Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 06:36 AM EDT

PDB ID	:	1Q3S
Title	:	Crystal structure of the chaperonin from Thermococcus strain KS-1 (FormIII crystal complexed with ADP)
Authors	:	Shomura, Y.; Yoshida, T.; Iizuka, R.; Maruyama, T.; Yohda, M.; Miki, K.
Deposited on	:	2003-07-31
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

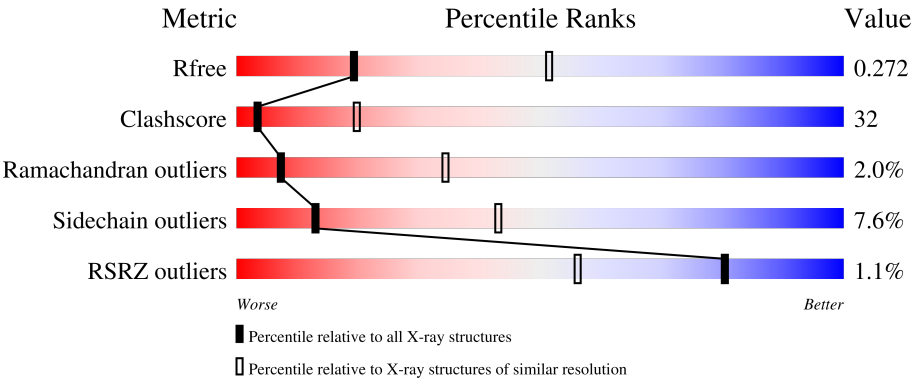
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	548	47% 42% 5% 6%
1	B	548	47% 43% · 6%
1	C	548	43% 47% · 6%
1	D	548	42% 46% 6% 6%
1	E	548	42% 48% 5% 6%

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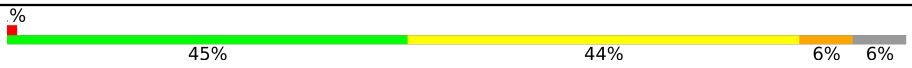
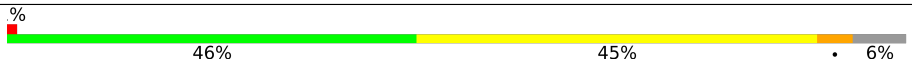
Mol	Chain	Length	Quality of chain
1	F	548	
1	G	548	
1	H	548	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31751 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 Thermosome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	B	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	C	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	D	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	E	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	F	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	G	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			
1	H	517	Total	C	N	O	S	0	0	0
			3941	2482	672	770	17			

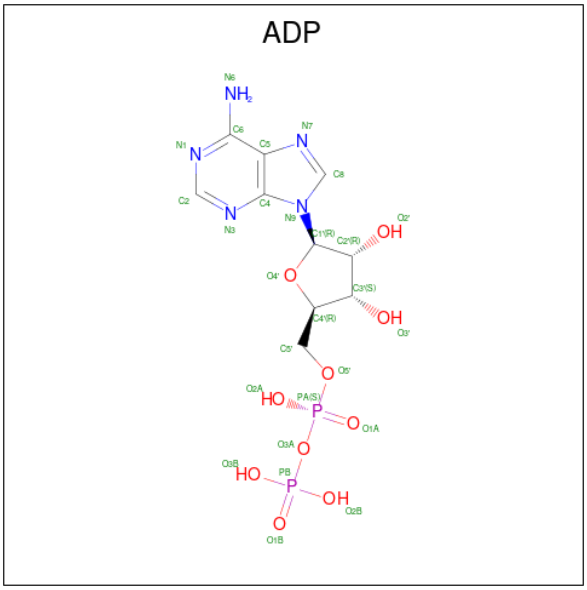
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	CYS	GLY	engineered mutation	UNP O24729
B	65	CYS	GLY	engineered mutation	UNP O24729
C	65	CYS	GLY	engineered mutation	UNP O24729
D	65	CYS	GLY	engineered mutation	UNP O24729
E	65	CYS	GLY	engineered mutation	UNP O24729
F	65	CYS	GLY	engineered mutation	UNP O24729
G	65	CYS	GLY	engineered mutation	UNP O24729
H	65	CYS	GLY	engineered mutation	UNP O24729

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

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

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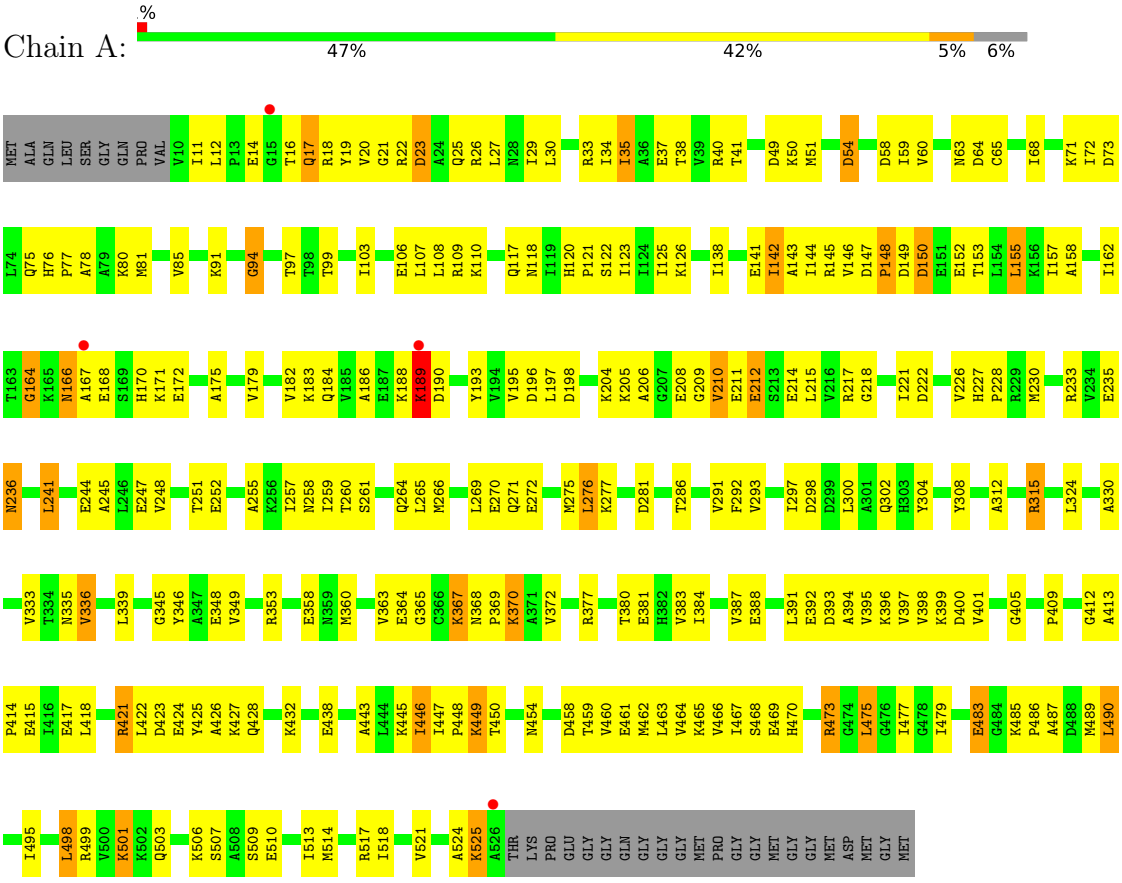
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

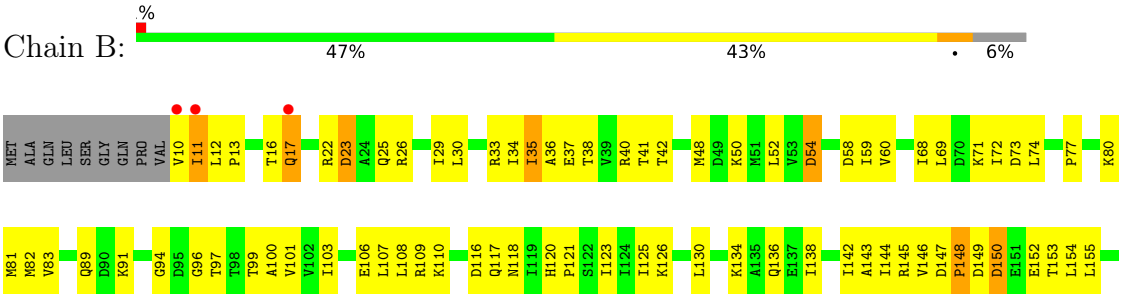
3 Residue-property plots (i)

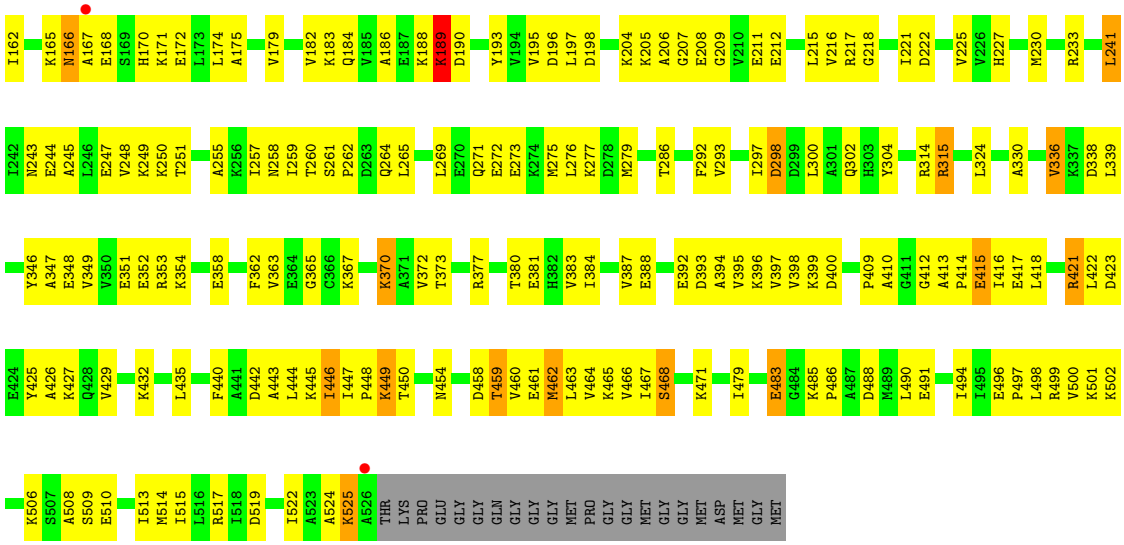
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Thermosome alpha subunit



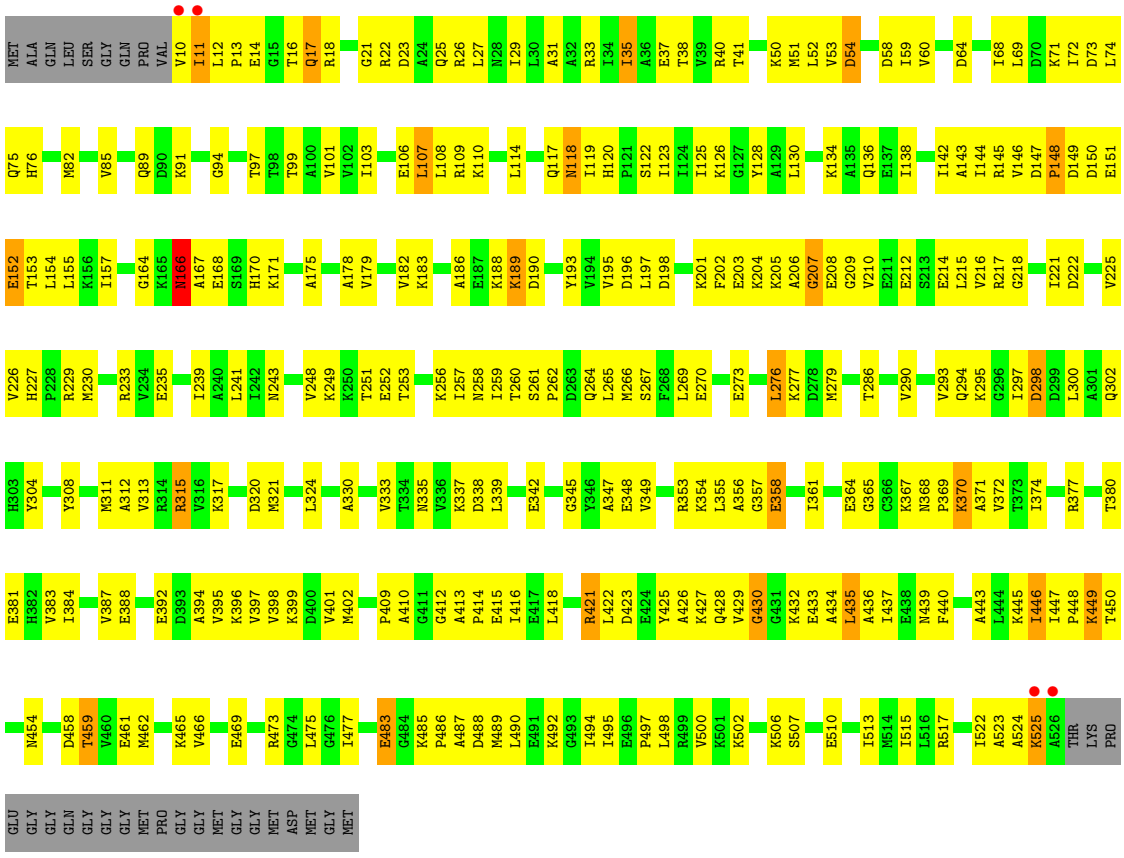
• Molecule 1: Thermosome alpha subunit





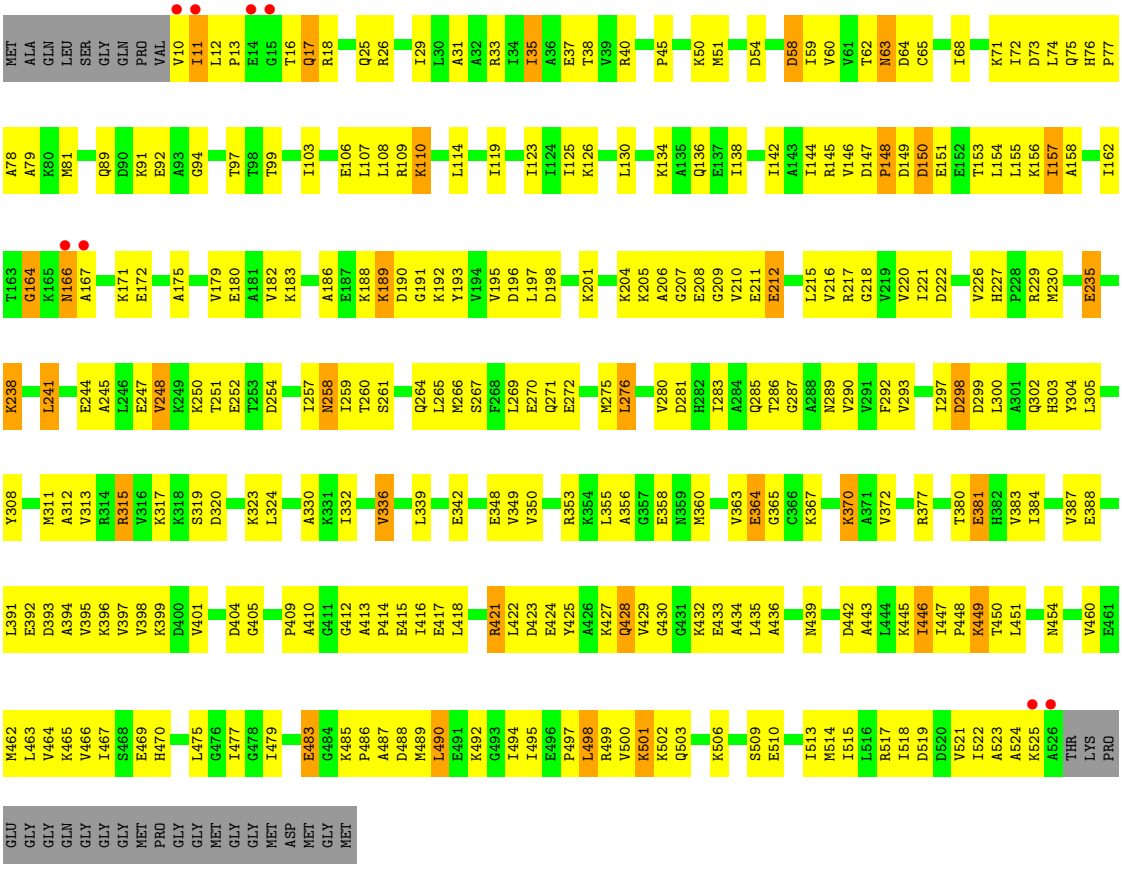
• Molecule 1: Thermosome alpha subunit

Chain C:



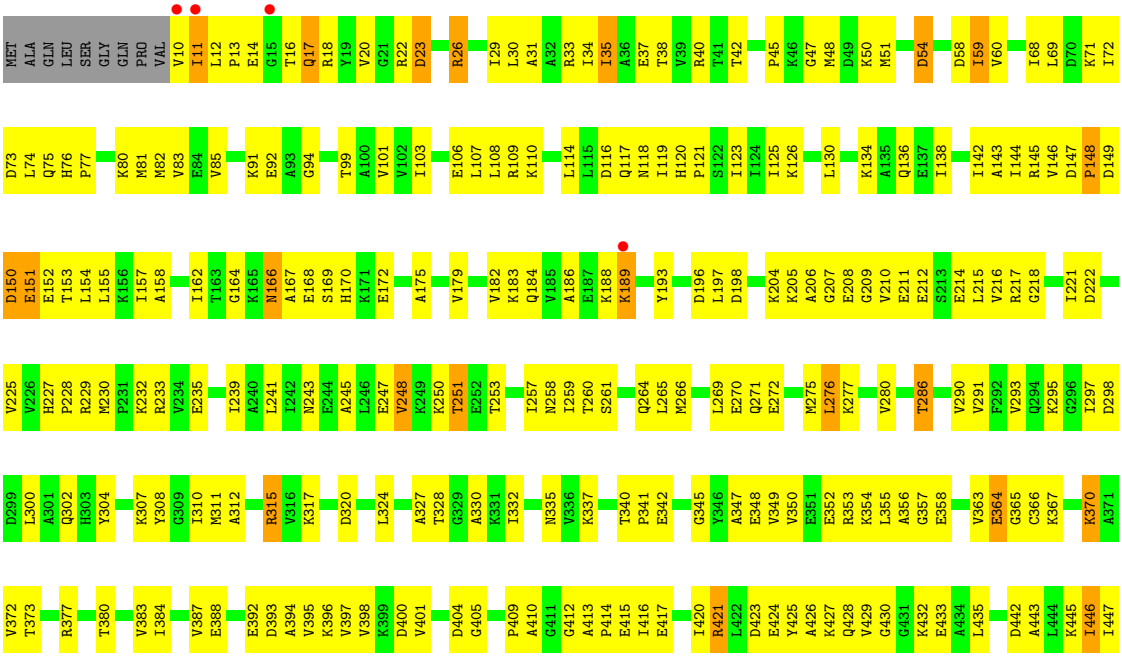
• Molecule 1: Thermosome alpha subunit

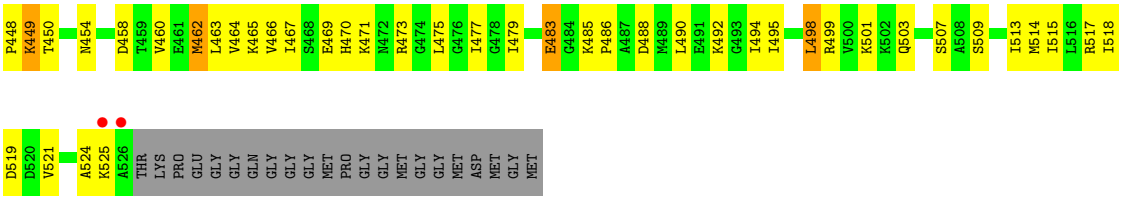
Chain D:



• Molecule 1: Thermosome alpha subunit

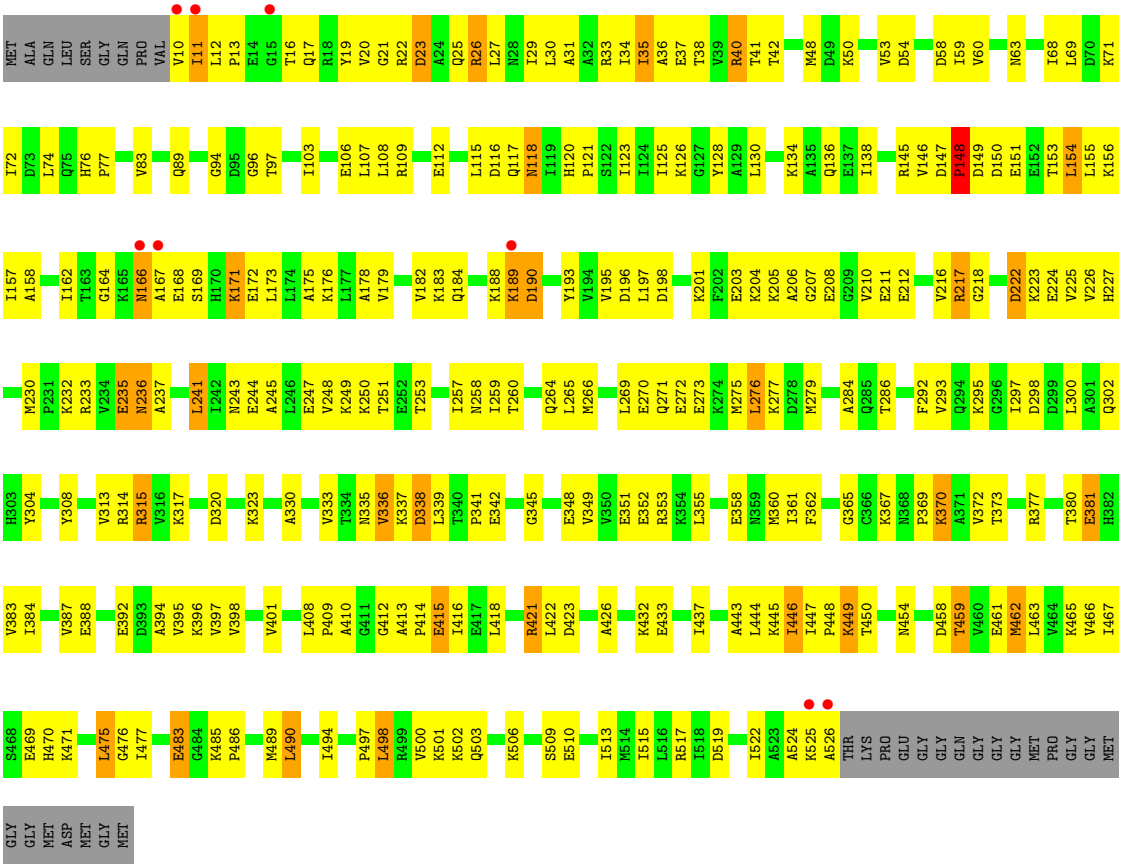
Chain E:





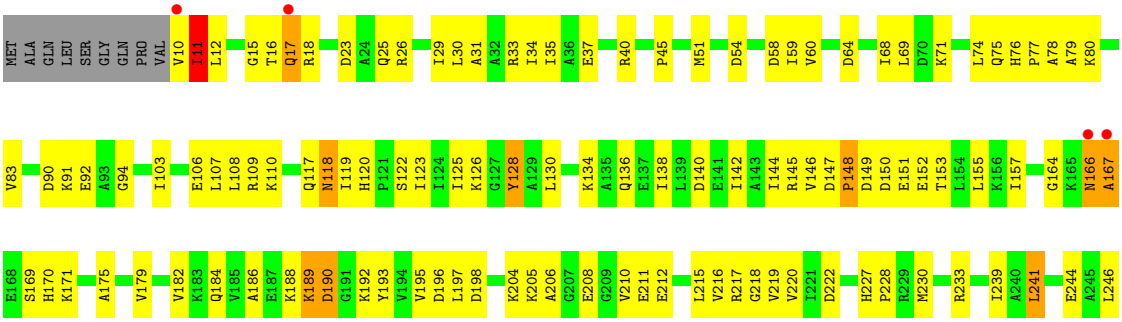
• Molecule 1: Thermosome alpha subunit

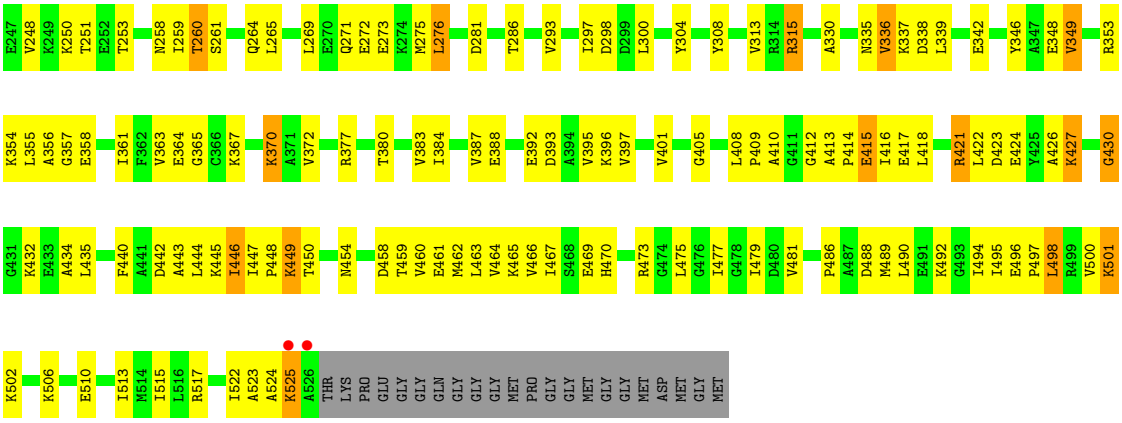
Chain F:



• Molecule 1: Thermosome alpha subunit

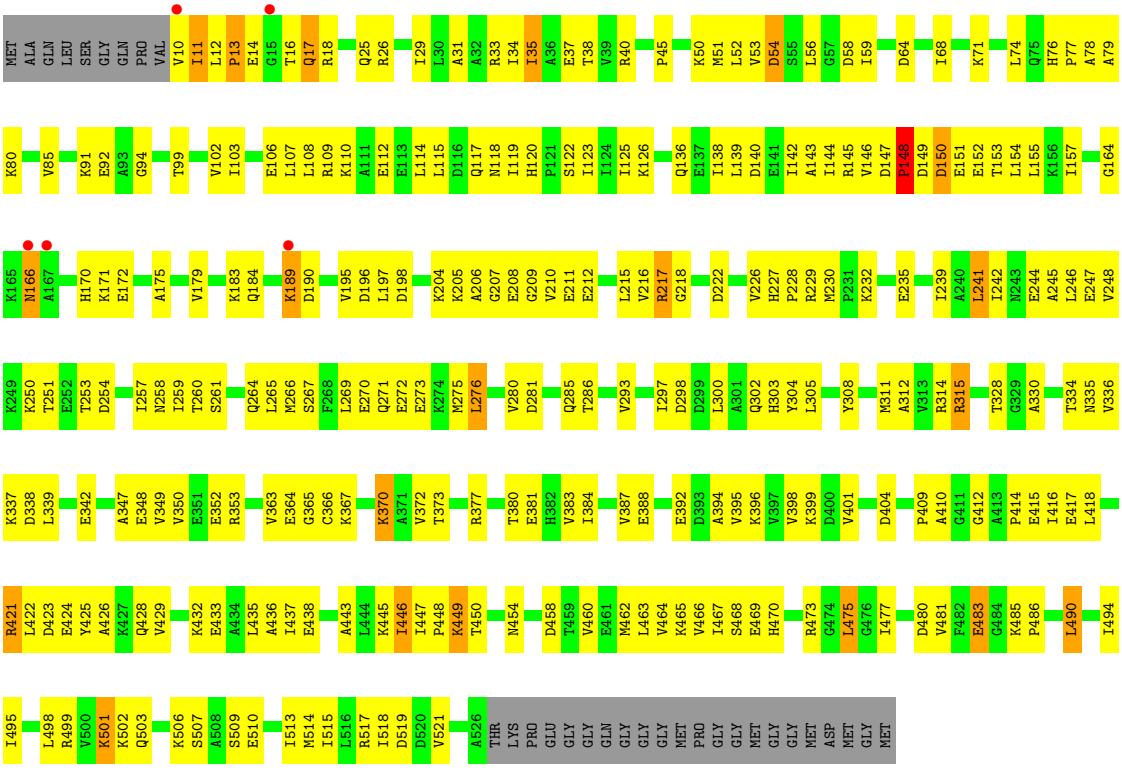
Chain G:





• Molecule 1: Thermosome alpha subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	207.43Å 236.23Å 234.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.62 – 3.00 155.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (73.62-3.00) 98.1 (155.87-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.288 0.233 , 0.272	Depositor DCC
R_{free} test set	5646 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	31751	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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

5.1 Standard geometry

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

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	0.43	0/3976	0.65	1/5358 (0.0%)
1	B	0.43	0/3976	0.66	0/5358
1	C	0.43	0/3976	0.65	1/5358 (0.0%)
1	D	0.42	0/3976	0.64	1/5358 (0.0%)
1	E	0.42	0/3976	0.66	0/5358
1	F	0.42	0/3976	0.65	0/5358
1	G	0.41	0/3976	0.64	0/5358
1	H	0.41	0/3976	0.64	0/5358
All	All	0.42	0/31808	0.65	3/42864 (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	C	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	207	GLY	O-C-N	-8.59	108.95	122.70
1	D	238	LYS	N-CA-C	-5.90	95.08	111.00
1	A	164	GLY	N-CA-C	-5.45	99.48	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	207	GLY	Mainchain
1	E	207	GLY	Mainchain

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	3941	0	4122	274	0
1	B	3941	0	4122	254	0
1	C	3941	0	4122	271	0
1	D	3941	0	4122	296	0
1	E	3941	0	4122	333	0
1	F	3941	0	4122	270	0
1	G	3941	0	4122	248	0
1	H	3941	0	4122	268	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	1	0
3	G	27	0	12	2	0
3	H	27	0	12	1	0
All	All	31751	0	33072	2088	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 32.

All (2088) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:THR:HG22	1:D:383:VAL:HG23	1.26	1.15
1:H:380:THR:HG22	1:H:383:VAL:HG23	1.27	1.14
1:E:380:THR:HG22	1:E:383:VAL:HG23	1.23	1.11
1:A:380:THR:HG22	1:A:383:VAL:HG23	1.10	1.09
1:B:380:THR:HG22	1:B:383:VAL:HG23	1.34	1.09
1:C:10:VAL:HG22	1:C:11:ILE:H	1.19	1.07
1:H:106:GLU:HG3	1:H:446:ILE:HG12	1.07	1.06
1:B:10:VAL:HG22	1:B:11:ILE:H	1.20	1.05
1:C:380:THR:HG22	1:C:383:VAL:HG23	1.39	1.05
1:D:10:VAL:HG22	1:D:11:ILE:H	1.22	1.03
1:E:10:VAL:HG22	1:E:11:ILE:H	1.19	1.03
1:C:258:ASN:HB3	1:D:258:ASN:HD21	1.25	1.02
1:H:261:SER:H	1:H:264:GLN:HE21	1.03	1.00
1:A:166:ASN:HA	1:B:517:ARG:HH12	1.25	1.00
1:C:60:VAL:HG21	1:C:71:LYS:HE2	1.42	0.99
1:A:258:ASN:HD21	1:H:258:ASN:HB3	1.27	0.99
1:G:380:THR:HG22	1:G:383:VAL:HG23	1.42	0.99
1:C:260:THR:H	1:C:264:GLN:HE21	1.01	0.98
1:G:421:ARG:HB2	1:G:421:ARG:HH11	1.24	0.98
1:E:421:ARG:HH11	1:E:421:ARG:HB2	1.23	0.98
1:E:12:LEU:HD23	1:E:13:PRO:HD2	1.47	0.97
1:F:10:VAL:HG22	1:F:11:ILE:H	1.30	0.96
1:H:260:THR:H	1:H:264:GLN:NE2	1.62	0.96
1:B:260:THR:H	1:B:264:GLN:HE22	1.01	0.94
1:E:125:ILE:HG23	1:E:513:ILE:HG23	1.46	0.94
1:F:421:ARG:HB2	1:F:421:ARG:HH11	1.29	0.94
1:G:10:VAL:HG13	1:G:11:ILE:H	1.31	0.94
1:D:258:ASN:HB3	1:E:258:ASN:HD21	1.30	0.94
1:E:227:HIS:HB3	1:E:230:MET:HG3	1.50	0.93
1:D:125:ILE:HG23	1:D:513:ILE:HG23	1.51	0.93
1:A:260:THR:H	1:A:264:GLN:HE21	1.17	0.92
1:D:260:THR:H	1:D:264:GLN:NE2	1.67	0.92
1:H:106:GLU:HG3	1:H:446:ILE:CG1	1.98	0.92
1:C:421:ARG:HB2	1:C:421:ARG:HH11	1.33	0.91
1:F:380:THR:HG22	1:F:383:VAL:HG23	1.52	0.91
1:F:125:ILE:HG23	1:F:513:ILE:HG23	1.50	0.90
1:B:260:THR:H	1:B:264:GLN:NE2	1.71	0.89
1:A:166:ASN:HA	1:B:517:ARG:NH1	1.88	0.89
1:E:260:THR:H	1:E:264:GLN:NE2	1.69	0.89
1:H:125:ILE:HG23	1:H:513:ILE:HG23	1.52	0.89
1:H:260:THR:H	1:H:264:GLN:HE22	1.19	0.89
1:A:125:ILE:HG23	1:A:513:ILE:HG23	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:GLU:CG	1:H:446:ILE:HG12	1.99	0.88
1:D:383:VAL:O	1:D:387:VAL:HG23	1.74	0.88
1:H:10:VAL:HG22	1:H:11:ILE:H	1.39	0.88
1:H:380:THR:CG2	1:H:383:VAL:HG23	2.02	0.88
1:G:258:ASN:HB3	1:H:258:ASN:HD21	1.36	0.88
1:F:108:LEU:HD11	1:F:515:ILE:HD12	1.54	0.87
1:B:184:GLN:NE2	1:B:217:ARG:HH21	1.72	0.87
1:H:204:LYS:HB3	1:H:384:ILE:HG21	1.56	0.87
1:A:212:GLU:HB2	1:A:377:ARG:HG3	1.56	0.86
1:C:380:THR:CG2	1:C:383:VAL:HG23	2.03	0.86
1:A:204:LYS:HD2	1:A:384:ILE:HG22	1.57	0.86
1:E:293:VAL:HG21	1:E:297:ILE:HD11	1.56	0.86
1:F:166:ASN:HA	1:G:517:ARG:HH12	1.41	0.86
1:G:260:THR:H	1:G:264:GLN:HE21	1.21	0.86
1:G:155:LEU:HD22	1:G:179:VAL:HG21	1.57	0.85
1:G:54:ASP:OD1	1:G:58:ASP:HB3	1.76	0.85
1:B:466:VAL:HG22	1:B:486:PRO:HG3	1.59	0.85
1:D:421:ARG:HB2	1:D:421:ARG:HH11	1.42	0.84
1:F:524:ALA:O	1:F:525:LYS:HG3	1.77	0.84
1:C:380:THR:HG23	1:C:383:VAL:H	1.40	0.84
1:D:212:GLU:HB2	1:D:377:ARG:HG3	1.58	0.84
1:E:72:ILE:HD11	1:F:522:ILE:HD12	1.56	0.84
1:G:462:MET:HA	1:G:462:MET:HE3	1.59	0.84
1:A:370:LYS:HE2	1:A:370:LYS:HA	1.60	0.84
1:G:123:ILE:HG21	1:G:432:LYS:HB3	1.60	0.84
1:G:260:THR:H	1:G:264:GLN:NE2	1.76	0.84
1:A:204:LYS:HD3	1:A:388:GLU:OE2	1.76	0.84
1:B:204:LYS:HB3	1:B:384:ILE:HG21	1.61	0.83
1:C:409:PRO:HB3	1:C:490:LEU:CD1	2.07	0.83
1:D:269:LEU:HD12	1:E:251:THR:HG23	1.58	0.83
1:C:260:THR:H	1:C:264:GLN:NE2	1.76	0.83
1:B:145:ARG:HG2	1:B:145:ARG:HH11	1.43	0.83
1:F:260:THR:H	1:F:264:GLN:NE2	1.76	0.83
1:A:206:ALA:HA	1:A:384:ILE:HD11	1.62	0.82
1:B:380:THR:HG23	1:B:383:VAL:H	1.43	0.82
1:G:265:LEU:O	1:G:269:LEU:HD13	1.79	0.82
1:G:206:ALA:HA	1:G:384:ILE:HD11	1.62	0.82
1:E:380:THR:CG2	1:E:383:VAL:HG23	2.07	0.82
1:F:370:LYS:HE2	1:F:370:LYS:HA	1.61	0.82
1:F:388:GLU:O	1:F:392:GLU:HG3	1.80	0.82
1:E:179:VAL:O	1:E:183:LYS:HG3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ALA:HB3	1:F:494:ILE:HG22	1.61	0.82
1:H:227:HIS:HB3	1:H:230:MET:HG3	1.62	0.82
1:A:469:GLU:HB2	1:A:477:ILE:HG21	1.60	0.81
1:A:11:ILE:HG13	1:H:34:ILE:HG21	1.62	0.81
1:B:421:ARG:HH11	1:B:421:ARG:HB2	1.44	0.81
1:F:233:ARG:HH12	1:F:349:VAL:CG1	1.93	0.81
1:F:380:THR:HG23	1:F:383:VAL:H	1.45	0.81
1:F:445:LYS:O	1:F:449:LYS:HB2	1.81	0.81
1:H:54:ASP:HB3	1:H:58:ASP:HB3	1.59	0.81
1:A:138:ILE:HD13	1:A:421:ARG:HG2	1.61	0.81
1:E:184:GLN:HA	1:E:184:GLN:HE21	1.45	0.81
1:A:462:MET:O	1:A:466:VAL:HG23	1.81	0.81
1:C:266:MET:O	1:C:270:GLU:HG3	1.81	0.81
1:E:204:LYS:HD3	1:E:388:GLU:OE2	1.81	0.81
1:A:38:THR:O	1:A:50:LYS:HE3	1.80	0.80
1:F:184:GLN:NE2	1:F:217:ARG:HH21	1.79	0.80
1:A:380:THR:CG2	1:A:383:VAL:HG23	2.03	0.80
1:B:315:ARG:HG3	1:B:315:ARG:HH11	1.45	0.80
1:F:269:LEU:HD12	1:G:251:THR:HG23	1.63	0.80
1:G:421:ARG:HB2	1:G:421:ARG:NH1	1.96	0.80
1:C:144:ILE:HD11	1:C:490:LEU:HD21	1.62	0.80
1:E:272:GLU:HA	1:E:275:MET:HE3	1.62	0.80
1:C:17:GLN:NE2	1:C:17:GLN:H	1.80	0.80
1:G:380:THR:HG23	1:G:383:VAL:H	1.47	0.80
1:G:370:LYS:HE2	1:G:370:LYS:HA	1.64	0.80
1:D:204:LYS:HD2	1:D:384:ILE:HG22	1.64	0.79
1:A:144:ILE:HD11	1:A:490:LEU:HD21	1.65	0.79
1:A:269:LEU:HD12	1:B:251:THR:HG23	1.65	0.79
1:E:348:GLU:HB3	1:E:365:GLY:HA3	1.64	0.79
1:A:388:GLU:O	1:A:392:GLU:HG3	1.83	0.79
1:A:421:ARG:HB2	1:A:421:ARG:HH11	1.48	0.79
1:B:409:PRO:HB3	1:B:490:LEU:CD1	2.13	0.79
1:D:241:LEU:HD22	1:D:330:ALA:HB3	1.65	0.79
1:C:54:ASP:OD1	1:C:58:ASP:HB3	1.83	0.78
1:C:483:GLU:HG3	1:C:485:LYS:NZ	1.97	0.78
1:G:125:ILE:HD13	1:G:517:ARG:HG2	1.65	0.78
1:B:445:LYS:O	1:B:448:PRO:HD2	1.82	0.78
1:G:60:VAL:HG21	1:G:71:LYS:HE2	1.65	0.78
1:G:125:ILE:HG23	1:G:513:ILE:HG23	1.66	0.78
1:H:370:LYS:HA	1:H:370:LYS:HE2	1.66	0.78
1:A:380:THR:HG22	1:A:383:VAL:CG2	2.05	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:PRO:HA	1:E:495:ILE:HG22	1.65	0.77
1:A:204:LYS:HB3	1:A:384:ILE:CG2	2.15	0.77
1:F:217:ARG:HA	1:F:372:VAL:HG23	1.67	0.77
1:H:204:LYS:HD3	1:H:388:GLU:OE2	1.83	0.77
1:C:10:VAL:HG22	1:C:11:ILE:N	1.99	0.77
1:B:370:LYS:HE2	1:B:370:LYS:HA	1.64	0.77
1:D:73:ASP:HB3	1:E:13:PRO:HG2	1.66	0.77
1:E:233:ARG:HH12	1:E:349:VAL:CG1	1.97	0.77
1:G:75:GLN:HG2	1:H:13:PRO:HD3	1.67	0.77
1:E:10:VAL:HG22	1:E:11:ILE:N	1.98	0.76
1:C:166:ASN:HA	1:D:517:ARG:HH12	1.50	0.76
1:C:462:MET:O	1:C:466:VAL:HG23	1.84	0.76
1:D:265:LEU:O	1:D:269:LEU:HD13	1.85	0.76
1:B:166:ASN:HA	1:C:517:ARG:HH12	1.50	0.76
1:C:348:GLU:O	1:C:349:VAL:HG23	1.85	0.76
1:F:260:THR:H	1:F:264:GLN:HE21	1.33	0.76
1:B:380:THR:CG2	1:B:383:VAL:HG23	2.16	0.76
1:C:206:ALA:HA	1:C:384:ILE:HD11	1.67	0.76
1:F:106:GLU:HG2	1:F:446:ILE:HG13	1.67	0.76
1:E:466:VAL:HG22	1:E:486:PRO:HG3	1.68	0.76
1:D:12:LEU:HD21	1:D:16:THR:HG21	1.68	0.76
1:F:462:MET:O	1:F:466:VAL:HG23	1.85	0.76
1:H:215:LEU:HD11	1:H:372:VAL:HG21	1.66	0.76
1:G:204:LYS:HB3	1:G:384:ILE:HG21	1.67	0.76
1:G:208:GLU:HB3	1:G:212:GLU:HG3	1.68	0.76
1:C:125:ILE:HG23	1:C:513:ILE:HG23	1.67	0.76
1:D:204:LYS:HB3	1:D:384:ILE:HG21	1.65	0.76
1:B:10:VAL:HG22	1:B:11:ILE:N	1.98	0.75
1:B:206:ALA:HA	1:B:384:ILE:HD11	1.68	0.75
1:D:91:LYS:HB2	1:D:91:LYS:NZ	2.01	0.75
1:E:380:THR:HG23	1:E:383:VAL:H	1.50	0.75
1:G:144:ILE:HD11	1:G:490:LEU:HD21	1.66	0.75
1:C:175:ALA:O	1:C:179:VAL:HG23	1.87	0.75
1:D:217:ARG:HB3	1:D:217:ARG:NH1	2.00	0.75
1:G:25:GLN:O	1:G:29:ILE:HG13	1.85	0.75
1:G:244:GLU:OE1	1:G:336:VAL:HG22	1.85	0.75
1:H:204:LYS:HB3	1:H:384:ILE:CG2	2.16	0.75
1:A:369:PRO:O	1:A:370:LYS:HE2	1.85	0.75
1:B:462:MET:HE1	1:B:486:PRO:HD3	1.67	0.75
1:B:380:THR:HG22	1:B:383:VAL:CG2	2.14	0.75
1:D:73:ASP:O	1:E:13:PRO:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ILE:HB	1:G:475:LEU:HD22	1.69	0.75
1:D:94:GLY:HA3	1:D:396:LYS:HD2	1.67	0.75
1:E:462:MET:O	1:E:466:VAL:HG23	1.86	0.75
1:C:204:LYS:HB3	1:C:384:ILE:HG21	1.68	0.74
1:D:380:THR:CG2	1:D:383:VAL:HG23	2.12	0.74
1:F:466:VAL:HG22	1:F:486:PRO:HG3	1.67	0.74
1:D:10:VAL:HG22	1:D:11:ILE:N	2.02	0.74
1:H:136:GLN:NE2	1:H:502:LYS:HE3	2.02	0.74
1:B:410:ALA:HB3	1:B:494:ILE:HG22	1.68	0.74
1:G:166:ASN:HA	1:H:517:ARG:HH12	1.52	0.74
1:D:94:GLY:CA	1:D:396:LYS:HD2	2.18	0.74
1:H:447:ILE:HB	1:H:448:PRO:HD3	1.68	0.74
1:E:233:ARG:HH12	1:E:349:VAL:HG11	1.52	0.74
1:D:469:GLU:HB2	1:D:477:ILE:HG21	1.69	0.74
1:E:125:ILE:HG23	1:E:513:ILE:CG2	2.18	0.74
1:A:447:ILE:HB	1:A:448:PRO:HD3	1.70	0.74
1:F:446:ILE:O	1:F:450:THR:HG23	1.87	0.74
1:D:205:LYS:HD2	1:D:356:ALA:HB3	1.69	0.73
1:E:175:ALA:O	1:E:179:VAL:HG23	1.88	0.73
1:F:315:ARG:HH11	1:F:315:ARG:HG3	1.52	0.73
1:H:353:ARG:NH2	1:H:364:GLU:OE2	2.21	0.73
1:A:251:THR:HG23	1:H:269:LEU:HD12	1.70	0.73
1:G:138:ILE:HD13	1:G:421:ARG:HG2	1.70	0.73
1:H:261:SER:H	1:H:264:GLN:NE2	1.83	0.73
1:H:469:GLU:HB2	1:H:477:ILE:HG21	1.71	0.73
1:A:258:ASN:HB3	1:B:258:ASN:HD21	1.52	0.73
1:D:445:LYS:O	1:D:449:LYS:HB2	1.87	0.73
1:G:466:VAL:HG22	1:G:486:PRO:HG3	1.69	0.73
1:H:144:ILE:HD11	1:H:490:LEU:HD21	1.70	0.73
1:C:447:ILE:HB	1:C:448:PRO:HD3	1.69	0.73
1:H:206:ALA:HA	1:H:384:ILE:HD11	1.69	0.73
1:E:204:LYS:HB3	1:E:384:ILE:HG21	1.68	0.73
1:H:421:ARG:HH11	1:H:421:ARG:HB2	1.53	0.73
1:A:155:LEU:HD22	1:A:179:VAL:HG21	1.71	0.73
1:B:460:VAL:O	1:B:464:VAL:HG23	1.87	0.73
1:A:204:LYS:HB3	1:A:384:ILE:HG21	1.69	0.73
1:D:276:LEU:HD23	1:D:300:LEU:HB2	1.69	0.73
1:B:488:ASP:HB3	1:B:491:GLU:HG3	1.71	0.72
1:F:506:LYS:O	1:F:510:GLU:HG3	1.89	0.72
1:H:443:ALA:O	1:H:446:ILE:HG13	1.89	0.72
1:G:413:ALA:HB3	1:G:414:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ARG:HH11	1:C:315:ARG:HG3	1.54	0.72
1:H:462:MET:O	1:H:466:VAL:HG23	1.88	0.72
1:B:204:LYS:HD3	1:B:388:GLU:OE2	1.89	0.72
1:G:134:LYS:O	1:G:138:ILE:HG13	1.90	0.72
1:E:146:VAL:HG22	1:E:147:ASP:H	1.55	0.72
1:A:383:VAL:O	1:A:387:VAL:HG23	1.88	0.72
1:E:103:ILE:O	1:E:107:LEU:HB2	1.89	0.72
1:B:125:ILE:HG23	1:B:513:ILE:HG23	1.70	0.72
1:B:506:LYS:O	1:B:510:GLU:HG3	1.89	0.72
1:D:60:VAL:HG21	1:D:71:LYS:HE2	1.71	0.72
1:D:125:ILE:HD13	1:D:517:ARG:HG2	1.69	0.72
1:A:462:MET:HE3	1:A:462:MET:HA	1.72	0.72
1:D:123:ILE:HG21	1:D:432:LYS:HB2	1.71	0.72
1:E:258:ASN:HB3	1:F:258:ASN:HD21	1.54	0.72
1:G:59:ILE:HD12	1:G:59:ILE:N	2.05	0.72
1:H:483:GLU:HG3	1:H:485:LYS:NZ	2.05	0.72
1:D:315:ARG:HH11	1:D:315:ARG:HG3	1.52	0.71
1:H:513:ILE:O	1:H:517:ARG:HG3	1.90	0.71
1:G:473:ARG:HB2	1:G:477:ILE:HG13	1.72	0.71
1:H:143:ALA:HB3	1:H:145:ARG:HH12	1.55	0.71
1:H:266:MET:O	1:H:270:GLU:HG3	1.90	0.71
1:F:54:ASP:OD1	1:F:58:ASP:HB3	1.90	0.71
1:D:37:GLU:HG2	1:D:40:ARG:NH1	2.05	0.71
1:A:22:ARG:HG3	1:A:23:ASP:N	2.06	0.71
1:C:506:LYS:O	1:C:510:GLU:HG3	1.91	0.71
1:E:147:ASP:HB3	1:E:150:ASP:HB2	1.71	0.71
1:G:108:LEU:HD11	1:G:515:ILE:HD12	1.71	0.71
1:B:286:THR:HG21	1:B:339:LEU:HG	1.72	0.71
1:D:380:THR:HG22	1:D:383:VAL:CG2	2.14	0.71
1:E:184:GLN:HA	1:E:184:GLN:NE2	2.06	0.71
1:D:123:ILE:HG21	1:D:432:LYS:CB	2.21	0.71
1:F:11:ILE:O	1:F:11:ILE:HD13	1.90	0.71
1:C:380:THR:HG22	1:C:383:VAL:CG2	2.19	0.70
1:F:412:GLY:O	1:F:415:GLU:HG2	1.90	0.70
1:F:29:ILE:O	1:F:33:ARG:HG3	1.91	0.70
1:C:383:VAL:O	1:C:387:VAL:HG23	1.91	0.70
1:F:178:ALA:O	1:F:182:VAL:HG23	1.92	0.70
1:F:147:ASP:HB3	1:F:150:ASP:HB2	1.73	0.70
1:G:383:VAL:O	1:G:387:VAL:HG23	1.92	0.70
1:H:445:LYS:O	1:H:449:LYS:HB2	1.92	0.70
1:B:73:ASP:HB3	1:C:13:PRO:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:O	1:B:396:LYS:HE3	1.92	0.70
1:H:506:LYS:O	1:H:510:GLU:HG3	1.91	0.70
1:C:25:GLN:O	1:C:29:ILE:HG13	1.92	0.70
1:C:125:ILE:HD13	1:C:517:ARG:HG2	1.73	0.70
1:C:466:VAL:HG22	1:C:486:PRO:HG3	1.71	0.70
1:H:380:THR:HG22	1:H:383:VAL:CG2	2.16	0.70
1:A:91:LYS:HB2	1:A:91:LYS:NZ	2.06	0.70
1:B:446:ILE:O	1:B:450:THR:HG23	1.92	0.70
1:E:483:GLU:HG3	1:E:485:LYS:NZ	2.06	0.70
1:F:10:VAL:HG22	1:F:11:ILE:N	2.06	0.70
1:F:509:SER:O	1:F:513:ILE:HG13	1.92	0.70
1:G:460:VAL:O	1:G:464:VAL:HG23	1.91	0.70
1:D:348:GLU:HB3	1:D:365:GLY:HA3	1.74	0.70
1:B:462:MET:HA	1:B:462:MET:HE3	1.73	0.70
1:H:261:SER:N	1:H:264:GLN:HE21	1.85	0.70
1:A:244:GLU:OE1	1:A:336:VAL:HG22	1.91	0.69
1:B:205:LYS:O	1:B:377:ARG:NH1	2.25	0.69
1:F:233:ARG:HH12	1:F:349:VAL:HG11	1.54	0.69
1:G:447:ILE:HB	1:G:448:PRO:HD3	1.74	0.69
1:H:241:LEU:HD22	1:H:330:ALA:HB3	1.73	0.69
1:H:394:ALA:O	1:H:398:VAL:HG23	1.91	0.69
1:A:394:ALA:O	1:A:398:VAL:HG23	1.92	0.69
1:B:42:THR:HG22	1:B:48:MET:O	1.90	0.69
1:B:244:GLU:OE1	1:B:336:VAL:HG22	1.91	0.69
1:C:412:GLY:O	1:C:415:GLU:HG2	1.91	0.69
1:C:488:ASP:O	1:C:492:LYS:HG2	1.92	0.69
1:D:37:GLU:HG2	1:D:40:ARG:HH12	1.58	0.69
1:H:501:LYS:HA	1:H:501:LYS:HE3	1.74	0.69
1:E:257:ILE:HG22	1:E:259:ILE:HD12	1.74	0.69
1:E:276:LEU:HD23	1:E:300:LEU:HB2	1.75	0.69
1:E:410:ALA:HB3	1:E:494:ILE:HG22	1.74	0.69
1:D:204:LYS:HB3	1:D:384:ILE:CG2	2.21	0.69
1:E:11:ILE:HD13	1:E:11:ILE:C	2.12	0.69
1:F:380:THR:CG2	1:F:383:VAL:HG23	2.20	0.69
1:B:30:LEU:O	1:B:34:ILE:HG13	1.93	0.69
1:D:460:VAL:O	1:D:464:VAL:HG23	1.92	0.69
1:F:227:HIS:HB3	1:F:230:MET:HG3	1.74	0.69
1:G:409:PRO:HB3	1:G:490:LEU:CD1	2.22	0.69
1:G:17:GLN:NE2	1:G:17:GLN:H	1.91	0.69
1:E:12:LEU:HD23	1:E:13:PRO:CD	2.22	0.69
1:E:421:ARG:HB2	1:E:421:ARG:NH1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:VAL:HG21	1:E:479:ILE:HG12	1.75	0.69
1:F:409:PRO:HB3	1:F:490:LEU:HD13	1.73	0.69
1:G:498:LEU:O	1:G:498:LEU:HD22	1.93	0.69
1:H:123:ILE:HG21	1:H:432:LYS:HB3	1.74	0.69
1:C:410:ALA:HB3	1:C:494:ILE:HG22	1.73	0.69
1:E:269:LEU:HD12	1:F:251:THR:HG23	1.74	0.69
1:A:196:ASP:OD1	1:A:198:ASP:HB2	1.92	0.69
1:B:204:LYS:HB3	1:B:384:ILE:CG2	2.22	0.69
1:H:226:VAL:HG12	1:H:312:ALA:O	1.93	0.69
1:G:29:ILE:HG23	1:G:108:LEU:HB3	1.74	0.68
1:E:166:ASN:HA	1:F:517:ARG:NH1	2.09	0.68
1:F:103:ILE:O	1:F:107:LEU:HB2	1.92	0.68
1:A:258:ASN:ND2	1:H:258:ASN:HB3	2.05	0.68
1:B:144:ILE:HD11	1:B:490:LEU:HD21	1.76	0.68
1:H:304:TYR:O	1:H:308:TYR:HD1	1.76	0.68
1:C:370:LYS:HE2	1:C:370:LYS:HA	1.74	0.68
1:D:261:SER:O	1:D:264:GLN:HG3	1.92	0.68
1:G:412:GLY:O	1:G:415:GLU:HG2	1.93	0.68
1:A:175:ALA:O	1:A:179:VAL:HG23	1.93	0.68
1:C:421:ARG:HB2	1:C:421:ARG:NH1	2.09	0.68
1:F:272:GLU:HA	1:F:275:MET:HE3	1.75	0.68
1:G:144:ILE:CD1	1:G:490:LEU:HD21	2.23	0.68
1:C:75:GLN:HG3	1:D:10:VAL:HG13	1.76	0.68
1:C:445:LYS:O	1:C:448:PRO:HD2	1.93	0.68
1:G:380:THR:CG2	1:G:383:VAL:HG23	2.23	0.68
1:D:506:LYS:O	1:D:510:GLU:HG3	1.94	0.68
1:E:416:ILE:O	1:E:420:ILE:HG13	1.94	0.68
1:A:260:THR:H	1:A:264:GLN:NE2	1.90	0.68
1:D:217:ARG:HA	1:D:372:VAL:HG23	1.76	0.68
1:D:443:ALA:O	1:D:446:ILE:HG13	1.93	0.68
1:A:353:ARG:NH2	1:A:364:GLU:OE2	2.26	0.68
1:C:446:ILE:O	1:C:450:THR:HG23	1.94	0.68
1:D:370:LYS:HE2	1:D:370:LYS:HA	1.74	0.68
1:A:75:GLN:HB2	1:B:11:ILE:C	2.14	0.67
1:A:315:ARG:HH11	1:A:315:ARG:HG3	1.60	0.67
1:F:125:ILE:HD13	1:F:517:ARG:HG2	1.77	0.67
1:F:276:LEU:HD23	1:F:300:LEU:HB2	1.75	0.67
1:F:449:LYS:HE3	1:F:459:THR:HG21	1.76	0.67
1:D:144:ILE:HD11	1:D:490:LEU:HD21	1.76	0.67
1:E:425:TYR:O	1:E:429:VAL:HG23	1.94	0.67
1:F:447:ILE:HB	1:F:448:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:ARG:HB3	1:G:217:ARG:NH1	2.09	0.67
1:G:315:ARG:HG3	1:G:315:ARG:HH11	1.59	0.67
1:D:230:MET:HE2	1:D:312:ALA:H	1.59	0.67
1:D:260:THR:H	1:D:264:GLN:HE21	1.40	0.67
1:H:38:THR:O	1:H:50:LYS:HE3	1.95	0.67
1:H:91:LYS:HB2	1:H:91:LYS:NZ	2.10	0.67
1:C:150:ASP:OD2	1:C:152:GLU:HB3	1.94	0.67
1:E:45:PRO:HA	1:E:164:GLY:HA2	1.75	0.67
1:E:206:ALA:HA	1:E:384:ILE:HD11	1.76	0.67
1:E:230:MET:HE1	1:E:312:ALA:HB3	1.76	0.67
1:F:205:LYS:HZ3	1:F:358:GLU:HB2	1.60	0.67
1:F:513:ILE:O	1:F:517:ARG:HG3	1.94	0.67
1:H:157:ILE:HG13	1:H:401:VAL:HG21	1.77	0.67
1:B:208:GLU:HB3	1:B:212:GLU:HG3	1.75	0.67
1:D:244:GLU:OE1	1:D:336:VAL:HG22	1.95	0.67
1:E:469:GLU:HB2	1:E:477:ILE:HG21	1.77	0.67
1:F:166:ASN:HA	1:G:517:ARG:NH1	2.10	0.67
1:H:265:LEU:O	1:H:269:LEU:HD13	1.95	0.67
1:A:60:VAL:HG21	1:A:71:LYS:HE2	1.77	0.67
1:G:348:GLU:O	1:G:349:VAL:HG23	1.93	0.67
1:G:418:LEU:O	1:G:422:LEU:HB2	1.95	0.67
1:E:35:ILE:HD11	1:E:74:LEU:HD21	1.77	0.66
1:G:227:HIS:HB3	1:G:230:MET:HG3	1.76	0.66
1:A:150:ASP:OD2	1:A:152:GLU:HB3	1.95	0.66
1:B:59:ILE:HD12	1:B:59:ILE:N	2.10	0.66
1:B:409:PRO:HB3	1:B:490:LEU:HD11	1.76	0.66
1:D:204:LYS:HD3	1:D:388:GLU:OE2	1.96	0.66
1:G:217:ARG:HB3	1:G:217:ARG:HH11	1.60	0.66
1:G:335:ASN:OD1	1:G:337:LYS:HB2	1.95	0.66
1:H:102:VAL:HG12	1:H:446:ILE:HD13	1.77	0.66
1:B:272:GLU:HA	1:B:275:MET:HE3	1.77	0.66
1:E:412:GLY:O	1:E:416:ILE:HG13	1.96	0.66
1:A:257:ILE:HB	1:B:255:ALA:HB2	1.78	0.66
1:H:125:ILE:HD13	1:H:517:ARG:HG2	1.76	0.66
1:E:94:GLY:HA3	1:E:396:LYS:HD2	1.77	0.66
1:G:29:ILE:O	1:G:33:ARG:HG3	1.96	0.66
1:H:37:GLU:HG2	1:H:40:ARG:NH1	2.10	0.66
1:A:109:ARG:NH2	1:A:110:LYS:HD3	2.10	0.66
1:A:483:GLU:HG3	1:A:485:LYS:NZ	2.09	0.66
1:H:35:ILE:HD11	1:H:74:LEU:HD21	1.78	0.66
1:A:469:GLU:CB	1:A:477:ILE:HG21	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:MET:O	1:B:466:VAL:HG23	1.95	0.66
1:A:230:MET:HE1	1:A:312:ALA:HB3	1.78	0.66
1:A:443:ALA:O	1:A:446:ILE:HG13	1.94	0.66
1:C:142:ILE:HB	1:C:475:LEU:CD2	2.26	0.66
1:D:197:LEU:HD22	1:D:395:VAL:HG12	1.78	0.66
1:E:59:ILE:N	1:E:59:ILE:HD12	2.11	0.66
1:F:126:LYS:NZ	1:F:126:LYS:HB3	2.10	0.66
1:E:370:LYS:HA	1:E:370:LYS:HE2	1.77	0.65
1:D:91:LYS:HB2	1:D:91:LYS:HZ2	1.59	0.65
1:E:94:GLY:CA	1:E:396:LYS:HD2	2.25	0.65
1:H:261:SER:O	1:H:264:GLN:HG3	1.95	0.65
1:B:94:GLY:HA3	1:B:396:LYS:HD2	1.77	0.65
1:B:413:ALA:HB3	1:B:414:PRO:HD3	1.78	0.65
1:E:383:VAL:O	1:E:387:VAL:HG23	1.95	0.65
1:H:380:THR:HG23	1:H:383:VAL:H	1.62	0.65
1:D:206:ALA:HA	1:D:384:ILE:HD11	1.76	0.65
1:D:445:LYS:O	1:D:448:PRO:HD2	1.95	0.65
1:E:307:LYS:HD2	1:F:338:ASP:OD2	1.97	0.65
1:G:145:ARG:HG2	1:G:145:ARG:HH11	1.61	0.65
1:B:445:LYS:O	1:B:449:LYS:HB2	1.96	0.65
1:D:446:ILE:O	1:D:450:THR:HG23	1.95	0.65
1:A:517:ARG:HH12	1:H:166:ASN:HA	1.61	0.65
1:B:380:THR:CG2	1:B:383:VAL:H	2.08	0.65
1:B:188:LYS:HB2	1:B:193:TYR:HA	1.79	0.65
1:D:524:ALA:O	1:D:525:LYS:HG2	1.97	0.65
1:E:380:THR:HG22	1:E:383:VAL:CG2	2.14	0.65
1:A:517:ARG:NH1	1:H:166:ASN:HA	2.11	0.65
1:B:108:LEU:HD11	1:B:515:ILE:HD12	1.79	0.65
1:C:155:LEU:HD13	1:C:179:VAL:HG21	1.78	0.65
1:E:73:ASP:O	1:F:13:PRO:HD3	1.97	0.65
1:F:258:ASN:HB3	1:G:258:ASN:HD21	1.61	0.65
1:F:272:GLU:HA	1:F:275:MET:CE	2.26	0.65
1:C:108:LEU:HD11	1:C:515:ILE:HD12	1.77	0.65
1:C:10:VAL:CG2	1:C:11:ILE:H	2.05	0.64
1:D:241:LEU:HD22	1:D:330:ALA:CB	2.27	0.64
1:D:304:TYR:O	1:D:308:TYR:HD1	1.80	0.64
1:E:205:LYS:NZ	1:E:358:GLU:HG2	2.12	0.64
1:E:394:ALA:O	1:E:398:VAL:HG23	1.96	0.64
1:C:166:ASN:HA	1:D:517:ARG:NH1	2.12	0.64
1:F:297:ILE:HG22	1:F:302:GLN:HG3	1.79	0.64
1:G:11:ILE:HG23	1:G:12:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HG21	1:C:432:LYS:HB3	1.79	0.64
1:G:37:GLU:HG2	1:G:40:ARG:NH1	2.12	0.64
1:A:208:GLU:HB3	1:A:212:GLU:HG3	1.77	0.64
1:D:138:ILE:HD13	1:D:421:ARG:HG2	1.79	0.64
1:D:465:LYS:O	1:D:469:GLU:HG2	1.97	0.64
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.11	0.64
1:H:372:VAL:HG22	1:H:373:THR:N	2.12	0.64
1:B:466:VAL:HG21	1:B:479:ILE:HG12	1.80	0.64
1:D:226:VAL:HG12	1:D:312:ALA:O	1.97	0.64
1:D:230:MET:HE1	1:D:312:ALA:HB3	1.79	0.64
1:C:189:LYS:HD2	1:C:189:LYS:C	2.18	0.64
1:E:99:THR:O	1:E:103:ILE:HG13	1.97	0.64
1:F:125:ILE:HG23	1:F:513:ILE:CG2	2.27	0.64
1:F:205:LYS:HZ3	1:F:358:GLU:CB	2.11	0.64
1:F:204:LYS:HD3	1:F:388:GLU:OE2	1.98	0.64
1:H:409:PRO:HB3	1:H:490:LEU:HD13	1.79	0.64
1:D:211:GLU:OE1	1:D:211:GLU:HA	1.98	0.64
1:E:272:GLU:HA	1:E:275:MET:CE	2.27	0.64
1:E:293:VAL:CG2	1:E:297:ILE:HD11	2.25	0.64
1:A:217:ARG:HB3	1:A:217:ARG:NH1	2.12	0.63
1:E:261:SER:H	1:E:264:GLN:HE21	1.45	0.63
1:F:225:VAL:HG21	1:F:232:LYS:HD3	1.80	0.63
1:G:423:ASP:OD1	1:G:427:LYS:HE2	1.98	0.63
1:A:30:LEU:O	1:A:34:ILE:HG13	1.98	0.63
1:D:11:ILE:HD13	1:D:12:LEU:HB2	1.80	0.63
1:E:447:ILE:HB	1:E:448:PRO:HD3	1.80	0.63
1:F:123:ILE:HG21	1:F:432:LYS:HB3	1.79	0.63
1:A:257:ILE:HG22	1:A:259:ILE:HD12	1.80	0.63
1:A:445:LYS:O	1:A:449:LYS:HB2	1.98	0.63
1:B:483:GLU:HG3	1:B:485:LYS:NZ	2.13	0.63
1:D:447:ILE:HB	1:D:448:PRO:HD3	1.79	0.63
1:H:383:VAL:O	1:H:387:VAL:HG23	1.98	0.63
1:B:60:VAL:HG21	1:B:71:LYS:HE2	1.78	0.63
1:F:235:GLU:HA	1:F:235:GLU:OE2	1.99	0.63
1:F:269:LEU:HD12	1:G:251:THR:CG2	2.28	0.63
1:H:11:ILE:HD13	1:H:11:ILE:C	2.18	0.63
1:B:11:ILE:C	1:B:11:ILE:HD13	2.19	0.63
1:E:227:HIS:ND1	1:E:228:PRO:HD2	2.13	0.63
1:F:277:LYS:HB2	1:F:304:TYR:CE2	2.33	0.63
1:B:29:ILE:O	1:B:33:ARG:HG3	1.98	0.63
1:C:142:ILE:HB	1:C:475:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:LEU:O	1:G:467:ILE:HG13	1.99	0.63
1:E:166:ASN:HA	1:F:517:ARG:HH12	1.62	0.63
1:E:513:ILE:O	1:E:517:ARG:HG3	1.99	0.63
1:G:423:ASP:O	1:G:426:ALA:HB3	1.98	0.63
1:A:85:VAL:HG13	1:A:507:SER:HB3	1.81	0.63
1:E:29:ILE:O	1:E:33:ARG:HG3	1.98	0.63
1:E:196:ASP:OD1	1:E:198:ASP:HB2	1.99	0.63
1:E:212:GLU:HB2	1:E:377:ARG:HG3	1.81	0.63
1:E:297:ILE:HG22	1:E:302:GLN:HG3	1.80	0.63
1:F:188:LYS:HD3	1:F:193:TYR:CE1	2.34	0.63
1:C:524:ALA:C	1:C:525:LYS:HD2	2.19	0.62
1:F:30:LEU:O	1:F:34:ILE:HG13	1.99	0.62
1:A:125:ILE:HG23	1:A:513:ILE:CG2	2.27	0.62
1:A:217:ARG:HB3	1:A:217:ARG:HH11	1.62	0.62
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.11	0.62
1:C:513:ILE:O	1:C:517:ARG:HG3	1.99	0.62
1:E:189:LYS:HD2	1:E:189:LYS:C	2.19	0.62
1:G:10:VAL:HG13	1:G:11:ILE:N	2.10	0.62
1:A:463:LEU:O	1:A:467:ILE:HG13	1.99	0.62
1:B:166:ASN:HA	1:C:517:ARG:NH1	2.13	0.62
1:D:409:PRO:HB3	1:D:490:LEU:HD13	1.80	0.62
1:E:445:LYS:O	1:E:449:LYS:HB2	1.99	0.62
1:F:383:VAL:O	1:F:387:VAL:HG23	1.99	0.62
1:C:497:PRO:HB2	1:C:500:VAL:HG23	1.80	0.62
1:E:265:LEU:O	1:E:269:LEU:HD13	1.99	0.62
1:F:233:ARG:NH1	1:F:349:VAL:HG13	2.14	0.62
1:C:22:ARG:HG3	1:C:23:ASP:N	2.14	0.62
1:F:335:ASN:OD1	1:F:337:LYS:HB2	1.99	0.62
1:G:465:LYS:O	1:G:469:GLU:HG2	1.99	0.62
1:G:497:PRO:HB2	1:G:500:VAL:HG23	1.81	0.62
1:A:59:ILE:HD12	1:A:59:ILE:N	2.15	0.62
1:D:11:ILE:HD13	1:D:11:ILE:C	2.20	0.62
1:G:204:LYS:HD2	1:G:384:ILE:HG22	1.81	0.62
1:G:354:LYS:HA	1:G:358:GLU:O	2.00	0.62
1:G:462:MET:HE1	1:G:486:PRO:HD3	1.80	0.62
1:H:64:ASP:O	1:H:68:ILE:HG13	1.99	0.62
1:D:109:ARG:NH2	1:D:110:LYS:HD3	2.13	0.62
1:H:281:ASP:OD1	1:H:308:TYR:OH	2.13	0.62
1:F:146:VAL:HG22	1:F:147:ASP:N	2.15	0.62
1:F:286:THR:HG21	1:F:339:LEU:HG	1.82	0.62
1:H:117:GLN:O	1:H:118:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HD13	1:A:517:ARG:HG2	1.82	0.62
1:A:257:ILE:HB	1:B:255:ALA:CB	2.30	0.62
1:B:249:LYS:HE2	1:B:279:MET:HE3	1.82	0.62
1:D:179:VAL:O	1:D:183:LYS:HG3	2.00	0.62
1:D:404:ASP:OD1	1:D:499:ARG:HB2	1.99	0.62
1:D:416:ILE:HD13	1:D:466:VAL:HG12	1.81	0.62
1:E:17:GLN:NE2	1:E:17:GLN:H	1.97	0.62
1:A:409:PRO:HB3	1:A:490:LEU:HD13	1.81	0.61
1:C:204:LYS:HD3	1:C:388:GLU:OE2	1.99	0.61
1:C:265:LEU:O	1:C:269:LEU:HD13	2.00	0.61
1:E:73:ASP:HB3	1:F:13:PRO:HG2	1.82	0.61
1:F:394:ALA:O	1:F:398:VAL:HG23	2.00	0.61
1:G:388:GLU:O	1:G:392:GLU:HG3	1.99	0.61
1:H:388:GLU:O	1:H:392:GLU:HG3	1.99	0.61
1:B:150:ASP:OD1	1:B:153:THR:HG23	1.99	0.61
1:B:509:SER:O	1:B:513:ILE:HG13	2.00	0.61
1:F:413:ALA:HB3	1:F:414:PRO:HD3	1.81	0.61
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.65	0.61
1:B:13:PRO:O	1:B:16:THR:HB	2.00	0.61
1:C:11:ILE:HD13	1:C:11:ILE:O	2.00	0.61
1:C:21:GLY:O	1:C:25:GLN:HG3	2.01	0.61
1:B:524:ALA:C	1:B:525:LYS:HD2	2.21	0.61
1:E:483:GLU:HG3	1:E:485:LYS:HZ3	1.64	0.61
1:B:447:ILE:HB	1:B:448:PRO:HD3	1.82	0.61
1:D:142:ILE:HB	1:D:475:LEU:HD22	1.81	0.61
1:E:144:ILE:HD11	1:E:490:LEU:HD21	1.82	0.61
1:A:11:ILE:HD11	1:H:31:ALA:HA	1.82	0.61
1:H:175:ALA:O	1:H:179:VAL:HG23	2.01	0.61
1:D:17:GLN:NE2	1:D:17:GLN:H	1.99	0.61
1:E:388:GLU:O	1:E:392:GLU:HG3	2.00	0.61
1:F:409:PRO:HB3	1:F:490:LEU:CD1	2.29	0.61
1:F:445:LYS:O	1:F:448:PRO:HD2	2.01	0.61
1:C:260:THR:N	1:C:264:GLN:HE21	1.86	0.61
1:D:106:GLU:HG2	1:D:446:ILE:CG1	2.31	0.61
1:E:125:ILE:HD13	1:E:517:ARG:HG2	1.82	0.61
1:E:151:GLU:O	1:E:155:LEU:HD23	2.01	0.61
1:H:125:ILE:HG23	1:H:513:ILE:CG2	2.27	0.61
1:H:126:LYS:NZ	1:H:126:LYS:HB3	2.16	0.61
1:B:120:HIS:ND1	1:B:121:PRO:HD2	2.15	0.61
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.01	0.61
1:E:60:VAL:HG21	1:E:71:LYS:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LEU:HB3	1:E:83:VAL:HG22	1.83	0.61
1:G:348:GLU:HB3	1:G:365:GLY:HA3	1.82	0.61
1:C:354:LYS:HE2	1:C:357:GLY:HA2	1.82	0.60
1:C:445:LYS:O	1:C:449:LYS:HB2	2.01	0.60
1:E:108:LEU:HD11	1:E:515:ILE:HD12	1.82	0.60
1:H:211:GLU:OE1	1:H:211:GLU:HA	2.00	0.60
1:B:103:ILE:O	1:B:107:LEU:HB2	2.00	0.60
1:D:241:LEU:CD2	1:D:330:ALA:HB3	2.31	0.60
1:F:106:GLU:HG2	1:F:446:ILE:CG1	2.31	0.60
1:C:11:ILE:HD13	1:C:11:ILE:C	2.21	0.60
1:E:354:LYS:HE2	1:E:357:GLY:HA2	1.83	0.60
1:F:243:ASN:OD1	1:F:295:LYS:HE3	2.00	0.60
1:A:106:GLU:HG2	1:A:446:ILE:HG13	1.82	0.60
1:B:261:SER:O	1:B:264:GLN:HB2	2.00	0.60
1:D:469:GLU:CB	1:D:477:ILE:HG21	2.31	0.60
1:E:205:LYS:HZ1	1:E:358:GLU:HG2	1.66	0.60
1:F:197:LEU:HD22	1:F:395:VAL:CG1	2.31	0.60
1:F:208:GLU:HB3	1:F:212:GLU:HG3	1.81	0.60
1:F:235:GLU:O	1:F:237:ALA:N	2.34	0.60
1:G:126:LYS:HB3	1:G:126:LYS:NZ	2.17	0.60
1:G:466:VAL:HG21	1:G:479:ILE:HG12	1.83	0.60
1:H:155:LEU:HD22	1:H:179:VAL:HG21	1.84	0.60
1:C:157:ILE:HG13	1:C:401:VAL:HG21	1.83	0.60
1:F:244:GLU:OE1	1:F:336:VAL:HG22	2.01	0.60
1:H:227:HIS:HD1	1:H:229:ARG:H	1.48	0.60
1:C:269:LEU:HD12	1:D:251:THR:HG23	1.83	0.60
1:D:151:GLU:O	1:D:155:LEU:HD23	2.02	0.60
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.67	0.60
1:A:179:VAL:O	1:A:183:LYS:HG3	2.02	0.60
1:A:261:SER:H	1:A:264:GLN:HG3	1.66	0.60
1:B:233:ARG:HD2	1:B:351:GLU:OE2	2.02	0.60
1:D:217:ARG:HB3	1:D:217:ARG:HH11	1.66	0.60
1:E:230:MET:HE2	1:E:312:ALA:N	2.17	0.60
1:G:269:LEU:HD12	1:H:251:THR:HG23	1.84	0.60
1:G:430:GLY:HA2	1:G:434:ALA:HB2	1.83	0.60
1:F:157:ILE:HG13	1:F:401:VAL:HG21	1.84	0.60
1:B:241:LEU:HD12	1:B:292:PHE:HB2	1.83	0.60
1:A:77:PRO:HB2	1:H:51:MET:CE	2.31	0.59
1:C:59:ILE:N	1:C:59:ILE:HD12	2.17	0.59
1:C:64:ASP:O	1:C:68:ILE:HG13	2.02	0.59
1:F:249:LYS:HE2	1:F:279:MET:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:THR:N	1:H:264:GLN:NE2	2.44	0.59
1:H:465:LYS:O	1:H:469:GLU:HG2	2.01	0.59
1:B:182:VAL:O	1:B:186:ALA:HB2	2.03	0.59
1:B:348:GLU:HB3	1:B:365:GLY:HA3	1.84	0.59
1:C:261:SER:O	1:C:264:GLN:HG3	2.02	0.59
1:E:142:ILE:HB	1:E:475:LEU:HD22	1.82	0.59
1:F:175:ALA:O	1:F:179:VAL:HG23	2.02	0.59
1:A:197:LEU:HD22	1:A:395:VAL:CG1	2.31	0.59
1:C:117:GLN:O	1:C:118:ASN:HB2	2.01	0.59
1:C:483:GLU:HG3	1:C:485:LYS:HZ1	1.68	0.59
1:H:59:ILE:N	1:H:59:ILE:HD12	2.16	0.59
1:H:136:GLN:NE2	1:H:136:GLN:HA	2.17	0.59
1:A:475:LEU:HD12	1:A:475:LEU:O	2.03	0.59
1:C:205:LYS:O	1:C:377:ARG:NH1	2.35	0.59
1:E:443:ALA:O	1:E:446:ILE:HG13	2.03	0.59
1:F:22:ARG:HG3	1:F:23:ASP:N	2.18	0.59
1:F:206:ALA:HA	1:F:384:ILE:HD11	1.83	0.59
1:G:136:GLN:HA	1:G:136:GLN:HE21	1.67	0.59
1:B:166:ASN:HD22	1:B:166:ASN:C	2.05	0.59
1:E:106:GLU:HG2	1:E:446:ILE:CG1	2.33	0.59
1:E:145:ARG:HG2	1:E:145:ARG:HH11	1.67	0.59
1:H:418:LEU:O	1:H:422:LEU:HB2	2.03	0.59
1:B:216:VAL:O	1:B:372:VAL:HG23	2.02	0.59
1:D:348:GLU:O	1:D:349:VAL:HG23	2.02	0.59
1:A:265:LEU:O	1:A:269:LEU:HD13	2.02	0.59
1:A:423:ASP:O	1:A:426:ALA:HB3	2.02	0.59
1:D:418:LEU:O	1:D:422:LEU:HB2	2.03	0.59
1:E:271:GLN:O	1:E:275:MET:HG3	2.02	0.59
1:F:257:ILE:HG22	1:F:259:ILE:HD12	1.85	0.59
1:F:465:LYS:O	1:F:469:GLU:HG2	2.03	0.59
1:A:12:LEU:HD13	1:A:16:THR:HG21	1.83	0.59
1:E:109:ARG:NH2	1:E:110:LYS:HD3	2.17	0.59
1:E:423:ASP:OD1	1:E:427:LYS:HE2	2.02	0.59
1:A:466:VAL:HG21	1:A:479:ILE:HG12	1.85	0.59
1:C:461:GLU:HG2	1:C:465:LYS:NZ	2.18	0.59
1:G:126:LYS:O	1:G:130:LEU:HG	2.02	0.59
1:G:353:ARG:NH2	1:G:364:GLU:OE2	2.35	0.59
1:H:328:THR:HG22	1:H:366:CYS:SG	2.43	0.59
1:H:509:SER:O	1:H:513:ILE:HG13	2.03	0.59
1:A:450:THR:O	1:A:454:ASN:ND2	2.36	0.59
1:C:433:GLU:O	1:C:437:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:HIS:HB3	1:E:230:MET:CG	2.30	0.59
1:G:205:LYS:NZ	1:G:358:GLU:HG2	2.17	0.59
1:G:409:PRO:HB3	1:G:490:LEU:HD13	1.85	0.59
1:C:226:VAL:HG12	1:C:312:ALA:O	2.03	0.58
1:D:182:VAL:O	1:D:186:ALA:HB2	2.03	0.58
1:G:157:ILE:HG13	1:G:401:VAL:HG21	1.85	0.58
1:G:276:LEU:HD23	1:G:300:LEU:HB2	1.84	0.58
1:A:266:MET:O	1:A:270:GLU:HG3	2.02	0.58
1:B:400:ASP:OD1	1:B:499:ARG:HD2	2.04	0.58
1:G:170:HIS:CE1	1:G:210:VAL:HB	2.38	0.58
1:G:416:ILE:HD13	1:G:466:VAL:HG12	1.84	0.58
1:H:120:HIS:ND1	1:H:122:SER:HB3	2.18	0.58
1:B:272:GLU:HA	1:B:275:MET:CE	2.33	0.58
1:D:106:GLU:HG2	1:D:446:ILE:HG13	1.83	0.58
1:E:91:LYS:HG2	1:E:91:LYS:O	2.04	0.58
1:G:513:ILE:O	1:G:517:ARG:HG3	2.03	0.58
1:C:204:LYS:HD2	1:C:384:ILE:HG22	1.86	0.58
1:D:315:ARG:HG3	1:D:315:ARG:NH1	2.19	0.58
1:F:233:ARG:NH1	1:F:349:VAL:CG1	2.65	0.58
1:H:264:GLN:HA	1:H:267:SER:OG	2.04	0.58
1:C:353:ARG:NH2	1:C:364:GLU:OE2	2.36	0.58
1:F:150:ASP:OD1	1:F:153:THR:HG23	2.03	0.58
1:F:271:GLN:O	1:F:275:MET:HG3	2.04	0.58
1:B:297:ILE:HG22	1:B:302:GLN:HG3	1.84	0.58
1:D:110:LYS:HE3	1:D:442:ASP:OD1	2.03	0.58
1:G:445:LYS:O	1:G:448:PRO:HD2	2.04	0.58
1:A:206:ALA:CA	1:A:384:ILE:HD11	2.32	0.58
1:D:303:HIS:CD2	1:E:335:ASN:HB3	2.39	0.58
1:D:409:PRO:HB3	1:D:490:LEU:CD1	2.33	0.58
1:A:226:VAL:HG12	1:A:312:ALA:O	2.03	0.58
1:A:400:ASP:OD1	1:A:499:ARG:HD2	2.04	0.58
1:D:188:LYS:HB2	1:D:193:TYR:HA	1.86	0.58
1:F:96:GLY:HA2	3:F:6528:ADP:O1B	2.04	0.58
1:F:184:GLN:NE2	1:F:217:ARG:NH2	2.52	0.58
1:F:469:GLU:HB2	1:F:477:ILE:HG21	1.85	0.58
1:G:370:LYS:HA	1:G:370:LYS:CE	2.34	0.58
1:H:216:VAL:O	1:H:218:GLY:N	2.36	0.58
1:B:277:LYS:HD2	1:B:304:TYR:CE1	2.39	0.57
1:B:513:ILE:O	1:B:517:ARG:HG3	2.02	0.57
1:D:29:ILE:HG23	1:D:108:LEU:HB3	1.86	0.57
1:D:280:VAL:HG13	1:D:305:LEU:HG	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD23	1:A:300:LEU:HB2	1.86	0.57
1:C:123:ILE:HG21	1:C:432:LYS:CB	2.34	0.57
1:D:45:PRO:HA	1:D:164:GLY:HA2	1.85	0.57
1:D:230:MET:HE2	1:D:312:ALA:N	2.19	0.57
1:E:136:GLN:HA	1:E:136:GLN:NE2	2.18	0.57
1:E:342:GLU:N	1:E:342:GLU:OE2	2.37	0.57
1:F:233:ARG:HH12	1:F:349:VAL:HG13	1.65	0.57
1:A:29:ILE:HG23	1:A:108:LEU:HB3	1.86	0.57
1:B:277:LYS:HB2	1:B:304:TYR:CE2	2.39	0.57
1:C:120:HIS:ND1	1:C:122:SER:HB3	2.18	0.57
1:D:466:VAL:HG22	1:D:486:PRO:HG3	1.86	0.57
1:E:154:LEU:HG	1:E:398:VAL:HG13	1.86	0.57
1:H:29:ILE:HG23	1:H:108:LEU:HB3	1.86	0.57
1:A:158:ALA:O	1:A:162:ILE:HG13	2.04	0.57
1:A:304:TYR:O	1:A:308:TYR:HD1	1.88	0.57
1:A:393:ASP:O	1:A:397:VAL:HG22	2.05	0.57
1:C:150:ASP:OD1	1:C:153:THR:HG23	2.04	0.57
1:H:280:VAL:HG13	1:H:305:LEU:HG	1.86	0.57
1:H:417:GLU:OE2	1:H:470:HIS:NE2	2.28	0.57
1:B:126:LYS:HB3	1:B:126:LYS:NZ	2.19	0.57
1:C:146:VAL:HG22	1:C:147:ASP:N	2.19	0.57
1:E:509:SER:O	1:E:513:ILE:HG13	2.05	0.57
1:G:188:LYS:HG3	1:G:192:LYS:C	2.24	0.57
1:A:230:MET:HE2	1:A:312:ALA:N	2.19	0.57
1:C:37:GLU:HG2	1:C:40:ARG:NH1	2.19	0.57
1:D:114:LEU:HD22	1:D:119:ILE:HD12	1.86	0.57
1:F:497:PRO:HB2	1:F:500:VAL:HG23	1.86	0.57
1:G:445:LYS:O	1:G:449:LYS:HB2	2.05	0.57
1:A:38:THR:O	1:A:50:LYS:CE	2.52	0.57
1:B:94:GLY:CA	1:B:396:LYS:HD2	2.34	0.57
1:B:394:ALA:O	1:B:398:VAL:HG23	2.04	0.57
1:D:388:GLU:O	1:D:392:GLU:HG3	2.05	0.57
1:F:204:LYS:HD2	1:F:384:ILE:HG22	1.86	0.57
1:G:11:ILE:CG2	1:G:12:LEU:N	2.67	0.57
1:H:241:LEU:HD22	1:H:330:ALA:CB	2.35	0.57
1:A:241:LEU:HD22	1:A:330:ALA:HB3	1.87	0.57
1:B:12:LEU:HD21	1:B:16:THR:HG21	1.87	0.57
1:B:227:HIS:HB3	1:B:230:MET:HG3	1.87	0.57
1:B:412:GLY:O	1:B:415:GLU:HG2	2.05	0.57
1:C:297:ILE:HG22	1:C:302:GLN:HG3	1.86	0.57
1:C:425:TYR:O	1:C:429:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ALA:O	1:C:446:ILE:HG13	2.04	0.57
1:D:259:ILE:HG22	1:E:257:ILE:HG23	1.85	0.57
1:D:261:SER:H	1:D:264:GLN:HE21	1.52	0.57
1:E:138:ILE:HD13	1:E:421:ARG:HG2	1.87	0.57
1:E:412:GLY:O	1:E:415:GLU:HG2	2.05	0.57
1:A:75:GLN:HB2	1:B:11:ILE:CA	2.35	0.57
1:H:205:LYS:O	1:H:377:ARG:NH1	2.38	0.57
1:A:37:GLU:HG2	1:A:40:ARG:NH1	2.20	0.56
1:D:197:LEU:HD22	1:D:395:VAL:CG1	2.35	0.56
1:E:355:LEU:O	1:E:356:ALA:HB3	2.05	0.56
1:F:59:ILE:HD12	1:F:59:ILE:N	2.20	0.56
1:G:147:ASP:O	1:G:149:ASP:N	2.38	0.56
1:G:261:SER:O	1:G:264:GLN:HG3	2.05	0.56
1:A:509:SER:O	1:A:513:ILE:HG13	2.05	0.56
1:F:13:PRO:O	1:F:16:THR:HB	2.05	0.56
1:F:270:GLU:HA	1:F:273:GLU:HG3	1.86	0.56
1:F:461:GLU:HG2	1:F:465:LYS:HZ2	1.71	0.56
1:H:76:HIS:CD2	1:H:78:ALA:HB3	2.40	0.56
1:H:125:ILE:CD1	1:H:517:ARG:HG2	2.34	0.56
1:A:99:THR:O	1:A:103:ILE:HG13	2.04	0.56
1:B:54:ASP:OD1	1:B:58:ASP:HB3	2.06	0.56
1:B:91:LYS:HB2	1:B:91:LYS:NZ	2.20	0.56
1:B:179:VAL:O	1:B:183:LYS:HG3	2.05	0.56
1:B:197:LEU:HD22	1:B:395:VAL:CG1	2.35	0.56
1:B:250:LYS:NZ	1:C:253:THR:HA	2.19	0.56
1:B:462:MET:CE	1:B:486:PRO:HD3	2.35	0.56
1:D:126:LYS:NZ	1:D:126:LYS:HB3	2.20	0.56
1:D:147:ASP:HB3	1:D:150:ASP:HB2	1.88	0.56
1:D:217:ARG:HH11	1:D:217:ARG:CB	2.17	0.56
1:D:497:PRO:HB2	1:D:500:VAL:HG23	1.86	0.56
1:F:134:LYS:O	1:F:138:ILE:HG13	2.05	0.56
1:F:179:VAL:O	1:F:183:LYS:HG3	2.04	0.56
1:H:189:LYS:HD2	1:H:189:LYS:C	2.25	0.56
1:A:138:ILE:CD1	1:A:421:ARG:HG2	2.34	0.56
1:C:413:ALA:HB3	1:C:414:PRO:HD3	1.87	0.56
1:E:150:ASP:OD2	1:E:152:GLU:HB3	2.05	0.56
1:E:266:MET:HG2	1:F:271:GLN:NE2	2.20	0.56
1:F:123:ILE:HG21	1:F:432:LYS:CB	2.35	0.56
1:F:204:LYS:HB3	1:F:384:ILE:HG21	1.87	0.56
1:F:210:VAL:HA	1:F:377:ARG:O	2.05	0.56
1:G:51:MET:HB2	1:H:518:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:ASP:O	1:G:68:ILE:HG13	2.05	0.56
1:A:182:VAL:O	1:A:186:ALA:HB2	2.06	0.56
1:C:409:PRO:HB3	1:C:490:LEU:HD12	1.88	0.56
1:D:513:ILE:O	1:D:517:ARG:HG3	2.05	0.56
1:H:348:GLU:O	1:H:349:VAL:HG23	2.06	0.56
1:F:184:GLN:HE22	1:F:217:ARG:HH21	1.54	0.56
1:B:241:LEU:CD2	1:B:330:ALA:HB3	2.35	0.56
1:C:257:ILE:HG22	1:C:259:ILE:HD12	1.87	0.56
1:D:175:ALA:O	1:D:179:VAL:HG23	2.06	0.56
1:D:226:VAL:HG22	1:D:302:GLN:OE1	2.06	0.56
1:E:233:ARG:HH11	1:E:233:ARG:HG3	1.71	0.56
1:G:196:ASP:OD1	1:G:198:ASP:HB2	2.06	0.56
1:B:276:LEU:HD23	1:B:300:LEU:HB2	1.87	0.56
1:E:38:THR:O	1:E:50:LYS:HE3	2.06	0.56
1:F:10:VAL:CG2	1:F:11:ILE:H	2.13	0.56
1:F:483:GLU:HG3	1:F:485:LYS:NZ	2.21	0.56
1:G:94:GLY:HA3	1:G:396:LYS:HD2	1.88	0.56
1:C:151:GLU:O	1:C:155:LEU:HD23	2.06	0.56
1:D:150:ASP:OD1	1:D:153:THR:HG23	2.06	0.56
1:D:196:ASP:OD1	1:D:198:ASP:HB2	2.06	0.56
1:E:11:ILE:HD13	1:E:11:ILE:O	2.05	0.56
1:E:218:GLY:HA3	1:E:363:VAL:O	2.06	0.56
1:H:54:ASP:OD1	1:H:56:LEU:HB2	2.06	0.56
1:A:81:MET:HE3	1:A:514:MET:SD	2.46	0.56
1:D:10:VAL:CG2	1:D:11:ILE:H	2.08	0.56
1:E:17:GLN:H	1:E:17:GLN:HE21	1.54	0.56
1:E:266:MET:O	1:E:270:GLU:HG3	2.06	0.56
1:F:146:VAL:HG22	1:F:147:ASP:H	1.70	0.56
1:G:125:ILE:CD1	1:G:517:ARG:HG2	2.33	0.56
1:D:423:ASP:OD1	1:D:427:LYS:HE2	2.06	0.55
1:E:372:VAL:HG22	1:E:373:THR:H	1.70	0.55
1:E:450:THR:O	1:E:454:ASN:ND2	2.38	0.55
1:G:315:ARG:HG3	1:G:315:ARG:NH1	2.20	0.55
1:C:315:ARG:HG3	1:C:315:ARG:NH1	2.21	0.55
1:D:501:LYS:HA	1:D:501:LYS:HE3	1.88	0.55
1:F:348:GLU:HB3	1:F:365:GLY:HA3	1.88	0.55
1:F:421:ARG:HH11	1:F:421:ARG:CB	2.11	0.55
1:G:166:ASN:HA	1:H:517:ARG:NH1	2.19	0.55
1:G:380:THR:HG22	1:G:383:VAL:CG2	2.26	0.55
1:H:54:ASP:CB	1:H:58:ASP:HB3	2.33	0.55
1:H:473:ARG:HB2	1:H:477:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HD2	1:B:384:ILE:HG22	1.87	0.55
1:C:233:ARG:HH12	1:C:349:VAL:HG11	1.71	0.55
1:G:208:GLU:HB3	1:G:212:GLU:CG	2.36	0.55
1:A:211:GLU:OE1	1:A:211:GLU:HA	2.06	0.55
1:E:197:LEU:HD22	1:E:395:VAL:CG1	2.36	0.55
1:G:204:LYS:HB3	1:G:384:ILE:CG2	2.36	0.55
1:A:209:GLY:C	1:A:211:GLU:N	2.60	0.55
1:E:123:ILE:HG21	1:E:432:LYS:HB3	1.89	0.55
1:E:400:ASP:O	1:E:404:ASP:HB2	2.07	0.55
1:E:409:PRO:HB3	1:E:490:LEU:CD1	2.36	0.55
1:F:208:GLU:HB3	1:F:212:GLU:CG	2.37	0.55
1:G:30:LEU:O	1:G:34:ILE:HG13	2.07	0.55
1:G:401:VAL:O	1:G:405:GLY:N	2.37	0.55
1:D:483:GLU:HG3	1:D:485:LYS:NZ	2.22	0.55
1:E:260:THR:H	1:E:264:GLN:HE22	1.53	0.55
1:F:60:VAL:HG21	1:F:71:LYS:HE2	1.89	0.55
1:G:443:ALA:O	1:G:446:ILE:HG13	2.06	0.55
1:B:463:LEU:O	1:B:467:ILE:HG13	2.07	0.55
1:C:423:ASP:OD1	1:C:427:LYS:HE2	2.07	0.55
1:D:250:LYS:NZ	1:E:253:THR:HA	2.22	0.55
1:D:293:VAL:CG2	1:D:297:ILE:HD11	2.36	0.55
1:D:394:ALA:O	1:D:398:VAL:HG23	2.07	0.55
1:E:412:GLY:HA2	1:E:415:GLU:OE2	2.06	0.55
1:G:269:LEU:HD12	1:H:251:THR:CG2	2.37	0.55
1:H:140:ASP:OD1	1:H:502:LYS:HD2	2.07	0.55
1:H:210:VAL:HA	1:H:377:ARG:O	2.07	0.55
1:B:241:LEU:HD22	1:B:330:ALA:HB3	1.88	0.55
1:C:16:THR:HG23	1:C:523:ALA:O	2.06	0.55
1:F:204:LYS:HB3	1:F:384:ILE:CG2	2.37	0.55
1:F:276:LEU:HD23	1:F:300:LEU:CB	2.36	0.55
1:G:35:ILE:HG13	1:G:79:ALA:HB1	1.89	0.55
1:G:128:TYR:CE2	1:G:440:PHE:HB2	2.42	0.55
1:A:205:LYS:O	1:A:377:ARG:NH1	2.40	0.55
1:D:392:GLU:O	1:D:396:LYS:HE3	2.07	0.55
1:E:142:ILE:HB	1:E:475:LEU:CD2	2.37	0.55
1:E:215:LEU:HD11	1:E:372:VAL:HG21	1.89	0.55
1:A:209:GLY:C	1:A:211:GLU:H	2.10	0.54
1:C:29:ILE:O	1:C:33:ARG:HG3	2.06	0.54
1:C:136:GLN:NE2	1:C:136:GLN:HA	2.22	0.54
1:G:125:ILE:HG23	1:G:513:ILE:CG2	2.37	0.54
1:H:215:LEU:HD11	1:H:372:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG21	1:A:339:LEU:HG	1.90	0.54
1:D:350:VAL:HG13	1:D:363:VAL:HG22	1.89	0.54
1:F:196:ASP:OD1	1:F:198:ASP:HB2	2.06	0.54
1:H:11:ILE:HG23	1:H:12:LEU:H	1.72	0.54
1:B:258:ASN:HB3	1:C:258:ASN:HD21	1.72	0.54
1:C:227:HIS:HB3	1:C:230:MET:HG3	1.89	0.54
1:D:238:LYS:HD2	1:D:287:GLY:O	2.08	0.54
1:D:248:VAL:HG11	1:D:272:GLU:OE2	2.07	0.54
1:D:466:VAL:HG21	1:D:479:ILE:HG12	1.89	0.54
1:D:488:ASP:O	1:D:492:LYS:HG2	2.07	0.54
1:F:461:GLU:HG2	1:F:465:LYS:NZ	2.22	0.54
1:A:235:GLU:O	1:A:236:ASN:C	2.45	0.54
1:A:417:GLU:OE2	1:A:470:HIS:NE2	2.34	0.54
1:B:209:GLY:O	1:B:212:GLU:HG2	2.07	0.54
1:D:380:THR:HG23	1:D:383:VAL:H	1.72	0.54
1:G:217:ARG:HA	1:G:372:VAL:HG23	1.89	0.54
1:G:370:LYS:HE2	1:G:370:LYS:CA	2.35	0.54
1:A:260:THR:N	1:A:264:GLN:HE21	1.97	0.54
1:D:166:ASN:HA	1:E:517:ARG:NH1	2.23	0.54
1:E:239:ILE:HD13	1:E:328:THR:HG21	1.90	0.54
1:E:488:ASP:O	1:E:492:LYS:HG2	2.07	0.54
1:E:503:GLN:HA	1:E:503:GLN:NE2	2.23	0.54
1:F:26:ARG:CB	1:F:26:ARG:HH11	2.20	0.54
1:H:138:ILE:O	1:H:142:ILE:HG12	2.08	0.54
1:D:108:LEU:HD11	1:D:515:ILE:HD12	1.89	0.54
1:E:42:THR:HG22	1:E:48:MET:O	2.08	0.54
1:H:206:ALA:CA	1:H:384:ILE:HD11	2.36	0.54
1:B:445:LYS:C	1:B:448:PRO:HD2	2.28	0.54
1:E:30:LEU:O	1:E:34:ILE:HG13	2.07	0.54
1:G:94:GLY:CA	1:G:396:LYS:HD2	2.38	0.54
1:A:233:ARG:HH12	1:A:349:VAL:HG11	1.72	0.54
1:E:205:LYS:O	1:E:377:ARG:NH1	2.41	0.54
1:G:142:ILE:HB	1:G:475:LEU:CD2	2.36	0.54
1:G:430:GLY:CA	1:G:434:ALA:HB2	2.37	0.54
1:A:462:MET:HE1	1:A:486:PRO:HD3	1.89	0.54
1:B:117:GLN:O	1:B:118:ASN:HB2	2.06	0.54
1:D:54:ASP:OD1	1:D:58:ASP:HB3	2.06	0.54
1:E:230:MET:HE2	1:E:312:ALA:H	1.72	0.54
1:F:380:THR:HG22	1:F:383:VAL:CG2	2.30	0.54
1:H:143:ALA:HB3	1:H:145:ARG:NH1	2.22	0.54
1:D:218:GLY:HA3	1:D:363:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:HD11	1:D:377:ARG:NH2	2.23	0.54
1:D:76:HIS:HB2	1:E:11:ILE:HA	1.91	0.53
1:D:134:LYS:O	1:D:138:ILE:HG13	2.08	0.53
1:E:372:VAL:HG22	1:E:373:THR:N	2.23	0.53
1:E:446:ILE:HG22	1:E:450:THR:HG23	1.91	0.53
1:H:348:GLU:HB3	1:H:365:GLY:HA3	1.91	0.53
1:B:189:LYS:HD2	1:B:189:LYS:C	2.28	0.53
1:C:136:GLN:HA	1:C:136:GLN:HE21	1.71	0.53
1:E:258:ASN:HB3	1:F:258:ASN:ND2	2.23	0.53
1:G:272:GLU:HA	1:G:275:MET:HE2	1.90	0.53
1:H:146:VAL:HG22	1:H:147:ASP:N	2.22	0.53
1:A:33:ARG:NH1	1:A:109:ARG:HG3	2.23	0.53
1:D:35:ILE:HD11	1:D:74:LEU:CD2	2.37	0.53
1:E:335:ASN:HD21	1:E:337:LYS:HB2	1.74	0.53
1:F:217:ARG:HA	1:F:372:VAL:CG2	2.36	0.53
1:F:317:LYS:O	1:F:320:ASP:N	2.41	0.53
1:G:18:ARG:HG3	1:G:522:ILE:HG12	1.90	0.53
1:G:146:VAL:HG22	1:G:147:ASP:N	2.24	0.53
1:H:426:ALA:HB1	1:H:438:GLU:HG3	1.91	0.53
1:A:94:GLY:CA	1:A:396:LYS:HD2	2.39	0.53
1:A:501:LYS:HA	1:A:501:LYS:HE3	1.88	0.53
1:B:216:VAL:O	1:B:372:VAL:CG2	2.56	0.53
1:C:31:ALA:CB	1:C:76:HIS:CD2	2.91	0.53
1:E:167:ALA:C	1:E:169:SER:H	2.11	0.53
1:E:233:ARG:HH12	1:E:349:VAL:HG13	1.72	0.53
1:F:11:ILE:HD13	1:F:11:ILE:C	2.29	0.53
1:F:12:LEU:HD23	1:F:13:PRO:HD2	1.90	0.53
1:F:138:ILE:HD13	1:F:421:ARG:HG2	1.91	0.53
1:G:11:ILE:CG2	1:G:12:LEU:H	2.21	0.53
1:H:151:GLU:O	1:H:155:LEU:HD23	2.08	0.53
1:D:391:LEU:O	1:D:395:VAL:HG23	2.08	0.53
1:E:50:LYS:HD2	1:E:68:ILE:HD13	1.90	0.53
1:E:146:VAL:HG22	1:E:147:ASP:N	2.21	0.53
1:F:38:THR:O	1:F:50:LYS:CE	2.57	0.53
1:F:147:ASP:O	1:F:149:ASP:N	2.41	0.53
1:F:418:LEU:O	1:F:422:LEU:HB2	2.09	0.53
1:G:409:PRO:HB2	1:G:489:MET:HB2	1.91	0.53
1:A:315:ARG:HG3	1:A:315:ARG:NH1	2.24	0.53
1:A:466:VAL:HG22	1:A:486:PRO:HG3	1.91	0.53
1:A:473:ARG:HB2	1:A:477:ILE:HG13	1.90	0.53
1:B:82:MET:CE	1:B:101:VAL:HG13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:LYS:HD2	1:H:352:GLU:OE2	2.09	0.53
1:H:315:ARG:HH11	1:H:315:ARG:HG3	1.73	0.53
1:C:259:ILE:HD12	1:C:259:ILE:N	2.24	0.53
1:C:313:VAL:HG21	1:C:361:ILE:CD1	2.38	0.53
1:C:354:LYS:HA	1:C:358:GLU:O	2.09	0.53
1:D:146:VAL:HG22	1:D:147:ASP:N	2.23	0.53
1:D:425:TYR:O	1:D:429:VAL:HG23	2.08	0.53
1:E:460:VAL:O	1:E:464:VAL:HG23	2.07	0.53
1:F:146:VAL:O	1:F:148:PRO:HD3	2.09	0.53
1:G:408:LEU:HD12	1:G:498:LEU:HA	1.89	0.53
1:G:417:GLU:OE2	1:G:470:HIS:NE2	2.42	0.53
1:B:106:GLU:HG2	1:B:446:ILE:HG13	1.91	0.53
1:E:184:GLN:NE2	1:E:217:ARG:NH2	2.57	0.53
1:E:208:GLU:HB3	1:E:212:GLU:CG	2.39	0.53
1:F:353:ARG:HD2	1:F:362:PHE:CD1	2.44	0.53
1:H:10:VAL:HG22	1:H:11:ILE:N	2.15	0.53
1:A:155:LEU:HA	1:A:179:VAL:HG21	1.91	0.53
1:B:354:LYS:HA	1:B:358:GLU:O	2.08	0.53
1:E:469:GLU:CB	1:E:477:ILE:HG21	2.38	0.53
1:F:154:LEU:HG	1:F:398:VAL:HG13	1.89	0.53
1:H:227:HIS:HB3	1:H:230:MET:CG	2.37	0.53
1:A:22:ARG:CG	1:A:23:ASP:N	2.72	0.52
1:A:189:LYS:HD2	1:A:189:LYS:C	2.28	0.52
1:B:146:VAL:HG22	1:B:147:ASP:N	2.24	0.52
1:D:463:LEU:O	1:D:467:ILE:HG13	2.09	0.52
1:E:353:ARG:NH2	1:E:364:GLU:OE2	2.40	0.52
1:E:421:ARG:HH11	1:E:421:ARG:CB	2.09	0.52
1:A:221:ILE:CD1	1:A:324:LEU:HD11	2.39	0.52
1:C:217:ARG:HA	1:C:372:VAL:HG23	1.90	0.52
1:G:208:GLU:HG3	1:G:377:ARG:HH21	1.74	0.52
1:H:245:ALA:HB1	1:H:247:GLU:OE1	2.09	0.52
1:A:227:HIS:HB3	1:A:230:MET:HG3	1.90	0.52
1:B:388:GLU:O	1:B:392:GLU:HG3	2.08	0.52
1:D:227:HIS:HB3	1:D:230:MET:SD	2.49	0.52
1:E:423:ASP:O	1:E:426:ALA:HB3	2.09	0.52
1:F:370:LYS:HA	1:F:370:LYS:CE	2.36	0.52
1:G:410:ALA:HB3	1:G:494:ILE:HG22	1.90	0.52
1:A:184:GLN:NE2	1:A:184:GLN:HA	2.24	0.52
1:A:465:LYS:O	1:A:468:SER:HB3	2.09	0.52
1:B:22:ARG:CG	1:B:23:ASP:N	2.71	0.52
1:B:425:TYR:O	1:B:429:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLU:O	1:C:392:GLU:HG3	2.09	0.52
1:D:286:THR:HG21	1:D:339:LEU:HG	1.92	0.52
1:F:205:LYS:O	1:F:377:ARG:NH1	2.42	0.52
1:H:372:VAL:HG22	1:H:373:THR:H	1.74	0.52
1:A:217:ARG:HA	1:A:372:VAL:HG23	1.92	0.52
1:B:25:GLN:O	1:B:29:ILE:HG13	2.10	0.52
1:B:315:ARG:HG3	1:B:315:ARG:NH1	2.16	0.52
1:C:506:LYS:O	1:C:510:GLU:CG	2.57	0.52
1:D:31:ALA:CB	1:D:76:HIS:CD2	2.93	0.52
1:H:38:THR:O	1:H:50:LYS:CE	2.57	0.52
1:A:195:VAL:HB	1:A:399:LYS:HG3	1.89	0.52
1:C:183:LYS:HG2	1:C:402:MET:HE3	1.92	0.52
1:C:335:ASN:OD1	1:C:337:LYS:HB2	2.09	0.52
1:D:293:VAL:HG21	1:D:297:ILE:HD11	1.92	0.52
1:D:342:GLU:OE2	1:D:342:GLU:N	2.40	0.52
1:E:286:THR:HA	1:E:341:PRO:HG3	1.91	0.52
1:G:462:MET:O	1:G:466:VAL:HG23	2.10	0.52
1:H:76:HIS:CD2	1:H:78:ALA:H	2.28	0.52
1:H:170:HIS:CE1	1:H:210:VAL:HB	2.44	0.52
1:H:460:VAL:O	1:H:464:VAL:HG23	2.09	0.52
1:B:81:MET:HE3	1:B:514:MET:SD	2.50	0.52
1:B:496:GLU:OE1	1:B:501:LYS:NZ	2.31	0.52
1:C:230:MET:HE1	1:C:312:ALA:HB3	1.91	0.52
1:C:368:ASN:ND2	1:C:370:LYS:HE3	2.24	0.52
1:C:394:ALA:O	1:C:398:VAL:HG23	2.09	0.52
1:D:209:GLY:C	1:D:211:GLU:H	2.11	0.52
1:E:22:ARG:CG	1:E:23:ASP:N	2.72	0.52
1:E:233:ARG:NH1	1:E:349:VAL:HG13	2.24	0.52
1:E:260:THR:H	1:E:264:GLN:HE21	1.56	0.52
1:F:380:THR:CG2	1:F:383:VAL:H	2.20	0.52
1:C:445:LYS:C	1:C:448:PRO:HD2	2.30	0.52
1:D:147:ASP:O	1:D:149:ASP:N	2.43	0.52
1:E:31:ALA:HA	1:E:34:ILE:HD12	1.91	0.52
1:G:227:HIS:HE2	1:H:334:THR:HB	1.75	0.52
1:G:524:ALA:O	1:G:525:LYS:HD2	2.09	0.52
1:A:182:VAL:HG22	1:A:395:VAL:HG13	1.92	0.52
1:A:461:GLU:HG2	1:A:465:LYS:NZ	2.25	0.52
1:C:13:PRO:O	1:C:16:THR:HB	2.10	0.52
1:D:424:GLU:O	1:D:428:GLN:HG2	2.10	0.52
1:F:29:ILE:HG23	1:F:108:LEU:HB3	1.92	0.52
1:G:380:THR:CG2	1:G:383:VAL:H	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASP:OD1	1:A:427:LYS:HE2	2.10	0.52
1:B:22:ARG:HG3	1:B:23:ASP:N	2.24	0.52
1:B:383:VAL:O	1:B:387:VAL:HG23	2.09	0.52
1:C:126:LYS:NZ	1:C:126:LYS:HB3	2.25	0.52
1:F:151:GLU:O	1:F:155:LEU:HD23	2.10	0.52
1:G:45:PRO:HA	1:G:164:GLY:HA2	1.92	0.52
1:H:483:GLU:HG3	1:H:485:LYS:HZ3	1.75	0.52
1:H:483:GLU:OE1	1:H:483:GLU:HA	2.09	0.52
1:D:59:ILE:HD12	1:D:59:ILE:N	2.25	0.51
1:E:330:ALA:HB2	1:E:345:GLY:HA3	1.92	0.51
1:E:470:HIS:CE1	1:E:475:LEU:HA	2.45	0.51
1:H:17:GLN:NE2	1:H:17:GLN:H	2.07	0.51
1:H:92:GLU:O	1:H:499:ARG:HD3	2.11	0.51
1:H:217:ARG:HB3	1:H:217:ARG:HH11	1.75	0.51
1:H:293:VAL:HG21	1:H:297:ILE:HD11	1.92	0.51
1:B:81:MET:CE	1:B:514:MET:SD	2.98	0.51
1:B:184:GLN:HE22	1:B:217:ARG:HH21	1.54	0.51
1:C:217:ARG:HB3	1:C:217:ARG:HH11	1.75	0.51
1:D:370:LYS:HE2	1:D:370:LYS:CA	2.39	0.51
1:E:327:ALA:O	1:E:366:CYS:HB3	2.10	0.51
1:F:458:ASP:O	1:F:459:THR:C	2.48	0.51
1:A:73:ASP:O	1:B:13:PRO:HD3	2.10	0.51
1:A:106:GLU:HG2	1:A:446:ILE:CG1	2.40	0.51
1:A:445:LYS:O	1:A:448:PRO:HD2	2.10	0.51
1:B:257:ILE:HG22	1:B:259:ILE:HD12	1.93	0.51
1:D:94:GLY:HA2	1:D:396:LYS:HD2	1.91	0.51
1:E:59:ILE:HD12	1:E:59:ILE:H	1.73	0.51
1:F:126:LYS:HB3	1:F:126:LYS:HZ2	1.74	0.51
1:F:201:LYS:HB2	1:F:323:LYS:HE3	1.92	0.51
1:A:170:HIS:HD2	1:A:211:GLU:OE1	1.93	0.51
1:B:154:LEU:HG	1:B:398:VAL:HG13	1.92	0.51
1:D:142:ILE:HB	1:D:475:LEU:CD2	2.41	0.51
1:E:33:ARG:NH1	1:E:109:ARG:HG3	2.26	0.51
1:E:94:GLY:HA2	1:E:396:LYS:HD2	1.93	0.51
1:E:147:ASP:O	1:E:149:ASP:N	2.43	0.51
1:G:184:GLN:NE2	1:G:217:ARG:NH2	2.59	0.51
1:G:250:LYS:NZ	1:H:253:THR:HA	2.26	0.51
1:D:75:GLN:HB2	1:E:10:VAL:C	2.31	0.51
1:E:417:GLU:OE1	1:E:421:ARG:NH1	2.43	0.51
1:H:136:GLN:HA	1:H:136:GLN:HE21	1.75	0.51
1:H:335:ASN:OD1	1:H:337:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:LYS:HE3	1:F:459:THR:CG2	2.40	0.51
1:H:239:ILE:HD11	1:H:347:ALA:CB	2.39	0.51
1:H:465:LYS:O	1:H:468:SER:HB3	2.09	0.51
1:A:460:VAL:O	1:A:464:VAL:HG23	2.11	0.51
1:B:217:ARG:HA	1:B:372:VAL:HG23	1.92	0.51
1:B:409:PRO:HB3	1:B:490:LEU:HD13	1.93	0.51
1:C:370:LYS:HE2	1:C:370:LYS:CA	2.41	0.51
1:C:392:GLU:O	1:C:396:LYS:HE3	2.11	0.51
1:D:188:LYS:HD3	1:D:193:TYR:CE1	2.45	0.51
1:E:446:ILE:HD12	1:E:446:ILE:H	1.76	0.51
1:G:136:GLN:HA	1:G:136:GLN:NE2	2.26	0.51
1:G:210:VAL:HA	1:G:377:ARG:O	2.11	0.51
1:G:313:VAL:HG21	1:G:361:ILE:HD13	1.92	0.51
1:H:429:VAL:HG21	1:H:437:ILE:CD1	2.41	0.51
1:B:348:GLU:CB	1:B:365:GLY:HA3	2.40	0.51
1:B:372:VAL:HG22	1:B:373:THR:N	2.26	0.51
1:C:22:ARG:CG	1:C:23:ASP:N	2.74	0.51
1:C:145:ARG:HG2	1:C:145:ARG:HH11	1.76	0.51
1:C:293:VAL:HG21	1:C:297:ILE:HD11	1.92	0.51
1:H:138:ILE:HD13	1:H:421:ARG:HG2	1.92	0.51
1:B:196:ASP:OD1	1:B:198:ASP:HB2	2.11	0.51
1:D:397:VAL:O	1:D:401:VAL:HG23	2.11	0.51
1:G:355:LEU:O	1:G:356:ALA:HB3	2.11	0.51
1:B:258:ASN:HB3	1:C:258:ASN:ND2	2.26	0.51
1:C:430:GLY:CA	1:C:434:ALA:HB2	2.41	0.51
1:D:292:PHE:CD1	1:D:324:LEU:HD13	2.45	0.51
1:E:51:MET:CE	1:F:77:PRO:HB2	2.41	0.51
1:G:59:ILE:HD12	1:G:59:ILE:H	1.76	0.51
1:A:146:VAL:HG22	1:A:147:ASP:H	1.75	0.50
1:B:412:GLY:HA2	1:B:415:GLU:CG	2.41	0.50
1:D:498:LEU:O	1:D:498:LEU:HD22	2.11	0.50
1:F:266:MET:O	1:F:270:GLU:HG3	2.11	0.50
1:F:498:LEU:O	1:F:498:LEU:HD22	2.11	0.50
1:B:269:LEU:HD12	1:C:251:THR:HG23	1.91	0.50
1:C:215:LEU:HD11	1:C:372:VAL:CG2	2.40	0.50
1:D:72:ILE:HG22	1:D:73:ASP:N	2.26	0.50
1:E:445:LYS:O	1:E:448:PRO:HD2	2.11	0.50
1:F:297:ILE:HD12	1:F:314:ARG:HB3	1.92	0.50
1:G:216:VAL:O	1:G:218:GLY:N	2.43	0.50
1:G:259:ILE:HG23	1:G:264:GLN:HB2	1.93	0.50
1:C:126:LYS:O	1:C:130:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LEU:HD22	1:D:179:VAL:HG21	1.93	0.50
1:D:210:VAL:O	1:D:210:VAL:HG12	2.12	0.50
1:D:271:GLN:O	1:D:275:MET:HG3	2.10	0.50
1:E:54:ASP:OD1	1:E:58:ASP:HB3	2.11	0.50
1:G:188:LYS:HD3	1:G:193:TYR:CE1	2.46	0.50
1:A:77:PRO:CG	1:H:53:VAL:HG21	2.41	0.50
1:B:233:ARG:HH11	1:B:233:ARG:HG3	1.77	0.50
1:B:461:GLU:HG2	1:B:465:LYS:NZ	2.25	0.50
1:C:227:HIS:HD1	1:C:229:ARG:H	1.58	0.50
1:E:106:GLU:HG2	1:E:446:ILE:HG13	1.93	0.50
1:E:204:LYS:HB3	1:E:384:ILE:CG2	2.40	0.50
1:E:315:ARG:HH11	1:E:315:ARG:HG3	1.76	0.50
1:F:117:GLN:O	1:F:118:ASN:HB2	2.10	0.50
1:G:17:GLN:NE2	1:G:17:GLN:N	2.57	0.50
1:G:117:GLN:O	1:G:118:ASN:HB2	2.10	0.50
1:G:189:LYS:HD2	1:G:189:LYS:C	2.32	0.50
1:A:271:GLN:O	1:A:275:MET:HG3	2.11	0.50
1:A:418:LEU:O	1:A:422:LEU:HB2	2.12	0.50
1:C:215:LEU:HD11	1:C:372:VAL:HG21	1.93	0.50
1:D:421:ARG:HB2	1:D:421:ARG:NH1	2.20	0.50
1:E:82:MET:CE	1:E:101:VAL:HG13	2.42	0.50
1:E:209:GLY:C	1:E:211:GLU:H	2.15	0.50
1:E:221:ILE:CD1	1:E:324:LEU:HD11	2.41	0.50
1:F:235:GLU:O	1:F:236:ASN:C	2.50	0.50
1:G:239:ILE:H	1:G:239:ILE:HD12	1.75	0.50
1:H:415:GLU:HG3	1:H:447:ILE:HB	1.94	0.50
1:A:182:VAL:CG2	1:A:395:VAL:HG13	2.42	0.50
1:D:51:MET:HB2	1:E:518:ILE:HD13	1.94	0.50
1:D:258:ASN:CB	1:E:258:ASN:HD21	2.14	0.50
1:D:450:THR:O	1:D:454:ASN:ND2	2.44	0.50
1:A:147:ASP:O	1:A:149:ASP:N	2.45	0.50
1:B:146:VAL:HG22	1:B:147:ASP:H	1.77	0.50
1:C:256:LYS:HE3	1:D:254:ASP:OD1	2.11	0.50
1:D:303:HIS:NE2	1:E:335:ASN:HB3	2.26	0.50
1:E:35:ILE:HD11	1:E:74:LEU:CD2	2.42	0.50
1:E:92:GLU:O	1:E:499:ARG:HD3	2.12	0.50
1:E:462:MET:HE3	1:E:465:LYS:HD2	1.94	0.50
1:G:138:ILE:O	1:G:142:ILE:HG23	2.12	0.50
1:G:175:ALA:O	1:G:179:VAL:HG23	2.11	0.50
1:H:29:ILE:O	1:H:33:ARG:HG3	2.11	0.50
1:A:218:GLY:HA3	1:A:363:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HD13	1:B:517:ARG:HG2	1.93	0.50
1:C:134:LYS:O	1:C:138:ILE:HG13	2.12	0.50
1:D:89:GLN:OE1	1:D:503:GLN:HG3	2.11	0.50
1:D:272:GLU:HA	1:D:275:MET:HE3	1.92	0.50
1:D:462:MET:O	1:D:466:VAL:HG23	2.12	0.50
1:E:277:LYS:HB2	1:E:304:TYR:CE2	2.47	0.50
1:G:10:VAL:CG1	1:G:11:ILE:H	2.13	0.50
1:G:215:LEU:HD11	1:G:372:VAL:HG21	1.94	0.50
1:H:138:ILE:CD1	1:H:421:ARG:HG2	2.42	0.50
1:H:286:THR:HG21	1:H:339:LEU:HG	1.93	0.50
1:E:126:LYS:NZ	1:E:126:LYS:HB3	2.27	0.50
1:E:167:ALA:O	1:E:169:SER:N	2.45	0.50
1:G:408:LEU:O	1:G:495:ILE:HB	2.12	0.50
1:A:91:LYS:HB2	1:A:91:LYS:HZ2	1.77	0.49
1:B:175:ALA:O	1:B:179:VAL:HG23	2.12	0.49
1:B:225:VAL:HG23	1:B:352:GLU:OE1	2.12	0.49
1:B:461:GLU:HG2	1:B:465:LYS:HZ2	1.77	0.49
1:C:217:ARG:HB3	1:C:217:ARG:NH1	2.27	0.49
1:E:106:GLU:HG2	1:E:446:ILE:HG12	1.93	0.49
1:E:462:MET:CE	1:E:486:PRO:HD3	2.42	0.49
1:H:244:GLU:OE1	1:H:336:VAL:HG22	2.12	0.49
1:A:150:ASP:OD1	1:A:153:THR:HG23	2.12	0.49
1:A:462:MET:HE3	1:A:462:MET:CA	2.41	0.49
1:A:513:ILE:O	1:A:517:ARG:HG3	2.12	0.49
1:B:120:HIS:CG	1:B:121:PRO:HD2	2.48	0.49
1:B:259:ILE:HD12	1:B:259:ILE:N	2.27	0.49
1:C:72:ILE:HG22	1:C:74:LEU:HD23	1.92	0.49
1:C:188:LYS:HD3	1:C:193:TYR:CE1	2.46	0.49
1:C:498:LEU:HD13	1:C:502:LYS:HD3	1.95	0.49
1:D:393:ASP:O	1:D:397:VAL:HG22	2.12	0.49
1:E:11:ILE:C	1:E:11:ILE:CD1	2.80	0.49
1:E:11:ILE:HG23	1:E:12:LEU:H	1.77	0.49
1:E:81:MET:HE3	1:E:514:MET:SD	2.51	0.49
1:E:110:LYS:HE3	1:E:442:ASP:OD1	2.11	0.49
1:E:394:ALA:O	1:E:397:VAL:HG22	2.12	0.49
1:F:72:ILE:HG22	1:F:74:LEU:HD23	1.95	0.49
1:A:123:ILE:HG21	1:A:432:LYS:HB2	1.95	0.49
1:A:227:HIS:ND1	1:A:228:PRO:HD2	2.28	0.49
1:C:75:GLN:HB2	1:D:11:ILE:C	2.32	0.49
1:E:247:GLU:HA	1:E:276:LEU:HD11	1.94	0.49
1:F:476:GLY:HA3	1:F:490:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:ILE:HD11	1:H:347:ALA:HB3	1.93	0.49
1:H:241:LEU:CD2	1:H:330:ALA:HB3	2.42	0.49
1:H:245:ALA:HB1	1:H:247:GLU:HG2	1.95	0.49
1:A:188:LYS:HB2	1:A:193:TYR:HA	1.94	0.49
1:A:209:GLY:O	1:A:211:GLU:N	2.45	0.49
1:A:251:THR:HG23	1:H:269:LEU:CD1	2.40	0.49
1:C:35:ILE:HD12	1:C:69:LEU:CD2	2.43	0.49
1:C:125:ILE:CD1	1:C:517:ARG:HG2	2.41	0.49
1:C:432:LYS:O	1:C:435:LEU:HB2	2.11	0.49
1:E:99:THR:HG23	1:E:447:ILE:HD12	1.95	0.49
1:F:216:VAL:O	1:F:218:GLY:N	2.45	0.49
1:F:462:MET:CE	1:F:465:LYS:HD2	2.42	0.49
1:C:138:ILE:O	1:C:142:ILE:HG23	2.12	0.49
1:C:293:VAL:CG2	1:C:297:ILE:HD11	2.42	0.49
1:C:304:TYR:O	1:C:308:TYR:HD1	1.96	0.49
1:D:12:LEU:HD23	1:D:13:PRO:HD2	1.93	0.49
1:D:409:PRO:HA	1:D:495:ILE:HG22	1.93	0.49
1:G:462:MET:CE	1:G:486:PRO:HD3	2.42	0.49
1:G:506:LYS:O	1:G:510:GLU:CG	2.60	0.49
1:H:146:VAL:HG22	1:H:147:ASP:H	1.76	0.49
1:A:205:LYS:HE3	1:A:360:MET:SD	2.52	0.49
1:D:136:GLN:HA	1:D:136:GLN:HE21	1.78	0.49
1:E:72:ILE:HD11	1:F:522:ILE:CD1	2.37	0.49
1:E:413:ALA:N	1:E:414:PRO:CD	2.76	0.49
1:A:103:ILE:O	1:A:107:LEU:HB2	2.12	0.49
1:A:208:GLU:HB3	1:A:212:GLU:CG	2.42	0.49
1:C:146:VAL:HG22	1:C:147:ASP:H	1.78	0.49
1:D:81:MET:HE3	1:D:514:MET:SD	2.53	0.49
1:E:170:HIS:HD2	1:E:211:GLU:OE1	1.96	0.49
1:F:38:THR:O	1:F:50:LYS:HE3	2.12	0.49
1:C:197:LEU:HD22	1:C:395:VAL:CG1	2.42	0.49
1:C:369:PRO:HB2	1:C:371:ALA:O	2.13	0.49
1:D:136:GLN:HA	1:D:136:GLN:NE2	2.27	0.49
1:E:248:VAL:HG11	1:E:272:GLU:OE2	2.12	0.49
1:E:400:ASP:OD1	1:E:499:ARG:HD2	2.12	0.49
1:G:126:LYS:HB3	1:G:126:LYS:HZ2	1.77	0.49
1:G:458:ASP:OD1	1:G:461:GLU:HB2	2.13	0.49
1:H:242:ILE:HD11	1:H:339:LEU:HD22	1.94	0.49
1:A:123:ILE:HG21	1:A:432:LYS:CB	2.43	0.49
1:A:272:GLU:HA	1:A:275:MET:CE	2.43	0.49
1:B:73:ASP:O	1:C:13:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:C	1:B:166:ASN:ND2	2.65	0.49
1:C:179:VAL:O	1:C:183:LYS:HG3	2.13	0.49
1:D:18:ARG:HG3	1:D:522:ILE:HG12	1.95	0.49
1:E:13:PRO:O	1:E:16:THR:HB	2.13	0.49
1:F:204:LYS:HD2	1:F:384:ILE:CG2	2.43	0.49
1:F:211:GLU:HA	1:F:211:GLU:OE1	2.13	0.49
1:G:123:ILE:HG21	1:G:432:LYS:CB	2.36	0.49
1:H:154:LEU:HG	1:H:398:VAL:HG13	1.93	0.49
1:E:477:ILE:HD13	1:E:488:ASP:HA	1.94	0.49
1:G:69:LEU:HB3	1:G:83:VAL:HG22	1.95	0.49
1:G:182:VAL:HG13	1:G:195:VAL:HG11	1.94	0.49
1:A:144:ILE:CD1	1:A:490:LEU:HD21	2.40	0.48
1:B:91:LYS:HB2	1:B:91:LYS:HZ2	1.77	0.48
1:C:99:THR:O	1:C:103:ILE:HG13	2.12	0.48
1:C:430:GLY:HA2	1:C:434:ALA:HB2	1.94	0.48
1:D:182:VAL:CG2	1:D:395:VAL:HG13	2.43	0.48
1:D:503:GLN:HA	1:D:503:GLN:NE2	2.28	0.48
1:E:109:ARG:HG2	1:E:109:ARG:NH1	2.24	0.48
1:E:145:ARG:HG2	1:E:145:ARG:NH1	2.28	0.48
1:F:333:VAL:HG21	1:F:339:LEU:HD13	1.95	0.48
1:G:304:TYR:O	1:G:308:TYR:HD1	1.95	0.48
1:H:404:ASP:OD1	1:H:499:ARG:HB2	2.13	0.48
1:B:143:ALA:HB3	1:B:145:ARG:NH1	2.28	0.48
1:B:215:LEU:HD11	1:B:372:VAL:HG21	1.96	0.48
1:C:82:MET:CE	1:C:101:VAL:HG13	2.43	0.48
1:C:348:GLU:O	1:C:349:VAL:CG2	2.59	0.48
1:D:221:ILE:CD1	1:D:324:LEU:HD11	2.43	0.48
1:G:54:ASP:OD1	1:G:58:ASP:CB	2.54	0.48
1:B:52:LEU:HD11	1:B:68:ILE:HA	1.95	0.48
1:B:91:LYS:HG2	1:B:91:LYS:O	2.14	0.48
1:B:250:LYS:HZ3	1:C:253:THR:HA	1.78	0.48
1:B:314:ARG:HD2	1:B:315:ARG:HD3	1.96	0.48
1:B:423:ASP:OD1	1:B:427:LYS:HE2	2.12	0.48
1:C:75:GLN:CG	1:D:10:VAL:HG13	2.42	0.48
1:A:49:ASP:OD1	1:A:63:ASN:HB2	2.13	0.48
1:A:94:GLY:HA3	1:A:396:LYS:HD2	1.94	0.48
1:A:146:VAL:HG22	1:A:147:ASP:N	2.29	0.48
1:A:197:LEU:HD22	1:A:395:VAL:HG12	1.96	0.48
1:A:235:GLU:O	1:A:236:ASN:O	2.32	0.48
1:D:123:ILE:HG21	1:D:432:LYS:HB3	1.91	0.48
1:D:487:ALA:HB3	1:D:489:MET:CE	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:GLN:HE21	1:F:13:PRO:HA	1.79	0.48
1:E:204:LYS:HD2	1:E:384:ILE:HG22	1.94	0.48
1:E:232:LYS:HD2	1:E:352:GLU:OE2	2.13	0.48
1:E:257:ILE:HG22	1:E:259:ILE:CD1	2.41	0.48
1:F:23:ASP:O	1:F:27:LEU:HG	2.14	0.48
1:G:450:THR:O	1:G:454:ASN:ND2	2.46	0.48
1:G:501:LYS:HA	1:G:501:LYS:HE3	1.95	0.48
1:A:397:VAL:HA	1:A:400:ASP:OD2	2.14	0.48
1:C:166:ASN:O	1:C:168:GLU:HG2	2.14	0.48
1:C:342:GLU:OE2	1:C:342:GLU:N	2.46	0.48
1:D:63:ASN:O	1:D:63:ASN:ND2	2.47	0.48
1:C:330:ALA:HB2	1:C:345:GLY:HA3	1.94	0.48
1:C:370:LYS:HA	1:C:370:LYS:CE	2.43	0.48
1:G:119:ILE:HD11	1:G:435:LEU:HD23	1.95	0.48
1:G:219:VAL:HG12	1:G:220:VAL:N	2.29	0.48
1:A:143:ALA:HB3	1:A:145:ARG:HH12	1.79	0.48
1:A:409:PRO:HA	1:A:495:ILE:HG22	1.94	0.48
1:B:35:ILE:HG21	1:B:82:MET:CB	2.44	0.48
1:B:100:ALA:O	1:B:508:ALA:HB2	2.14	0.48
1:B:450:THR:O	1:B:454:ASN:ND2	2.47	0.48
1:C:243:ASN:OD1	1:C:295:LYS:HE3	2.14	0.48
1:E:304:TYR:O	1:E:308:TYR:HD1	1.97	0.48
1:E:475:LEU:HD12	1:E:475:LEU:O	2.13	0.48
1:F:315:ARG:HG3	1:F:315:ARG:NH1	2.22	0.48
1:F:369:PRO:O	1:F:370:LYS:HE2	2.13	0.48
1:G:273:GLU:HG2	1:G:300:LEU:CD1	2.43	0.48
1:A:297:ILE:HG22	1:A:302:GLN:HG3	1.96	0.48
1:B:143:ALA:HB3	1:B:145:ARG:HH12	1.79	0.48
1:B:212:GLU:HB2	1:B:377:ARG:HG3	1.96	0.48
1:B:524:ALA:O	1:B:525:LYS:HD2	2.12	0.48
1:C:120:HIS:ND1	1:C:122:SER:CB	2.76	0.48
1:C:423:ASP:O	1:C:426:ALA:HB3	2.13	0.48
1:D:158:ALA:O	1:D:162:ILE:HG13	2.13	0.48
1:E:22:ARG:HG3	1:E:23:ASP:N	2.29	0.48
1:E:158:ALA:O	1:E:162:ILE:HG13	2.12	0.48
1:E:280:VAL:HG11	1:E:304:TYR:HB3	1.96	0.48
1:E:317:LYS:O	1:E:320:ASP:N	2.47	0.48
1:H:50:LYS:HD2	1:H:68:ILE:HD13	1.96	0.48
1:B:269:LEU:HD12	1:C:251:THR:CG2	2.44	0.48
1:E:432:LYS:O	1:E:435:LEU:HB2	2.13	0.48
1:F:226:VAL:O	1:F:226:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:LEU:HD22	1:F:330:ALA:HB3	1.95	0.48
1:G:16:THR:HG23	1:G:523:ALA:O	2.14	0.48
1:G:146:VAL:HG22	1:G:147:ASP:H	1.79	0.48
1:H:99:THR:O	1:H:103:ILE:HG13	2.13	0.48
1:C:524:ALA:O	1:C:525:LYS:HE2	2.14	0.48
1:D:509:SER:O	1:D:513:ILE:HG13	2.13	0.48
1:F:38:THR:HG22	1:F:50:LYS:HE3	1.95	0.48
1:F:89:GLN:HG2	1:F:97:THR:HA	1.95	0.48
1:F:233:ARG:HH11	1:F:233:ARG:HG3	1.78	0.48
1:F:355:LEU:HB3	1:F:360:MET:SD	2.54	0.48
1:F:421:ARG:HB2	1:F:421:ARG:NH1	2.12	0.48
1:H:449:LYS:HG3	1:H:463:LEU:HD22	1.95	0.48
1:A:424:GLU:OE1	1:A:424:GLU:HA	2.14	0.47
1:B:37:GLU:HG2	1:B:40:ARG:NH1	2.29	0.47
1:B:82:MET:HE2	1:B:101:VAL:HG13	1.96	0.47
1:C:204:LYS:HB3	1:C:384:ILE:CG2	2.41	0.47
1:E:465:LYS:O	1:E:469:GLU:HG2	2.13	0.47
1:F:42:THR:HG22	1:F:48:MET:O	2.14	0.47
1:G:189:LYS:HD2	1:G:190:ASP:N	2.28	0.47
1:G:281:ASP:OD1	1:G:308:TYR:OH	2.20	0.47
1:A:333:VAL:HG21	1:A:339:LEU:HD13	1.96	0.47
1:C:11:ILE:HD13	1:C:12:LEU:HB2	1.96	0.47
1:E:239:ILE:HD11	1:E:347:ALA:CB	2.43	0.47
1:F:53:VAL:HG21	1:G:77:PRO:CG	2.44	0.47
1:F:145:ARG:HH11	1:F:145:ARG:HG2	1.79	0.47
1:F:207:GLY:HA2	1:G:92:GLU:OE1	2.14	0.47
1:F:293:VAL:HG21	1:F:297:ILE:HD11	1.96	0.47
1:F:463:LEU:O	1:F:467:ILE:HG13	2.14	0.47
1:G:217:ARG:HH11	1:G:217:ARG:CB	2.24	0.47
1:H:281:ASP:O	1:H:285:GLN:HG3	2.14	0.47
1:A:412:GLY:O	1:A:415:GLU:HG2	2.14	0.47
1:B:134:LYS:O	1:B:138:ILE:HG13	2.14	0.47
1:C:249:LYS:HE2	1:C:279:MET:CE	2.45	0.47
1:D:125:ILE:CD1	1:D:517:ARG:HG2	2.42	0.47
1:D:311:MET:HE3	1:D:350:VAL:HG12	1.97	0.47
1:F:498:LEU:HD13	1:F:502:LYS:HD3	1.95	0.47
1:G:409:PRO:HA	1:G:495:ILE:HG22	1.95	0.47
1:E:120:HIS:CG	1:E:121:PRO:HD2	2.49	0.47
1:H:272:GLU:HA	1:H:275:MET:CE	2.43	0.47
1:H:414:PRO:HD2	1:H:415:GLU:OE2	2.15	0.47
1:A:487:ALA:HB3	1:A:489:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:HD22	1:B:330:ALA:CB	2.45	0.47
1:E:197:LEU:HD22	1:E:395:VAL:HG12	1.96	0.47
1:E:498:LEU:HD22	1:E:498:LEU:O	2.15	0.47
1:G:150:ASP:OD1	1:G:153:THR:HG23	2.14	0.47
1:G:481:VAL:HG22	3:G:7528:ADP:N1	2.29	0.47
1:H:184:GLN:NE2	1:H:217:ARG:NH2	2.61	0.47
1:A:230:MET:HE2	1:A:312:ALA:H	1.77	0.47
1:A:272:GLU:HA	1:A:275:MET:HE3	1.96	0.47
1:A:518:ILE:HD13	1:H:51:MET:HB2	1.96	0.47
1:B:54:ASP:OD1	1:B:58:ASP:CB	2.62	0.47
1:B:123:ILE:HG21	1:B:432:LYS:HB3	1.95	0.47
1:C:51:MET:CE	1:D:77:PRO:HB2	2.44	0.47
1:C:229:ARG:NH1	1:D:332:ILE:O	2.47	0.47
1:C:286:THR:HG21	1:C:339:LEU:HG	1.95	0.47
1:C:298:ASP:O	1:C:302:GLN:HG3	2.14	0.47
1:F:22:ARG:CG	1:F:23:ASP:N	2.78	0.47
1:F:370:LYS:HE2	1:F:370:LYS:CA	2.39	0.47
1:G:91:LYS:HB2	1:G:91:LYS:NZ	2.29	0.47
1:H:425:TYR:O	1:H:429:VAL:HG23	2.15	0.47
1:A:257:ILE:HG12	1:H:259:ILE:HG21	1.95	0.47
1:A:367:LYS:HG2	1:A:368:ASN:N	2.29	0.47
1:B:150:ASP:OD2	1:B:152:GLU:HB3	2.14	0.47
1:B:260:THR:N	1:B:264:GLN:HE22	1.86	0.47
1:B:397:VAL:HG23	1:B:398:VAL:N	2.30	0.47
1:B:497:PRO:HB2	1:B:500:VAL:HG23	1.95	0.47
1:C:75:GLN:HG2	1:D:13:PRO:HD3	1.97	0.47
1:C:94:GLY:CA	1:C:396:LYS:HD2	2.45	0.47
1:C:276:LEU:HD23	1:C:300:LEU:HB2	1.97	0.47
1:D:51:MET:CE	1:E:77:PRO:HB2	2.44	0.47
1:E:103:ILE:O	1:E:103:ILE:HG22	2.14	0.47
1:F:26:ARG:HH11	1:F:26:ARG:HB3	1.78	0.47
1:F:37:GLU:HG2	1:F:40:ARG:NH1	2.30	0.47
1:F:222:ASP:O	1:F:223:LYS:HG2	2.15	0.47
1:G:59:ILE:HD11	1:H:80:LYS:HE2	1.96	0.47
1:G:188:LYS:HB2	1:G:193:TYR:HA	1.97	0.47
1:G:227:HIS:HE2	1:H:334:THR:CB	2.26	0.47
1:G:269:LEU:CD1	1:H:251:THR:HG23	2.44	0.47
1:H:13:PRO:O	1:H:16:THR:HB	2.15	0.47
1:H:18:ARG:HA	1:H:521:VAL:O	2.15	0.47
1:A:370:LYS:HE2	1:A:370:LYS:CA	2.40	0.47
1:B:208:GLU:HB3	1:B:212:GLU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ALA:HB3	1:D:414:PRO:HD3	1.95	0.47
1:C:106:GLU:HB2	1:C:446:ILE:HG12	1.97	0.47
1:C:208:GLU:OE2	1:C:212:GLU:HG3	2.15	0.47
1:D:16:THR:HA	1:D:523:ALA:O	2.15	0.47
1:D:38:THR:O	1:D:50:LYS:HE3	2.15	0.47
1:D:215:LEU:HD11	1:D:372:VAL:CG2	2.45	0.47
1:D:283:ILE:HA	1:D:339:LEU:HD23	1.96	0.47
1:G:241:LEU:HD22	1:G:330:ALA:HB3	1.97	0.47
1:H:208:GLU:HB3	1:H:212:GLU:HG3	1.95	0.47
1:B:99:THR:O	1:B:103:ILE:HG13	2.14	0.47
1:C:144:ILE:CD1	1:C:490:LEU:HD21	2.39	0.47
1:D:25:GLN:O	1:D:29:ILE:HG13	2.15	0.47
1:D:92:GLU:O	1:D:499:ARG:HD3	2.15	0.47
1:E:29:ILE:HG23	1:E:108:LEU:HB3	1.97	0.47
1:E:269:LEU:CD1	1:F:251:THR:HG23	2.45	0.47
1:G:120:HIS:ND1	1:G:122:SER:HB3	2.30	0.47
1:H:91:LYS:HG2	1:H:91:LYS:O	2.15	0.47
1:H:150:ASP:OD1	1:H:153:THR:HG23	2.14	0.47
1:A:146:VAL:HG21	1:A:153:THR:HG21	1.97	0.46
1:A:370:LYS:HA	1:A:370:LYS:CE	2.40	0.46
1:B:126:LYS:O	1:B:130:LEU:HG	2.14	0.46
1:B:314:ARG:HD2	1:B:315:ARG:CD	2.45	0.46
1:C:210:VAL:HA	1:C:377:ARG:O	2.15	0.46
1:D:483:GLU:O	1:D:485:LYS:HG2	2.14	0.46
1:F:446:ILE:N	1:F:446:ILE:HD12	2.29	0.46
1:H:253:THR:O	1:H:254:ASP:C	2.54	0.46
1:H:417:GLU:HG3	1:H:421:ARG:HH12	1.80	0.46
1:A:221:ILE:HD11	1:A:324:LEU:HD11	1.96	0.46
1:A:449:LYS:HE3	1:A:459:THR:HG21	1.98	0.46
1:A:483:GLU:HG3	1:A:485:LYS:HZ1	1.78	0.46
1:B:89:GLN:HG2	1:B:97:THR:HA	1.97	0.46
1:C:18:ARG:HG3	1:C:522:ILE:HG12	1.98	0.46
1:C:225:VAL:HG11	1:C:230:MET:HB2	1.97	0.46
1:C:249:LYS:HE2	1:C:279:MET:HE3	1.97	0.46
1:D:412:GLY:O	1:D:415:GLU:HG2	2.15	0.46
1:G:15:GLY:O	1:G:525:LYS:HE2	2.14	0.46
1:G:211:GLU:OE1	1:G:211:GLU:HA	2.15	0.46
1:B:144:ILE:HG22	1:B:144:ILE:O	2.14	0.46
1:C:35:ILE:HG13	1:C:74:LEU:HD13	1.97	0.46
1:D:208:GLU:HB3	1:D:212:GLU:CG	2.45	0.46
1:D:259:ILE:HG21	1:E:257:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:LYS:HZ1	1:G:358:GLU:HG2	1.80	0.46
1:G:239:ILE:HD12	1:G:239:ILE:N	2.30	0.46
1:H:150:ASP:OD2	1:H:152:GLU:HB3	2.16	0.46
1:H:432:LYS:O	1:H:435:LEU:HB2	2.14	0.46
1:A:483:GLU:HG3	1:A:485:LYS:HZ3	1.79	0.46
1:B:372:VAL:HG22	1:B:373:THR:H	1.79	0.46
1:D:75:GLN:HG3	1:E:10:VAL:HG13	1.96	0.46
1:G:59:ILE:N	1:G:59:ILE:CD1	2.76	0.46
1:H:11:ILE:HG23	1:H:12:LEU:N	2.30	0.46
1:H:450:THR:O	1:H:454:ASN:ND2	2.48	0.46
1:B:348:GLU:O	1:B:349:VAL:HG23	2.15	0.46
1:C:239:ILE:HD11	1:C:347:ALA:HB3	1.98	0.46
1:D:182:VAL:HG22	1:D:395:VAL:HG13	1.98	0.46
1:G:35:ILE:HD11	1:G:74:LEU:HD22	1.97	0.46
1:G:106:GLU:HG2	1:G:446:ILE:HG13	1.97	0.46
1:H:370:LYS:HE2	1:H:370:LYS:CA	2.43	0.46
1:A:91:LYS:HB2	1:A:91:LYS:HZ3	1.79	0.46
1:A:465:LYS:O	1:A:469:GLU:HG2	2.15	0.46
1:B:421:ARG:HB2	1:B:421:ARG:NH1	2.21	0.46
1:E:208:GLU:HB3	1:E:212:GLU:HG3	1.98	0.46
1:E:229:ARG:HG2	1:E:229:ARG:HH11	1.81	0.46
1:E:401:VAL:O	1:E:405:GLY:N	2.44	0.46
1:F:293:VAL:CG2	1:F:297:ILE:HD11	2.46	0.46
1:G:103:ILE:HG12	1:G:446:ILE:HD11	1.97	0.46
1:G:271:GLN:O	1:G:275:MET:HG3	2.16	0.46
1:G:286:THR:HG21	1:G:339:LEU:HG	1.97	0.46
1:H:426:ALA:CB	1:H:438:GLU:HG3	2.45	0.46
1:H:515:ILE:C	1:H:517:ARG:H	2.19	0.46
1:A:392:GLU:O	1:A:396:LYS:HE3	2.16	0.46
1:A:524:ALA:O	1:A:525:LYS:HD2	2.16	0.46
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.83	0.46
1:B:162:ILE:HD13	1:B:174:LEU:HB2	1.98	0.46
1:D:11:ILE:HD13	1:D:11:ILE:O	2.15	0.46
1:D:106:GLU:HG2	1:D:446:ILE:HG12	1.97	0.46
1:E:20:VAL:O	1:E:23:ASP:HB2	2.15	0.46
1:G:103:ILE:O	1:G:107:LEU:HB2	2.16	0.46
1:H:480:ASP:HB3	1:H:483:GLU:HB2	1.98	0.46
1:A:170:HIS:HD2	1:A:211:GLU:CD	2.19	0.46
1:B:498:LEU:O	1:B:498:LEU:HD22	2.16	0.46
1:C:38:THR:O	1:C:50:LYS:HE3	2.16	0.46
1:C:114:LEU:HG	1:C:439:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:O	1:D:33:ARG:HG3	2.15	0.46
1:H:119:ILE:HD11	1:H:435:LEU:HD23	1.97	0.46
1:A:126:LYS:HB3	1:A:126:LYS:HZ2	1.79	0.46
1:A:276:LEU:HD23	1:A:300:LEU:CB	2.46	0.46
1:B:443:ALA:O	1:B:446:ILE:HG13	2.16	0.46
1:C:91:LYS:O	1:C:91:LYS:HG2	2.15	0.46
1:C:154:LEU:HG	1:C:398:VAL:HG13	1.97	0.46
1:E:424:GLU:O	1:E:428:GLN:HG2	2.16	0.46
1:G:147:ASP:HB3	1:G:150:ASP:HB2	1.97	0.46
1:H:514:MET:O	1:H:514:MET:HG2	2.16	0.46
1:A:255:ALA:HB2	1:H:257:ILE:HB	1.98	0.46
1:A:466:VAL:HG21	1:A:479:ILE:CG1	2.46	0.46
1:B:11:ILE:HD13	1:B:11:ILE:O	2.16	0.46
1:B:165:LYS:NZ	1:B:393:ASP:OD2	2.34	0.46
1:D:188:LYS:HD3	1:D:193:TYR:CD1	2.51	0.46
1:D:290:VAL:HG22	1:D:311:MET:HE2	1.98	0.46
1:H:91:LYS:HB2	1:H:91:LYS:HZ2	1.79	0.46
1:H:195:VAL:HB	1:H:399:LYS:HG3	1.98	0.46
1:A:506:LYS:O	1:A:510:GLU:CG	2.63	0.45
1:B:109:ARG:NH2	1:B:110:LYS:HD3	2.31	0.45
1:C:290:VAL:HG13	1:C:311:MET:HE2	1.97	0.45
1:D:38:THR:HG22	1:D:50:LYS:HE3	1.97	0.45
1:D:99:THR:O	1:D:103:ILE:HG13	2.16	0.45
1:D:432:LYS:O	1:D:435:LEU:HB2	2.16	0.45
1:E:123:ILE:HG21	1:E:432:LYS:CB	2.46	0.45
1:F:162:ILE:HG21	1:F:171:LYS:HA	1.98	0.45
1:F:416:ILE:HD13	1:F:466:VAL:HG12	1.98	0.45
1:H:412:GLY:O	1:H:416:ILE:HG13	2.17	0.45
1:H:424:GLU:O	1:H:428:GLN:HG3	2.16	0.45
1:A:252:GLU:O	1:H:250:LYS:NZ	2.47	0.45
1:A:255:ALA:CB	1:H:257:ILE:HB	2.46	0.45
1:A:461:GLU:HG2	1:A:465:LYS:HZ2	1.81	0.45
1:C:128:TYR:CE2	1:C:440:PHE:HB2	2.51	0.45
1:C:178:ALA:O	1:C:182:VAL:HG23	2.15	0.45
1:D:272:GLU:HA	1:D:275:MET:CE	2.46	0.45
1:E:134:LYS:O	1:E:138:ILE:HG13	2.16	0.45
1:E:462:MET:HE1	1:E:485:LYS:HA	1.97	0.45
1:A:120:HIS:ND1	1:A:122:SER:HB3	2.31	0.45
1:A:469:GLU:HG3	1:A:486:PRO:CB	2.46	0.45
1:B:211:GLU:OE1	1:B:211:GLU:HA	2.16	0.45
1:C:369:PRO:O	1:C:370:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ILE:HG23	1:D:433:GLU:OE2	2.15	0.45
1:D:188:LYS:HD2	1:D:191:GLY:O	2.17	0.45
1:D:410:ALA:HB3	1:D:494:ILE:HG22	1.97	0.45
1:E:243:ASN:OD1	1:E:295:LYS:HE3	2.16	0.45
1:E:245:ALA:HB1	1:E:247:GLU:HG2	1.97	0.45
1:E:469:GLU:HA	1:E:469:GLU:OE2	2.16	0.45
1:F:120:HIS:ND1	1:F:121:PRO:HD2	2.31	0.45
1:G:488:ASP:O	1:G:492:LYS:HG2	2.16	0.45
1:H:12:LEU:HD23	1:H:13:PRO:HD2	1.96	0.45
1:H:139:LEU:HD23	1:H:142:ILE:HD11	1.98	0.45
1:H:166:ASN:C	1:H:166:ASN:HD22	2.20	0.45
1:A:37:GLU:HA	1:A:40:ARG:HG2	1.97	0.45
1:A:54:ASP:OD1	1:A:58:ASP:HB3	2.15	0.45
1:C:418:LEU:O	1:C:422:LEU:HB2	2.16	0.45
1:D:35:ILE:HD11	1:D:74:LEU:HD22	1.98	0.45
1:D:38:THR:O	1:D:50:LYS:CE	2.64	0.45
1:E:466:VAL:HG21	1:E:479:ILE:CG1	2.46	0.45
1:E:469:GLU:O	1:E:473:ARG:N	2.48	0.45
1:F:116:ASP:C	1:F:118:ASN:H	2.19	0.45
1:F:259:ILE:HD12	1:F:259:ILE:N	2.30	0.45
1:G:182:VAL:O	1:G:186:ALA:HB2	2.16	0.45
1:H:142:ILE:HB	1:H:475:LEU:HD22	1.99	0.45
1:H:149:ASP:O	1:H:151:GLU:N	2.49	0.45
1:H:297:ILE:HD12	1:H:314:ARG:HB3	1.98	0.45
1:B:293:VAL:CG2	1:B:297:ILE:HD11	2.46	0.45
1:C:91:LYS:HB2	1:C:91:LYS:NZ	2.31	0.45
1:D:483:GLU:HG3	1:D:485:LYS:CE	2.47	0.45
1:E:136:GLN:HA	1:E:136:GLN:HE21	1.81	0.45
1:E:208:GLU:HB3	1:E:212:GLU:HG2	1.98	0.45
1:G:313:VAL:HG21	1:G:361:ILE:CD1	2.47	0.45
1:G:449:LYS:HG3	1:G:463:LEU:HD22	1.98	0.45
1:G:470:HIS:HA	1:G:477:ILE:HB	1.99	0.45
1:H:114:LEU:HD11	1:H:436:ALA:HA	1.98	0.45
1:H:204:LYS:HD2	1:H:384:ILE:HG22	1.99	0.45
1:A:77:PRO:HG2	1:H:53:VAL:HG21	1.98	0.45
1:A:230:MET:CE	1:A:312:ALA:HB3	2.47	0.45
1:A:458:ASP:C	1:A:458:ASP:OD2	2.55	0.45
1:D:195:VAL:HB	1:D:399:LYS:HG3	1.98	0.45
1:E:145:ARG:HD3	1:E:145:ARG:HA	1.76	0.45
1:E:209:GLY:C	1:E:211:GLU:N	2.69	0.45
1:E:394:ALA:O	1:E:397:VAL:CG2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:HE2	1:F:203:GLU:OE1	2.17	0.45
1:F:241:LEU:HD12	1:F:292:PHE:HB2	1.98	0.45
1:F:276:LEU:CD2	1:F:300:LEU:HB2	2.43	0.45
1:G:146:VAL:HG21	1:G:153:THR:HG21	1.99	0.45
1:G:205:LYS:O	1:G:377:ARG:NH1	2.49	0.45
1:G:393:ASP:O	1:G:397:VAL:HG13	2.17	0.45
1:H:462:MET:HA	1:H:462:MET:HE3	1.98	0.45
1:H:463:LEU:O	1:H:467:ILE:HG13	2.17	0.45
1:A:76:HIS:CD2	1:A:78:ALA:H	2.35	0.45
1:B:17:GLN:NE2	1:B:17:GLN:H	2.15	0.45
1:B:123:ILE:HG21	1:B:432:LYS:CB	2.47	0.45
1:D:12:LEU:CD2	1:D:16:THR:HG21	2.43	0.45
1:D:35:ILE:HD13	1:D:35:ILE:HA	1.80	0.45
1:F:408:LEU:HD11	1:F:498:LEU:HD23	1.99	0.45
1:G:90:ASP:O	1:G:94:GLY:HA2	2.17	0.45
1:G:109:ARG:NH2	1:G:110:LYS:HD3	2.32	0.45
1:G:110:LYS:HE3	1:G:442:ASP:OD1	2.17	0.45
1:H:45:PRO:HB2	1:H:481:VAL:HG21	1.99	0.45
1:A:35:ILE:HD13	1:A:35:ILE:HA	1.82	0.45
1:B:215:LEU:HD11	1:B:372:VAL:CG2	2.47	0.45
1:B:265:LEU:O	1:B:269:LEU:HD13	2.16	0.45
1:C:262:PRO:O	1:D:271:GLN:HG2	2.17	0.45
1:D:235:GLU:O	1:D:348:GLU:O	2.35	0.45
1:E:76:HIS:HB2	1:F:11:ILE:HA	1.98	0.45
1:E:414:PRO:HD2	1:E:415:GLU:OE2	2.17	0.45
1:G:410:ALA:O	1:G:489:MET:HG3	2.17	0.45
1:H:260:THR:N	1:H:264:GLN:HE22	1.99	0.45
1:H:372:VAL:CG2	1:H:373:THR:N	2.79	0.45
1:A:77:PRO:HB2	1:H:51:MET:HE1	1.99	0.45
1:B:69:LEU:HB3	1:B:83:VAL:HG22	1.98	0.45
1:C:89:GLN:HG2	1:C:97:THR:HA	1.98	0.45
1:C:143:ALA:HB3	1:C:145:ARG:NH1	2.31	0.45
1:C:355:LEU:O	1:C:356:ALA:HB3	2.17	0.45
1:C:461:GLU:HG2	1:C:465:LYS:HZ2	1.80	0.45
1:D:241:LEU:HD12	1:D:292:PHE:HB2	1.99	0.45
1:E:269:LEU:HD12	1:F:251:THR:CG2	2.43	0.45
1:F:167:ALA:O	1:F:169:SER:N	2.50	0.45
1:G:215:LEU:HD11	1:G:372:VAL:CG2	2.47	0.45
1:A:25:GLN:O	1:A:29:ILE:HG13	2.16	0.45
1:A:37:GLU:HG2	1:A:40:ARG:CZ	2.47	0.45
1:A:117:GLN:O	1:A:118:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:O	1:A:143:ALA:N	2.50	0.45
1:A:210:VAL:HA	1:A:377:ARG:O	2.16	0.45
1:A:503:GLN:NE2	1:A:503:GLN:HA	2.32	0.45
1:C:412:GLY:HA2	1:C:415:GLU:CG	2.47	0.45
1:E:227:HIS:HD2	1:E:302:GLN:HB3	1.82	0.45
1:E:286:THR:HG22	1:E:341:PRO:CD	2.47	0.45
1:E:335:ASN:ND2	1:E:337:LYS:HB2	2.30	0.45
1:F:409:PRO:HB2	1:F:489:MET:HB2	1.99	0.45
1:G:17:GLN:H	1:G:17:GLN:HE21	1.62	0.45
1:A:215:LEU:HD11	1:A:372:VAL:CG2	2.47	0.44
1:B:29:ILE:HG23	1:B:108:LEU:HB3	1.97	0.44
1:B:218:GLY:HA3	1:B:363:VAL:O	2.16	0.44
1:B:353:ARG:HD2	1:B:362:PHE:CD1	2.52	0.44
1:B:458:ASP:OD2	1:B:458:ASP:C	2.55	0.44
1:C:52:LEU:HD11	1:C:68:ILE:HA	1.98	0.44
1:C:415:GLU:HG3	1:C:447:ILE:HB	1.99	0.44
1:D:144:ILE:CD1	1:D:490:LEU:HD21	2.45	0.44
1:D:207:GLY:O	1:D:208:GLU:HB2	2.16	0.44
1:E:17:GLN:NE2	1:E:17:GLN:N	2.63	0.44
1:E:157:ILE:HD11	1:E:495:ILE:HD12	2.00	0.44
1:F:206:ALA:HA	1:F:384:ILE:CD1	2.47	0.44
1:F:225:VAL:HG23	1:F:352:GLU:OE1	2.18	0.44
1:F:397:VAL:HG23	1:F:398:VAL:N	2.31	0.44
1:H:11:ILE:HD13	1:H:12:LEU:HB2	1.99	0.44
1:H:273:GLU:HG2	1:H:300:LEU:HD13	1.99	0.44
1:A:281:ASP:OD1	1:A:308:TYR:OH	2.17	0.44
1:B:221:ILE:HD11	1:B:324:LEU:HD11	1.99	0.44
1:C:182:VAL:CG2	1:C:395:VAL:HG13	2.47	0.44
1:D:13:PRO:O	1:D:16:THR:HB	2.17	0.44
1:D:445:LYS:C	1:D:448:PRO:HD2	2.37	0.44
1:E:38:THR:O	1:E:50:LYS:CE	2.64	0.44
1:E:85:VAL:HG13	1:E:507:SER:HB3	1.99	0.44
1:E:144:ILE:CD1	1:E:490:LEU:HD21	2.47	0.44
1:E:216:VAL:O	1:E:372:VAL:HG23	2.17	0.44
1:F:136:GLN:NE2	1:F:136:GLN:HA	2.33	0.44
1:F:158:ALA:HB2	1:F:398:VAL:CG2	2.48	0.44
1:F:333:VAL:HG12	1:F:335:ASN:H	1.82	0.44
1:G:205:LYS:HD3	1:G:205:LYS:HA	1.74	0.44
1:G:461:GLU:HG2	1:G:465:LYS:NZ	2.32	0.44
1:H:52:LEU:HD11	1:H:68:ILE:HA	1.98	0.44
1:A:142:ILE:HB	1:A:475:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLU:HB2	1:C:377:ARG:HG3	2.00	0.44
1:C:230:MET:CE	1:C:312:ALA:HB3	2.47	0.44
1:C:333:VAL:HG21	1:C:339:LEU:CD1	2.47	0.44
1:C:498:LEU:O	1:C:498:LEU:HD22	2.17	0.44
1:D:145:ARG:HG2	1:D:145:ARG:HH11	1.82	0.44
1:E:446:ILE:H	1:E:446:ILE:CD1	2.28	0.44
1:G:184:GLN:NE2	1:G:217:ARG:HH21	2.15	0.44
1:H:108:LEU:HD11	1:H:515:ILE:HD12	1.99	0.44
1:A:145:ARG:HG2	1:A:145:ARG:NH1	2.28	0.44
1:B:245:ALA:HB1	1:B:247:GLU:HG2	1.98	0.44
1:C:17:GLN:H	1:C:17:GLN:CD	2.21	0.44
1:C:449:LYS:HE3	1:C:459:THR:CG2	2.48	0.44
1:D:217:ARG:NH1	1:D:217:ARG:CB	2.74	0.44
1:E:458:ASP:OD2	1:E:458:ASP:C	2.56	0.44
1:F:412:GLY:O	1:F:416:ILE:HG13	2.17	0.44
1:G:218:GLY:HA3	1:G:363:VAL:O	2.17	0.44
1:G:354:LYS:HE2	1:G:357:GLY:HA2	2.00	0.44
1:G:517:ARG:HE	1:G:517:ARG:HB3	1.65	0.44
1:A:18:ARG:HA	1:A:521:VAL:O	2.17	0.44
1:A:251:THR:CG2	1:H:269:LEU:HD12	2.45	0.44
1:B:136:GLN:HE21	1:B:502:LYS:NZ	2.14	0.44
1:B:446:ILE:HD12	1:B:446:ILE:N	2.33	0.44
1:C:227:HIS:HB3	1:C:230:MET:SD	2.57	0.44
1:D:215:LEU:HD11	1:D:372:VAL:HG21	2.00	0.44
1:E:488:ASP:OD1	1:E:490:LEU:HB2	2.16	0.44
1:F:156:LYS:O	1:F:157:ILE:C	2.56	0.44
1:G:140:ASP:OD1	1:G:502:LYS:HD2	2.17	0.44
1:G:145:ARG:HG2	1:G:145:ARG:NH1	2.30	0.44
1:G:151:GLU:O	1:G:155:LEU:HD23	2.17	0.44
1:H:37:GLU:HG2	1:H:40:ARG:HH12	1.79	0.44
1:H:112:GLU:HA	1:H:115:LEU:HD12	2.00	0.44
1:H:147:ASP:HB3	1:H:150:ASP:HB2	1.99	0.44
1:A:142:ILE:HB	1:A:475:LEU:CD2	2.48	0.44
1:A:204:LYS:HD2	1:A:384:ILE:CG2	2.40	0.44
1:A:209:GLY:O	1:A:212:GLU:HG2	2.17	0.44
1:B:35:ILE:HD12	1:B:69:LEU:CD2	2.47	0.44
1:B:96:GLY:HA2	3:B:2528:ADP:O1B	2.18	0.44
1:C:202:PHE:CE2	1:C:374:ILE:HD12	2.53	0.44
1:D:81:MET:CE	1:D:514:MET:SD	3.06	0.44
1:D:154:LEU:HG	1:D:398:VAL:HG13	1.99	0.44
1:D:209:GLY:C	1:D:211:GLU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:VAL:CG2	1:E:11:ILE:N	2.72	0.44
1:E:11:ILE:HG23	1:E:12:LEU:N	2.33	0.44
1:E:75:GLN:HG3	1:F:12:LEU:C	2.38	0.44
1:E:149:ASP:O	1:E:151:GLU:N	2.50	0.44
1:F:35:ILE:HD13	1:F:35:ILE:HA	1.78	0.44
1:F:205:LYS:HB3	1:F:377:ARG:NH1	2.33	0.44
1:F:313:VAL:HG21	1:F:361:ILE:CD1	2.46	0.44
1:G:424:GLU:OE1	1:G:424:GLU:HA	2.17	0.44
1:H:217:ARG:HB3	1:H:217:ARG:NH1	2.32	0.44
1:H:342:GLU:H	1:H:342:GLU:CD	2.21	0.44
1:B:12:LEU:HD23	1:B:13:PRO:HD2	1.99	0.44
1:B:146:VAL:O	1:B:148:PRO:HD3	2.18	0.44
1:B:204:LYS:O	1:B:205:LYS:HD3	2.18	0.44
1:B:416:ILE:CD1	1:B:466:VAL:HG12	2.48	0.44
1:D:319:SER:O	1:D:323:LYS:HG3	2.18	0.44
1:F:12:LEU:HD21	1:F:16:THR:HG21	2.00	0.44
1:F:284:ALA:HB2	1:F:308:TYR:CD1	2.52	0.44
1:F:372:VAL:HG22	1:F:373:THR:N	2.33	0.44
1:F:415:GLU:HG3	1:F:447:ILE:HB	1.99	0.44
1:H:272:GLU:HA	1:H:275:MET:HE3	1.98	0.44
1:A:65:CYS:HB3	1:A:97:THR:OG1	2.17	0.44
1:A:277:LYS:HB2	1:A:304:TYR:CE2	2.52	0.44
1:C:109:ARG:HG2	1:C:109:ARG:HH11	1.83	0.44
1:E:182:VAL:O	1:E:186:ALA:HB2	2.18	0.44
1:E:208:GLU:HB2	1:E:377:ARG:HB3	1.99	0.44
1:E:433:GLU:H	1:E:433:GLU:CD	2.21	0.44
1:F:94:GLY:HA2	1:F:396:LYS:HD2	1.99	0.44
1:G:80:LYS:O	1:G:83:VAL:HB	2.17	0.44
1:G:205:LYS:HZ3	1:G:358:GLU:HG2	1.83	0.44
1:G:233:ARG:HH12	1:G:349:VAL:HG11	1.83	0.44
1:A:59:ILE:HD11	1:B:80:LYS:HE2	1.99	0.44
1:B:233:ARG:HH12	1:B:349:VAL:CG1	2.29	0.44
1:B:271:GLN:O	1:B:275:MET:HG3	2.18	0.44
1:B:370:LYS:HA	1:B:370:LYS:CE	2.40	0.44
1:C:450:THR:O	1:C:454:ASN:ND2	2.51	0.44
1:C:483:GLU:HG3	1:C:485:LYS:CE	2.48	0.44
1:D:119:ILE:HD11	1:D:435:LEU:HD23	1.99	0.44
1:D:266:MET:O	1:D:270:GLU:HG3	2.18	0.44
1:F:69:LEU:HB3	1:F:83:VAL:HG22	1.99	0.44
1:F:450:THR:O	1:F:454:ASN:ND2	2.51	0.44
1:H:245:ALA:HB1	1:H:247:GLU:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:ILE:HG22	1:H:302:GLN:HG3	2.00	0.44
1:A:380:THR:HG23	1:A:383:VAL:H	1.83	0.43
1:A:425:TYR:O	1:A:428:GLN:HG3	2.18	0.43
1:B:458:ASP:O	1:B:459:THR:C	2.57	0.43
1:D:110:LYS:HB3	1:D:439:ASN:HD22	1.83	0.43
1:E:233:ARG:NH1	1:E:349:VAL:CG1	2.72	0.43
1:F:31:ALA:CB	1:F:76:HIS:CD2	3.01	0.43
1:F:146:VAL:CG2	1:F:147:ASP:N	2.81	0.43
1:F:416:ILE:CD1	1:F:466:VAL:HG12	2.48	0.43
1:G:75:GLN:CG	1:H:13:PRO:HD3	2.41	0.43
1:G:392:GLU:O	1:G:396:LYS:HB2	2.17	0.43
1:A:19:TYR:HB3	1:A:23:ASP:HB3	2.00	0.43
1:A:217:ARG:HH11	1:A:217:ARG:CB	2.30	0.43
1:C:17:GLN:NE2	1:C:17:GLN:N	2.59	0.43
1:D:62:THR:OG1	1:D:63:ASN:N	2.51	0.43
1:D:430:GLY:CA	1:D:434:ALA:HB2	2.48	0.43
1:E:35:ILE:HG21	1:E:82:MET:CB	2.47	0.43
1:E:167:ALA:C	1:E:169:SER:N	2.71	0.43
1:G:31:ALA:CB	1:G:76:HIS:CD2	3.01	0.43
1:G:392:GLU:O	1:G:396:LYS:HE3	2.18	0.43
1:A:64:ASP:O	1:A:68:ILE:HG13	2.18	0.43
1:A:413:ALA:N	1:A:414:PRO:CD	2.81	0.43
1:C:147:ASP:O	1:C:149:ASP:N	2.51	0.43
1:D:201:LYS:HB2	1:D:323:LYS:HE3	2.00	0.43
1:D:220:VAL:HG11	1:D:360:MET:CE	2.48	0.43
1:E:143:ALA:HB3	1:E:145:ARG:NH1	2.34	0.43
1:F:467:ILE:HG22	1:F:471:LYS:HD2	1.99	0.43
1:G:138:ILE:O	1:G:142:ILE:HG12	2.18	0.43
1:H:25:GLN:O	1:H:29:ILE:HG13	2.17	0.43
1:A:80:LYS:HE2	1:H:59:ILE:HD11	1.99	0.43
1:B:262:PRO:HG2	1:C:267:SER:HB2	2.01	0.43
1:B:483:GLU:HG3	1:B:485:LYS:HZ3	1.80	0.43
1:C:221:ILE:HD11	1:C:324:LEU:HD11	2.01	0.43
1:C:262:PRO:HG2	1:D:267:SER:HB2	2.00	0.43
1:C:446:ILE:HA	1:C:449:LYS:HB2	2.00	0.43
1:D:180:GLU:HG2	1:D:215:LEU:CD2	2.48	0.43
1:D:353:ARG:NH2	1:D:364:GLU:OE2	2.52	0.43
1:E:393:ASP:O	1:E:397:VAL:HG22	2.19	0.43
1:F:265:LEU:O	1:F:269:LEU:HD13	2.18	0.43
1:H:458:ASP:OD2	1:H:458:ASP:C	2.56	0.43
1:A:94:GLY:HA3	1:A:396:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:O	1:B:103:ILE:HG22	2.18	0.43
1:B:106:GLU:HG2	1:B:446:ILE:CG1	2.48	0.43
1:D:51:MET:HE1	1:E:77:PRO:HB2	2.00	0.43
1:E:239:ILE:HD11	1:E:347:ALA:HB3	2.00	0.43
1:E:446:ILE:HD12	1:E:446:ILE:N	2.33	0.43
1:E:462:MET:HE3	1:E:462:MET:HA	2.00	0.43
1:F:146:VAL:HG21	1:F:153:THR:HG21	1.99	0.43
1:F:423:ASP:O	1:F:426:ALA:HB3	2.18	0.43
1:G:106:GLU:OE1	1:G:106:GLU:HA	2.18	0.43
1:H:94:GLY:HA2	1:H:396:LYS:HD2	1.99	0.43
1:A:257:ILE:HG22	1:A:259:ILE:CD1	2.47	0.43
1:B:155:LEU:HD22	1:B:179:VAL:HG21	1.99	0.43
1:B:207:GLY:O	1:B:208:GLU:HB2	2.18	0.43
1:C:206:ALA:CA	1:C:384:ILE:HD11	2.44	0.43
1:E:286:THR:HG22	1:E:341:PRO:HG3	2.00	0.43
1:E:392:GLU:O	1:E:396:LYS:HB2	2.19	0.43
1:F:19:TYR:N	1:F:19:TYR:CD1	2.86	0.43
1:F:20:VAL:HG12	1:F:21:GLY:N	2.33	0.43
1:F:217:ARG:HB3	1:F:217:ARG:NH1	2.33	0.43
1:A:261:SER:O	1:A:264:GLN:HG3	2.19	0.43
1:A:426:ALA:HB1	1:A:438:GLU:HG3	2.00	0.43
1:B:147:ASP:O	1:B:149:ASP:N	2.52	0.43
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.92	0.43
1:C:333:VAL:HG21	1:C:339:LEU:HD13	2.00	0.43
1:D:281:ASP:O	1:D:285:GLN:HG3	2.18	0.43
1:E:297:ILE:CG2	1:E:302:GLN:HG3	2.47	0.43
1:F:445:LYS:C	1:F:448:PRO:HD2	2.39	0.43
1:H:35:ILE:HG13	1:H:79:ALA:HB1	2.01	0.43
1:H:271:GLN:O	1:H:275:MET:HG3	2.19	0.43
1:H:293:VAL:CG2	1:H:297:ILE:HD11	2.49	0.43
1:A:409:PRO:HB3	1:A:490:LEU:CD1	2.46	0.43
1:B:149:ASP:N	1:B:149:ASP:OD2	2.50	0.43
1:B:195:VAL:HB	1:B:399:LYS:HG3	2.01	0.43
1:D:156:LYS:O	1:D:157:ILE:C	2.56	0.43
1:E:210:VAL:HA	1:E:377:ARG:O	2.19	0.43
1:F:443:ALA:O	1:F:446:ILE:HG13	2.18	0.43
1:H:207:GLY:O	1:H:208:GLU:HB2	2.18	0.43
1:A:17:GLN:N	1:A:17:GLN:NE2	2.67	0.43
1:E:81:MET:CE	1:E:514:MET:SD	3.07	0.43
1:E:126:LYS:O	1:E:130:LEU:HG	2.19	0.43
1:E:204:LYS:CD	1:E:388:GLU:OE2	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:LYS:HD2	1:F:190:ASP:N	2.33	0.43
1:H:462:MET:O	1:H:462:MET:HE3	2.19	0.43
1:H:469:GLU:O	1:H:473:ARG:N	2.52	0.43
1:H:503:GLN:HA	1:H:503:GLN:NE2	2.33	0.43
1:B:110:LYS:HE3	1:B:442:ASP:OD1	2.19	0.43
1:D:205:LYS:O	1:D:377:ARG:NH1	2.51	0.43
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.88	0.43
1:E:291:VAL:HG23	1:E:310:ILE:CG2	2.48	0.43
1:F:224:GLU:O	1:F:313:VAL:HG13	2.19	0.43
1:F:269:LEU:CD1	1:G:251:THR:HG23	2.40	0.43
1:F:272:GLU:HA	1:F:275:MET:HE2	2.00	0.43
1:F:433:GLU:O	1:F:437:ILE:HG13	2.18	0.43
1:A:462:MET:CE	1:A:486:PRO:HD3	2.47	0.42
1:B:59:ILE:HD12	1:B:59:ILE:H	1.81	0.42
1:C:182:VAL:O	1:C:186:ALA:HB2	2.19	0.42
1:E:300:LEU:HD23	1:E:300:LEU:HA	1.84	0.42
1:C:75:GLN:HB2	1:D:11:ILE:CA	2.49	0.42
1:C:196:ASP:OD1	1:C:198:ASP:HB2	2.19	0.42
1:C:205:LYS:HZ1	1:C:358:GLU:HG2	1.84	0.42
1:D:425:TYR:O	1:D:428:GLN:HG3	2.19	0.42
1:D:517:ARG:HE	1:D:517:ARG:HB3	1.68	0.42
1:E:72:ILE:HG22	1:E:74:LEU:HD23	2.01	0.42
1:E:215:LEU:HD11	1:E:372:VAL:CG2	2.48	0.42
1:E:217:ARG:HA	1:E:372:VAL:HG23	2.01	0.42
1:E:221:ILE:HD11	1:E:324:LEU:HD11	2.00	0.42
1:E:286:THR:CA	1:E:341:PRO:HG3	2.49	0.42
1:E:404:ASP:OD1	1:E:499:ARG:HB2	2.18	0.42
1:E:410:ALA:CB	1:E:494:ILE:HG22	2.46	0.42
1:E:443:ALA:O	1:E:446:ILE:CD1	2.68	0.42
1:F:50:LYS:HD2	1:F:68:ILE:HD13	2.01	0.42
1:F:182:VAL:HG13	1:F:195:VAL:HG11	1.99	0.42
1:G:197:LEU:HD22	1:G:395:VAL:CG1	2.49	0.42
1:H:172:GLU:OE1	1:H:172:GLU:HA	2.19	0.42
1:H:218:GLY:HA3	1:H:363:VAL:O	2.19	0.42
1:H:446:ILE:O	1:H:450:THR:HG23	2.19	0.42
1:A:269:LEU:CD1	1:B:251:THR:HG23	2.42	0.42
1:A:348:GLU:HB3	1:A:365:GLY:HA3	2.00	0.42
1:B:72:ILE:HG22	1:B:74:LEU:HD23	2.02	0.42
1:B:116:ASP:C	1:B:118:ASN:H	2.22	0.42
1:C:114:LEU:HD11	1:C:436:ALA:HA	2.01	0.42
1:C:477:ILE:HA	1:C:487:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:ALA:C	1:G:169:SER:H	2.23	0.42
1:A:20:VAL:HG12	1:A:21:GLY:N	2.35	0.42
1:A:391:LEU:O	1:A:394:ALA:HB3	2.19	0.42
1:B:17:GLN:H	1:B:17:GLN:HE21	1.67	0.42
1:B:144:ILE:CD1	1:B:490:LEU:HD21	2.47	0.42
1:C:397:VAL:HG23	1:C:398:VAL:N	2.34	0.42
1:C:449:LYS:HE2	1:C:449:LYS:HB3	1.85	0.42
1:E:37:GLU:HG2	1:E:40:ARG:CZ	2.49	0.42
1:E:503:GLN:HA	1:E:503:GLN:HE21	1.84	0.42
1:E:524:ALA:O	1:E:525:LYS:HD3	2.19	0.42
1:F:146:VAL:CG2	1:F:147:ASP:H	2.32	0.42
1:F:197:LEU:HD22	1:F:395:VAL:HG12	2.01	0.42
1:F:245:ALA:HB1	1:F:247:GLU:HG2	2.01	0.42
1:F:503:GLN:NE2	1:F:506:LYS:HD2	2.35	0.42
1:H:52:LEU:HD13	1:H:71:LYS:HB2	2.02	0.42
1:A:23:ASP:O	1:A:27:LEU:HG	2.19	0.42
1:A:94:GLY:HA2	1:A:396:LYS:HD2	2.00	0.42
1:C:29:ILE:HG23	1:C:108:LEU:HB3	2.01	0.42
1:C:209:GLY:H	1:C:212:GLU:HG2	1.83	0.42
1:C:259:ILE:HG12	1:C:265:LEU:HD23	2.02	0.42
1:C:261:SER:H	1:C:264:GLN:HG3	1.83	0.42
1:D:74:LEU:HD13	1:D:79:ALA:HB1	2.01	0.42
1:D:138:ILE:O	1:D:142:ILE:HG12	2.20	0.42
1:D:144:ILE:O	1:D:144:ILE:HG22	2.19	0.42
1:E:276:LEU:HD23	1:E:300:LEU:CB	2.46	0.42
1:F:72:ILE:HG22	1:F:74:LEU:CD2	2.50	0.42
1:F:109:ARG:HG2	1:F:109:ARG:HH11	1.84	0.42
1:F:112:GLU:HA	1:F:115:LEU:HD12	2.00	0.42
1:G:293:VAL:HG21	1:G:297:ILE:HD11	2.01	0.42
1:H:91:LYS:O	1:H:91:LYS:CG	2.67	0.42
1:C:270:GLU:HA	1:C:273:GLU:HG3	2.02	0.42
1:E:250:LYS:NZ	1:F:253:THR:HA	2.35	0.42
1:H:109:ARG:NH2	1:H:110:LYS:HD3	2.34	0.42
1:H:147:ASP:O	1:H:149:ASP:N	2.53	0.42
1:H:304:TYR:O	1:H:308:TYR:CD1	2.65	0.42
1:H:462:MET:HE2	1:H:486:PRO:HG3	2.02	0.42
1:A:236:ASN:HA	1:A:346:TYR:HE1	1.85	0.42
1:B:35:ILE:HD13	1:B:35:ILE:HA	1.89	0.42
1:C:23:ASP:O	1:C:27:LEU:HG	2.19	0.42
1:C:462:MET:CE	1:C:486:PRO:HD3	2.50	0.42
1:D:76:HIS:HA	1:D:77:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LYS:O	1:F:130:LEU:HG	2.20	0.42
1:F:286:THR:HA	1:F:341:PRO:HG3	2.01	0.42
1:F:467:ILE:O	1:F:471:LYS:HG3	2.20	0.42
1:G:45:PRO:HB2	1:G:481:VAL:HG21	2.00	0.42
1:H:498:LEU:HD22	1:H:498:LEU:O	2.19	0.42
1:A:76:HIS:CD2	1:A:78:ALA:HB3	2.55	0.42
1:A:143:ALA:HB3	1:A:145:ARG:NH1	2.35	0.42
1:A:245:ALA:HB1	1:A:247:GLU:HG2	2.00	0.42
1:A:446:ILE:N	1:A:446:ILE:HD12	2.34	0.42
1:B:35:ILE:HG22	1:B:36:ALA:N	2.35	0.42
1:C:461:GLU:HG2	1:C:465:LYS:HZ1	1.83	0.42
1:D:76:HIS:CD2	1:D:78:ALA:HB3	2.55	0.42
1:E:239:ILE:HG23	1:E:290:VAL:HG12	2.01	0.42
1:E:348:GLU:O	1:E:349:VAL:HG23	2.19	0.42
1:F:25:GLN:O	1:F:29:ILE:HG13	2.20	0.42
1:F:446:ILE:HD12	1:F:446:ILE:H	1.85	0.42
1:H:433:GLU:CD	1:H:433:GLU:H	2.22	0.42
1:A:227:HIS:HB3	1:A:230:MET:SD	2.59	0.42
1:A:469:GLU:HG3	1:A:486:PRO:HB2	2.01	0.42
1:B:370:LYS:HE2	1:B:370:LYS:CA	2.42	0.42
1:B:446:ILE:HD12	1:B:446:ILE:H	1.85	0.42
1:D:212:GLU:CA	1:D:212:GLU:OE2	2.68	0.42
1:C:37:GLU:HA	1:C:40:ARG:HG2	2.01	0.42
1:C:277:LYS:HB2	1:C:304:TYR:CE2	2.55	0.42
1:C:315:ARG:NH1	1:C:315:ARG:CG	2.82	0.42
1:C:409:PRO:HA	1:C:495:ILE:HG22	2.02	0.42
1:E:114:LEU:HD22	1:E:119:ILE:HD12	2.00	0.42
1:E:117:GLN:O	1:E:118:ASN:HB2	2.19	0.42
1:E:152:GLU:HG3	1:E:153:THR:N	2.34	0.42
1:E:188:LYS:HD3	1:E:193:TYR:CE1	2.54	0.42
1:E:233:ARG:HG3	1:E:233:ARG:NH1	2.32	0.42
1:F:37:GLU:HA	1:F:40:ARG:HG2	2.01	0.42
1:F:342:GLU:OE2	1:F:342:GLU:N	2.50	0.42
1:G:37:GLU:HA	1:G:40:ARG:HG2	2.01	0.42
1:G:227:HIS:HA	1:G:228:PRO:HD3	1.91	0.42
1:H:197:LEU:HD22	1:H:395:VAL:CG1	2.50	0.42
1:H:370:LYS:HA	1:H:370:LYS:CE	2.45	0.42
1:D:40:ARG:HE	1:D:450:THR:HG21	1.85	0.41
1:D:462:MET:HE2	1:D:486:PRO:HG3	2.01	0.41
1:E:340:THR:HG1	1:E:342:GLU:HB2	1.85	0.41
1:F:250:LYS:NZ	1:G:253:THR:HA	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:ALA:HB2	1:F:345:GLY:HA3	2.01	0.41
1:G:204:LYS:HD3	1:G:388:GLU:OE2	2.19	0.41
1:G:481:VAL:HG13	3:G:7528:ADP:C2	2.55	0.41
1:H:412:GLY:O	1:H:415:GLU:HG2	2.20	0.41
1:C:51:MET:HB2	1:D:518:ILE:HD13	2.01	0.41
1:D:208:GLU:HB3	1:D:212:GLU:HG3	2.01	0.41
1:D:292:PHE:CE2	1:D:313:VAL:HG21	2.56	0.41
1:E:144:ILE:O	1:E:144:ILE:HG22	2.19	0.41
1:E:210:VAL:O	1:E:210:VAL:HG12	2.20	0.41
1:G:208:GLU:CG	1:G:377:ARG:HH21	2.33	0.41
1:G:412:GLY:HA2	1:G:415:GLU:CG	2.50	0.41
1:A:17:GLN:NE2	1:A:17:GLN:H	2.18	0.41
1:A:401:VAL:O	1:A:405:GLY:N	2.51	0.41
1:B:106:GLU:CB	1:B:446:ILE:HG12	2.51	0.41
1:C:94:GLY:HA2	1:C:396:LYS:HD2	2.01	0.41
1:C:469:GLU:O	1:C:473:ARG:N	2.53	0.41
1:E:463:LEU:O	1:E:467:ILE:HG13	2.21	0.41
1:G:76:HIS:CD2	1:G:78:ALA:HB3	2.55	0.41
1:G:346:TYR:OH	1:G:348:GLU:HA	2.20	0.41
1:A:138:ILE:O	1:A:142:ILE:HG12	2.20	0.41
1:A:241:LEU:HD12	1:A:292:PHE:HB2	2.02	0.41
1:A:369:PRO:O	1:A:370:LYS:CE	2.62	0.41
1:A:483:GLU:OE1	1:A:483:GLU:HA	2.21	0.41
1:B:346:TYR:CG	1:B:347:ALA:N	2.88	0.41
1:C:114:LEU:HD22	1:C:119:ILE:HD12	2.02	0.41
1:D:145:ARG:HD3	1:D:145:ARG:HA	1.83	0.41
1:D:216:VAL:O	1:D:372:VAL:CG2	2.68	0.41
1:D:417:GLU:OE2	1:D:470:HIS:NE2	2.42	0.41
1:D:462:MET:O	1:D:462:MET:HE3	2.21	0.41
1:E:211:GLU:OE1	1:E:211:GLU:HA	2.21	0.41
1:F:54:ASP:OD1	1:F:58:ASP:CB	2.64	0.41
1:G:15:GLY:O	1:G:524:ALA:O	2.39	0.41
1:G:167:ALA:HB2	1:G:387:VAL:HG22	2.01	0.41
1:H:94:GLY:HA3	1:H:396:LYS:HB3	2.02	0.41
1:A:72:ILE:HD11	1:B:522:ILE:HD12	2.02	0.41
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.35	0.41
1:A:293:VAL:HG21	1:A:297:ILE:HD11	2.03	0.41
1:B:293:VAL:HG21	1:B:297:ILE:HD11	2.02	0.41
1:B:483:GLU:HG3	1:B:485:LYS:HZ1	1.86	0.41
1:C:35:ILE:HD12	1:C:69:LEU:HD22	2.02	0.41
1:D:498:LEU:HD13	1:D:502:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:LEU:CD1	1:E:396:LYS:HG3	2.51	0.41
1:E:420:ILE:HD13	1:E:471:LYS:HG3	2.02	0.41
1:E:498:LEU:C	1:E:498:LEU:HD13	2.41	0.41
1:F:94:GLY:HA3	1:F:396:LYS:HB3	2.02	0.41
1:F:173:LEU:O	1:F:176:LYS:HB3	2.19	0.41
1:G:524:ALA:O	1:G:525:LYS:CD	2.69	0.41
1:H:273:GLU:HG2	1:H:300:LEU:CD1	2.50	0.41
1:H:498:LEU:C	1:H:498:LEU:HD13	2.40	0.41
1:A:51:MET:CE	1:B:77:PRO:HB2	2.50	0.41
1:A:266:MET:HG2	1:B:271:GLN:NE2	2.36	0.41
1:A:335:ASN:HB2	1:H:303:HIS:CD2	2.54	0.41
1:B:91:LYS:O	1:B:91:LYS:CG	2.68	0.41
1:C:12:LEU:HD23	1:C:13:PRO:N	2.34	0.41
1:C:201:LYS:HE2	1:C:203:GLU:OE1	2.21	0.41
1:C:259:ILE:N	1:C:259:ILE:CD1	2.84	0.41
1:D:304:TYR:O	1:D:308:TYR:CD1	2.67	0.41
1:E:35:ILE:HA	1:E:35:ILE:HD13	1.85	0.41
1:E:75:GLN:HB2	1:F:11:ILE:C	2.41	0.41
1:E:380:THR:CG2	1:E:383:VAL:H	2.28	0.41
1:E:462:MET:HE1	1:E:486:PRO:HD3	2.02	0.41
1:F:109:ARG:HG2	1:F:109:ARG:NH1	2.36	0.41
1:F:470:HIS:CE1	1:F:475:LEU:HA	2.55	0.41
1:G:192:LYS:HE2	1:G:192:LYS:HB3	1.87	0.41
1:G:342:GLU:OE2	1:G:342:GLU:N	2.52	0.41
1:H:209:GLY:C	1:H:211:GLU:H	2.24	0.41
1:A:103:ILE:O	1:A:103:ILE:HG22	2.20	0.41
1:A:157:ILE:HG13	1:A:401:VAL:HG21	2.03	0.41
1:A:257:ILE:HG12	1:H:259:ILE:CG2	2.51	0.41
1:A:291:VAL:O	1:A:312:ALA:HA	2.21	0.41
1:B:142:ILE:HD13	1:B:417:GLU:HG2	2.03	0.41
1:C:317:LYS:O	1:C:320:ASP:HB2	2.21	0.41
1:C:409:PRO:HB2	1:C:489:MET:HB2	2.02	0.41
1:C:458:ASP:O	1:C:459:THR:C	2.59	0.41
1:D:126:LYS:O	1:D:130:LEU:HG	2.21	0.41
1:D:317:LYS:O	1:D:320:ASP:N	2.53	0.41
1:D:381:GLU:O	1:D:384:ILE:HB	2.21	0.41
1:E:37:GLU:HA	1:E:40:ARG:HG2	2.03	0.41
1:E:103:ILE:CG1	1:E:447:ILE:HD11	2.51	0.41
1:F:35:ILE:HG22	1:F:36:ALA:N	2.35	0.41
1:F:154:LEU:HD12	1:F:154:LEU:HA	1.83	0.41
1:F:189:LYS:HD2	1:F:189:LYS:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:GLY:CA	1:H:396:LYS:HD2	2.51	0.41
1:A:12:LEU:HD13	1:A:16:THR:CG2	2.50	0.41
1:B:490:LEU:CD1	1:B:490:LEU:N	2.84	0.41
1:C:103:ILE:O	1:C:107:LEU:HB2	2.21	0.41
1:D:72:ILE:CG2	1:D:73:ASP:N	2.83	0.41
1:D:73:ASP:O	1:E:13:PRO:CD	2.64	0.41
1:D:114:LEU:CD1	1:D:436:ALA:HA	2.51	0.41
1:D:206:ALA:CA	1:D:384:ILE:HD11	2.47	0.41
1:E:146:VAL:HG21	1:E:153:THR:HG21	2.03	0.41
1:F:31:ALA:HB2	1:F:76:HIS:CD2	2.56	0.41
1:H:227:HIS:ND1	1:H:228:PRO:HD2	2.36	0.41
1:H:311:MET:CE	1:H:350:VAL:HG12	2.50	0.41
1:H:410:ALA:HB3	1:H:494:ILE:HG22	2.02	0.41
1:A:81:MET:CE	1:A:514:MET:SD	3.09	0.41
1:A:141:GLU:C	1:A:143:ALA:H	2.23	0.41
1:A:330:ALA:HB2	1:A:345:GLY:HA3	2.03	0.41
1:A:446:ILE:HD12	1:A:446:ILE:H	1.86	0.41
1:A:498:LEU:HD13	1:A:498:LEU:C	2.41	0.41
1:B:59:ILE:N	1:B:59:ILE:CD1	2.79	0.41
1:C:85:VAL:HG13	1:C:507:SER:HB3	2.02	0.41
1:C:202:PHE:HE2	1:C:374:ILE:HD12	1.86	0.41
1:C:216:VAL:O	1:C:218:GLY:N	2.52	0.41
1:D:65:CYS:HB3	1:D:97:THR:OG1	2.21	0.41
1:D:188:LYS:HG3	1:D:192:LYS:C	2.40	0.41
1:D:189:LYS:HD2	1:D:189:LYS:C	2.40	0.41
1:D:483:GLU:HG3	1:D:485:LYS:HE2	2.03	0.41
1:F:217:ARG:CA	1:F:372:VAL:HG23	2.44	0.41
1:F:233:ARG:HD2	1:F:351:GLU:OE2	2.21	0.41
1:G:75:GLN:NE2	1:H:13:PRO:HG3	2.36	0.41
1:G:502:LYS:HB3	1:G:502:LYS:HE3	1.90	0.41
1:H:29:ILE:CD1	1:H:112:GLU:HB2	2.50	0.41
1:H:481:VAL:HG13	3:H:8528:ADP:C2	2.56	0.41
1:C:109:ARG:HG2	1:C:109:ARG:NH1	2.36	0.41
1:C:119:ILE:HD11	1:C:435:LEU:HD23	2.02	0.41
1:D:18:ARG:HA	1:D:521:VAL:O	2.21	0.41
1:D:64:ASP:O	1:D:68:ILE:HG13	2.21	0.41
1:D:172:GLU:OE1	1:D:172:GLU:CA	2.69	0.41
1:E:81:MET:HE2	1:E:515:ILE:HG12	2.03	0.41
1:F:216:VAL:O	1:F:372:VAL:HG23	2.20	0.41
1:H:209:GLY:C	1:H:211:GLU:N	2.73	0.41
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:O	1:B:50:LYS:CE	2.69	0.40
1:B:166:ASN:O	1:B:168:GLU:N	2.54	0.40
1:B:468:SER:O	1:B:471:LYS:N	2.54	0.40
1:C:33:ARG:O	1:C:37:GLU:HG3	2.21	0.40
1:C:82:MET:HE2	1:C:101:VAL:HG13	2.01	0.40
1:D:348:GLU:O	1:D:349:VAL:CG2	2.67	0.40
1:D:401:VAL:O	1:D:405:GLY:N	2.51	0.40
1:E:232:LYS:HD3	1:E:232:LYS:HA	1.85	0.40
1:F:13:PRO:HB2	1:F:16:THR:OG1	2.21	0.40
1:F:300:LEU:HD23	1:F:300:LEU:HA	1.81	0.40
1:G:136:GLN:HE21	1:G:136:GLN:CA	2.31	0.40
1:G:524:ALA:C	1:G:525:LYS:HD2	2.42	0.40
1:H:76:HIS:HA	1:H:77:PRO:HD3	1.86	0.40
1:H:85:VAL:HG13	1:H:507:SER:HB3	2.03	0.40
1:H:196:ASP:OD1	1:H:198:ASP:HB2	2.21	0.40
1:H:276:LEU:HD23	1:H:300:LEU:HB2	2.03	0.40
1:B:423:ASP:O	1:B:426:ALA:HB3	2.20	0.40
1:C:53:VAL:HG21	1:D:77:PRO:HG2	2.02	0.40
1:C:195:VAL:HB	1:C:399:LYS:HG3	2.03	0.40
1:D:370:LYS:HA	1:D:370:LYS:CE	2.46	0.40
1:E:116:ASP:C	1:E:118:ASN:H	2.24	0.40
1:F:54:ASP:OD1	1:F:58:ASP:N	2.54	0.40
1:F:380:THR:OG1	1:F:381:GLU:N	2.53	0.40
1:G:75:GLN:HB2	1:H:11:ILE:C	2.42	0.40
1:G:204:LYS:HB2	1:G:204:LYS:HE3	1.90	0.40
1:G:496:GLU:OE1	1:G:501:LYS:NZ	2.48	0.40
1:H:469:GLU:CB	1:H:477:ILE:HG21	2.46	0.40
1:A:106:GLU:HB2	1:A:446:ILE:HG12	2.03	0.40
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.87	0.40
1:B:273:GLU:HG2	1:B:300:LEU:CD1	2.51	0.40
1:B:466:VAL:CG2	1:B:486:PRO:HG3	2.42	0.40
1:B:488:ASP:HB3	1:B:491:GLU:CG	2.48	0.40
1:C:73:ASP:O	1:D:13:PRO:HD3	2.21	0.40
1:C:136:GLN:NE2	1:C:502:LYS:HG2	2.36	0.40
1:C:462:MET:HE1	1:C:486:PRO:HD3	2.04	0.40
1:C:469:GLU:HA	1:C:469:GLU:OE2	2.20	0.40
1:D:475:LEU:HD12	1:D:475:LEU:O	2.21	0.40
1:E:172:GLU:HA	1:E:172:GLU:OE1	2.21	0.40
1:E:229:ARG:HG2	1:E:229:ARG:NH1	2.37	0.40
1:E:311:MET:CE	1:E:350:VAL:HG12	2.51	0.40
1:F:525:LYS:O	1:F:526:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ILE:HD13	1:H:35:ILE:HA	1.93	0.40
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.80	0.40
1:B:81:MET:HE1	1:B:514:MET:SD	2.60	0.40
1:B:145:ARG:NH1	1:B:145:ARG:CG	2.78	0.40
1:C:304:TYR:O	1:C:308:TYR:CD1	2.75	0.40
1:C:356:ALA:C	1:C:358:GLU:H	2.24	0.40
1:C:483:GLU:HA	1:C:483:GLU:OE1	2.21	0.40
1:C:525:LYS:HD2	1:C:525:LYS:N	2.35	0.40
1:D:227:HIS:HB3	1:D:230:MET:HG3	2.03	0.40
1:D:229:ARG:HH12	1:E:332:ILE:H	1.69	0.40
1:D:451:LEU:HD23	1:D:451:LEU:HA	1.97	0.40
1:E:18:ARG:HA	1:E:521:VAL:O	2.22	0.40
1:E:225:VAL:CG1	1:E:230:MET:HB2	2.52	0.40
1:E:311:MET:HE1	1:E:350:VAL:CG1	2.51	0.40
1:H:76:HIS:HD2	1:H:78:ALA:HB3	1.84	0.40
1:H:123:ILE:HG21	1:H:432:LYS:CB	2.45	0.40
1:A:75:GLN:HG3	1:B:10:VAL:HG13	2.04	0.40
1:A:227:HIS:HA	1:A:228:PRO:HD3	1.90	0.40
1:B:243:ASN:O	1:B:243:ASN:CG	2.59	0.40
1:B:418:LEU:O	1:B:422:LEU:HB2	2.22	0.40
1:C:118:ASN:HD22	1:C:118:ASN:HA	1.57	0.40
1:C:142:ILE:HB	1:C:475:LEU:HD21	2.01	0.40
1:C:294:GLN:OE1	1:C:321:MET:HG3	2.21	0.40
1:C:348:GLU:HB3	1:C:365:GLY:HA3	2.02	0.40
1:C:416:ILE:HD13	1:C:466:VAL:HG12	2.03	0.40
1:D:91:LYS:O	1:D:91:LYS:CG	2.70	0.40
1:D:106:GLU:HG3	1:D:443:ALA:HB1	2.03	0.40
1:D:106:GLU:HB2	1:D:446:ILE:HG12	2.03	0.40
1:D:245:ALA:HB1	1:D:247:GLU:HG2	2.04	0.40
1:D:257:ILE:HG22	1:D:259:ILE:HD12	2.04	0.40
1:D:299:ASP:O	1:D:302:GLN:HB2	2.21	0.40
1:E:26:ARG:CG	1:E:26:ARG:HH11	2.35	0.40
1:E:143:ALA:HB3	1:E:145:ARG:HH12	1.87	0.40
1:E:184:GLN:HE21	1:E:184:GLN:CA	2.11	0.40
1:H:147:ASP:OD2	1:H:148:PRO:HD2	2.20	0.40
1:H:179:VAL:O	1:H:183:LYS:HG3	2.22	0.40
1:H:409:PRO:HA	1:H:495:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/548 (94%)	468 (91%)	34 (7%)	13 (2%)	5	28
1	B	515/548 (94%)	464 (90%)	41 (8%)	10 (2%)	8	36
1	C	515/548 (94%)	463 (90%)	42 (8%)	10 (2%)	8	36
1	D	515/548 (94%)	459 (89%)	46 (9%)	10 (2%)	8	36
1	E	515/548 (94%)	468 (91%)	38 (7%)	9 (2%)	9	39
1	F	515/548 (94%)	467 (91%)	36 (7%)	12 (2%)	6	30
1	G	515/548 (94%)	452 (88%)	52 (10%)	11 (2%)	7	33
1	H	515/548 (94%)	459 (89%)	47 (9%)	9 (2%)	9	39
All	All	4120/4384 (94%)	3700 (90%)	336 (8%)	84 (2%)	7	34

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	PRO
1	A	367	LYS
1	B	167	ALA
1	B	248	VAL
1	C	148	PRO
1	C	167	ALA
1	D	148	PRO
1	D	367	LYS
1	E	150	ASP
1	E	248	VAL
1	E	367	LYS
1	F	148	PRO
1	F	367	LYS
1	G	11	ILE
1	G	148	PRO
1	H	367	LYS
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	473	ARG
1	A	475	LEU
1	B	367	LYS
1	C	152	GLU
1	C	235	GLU
1	C	367	LYS
1	C	430	GLY
1	D	167	ALA
1	D	248	VAL
1	E	47	GLY
1	E	148	PRO
1	E	168	GLU
1	E	235	GLU
1	F	168	GLU
1	F	236	ASN
1	F	459	THR
1	G	167	ALA
1	G	367	LYS
1	G	430	GLY
1	H	148	PRO
1	H	150	ASP
1	H	248	VAL
1	A	142	ILE
1	A	189	LYS
1	B	150	ASP
1	B	189	LYS
1	C	164	GLY
1	D	298	ASP
1	E	151	GLU
1	F	172	GLU
1	F	217	ARG
1	F	444	LEU
1	F	475	LEU
1	G	444	LEU
1	G	459	THR
1	H	164	GLY
1	H	235	GLU
1	H	475	LEU
1	A	167	ALA
1	B	459	THR
1	C	248	VAL
1	C	459	THR

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Mol	Chain	Res	Type
1	D	58	ASP
1	D	235	GLU
1	F	235	GLU
1	F	248	VAL
1	G	152	GLU
1	G	427	LYS
1	H	13	PRO
1	A	164	GLY
1	A	248	VAL
1	B	172	GLU
1	B	298	ASP
1	B	444	LEU
1	C	166	ASN
1	D	150	ASP
1	D	164	GLY
1	H	217	ARG
1	A	150	ASP
1	D	157	ILE
1	F	164	GLY
1	G	248	VAL
1	A	94	GLY
1	A	210	VAL
1	E	430	GLY
1	G	349	VAL
1	B	148	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	422/441 (96%)	389 (92%)	33 (8%)	12	42
1	B	422/441 (96%)	391 (93%)	31 (7%)	14	44
1	C	422/441 (96%)	388 (92%)	34 (8%)	11	40
1	D	422/441 (96%)	387 (92%)	35 (8%)	11	39
1	E	422/441 (96%)	392 (93%)	30 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	422/441 (96%)	387 (92%)	35 (8%)	11 39
1	G	422/441 (96%)	394 (93%)	28 (7%)	16 49
1	H	422/441 (96%)	393 (93%)	29 (7%)	15 48
All	All	3376/3528 (96%)	3121 (92%)	255 (8%)	13 43

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	17	GLN
1	A	23	ASP
1	A	26	ARG
1	A	35	ILE
1	A	41	THR
1	A	54	ASP
1	A	148	PRO
1	A	155	LEU
1	A	166	ASN
1	A	168	GLU
1	A	171	LYS
1	A	189	LYS
1	A	190	ASP
1	A	212	GLU
1	A	214	GLU
1	A	222	ASP
1	A	241	LEU
1	A	276	LEU
1	A	298	ASP
1	A	315	ARG
1	A	336	VAL
1	A	358	GLU
1	A	370	LYS
1	A	381	GLU
1	A	421	ARG
1	A	446	ILE
1	A	449	LYS
1	A	483	GLU
1	A	490	LEU
1	A	498	LEU
1	A	501	LYS
1	A	525	LYS

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Mol	Chain	Res	Type
1	B	11	ILE
1	B	17	GLN
1	B	23	ASP
1	B	26	ARG
1	B	35	ILE
1	B	41	THR
1	B	54	ASP
1	B	166	ASN
1	B	170	HIS
1	B	171	LYS
1	B	189	LYS
1	B	190	ASP
1	B	222	ASP
1	B	241	LEU
1	B	298	ASP
1	B	315	ARG
1	B	336	VAL
1	B	338	ASP
1	B	370	LYS
1	B	381	GLU
1	B	415	GLU
1	B	421	ARG
1	B	435	LEU
1	B	440	PHE
1	B	446	ILE
1	B	449	LYS
1	B	462	MET
1	B	468	SER
1	B	483	GLU
1	B	519	ASP
1	B	525	LYS
1	C	11	ILE
1	C	14	GLU
1	C	17	GLN
1	C	26	ARG
1	C	35	ILE
1	C	41	THR
1	C	54	ASP
1	C	107	LEU
1	C	110	LYS
1	C	118	ASN
1	C	148	PRO

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Mol	Chain	Res	Type
1	C	166	ASN
1	C	170	HIS
1	C	171	LYS
1	C	189	LYS
1	C	190	ASP
1	C	214	GLU
1	C	222	ASP
1	C	241	LEU
1	C	252	GLU
1	C	276	LEU
1	C	298	ASP
1	C	315	ARG
1	C	338	ASP
1	C	358	GLU
1	C	370	LYS
1	C	381	GLU
1	C	421	ARG
1	C	428	GLN
1	C	435	LEU
1	C	446	ILE
1	C	449	LYS
1	C	483	GLU
1	C	525	LYS
1	D	11	ILE
1	D	17	GLN
1	D	26	ARG
1	D	35	ILE
1	D	63	ASN
1	D	107	LEU
1	D	110	LYS
1	D	148	PRO
1	D	166	ASN
1	D	171	LYS
1	D	189	LYS
1	D	190	ASP
1	D	212	GLU
1	D	222	ASP
1	D	241	LEU
1	D	252	GLU
1	D	258	ASN
1	D	276	LEU
1	D	289	ASN

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Mol	Chain	Res	Type
1	D	298	ASP
1	D	315	ARG
1	D	336	VAL
1	D	358	GLU
1	D	364	GLU
1	D	370	LYS
1	D	381	GLU
1	D	421	ARG
1	D	428	GLN
1	D	446	ILE
1	D	449	LYS
1	D	483	GLU
1	D	490	LEU
1	D	498	LEU
1	D	501	LYS
1	D	519	ASP
1	E	11	ILE
1	E	14	GLU
1	E	17	GLN
1	E	23	ASP
1	E	26	ARG
1	E	35	ILE
1	E	54	ASP
1	E	59	ILE
1	E	80	LYS
1	E	148	PRO
1	E	166	ASN
1	E	189	LYS
1	E	214	GLU
1	E	222	ASP
1	E	241	LEU
1	E	251	THR
1	E	276	LEU
1	E	286	THR
1	E	298	ASP
1	E	315	ARG
1	E	364	GLU
1	E	370	LYS
1	E	421	ARG
1	E	446	ILE
1	E	449	LYS
1	E	462	MET

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Mol	Chain	Res	Type
1	E	483	GLU
1	E	498	LEU
1	E	501	LYS
1	E	519	ASP
1	F	11	ILE
1	F	17	GLN
1	F	23	ASP
1	F	26	ARG
1	F	35	ILE
1	F	40	ARG
1	F	41	THR
1	F	63	ASN
1	F	118	ASN
1	F	128	TYR
1	F	148	PRO
1	F	154	LEU
1	F	166	ASN
1	F	171	LYS
1	F	189	LYS
1	F	190	ASP
1	F	222	ASP
1	F	241	LEU
1	F	276	LEU
1	F	298	ASP
1	F	315	ARG
1	F	336	VAL
1	F	338	ASP
1	F	370	LYS
1	F	381	GLU
1	F	415	GLU
1	F	421	ARG
1	F	446	ILE
1	F	449	LYS
1	F	462	MET
1	F	483	GLU
1	F	490	LEU
1	F	498	LEU
1	F	501	LYS
1	F	519	ASP
1	G	11	ILE
1	G	17	GLN
1	G	23	ASP

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Mol	Chain	Res	Type
1	G	26	ARG
1	G	118	ASN
1	G	128	TYR
1	G	148	PRO
1	G	166	ASN
1	G	171	LYS
1	G	189	LYS
1	G	190	ASP
1	G	222	ASP
1	G	241	LEU
1	G	246	LEU
1	G	260	THR
1	G	276	LEU
1	G	298	ASP
1	G	315	ARG
1	G	336	VAL
1	G	338	ASP
1	G	370	LYS
1	G	415	GLU
1	G	421	ARG
1	G	446	ILE
1	G	449	LYS
1	G	498	LEU
1	G	501	LYS
1	G	525	LYS
1	H	11	ILE
1	H	14	GLU
1	H	17	GLN
1	H	26	ARG
1	H	35	ILE
1	H	54	ASP
1	H	107	LEU
1	H	148	PRO
1	H	166	ASN
1	H	171	LYS
1	H	189	LYS
1	H	190	ASP
1	H	222	ASP
1	H	241	LEU
1	H	246	LEU
1	H	276	LEU
1	H	298	ASP

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Mol	Chain	Res	Type
1	H	315	ARG
1	H	338	ASP
1	H	370	LYS
1	H	381	GLU
1	H	421	ARG
1	H	423	ASP
1	H	446	ILE
1	H	449	LYS
1	H	483	GLU
1	H	490	LEU
1	H	501	LYS
1	H	519	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	28	ASN
1	A	63	ASN
1	A	75	GLN
1	A	76	HIS
1	A	117	GLN
1	A	118	ASN
1	A	136	GLN
1	A	166	ASN
1	A	184	GLN
1	A	258	ASN
1	A	264	GLN
1	A	285	GLN
1	A	439	ASN
1	A	503	GLN
1	B	17	GLN
1	B	28	ASN
1	B	76	HIS
1	B	118	ASN
1	B	136	GLN
1	B	166	ASN
1	B	170	HIS
1	B	184	GLN
1	B	258	ASN
1	B	264	GLN
1	B	285	GLN

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Mol	Chain	Res	Type
1	B	503	GLN
1	C	17	GLN
1	C	28	ASN
1	C	75	GLN
1	C	76	HIS
1	C	118	ASN
1	C	136	GLN
1	C	166	ASN
1	C	258	ASN
1	C	264	GLN
1	C	285	GLN
1	C	368	ASN
1	D	17	GLN
1	D	28	ASN
1	D	63	ASN
1	D	76	HIS
1	D	118	ASN
1	D	136	GLN
1	D	166	ASN
1	D	170	HIS
1	D	184	GLN
1	D	258	ASN
1	D	264	GLN
1	D	285	GLN
1	D	439	ASN
1	E	17	GLN
1	E	28	ASN
1	E	75	GLN
1	E	76	HIS
1	E	118	ASN
1	E	136	GLN
1	E	166	ASN
1	E	170	HIS
1	E	184	GLN
1	E	258	ASN
1	E	264	GLN
1	E	285	GLN
1	E	335	ASN
1	E	439	ASN
1	F	17	GLN
1	F	28	ASN
1	F	63	ASN

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Mol	Chain	Res	Type
1	F	76	HIS
1	F	118	ASN
1	F	136	GLN
1	F	166	ASN
1	F	170	HIS
1	F	184	GLN
1	F	258	ASN
1	F	264	GLN
1	F	271	GLN
1	F	285	GLN
1	F	503	GLN
1	G	17	GLN
1	G	28	ASN
1	G	76	HIS
1	G	118	ASN
1	G	136	GLN
1	G	166	ASN
1	G	184	GLN
1	G	258	ASN
1	G	264	GLN
1	G	285	GLN
1	G	503	GLN
1	H	17	GLN
1	H	28	ASN
1	H	76	HIS
1	H	118	ASN
1	H	136	GLN
1	H	166	ASN
1	H	170	HIS
1	H	184	GLN
1	H	258	ASN
1	H	264	GLN
1	H	285	GLN
1	H	503	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	H	8528	2	24,29,29	1.60	7 (29%)	29,45,45	1.53	2 (6%)
3	ADP	E	5528	2	24,29,29	1.55	5 (20%)	29,45,45	1.57	2 (6%)
3	ADP	G	7528	2	24,29,29	1.60	6 (25%)	29,45,45	1.54	2 (6%)
3	ADP	A	1528	2	24,29,29	1.62	6 (25%)	29,45,45	1.54	2 (6%)
3	ADP	D	4528	2	24,29,29	1.64	4 (16%)	29,45,45	1.62	2 (6%)
3	ADP	C	3528	2	24,29,29	1.52	5 (20%)	29,45,45	1.59	2 (6%)
3	ADP	F	6528	-	24,29,29	1.62	6 (25%)	29,45,45	1.55	2 (6%)
3	ADP	B	2528	2	24,29,29	1.54	6 (25%)	29,45,45	1.57	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	H	8528	2	-	2/12/32/32	0/3/3/3
3	ADP	E	5528	2	-	2/12/32/32	0/3/3/3
3	ADP	G	7528	2	-	2/12/32/32	0/3/3/3
3	ADP	A	1528	2	-	2/12/32/32	0/3/3/3
3	ADP	D	4528	2	-	2/12/32/32	0/3/3/3
3	ADP	C	3528	2	-	2/12/32/32	0/3/3/3
3	ADP	F	6528	-	-	2/12/32/32	0/3/3/3
3	ADP	B	2528	2	-	2/12/32/32	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6528	ADP	C2-N3	3.97	1.38	1.32
3	C	3528	ADP	C2-N3	3.97	1.38	1.32
3	G	7528	ADP	C2-N3	3.96	1.38	1.32
3	D	4528	ADP	C2-N3	3.89	1.38	1.32
3	A	1528	ADP	C2-N3	3.79	1.38	1.32
3	H	8528	ADP	C2-N3	3.72	1.38	1.32
3	B	2528	ADP	C2-N3	3.54	1.37	1.32
3	D	4528	ADP	PB-O3B	3.46	1.68	1.54
3	E	5528	ADP	C2-N3	3.44	1.37	1.32
3	H	8528	ADP	PB-O3B	3.32	1.67	1.54
3	E	5528	ADP	PB-O3B	3.30	1.67	1.54
3	C	3528	ADP	PB-O3B	3.25	1.67	1.54
3	A	1528	ADP	PB-O3B	3.24	1.67	1.54
3	F	6528	ADP	PB-O3B	3.24	1.67	1.54
3	G	7528	ADP	C2'-C1'	-3.13	1.49	1.53
3	D	4528	ADP	C4-N3	3.10	1.39	1.35
3	B	2528	ADP	PB-O3B	3.03	1.66	1.54
3	G	7528	ADP	PB-O3B	2.82	1.65	1.54
3	B	2528	ADP	C2'-C1'	-2.56	1.49	1.53
3	D	4528	ADP	C2-N1	2.54	1.38	1.33
3	G	7528	ADP	C2-N1	2.54	1.38	1.33
3	A	1528	ADP	C2-N1	2.52	1.38	1.33
3	H	8528	ADP	O4'-C1'	2.51	1.44	1.41
3	F	6528	ADP	C4-N3	2.39	1.39	1.35
3	F	6528	ADP	C2-N1	2.38	1.38	1.33
3	B	2528	ADP	C2-N1	2.36	1.38	1.33
3	F	6528	ADP	C5-N7	-2.36	1.31	1.39
3	E	5528	ADP	C2-N1	2.34	1.38	1.33
3	A	1528	ADP	C5-N7	-2.33	1.31	1.39
3	H	8528	ADP	C2-N1	2.30	1.38	1.33
3	E	5528	ADP	C4-N3	2.28	1.38	1.35
3	A	1528	ADP	C4-N3	2.28	1.38	1.35
3	B	2528	ADP	C4-N3	2.28	1.38	1.35
3	H	8528	ADP	C4-N3	2.25	1.38	1.35
3	H	8528	ADP	C5-N7	-2.25	1.31	1.39
3	G	7528	ADP	C4-N3	2.24	1.38	1.35
3	B	2528	ADP	C5-N7	-2.23	1.31	1.39
3	C	3528	ADP	C2-N1	2.23	1.38	1.33
3	A	1528	ADP	O4'-C1'	2.16	1.44	1.41
3	F	6528	ADP	O4'-C1'	2.14	1.44	1.41
3	H	8528	ADP	C2'-C1'	-2.13	1.50	1.53
3	C	3528	ADP	C4-N3	2.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7528	ADP	C5-N7	-2.05	1.32	1.39
3	C	3528	ADP	C5-N7	-2.05	1.32	1.39
3	E	5528	ADP	O3'-C3'	2.02	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	8528	ADP	N3-C2-N1	-6.61	118.35	128.68
3	D	4528	ADP	N3-C2-N1	-6.59	118.37	128.68
3	A	1528	ADP	N3-C2-N1	-6.54	118.45	128.68
3	G	7528	ADP	N3-C2-N1	-6.54	118.46	128.68
3	B	2528	ADP	N3-C2-N1	-6.54	118.46	128.68
3	F	6528	ADP	N3-C2-N1	-6.50	118.51	128.68
3	C	3528	ADP	N3-C2-N1	-6.49	118.53	128.68
3	E	5528	ADP	N3-C2-N1	-6.42	118.64	128.68
3	E	5528	ADP	C4-C5-N7	-3.15	106.12	109.40
3	C	3528	ADP	C4-C5-N7	-3.12	106.14	109.40
3	D	4528	ADP	C4-C5-N7	-3.10	106.17	109.40
3	G	7528	ADP	C4-C5-N7	-2.94	106.33	109.40
3	H	8528	ADP	C4-C5-N7	-2.92	106.36	109.40
3	F	6528	ADP	C4-C5-N7	-2.91	106.37	109.40
3	B	2528	ADP	C4-C5-N7	-2.86	106.42	109.40
3	A	1528	ADP	C4-C5-N7	-2.84	106.44	109.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1528	ADP	PA-O3A-PB-O3B
3	B	2528	ADP	PA-O3A-PB-O3B
3	C	3528	ADP	PA-O3A-PB-O3B
3	D	4528	ADP	PA-O3A-PB-O3B
3	E	5528	ADP	PA-O3A-PB-O3B
3	F	6528	ADP	PA-O3A-PB-O3B
3	G	7528	ADP	PA-O3A-PB-O3B
3	H	8528	ADP	PA-O3A-PB-O3B
3	A	1528	ADP	PA-O3A-PB-O2B
3	B	2528	ADP	PA-O3A-PB-O2B
3	C	3528	ADP	PA-O3A-PB-O2B
3	D	4528	ADP	PA-O3A-PB-O2B
3	E	5528	ADP	PA-O3A-PB-O2B
3	F	6528	ADP	PA-O3A-PB-O2B

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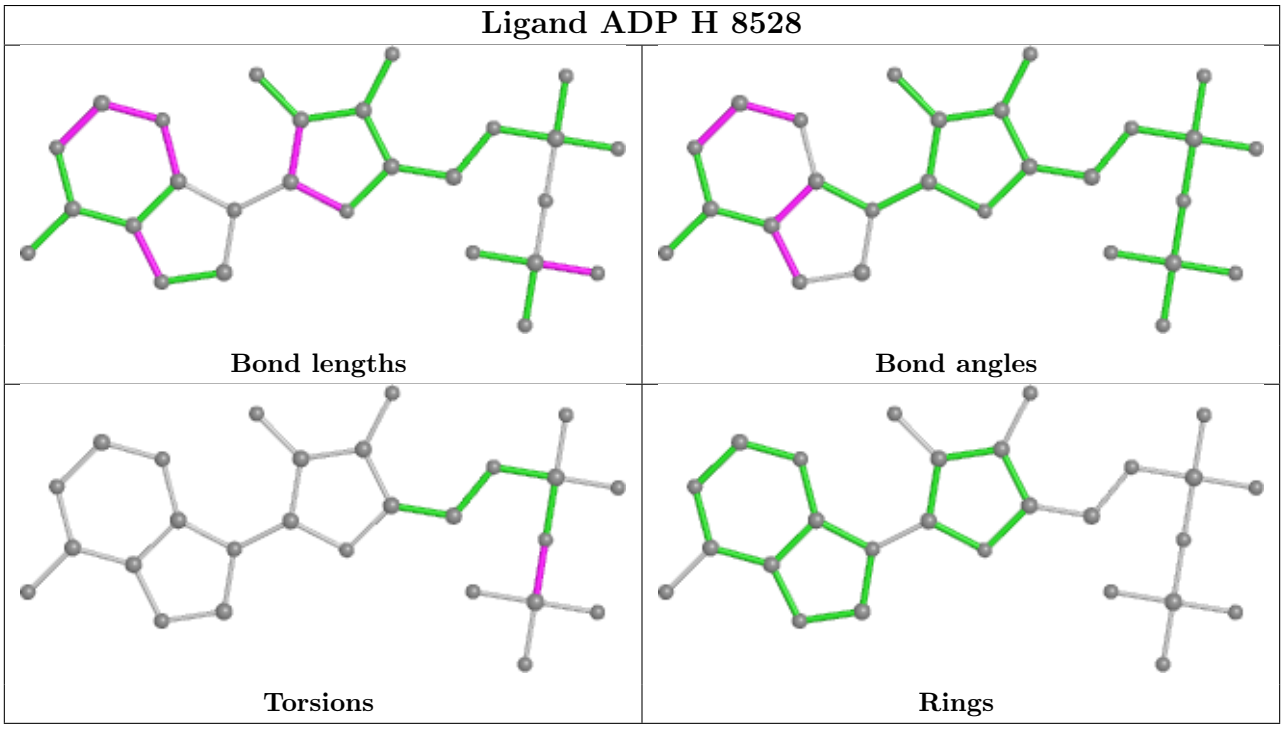
Mol	Chain	Res	Type	Atoms
3	G	7528	ADP	PA-O3A-PB-O2B
3	H	8528	ADP	PA-O3A-PB-O2B

There are no ring outliers.

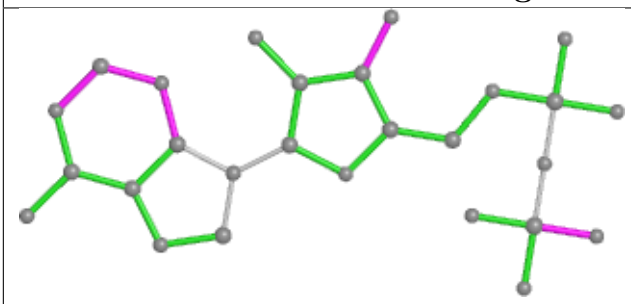
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	8528	ADP	1	0
3	G	7528	ADP	2	0
3	F	6528	ADP	1	0
3	B	2528	ADP	1	0

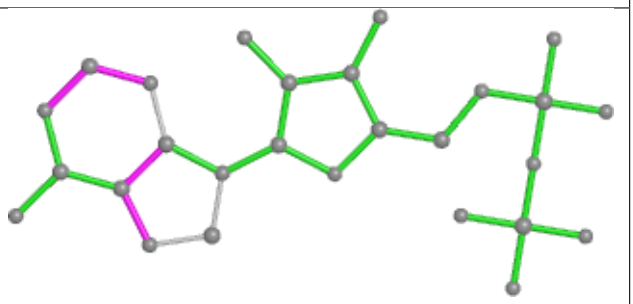
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



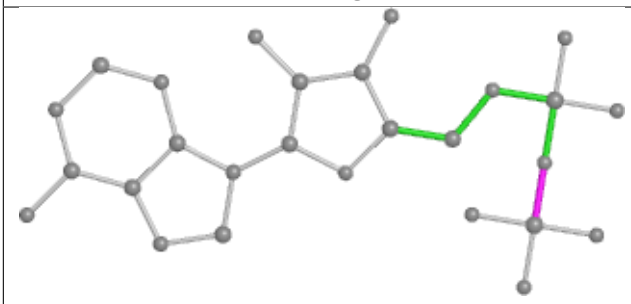
Ligand ADP E 5528



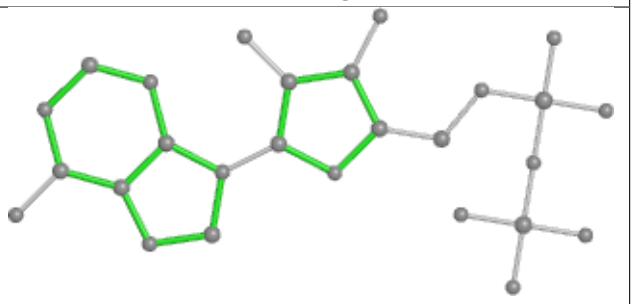
Bond lengths



Bond angles

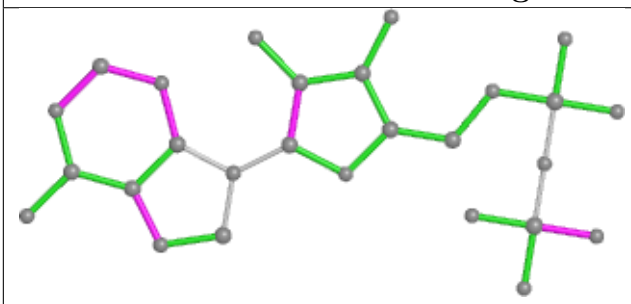


Torsions

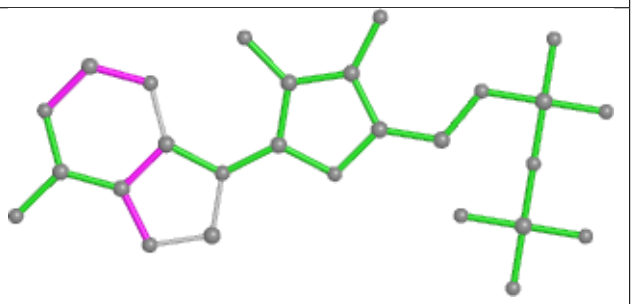


Rings

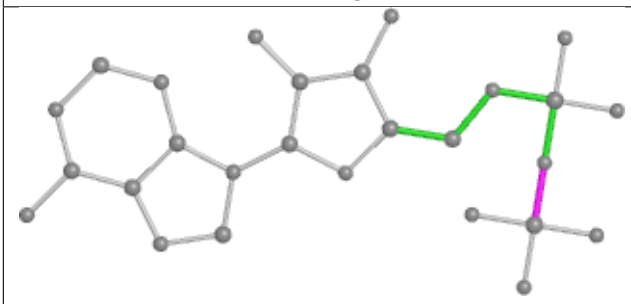
Ligand ADP G 7528



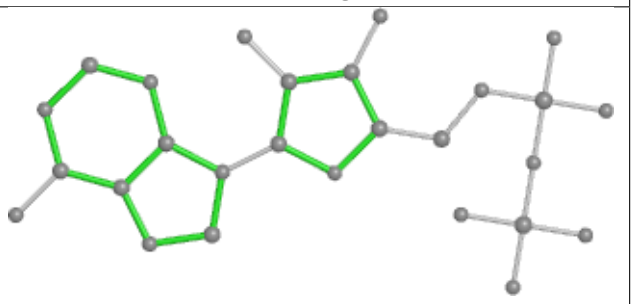
Bond lengths



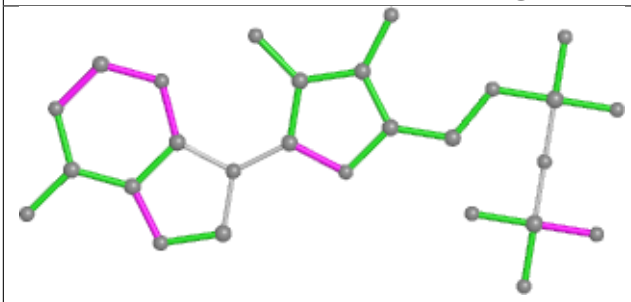
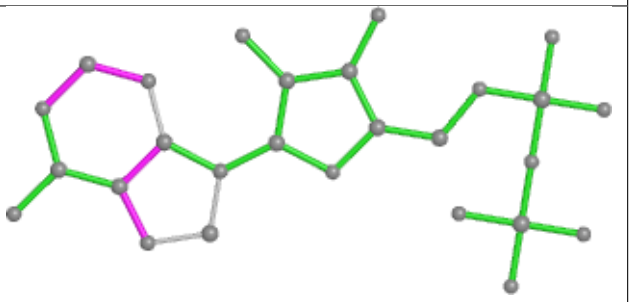
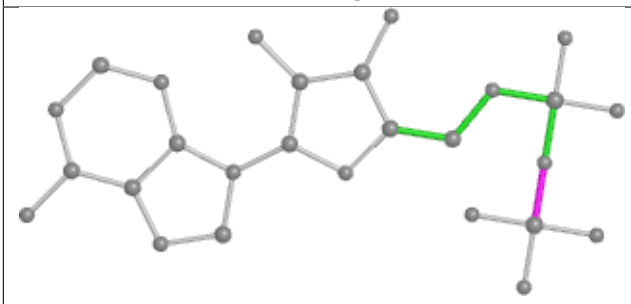
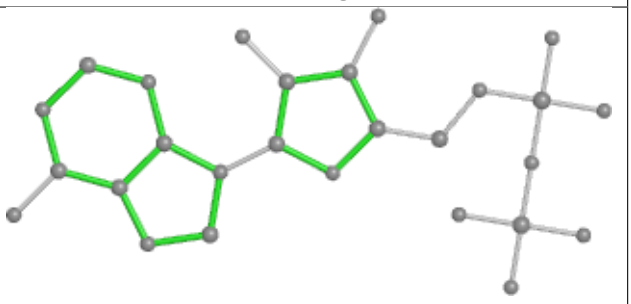
Bond angles

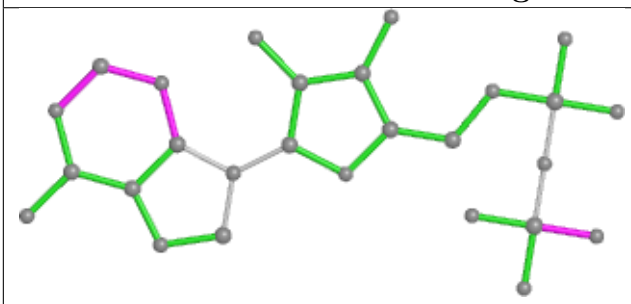
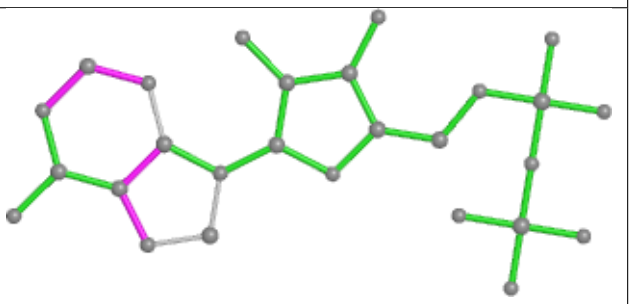
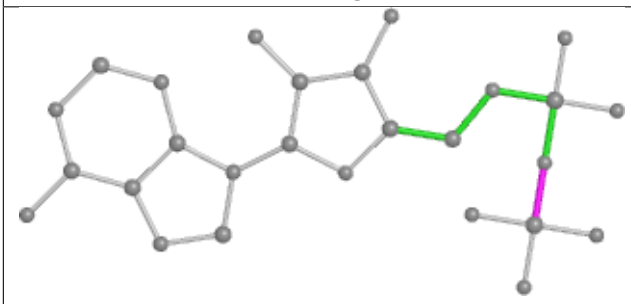
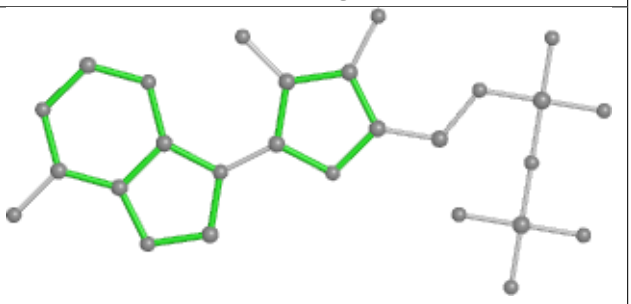


Torsions

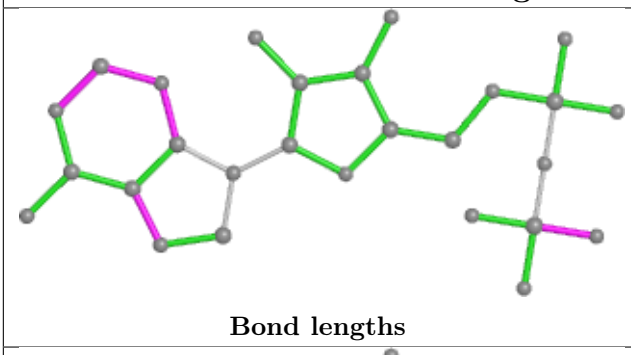


Rings

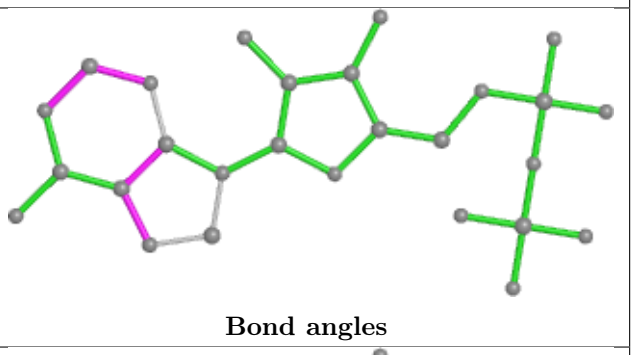
Ligand ADP A 1528	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 4528	
 Bond lengths	 Bond angles
 Torsions	 Rings

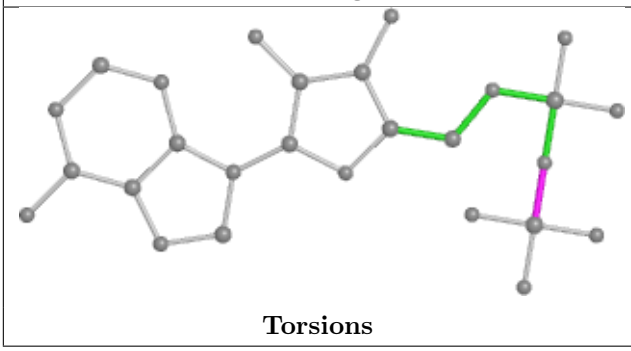
Ligand ADP C 3528



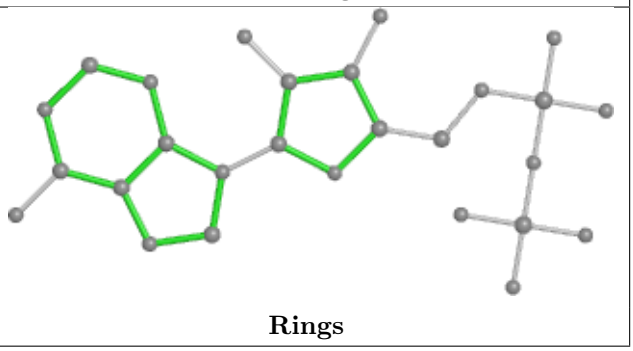
Bond lengths



Bond angles

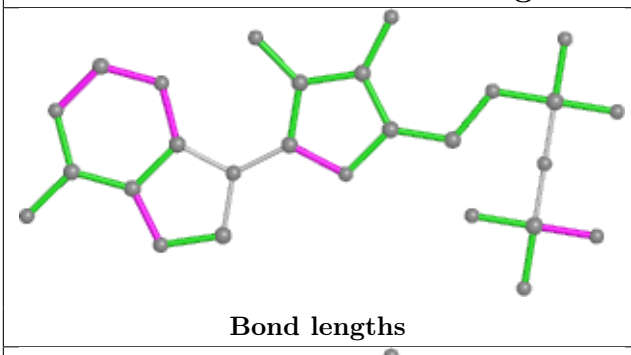


Torsions

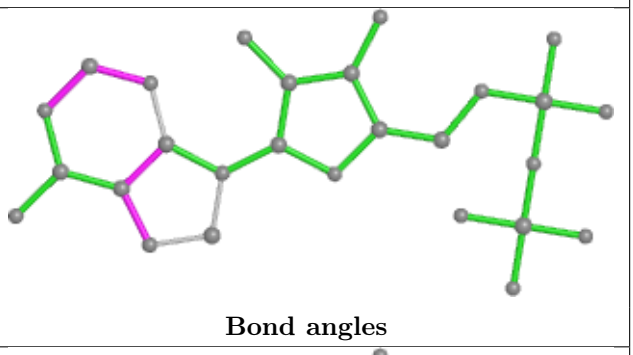


Rings

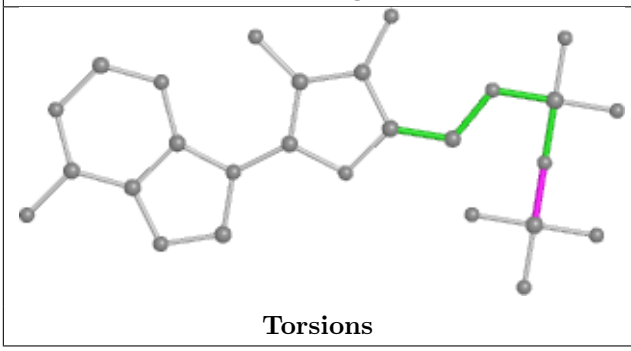
Ligand ADP F 6528



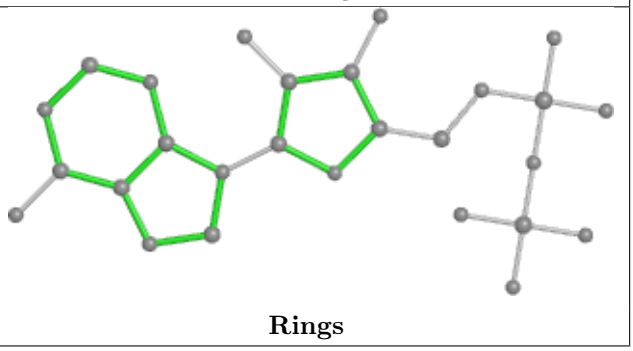
Bond lengths



Bond angles

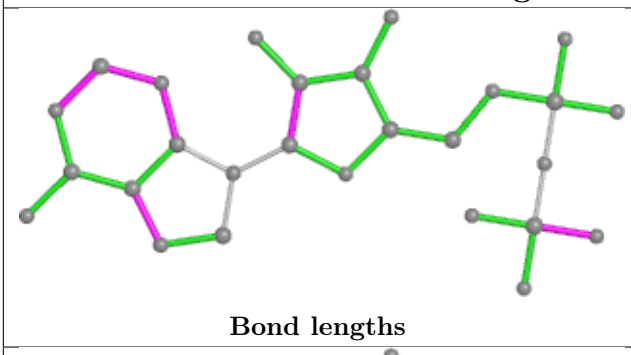


Torsions

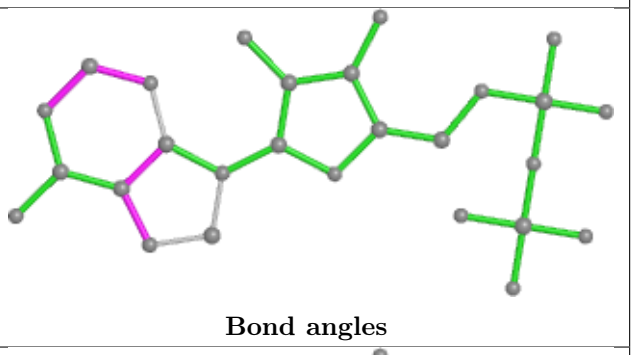


Rings

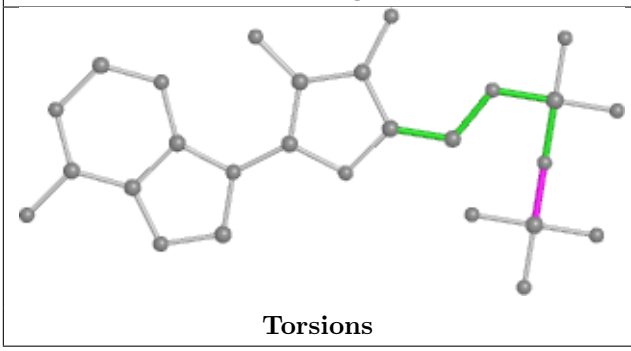
Ligand ADP B 2528



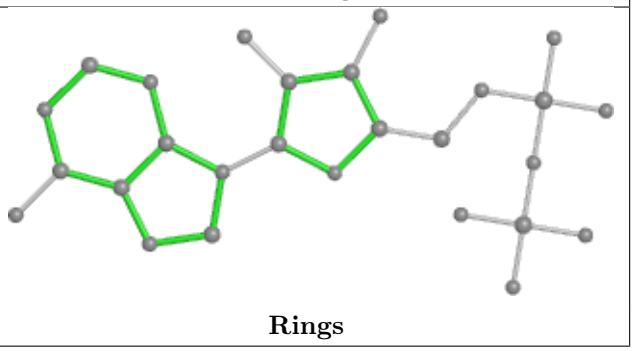
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	517/548 (94%)	-0.17	4 (0%)	86	65	10, 30, 62, 102	0
1	B	517/548 (94%)	-0.12	5 (0%)	82	59	8, 28, 62, 105	0
1	C	517/548 (94%)	-0.10	4 (0%)	86	65	16, 40, 70, 100	0
1	D	517/548 (94%)	-0.02	8 (1%)	73	46	13, 41, 70, 102	0
1	E	517/548 (94%)	-0.06	6 (1%)	79	54	16, 41, 67, 108	0
1	F	517/548 (94%)	-0.08	8 (1%)	73	46	14, 34, 65, 109	0
1	G	517/548 (94%)	-0.08	6 (1%)	79	54	12, 35, 65, 98	0
1	H	517/548 (94%)	-0.14	5 (0%)	82	59	8, 29, 56, 96	0
All	All	4136/4384 (94%)	-0.10	46 (1%)	80	56	8, 35, 66, 109	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	VAL	10.7
1	E	526	ALA	10.3
1	D	526	ALA	9.3
1	A	526	ALA	8.2
1	C	10	VAL	7.0
1	D	10	VAL	6.5
1	F	10	VAL	6.3
1	H	10	VAL	6.1
1	B	526	ALA	5.9
1	E	10	VAL	5.8
1	G	526	ALA	5.0
1	F	526	ALA	5.0
1	A	189	LYS	4.6
1	B	11	ILE	4.6
1	C	526	ALA	4.6
1	F	15	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	4.1
1	D	525	LYS	3.8
1	D	166	ASN	3.8
1	G	167	ALA	3.6
1	E	525	LYS	3.3
1	D	15	GLY	3.2
1	E	189	LYS	2.9
1	B	17	GLN	2.9
1	H	189	LYS	2.8
1	F	167	ALA	2.8
1	G	10	VAL	2.7
1	D	14	GLU	2.6
1	H	166	ASN	2.6
1	F	11	ILE	2.6
1	C	525	LYS	2.5
1	H	167	ALA	2.5
1	G	166	ASN	2.3
1	H	15	GLY	2.3
1	A	167	ALA	2.3
1	F	189	LYS	2.3
1	A	15	GLY	2.2
1	E	15	GLY	2.2
1	F	166	ASN	2.2
1	C	11	ILE	2.1
1	B	167	ALA	2.1
1	F	525	LYS	2.0
1	D	11	ILE	2.0
1	E	11	ILE	2.0
1	G	17	GLN	2.0
1	G	525	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

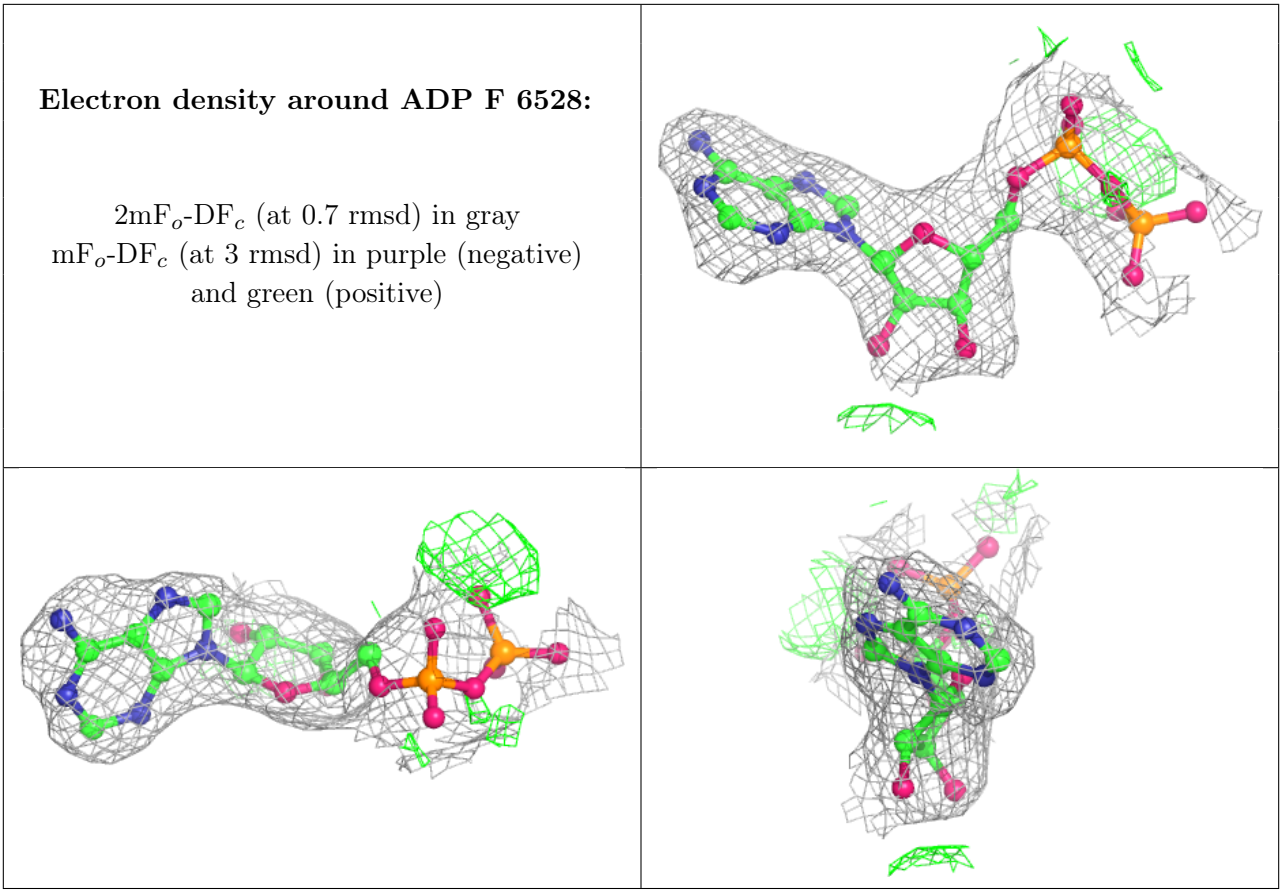
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MG	A	1527	1/1	0.84	0.18	15,15,15,15	0
2	MG	C	3527	1/1	0.88	0.16	18,18,18,18	0
2	MG	H	8527	1/1	0.91	0.21	25,25,25,25	0
3	ADP	F	6528	27/27	0.93	0.21	21,27,34,35	0
3	ADP	D	4528	27/27	0.94	0.20	32,37,44,45	0
2	MG	E	5527	1/1	0.94	0.20	14,14,14,14	0
3	ADP	G	7528	27/27	0.94	0.21	30,39,44,45	0
3	ADP	A	1528	27/27	0.95	0.20	21,33,39,41	0
3	ADP	E	5528	27/27	0.95	0.18	30,32,35,36	0
3	ADP	B	2528	27/27	0.95	0.19	17,24,28,29	0
3	ADP	C	3528	27/27	0.95	0.20	32,35,37,38	0
3	ADP	H	8528	27/27	0.95	0.21	26,28,31,32	0
2	MG	D	4527	1/1	0.97	0.17	17,17,17,17	0
2	MG	B	2527	1/1	0.97	0.21	10,10,10,10	0
2	MG	G	6527	1/1	0.97	0.16	16,16,16,16	0

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

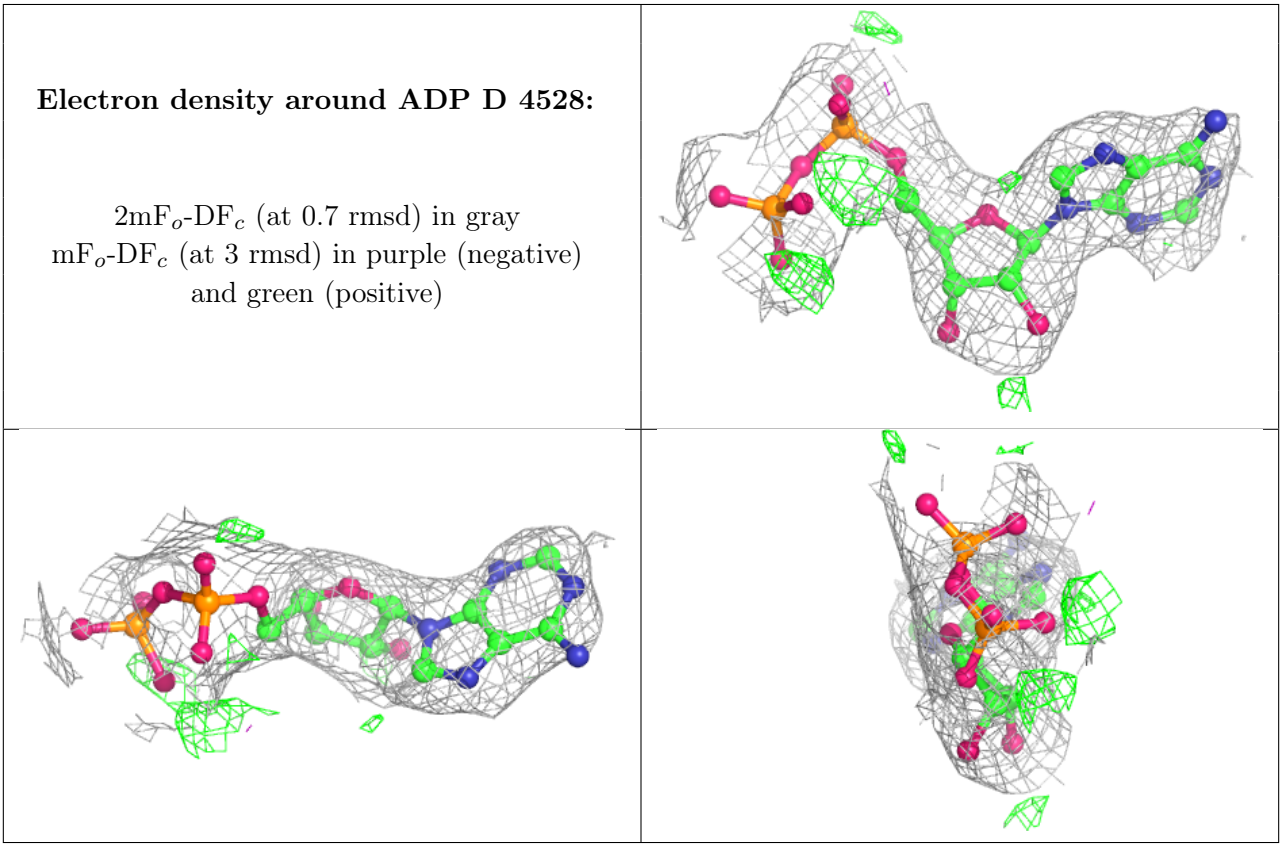
Electron density around ADP F 6528:

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



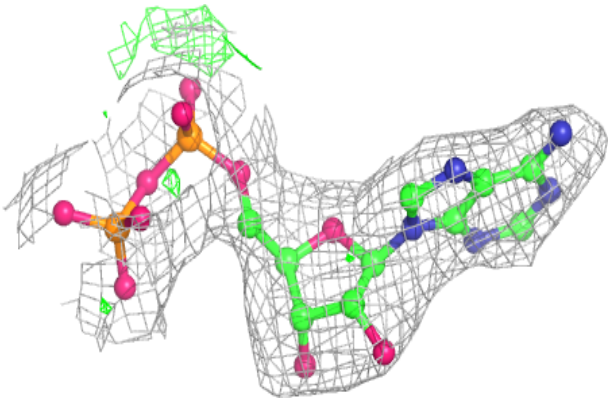
Electron density around ADP D 4528:

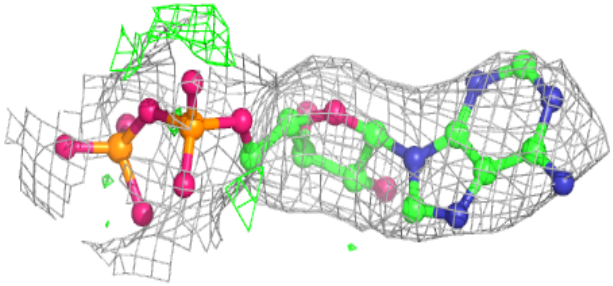
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

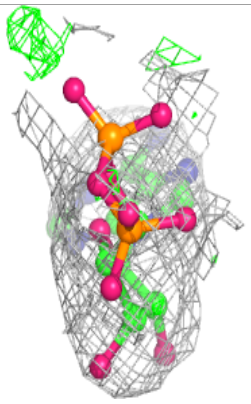


Electron density around ADP G 7528:

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

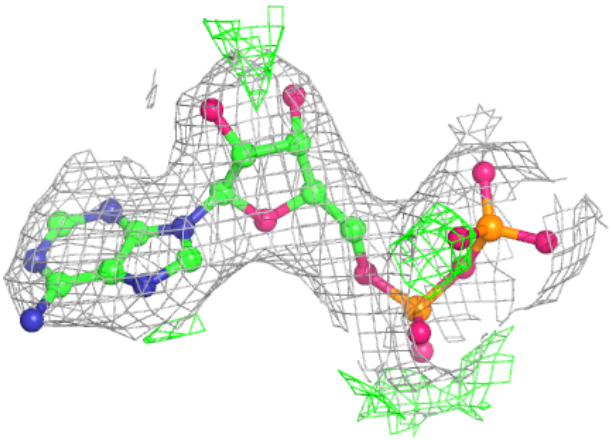


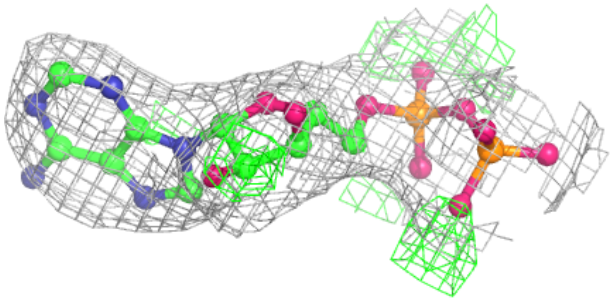




Electron density around ADP A 1528:

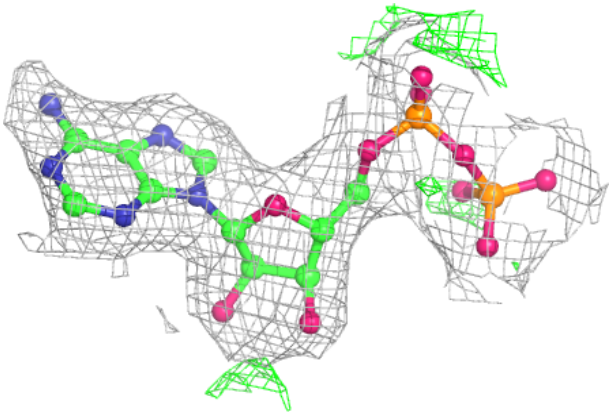
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

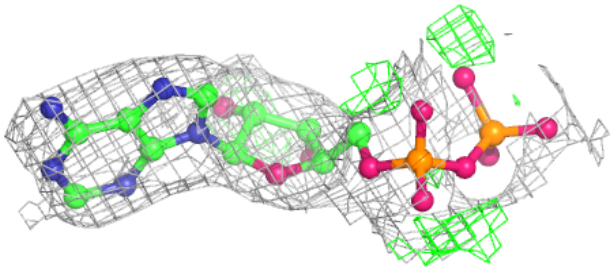


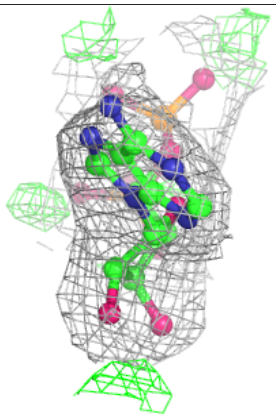


Electron density around ADP E 5528:

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

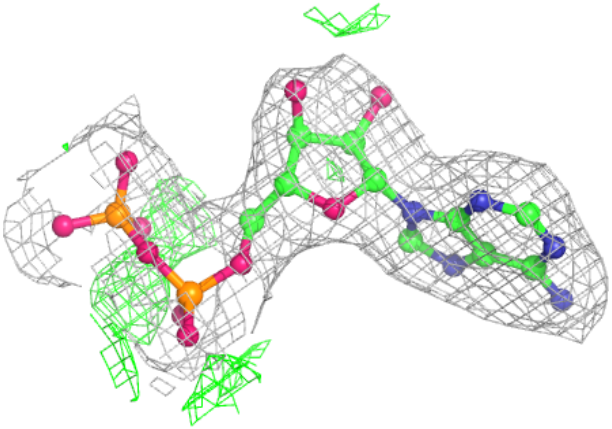


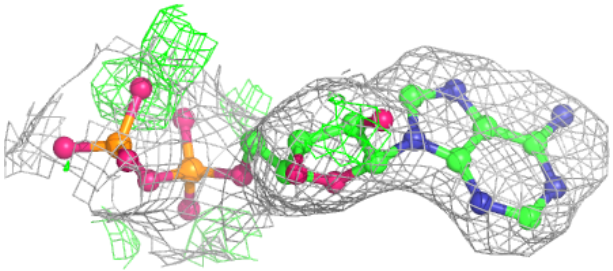


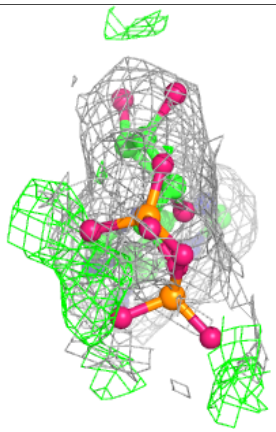


Electron density around ADP B 2528:

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

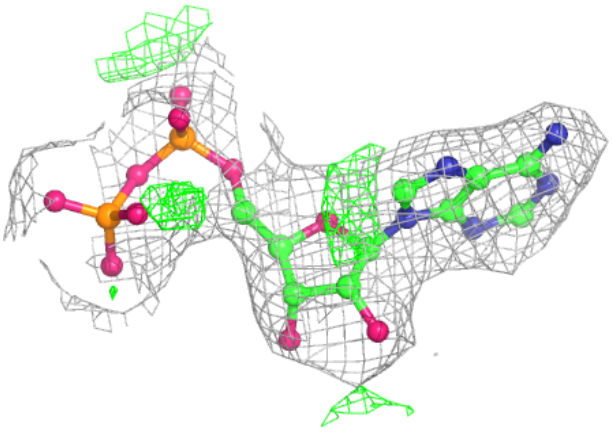


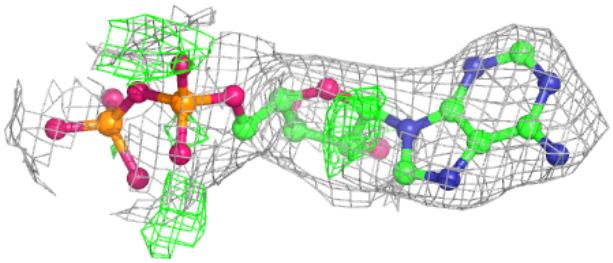


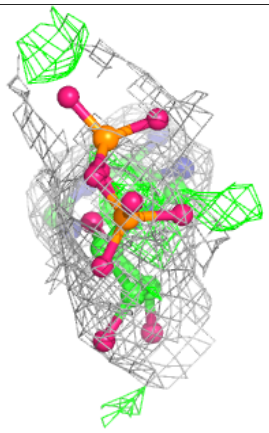


Electron density around ADP C 3528:

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

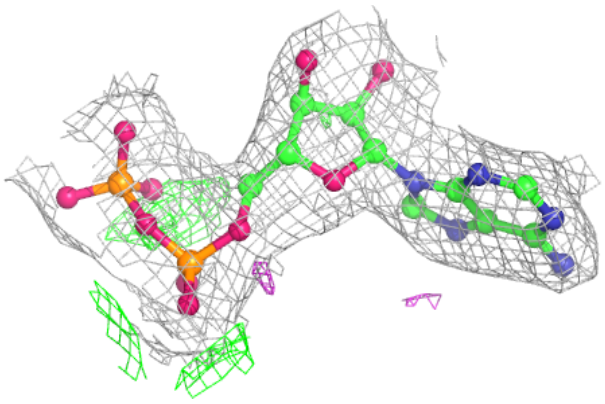


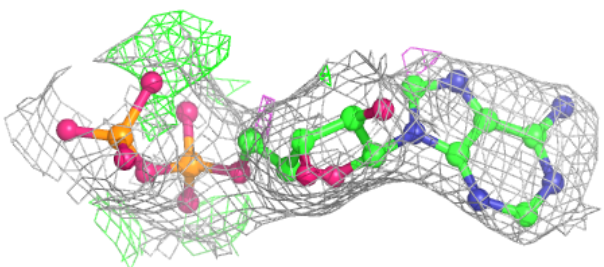


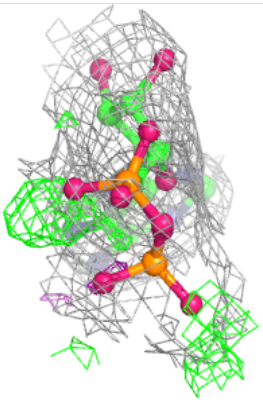


Electron density around ADP H 8528:

$2mF_o$-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.