:HG3	2.14	0.47
1:D:425:ASP:HB2	1:D:476:THR:HB	1.95	0.47
1:E:265:LYS:HZ1	1:E:268:LYS:HB3	1.79	0.47
1:E:406:ILE:HG12	1:E:453:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:LYS:O	1:E:410:LYS:HE3	2.15	0.47
1:E:508:PRO:O	1:E:511:VAL:HB	2.14	0.47
1:B:363:SER:O	1:B:366:ARG:HB2	2.14	0.47
1:C:302:ASP:HB3	1:C:414:VAL:HG11	1.95	0.47
1:C:526:ALA:CB	1:C:571:ALA:CB	2.93	0.47
1:D:416:ASN:CB	1:D:464:LYS:CG	2.93	0.47
1:D:493:TYR:O	1:D:727:GLN:NE2	2.48	0.47
1:B:619:GLY:O	1:B:660:LYS:O	2.33	0.47
1:B:746:LEU:HD12	1:B:751:LEU:CD2	2.39	0.47
1:E:397:TYR:O	1:E:398:ILE:HD13	2.15	0.47
1:A:584:ARG:HE	1:A:584:ARG:HB3	1.58	0.47
1:B:325:VAL:HG13	1:B:488:ILE:HG21	1.96	0.47
1:B:658:TYR:CD1	1:B:659:ASN:HB3	2.49	0.47
1:D:523:THR:CG2	1:D:570:ASP:OD1	2.63	0.47
1:D:584:ARG:N	1:D:585:PRO:CD	2.78	0.47
1:A:416:ASN:N	1:A:417:PRO:HD3	2.29	0.46
1:B:273:LEU:O	1:B:276:MET:CG	2.62	0.46
1:B:710:GLY:O	1:B:762:VAL:HG12	2.15	0.46
1:C:556:LYS:C	1:C:559:LEU:HD22	2.28	0.46
1:F:619:GLY:N	1:F:660:LYS:O	2.39	0.46
1:D:397:TYR:O	1:D:400:ALA:HB2	2.14	0.46
1:D:424:ILE:HG22	1:D:471:ALA:HB2	1.96	0.46
1:D:451:PHE:O	1:D:460:TYR:N	2.40	0.46
1:E:406:ILE:HG23	1:E:407:HIS:N	2.30	0.46
1:E:516:MET:HA	1:E:519:ARG:HE	1.79	0.46
1:E:679:ALA:O	1:E:680:GLY:C	2.52	0.46
1:A:526:ALA:HB2	1:A:571:ALA:H	1.80	0.46
1:A:526:ALA:CB	1:A:570:ASP:HA	2.45	0.46
1:C:378:ARG:O	1:C:378:ARG:HG3	2.14	0.46
1:C:401:MET:CB	1:C:402:PRO:CA	2.93	0.46
1:F:393:HIS:O	1:F:454:HIS:CB	2.63	0.46
1:D:297:PRO:CD	1:D:409:MET:O	2.64	0.46
1:D:314:VAL:O	1:D:317:GLU:HB3	2.15	0.46
1:E:510:GLN:OE1	1:E:510:GLN:HA	2.15	0.46
1:E:559:LEU:HD12	1:E:559:LEU:HA	1.79	0.46
1:A:343:ASP:HB3	1:A:346:ASN:HB3	1.96	0.46
1:A:478:PRO:CB	1:A:480:PRO:HD2	2.45	0.46
1:C:380:SER:O	1:C:381:LEU:HD12	2.16	0.46
1:C:393:HIS:HB2	1:C:402:PRO:HD3	0.54	0.46
1:F:249:LEU:HD12	1:F:249:LEU:C	2.34	0.46
1:D:580:ILE:CG2	1:D:581:PRO:HD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:TYR:C	1:D:585:PRO:HD2	2.36	0.46
1:D:733:ILE:HG22	1:D:734:VAL:H	1.81	0.46
1:E:252:LYS:O	1:E:256:VAL:HG22	2.16	0.46
1:E:377:HIS:CE1	1:E:408:ALA:HB1	2.49	0.46
1:A:256:VAL:HG22	1:A:257:GLY:N	2.30	0.46
1:A:523:THR:O	1:A:526:ALA:N	2.48	0.46
1:A:677:PRO:O	1:A:705:GLU:HA	2.16	0.46
1:B:298:TRP:H	1:B:298:TRP:HD1	1.60	0.46
1:B:630:GLY:O	1:B:633:MET:N	2.48	0.46
1:F:308:ILE:HG12	1:F:310:HIS:H	1.80	0.46
1:D:506:LEU:CD2	1:D:544:GLU:OE1	2.63	0.46
1:E:336:ARG:HH21	1:E:336:ARG:CG	2.29	0.46
1:E:558:TRP:CE3	1:E:563:TRP:CE2	3.04	0.46
1:A:335:VAL:O	1:A:336:ARG:C	2.53	0.46
1:A:643:TYR:O	1:A:646:ALA:HB3	2.15	0.46
1:B:391:ARG:CA	1:B:453:ASP:HB2	2.43	0.46
1:B:658:TYR:CD1	1:B:658:TYR:C	2.89	0.46
1:F:445:PRO:HA	1:F:448:ASN:CB	2.45	0.46
1:F:668:PRO:HA	1:F:669:ASP:C	2.36	0.46
1:F:675:ASP:OD1	1:F:676:GLY:N	2.48	0.46
1:D:308:ILE:O	1:D:311:THR:HG23	2.16	0.46
1:D:588:ALA:N	1:D:589:GLU:CA	2.79	0.46
1:E:336:ARG:O	1:E:339:THR:HG23	2.16	0.46
1:E:512:ARG:HG3	1:E:513:GLU:N	2.30	0.46
1:C:246:LEU:CA	1:C:249:LEU:HB3	2.45	0.46
1:C:268:LYS:O	1:C:271:ASP:HB2	2.15	0.46
1:C:340:GLN:HE21	1:C:340:GLN:CA	2.26	0.46
1:C:350:ILE:HG21	1:C:443:LEU:CD1	2.46	0.46
1:C:609:LEU:HD12	1:C:728:ALA:CB	2.46	0.46
1:F:258:MET:HB2	1:F:263:LYS:HG2	1.98	0.46
1:D:332:TYR:CZ	1:D:351:LEU:HD12	2.50	0.46
1:D:495:ASN:HD21	1:D:727:GLN:HA	1.81	0.46
1:E:267:LEU:HD13	1:E:268:LYS:HA	1.98	0.46
1:E:382:GLY:N	1:E:423:GLN:O	2.49	0.46
1:A:381:LEU:HB3	1:A:427:MET:HE3	1.97	0.46
1:A:741:ALA:HA	1:F:580:ILE:HB	1.98	0.46
1:B:325:VAL:HG13	1:B:488:ILE:CG2	2.46	0.46
1:B:666:HIS:HB2	1:C:708:LEU:HD13	1.97	0.46
1:C:386:ASP:O	1:C:435:PRO:CG	2.57	0.46
1:C:450:THR:CG2	1:C:462:LEU:H	2.27	0.46
1:C:479:ARG:HG2	1:C:479:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:612:ILE:HD12	1:F:682:THR:CG2	2.45	0.46
1:F:657:PHE:O	1:F:660:LYS:N	2.47	0.46
1:E:315:LEU:C	1:E:326:LYS:HZ2	2.19	0.46
1:E:707:SER:OG	1:E:711:LYS:HB2	2.16	0.46
1:A:257:GLY:HA2	1:A:298:TRP:HB2	1.97	0.46
1:B:494:THR:OG1	1:B:726:HIS:CE1	2.67	0.46
1:C:667:VAL:O	1:C:674:LYS:HE2	2.16	0.46
1:F:277:GLN:HG3	1:F:280:SER:CB	2.46	0.46
1:F:412:VAL:CG1	1:F:414:VAL:H	2.29	0.46
1:D:439:MET:O	1:D:442:VAL:HB	2.16	0.46
1:E:336:ARG:HH21	1:E:336:ARG:HG3	1.81	0.46
1:E:366:ARG:N	1:E:376:PHE:CE2	2.69	0.46
1:E:462:LEU:O	1:E:465:VAL:HG23	2.16	0.46
1:E:534:TYR:HE2	1:E:579:GLY:HA2	1.80	0.46
1:E:556:LYS:HG3	1:E:557:PHE:N	2.29	0.46
1:B:278:GLN:HA	1:B:283:ALA:CB	2.46	0.46
1:B:389:GLU:OE1	1:B:404:LYS:NZ	2.38	0.46
1:B:609:LEU:HD11	1:B:725:ALA:HA	1.98	0.46
1:C:256:VAL:O	1:C:258:MET:HG3	2.16	0.46
1:C:258:MET:CG	1:C:262:VAL:CG1	2.94	0.46
1:F:272:ARG:O	1:F:276:MET:HG2	2.16	0.46
1:F:593:GLN:CB	1:F:596:THR:HG21	2.46	0.46
1:D:307:ASP:OD1	1:D:309:ASN:OD1	2.33	0.46
1:D:332:TYR:CD1	1:D:351:LEU:HD11	2.51	0.46
1:E:289:TYR:CZ	1:E:456:LEU:HG	2.49	0.46
1:E:390:ILE:HG22	1:E:390:ILE:O	2.16	0.46
1:B:374:ARG:NE	1:B:416:ASN:ND2	2.63	0.46
1:C:268:LYS:NZ	1:C:271:ASP:OD2	2.38	0.46
1:C:351:LEU:O	1:C:469:THR:HB	2.16	0.46
1:C:366:ARG:O	1:C:369:ALA:HB3	2.16	0.46
1:D:651:TYR:OH	1:D:763:GLY:CA	2.55	0.46
1:E:292:TRP:CH2	1:E:407:HIS:HB2	2.36	0.46
1:B:430:ASP:OD1	1:B:432:ARG:HG3	2.16	0.45
1:C:380:SER:C	1:C:381:LEU:HD12	2.35	0.45
1:C:395:ARG:HD3	1:C:397:TYR:HD1	1.81	0.45
1:C:406:ILE:HA	1:C:409:MET:HB2	1.98	0.45
1:F:356:PRO:O	1:F:359:VAL:HG22	2.16	0.45
1:D:275:ARG:O	1:D:276:MET:C	2.52	0.45
1:D:503:ARG:CZ	1:D:524:ASP:OD1	2.63	0.45
1:D:523:THR:HG21	1:D:570:ASP:OD1	2.15	0.45
1:E:289:TYR:O	1:E:293:LEU:HD12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:ARG:CZ	1:E:428:SER:HB2	2.45	0.45
1:A:421:LEU:HD12	1:A:469:THR:HG22	1.98	0.45
1:B:695:PRO:HD3	1:B:775:THR:HG23	1.98	0.45
1:C:246:LEU:HA	1:C:249:LEU:CB	2.47	0.45
1:C:574:ILE:N	1:C:575:PRO:CD	2.80	0.45
1:F:277:GLN:HG3	1:F:280:SER:OG	2.16	0.45
1:E:282:GLU:N	1:E:282:GLU:OE2	2.49	0.45
1:E:501:ILE:HD12	1:E:501:ILE:C	2.36	0.45
1:B:625:LEU:HB3	1:B:629:LEU:HD12	1.98	0.45
1:C:296:VAL:O	1:C:296:VAL:CG2	2.65	0.45
1:F:338:LEU:O	1:F:341:GLY:N	2.48	0.45
1:F:532:SER:HB2	1:F:585:PRO:HB3	1.98	0.45
1:D:327:GLU:HA	1:D:330:LEU:HD12	1.97	0.45
1:D:430:ASP:CG	1:D:434:ASP:HA	2.37	0.45
1:D:523:THR:HG22	1:D:525:ALA:H	1.80	0.45
1:E:386:ASP:CB	1:E:389:GLU:HB2	2.46	0.45
1:E:401:MET:O	1:E:455:TYR:HB2	2.16	0.45
1:E:558:TRP:O	1:E:558:TRP:CG	2.65	0.45
1:C:298:TRP:CD1	1:C:298:TRP:C	2.89	0.45
1:C:414:VAL:O	1:C:417:PRO:HD3	2.16	0.45
1:A:319:HIS:O	1:A:326:LYS:NZ	2.33	0.45
1:A:375:LYS:HB2	1:A:417:PRO:HB3	1.99	0.45
1:B:350:ILE:CD1	1:B:443:LEU:HD23	2.47	0.45
1:B:432:ARG:NH2	1:B:432:ARG:HB3	2.31	0.45
1:C:425:ASP:OD2	1:C:472:ASN:N	2.47	0.45
1:C:558:TRP:O	1:C:562:ALA:HB2	2.17	0.45
1:D:293:LEU:HD23	1:D:293:LEU:C	2.36	0.45
1:E:406:ILE:HG23	1:E:407:HIS:H	1.82	0.45
1:A:339:THR:HB	1:A:344:VAL:HG21	1.99	0.45
1:A:429:SER:HB3	1:A:434:ASP:HA	1.99	0.45
1:A:507:TRP:HB3	1:A:508:PRO:HD3	1.99	0.45
1:A:677:PRO:HG3	1:F:671:ALA:HB2	1.98	0.45
1:C:309:ASN:N	1:C:309:ASN:HD22	2.13	0.45
1:C:596:THR:HG23	1:C:613:GLU:HB3	1.98	0.45
1:F:289:TYR:O	1:F:290:LEU:C	2.54	0.45
1:F:402:PRO:CB	1:F:453:ASP:OD2	2.64	0.45
1:F:449:ASN:OD1	1:F:449:ASN:N	2.41	0.45
1:D:559:LEU:CD1	1:E:334:ALA:HB1	2.47	0.45
1:D:681:ILE:CG1	1:D:682:THR:N	2.80	0.45
1:E:779:VAL:O	1:E:780:VAL:HB	2.16	0.45
1:A:375:LYS:O	1:A:418:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:HB2	1:A:432:ARG:HG3	1.98	0.45
1:B:390:ILE:HG23	1:B:405:LEU:HD13	1.99	0.45
1:B:523:THR:HG22	1:B:526:ALA:HB2	1.99	0.45
1:C:312:ARG:NH2	1:C:327:GLU:OE2	2.50	0.45
1:C:460:TYR:HD1	1:C:460:TYR:O	2.00	0.45
1:C:766:LEU:CD2	1:C:770:LEU:HD11	2.47	0.45
1:F:246:LEU:CA	1:F:249:LEU:HG	2.46	0.45
1:F:354:VAL:CG2	1:F:489:GLU:HG2	2.47	0.45
1:F:424:ILE:HG22	1:F:471:ALA:HB2	1.98	0.45
1:D:261:ALA:O	1:D:264:THR:OG1	2.29	0.45
1:E:296:VAL:HG13	1:E:410:LYS:HB2	1.99	0.45
1:E:375:LYS:HD3	1:E:412:VAL:HB	1.99	0.45
1:E:392:GLY:HA3	1:E:455:TYR:N	2.31	0.45
1:A:531:ILE:HA	1:A:535:THR:HG22	1.93	0.45
1:B:319:HIS:CD2	1:B:364:LEU:HD23	2.52	0.45
1:B:439:MET:O	1:B:442:VAL:HG22	2.17	0.45
1:C:393:HIS:HD2	1:C:402:PRO:HB3	1.71	0.45
1:C:440:LEU:HD22	1:C:481:LEU:HD23	1.98	0.45
1:C:521:GLU:N	1:C:567:ARG:O	2.47	0.45
1:C:653:LEU:HD22	1:C:691:LEU:HB2	1.98	0.45
1:F:439:MET:O	1:F:443:LEU:N	2.45	0.45
1:F:558:TRP:O	1:F:561:GLY:O	2.34	0.45
1:E:451:PHE:CD1	1:E:452:THR:CA	3.00	0.45
1:E:558:TRP:CE3	1:E:563:TRP:CE3	3.04	0.45
1:A:401:MET:HB2	1:A:402:PRO:CD	2.47	0.45
1:A:653:LEU:CD2	1:A:692:SER:OG	2.65	0.45
1:B:757:LYS:C	1:B:758:LEU:HD23	2.37	0.45
1:C:439:MET:SD	1:C:442:VAL:CG2	3.04	0.45
1:C:612:ILE:HD13	1:C:682:THR:HG21	1.99	0.45
1:F:258:MET:HB2	1:F:263:LYS:CG	2.47	0.45
1:F:478:PRO:O	1:F:481:LEU:N	2.49	0.45
1:D:558:TRP:C	1:D:561:GLY:HA3	2.38	0.45
1:E:272:ARG:O	1:E:276:MET:HG2	2.17	0.45
1:A:429:SER:OG	1:A:434:ASP:HB2	2.17	0.45
1:B:297:PRO:CD	1:B:460:TYR:OH	2.65	0.45
1:B:342:LEU:C	1:B:342:LEU:HD13	2.37	0.45
1:C:456:LEU:N	1:C:456:LEU:CD1	2.76	0.45
1:C:693:ARG:HD2	1:C:776:MET:CB	2.47	0.45
1:F:418:VAL:HG22	1:F:466:PHE:CD2	2.53	0.45
1:F:563:TRP:N	1:F:563:TRP:CD2	2.85	0.45
1:D:281:PRO:O	1:D:285:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:PHE:HD1	1:E:377:HIS:N	2.15	0.45
1:E:503:ARG:NH1	1:E:524:ASP:OD1	2.49	0.45
1:A:252:LYS:HD2	1:A:255:GLU:OE2	2.16	0.44
1:A:678:SER:HB3	2:A:801:4KZ:O31	2.16	0.44
1:A:706:VAL:HG22	1:A:707:SER:N	2.32	0.44
1:C:392:GLY:N	1:C:453:ASP:CB	2.66	0.44
1:F:453:ASP:OD1	1:F:453:ASP:C	2.56	0.44
1:F:663:LEU:CD2	1:F:691:LEU:HD21	2.47	0.44
1:D:307:ASP:CG	1:D:310:HIS:H	2.20	0.44
1:D:308:ILE:CA	1:D:311:THR:HG22	2.47	0.44
1:D:369:ALA:HB2	1:D:418:VAL:CG2	2.47	0.44
1:D:369:ALA:HB2	1:D:418:VAL:HG21	1.99	0.44
1:D:417:PRO:O	1:D:465:VAL:HG13	2.17	0.44
1:D:613:GLU:OE1	1:E:707:SER:HB2	2.17	0.44
1:D:676:GLY:HA3	2:D:802:4KZ:C14	2.47	0.44
1:E:614:VAL:CG1	1:E:663:LEU:HD21	2.47	0.44
1:E:708:LEU:HD23	1:E:708:LEU:C	2.36	0.44
1:E:731:HIS:HB3	1:E:753:GLY:O	2.17	0.44
1:A:651:TYR:O	1:A:694:ARG:NH2	2.50	0.44
1:B:320:TYR:CD1	1:B:320:TYR:C	2.90	0.44
1:B:482:LEU:HA	1:B:485:MET:HG3	1.99	0.44
1:C:478:PRO:CB	1:C:480:PRO:HD2	2.47	0.44
1:C:600:LEU:HD11	1:C:701:ALA:HB1	1.99	0.44
1:D:327:GLU:HA	1:D:330:LEU:CD1	2.47	0.44
1:D:416:ASN:CB	1:D:464:LYS:HG3	2.48	0.44
1:D:545:ARG:NH2	1:D:546:GLU:OE2	2.51	0.44
1:E:523:THR:O	1:E:526:ALA:HB3	2.16	0.44
1:A:509:LYS:O	1:A:513:GLU:HG2	2.18	0.44
1:B:452:THR:HG22	1:B:458:VAL:O	2.17	0.44
1:C:401:MET:HB3	1:C:402:PRO:C	2.38	0.44
1:F:246:LEU:HD23	1:F:247:GLU:N	2.32	0.44
1:F:252:LYS:O	1:F:255:GLU:N	2.47	0.44
1:F:441:GLU:CD	1:F:451:PHE:HB2	2.37	0.44
1:F:523:THR:HB	1:F:570:ASP:HA	1.98	0.44
1:D:246:LEU:O	1:D:249:LEU:HB3	2.18	0.44
1:D:369:ALA:HB2	1:D:418:VAL:CB	2.48	0.44
1:D:510:GLN:NE2	1:D:544:GLU:O	2.50	0.44
1:E:507:TRP:N	1:E:508:PRO:HD2	2.33	0.44
1:A:527:ILE:O	1:A:530:VAL:N	2.49	0.44
1:B:700:ILE:CG2	1:B:769:LEU:HD21	2.47	0.44
1:B:748:LYS:O	1:B:752:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:VAL:O	1:C:339:THR:HG22	2.18	0.44
1:C:390:ILE:CG1	1:C:391:ARG:N	2.80	0.44
1:C:544:GLU:O	1:C:548:GLY:N	2.48	0.44
1:F:410:LYS:HG3	1:F:411:GLN:H	1.82	0.44
1:F:591:GLU:O	1:F:593:GLN:HG2	2.18	0.44
1:D:416:ASN:HB2	1:D:464:LYS:HG3	1.98	0.44
1:B:273:LEU:O	1:B:276:MET:HG3	2.17	0.44
1:C:273:LEU:HD21	1:C:286:ALA:CB	2.44	0.44
1:C:304:GLU:OE2	1:C:374:ARG:NH2	2.51	0.44
1:C:392:GLY:HA3	1:C:454:HIS:HB2	1.94	0.44
1:C:454:HIS:HD2	1:C:455:TYR:O	2.00	0.44
1:F:263:LYS:HG2	1:F:263:LYS:H	1.66	0.44
1:F:452:THR:CB	1:F:458:VAL:O	2.65	0.44
1:F:584:ARG:HH22	1:F:589:GLU:CD	2.21	0.44
1:D:661:VAL:HG12	1:D:662:ASP:N	2.32	0.44
1:D:692:SER:OG	1:D:694:ARG:HG3	2.18	0.44
1:E:345:ARG:NH1	1:E:347:LYS:CD	2.81	0.44
1:E:456:LEU:HD23	1:E:458:VAL:HG12	1.99	0.44
1:A:550:ILE:HD11	1:A:578:LEU:HD11	2.00	0.44
1:B:278:GLN:NE2	1:C:396:THR:CG2	2.79	0.44
1:B:585:PRO:O	1:B:587:LYS:HB2	2.17	0.44
1:C:481:LEU:HD23	1:C:481:LEU:N	2.32	0.44
1:F:311:THR:HG23	1:F:371:SER:CB	2.48	0.44
1:F:499:GLN:NE2	1:F:528:LEU:HD13	2.32	0.44
1:D:387:GLU:HG2	1:D:434:ASP:O	2.18	0.44
1:A:390:ILE:CG2	1:A:438:ALA:HB1	2.48	0.44
1:A:723:LEU:O	1:A:726:HIS:N	2.48	0.44
1:B:297:PRO:HG2	1:B:460:TYR:HH	1.78	0.44
1:B:700:ILE:HG12	1:B:734:VAL:HG23	2.00	0.44
1:C:292:TRP:HZ3	1:C:455:TYR:CG	2.36	0.44
1:C:762:VAL:O	1:C:766:LEU:HD12	2.17	0.44
1:F:277:GLN:CB	1:F:280:SER:HB3	2.40	0.44
1:F:452:THR:OG1	1:F:460:TYR:N	2.50	0.44
1:E:327:GLU:O	1:E:330:LEU:N	2.51	0.44
1:E:402:PRO:HG3	1:E:456:LEU:HD11	1.99	0.44
1:E:431:TRP:O	1:E:432:ARG:HB2	2.17	0.44
1:E:451:PHE:HB3	1:E:460:TYR:O	2.18	0.44
1:E:510:GLN:HG2	1:E:548:GLY:HA2	2.00	0.44
1:A:762:VAL:HG12	1:A:762:VAL:O	2.18	0.44
1:B:692:SER:O	1:B:693:ARG:CB	2.65	0.44
1:C:416:ASN:N	1:C:417:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:ILE:C	1:C:715:ILE:HD12	2.38	0.44
1:F:441:GLU:HG3	1:F:447:GLN:HB3	2.00	0.44
1:D:308:ILE:O	1:D:312:ARG:N	2.35	0.44
1:D:374:ARG:NH2	1:D:416:ASN:C	2.65	0.44
1:E:385:ARG:HA	1:E:428:SER:HB3	1.99	0.44
1:E:444:ASP:OD1	1:E:445:PRO:HD2	2.17	0.44
1:E:447:GLN:CG	1:E:450:THR:HB	2.47	0.44
1:B:356:PRO:HD2	1:B:359:VAL:HG11	1.99	0.44
1:C:617:VAL:O	1:C:618:PRO:C	2.54	0.44
1:D:527:ILE:O	1:D:530:VAL:N	2.51	0.44
1:D:549:LYS:HE2	1:D:578:LEU:HD23	2.00	0.44
1:E:534:TYR:CE2	1:E:579:GLY:HA2	2.51	0.44
1:A:503:ARG:HH21	1:A:524:ASP:HB3	1.83	0.43
1:A:575:PRO:O	1:A:579:GLY:O	2.36	0.43
1:B:259:PRO:O	1:B:262:VAL:N	2.51	0.43
1:B:358:GLY:O	1:B:540:VAL:HG22	2.18	0.43
1:B:477:ILE:HB	1:B:482:LEU:CD1	2.48	0.43
1:B:596:THR:HA	1:B:612:ILE:O	2.18	0.43
1:B:721:LYS:NZ	2:B:802:4KZ:O31	2.50	0.43
1:C:402:PRO:HG2	1:C:403:GLY:HA2	1.87	0.43
1:D:244:SER:O	1:D:247:GLU:CD	2.56	0.43
1:D:693:ARG:HD2	1:D:778:PRO:HA	1.99	0.43
1:E:722:LEU:HD21	1:E:733:ILE:HG21	2.00	0.43
1:B:244:SER:HA	1:B:247:GLU:OE2	2.18	0.43
1:C:278:GLN:N	1:C:280:SER:OG	2.51	0.43
1:C:594:VAL:CG2	1:C:775:THR:CG2	2.96	0.43
1:F:382:GLY:HA2	1:F:383:GLY:HA2	1.80	0.43
1:D:339:THR:CG2	1:D:343:ASP:HB2	2.35	0.43
1:D:526:ALA:O	1:D:529:ARG:HB3	2.18	0.43
1:A:617:VAL:HG12	1:B:646:ALA:HB2	2.00	0.43
1:A:624:SER:CB	1:A:664:HIS:HD1	2.29	0.43
1:B:518:GLY:O	1:B:566:LEU:HD22	2.18	0.43
1:B:648:THR:HA	1:B:653:LEU:HD12	2.00	0.43
1:B:672:THR:HG23	1:B:674:LYS:NZ	2.33	0.43
1:C:406:ILE:CA	1:C:409:MET:HB3	2.45	0.43
1:F:448:ASN:ND2	1:F:462:LEU:CB	2.79	0.43
1:D:350:ILE:HD13	1:D:443:LEU:HD22	1.99	0.43
1:D:386:ASP:OD2	1:D:388:ALA:CB	2.65	0.43
1:A:395:ARG:HG3	1:A:395:ARG:O	2.18	0.43
1:C:287:ARG:O	1:C:290:LEU:N	2.51	0.43
1:F:350:ILE:O	1:F:485:MET:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ILE:O	1:D:421:LEU:HA	2.18	0.43
1:E:314:VAL:HG13	1:E:370:ARG:HD3	2.00	0.43
1:E:334:ALA:O	1:E:338:LEU:HD13	2.18	0.43
1:E:386:ASP:C	1:E:389:GLU:HB3	2.35	0.43
1:E:395:ARG:O	1:E:455:TYR:CE1	2.71	0.43
1:E:619:GLY:HA3	1:E:662:ASP:N	2.33	0.43
1:A:318:ASP:OD2	1:A:367:SER:HB3	2.17	0.43
1:A:678:SER:N	2:A:801:4KZ:O30	2.45	0.43
1:B:343:ASP:O	1:B:345:ARG:N	2.40	0.43
1:B:658:TYR:CD1	1:B:659:ASN:N	2.86	0.43
1:B:723:LEU:C	1:B:723:LEU:HD23	2.39	0.43
1:C:395:ARG:CG	1:C:395:ARG:NH1	2.79	0.43
1:C:555:ALA:O	1:C:558:TRP:HB2	2.18	0.43
1:C:617:VAL:HG11	1:D:645:ARG:HE	1.84	0.43
1:C:715:ILE:HD12	1:C:716:GLY:N	2.34	0.43
1:F:308:ILE:CG2	1:F:310:HIS:HB3	2.48	0.43
1:F:452:THR:CG2	1:F:458:VAL:O	2.65	0.43
1:F:706:VAL:O	1:F:706:VAL:CG1	2.67	0.43
1:D:260:GLU:O	1:D:264:THR:HG23	2.18	0.43
1:E:479:ARG:N	1:E:480:PRO:HD2	2.33	0.43
1:E:619:GLY:HA3	1:E:662:ASP:OD2	2.17	0.43
1:A:306:LEU:O	1:A:337:GLN:NE2	2.50	0.43
2:A:801:4KZ:O30	2:A:801:4KZ:C22	2.65	0.43
1:B:503:ARG:HH21	1:B:524:ASP:CG	2.21	0.43
1:B:559:LEU:HD21	1:C:337:GLN:NE2	2.33	0.43
1:C:329:ILE:O	1:C:333:LEU:HD13	2.19	0.43
1:C:393:HIS:CD2	1:C:401:MET:H	2.37	0.43
1:C:479:ARG:HA	1:C:479:ARG:HD3	1.87	0.43
1:C:617:VAL:HG11	1:D:645:ARG:NE	2.34	0.43
1:C:693:ARG:NH2	1:C:779:VAL:HG22	2.34	0.43
1:F:367:SER:O	1:F:367:SER:OG	2.36	0.43
1:F:653:LEU:CD2	1:F:691:LEU:HB2	2.48	0.43
1:D:416:ASN:CB	1:D:464:LYS:HG2	2.49	0.43
1:E:314:VAL:O	1:E:317:GLU:HB2	2.19	0.43
1:E:603:THR:HG22	1:E:604:PRO:HD2	2.01	0.43
1:A:534:TYR:CZ	1:A:581:PRO:HA	2.53	0.43
1:A:626:THR:HG22	1:B:635:GLU:CG	2.49	0.43
1:A:679:ALA:O	1:A:680:GLY:C	2.57	0.43
1:B:692:SER:O	1:B:693:ARG:HG2	2.18	0.43
1:C:389:GLU:C	1:C:391:ARG:O	2.57	0.43
1:C:410:LYS:O	1:C:411:GLN:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:622:LYS:HB2	1:F:662:ASP:OD2	2.19	0.43
1:B:458:VAL:HG12	1:B:459:PRO:HD2	2.00	0.43
1:C:474:LEU:HD21	1:C:482:LEU:CD1	2.49	0.43
1:C:678:SER:O	1:C:704:GLY:O	2.36	0.43
1:F:393:HIS:O	1:F:455:TYR:N	2.52	0.43
1:E:274:GLU:O	1:E:276:MET:N	2.52	0.43
1:E:336:ARG:O	1:E:339:THR:CG2	2.67	0.43
1:E:422:ASP:OD1	1:E:422:ASP:N	2.52	0.43
1:E:502:ALA:HA	1:E:506:LEU:HB3	2.00	0.43
1:A:608:THR:HG22	1:A:609:LEU:N	2.34	0.43
1:A:713:MET:HB3	1:A:714:PRO:HD2	2.00	0.43
1:B:494:THR:HG22	1:B:497:GLU:OE1	2.19	0.43
1:B:678:SER:O	1:B:704:GLY:O	2.37	0.43
1:B:700:ILE:HD13	1:B:768:TYR:HE1	1.79	0.43
1:C:413:GLY:C	1:C:414:VAL:HG23	2.38	0.43
1:C:577:TYR:C	1:C:578:LEU:HD12	2.39	0.43
1:F:352:VAL:O	1:F:353:LEU:HD12	2.19	0.43
1:E:250:ARG:NH1	1:E:254:GLU:HG3	2.34	0.43
1:E:530:VAL:HG13	1:E:543:LEU:HD21	2.00	0.43
1:A:529:ARG:NH2	1:A:533:GLU:OE1	2.52	0.43
1:B:289:TYR:CE2	1:B:395:ARG:NE	2.86	0.43
1:B:757:LYS:HD3	1:B:768:TYR:CD2	2.54	0.43
1:C:244:SER:O	1:C:247:GLU:HB3	2.18	0.43
1:C:277:GLN:HG2	1:C:282:GLU:OE1	2.18	0.43
1:C:494:THR:CB	1:C:497:GLU:HG3	2.49	0.43
1:C:612:ILE:N	1:C:612:ILE:HD12	2.33	0.43
1:F:252:LYS:O	1:F:255:GLU:HB3	2.19	0.43
1:F:273:LEU:O	1:F:276:MET:HG2	2.17	0.43
1:F:394:ARG:CD	1:F:397:TYR:CD1	3.01	0.43
1:F:506:LEU:HD21	3:F:801:ADP:H1'	2.01	0.43
1:F:709:ARG:NH2	1:E:611:THR:HG21	2.34	0.43
1:D:412:VAL:HG21	1:D:417:PRO:HG3	2.00	0.43
1:D:432:ARG:HG3	1:D:433:GLY:N	2.32	0.43
1:E:332:TYR:O	1:E:335:VAL:HG13	2.19	0.43
1:E:390:ILE:CD1	1:E:435:PRO:HB2	2.48	0.43
1:E:447:GLN:O	1:E:447:GLN:HG2	2.18	0.43
1:E:619:GLY:O	1:E:660:LYS:C	2.57	0.43
1:A:598:GLN:HG2	1:A:609:LEU:HD13	2.01	0.42
1:A:669:ASP:OD1	1:A:670:GLY:N	2.52	0.42
1:B:408:ALA:O	1:B:412:VAL:CG1	2.59	0.42
1:B:494:THR:OG1	1:B:726:HIS:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:VAL:HG23	1:B:695:PRO:HA	2.01	0.42
1:C:389:GLU:HB3	1:C:404:LYS:N	2.34	0.42
1:C:430:ASP:O	1:C:431:TRP:HE3	2.01	0.42
1:D:345:ARG:O	1:D:346:ASN:HB2	2.19	0.42
1:D:585:PRO:CA	1:D:586:ASP:CB	2.96	0.42
1:E:397:TYR:C	1:E:398:ILE:HD13	2.39	0.42
1:B:450:THR:O	1:B:450:THR:OG1	2.34	0.42
1:C:575:PRO:HA	1:C:579:GLY:CA	2.49	0.42
1:F:381:LEU:O	1:F:384:VAL:HG13	2.19	0.42
1:F:447:GLN:CG	1:F:451:PHE:CD2	3.02	0.42
1:F:450:THR:O	1:F:459:PRO:HA	2.18	0.42
1:E:435:PRO:CD	1:E:436:ALA:H	2.32	0.42
1:E:589:GLU:N	1:E:589:GLU:OE2	2.52	0.42
1:A:715:ILE:HG13	1:A:739:ASN:HD21	1.83	0.42
1:B:245:ASP:O	1:B:249:LEU:HD12	2.20	0.42
1:B:597:ALA:HB1	1:B:702:MET:CE	2.50	0.42
1:C:279:GLY:N	1:C:280:SER:CB	2.82	0.42
1:C:350:ILE:CD1	1:C:443:LEU:CD1	2.97	0.42
1:C:423:GLN:N	1:C:470:THR:O	2.52	0.42
1:C:558:TRP:O	1:C:562:ALA:CA	2.67	0.42
1:C:580:ILE:CD1	1:D:742:GLN:HA	2.50	0.42
1:F:246:LEU:HA	1:F:249:LEU:HD21	1.97	0.42
1:F:448:ASN:HD21	1:F:462:LEU:CB	2.32	0.42
1:F:558:TRP:O	1:F:561:GLY:N	2.43	0.42
1:F:562:ALA:C	1:F:563:TRP:CE3	2.93	0.42
1:F:737:LYS:O	1:F:740:GLU:HB2	2.19	0.42
1:D:507:TRP:HB3	1:D:508:PRO:HD3	2.00	0.42
1:D:643:TYR:CZ	1:D:762:VAL:CG1	2.99	0.42
1:E:265:LYS:O	1:E:266:ALA:C	2.54	0.42
1:E:295:GLU:O	1:E:410:LYS:HD3	2.19	0.42
1:E:546:GLU:OE2	1:E:549:LYS:HD3	2.19	0.42
1:E:580:ILE:HG12	1:E:581:PRO:CD	2.50	0.42
1:A:270:LEU:O	1:A:270:LEU:HD23	2.20	0.42
1:A:385:ARG:HG2	1:A:431:TRP:CH2	2.55	0.42
1:A:405:LEU:HD21	1:A:442:VAL:HG21	2.00	0.42
1:A:531:ILE:CA	1:A:535:THR:CG2	2.91	0.42
1:B:308:ILE:C	1:B:308:ILE:HD12	2.39	0.42
1:B:580:ILE:HB	1:C:741:ALA:HA	2.01	0.42
1:B:779:VAL:O	1:B:780:VAL:HB	2.18	0.42
1:F:331:GLU:HG2	1:E:556:LYS:HD2	2.01	0.42
1:F:386:ASP:CG	1:F:388:ALA:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HG23	1:A:337:GLN:OE1	2.18	0.42
1:A:733:ILE:HG22	1:A:734:VAL:N	2.34	0.42
1:C:294:THR:HG23	1:C:295:GLU:CD	2.40	0.42
1:F:753:GLY:C	1:F:754:LEU:HD12	2.40	0.42
1:E:262:VAL:O	1:E:265:LYS:HB3	2.19	0.42
1:E:264:THR:O	1:E:267:LEU:HB3	2.19	0.42
1:E:401:MET:O	1:E:455:TYR:CB	2.67	0.42
1:E:613:GLU:OE1	1:E:668:PRO:CG	2.68	0.42
1:A:348:ALA:O	1:A:484:ARG:NH2	2.53	0.42
1:A:351:LEU:CD1	1:A:488:ILE:HD12	2.46	0.42
1:B:499:GLN:OE1	1:B:528:LEU:HD12	2.18	0.42
1:F:246:LEU:C	1:F:246:LEU:CD2	2.88	0.42
1:E:584:ARG:HG2	1:E:585:PRO:HD2	2.02	0.42
1:E:703:THR:CG2	1:E:735:LEU:HD12	2.49	0.42
1:A:614:VAL:HG22	1:A:665:VAL:HG13	2.00	0.42
1:A:735:LEU:HD12	1:A:736:PRO:HD3	2.02	0.42
1:B:263:LYS:O	1:B:267:LEU:HD13	2.19	0.42
1:B:350:ILE:HD13	1:B:443:LEU:CD2	2.49	0.42
1:B:575:PRO:HB3	1:B:579:GLY:O	2.20	0.42
1:B:586:ASP:CA	1:B:587:LYS:HB2	2.25	0.42
1:C:374:ARG:CD	1:C:418:VAL:HG23	2.49	0.42
1:C:453:ASP:HA	1:C:457:ASP:O	2.20	0.42
1:C:479:ARG:HG2	1:C:479:ARG:NH2	2.35	0.42
1:F:276:MET:HB2	1:F:283:ALA:HB2	2.01	0.42
1:F:441:GLU:CD	1:F:451:PHE:CB	2.87	0.42
1:F:451:PHE:C	1:F:452:THR:HG1	2.23	0.42
1:F:766:LEU:O	1:F:770:LEU:HB2	2.20	0.42
1:D:559:LEU:HD22	1:E:337:GLN:OE1	2.20	0.42
1:E:286:ALA:O	1:E:290:LEU:HD12	2.19	0.42
1:E:444:ASP:CG	1:E:446:GLU:H	2.23	0.42
1:A:389:GLU:O	1:A:390:ILE:HB	2.20	0.42
1:A:432:ARG:CD	1:A:432:ARG:C	2.88	0.42
1:B:278:GLN:HA	1:B:283:ALA:HB1	2.01	0.42
1:C:255:GLU:OE2	1:C:255:GLU:N	2.52	0.42
1:C:507:TRP:N	1:C:508:PRO:HD2	2.34	0.42
1:C:596:THR:HG21	1:D:709:ARG:HD3	2.01	0.42
1:C:619:GLY:O	1:C:660:LYS:O	2.37	0.42
1:D:249:LEU:HA	1:D:252:LYS:HG2	2.01	0.42
1:D:264:THR:OG1	1:D:265:LYS:N	2.53	0.42
1:D:374:ARG:NE	1:D:416:ASN:O	2.52	0.42
1:D:386:ASP:C	1:D:435:PRO:HB3	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ASP:CB	1:D:470:THR:OG1	2.67	0.42
1:D:439:MET:O	1:D:442:VAL:N	2.53	0.42
1:E:315:LEU:C	1:E:326:LYS:NZ	2.73	0.42
1:E:351:LEU:HD12	1:E:351:LEU:HA	1.93	0.42
1:E:401:MET:C	1:E:455:TYR:CG	2.93	0.42
1:E:553:LYS:O	1:E:553:LYS:HG3	2.18	0.42
1:E:730:ILE:O	1:E:730:ILE:HG13	2.19	0.42
1:A:338:LEU:HD11	1:F:559:LEU:HD21	2.01	0.42
1:B:292:TRP:CE2	1:B:402:PRO:HG3	2.55	0.42
1:B:442:VAL:HG23	1:B:443:LEU:HD12	2.02	0.42
1:B:449:ASN:O	1:B:461:ASP:HA	2.19	0.42
1:B:497:GLU:O	1:B:501:ILE:HG12	2.19	0.42
1:B:733:ILE:CG1	1:B:754:LEU:HD22	2.50	0.42
1:C:346:ASN:OD1	1:C:346:ASN:N	2.53	0.42
1:C:523:THR:HB	1:C:526:ALA:HB3	2.01	0.42
1:F:247:GLU:O	1:F:250:ARG:N	2.53	0.42
1:F:580:ILE:HG23	1:F:581:PRO:CD	2.50	0.42
1:D:320:TYR:CD1	1:D:320:TYR:C	2.93	0.42
1:E:392:GLY:H	1:E:453:ASP:HB3	1.85	0.42
1:A:381:LEU:HD13	1:A:427:MET:HE3	2.02	0.42
1:A:526:ALA:HB2	1:A:571:ALA:N	2.35	0.42
1:B:307:ASP:O	1:B:310:HIS:HB3	2.19	0.42
1:C:434:ASP:OD1	1:C:434:ASP:N	2.53	0.42
1:C:508:PRO:O	1:C:511:VAL:HB	2.20	0.42
1:C:546:GLU:HA	1:C:549:LYS:HG3	2.02	0.42
1:F:584:ARG:NH1	1:F:589:GLU:OE1	2.45	0.42
1:D:314:VAL:HG13	1:D:370:ARG:NH2	2.35	0.42
1:D:528:LEU:O	1:D:532:SER:OG	2.38	0.42
1:E:286:ALA:C	1:E:290:LEU:CD1	2.88	0.42
1:A:320:TYR:CD1	1:A:320:TYR:C	2.92	0.41
1:A:521:GLU:O	1:A:569:ILE:CG1	2.66	0.41
1:B:374:ARG:CZ	1:B:416:ASN:ND2	2.83	0.41
1:B:385:ARG:HB3	1:B:428:SER:CB	2.50	0.41
1:B:723:LEU:HD23	1:B:723:LEU:O	2.20	0.41
1:C:409:MET:SD	1:C:410:LYS:HA	2.60	0.41
1:F:271:ASP:CA	1:F:274:GLU:HG3	2.50	0.41
1:D:280:SER:O	1:D:283:ALA:HB3	2.20	0.41
1:D:375:LYS:O	1:D:418:VAL:N	2.50	0.41
1:E:342:LEU:HD12	1:E:342:LEU:O	2.19	0.41
1:A:431:TRP:CD1	1:A:432:ARG:N	2.89	0.41
1:B:449:ASN:HA	1:B:461:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:O	1:B:546:GLU:N	2.53	0.41
1:B:615:ALA:O	1:B:663:LEU:HD23	2.20	0.41
1:C:575:PRO:HA	1:C:579:GLY:N	2.35	0.41
1:D:258:MET:HB2	1:D:262:VAL:CG2	2.39	0.41
1:D:343:ASP:N	1:D:344:VAL:CA	2.75	0.41
1:A:558:TRP:HE3	1:A:563:TRP:CZ3	2.38	0.41
1:A:643:TYR:CE1	1:A:647:HIS:NE2	2.88	0.41
1:B:269:GLU:OE1	1:B:272:ARG:NE	2.45	0.41
1:B:277:GLN:O	1:B:280:SER:N	2.53	0.41
1:B:424:ILE:HD12	1:B:469:THR:HG23	2.01	0.41
1:B:507:TRP:CH2	1:B:522:VAL:CG2	3.03	0.41
1:F:626:THR:CG2	1:F:627:GLY:N	2.82	0.41
1:E:262:VAL:HG11	1:E:458:VAL:CG2	2.51	0.41
1:E:349:PRO:O	1:E:350:ILE:HD12	2.20	0.41
1:A:423:GLN:CA	1:A:470:THR:O	2.68	0.41
1:A:494:THR:O	1:A:497:GLU:N	2.54	0.41
1:A:514:SER:CB	1:A:551:ALA:CB	2.97	0.41
1:C:450:THR:HG23	1:C:462:LEU:N	2.35	0.41
1:C:519:ARG:HG2	1:C:565:GLY:O	2.19	0.41
1:C:596:THR:HG23	1:C:613:GLU:CB	2.50	0.41
1:F:273:LEU:HA	1:F:276:MET:CG	2.50	0.41
1:E:297:PRO:HD3	1:E:410:LYS:CD	2.50	0.41
1:E:422:ASP:HA	1:E:470:THR:HB	2.02	0.41
1:E:451:PHE:CD1	1:E:451:PHE:C	2.92	0.41
1:E:545:ARG:O	1:E:548:GLY:N	2.54	0.41
1:A:298:TRP:O	1:A:299:SER:HB3	2.20	0.41
1:B:558:TRP:HZ3	1:B:563:TRP:O	2.04	0.41
1:C:310:HIS:O	1:C:314:VAL:HG23	2.19	0.41
1:C:442:VAL:CG2	1:C:443:LEU:HD23	2.50	0.41
1:F:397:TYR:N	1:F:398:ILE:CA	2.83	0.41
1:F:523:THR:HG22	1:F:526:ALA:CB	2.51	0.41
1:D:625:LEU:HB3	1:D:629:LEU:HD12	2.03	0.41
1:E:342:LEU:HB2	1:E:346:ASN:CB	2.31	0.41
1:E:351:LEU:HB3	1:E:468:ILE:HG22	2.02	0.41
1:A:370:ARG:HE	1:A:370:ARG:HB2	1.70	0.41
1:A:494:THR:HG22	1:A:497:GLU:CD	2.40	0.41
1:A:520:ILE:HG12	1:A:569:ILE:HD11	2.02	0.41
1:B:700:ILE:HG23	1:B:769:LEU:HD21	2.03	0.41
1:B:712:VAL:HG12	1:B:736:PRO:HB3	2.02	0.41
1:C:252:LYS:O	1:C:256:VAL:HG12	2.20	0.41
1:C:415:ILE:C	1:C:417:PRO:CD	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:LEU:N	1:C:600:LEU:CD1	2.84	0.41
1:F:584:ARG:HG3	1:F:586:ASP:O	2.21	0.41
1:F:694:ARG:NH1	1:F:772:PRO:HA	2.35	0.41
1:D:253:ILE:HG12	1:D:258:MET:CE	2.50	0.41
1:D:661:VAL:CG1	1:D:662:ASP:N	2.84	0.41
1:A:405:LEU:O	1:A:408:ALA:HB3	2.19	0.41
1:A:545:ARG:O	1:A:548:GLY:N	2.54	0.41
1:B:590:THR:HG22	1:B:590:THR:O	2.20	0.41
1:B:642:THR:HA	1:B:645:ARG:HG3	2.02	0.41
1:C:272:ARG:CA	1:C:275:ARG:NH1	2.82	0.41
1:C:409:MET:SD	1:C:409:MET:C	2.99	0.41
1:C:424:ILE:HG21	1:C:469:THR:HG23	2.02	0.41
1:C:444:ASP:HB3	1:C:447:GLN:CB	2.51	0.41
1:C:511:VAL:HG12	1:C:517:GLU:HA	2.03	0.41
1:C:608:THR:HG22	1:C:609:LEU:N	2.36	0.41
1:C:721:LYS:O	1:C:724:ALA:HB3	2.21	0.41
1:F:396:THR:O	1:F:398:ILE:HD12	2.20	0.41
1:D:244:SER:O	1:D:247:GLU:CG	2.69	0.41
1:D:388:ALA:O	1:D:392:GLY:HA2	2.20	0.41
1:D:436:ALA:O	1:D:439:MET:N	2.54	0.41
1:A:297:PRO:HD2	1:A:460:TYR:CZ	2.54	0.41
1:A:305:VAL:C	1:A:306:LEU:HD12	2.41	0.41
1:A:551:ALA:O	1:A:555:ALA:N	2.45	0.41
1:A:593:GLN:OE1	1:B:709:ARG:NH2	2.53	0.41
1:C:292:TRP:HE3	1:C:455:TYR:CZ	2.31	0.41
1:C:559:LEU:N	1:C:559:LEU:CD1	2.81	0.41
1:F:272:ARG:HE	1:F:275:ARG:NH2	2.17	0.41
1:F:276:MET:HG2	1:F:276:MET:H	1.62	0.41
1:F:331:GLU:CG	1:E:556:LYS:HD2	2.51	0.41
1:E:286:ALA:C	1:E:290:LEU:HD11	2.41	0.41
1:E:287:ARG:C	1:E:290:LEU:HD12	2.35	0.41
1:E:385:ARG:CG	1:E:431:TRP:CD1	3.04	0.41
1:E:386:ASP:HB3	1:E:389:GLU:N	2.35	0.41
1:E:715:ILE:H	1:E:739:ASN:CG	2.24	0.41
1:A:318:ASP:HB2	1:A:319:HIS:CD2	2.56	0.41
1:B:273:LEU:HA	1:B:276:MET:CE	2.18	0.41
1:B:599:GLY:HA3	1:B:682:THR:HG21	2.02	0.41
1:B:601:ALA:HB3	1:B:610:LEU:HD12	2.03	0.41
1:B:692:SER:OG	1:B:694:ARG:HB2	2.21	0.41
1:B:707:SER:OG	1:B:713:MET:SD	2.79	0.41
1:C:347:LYS:HG2	1:C:446:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ALA:CB	1:C:376:PHE:HB2	2.51	0.41
1:C:411:GLN:O	1:C:413:GLY:N	2.54	0.41
1:C:424:ILE:CG2	1:C:469:THR:HG23	2.51	0.41
1:C:440:LEU:HB2	1:C:481:LEU:HD22	1.92	0.41
1:C:494:THR:HG23	1:C:723:LEU:HD22	2.03	0.41
1:F:273:LEU:HA	1:F:276:MET:SD	2.61	0.41
1:F:289:TYR:CD1	1:F:289:TYR:C	2.93	0.41
1:F:320:TYR:CD1	1:F:320:TYR:C	2.94	0.41
1:F:582:ARG:O	1:F:583:TYR:HD1	1.98	0.41
1:F:643:TYR:CE2	1:F:710:GLY:HA3	2.56	0.41
1:D:334:ALA:O	1:D:337:GLN:HB3	2.21	0.41
1:D:430:ASP:OD1	1:D:434:ASP:HA	2.21	0.41
1:D:444:ASP:HB3	1:D:447:GLN:CB	2.50	0.41
1:D:494:THR:HG22	1:D:497:GLU:OE1	2.20	0.41
1:D:692:SER:O	1:D:693:ARG:CB	2.69	0.41
1:E:289:TYR:HE1	1:E:456:LEU:HG	1.85	0.41
1:E:340:GLN:NE2	1:E:340:GLN:N	2.66	0.41
1:E:387:GLU:C	1:E:391:ARG:HD3	2.41	0.41
1:E:410:LYS:CG	1:E:410:LYS:O	2.68	0.41
1:A:386:ASP:HB2	1:A:432:ARG:CB	2.49	0.41
1:A:699:ASP:O	1:A:730:ILE:HG23	2.21	0.41
1:B:503:ARG:HH21	1:B:524:ASP:CB	2.34	0.41
1:B:758:LEU:N	1:B:758:LEU:CD2	2.84	0.41
1:C:257:GLY:HA2	1:C:299:SER:HB2	2.03	0.41
1:C:312:ARG:HG3	1:C:330:LEU:HD11	2.03	0.41
1:C:524:ASP:N	1:C:524:ASP:OD1	2.54	0.41
1:C:537:GLU:OE1	1:C:542:GLY:N	2.50	0.41
1:D:248:ALA:O	1:D:252:LYS:HG2	2.20	0.41
1:D:253:ILE:HD13	1:D:253:ILE:C	2.42	0.41
1:D:305:VAL:HG22	1:D:306:LEU:N	2.36	0.41
1:D:318:ASP:CG	1:D:370:ARG:HH21	2.25	0.41
1:D:718:VAL:HG21	1:D:742:GLN:CB	2.51	0.41
1:E:261:ALA:HA	1:E:264:THR:HB	2.02	0.41
1:E:296:VAL:HB	1:E:298:TRP:CH2	2.56	0.41
1:E:355:GLY:O	1:E:472:ASN:HA	2.21	0.41
1:E:391:ARG:HD2	1:E:391:ARG:N	2.36	0.41
1:E:510:GLN:NE2	1:E:551:ALA:CB	2.55	0.41
1:E:510:GLN:CD	1:E:548:GLY:HA2	2.41	0.41
1:E:661:VAL:HG12	1:E:662:ASP:O	2.21	0.41
1:E:751:LEU:HA	1:E:754:LEU:HD12	2.03	0.41
1:A:390:ILE:CD1	1:A:435:PRO:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ARG:HD2	1:A:776:MET:HB3	2.02	0.40
1:B:580:ILE:CG2	1:B:581:PRO:HD2	2.50	0.40
1:C:670:GLY:O	1:D:632:VAL:HG13	2.21	0.40
1:C:731:HIS:HA	1:C:754:LEU:HD23	2.04	0.40
1:C:773:GLU:HA	1:C:774:PRO:HD3	1.91	0.40
1:F:271:ASP:C	1:F:274:GLU:HG3	2.41	0.40
1:E:311:THR:HG23	1:E:371:SER:HG	1.83	0.40
1:E:354:VAL:HG12	1:E:489:GLU:HA	2.03	0.40
1:E:747:PRO:HG2	1:E:750:VAL:CG2	2.51	0.40
1:A:389:GLU:HB3	1:A:404:LYS:HG3	2.04	0.40
1:A:566:LEU:O	1:A:566:LEU:HD23	2.21	0.40
1:C:291:ASP:HA	1:C:294:THR:HG22	2.02	0.40
1:C:460:TYR:O	1:C:460:TYR:CD1	2.74	0.40
1:F:453:ASP:O	1:F:456:LEU:O	2.39	0.40
1:F:469:THR:HG22	1:F:470:THR:N	2.35	0.40
1:F:528:LEU:O	1:F:531:ILE:N	2.54	0.40
1:F:656:ASP:O	1:F:660:LYS:CD	2.69	0.40
1:D:334:ALA:O	1:D:337:GLN:CB	2.70	0.40
1:E:392:GLY:HA2	1:E:401:MET:O	2.22	0.40
1:E:474:LEU:HA	1:E:477:ILE:HD12	2.02	0.40
1:E:556:LYS:O	1:E:560:GLU:N	2.42	0.40
1:B:345:ARG:O	1:B:345:ARG:HD3	2.21	0.40
1:C:379:ILE:CG2	1:C:405:LEU:HG	2.52	0.40
1:C:401:MET:HE3	1:C:407:HIS:HE1	1.79	0.40
1:F:393:HIS:O	1:F:454:HIS:HB3	2.21	0.40
1:F:472:ASN:OD1	1:F:472:ASN:N	2.55	0.40
1:E:309:ASN:O	1:E:312:ARG:HB3	2.22	0.40
1:E:701:ALA:HB2	1:E:730:ILE:HD11	2.01	0.40
1:A:425:ASP:OD1	1:A:471:ALA:HB1	2.13	0.40
1:A:431:TRP:CD1	1:A:431:TRP:C	2.94	0.40
1:A:617:VAL:O	1:A:661:VAL:HG13	2.21	0.40
1:B:292:TRP:CD2	1:B:402:PRO:HG3	2.57	0.40
1:B:669:ASP:OD1	1:B:672:THR:HG22	2.19	0.40
1:B:770:LEU:N	1:B:770:LEU:HD12	2.36	0.40
1:C:243:LEU:HA	1:C:246:LEU:CD1	2.49	0.40
1:C:257:GLY:HA3	1:C:258:MET:HA	1.86	0.40
1:C:272:ARG:HG3	1:C:273:LEU:N	2.36	0.40
1:C:292:TRP:CZ3	1:C:455:TYR:CG	3.10	0.40
1:C:342:LEU:CD1	1:C:342:LEU:N	2.84	0.40
1:C:524:ASP:HA	1:C:527:ILE:HG22	2.02	0.40
1:F:508:PRO:HA	1:F:511:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:GLY:HA2	1:D:423:GLN:HB3	2.02	0.40
1:D:478:PRO:HB2	1:D:480:PRO:HD2	2.04	0.40
1:D:558:TRP:HE3	1:D:563:TRP:CD1	2.40	0.40
1:D:596:THR:HG22	1:D:698:MET:SD	2.62	0.40
1:D:678:SER:HB3	2:D:802:4KZ:O31	2.22	0.40
1:D:765:VAL:O	1:D:769:LEU:HD22	2.20	0.40
1:E:307:ASP:HB3	1:E:310:HIS:CB	2.45	0.40
1:E:502:ALA:HA	1:E:506:LEU:HB2	2.03	0.40
1:A:385:ARG:H	1:A:385:ARG:HD2	1.85	0.40
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.92	0.40
1:B:575:PRO:O	1:B:579:GLY:N	2.55	0.40
1:B:687:ILE:O	1:B:691:LEU:HD12	2.22	0.40
1:B:747:PRO:HB2	1:B:750:VAL:CG2	2.52	0.40
1:C:357:PRO:HD3	1:C:472:ASN:HD22	1.87	0.40
1:C:425:ASP:HB3	1:C:471:ALA:CB	2.48	0.40
1:F:252:LYS:O	1:F:255:GLU:CB	2.70	0.40
1:F:297:PRO:O	1:F:460:TYR:OH	2.24	0.40
1:D:302:ASP:OD1	1:D:303:PRO:HD2	2.21	0.40
1:D:396:THR:OG1	1:D:397:TYR:N	2.54	0.40
1:D:424:ILE:CB	1:D:469:THR:HG23	2.49	0.40
1:D:735:LEU:HG	1:D:736:PRO:HD2	2.03	0.40
1:E:319:HIS:CE1	1:E:363:SER:CB	2.95	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	535/555 (96%)	498 (93%)	36 (7%)	1 (0%)	47	80
1	B	535/555 (96%)	501 (94%)	33 (6%)	1 (0%)	47	80
1	C	536/555 (97%)	492 (92%)	42 (8%)	2 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	535/555 (96%)	499 (93%)	36 (7%)	0	100	100
1	E	535/555 (96%)	505 (94%)	27 (5%)	3 (1%)	25	62
1	F	536/555 (97%)	499 (93%)	35 (6%)	2 (0%)	34	70
All	All	3212/3330 (96%)	2994 (93%)	209 (6%)	9 (0%)	41	75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	ALA
1	C	401	MET
1	F	308	ILE
1	E	416	ASN
1	B	416	ASN
1	C	416	ASN
1	E	402	PRO
1	E	677	PRO
1	F	491	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/460 (97%)	388 (87%)	60 (13%)	4	19
1	B	448/460 (97%)	398 (89%)	50 (11%)	6	25
1	C	449/460 (98%)	370 (82%)	79 (18%)	2	9
1	D	448/460 (97%)	387 (86%)	61 (14%)	3	18
1	E	448/460 (97%)	363 (81%)	85 (19%)	1	7
1	F	449/460 (98%)	389 (87%)	60 (13%)	4	19
All	All	2690/2760 (98%)	2295 (85%)	395 (15%)	3	16

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ASP
1	A	246	LEU
1	A	251	LYS
1	A	254	GLU
1	A	258	MET
1	A	260	GLU
1	A	273	LEU
1	A	275	ARG
1	A	276	MET
1	A	278	GLN
1	A	294	THR
1	A	304	GLU
1	A	305	VAL
1	A	322	LEU
1	A	339	THR
1	A	363	SER
1	A	371	SER
1	A	380	SER
1	A	385	ARG
1	A	409	MET
1	A	420	LEU
1	A	421	LEU
1	A	424	ILE
1	A	432	ARG
1	A	458	VAL
1	A	464	LYS
1	A	470	THR
1	A	472	ASN
1	A	483	ASP
1	A	484	ARG
1	A	495	ASN
1	A	514	SER
1	A	523	THR
1	A	532	SER
1	A	533	GLU
1	A	543	LEU
1	A	545	ARG
1	A	559	LEU
1	A	566	LEU
1	A	569	ILE
1	A	580	ILE
1	A	584	ARG
1	A	589	GLU

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Mol	Chain	Res	Type
1	A	591	GLU
1	A	603	THR
1	A	609	LEU
1	A	620	SER
1	A	624	SER
1	A	626	THR
1	A	636	SER
1	A	649	GLN
1	A	650	ASP
1	A	674	LYS
1	A	689	SER
1	A	694	ARG
1	A	699	ASP
1	A	707	SER
1	A	718	VAL
1	A	742	GLN
1	A	751	LEU
1	B	247	GLU
1	B	262	VAL
1	B	264	THR
1	B	272	ARG
1	B	278	GLN
1	B	299	SER
1	B	311	THR
1	B	327	GLU
1	B	328	ARG
1	B	339	THR
1	B	340	GLN
1	B	345	ARG
1	B	346	ASN
1	B	391	ARG
1	B	395	ARG
1	B	416	ASN
1	B	422	ASP
1	B	424	ILE
1	B	428	SER
1	B	432	ARG
1	B	440	LEU
1	B	447	GLN
1	B	450	THR
1	B	453	ASP
1	B	457	ASP

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Mol	Chain	Res	Type
1	B	460	TYR
1	B	470	THR
1	B	472	ASN
1	B	479	ARG
1	B	482	LEU
1	B	485	MET
1	B	501	ILE
1	B	512	ARG
1	B	513	GLU
1	B	523	THR
1	B	541	ARG
1	B	546	GLU
1	B	566	LEU
1	B	570	ASP
1	B	603	THR
1	B	624	SER
1	B	647	HIS
1	B	653	LEU
1	B	672	THR
1	B	687	ILE
1	B	699	ASP
1	B	748	LYS
1	B	749	GLU
1	B	751	LEU
1	B	758	LEU
1	C	245	ASP
1	C	249	LEU
1	C	255	GLU
1	C	258	MET
1	C	260	GLU
1	C	262	VAL
1	C	267	LEU
1	C	268	LYS
1	C	273	LEU
1	C	275	ARG
1	C	276	MET
1	C	277	GLN
1	C	280	SER
1	C	282	GLU
1	C	291	ASP
1	C	292	TRP
1	C	293	LEU

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Mol	Chain	Res	Type
1	C	294	THR
1	C	296	VAL
1	C	307	ASP
1	C	338	LEU
1	C	340	GLN
1	C	342	LEU
1	C	343	ASP
1	C	346	ASN
1	C	363	SER
1	C	375	LYS
1	C	378	ARG
1	C	385	ARG
1	C	387	GLU
1	C	389	GLU
1	C	390	ILE
1	C	401	MET
1	C	407	HIS
1	C	409	MET
1	C	412	VAL
1	C	420	LEU
1	C	430	ASP
1	C	431	TRP
1	C	434	ASP
1	C	444	ASP
1	C	452	THR
1	C	455	TYR
1	C	456	LEU
1	C	457	ASP
1	C	459	PRO
1	C	460	TYR
1	C	463	SER
1	C	469	THR
1	C	472	ASN
1	C	474	LEU
1	C	479	ARG
1	C	483	ASP
1	C	496	MET
1	C	498	LYS
1	C	536	ARG
1	C	537	GLU
1	C	552	ARG
1	C	558	TRP

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Mol	Chain	Res	Type
1	C	559	LEU
1	C	566	LEU
1	C	567	ARG
1	C	596	THR
1	C	600	LEU
1	C	609	LEU
1	C	650	ASP
1	C	672	THR
1	C	689	SER
1	C	693	ARG
1	C	706	VAL
1	C	707	SER
1	C	708	LEU
1	C	711	LYS
1	C	737	LYS
1	C	744	GLU
1	C	761	ASP
1	C	764	GLU
1	C	769	LEU
1	C	779	VAL
1	F	245	ASP
1	F	246	LEU
1	F	247	GLU
1	F	250	ARG
1	F	258	MET
1	F	272	ARG
1	F	274	GLU
1	F	275	ARG
1	F	276	MET
1	F	278	GLN
1	F	289	TYR
1	F	299	SER
1	F	302	ASP
1	F	304	GLU
1	F	307	ASP
1	F	313	GLN
1	F	316	ASP
1	F	324	ASP
1	F	330	LEU
1	F	331	GLU
1	F	339	THR
1	F	342	LEU

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Mol	Chain	Res	Type
1	F	345	ARG
1	F	347	LYS
1	F	351	LEU
1	F	367	SER
1	F	373	ASN
1	F	391	ARG
1	F	394	ARG
1	F	395	ARG
1	F	410	LYS
1	F	415	ILE
1	F	444	ASP
1	F	446	GLU
1	F	450	THR
1	F	457	ASP
1	F	472	ASN
1	F	479	ARG
1	F	496	MET
1	F	523	THR
1	F	537	GLU
1	F	544	GLU
1	F	550	ILE
1	F	563	TRP
1	F	566	LEU
1	F	572	SER
1	F	582	ARG
1	F	584	ARG
1	F	587	LYS
1	F	598	GLN
1	F	603	THR
1	F	620	SER
1	F	624	SER
1	F	650	ASP
1	F	662	ASP
1	F	692	SER
1	F	699	ASP
1	F	715	ILE
1	F	719	LYS
1	F	760	GLU
1	D	244	SER
1	D	246	LEU
1	D	247	GLU
1	D	251	LYS

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Mol	Chain	Res	Type
1	D	253	ILE
1	D	254	GLU
1	D	258	MET
1	D	262	VAL
1	D	270	LEU
1	D	274	GLU
1	D	275	ARG
1	D	276	MET
1	D	277	GLN
1	D	300	LYS
1	D	309	ASN
1	D	324	ASP
1	D	347	LYS
1	D	398	ILE
1	D	401	MET
1	D	412	VAL
1	D	429	SER
1	D	430	ASP
1	D	432	ARG
1	D	440	LEU
1	D	448	ASN
1	D	449	ASN
1	D	457	ASP
1	D	466	PHE
1	D	470	THR
1	D	472	ASN
1	D	513	GLU
1	D	532	SER
1	D	541	ARG
1	D	543	LEU
1	D	558	TRP
1	D	559	LEU
1	D	564	GLU
1	D	568	THR
1	D	572	SER
1	D	591	GLU
1	D	600	LEU
1	D	603	THR
1	D	608	THR
1	D	624	SER
1	D	636	SER
1	D	648	THR

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Mol	Chain	Res	Type
1	D	650	ASP
1	D	693	ARG
1	D	699	ASP
1	D	703	THR
1	D	718	VAL
1	D	723	LEU
1	D	737	LYS
1	D	738	ASP
1	D	739	ASN
1	D	744	GLU
1	D	748	LYS
1	D	749	GLU
1	D	750	VAL
1	D	769	LEU
1	D	775	THR
1	E	247	GLU
1	E	249	LEU
1	E	250	ARG
1	E	253	ILE
1	E	254	GLU
1	E	256	VAL
1	E	260	GLU
1	E	265	LYS
1	E	267	LEU
1	E	268	LYS
1	E	270	LEU
1	E	272	ARG
1	E	273	LEU
1	E	278	GLN
1	E	282	GLU
1	E	287	ARG
1	E	290	LEU
1	E	292	TRP
1	E	293	LEU
1	E	300	LYS
1	E	312	ARG
1	E	318	ASP
1	E	323	LYS
1	E	328	ARG
1	E	336	ARG
1	E	337	GLN
1	E	340	GLN

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Mol	Chain	Res	Type
1	E	342	LEU
1	E	343	ASP
1	E	347	LYS
1	E	354	VAL
1	E	363	SER
1	E	370	ARG
1	E	371	SER
1	E	372	MET
1	E	374	ARG
1	E	376	PHE
1	E	380	SER
1	E	381	LEU
1	E	386	ASP
1	E	387	GLU
1	E	391	ARG
1	E	393	HIS
1	E	394	ARG
1	E	395	ARG
1	E	398	ILE
1	E	405	LEU
1	E	432	ARG
1	E	443	LEU
1	E	449	ASN
1	E	457	ASP
1	E	462	LEU
1	E	479	ARG
1	E	486	GLU
1	E	496	MET
1	E	503	ARG
1	E	504	GLN
1	E	506	LEU
1	E	521	GLU
1	E	530	VAL
1	E	545	ARG
1	E	556	LYS
1	E	559	LEU
1	E	564	GLU
1	E	572	SER
1	E	573	ASP
1	E	580	ILE
1	E	582	ARG
1	E	587	LYS

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Mol	Chain	Res	Type
1	E	589	GLU
1	E	602	TRP
1	E	603	THR
1	E	624	SER
1	E	625	LEU
1	E	655	GLU
1	E	663	LEU
1	E	674	LYS
1	E	691	LEU
1	E	692	SER
1	E	707	SER
1	E	718	VAL
1	E	761	ASP
1	E	767	GLU
1	E	769	LEU
1	E	771	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	A	313	GLN
1	A	319	HIS
1	A	454	HIS
1	A	495	ASN
1	A	510	GLN
1	A	598	GLN
1	A	649	GLN
1	A	726	HIS
1	A	727	GLN
1	A	731	HIS
1	B	319	HIS
1	B	346	ASN
1	B	454	HIS
1	B	510	GLN
1	B	649	GLN
1	B	726	HIS
1	B	739	ASN
1	C	309	ASN
1	C	340	GLN
1	C	393	HIS
1	C	407	HIS

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Mol	Chain	Res	Type
1	C	447	GLN
1	C	448	ASN
1	C	454	HIS
1	C	510	GLN
1	C	726	HIS
1	C	731	HIS
1	C	739	ASN
1	F	448	ASN
1	F	495	ASN
1	F	598	GLN
1	F	666	HIS
1	F	726	HIS
1	D	448	ASN
1	D	449	ASN
1	D	495	ASN
1	D	727	GLN
1	E	310	HIS
1	E	346	ASN
1	E	377	HIS
1	E	393	HIS
1	E	411	GLN
1	E	449	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4KZ	A	801	1	30,33,33	0.63	0	39,43,43	1.54	5 (12%)
3	ADP	F	801	-	24,29,29	1.01	1 (4%)	29,45,45	1.55	5 (17%)
2	4KZ	F	802	1	30,33,33	0.62	0	39,43,43	1.06	3 (7%)
2	4KZ	B	802	1	30,33,33	0.81	0	39,43,43	1.78	5 (12%)
2	4KZ	C	801	1	30,33,33	0.48	0	39,43,43	1.23	5 (12%)
2	4KZ	D	802	1	30,33,33	0.78	1 (3%)	39,43,43	1.58	4 (10%)
2	4KZ	E	801	1	30,33,33	0.90	2 (6%)	39,43,43	1.72	8 (20%)
3	ADP	B	801	-	24,29,29	0.99	1 (4%)	29,45,45	1.50	5 (17%)
3	ADP	D	801	-	24,29,29	0.91	1 (4%)	29,45,45	1.55	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4KZ	A	801	1	-	9/23/28/28	0/3/3/3
3	ADP	F	801	-	-	5/12/32/32	0/3/3/3
2	4KZ	F	802	1	-	0/23/28/28	0/3/3/3
2	4KZ	B	802	1	-	13/23/28/28	0/3/3/3
2	4KZ	C	801	1	-	5/23/28/28	0/3/3/3
2	4KZ	D	802	1	-	13/23/28/28	0/3/3/3
2	4KZ	E	801	1	-	6/23/28/28	0/3/3/3
3	ADP	B	801	-	-	3/12/32/32	0/3/3/3
3	ADP	D	801	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	4KZ	C21-N20	-2.71	1.41	1.46
2	E	801	4KZ	C21-N20	-2.47	1.41	1.46
3	B	801	ADP	C5-C4	2.45	1.47	1.40
2	E	801	4KZ	C10-C18	-2.27	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	801	ADP	C5-C4	2.02	1.46	1.40
3	D	801	ADP	C5-C4	2.01	1.46	1.40

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	4KZ	C22-C21-N20	-8.30	99.66	110.39
2	E	801	4KZ	C22-C21-N20	-7.63	100.52	110.39
2	D	802	4KZ	C22-C21-N20	-6.98	101.36	110.39
2	A	801	4KZ	C22-C21-N20	-6.05	102.56	110.39
3	F	801	ADP	N3-C2-N1	-3.94	122.53	128.68
3	D	801	ADP	N3-C2-N1	-3.91	122.57	128.68
3	B	801	ADP	C4-C5-N7	-3.56	105.69	109.40
3	F	801	ADP	PA-O3A-PB	-3.48	120.88	132.83
3	B	801	ADP	N3-C2-N1	-3.38	123.39	128.68
3	F	801	ADP	C4-C5-N7	-3.32	105.94	109.40
3	D	801	ADP	C4-C5-N7	-3.11	106.15	109.40
3	D	801	ADP	PA-O3A-PB	-3.06	122.34	132.83
3	B	801	ADP	PA-O3A-PB	-3.00	122.54	132.83
2	C	801	4KZ	C6-N1-C2	2.96	120.78	116.93
3	B	801	ADP	C3'-C2'-C1'	2.96	105.43	100.98
2	A	801	4KZ	C6-N1-C2	2.87	120.65	116.93
2	E	801	4KZ	C2-C3-N4	-2.78	118.59	122.05
2	F	802	4KZ	C6-N1-C2	2.74	120.48	116.93
2	B	802	4KZ	O19-C18-N20	2.71	127.95	122.93
2	E	801	4KZ	O19-C18-N20	2.63	127.81	122.93
3	F	801	ADP	C3'-C2'-C1'	2.62	104.92	100.98
2	C	801	4KZ	C5-N4-C3	2.52	121.22	116.85
2	B	802	4KZ	C6-N1-C2	2.49	120.16	116.93
2	A	801	4KZ	O19-C18-N20	2.45	127.47	122.93
2	E	801	4KZ	C6-N1-C2	2.42	120.07	116.93
2	F	802	4KZ	C5-N4-C3	2.32	120.86	116.85
2	C	801	4KZ	C22-C21-N20	-2.31	107.39	110.39
2	D	802	4KZ	C10-C18-N20	-2.29	111.68	116.70
2	F	802	4KZ	C7-C2-N1	2.29	120.18	117.48
3	D	801	ADP	C2'-C3'-C4'	2.28	107.07	102.64
2	E	801	4KZ	C5-N4-C3	2.27	120.78	116.85
2	A	801	4KZ	C5-N4-C3	2.24	120.72	116.85
2	D	802	4KZ	C6-N1-C2	2.24	119.83	116.93
3	D	801	ADP	C3'-C2'-C1'	2.23	104.34	100.98
2	C	801	4KZ	C3-C2-N1	-2.18	119.02	121.61
2	C	801	4KZ	C6-C5-N4	-2.18	119.23	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	4KZ	C5-C6-N1	-2.08	119.18	122.17
2	A	801	4KZ	C2-C3-N4	-2.08	119.47	122.05
2	B	802	4KZ	C18-C10-N9	-2.06	105.55	111.16
3	F	801	ADP	C2'-C3'-C4'	2.06	106.64	102.64
3	B	801	ADP	C2'-C3'-C4'	2.06	106.64	102.64
2	B	802	4KZ	C2-C3-N4	-2.05	119.50	122.05
2	E	801	4KZ	C10-C18-N20	-2.02	112.27	116.70
2	E	801	4KZ	C21-N20-C18	-2.01	117.57	122.77
2	D	802	4KZ	C2-C7-N9	2.01	118.94	115.20

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	4KZ	C3-C2-C7-N9
2	A	801	4KZ	C3-C2-C7-O8
2	A	801	4KZ	O19-C18-N20-C21
2	A	801	4KZ	N20-C21-C22-C23
2	A	801	4KZ	B29-C21-C22-C23
2	B	802	4KZ	C3-C2-C7-N9
2	B	802	4KZ	C3-C2-C7-O8
2	B	802	4KZ	O19-C18-N20-C21
2	B	802	4KZ	N20-C21-C22-C23
2	B	802	4KZ	B29-C21-C22-C23
2	B	802	4KZ	C21-C22-C23-C24
2	B	802	4KZ	C21-C22-C23-C28
2	D	802	4KZ	O19-C18-N20-C21
2	D	802	4KZ	N20-C21-C22-C23
2	D	802	4KZ	B29-C21-C22-C23
2	E	801	4KZ	O19-C18-N20-C21
2	E	801	4KZ	N20-C21-C22-C23
2	E	801	4KZ	B29-C21-C22-C23
3	F	801	ADP	C5'-O5'-PA-O1A
3	D	801	ADP	C5'-O5'-PA-O1A
3	D	801	ADP	C5'-O5'-PA-O2A
2	A	801	4KZ	C10-C18-N20-C21
2	E	801	4KZ	C10-C18-N20-C21
2	A	801	4KZ	N1-C2-C7-O8
2	B	802	4KZ	N1-C2-C7-O8
2	A	801	4KZ	N1-C2-C7-N9
2	B	802	4KZ	N1-C2-C7-N9
2	D	802	4KZ	N1-C2-C7-N9

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Mol	Chain	Res	Type	Atoms
2	C	801	4KZ	N1-C2-C7-O8
2	D	802	4KZ	N1-C2-C7-O8
2	D	802	4KZ	C10-C18-N20-C21
2	C	801	4KZ	N1-C2-C7-N9
2	B	802	4KZ	C10-C18-N20-C21
2	C	801	4KZ	C3-C2-C7-O8
2	D	802	4KZ	C3-C2-C7-O8
2	C	801	4KZ	C3-C2-C7-N9
2	D	802	4KZ	C3-C2-C7-N9
3	B	801	ADP	O4'-C4'-C5'-O5'
2	D	802	4KZ	N9-C10-C18-O19
3	F	801	ADP	O4'-C4'-C5'-O5'
3	B	801	ADP	C3'-C4'-C5'-O5'
2	D	802	4KZ	C11-C10-C18-O19
3	F	801	ADP	C5'-O5'-PA-O3A
2	D	802	4KZ	C22-C21-N20-C18
3	F	801	ADP	C5'-O5'-PA-O2A
3	B	801	ADP	C4'-C5'-O5'-PA
3	F	801	ADP	C3'-C4'-C5'-O5'
2	B	802	4KZ	C10-C11-C12-C17
2	A	801	4KZ	C21-C22-C23-C28
2	C	801	4KZ	C21-C22-C23-C24
2	E	801	4KZ	C21-C22-C23-C24
2	E	801	4KZ	C21-C22-C23-C28
2	D	802	4KZ	N9-C10-C18-N20
2	B	802	4KZ	C10-C11-C12-C13
2	B	802	4KZ	C18-C10-N9-C7
3	D	801	ADP	C5'-O5'-PA-O3A
2	D	802	4KZ	N9-C10-C11-C12

There are no ring outliers.

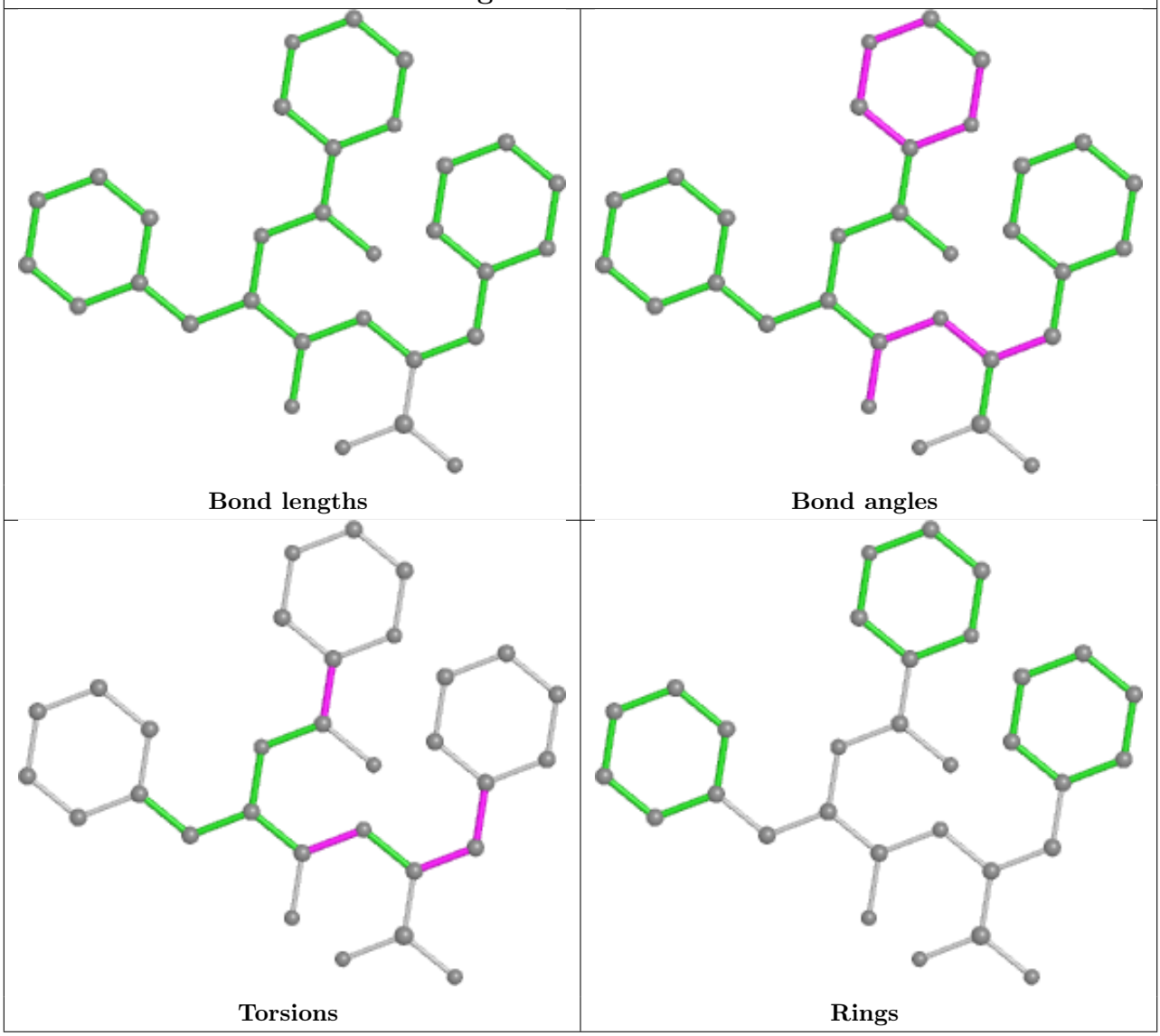
5 monomers are involved in 14 short contacts:

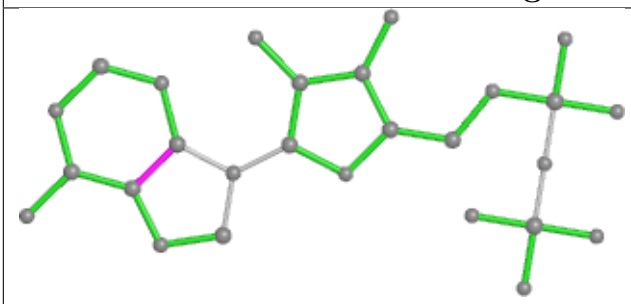
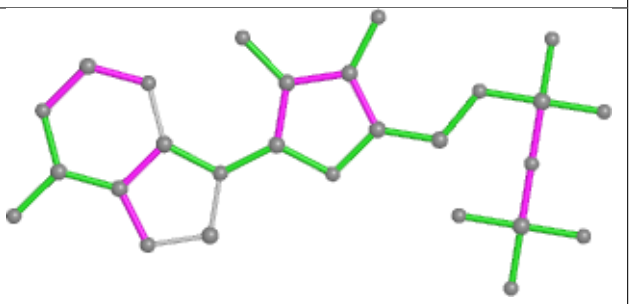
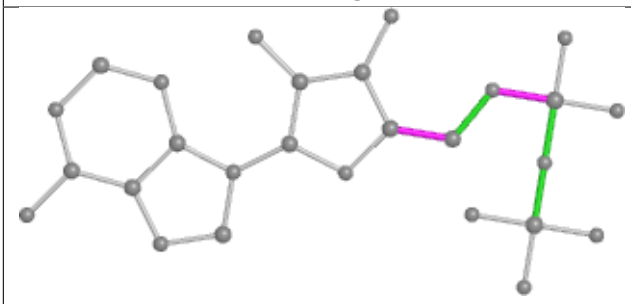
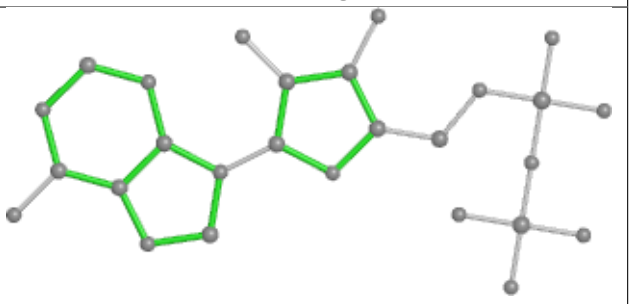
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	4KZ	4	0
3	F	801	ADP	3	0
2	F	802	4KZ	1	0
2	B	802	4KZ	2	0
2	D	802	4KZ	4	0

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

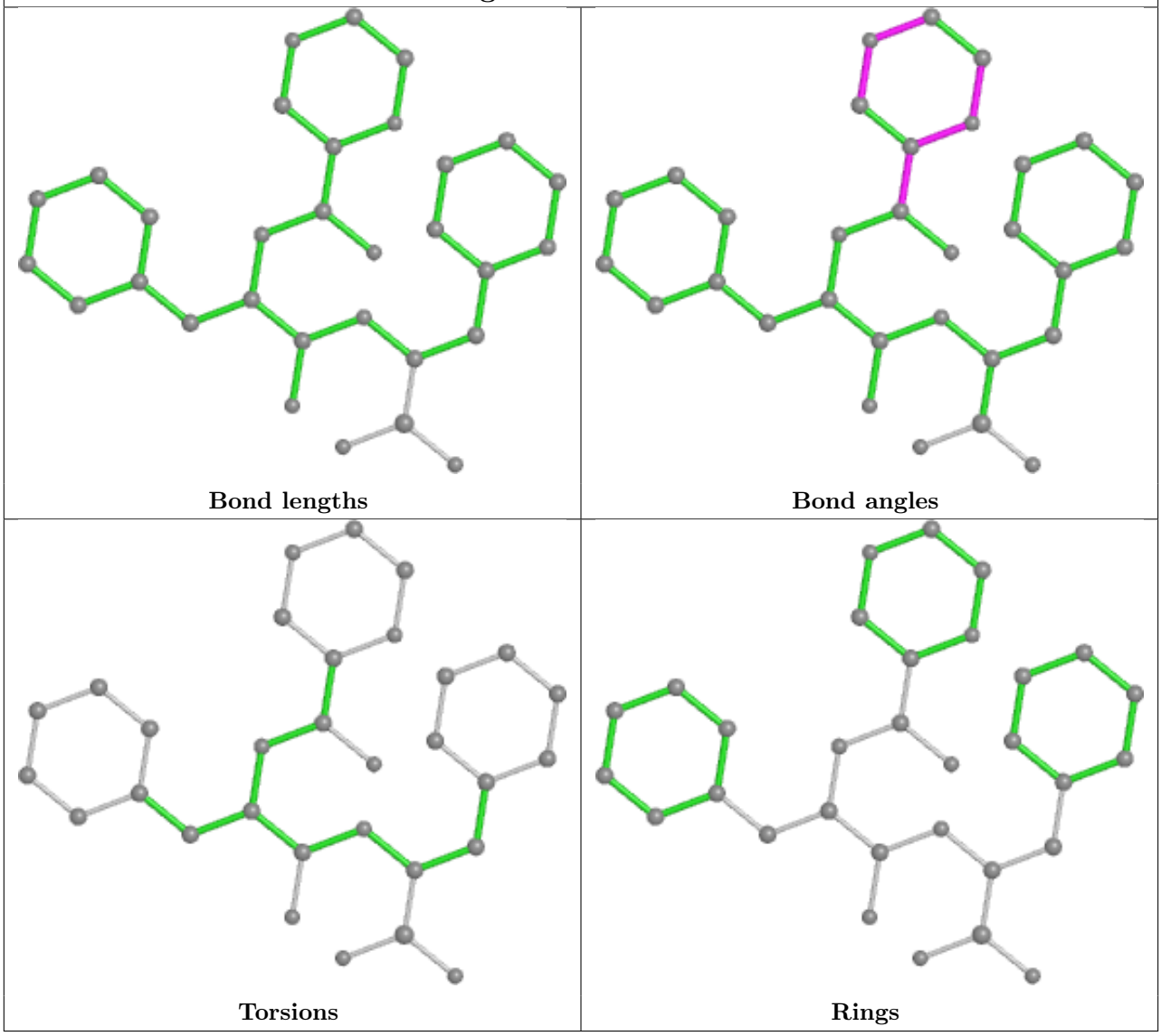
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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 4KZ A 801

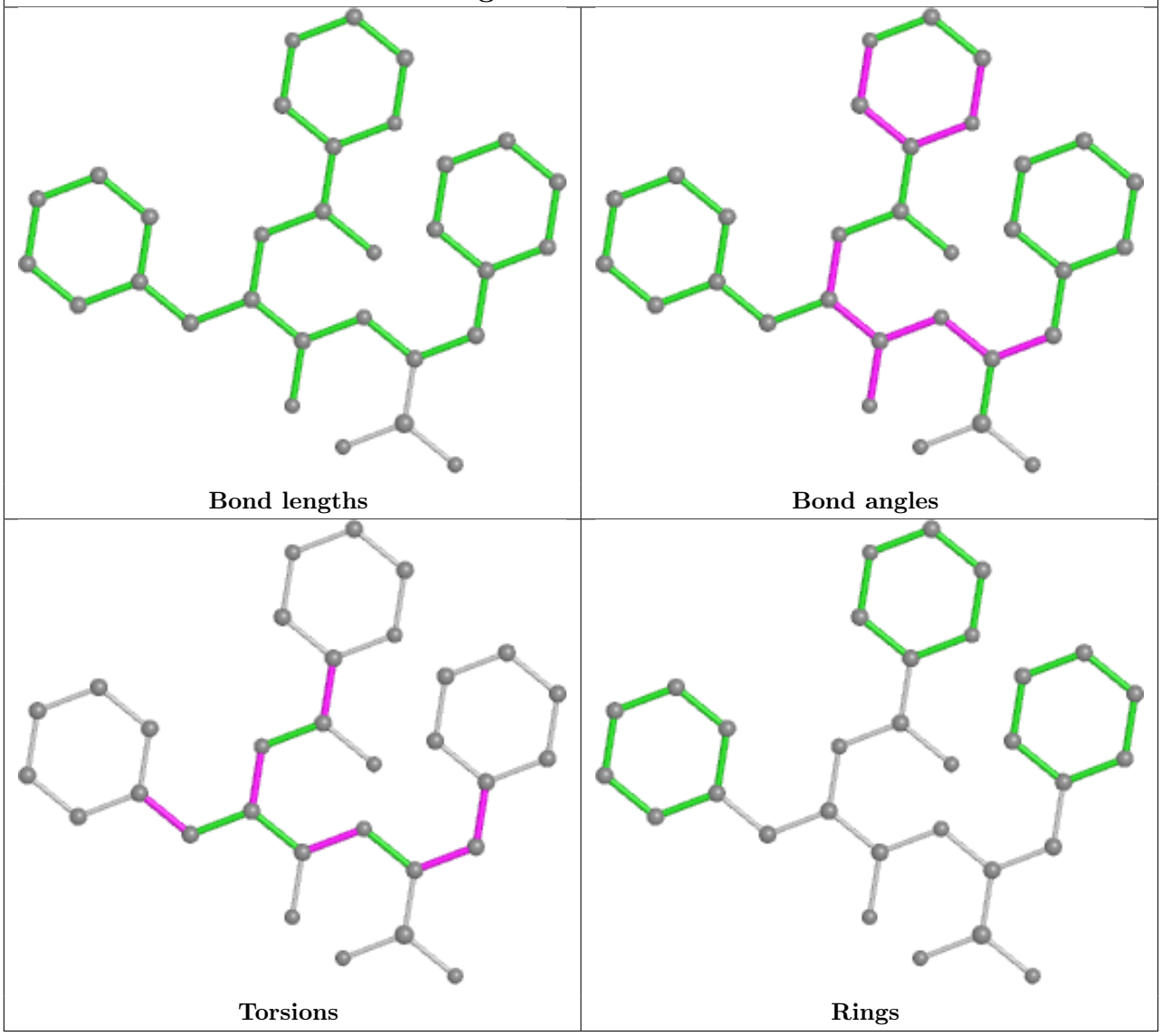


Ligand ADP F 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

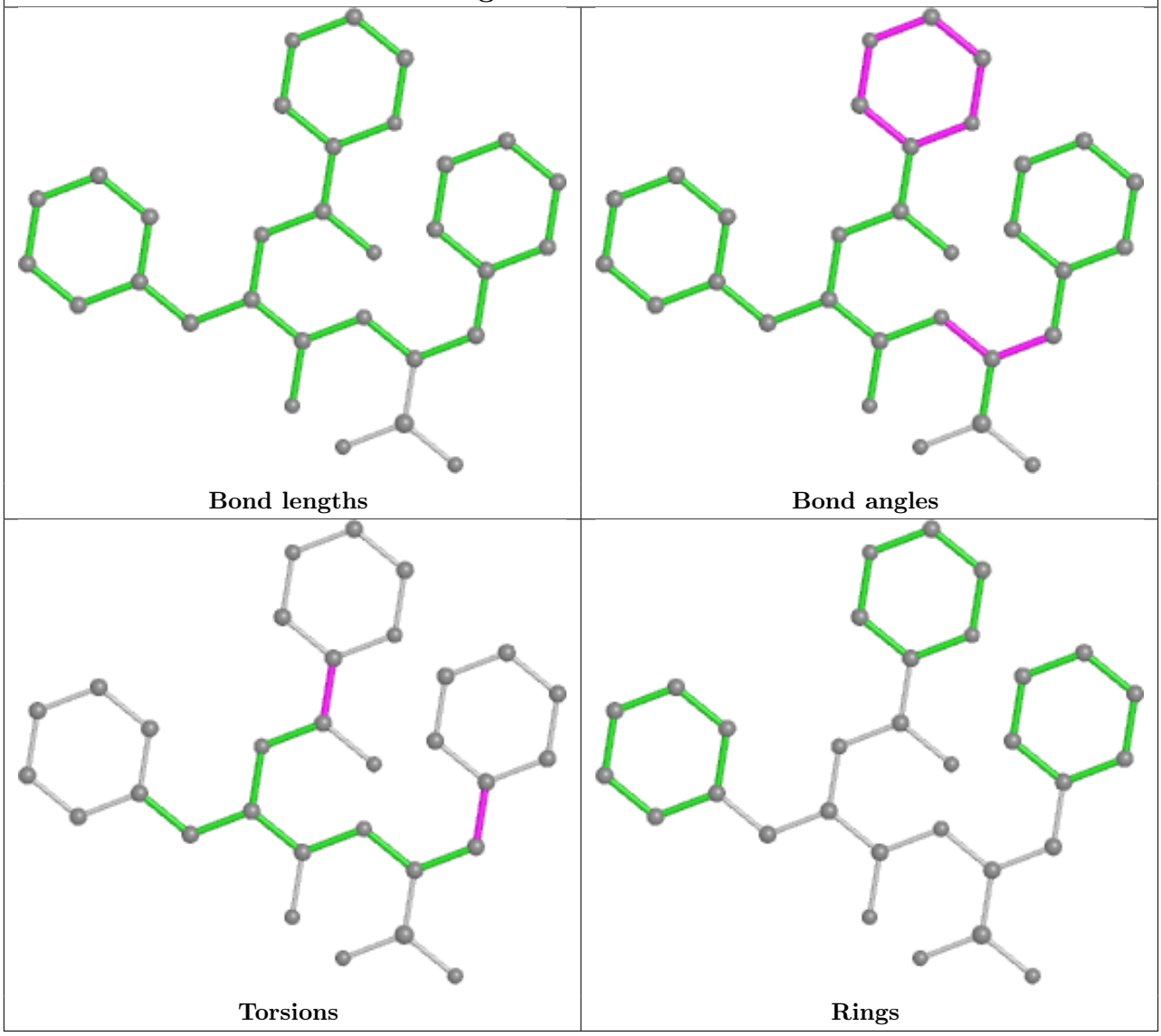
Ligand 4KZ F 802



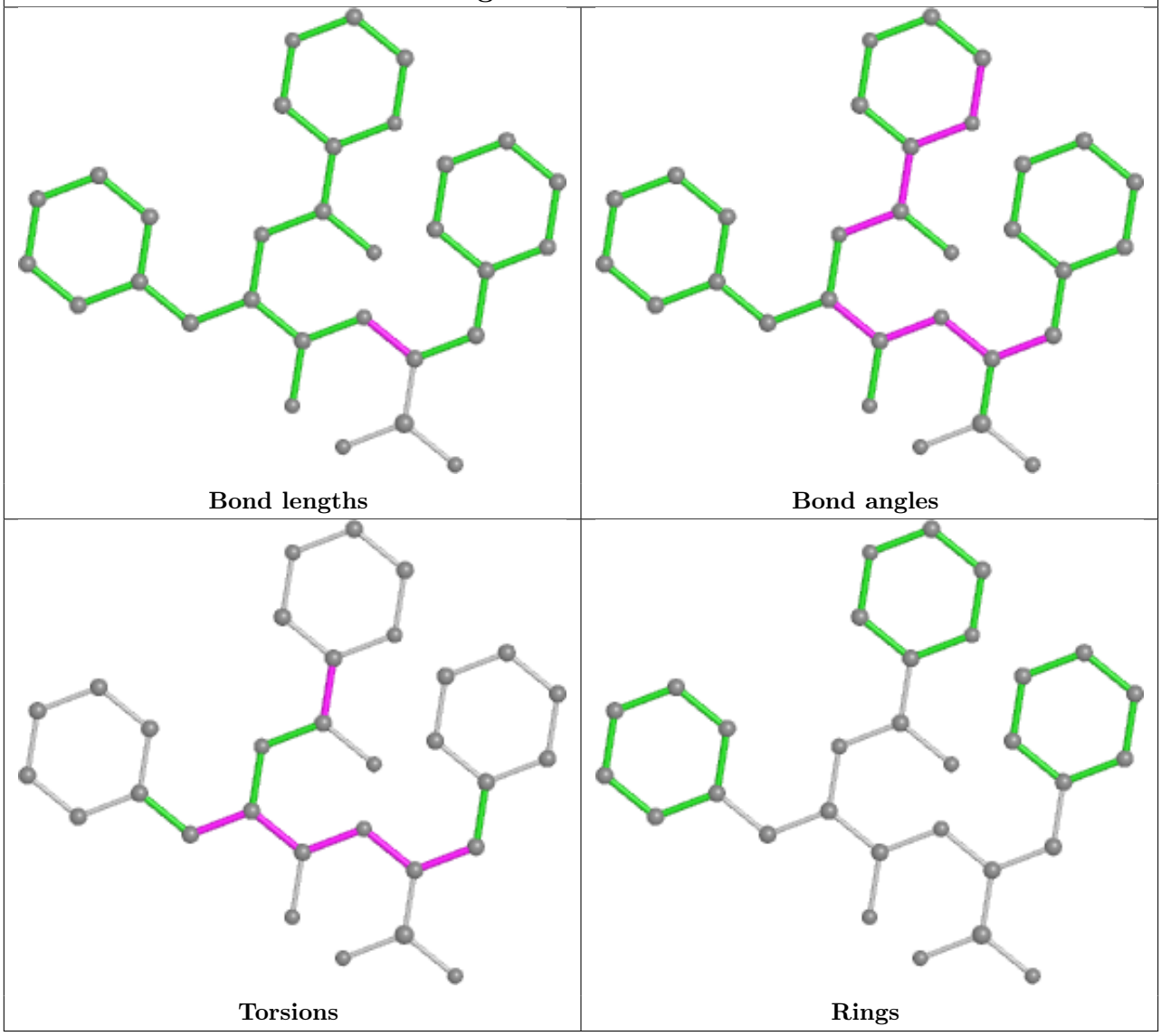
Ligand 4KZ B 802



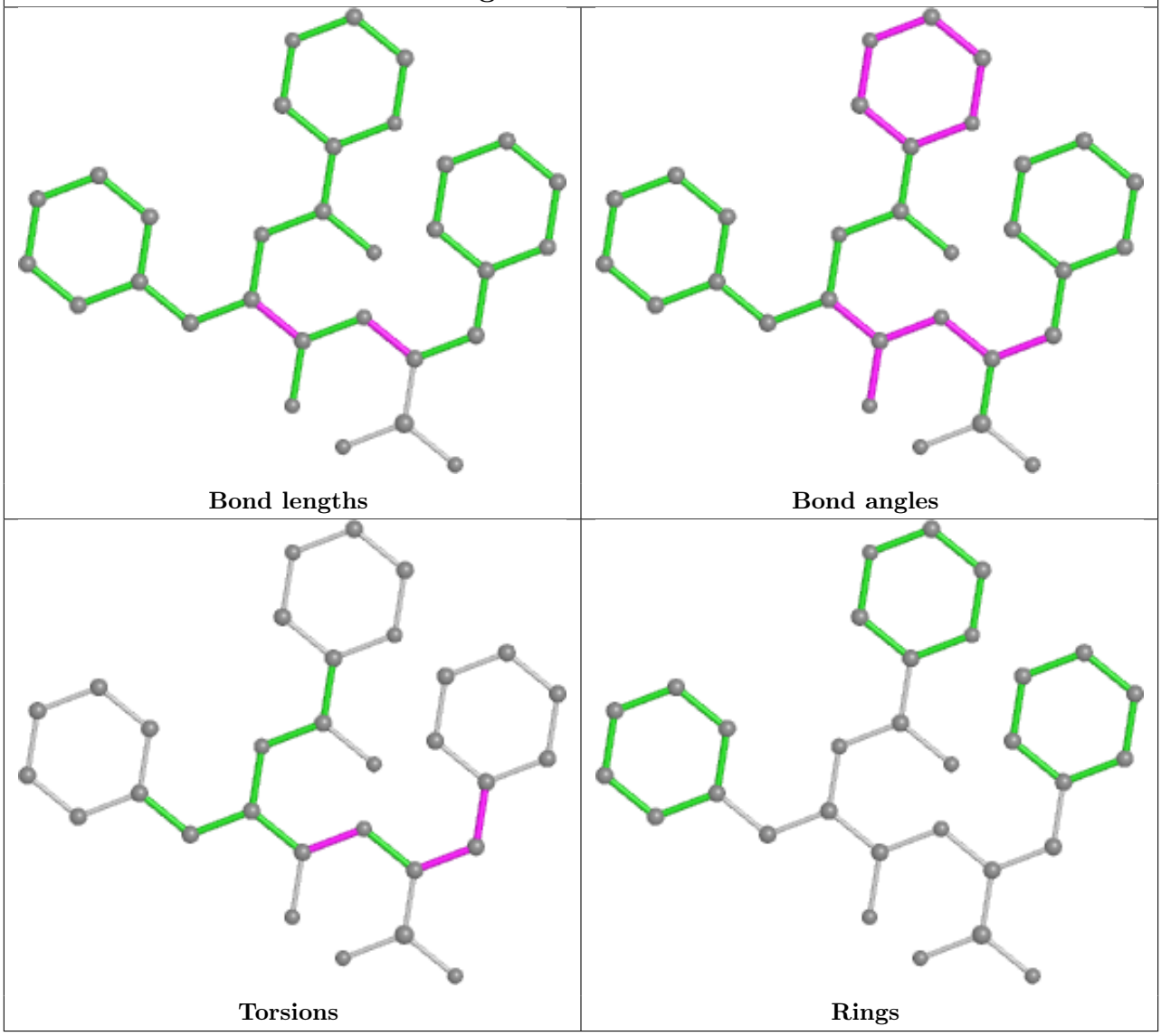
Ligand 4KZ C 801



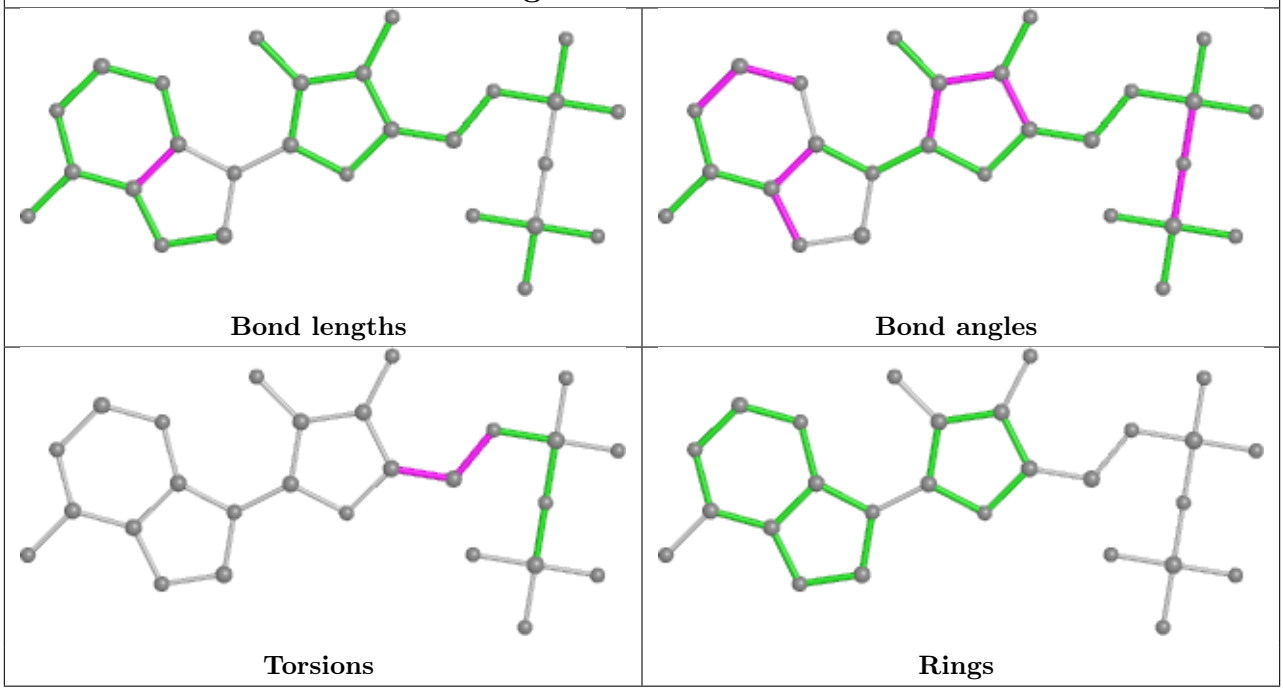
Ligand 4KZ D 802



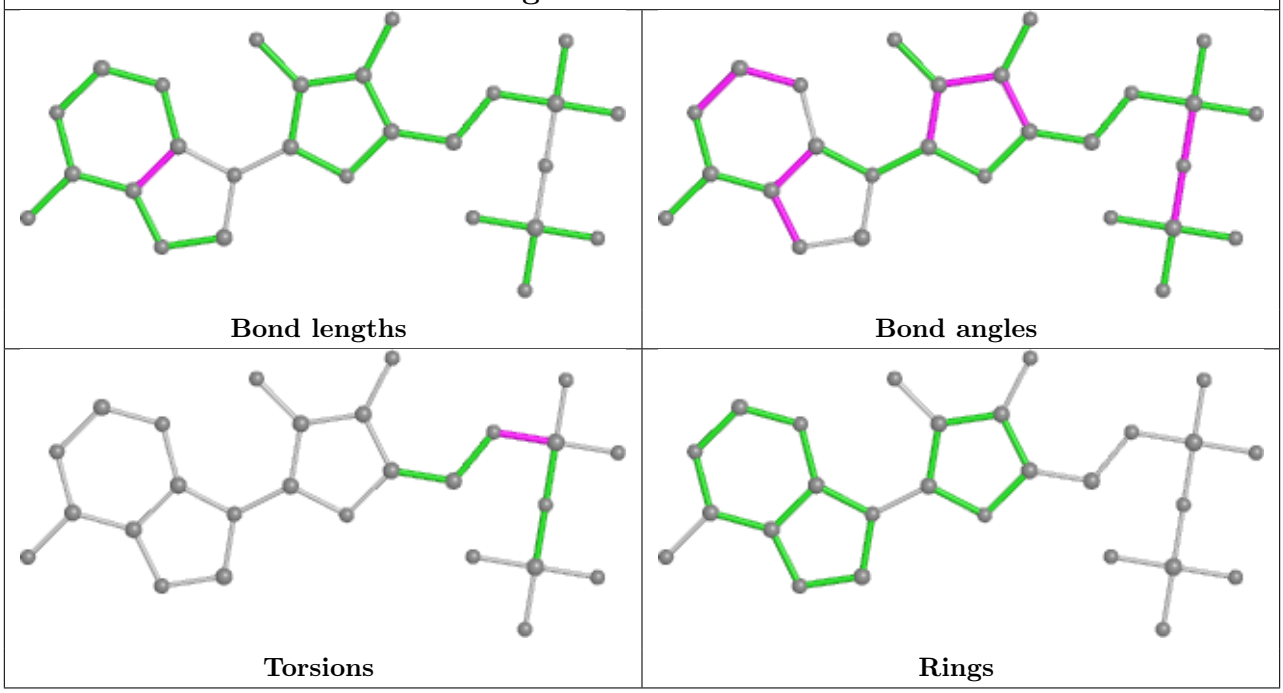
Ligand 4KZ E 801



Ligand ADP B 801



Ligand ADP D 801



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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	537/555 (96%)	-0.06	3 (0%)	89	87	31, 57, 94, 130	0
1	B	537/555 (96%)	0.01	7 (1%)	77	73	32, 62, 112, 141	0
1	C	538/555 (96%)	0.23	30 (5%)	24	24	27, 63, 121, 148	0
1	D	537/555 (96%)	0.01	11 (2%)	65	63	27, 59, 109, 127	0
1	E	537/555 (96%)	0.28	28 (5%)	27	27	30, 75, 132, 155	0
1	F	538/555 (96%)	-0.11	11 (2%)	65	63	25, 55, 104, 129	0
All	All	3224/3330 (96%)	0.06	90 (2%)	53	51	25, 61, 115, 155	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	GLU	4.3
1	C	281	PRO	4.0
1	C	429	SER	3.9
1	C	396	THR	3.6
1	E	273	LEU	3.5
1	A	399	GLY	3.4
1	C	430	ASP	3.2
1	C	428	SER	3.2
1	C	402	PRO	3.1
1	A	398	ILE	3.0
1	F	307	ASP	3.0
1	E	272	ARG	2.9
1	C	278	GLN	2.9
1	F	343	ASP	2.9
1	C	274	GLU	2.9
1	D	776	MET	2.8
1	B	431	TRP	2.8
1	C	291	ASP	2.7
1	C	270	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	251	LYS	2.7
1	C	273	LEU	2.6
1	E	301	ALA	2.6
1	B	299	SER	2.6
1	E	397	TYR	2.6
1	B	780	VAL	2.6
1	B	393	HIS	2.6
1	D	775	THR	2.5
1	E	399	GLY	2.5
1	D	777	PRO	2.5
1	C	400	ALA	2.5
1	D	339	THR	2.5
1	D	341	GLY	2.5
1	F	430	ASP	2.5
1	E	454	HIS	2.5
1	D	301	ALA	2.5
1	D	778	PRO	2.5
1	C	284	THR	2.5
1	B	282	GLU	2.4
1	A	780	VAL	2.4
1	C	248	ALA	2.4
1	E	346	ASN	2.4
1	C	243	LEU	2.4
1	C	244	SER	2.4
1	E	400	ALA	2.4
1	E	455	TYR	2.4
1	F	397	TYR	2.4
1	C	565	GLY	2.4
1	E	264	THR	2.3
1	C	401	MET	2.3
1	E	552	ARG	2.3
1	E	297	PRO	2.3
1	E	284	THR	2.3
1	E	492	GLY	2.3
1	E	304	GLU	2.3
1	C	563	TRP	2.3
1	C	780	VAL	2.3
1	E	780	VAL	2.3
1	D	337	GLN	2.3
1	B	777	PRO	2.2
1	E	244	SER	2.2
1	F	433	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	588	ALA	2.2
1	C	258	MET	2.2
1	F	385	ARG	2.2
1	E	298	TRP	2.2
1	E	286	ALA	2.2
1	E	245	ASP	2.2
1	C	292	TRP	2.2
1	C	259	PRO	2.2
1	E	266	ALA	2.2
1	E	452	THR	2.2
1	C	342	LEU	2.1
1	F	260	GLU	2.1
1	B	273	LEU	2.1
1	E	775	THR	2.1
1	D	303	PRO	2.1
1	E	274	GLU	2.1
1	E	453	ASP	2.1
1	C	280	SER	2.1
1	F	344	VAL	2.1
1	C	431	TRP	2.0
1	C	260	GLU	2.0
1	C	460	TYR	2.0
1	E	283	ALA	2.0
1	C	257	GLY	2.0
1	D	774	PRO	2.0
1	D	433	GLY	2.0
1	E	457	ASP	2.0
1	F	244	SER	2.0
1	F	428	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

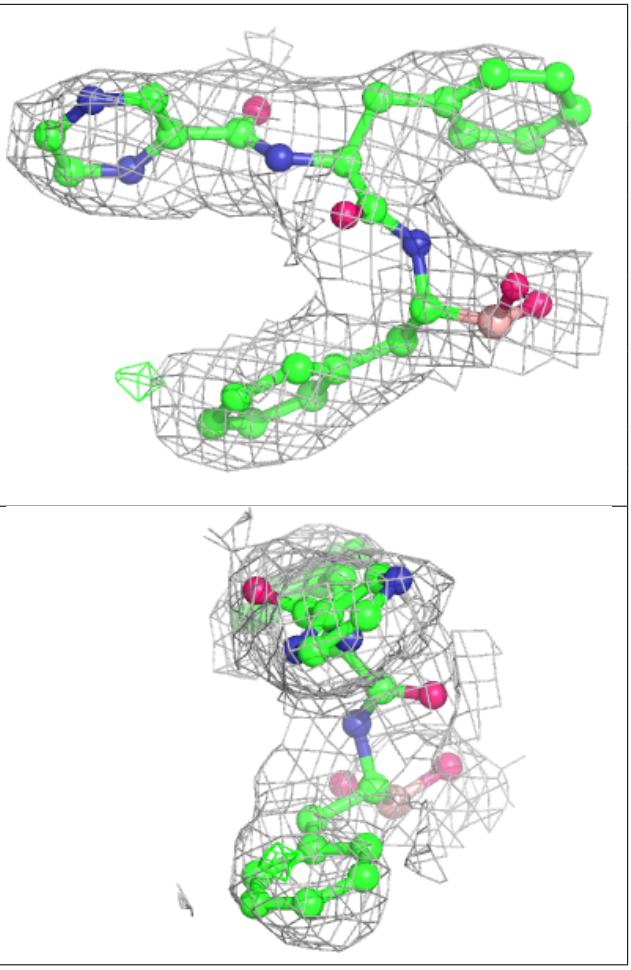
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4KZ	B	802	31/31	0.92	0.24	42,47,64,70	0
2	4KZ	D	802	31/31	0.92	0.24	31,38,50,55	0
2	4KZ	C	801	31/31	0.94	0.28	31,32,37,39	0
2	4KZ	F	802	31/31	0.94	0.21	34,41,44,44	0
2	4KZ	A	801	31/31	0.94	0.30	46,52,58,59	0
2	4KZ	E	801	31/31	0.94	0.26	37,42,47,48	0
3	ADP	B	801	27/27	0.95	0.19	38,45,52,55	0
3	ADP	F	801	27/27	0.96	0.18	38,46,50,52	0
3	ADP	D	801	27/27	0.96	0.17	41,45,49,51	0

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

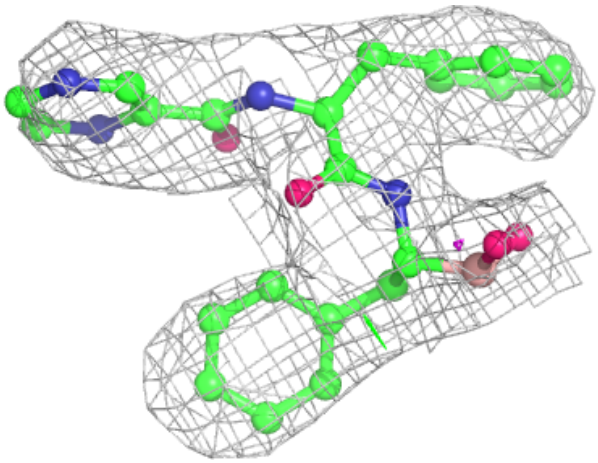
Electron density around 4KZ B 802:

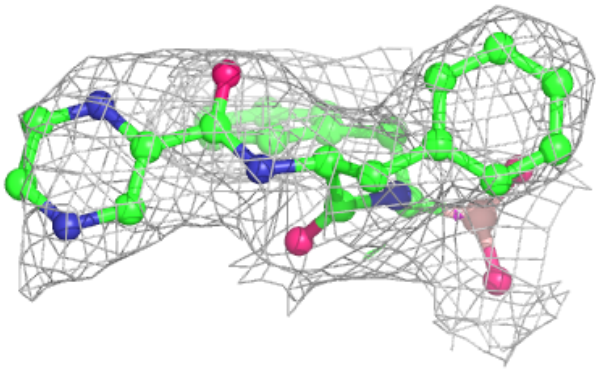
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

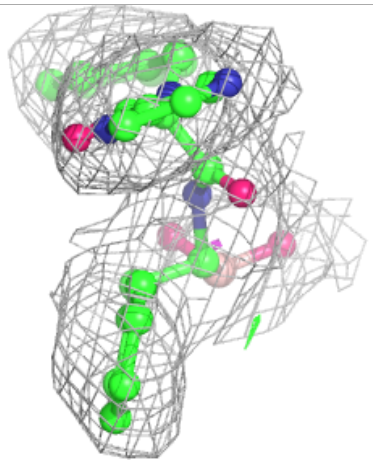


Electron density around 4KZ D 802:

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

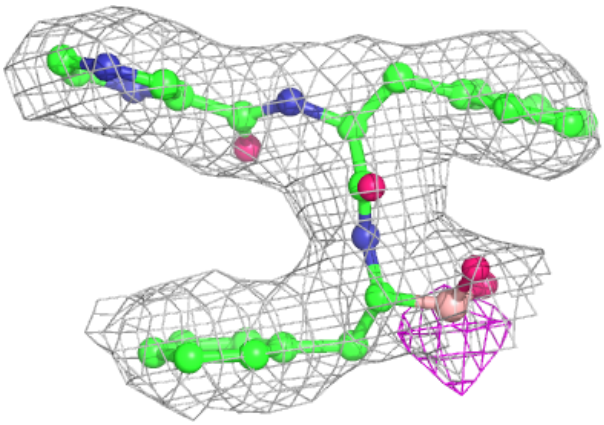


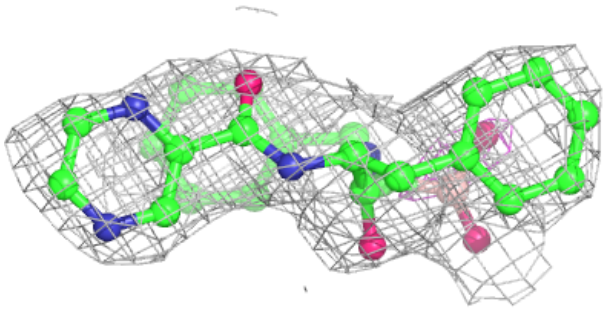


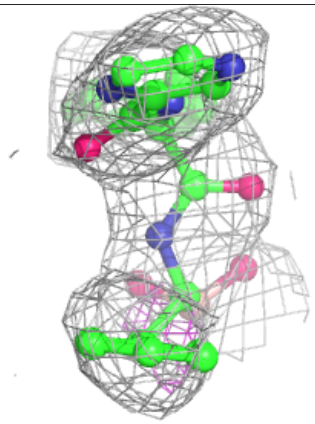


Electron density around 4KZ C 801:

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

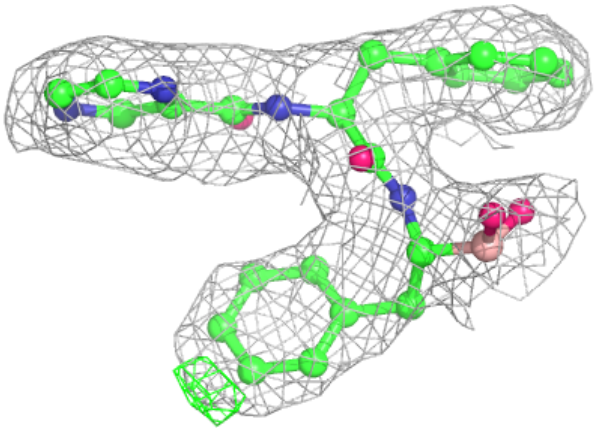


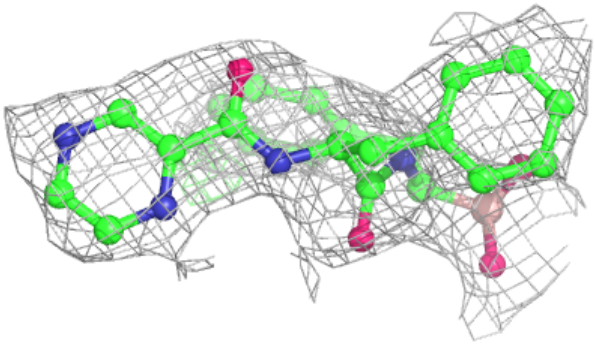


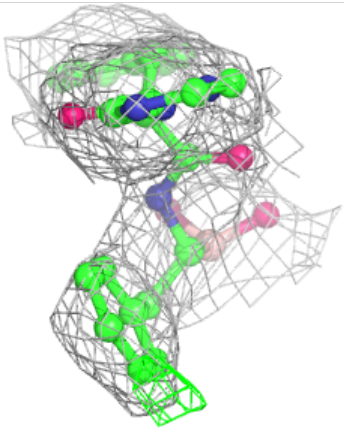


Electron density around 4KZ F 802:

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

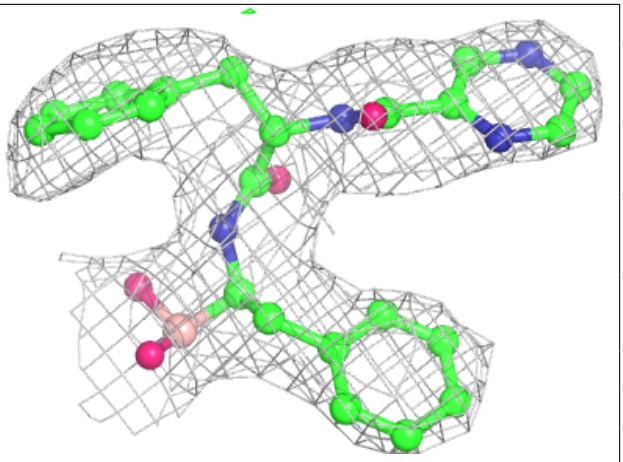


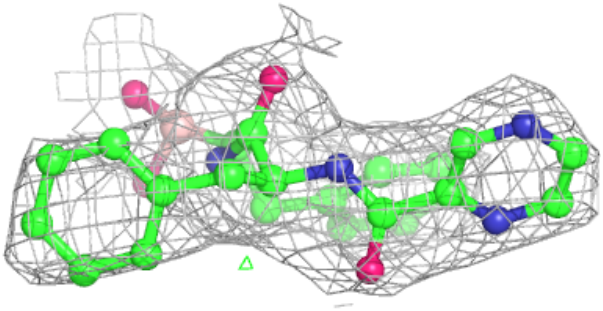


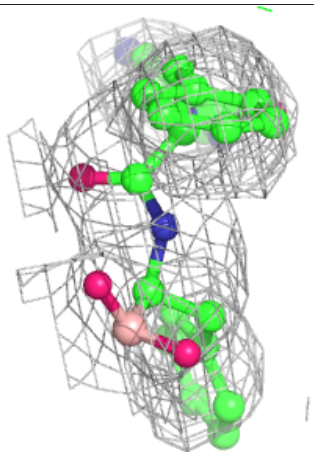


Electron density around 4KZ A 801:

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

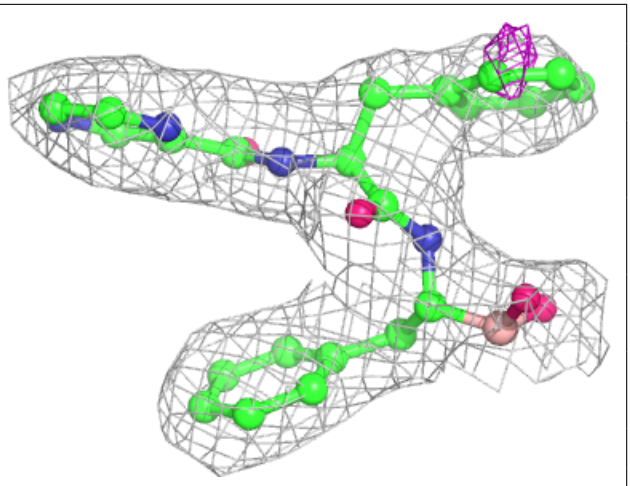


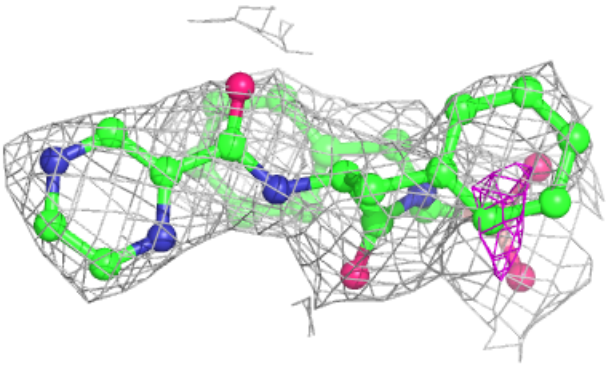


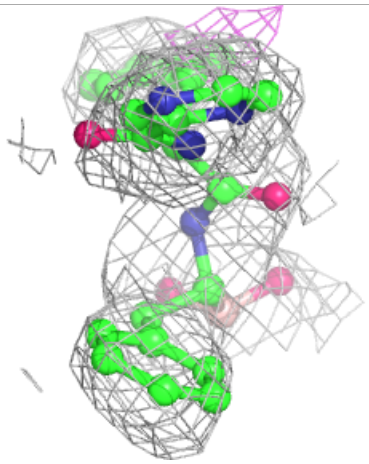


Electron density around 4KZ E 801:

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

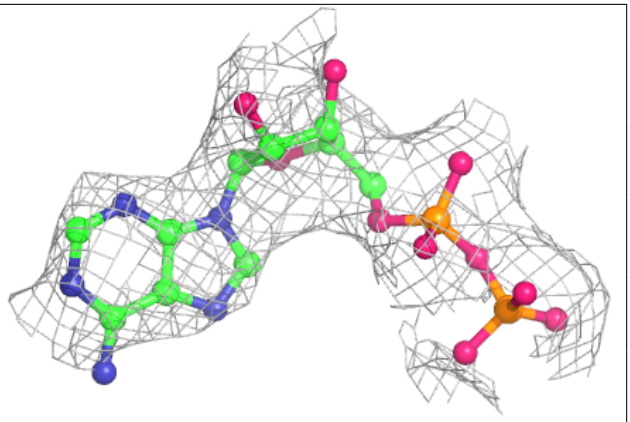


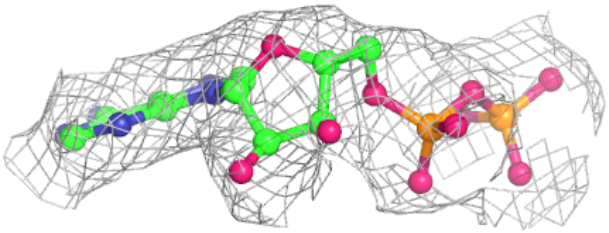


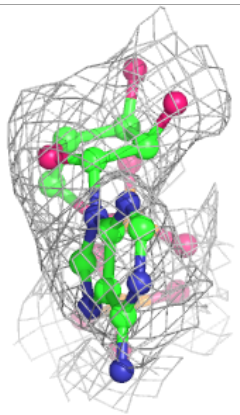


Electron density around ADP B 801:

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

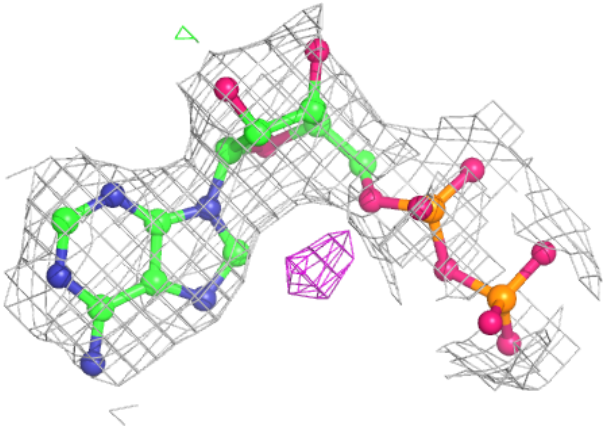


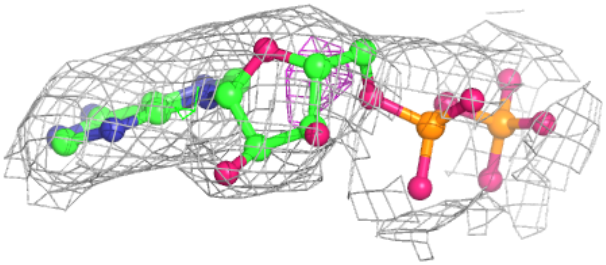


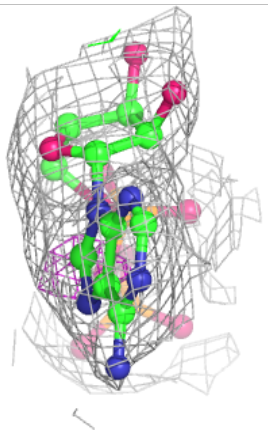


Electron density around ADP F 801:

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

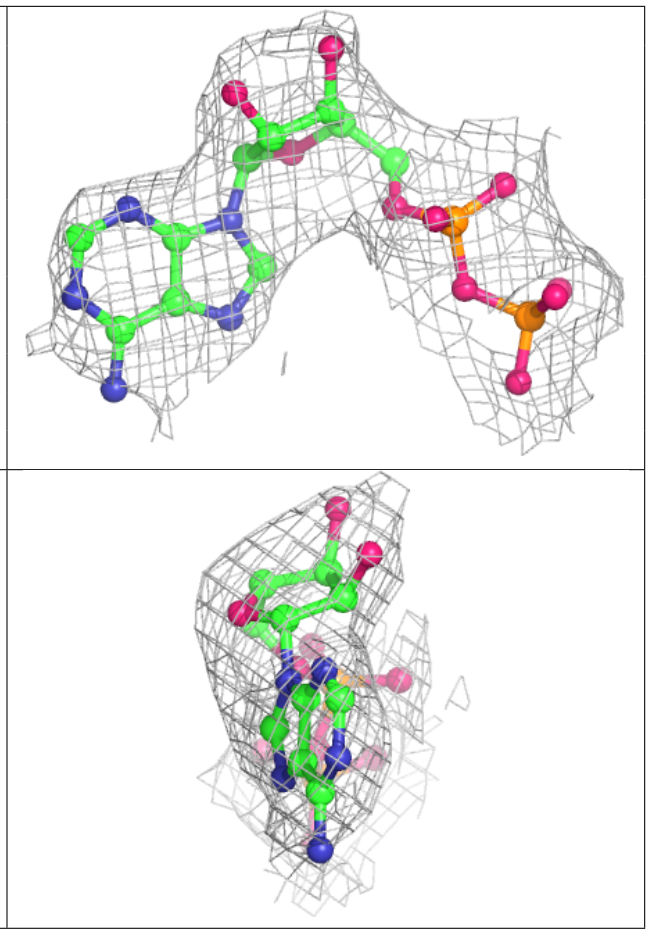






Electron density around ADP D 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.