Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 07:23 AM EST

PDB ID	:	3PDI
Title	:	Precursor bound NifEN
Authors	:	Kaiser, J.T.; Hu, Y.; Wiig, J.A.; Rees, D.C.; Ribbe, M.W.
Deposited on	:	2010-10-22
Resolution	:	2.40 Å(reported)

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

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

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

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

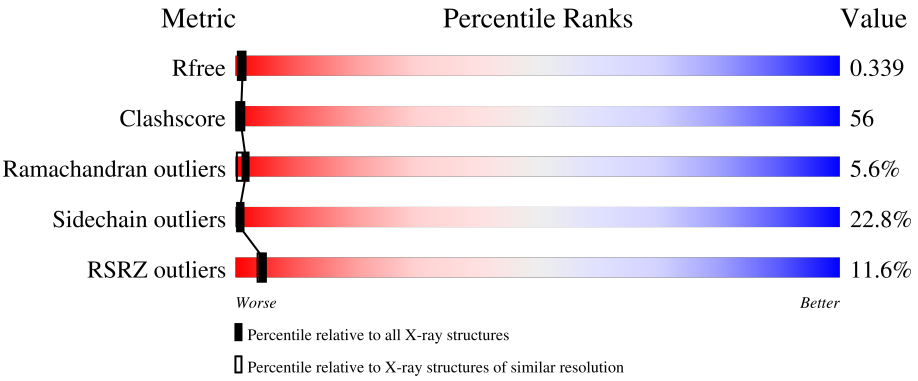
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	483	11% 33% 40% 14% • 12%
1	C	483	16% 30% 42% 15% • 12%
1	E	483	13% 32% 42% 13% • 12%
1	G	483	15% 29% 44% 14% • 12%
2	B	458	5% 38% 41% 14% • 6%

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Mol	Chain	Length	Quality of chain
2	D	458	6% 40% 39% 13% 6%
2	F	458	9% 37% 41% 13% 6%
2	H	458	8% 38% 40% 14% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
3	SF4	E	501	-	-	X	-
3	SF4	G	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26112 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 Nitrogenase MoFe cofactor biosynthesis protein NifE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	C	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	E	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			
1	G	427	Total	C	N	O	S	0	0	0
			3280	2064	577	618	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP C1DH03
A	-6	HIS	-	expression tag	UNP C1DH03
A	-5	HIS	-	expression tag	UNP C1DH03
A	-4	HIS	-	expression tag	UNP C1DH03
A	-3	HIS	-	expression tag	UNP C1DH03
A	-2	HIS	-	expression tag	UNP C1DH03
A	-1	HIS	-	expression tag	UNP C1DH03
A	0	HIS	-	expression tag	UNP C1DH03
C	-7	MET	-	expression tag	UNP C1DH03
C	-6	HIS	-	expression tag	UNP C1DH03
C	-5	HIS	-	expression tag	UNP C1DH03
C	-4	HIS	-	expression tag	UNP C1DH03
C	-3	HIS	-	expression tag	UNP C1DH03
C	-2	HIS	-	expression tag	UNP C1DH03
C	-1	HIS	-	expression tag	UNP C1DH03
C	0	HIS	-	expression tag	UNP C1DH03
E	-7	MET	-	expression tag	UNP C1DH03
E	-6	HIS	-	expression tag	UNP C1DH03
E	-5	HIS	-	expression tag	UNP C1DH03
E	-4	HIS	-	expression tag	UNP C1DH03
E	-3	HIS	-	expression tag	UNP C1DH03

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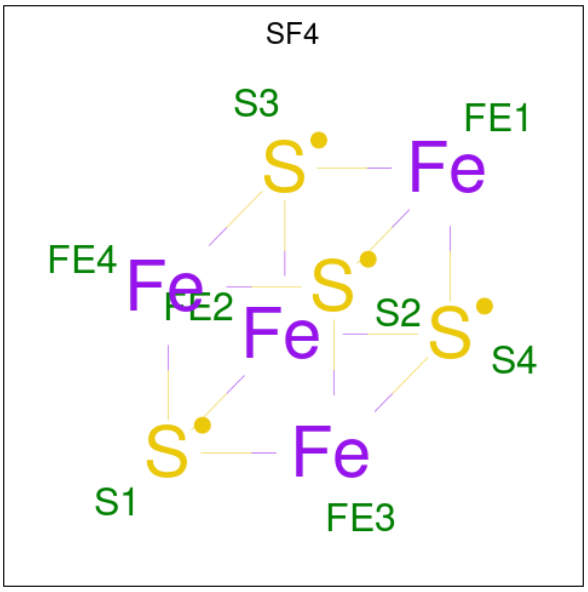
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	expression tag	UNP C1DH03
E	-1	HIS	-	expression tag	UNP C1DH03
E	0	HIS	-	expression tag	UNP C1DH03
G	-7	MET	-	expression tag	UNP C1DH03
G	-6	HIS	-	expression tag	UNP C1DH03
G	-5	HIS	-	expression tag	UNP C1DH03
G	-4	HIS	-	expression tag	UNP C1DH03
G	-3	HIS	-	expression tag	UNP C1DH03
G	-2	HIS	-	expression tag	UNP C1DH03
G	-1	HIS	-	expression tag	UNP C1DH03
G	0	HIS	-	expression tag	UNP C1DH03

- Molecule 2 is a protein called Nitrogenase MoFe cofactor biosynthesis protein NifN.

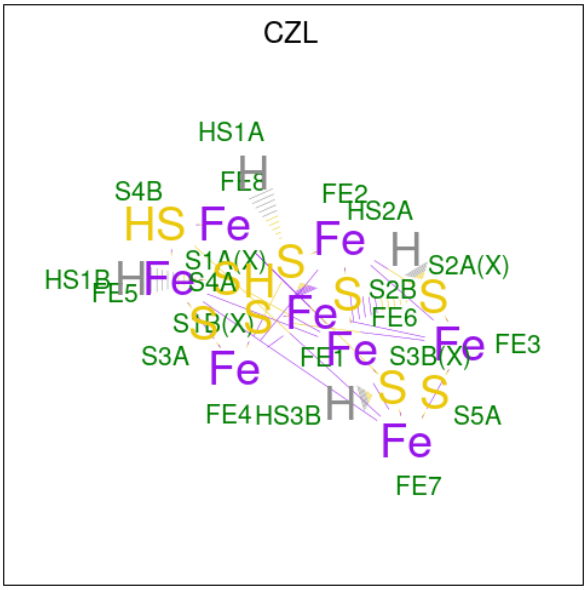
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	D	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	F	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			
2	H	432	Total	C	N	O	S	0	0	0
			3223	2025	573	610	15			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	E	1	Total Fe S 8 4 4	0	0
3	G	1	Total Fe S 8 4 4	0	0

- Molecule 4 is L-Cluster (Fe8S9) (three-letter code: CZL) (formula: $Fe_8H_6S_9$).

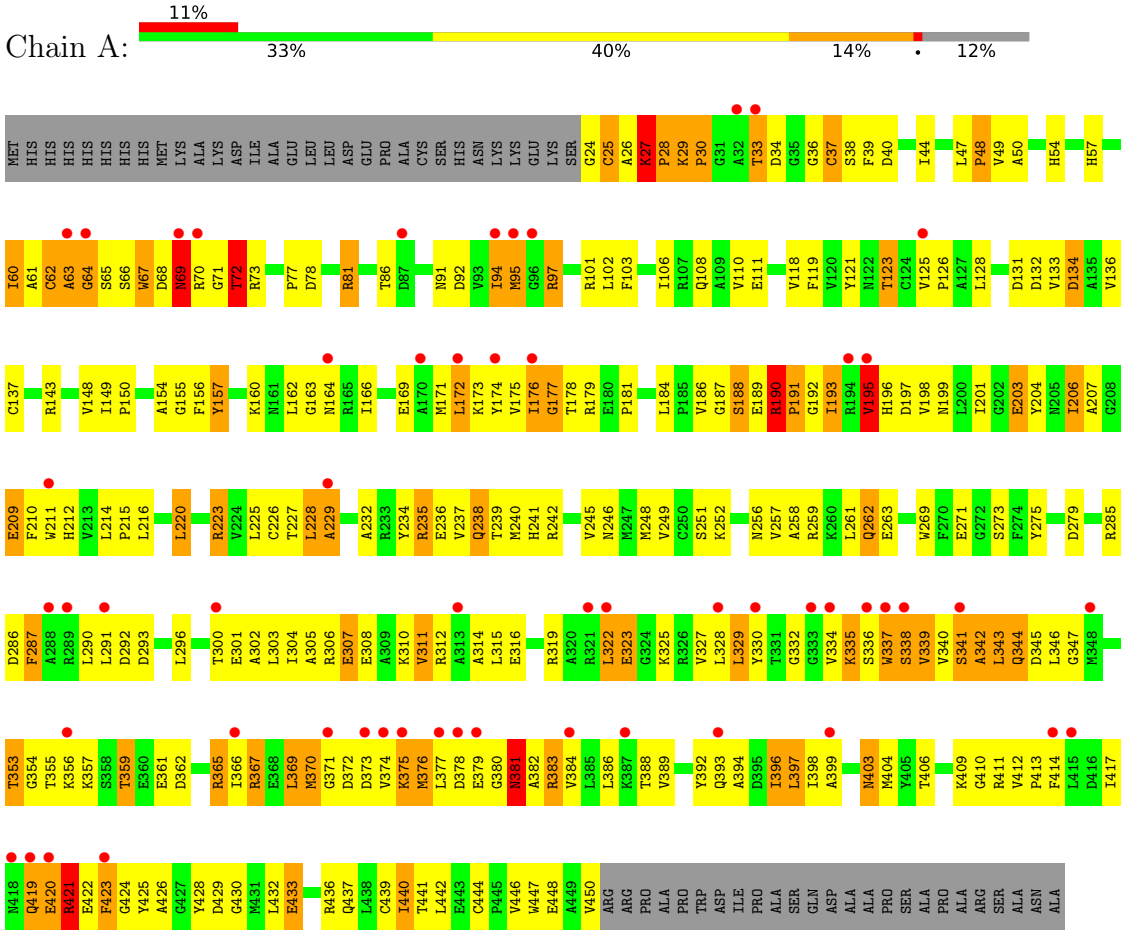


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 17 8 9	0	0
4	C	1	Total Fe S 17 8 9	0	0
4	E	1	Total Fe S 17 8 9	0	0
4	G	1	Total Fe S 17 8 9	0	0

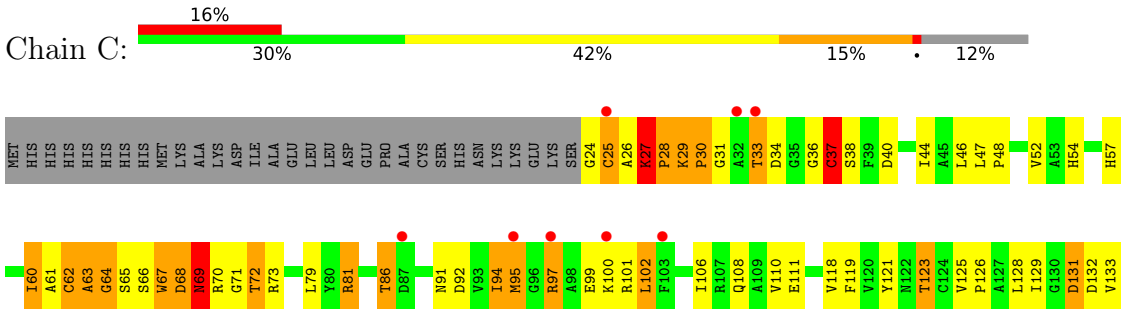
3 Residue-property plots (i)

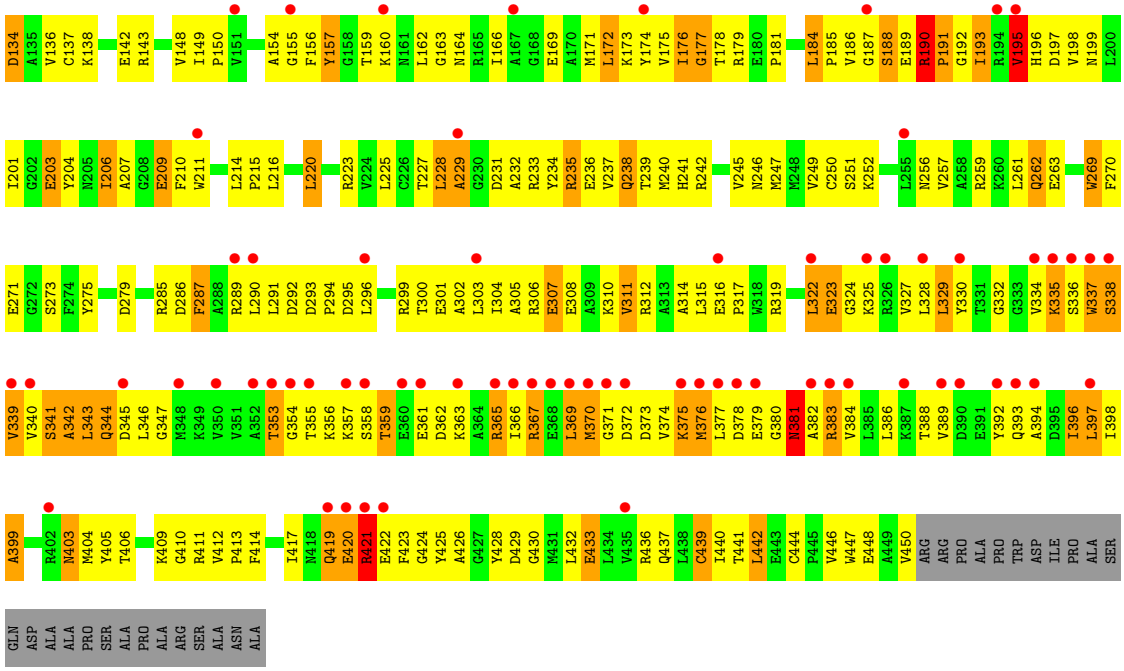
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE



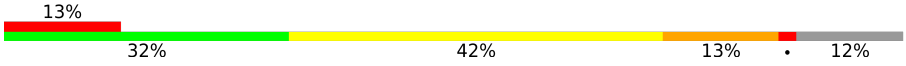
• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE

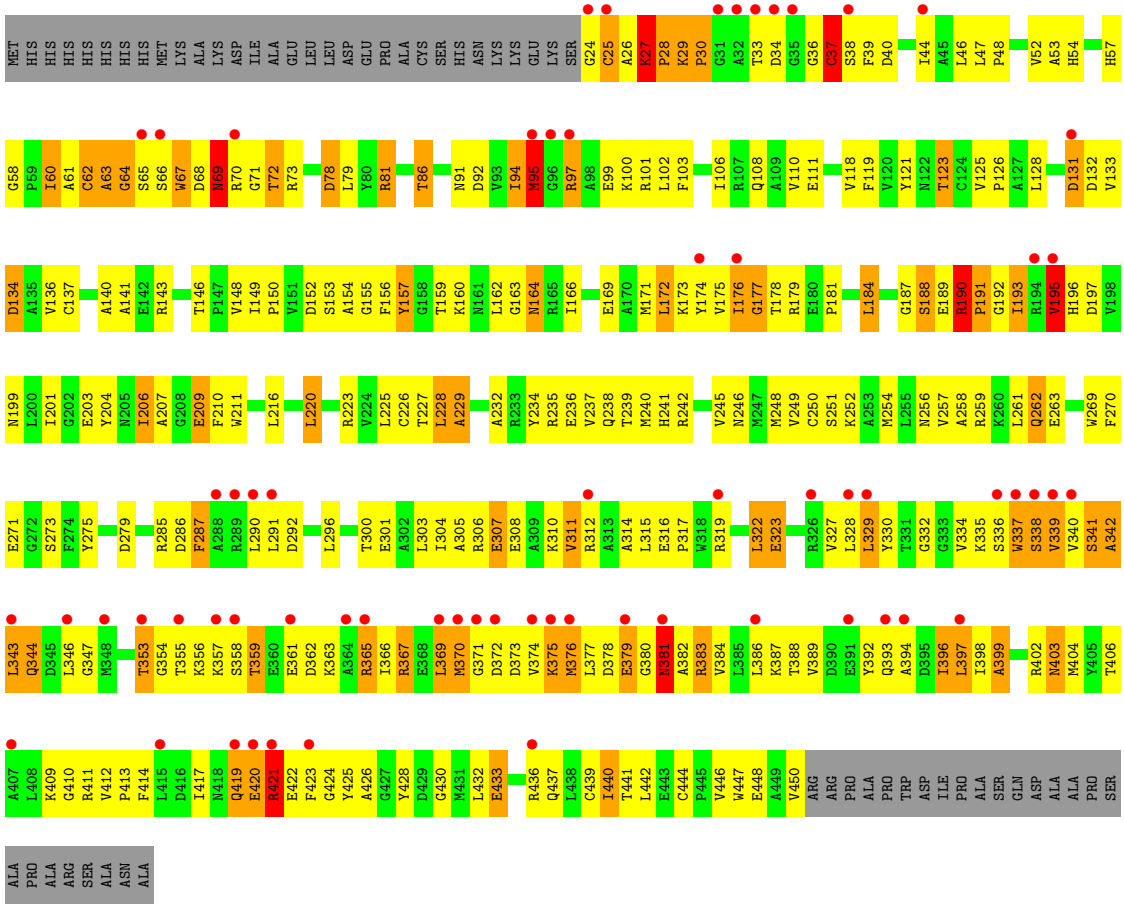




• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE

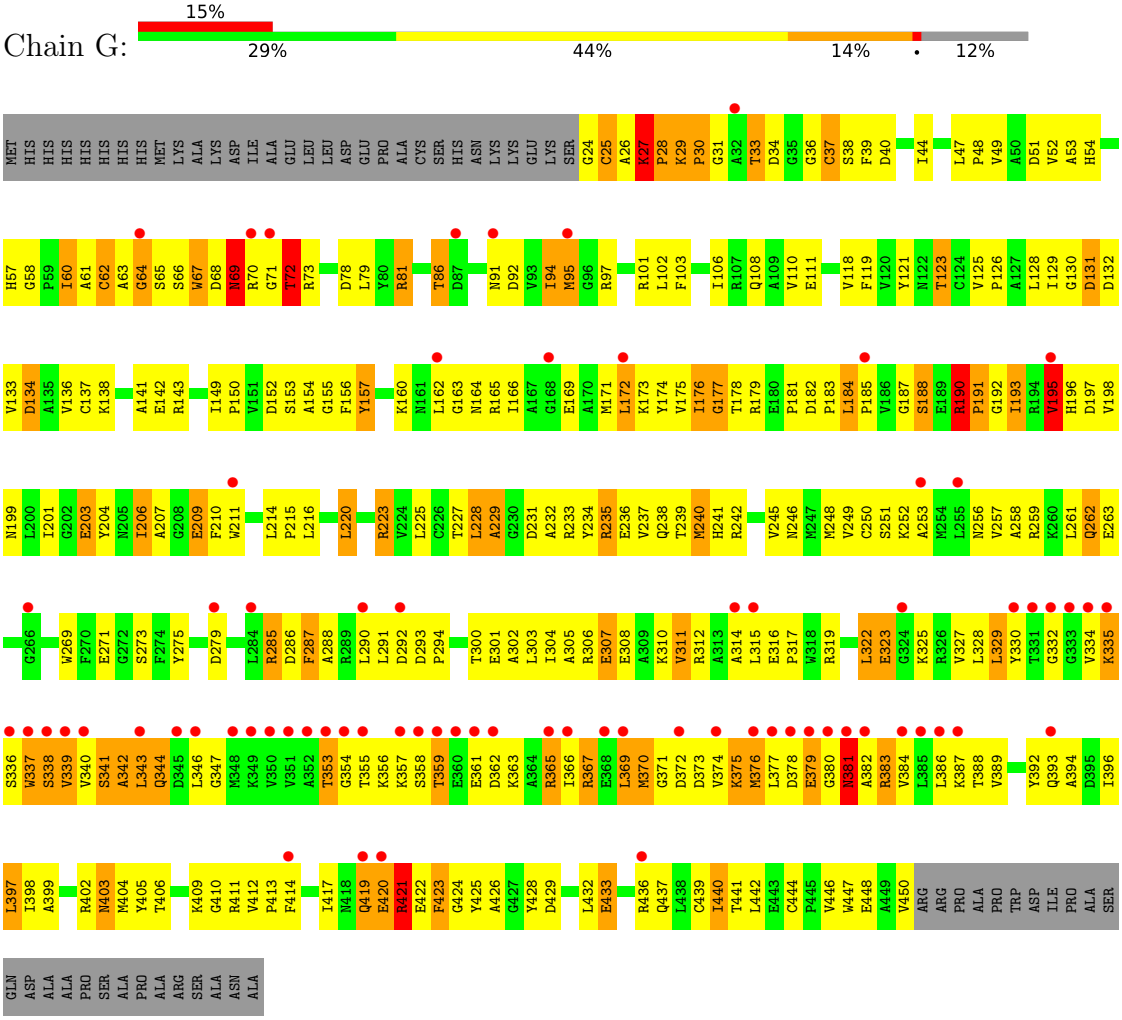
Chain E:





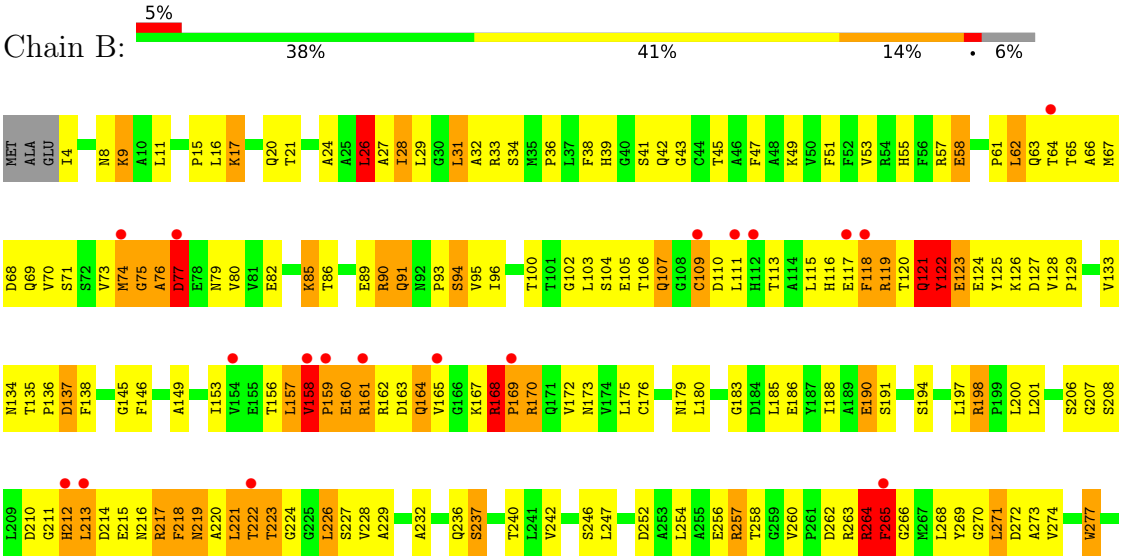
• Molecule 1: Nitrogenase MoFe cofactor biosynthesis protein NifE

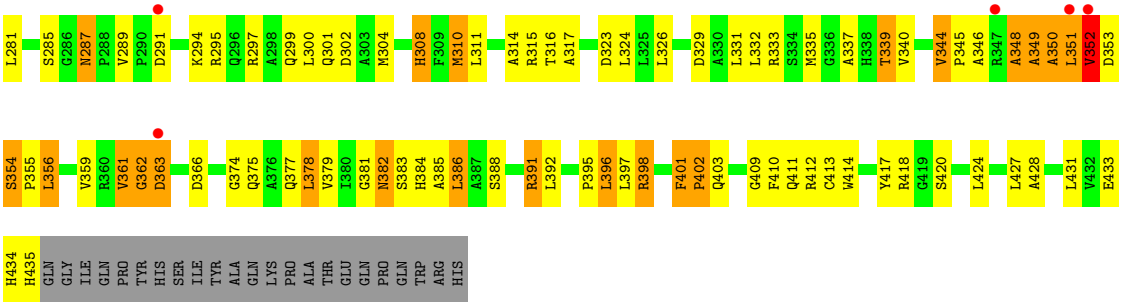
Chain G:



• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

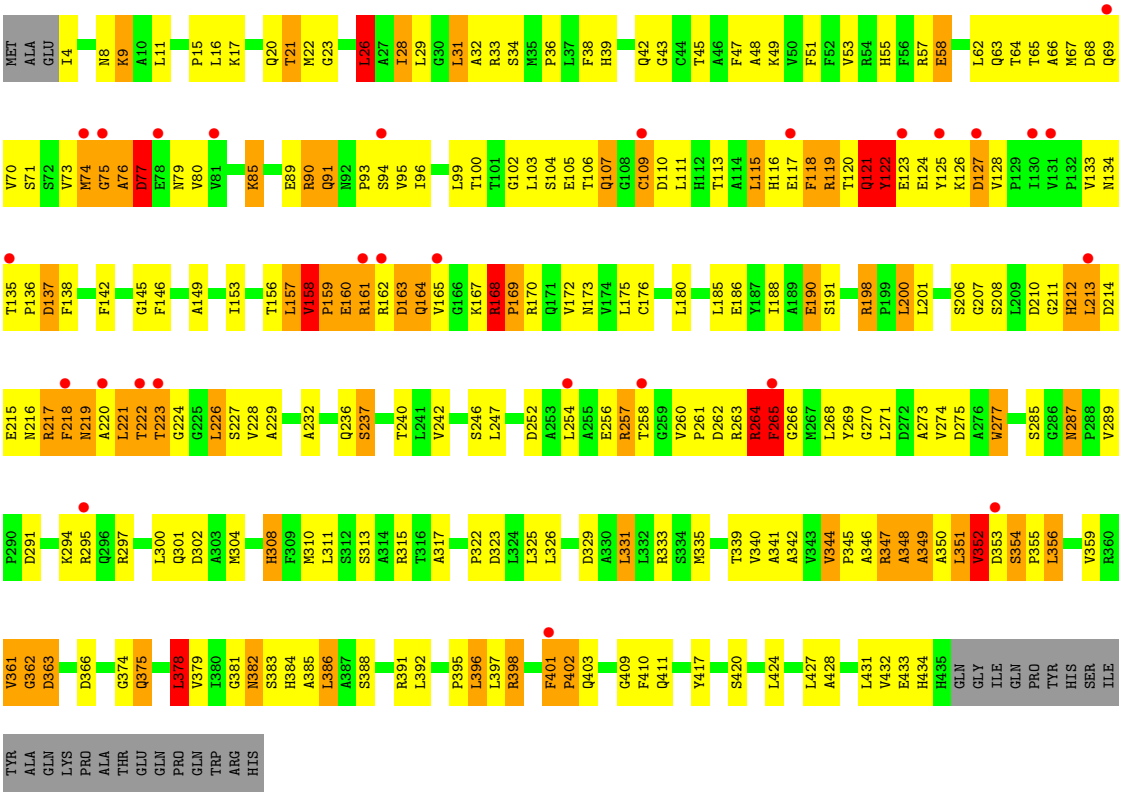
Chain B:





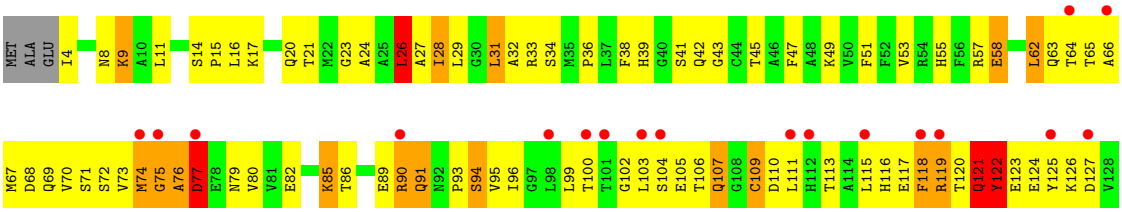
• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

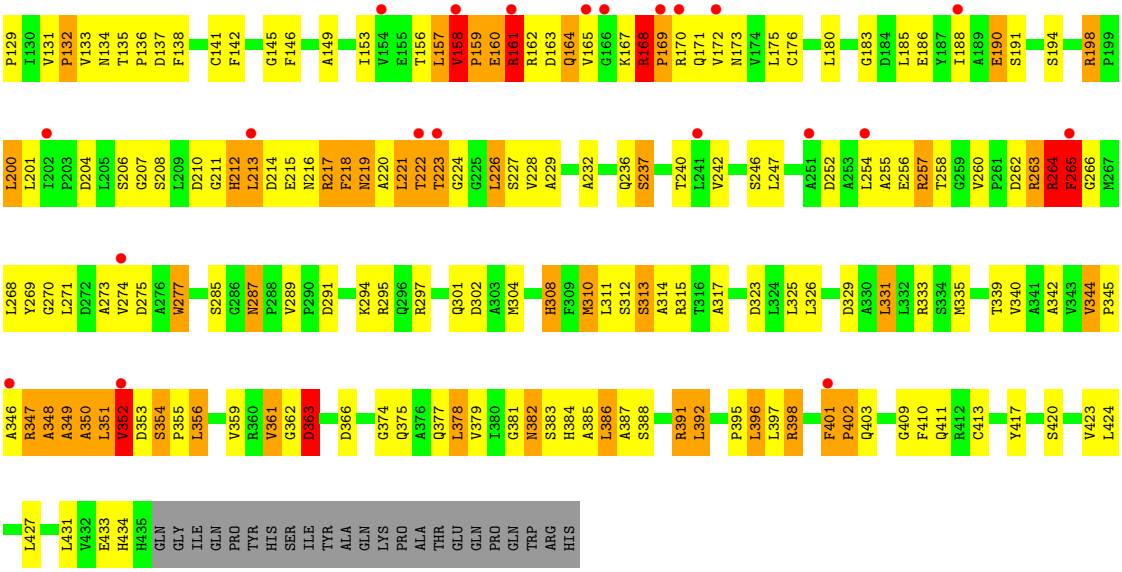
Chain D:



• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

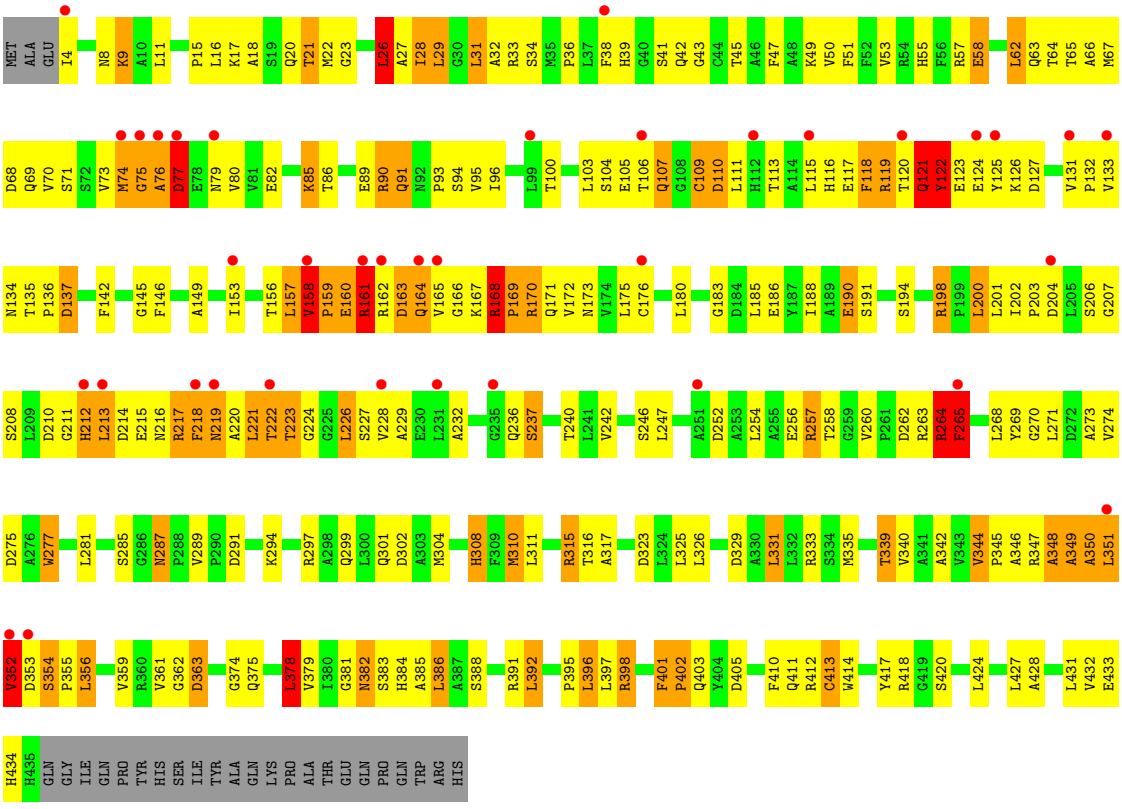
Chain F:





• Molecule 2: Nitrogenase MoFe cofactor biosynthesis protein NifN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.07Å 95.22Å 149.98Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	39.83 – 2.40 39.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.83-2.40) 87.2 (39.83-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.294 , 0.341 0.291 , 0.339	Depositor DCC
R_{free} test set	13821 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 22.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.075 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	26112	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: SF4, CZL

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	0.61	0/3342	0.76	1/4531 (0.0%)
1	C	0.58	2/3342 (0.1%)	0.76	0/4531
1	E	0.61	1/3342 (0.0%)	0.77	0/4531
1	G	0.58	0/3342	0.77	2/4531 (0.0%)
2	B	0.68	2/3283 (0.1%)	0.85	2/4466 (0.0%)
2	D	0.71	4/3283 (0.1%)	0.87	4/4466 (0.1%)
2	F	0.69	4/3283 (0.1%)	0.85	3/4466 (0.1%)
2	H	0.70	4/3283 (0.1%)	0.87	4/4466 (0.1%)
All	All	0.65	17/26500 (0.1%)	0.81	16/35988 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
2	B	0	4
2	D	0	4
2	F	0	5
2	H	0	4
All	All	0	21

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	122	TYR	CD1-CE1	-7.62	1.27	1.39
2	B	122	TYR	CD1-CE1	-7.59	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	122	TYR	CD1-CE1	-7.51	1.28	1.39
2	H	122	TYR	CD1-CE1	-7.16	1.28	1.39
2	H	413	CYS	CB-SG	6.81	1.93	1.82
2	D	122	TYR	CD2-CE2	-6.26	1.29	1.39
2	D	122	TYR	CE1-CZ	-6.21	1.30	1.38
2	F	122	TYR	CE1-CZ	-6.15	1.30	1.38
2	F	122	TYR	CD2-CE2	-6.00	1.30	1.39
2	B	122	TYR	CD2-CE2	-5.99	1.30	1.39
1	C	37	CYS	CB-SG	-5.66	1.72	1.81
2	H	122	TYR	CD2-CE2	-5.54	1.31	1.39
2	F	122	TYR	CB-CG	-5.46	1.43	1.51
2	H	122	TYR	CE1-CZ	-5.42	1.31	1.38
1	E	37	CYS	CB-SG	-5.25	1.73	1.81
2	D	122	TYR	CB-CG	-5.10	1.44	1.51
1	C	439	CYS	CB-SG	-5.02	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	26	LEU	CA-CB-CG	7.03	131.47	115.30
2	F	26	LEU	CA-CB-CG	6.89	131.14	115.30
2	B	122	TYR	CB-CG-CD1	-6.70	116.98	121.00
2	B	26	LEU	CA-CB-CG	6.53	130.32	115.30
2	H	26	LEU	CA-CB-CG	6.25	129.67	115.30
2	H	122	TYR	CB-CG-CD1	-6.15	117.31	121.00
2	D	122	TYR	CB-CG-CD1	-6.10	117.34	121.00
2	F	122	TYR	CB-CG-CD1	-5.79	117.53	121.00
2	H	392	LEU	CA-CB-CG	5.64	128.28	115.30
1	G	223	ARG	NE-CZ-NH1	-5.33	117.63	120.30
2	F	392	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	223	ARG	NE-CZ-NH1	-5.23	117.68	120.30
2	H	378	LEU	CA-CB-CG	5.22	127.31	115.30
1	G	62	CYS	CA-CB-SG	-5.12	104.78	114.00
2	D	378	LEU	CA-CB-CG	5.10	127.04	115.30
2	D	122	TYR	CG-CD2-CE2	-5.02	117.29	121.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ILE	Peptide
2	B	118	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	121	GLN	Peptide
2	B	159	PRO	Peptide
2	B	264	ARG	Peptide
1	C	94	ILE	Peptide
2	D	118	PHE	Peptide
2	D	121	GLN	Peptide
2	D	159	PRO	Peptide
2	D	264	ARG	Peptide
1	E	94	ILE	Peptide
2	F	118	PHE	Peptide
2	F	121	GLN	Peptide
2	F	159	PRO	Peptide
2	F	264	ARG	Peptide
2	F	363	ASP	Peptide
1	G	94	ILE	Peptide
2	H	118	PHE	Peptide
2	H	121	GLN	Peptide
2	H	159	PRO	Peptide
2	H	264	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3280	0	3271	383	0
1	C	3280	0	3271	406	0
1	E	3280	0	3270	396	0
1	G	3280	0	3271	385	0
2	B	3223	0	3197	404	5
2	D	3223	0	3197	399	2
2	F	3223	0	3197	394	0
2	H	3223	0	3197	388	7
3	A	8	0	0	2	0
3	C	8	0	0	2	0
3	E	8	0	0	3	0
3	G	8	0	0	4	0
4	A	17	0	0	3	0
4	C	17	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	17	0	0	2	0
4	G	17	0	0	4	0
All	All	26112	0	25871	2918	7

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 56.

All (2918) 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:A:190:ARG:CB	1:A:191:PRO:HD2	1.56	1.33
1:A:190:ARG:HB3	1:A:191:PRO:CD	1.54	1.31
2:H:119:ARG:HA	2:H:122:TYR:CE2	1.66	1.30
2:B:119:ARG:CA	2:B:122:TYR:HE2	1.42	1.29
2:B:119:ARG:HA	2:B:122:TYR:CE2	1.64	1.29
2:H:119:ARG:CA	2:H:122:TYR:HE2	1.44	1.28
1:E:190:ARG:CB	1:E:191:PRO:HD2	1.62	1.27
2:F:119:ARG:CA	2:F:122:TYR:HE2	1.47	1.27
1:E:190:ARG:HB3	1:E:191:PRO:CD	1.63	1.26
1:G:190:ARG:HB3	1:G:191:PRO:CD	1.64	1.26
1:C:190:ARG:HB3	1:C:191:PRO:CD	1.63	1.26
2:D:119:ARG:HA	2:D:122:TYR:CE2	1.69	1.26
2:D:119:ARG:CA	2:D:122:TYR:HE2	1.46	1.25
1:G:190:ARG:CB	1:G:191:PRO:HD2	1.64	1.23
2:F:119:ARG:HA	2:F:122:TYR:CE2	1.72	1.22
1:C:190:ARG:CB	1:C:191:PRO:HD2	1.64	1.21
2:D:122:TYR:N	2:D:122:TYR:HD1	1.37	1.19
2:B:122:TYR:N	2:B:122:TYR:HD1	1.36	1.16
2:B:308:HIS:CE1	1:C:441:THR:HG22	1.82	1.14
1:A:29:LYS:NZ	1:A:29:LYS:H	1.44	1.13
1:A:441:THR:HG22	2:D:308:HIS:CE1	1.84	1.13
1:E:441:THR:HG22	2:H:308:HIS:CE1	1.84	1.13
2:B:173:ASN:HB2	2:B:240:THR:HG22	1.30	1.12
2:F:122:TYR:N	2:F:122:TYR:HD1	1.34	1.11
1:E:29:LYS:NZ	1:E:29:LYS:H	1.46	1.11
2:F:308:HIS:HE1	1:G:441:THR:HG22	1.08	1.11
2:H:173:ASN:HB2	2:H:240:THR:HG22	1.32	1.11
1:A:419:GLN:HA	1:A:419:GLN:HE21	0.96	1.10
1:C:29:LYS:NZ	1:C:29:LYS:H	1.47	1.10
2:H:242:VAL:HB	2:H:264:ARG:HB3	1.33	1.10
2:F:173:ASN:HB2	2:F:240:THR:HG22	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:THR:HG22	2:H:308:HIS:HE1	0.92	1.08
2:D:119:ARG:CA	2:D:122:TYR:CE2	2.32	1.08
2:B:118:PHE:O	2:B:119:ARG:HD2	1.52	1.08
2:D:173:ASN:HB2	2:D:240:THR:HG22	1.34	1.08
2:F:122:TYR:N	2:F:122:TYR:CD1	2.10	1.08
1:G:419:GLN:HE21	1:G:419:GLN:HA	0.97	1.07
2:H:122:TYR:N	2:H:122:TYR:HD1	1.38	1.07
2:B:122:TYR:N	2:B:122:TYR:CD1	2.13	1.07
1:A:419:GLN:HA	1:A:419:GLN:NE2	1.66	1.07
2:H:68:ASP:HB3	2:H:70:VAL:HG22	1.35	1.06
1:E:419:GLN:HA	1:E:419:GLN:NE2	1.69	1.06
1:E:419:GLN:HA	1:E:419:GLN:HE21	0.97	1.06
2:H:122:TYR:N	2:H:122:TYR:CD1	2.15	1.06
2:D:242:VAL:HB	2:D:264:ARG:HB3	1.34	1.05
2:H:119:ARG:CA	2:H:122:TYR:CE2	2.29	1.05
2:D:122:TYR:N	2:D:122:TYR:CD1	2.15	1.05
1:A:441:THR:HG22	2:D:308:HIS:HE1	0.92	1.04
2:F:107:GLN:N	2:F:107:GLN:HE21	1.54	1.04
2:F:118:PHE:O	2:F:119:ARG:HD2	1.56	1.04
1:G:29:LYS:H	1:G:29:LYS:NZ	1.53	1.04
2:F:68:ASP:HB3	2:F:70:VAL:HG22	1.35	1.04
1:C:419:GLN:HA	1:C:419:GLN:HE21	0.90	1.04
2:D:118:PHE:O	2:D:119:ARG:HD2	1.56	1.04
1:A:57:HIS:HD2	1:A:86:THR:HG21	1.19	1.03
1:C:419:GLN:HA	1:C:419:GLN:NE2	1.65	1.03
2:F:119:ARG:CA	2:F:122:TYR:CE2	2.33	1.03
1:A:322:LEU:HD21	1:A:439:CYS:SG	1.99	1.03
2:F:242:VAL:HB	2:F:264:ARG:HB3	1.40	1.03
2:H:208:SER:HA	2:H:223:THR:O	1.59	1.03
2:B:119:ARG:CA	2:B:122:TYR:CE2	2.28	1.02
1:E:206:ILE:HG13	1:E:419:GLN:HB3	1.39	1.02
1:E:57:HIS:CD2	1:E:86:THR:HG21	1.95	1.02
2:B:242:VAL:HB	2:B:264:ARG:HB3	1.38	1.02
2:B:308:HIS:HE1	1:C:441:THR:HG22	0.92	1.02
2:H:118:PHE:O	2:H:119:ARG:HD2	1.60	1.02
2:B:107:GLN:N	2:B:107:GLN:HE21	1.57	1.01
2:D:208:SER:HA	2:D:223:THR:O	1.61	1.00
2:B:68:ASP:HB3	2:B:70:VAL:HG22	1.40	1.00
1:A:57:HIS:CD2	1:A:86:THR:HG21	1.96	1.00
1:G:419:GLN:HA	1:G:419:GLN:NE2	1.69	1.00
2:H:34:SER:H	2:H:221:LEU:HD22	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:HIS:CD2	1:G:86:THR:HG21	1.98	0.99
1:G:57:HIS:HD2	1:G:86:THR:HG21	1.21	0.99
2:B:301:GLN:HE21	1:C:450:VAL:HG12	1.20	0.99
2:F:208:SER:HA	2:F:223:THR:O	1.61	0.99
2:B:34:SER:H	2:B:221:LEU:HD22	1.28	0.99
1:A:172:LEU:HD12	1:A:173:LYS:N	1.76	0.99
2:D:107:GLN:HE21	2:D:107:GLN:N	1.59	0.99
2:D:16:LEU:H	2:D:363:ASP:HB3	1.27	0.98
1:G:172:LEU:HD12	1:G:173:LYS:N	1.76	0.98
1:E:172:LEU:HD12	1:E:173:LYS:N	1.78	0.98
2:D:68:ASP:HB3	2:D:70:VAL:HG22	1.42	0.98
2:F:119:ARG:HA	2:F:122:TYR:HE2	0.83	0.97
1:G:319:ARG:O	1:G:323:GLU:HB2	1.64	0.97
2:H:107:GLN:N	2:H:107:GLN:HE21	1.62	0.97
2:D:34:SER:H	2:D:221:LEU:HD22	1.27	0.97
1:E:450:VAL:HG12	2:H:301:GLN:HE21	1.27	0.97
1:E:176:ILE:O	1:E:178:THR:N	1.98	0.97
1:A:174:TYR:CE2	1:A:238:GLN:HG2	2.00	0.96
2:D:119:ARG:HA	2:D:122:TYR:HE2	0.79	0.96
1:G:206:ILE:HG13	1:G:419:GLN:HB3	1.45	0.96
2:F:308:HIS:CE1	1:G:441:THR:HG22	2.00	0.96
2:F:34:SER:H	2:F:221:LEU:HD22	1.31	0.96
1:C:57:HIS:CD2	1:C:86:THR:HG21	2.00	0.96
1:E:57:HIS:HD2	1:E:86:THR:HG21	1.23	0.96
2:B:16:LEU:H	2:B:363:ASP:HB3	1.31	0.96
1:C:57:HIS:HD2	1:C:86:THR:HG21	1.31	0.96
1:C:174:TYR:CE2	1:C:238:GLN:HG2	2.01	0.95
1:A:450:VAL:HG12	2:D:301:GLN:HE21	1.27	0.95
1:C:206:ILE:HG13	1:C:419:GLN:HB3	1.47	0.95
1:A:206:ILE:HG13	1:A:419:GLN:HB3	1.47	0.95
2:B:20:GLN:HG3	2:B:145:GLY:HA2	1.46	0.95
1:E:201:ILE:HG23	1:E:228:LEU:HD23	1.48	0.95
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.31	0.95
1:E:108:GLN:HE22	2:F:11:LEU:H	1.07	0.95
2:F:100:THR:HG22	2:F:135:THR:H	1.32	0.95
2:D:39:HIS:CD2	2:D:65:THR:HG21	2.01	0.94
1:E:154:ALA:HB3	1:E:157:TYR:HE1	1.32	0.94
1:A:29:LYS:H	1:A:29:LYS:HZ2	1.12	0.94
1:E:319:ARG:O	1:E:323:GLU:HB2	1.66	0.94
1:C:367:ARG:HH11	1:C:367:ARG:HG2	1.31	0.94
2:H:118:PHE:CA	2:H:122:TYR:OH	2.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:O	1:A:323:GLU:HB2	1.66	0.94
2:F:20:GLN:HG3	2:F:145:GLY:HA2	1.47	0.94
1:A:176:ILE:O	1:A:178:THR:N	2.00	0.94
2:H:32:ALA:HA	2:H:224:GLY:HA3	1.49	0.94
1:E:193:ILE:H	1:E:193:ILE:HD12	1.29	0.94
2:F:32:ALA:HA	2:F:224:GLY:HA3	1.50	0.94
1:C:29:LYS:H	1:C:29:LYS:HZ1	1.13	0.93
1:G:174:TYR:CE2	1:G:238:GLN:HG2	2.03	0.93
2:H:119:ARG:HA	2:H:122:TYR:HE2	0.77	0.93
1:C:319:ARG:O	1:C:323:GLU:HB2	1.68	0.93
2:D:158:VAL:HG11	2:D:232:ALA:O	1.69	0.93
1:C:419:GLN:HE21	1:C:419:GLN:CA	1.80	0.93
1:G:176:ILE:O	1:G:178:THR:N	2.02	0.93
2:B:208:SER:HA	2:B:223:THR:O	1.69	0.93
1:C:172:LEU:HD12	1:C:173:LYS:N	1.84	0.93
1:C:322:LEU:HD21	1:C:439:CYS:SG	2.08	0.92
1:G:201:ILE:HG23	1:G:228:LEU:HD23	1.51	0.92
1:E:322:LEU:HD21	1:E:439:CYS:SG	2.09	0.92
1:C:37:CYS:SG	2:D:43:GLY:HA3	2.09	0.92
1:G:37:CYS:CB	1:G:155:GLY:HA2	1.99	0.92
1:G:367:ARG:HG2	1:G:367:ARG:HH11	1.31	0.92
1:C:37:CYS:HB3	1:C:155:GLY:CA	2.00	0.92
1:G:322:LEU:HD21	1:G:439:CYS:SG	2.09	0.92
1:E:29:LYS:H	1:E:29:LYS:HZ1	1.13	0.92
1:E:174:TYR:CE2	1:E:238:GLN:HG2	2.05	0.92
1:G:209:GLU:OE1	1:G:426:ALA:HB2	1.70	0.92
1:A:419:GLN:HE21	1:A:419:GLN:CA	1.83	0.92
2:F:39:HIS:CD2	2:F:65:THR:HG21	2.05	0.92
2:F:158:VAL:HG11	2:F:232:ALA:O	1.70	0.92
2:H:118:PHE:HA	2:H:122:TYR:CZ	2.05	0.92
2:D:351:LEU:C	2:D:353:ASP:H	1.74	0.92
1:A:206:ILE:HB	1:A:419:GLN:C	1.90	0.91
2:H:100:THR:HG22	2:H:135:THR:H	1.35	0.91
2:D:100:THR:HG22	2:D:135:THR:H	1.34	0.91
2:F:16:LEU:H	2:F:363:ASP:HB3	1.34	0.91
2:H:118:PHE:C	2:H:122:TYR:CE2	2.44	0.91
1:G:37:CYS:HB3	1:G:155:GLY:CA	2.01	0.91
1:G:206:ILE:HB	1:G:419:GLN:C	1.90	0.91
2:H:16:LEU:H	2:H:363:ASP:HB3	1.33	0.91
2:D:39:HIS:HD2	2:D:65:THR:HG21	1.35	0.91
1:A:209:GLU:OE1	1:A:426:ALA:HB2	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:ALA:HA	2:B:224:GLY:HA3	1.53	0.90
1:E:37:CYS:HB3	1:E:155:GLY:CA	2.00	0.90
2:H:158:VAL:HG11	2:H:232:ALA:O	1.71	0.90
2:H:217:ARG:HD3	2:H:219:ASN:H	1.36	0.90
1:C:199:ASN:HD21	1:C:225:LEU:HB2	1.36	0.90
1:E:206:ILE:HB	1:E:419:GLN:C	1.91	0.90
1:E:367:ARG:HG2	1:E:367:ARG:HH11	1.35	0.90
2:B:351:LEU:C	2:B:353:ASP:H	1.74	0.90
1:C:176:ILE:O	1:C:178:THR:N	2.04	0.90
2:B:119:ARG:HA	2:B:122:TYR:HE2	0.74	0.90
1:C:193:ILE:H	1:C:193:ILE:HD12	1.35	0.90
2:D:120:THR:N	2:D:122:TYR:CZ	2.40	0.90
2:H:20:GLN:HG3	2:H:145:GLY:HA2	1.52	0.90
2:B:118:PHE:CA	2:B:122:TYR:OH	2.19	0.90
1:C:154:ALA:HB3	1:C:157:TYR:HE1	1.35	0.90
2:F:118:PHE:O	2:F:119:ARG:CD	2.20	0.90
1:A:29:LYS:HB3	1:A:30:PRO:HD2	1.53	0.89
2:B:158:VAL:HG11	2:B:232:ALA:O	1.73	0.89
2:B:120:THR:N	2:B:122:TYR:CZ	2.41	0.89
1:C:206:ILE:HB	1:C:419:GLN:C	1.93	0.89
2:H:39:HIS:CD2	2:H:65:THR:HG21	2.08	0.89
2:F:118:PHE:CA	2:F:122:TYR:OH	2.22	0.88
1:A:37:CYS:HB3	1:A:155:GLY:CA	2.03	0.88
2:F:351:LEU:C	2:F:353:ASP:H	1.75	0.88
1:E:37:CYS:CB	1:E:155:GLY:HA2	2.03	0.88
2:B:39:HIS:CD2	2:B:65:THR:HG21	2.08	0.88
1:E:199:ASN:HD21	1:E:225:LEU:HB2	1.38	0.88
2:D:217:ARG:HD3	2:D:219:ASN:H	1.37	0.88
1:A:191:PRO:HB3	1:E:314:ALA:HB2	1.53	0.88
1:A:174:TYR:OH	1:A:234:TYR:O	1.91	0.88
2:H:351:LEU:C	2:H:353:ASP:H	1.75	0.88
1:E:419:GLN:HE21	1:E:419:GLN:CA	1.86	0.87
2:F:212:HIS:HB3	2:F:223:THR:CG2	2.05	0.87
2:H:17:LYS:HG3	2:H:345:PRO:HB2	1.54	0.87
2:B:85:LYS:HD2	2:B:118:PHE:CE1	2.10	0.87
2:B:118:PHE:C	2:B:122:TYR:CE2	2.47	0.87
1:G:29:LYS:H	1:G:29:LYS:HZ1	1.13	0.87
1:G:108:GLN:HE22	2:H:11:LEU:H	1.19	0.87
1:A:199:ASN:HD21	1:A:225:LEU:HB2	1.37	0.87
2:B:118:PHE:O	2:B:119:ARG:CD	2.22	0.87
2:F:118:PHE:HA	2:F:122:TYR:CZ	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:GLN:HG3	2:D:145:GLY:HA2	1.56	0.87
1:E:37:CYS:HB3	1:E:155:GLY:HA2	1.54	0.87
2:F:122:TYR:HD1	2:F:122:TYR:H	1.21	0.87
2:B:118:PHE:HA	2:B:122:TYR:CZ	2.10	0.87
2:B:382:ASN:HD21	2:B:384:HIS:HB2	1.37	0.87
2:D:118:PHE:C	2:D:122:TYR:CE2	2.48	0.87
2:F:120:THR:N	2:F:122:TYR:CZ	2.43	0.86
1:E:206:ILE:HG13	1:E:419:GLN:CB	2.05	0.86
1:A:307:GLU:O	1:A:311:VAL:HG23	1.75	0.86
2:D:118:PHE:HA	2:D:122:TYR:CZ	2.10	0.86
1:A:201:ILE:HG23	1:A:228:LEU:HD23	1.57	0.86
2:D:32:ALA:HA	2:D:224:GLY:HA3	1.56	0.86
2:D:118:PHE:CA	2:D:122:TYR:OH	2.22	0.86
1:G:193:ILE:H	1:G:193:ILE:HD12	1.39	0.86
2:H:118:PHE:C	2:H:122:TYR:CZ	2.48	0.86
1:A:29:LYS:H	1:A:29:LYS:HZ1	1.24	0.86
2:B:308:HIS:HE1	1:C:441:THR:CG2	1.86	0.86
1:E:307:GLU:O	1:E:311:VAL:HG23	1.76	0.86
2:F:17:LYS:HG3	2:F:345:PRO:HB2	1.57	0.86
2:H:118:PHE:O	2:H:119:ARG:CD	2.22	0.86
2:F:217:ARG:HD3	2:F:219:ASN:H	1.39	0.86
1:C:177:GLY:HA3	1:C:241:HIS:NE2	1.90	0.85
2:H:213:LEU:HD23	2:H:214:ASP:H	1.41	0.85
2:B:118:PHE:C	2:B:122:TYR:CZ	2.50	0.85
2:D:118:PHE:O	2:D:119:ARG:CD	2.22	0.85
1:E:29:LYS:HB3	1:E:30:PRO:HD2	1.58	0.85
1:G:209:GLU:OE1	1:G:419:GLN:OE1	1.94	0.85
2:B:242:VAL:HB	2:B:264:ARG:CB	2.07	0.85
1:E:209:GLU:OE1	1:E:419:GLN:OE1	1.93	0.85
2:F:118:PHE:C	2:F:122:TYR:CE2	2.50	0.85
2:D:382:ASN:HD21	2:D:384:HIS:HB2	1.40	0.85
2:F:39:HIS:HD2	2:F:65:THR:HG21	1.39	0.85
1:G:29:LYS:HB3	1:G:30:PRO:HD2	1.59	0.85
2:D:17:LYS:HG3	2:D:345:PRO:HB2	1.57	0.85
2:H:264:ARG:O	2:H:265:PHE:HB2	1.74	0.85
1:C:209:GLU:OE1	1:C:426:ALA:HB2	1.76	0.85
1:C:30:PRO:HA	2:D:63:GLN:OE1	1.77	0.85
1:A:154:ALA:HB3	1:A:157:TYR:HE1	1.39	0.85
2:H:351:LEU:O	2:H:352:VAL:HG12	1.77	0.85
1:C:307:GLU:HG2	1:C:428:TYR:CD2	2.12	0.84
2:H:382:ASN:HD21	2:H:384:HIS:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:VAL:HB	2:D:264:ARG:CB	2.07	0.84
2:B:163:ASP:O	2:B:165:VAL:N	2.11	0.84
1:A:307:GLU:HG2	1:A:428:TYR:CD2	2.12	0.84
1:C:201:ILE:HG23	1:C:228:LEU:HD23	1.57	0.84
1:A:193:ILE:HD12	1:A:193:ILE:H	1.43	0.84
1:E:307:GLU:HG2	1:E:428:TYR:CD2	2.12	0.84
1:A:30:PRO:HA	2:B:63:GLN:OE1	1.76	0.84
1:C:411:ARG:HH22	2:D:214:ASP:HA	1.43	0.84
1:G:154:ALA:HB3	1:G:157:TYR:HE1	1.43	0.84
1:A:209:GLU:OE1	1:A:426:ALA:CB	2.26	0.83
1:E:29:LYS:H	1:E:29:LYS:HZ2	1.26	0.83
1:E:37:CYS:SG	2:F:43:GLY:HA3	2.18	0.83
1:G:419:GLN:HE21	1:G:419:GLN:CA	1.88	0.83
1:A:37:CYS:CB	1:A:155:GLY:HA2	2.08	0.83
1:C:386:LEU:HD21	2:D:216:ASN:HB3	1.59	0.83
2:H:242:VAL:HB	2:H:264:ARG:CB	2.08	0.83
2:D:85:LYS:HD2	2:D:118:PHE:CE1	2.13	0.83
2:B:39:HIS:HD2	2:B:65:THR:HG21	1.41	0.83
2:B:100:THR:HG22	2:B:135:THR:H	1.42	0.83
2:F:301:GLN:HE21	1:G:450:VAL:HG12	1.44	0.83
2:B:201:LEU:O	2:B:226:LEU:HD21	1.79	0.83
2:D:264:ARG:O	2:D:265:PHE:HB2	1.76	0.83
1:E:30:PRO:HA	2:F:63:GLN:OE1	1.78	0.83
2:F:351:LEU:O	2:F:352:VAL:HG12	1.78	0.83
2:D:85:LYS:HD2	2:D:118:PHE:HE1	1.44	0.83
1:E:154:ALA:HB3	1:E:157:TYR:CE1	2.14	0.83
2:B:122:TYR:HD1	2:B:122:TYR:H	1.25	0.83
1:C:361:GLU:HG3	4:C:502:CZL:S3B	2.19	0.82
1:G:307:GLU:HG2	1:G:428:TYR:CD2	2.13	0.82
2:B:217:ARG:HD3	2:B:219:ASN:H	1.43	0.82
1:G:199:ASN:HD21	1:G:225:LEU:HB2	1.41	0.82
1:C:307:GLU:O	1:C:311:VAL:HG23	1.78	0.82
1:E:209:GLU:OE1	1:E:426:ALA:HB2	1.78	0.82
2:B:264:ARG:O	2:B:265:PHE:HB2	1.75	0.82
1:C:37:CYS:HB3	1:C:155:GLY:HA2	1.62	0.82
1:G:177:GLY:HA3	1:G:241:HIS:NE2	1.95	0.82
2:H:85:LYS:HD2	2:H:118:PHE:CE1	2.13	0.82
2:D:126:LYS:NZ	2:D:127:ASP:H	1.78	0.82
1:A:206:ILE:HB	1:A:419:GLN:O	1.80	0.82
1:E:123:THR:HG22	3:E:501:SF4:S4	2.19	0.82
2:H:122:TYR:HD1	2:H:122:TYR:H	1.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:ASP:O	1:G:366:ILE:HG13	1.80	0.82
2:B:85:LYS:HD2	2:B:118:PHE:HE1	1.44	0.82
2:H:39:HIS:HD2	2:H:65:THR:HG21	1.43	0.82
1:A:206:ILE:HG13	1:A:419:GLN:CB	2.09	0.81
2:F:85:LYS:HD2	2:F:118:PHE:CE1	2.15	0.81
2:H:119:ARG:N	2:H:122:TYR:CE2	2.47	0.81
1:A:209:GLU:OE1	1:A:419:GLN:OE1	1.99	0.81
2:D:118:PHE:C	2:D:122:TYR:CZ	2.53	0.81
1:C:206:ILE:HG13	1:C:419:GLN:CB	2.10	0.81
2:F:159:PRO:HG3	2:F:257:ARG:HH11	1.46	0.81
2:F:212:HIS:HB3	2:F:223:THR:HG22	1.59	0.81
2:H:120:THR:N	2:H:122:TYR:CZ	2.47	0.81
2:D:381:GLY:O	2:D:398:ARG:HA	1.78	0.81
1:C:29:LYS:H	1:C:29:LYS:HZ2	1.28	0.81
1:A:66:SER:O	1:A:69:ASN:ND2	2.14	0.81
2:F:118:PHE:C	2:F:122:TYR:CZ	2.54	0.81
1:G:206:ILE:HG13	1:G:419:GLN:CB	2.10	0.81
2:D:159:PRO:HG3	2:D:257:ARG:HH11	1.46	0.81
1:G:72:THR:HG23	1:G:204:TYR:O	1.79	0.81
2:H:163:ASP:O	2:H:165:VAL:N	2.14	0.81
2:F:264:ARG:O	2:F:265:PHE:HB2	1.79	0.81
2:H:397:LEU:HD23	2:H:427:LEU:HD21	1.62	0.81
1:E:174:TYR:CE2	1:E:234:TYR:CZ	2.69	0.80
2:B:126:LYS:NZ	2:B:127:ASP:H	1.79	0.80
1:C:209:GLU:OE1	1:C:419:GLN:OE1	1.98	0.80
1:E:29:LYS:HZ1	1:E:29:LYS:N	1.79	0.80
1:E:91:ASN:O	1:E:94:ILE:HG13	1.81	0.80
2:F:242:VAL:HB	2:F:264:ARG:CB	2.10	0.80
2:H:212:HIS:HB3	2:H:223:THR:CG2	2.11	0.80
1:C:37:CYS:CB	1:C:155:GLY:HA2	2.10	0.80
1:G:367:ARG:HG2	1:G:367:ARG:NH1	1.93	0.80
2:B:213:LEU:HD23	2:B:214:ASP:H	1.44	0.80
1:G:209:GLU:OE1	1:G:426:ALA:CB	2.29	0.80
2:D:133:VAL:HG12	2:D:135:THR:HG23	1.63	0.80
2:H:315:ARG:CG	2:H:340:VAL:HG21	2.11	0.80
1:G:57:HIS:HA	1:G:86:THR:CG2	2.12	0.80
2:D:163:ASP:O	2:D:165:VAL:N	2.14	0.80
1:G:26:ALA:O	1:G:27:LYS:HB3	1.80	0.80
1:C:29:LYS:HB3	1:C:30:PRO:HD2	1.61	0.80
1:E:29:LYS:NZ	1:E:29:LYS:N	2.30	0.79
1:C:154:ALA:HB3	1:C:157:TYR:CE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:LEU:HD23	2:D:214:ASP:H	1.46	0.79
1:E:206:ILE:HB	1:E:419:GLN:O	1.80	0.79
2:D:201:LEU:O	2:D:226:LEU:HD21	1.81	0.79
1:E:177:GLY:HA3	1:E:241:HIS:NE2	1.97	0.79
1:C:91:ASN:O	1:C:94:ILE:HG13	1.82	0.79
2:D:120:THR:N	2:D:122:TYR:CE2	2.50	0.79
2:H:168:ARG:HE	2:H:169:PRO:HD3	1.45	0.79
2:B:212:HIS:HB3	2:B:223:THR:CG2	2.13	0.79
1:C:383:ARG:CA	2:D:217:ARG:HH12	1.96	0.79
2:H:159:PRO:CG	2:H:257:ARG:HH11	1.94	0.79
2:B:258:THR:OG1	2:B:260:VAL:HG23	1.82	0.79
2:F:85:LYS:HD2	2:F:118:PHE:HE1	1.46	0.79
2:F:159:PRO:CG	2:F:257:ARG:HH11	1.94	0.79
1:G:37:CYS:HB3	1:G:155:GLY:HA2	1.61	0.79
1:G:206:ILE:HB	1:G:419:GLN:O	1.83	0.79
2:B:120:THR:N	2:B:122:TYR:CE2	2.51	0.79
2:F:163:ASP:O	2:F:165:VAL:N	2.15	0.79
1:C:27:LYS:HD3	2:D:66:ALA:HB1	1.65	0.79
1:C:409:LYS:HB3	2:D:218:PHE:CZ	2.18	0.79
2:D:42:GLN:HA	2:D:64:THR:HG21	1.62	0.79
2:H:85:LYS:HD2	2:H:118:PHE:HE1	1.48	0.79
2:B:221:LEU:O	2:B:223:THR:N	2.16	0.79
1:C:29:LYS:HZ1	1:C:29:LYS:N	1.81	0.79
2:F:42:GLN:HA	2:F:64:THR:HG21	1.65	0.79
2:H:118:PHE:CA	2:H:122:TYR:CZ	2.65	0.79
1:C:206:ILE:HB	1:C:419:GLN:O	1.83	0.79
2:F:213:LEU:HD23	2:F:214:ASP:H	1.48	0.79
1:E:193:ILE:HD12	1:E:193:ILE:N	1.97	0.78
2:F:118:PHE:HA	2:F:122:TYR:OH	1.83	0.78
2:H:126:LYS:NZ	2:H:127:ASP:H	1.80	0.78
2:B:17:LYS:HG3	2:B:345:PRO:HB2	1.64	0.78
2:B:159:PRO:HG3	2:B:257:ARG:HH11	1.47	0.78
2:B:351:LEU:O	2:B:352:VAL:HG12	1.82	0.78
1:G:29:LYS:HZ1	1:G:29:LYS:N	1.81	0.78
1:A:29:LYS:NZ	1:A:29:LYS:N	2.27	0.78
1:A:174:TYR:CE2	1:A:234:TYR:CZ	2.71	0.78
1:A:252:LYS:HB2	1:A:361:GLU:OE2	1.82	0.78
2:F:119:ARG:N	2:F:122:TYR:CE2	2.51	0.78
2:B:119:ARG:N	2:B:122:TYR:CE2	2.50	0.78
2:F:315:ARG:CG	2:F:340:VAL:HG21	2.13	0.78
1:G:177:GLY:CA	1:G:241:HIS:CE1	2.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:CYS:HB2	1:G:155:GLY:HA2	1.63	0.78
2:H:118:PHE:HA	2:H:122:TYR:OH	1.80	0.78
1:E:66:SER:O	1:E:69:ASN:ND2	2.16	0.78
2:F:133:VAL:HG12	2:F:135:THR:HG23	1.66	0.78
2:F:201:LEU:O	2:F:226:LEU:HD21	1.84	0.78
2:F:382:ASN:HD21	2:F:384:HIS:HB2	1.49	0.78
1:A:27:LYS:HD3	2:B:66:ALA:HB1	1.64	0.78
1:A:386:LEU:HD21	2:B:216:ASN:HB3	1.63	0.78
1:C:57:HIS:HA	1:C:86:THR:HG22	1.66	0.78
2:F:126:LYS:NZ	2:F:127:ASP:H	1.82	0.78
1:G:413:PRO:HA	1:G:447:TRP:CZ2	2.19	0.78
1:E:386:LEU:HD21	2:F:216:ASN:HB3	1.65	0.78
2:F:240:THR:HG21	2:F:254:LEU:HD11	1.66	0.78
1:A:362:ASP:O	1:A:366:ILE:HG13	1.83	0.77
2:D:168:ARG:HE	2:D:169:PRO:HD3	1.48	0.77
1:E:72:THR:HG23	1:E:204:TYR:O	1.85	0.77
2:H:159:PRO:HG3	2:H:257:ARG:HH11	1.49	0.77
2:H:270:GLY:O	2:H:274:VAL:HG23	1.84	0.77
1:A:91:ASN:O	1:A:94:ILE:HG13	1.84	0.77
2:B:64:THR:HG22	2:B:66:ALA:H	1.50	0.77
2:B:326:LEU:HD11	2:B:350:ALA:HB1	1.66	0.77
1:C:177:GLY:CA	1:C:241:HIS:CE1	2.67	0.77
2:D:351:LEU:O	2:D:352:VAL:HG12	1.84	0.77
2:H:133:VAL:HG12	2:H:135:THR:HG23	1.66	0.77
1:A:26:ALA:O	1:A:27:LYS:HB3	1.85	0.77
2:D:122:TYR:HD1	2:D:122:TYR:H	1.28	0.77
1:E:361:GLU:HG3	4:E:502:CZL:S3B	2.25	0.77
2:B:168:ARG:HE	2:B:169:PRO:HD3	1.49	0.77
1:C:174:TYR:OH	1:C:234:TYR:O	2.02	0.77
2:B:119:ARG:N	2:B:122:TYR:OH	2.16	0.77
2:D:119:ARG:N	2:D:122:TYR:CE2	2.52	0.77
1:E:362:ASP:O	1:E:366:ILE:HG13	1.85	0.77
2:F:39:HIS:HA	2:F:65:THR:OG1	1.84	0.77
2:H:64:THR:HG22	2:H:66:ALA:H	1.48	0.77
1:E:94:ILE:HD12	1:E:94:ILE:O	1.85	0.77
1:A:27:LYS:HD3	2:B:66:ALA:CB	2.15	0.77
1:C:26:ALA:O	1:C:27:LYS:HB3	1.85	0.77
1:E:26:ALA:O	1:E:27:LYS:HB3	1.82	0.77
1:A:206:ILE:C	1:A:419:GLN:O	2.24	0.76
2:F:120:THR:N	2:F:122:TYR:CE2	2.52	0.76
2:D:212:HIS:HB3	2:D:223:THR:CG2	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:THR:HG21	2:D:254:LEU:HD11	1.67	0.76
1:A:57:HIS:HA	1:A:86:THR:CG2	2.16	0.76
2:D:118:PHE:HA	2:D:122:TYR:OH	1.85	0.76
2:F:26:LEU:HA	2:F:29:LEU:HB2	1.67	0.76
1:A:72:THR:HG23	1:A:204:TYR:O	1.85	0.76
2:F:64:THR:HG22	2:F:66:ALA:H	1.49	0.76
2:H:173:ASN:CB	2:H:240:THR:HG22	2.14	0.76
2:H:212:HIS:HB3	2:H:223:THR:HG22	1.66	0.76
2:H:381:GLY:O	2:H:398:ARG:HA	1.84	0.76
1:E:206:ILE:CG1	1:E:419:GLN:HB3	2.13	0.76
2:H:119:ARG:N	2:H:122:TYR:OH	2.19	0.76
2:B:118:PHE:CA	2:B:122:TYR:CZ	2.69	0.76
2:B:315:ARG:CG	2:B:340:VAL:HG21	2.15	0.76
1:C:57:HIS:HA	1:C:86:THR:CG2	2.16	0.76
1:A:177:GLY:HA2	1:A:241:HIS:CE1	2.21	0.75
2:B:42:GLN:HA	2:B:64:THR:HG21	1.67	0.75
2:B:159:PRO:CG	2:B:257:ARG:HH11	1.99	0.75
1:G:177:GLY:HA2	1:G:241:HIS:CE1	2.20	0.75
1:A:37:CYS:HB3	1:A:155:GLY:HA2	1.65	0.75
1:A:154:ALA:HB3	1:A:157:TYR:CE1	2.21	0.75
1:A:191:PRO:HG2	1:E:310:LYS:NZ	2.01	0.75
1:C:174:TYR:CE2	1:C:234:TYR:CZ	2.75	0.75
2:F:125:TYR:O	2:F:126:LYS:HB3	1.86	0.75
1:G:91:ASN:O	1:G:94:ILE:HG13	1.86	0.75
1:G:252:LYS:HB2	1:G:361:GLU:OE2	1.85	0.75
2:F:173:ASN:CB	2:F:240:THR:HG22	2.15	0.75
2:B:118:PHE:HA	2:B:122:TYR:OH	1.86	0.75
2:D:159:PRO:CG	2:D:257:ARG:HH11	1.98	0.75
2:D:168:ARG:HG3	2:D:236:GLN:HB2	1.67	0.75
2:H:201:LEU:O	2:H:226:LEU:HD21	1.85	0.75
2:B:212:HIS:HB3	2:B:223:THR:HG22	1.68	0.75
1:C:209:GLU:OE1	1:C:426:ALA:CB	2.34	0.75
1:E:66:SER:HB3	2:F:47:PHE:CE1	2.22	0.75
1:E:381:ASN:HD22	1:E:381:ASN:H	1.34	0.75
2:B:168:ARG:HG3	2:B:236:GLN:HB2	1.67	0.75
2:H:168:ARG:HG3	2:H:236:GLN:HB2	1.67	0.75
2:D:39:HIS:HA	2:D:65:THR:OG1	1.87	0.75
2:D:159:PRO:CB	2:D:257:ARG:HD3	2.17	0.75
1:G:190:ARG:O	1:G:192:GLY:N	2.20	0.75
1:A:191:PRO:CB	1:E:314:ALA:HB2	2.17	0.74
2:D:212:HIS:HB3	2:D:223:THR:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:NE2	2:F:11:LEU:H	1.81	0.74
2:F:168:ARG:HG3	2:F:236:GLN:HB2	1.68	0.74
1:E:57:HIS:HA	1:E:86:THR:CG2	2.17	0.74
1:C:220:LEU:HG	1:C:300:THR:HG22	1.69	0.74
2:F:20:GLN:HG3	2:F:145:GLY:CA	2.17	0.74
2:H:117:GLU:C	2:H:122:TYR:OH	2.25	0.74
2:B:107:GLN:N	2:B:107:GLN:NE2	2.34	0.74
2:B:20:GLN:HG3	2:B:145:GLY:CA	2.17	0.74
2:B:173:ASN:CB	2:B:240:THR:HG22	2.12	0.74
2:B:351:LEU:C	2:B:353:ASP:N	2.40	0.74
2:D:16:LEU:H	2:D:363:ASP:CB	1.98	0.74
2:D:118:PHE:CA	2:D:122:TYR:CZ	2.70	0.74
2:F:168:ARG:HE	2:F:169:PRO:HD3	1.51	0.74
1:A:190:ARG:O	1:A:192:GLY:N	2.19	0.74
1:A:361:GLU:HG3	4:A:502:CZL:S3B	2.27	0.74
1:E:67:TRP:CZ3	2:F:15:PRO:O	2.40	0.74
2:F:121:GLN:N	2:F:122:TYR:CE1	2.56	0.74
2:F:159:PRO:HB2	2:F:257:ARG:HB2	1.67	0.74
2:H:125:TYR:O	2:H:126:LYS:HB3	1.86	0.74
2:D:16:LEU:N	2:D:363:ASP:HB3	2.00	0.74
2:D:382:ASN:ND2	2:D:384:HIS:HB2	2.03	0.74
1:A:383:ARG:CA	2:B:217:ARG:HH12	2.00	0.74
1:C:206:ILE:CG1	1:C:419:GLN:HB3	2.17	0.74
1:E:174:TYR:OH	1:E:234:TYR:O	2.04	0.74
1:G:38:SER:OG	1:G:162:LEU:HD12	1.87	0.74
2:B:159:PRO:HB2	2:B:257:ARG:HB2	1.69	0.74
2:B:363:ASP:OD2	2:B:363:ASP:N	2.20	0.74
1:C:367:ARG:HG2	1:C:367:ARG:NH1	1.94	0.74
1:G:30:PRO:HA	2:H:63:GLN:OE1	1.87	0.74
2:B:302:ASP:CB	2:D:211:GLY:HA3	2.17	0.74
1:E:106:ILE:O	1:E:110:VAL:HG22	1.87	0.73
1:E:417:ILE:HG22	1:E:417:ILE:O	1.87	0.73
2:F:107:GLN:N	2:F:107:GLN:NE2	2.36	0.73
1:G:175:VAL:O	1:G:176:ILE:C	2.26	0.73
2:B:198:ARG:HG3	2:B:198:ARG:O	1.88	0.73
2:D:168:ARG:HB2	2:D:169:PRO:HD3	1.69	0.73
1:G:67:TRP:CZ3	2:H:15:PRO:O	2.41	0.73
2:H:351:LEU:C	2:H:353:ASP:N	2.42	0.73
1:A:57:HIS:HA	1:A:86:THR:HG22	1.70	0.73
1:A:66:SER:HB3	2:B:47:PHE:CE1	2.23	0.73
2:B:119:ARG:C	2:B:122:TYR:CE2	2.61	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:TYR:O	2:B:126:LYS:HB3	1.87	0.73
2:H:297:ARG:HD2	2:H:417:TYR:OH	1.88	0.73
2:B:382:ASN:ND2	2:B:384:HIS:HB2	2.03	0.73
2:D:121:GLN:N	2:D:122:TYR:CE1	2.57	0.73
2:D:125:TYR:O	2:D:126:LYS:HB3	1.87	0.73
1:E:209:GLU:OE1	1:E:426:ALA:CB	2.36	0.73
1:G:62:CYS:SG	1:G:123:THR:HG21	2.28	0.73
1:G:154:ALA:HB3	1:G:157:TYR:CE1	2.24	0.73
1:E:206:ILE:C	1:E:419:GLN:O	2.27	0.73
1:A:367:ARG:HG2	1:A:367:ARG:NH1	1.93	0.73
1:C:67:TRP:CZ3	2:D:15:PRO:O	2.42	0.73
1:C:175:VAL:O	1:C:176:ILE:C	2.26	0.73
1:E:38:SER:OG	1:E:162:LEU:HD12	1.87	0.73
1:E:175:VAL:O	1:E:176:ILE:C	2.23	0.73
1:G:174:TYR:CE2	1:G:234:TYR:CZ	2.76	0.73
2:H:242:VAL:CB	2:H:264:ARG:HB3	2.16	0.73
1:C:193:ILE:HD12	1:C:193:ILE:N	2.03	0.73
1:C:413:PRO:HA	1:C:447:TRP:CZ2	2.23	0.73
1:A:206:ILE:HG13	1:A:419:GLN:CG	2.19	0.73
1:E:177:GLY:CA	1:E:241:HIS:CE1	2.72	0.73
1:A:314:ALA:HB2	1:E:191:PRO:HB3	1.70	0.73
1:C:29:LYS:NZ	1:C:29:LYS:N	2.31	0.73
2:F:119:ARG:N	2:F:122:TYR:OH	2.21	0.73
2:H:149:ALA:O	2:H:153:ILE:HG13	1.88	0.73
2:B:240:THR:HG21	2:B:254:LEU:HD11	1.71	0.72
2:D:107:GLN:N	2:D:107:GLN:NE2	2.36	0.72
1:G:174:TYR:OH	1:G:234:TYR:O	2.06	0.72
1:G:307:GLU:O	1:G:311:VAL:HG23	1.87	0.72
1:G:367:ARG:HH11	1:G:367:ARG:CG	2.02	0.72
2:B:121:GLN:N	2:B:122:TYR:CE1	2.57	0.72
1:C:191:PRO:HB3	1:G:314:ALA:HB2	1.69	0.72
2:D:315:ARG:CG	2:D:340:VAL:HG21	2.18	0.72
1:E:57:HIS:HA	1:E:86:THR:HG22	1.70	0.72
2:F:118:PHE:CA	2:F:122:TYR:CZ	2.71	0.72
2:F:270:GLY:O	2:F:274:VAL:HG23	1.90	0.72
1:G:206:ILE:CG1	1:G:419:GLN:HB3	2.18	0.72
1:A:177:GLY:CA	1:A:241:HIS:CE1	2.72	0.72
1:A:367:ARG:HH11	1:A:367:ARG:CG	2.01	0.72
1:C:108:GLN:HE22	2:D:11:LEU:H	1.37	0.72
1:C:177:GLY:HA2	1:C:241:HIS:CE1	2.24	0.72
1:E:252:LYS:HB2	1:E:361:GLU:OE2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:THR:N	2:H:122:TYR:CE2	2.57	0.72
1:A:436:ARG:O	1:A:440:ILE:HG23	1.88	0.72
1:C:66:SER:O	1:C:69:ASN:ND2	2.21	0.72
1:C:383:ARG:HG2	1:C:384:VAL:H	1.55	0.72
2:D:351:LEU:C	2:D:353:ASP:N	2.40	0.72
2:B:302:ASP:HB2	2:D:211:GLY:HA3	1.70	0.72
1:C:190:ARG:O	1:C:192:GLY:N	2.22	0.72
1:G:301:GLU:O	1:G:304:ILE:HG13	1.90	0.72
2:H:240:THR:HG21	2:H:254:LEU:HD11	1.72	0.72
1:E:382:ALA:HB3	2:F:217:ARG:HG3	1.71	0.72
1:E:441:THR:CG2	2:H:308:HIS:HE1	1.87	0.72
1:G:193:ILE:HD12	1:G:193:ILE:N	2.04	0.72
1:C:382:ALA:HB3	2:D:217:ARG:HG3	1.70	0.72
1:A:174:TYR:HE2	1:A:238:GLN:HG2	1.53	0.72
1:C:66:SER:HB3	2:D:47:PHE:CE1	2.25	0.72
2:F:159:PRO:CB	2:F:257:ARG:HD3	2.19	0.72
2:F:351:LEU:C	2:F:353:ASP:N	2.42	0.72
1:G:29:LYS:H	1:G:29:LYS:HZ2	1.37	0.72
1:A:383:ARG:HA	2:B:217:ARG:HH12	1.55	0.72
2:B:218:PHE:CD2	2:B:218:PHE:N	2.58	0.72
1:C:362:ASP:O	1:C:366:ILE:HG13	1.90	0.72
2:D:119:ARG:N	2:D:122:TYR:OH	2.23	0.72
2:H:168:ARG:HB2	2:H:169:PRO:HD3	1.71	0.72
1:G:27:LYS:HD3	2:H:66:ALA:HB1	1.71	0.71
1:A:177:GLY:HA3	1:A:241:HIS:NE2	2.05	0.71
1:C:94:ILE:HD12	1:C:94:ILE:O	1.90	0.71
1:E:367:ARG:HG2	1:E:367:ARG:NH1	1.97	0.71
2:H:119:ARG:N	2:H:122:TYR:CZ	2.59	0.71
2:B:26:LEU:HA	2:B:29:LEU:HB2	1.72	0.71
2:B:344:VAL:HG22	2:B:345:PRO:HD2	1.71	0.71
2:D:39:HIS:HD2	2:D:65:THR:CG2	2.01	0.71
1:A:108:GLN:HE22	2:B:11:LEU:H	1.37	0.71
1:C:27:LYS:HD3	2:D:66:ALA:CB	2.19	0.71
2:D:397:LEU:HD23	2:D:427:LEU:HD21	1.71	0.71
1:E:397:LEU:HD22	1:E:398:ILE:N	2.06	0.71
1:G:381:ASN:HD22	1:G:381:ASN:H	1.38	0.71
2:H:159:PRO:CB	2:H:257:ARG:HD3	2.20	0.71
1:A:409:LYS:HB3	2:B:218:PHE:CZ	2.25	0.71
2:B:67:MET:CE	2:B:71:SER:HB2	2.20	0.71
2:D:64:THR:HG22	2:D:66:ALA:H	1.55	0.71
2:D:117:GLU:C	2:D:122:TYR:OH	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:363:ASP:N	2:D:363:ASP:OD2	2.22	0.71
2:F:397:LEU:HD23	2:F:427:LEU:HD21	1.70	0.71
1:A:175:VAL:O	1:A:176:ILE:C	2.29	0.71
2:B:133:VAL:HG12	2:B:135:THR:HG23	1.72	0.71
2:B:117:GLU:C	2:B:122:TYR:OH	2.29	0.71
2:B:159:PRO:CB	2:B:257:ARG:HD3	2.21	0.71
2:B:381:GLY:O	2:B:398:ARG:HA	1.90	0.71
2:D:218:PHE:CD2	2:D:218:PHE:N	2.58	0.71
2:F:159:PRO:HB3	2:F:257:ARG:HD3	1.72	0.71
2:H:221:LEU:O	2:H:223:THR:N	2.23	0.71
2:H:344:VAL:HG22	2:H:345:PRO:HD2	1.70	0.71
1:A:383:ARG:HG2	1:A:384:VAL:H	1.56	0.71
1:A:62:CYS:SG	1:A:123:THR:HG21	2.30	0.70
2:D:217:ARG:C	2:D:218:PHE:HD2	1.94	0.70
2:H:16:LEU:H	2:H:363:ASP:CB	2.03	0.70
2:D:159:PRO:HB2	2:D:257:ARG:HB2	1.73	0.70
1:E:193:ILE:H	1:E:193:ILE:CD1	2.02	0.70
1:E:262:GLN:HG3	1:E:263:GLU:N	2.05	0.70
2:H:121:GLN:N	2:H:122:TYR:CE1	2.59	0.70
1:A:301:GLU:O	1:A:304:ILE:HG13	1.91	0.70
2:D:20:GLN:HG2	2:D:135:THR:HB	1.73	0.70
2:D:221:LEU:O	2:D:223:THR:N	2.24	0.70
1:E:108:GLN:CD	2:F:11:LEU:HB3	2.11	0.70
1:E:220:LEU:HG	1:E:300:THR:HG22	1.72	0.70
2:F:221:LEU:O	2:F:223:THR:N	2.24	0.70
2:H:382:ASN:ND2	2:H:384:HIS:HB2	2.05	0.70
1:C:174:TYR:HE2	1:C:238:GLN:HG2	1.51	0.70
1:E:108:GLN:NE2	2:F:11:LEU:HB3	2.06	0.70
1:A:383:ARG:H	2:B:217:ARG:HH22	1.39	0.70
2:D:220:ALA:O	2:D:221:LEU:HB3	1.89	0.70
1:E:67:TRP:CH2	2:F:15:PRO:O	2.44	0.70
2:F:16:LEU:H	2:F:363:ASP:CB	2.04	0.70
1:G:332:GLY:H	1:G:334:VAL:HG22	1.56	0.70
2:H:198:ARG:O	2:H:198:ARG:HG3	1.91	0.70
1:C:397:LEU:HD22	1:C:398:ILE:N	2.06	0.70
1:E:367:ARG:HH11	1:E:367:ARG:CG	2.04	0.70
2:F:363:ASP:OD2	2:F:363:ASP:N	2.24	0.70
2:F:381:GLY:O	2:F:398:ARG:HA	1.91	0.70
2:D:173:ASN:CB	2:D:240:THR:HG22	2.16	0.70
2:H:20:GLN:HG3	2:H:145:GLY:CA	2.21	0.70
1:C:191:PRO:CB	1:G:314:ALA:HB2	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ALA:HB2	1:G:191:PRO:HB3	1.73	0.69
1:G:410:GLY:O	1:G:412:VAL:HG23	1.91	0.69
2:B:119:ARG:N	2:B:122:TYR:CZ	2.61	0.69
1:C:206:ILE:HG13	1:C:419:GLN:CG	2.21	0.69
2:D:119:ARG:C	2:D:122:TYR:CE2	2.65	0.69
1:E:329:LEU:HD13	1:E:340:VAL:HG22	1.74	0.69
2:H:218:PHE:N	2:H:218:PHE:CD2	2.56	0.69
2:H:379:VAL:O	2:H:396:LEU:HD23	1.92	0.69
1:C:383:ARG:HA	2:D:217:ARG:HH12	1.58	0.69
2:D:242:VAL:CB	2:D:264:ARG:HB3	2.17	0.69
2:F:168:ARG:HH21	2:F:169:PRO:HG3	1.56	0.69
1:G:197:ASP:OD2	1:G:223:ARG:HD3	1.92	0.69
1:G:383:ARG:HG2	1:G:384:VAL:H	1.56	0.69
1:E:413:PRO:HA	1:E:447:TRP:CZ2	2.27	0.69
1:A:106:ILE:O	1:A:110:VAL:HG22	1.92	0.69
2:F:39:HIS:HD2	2:F:65:THR:CG2	2.04	0.69
2:B:16:LEU:H	2:B:363:ASP:CB	2.03	0.69
1:C:367:ARG:HH11	1:C:367:ARG:CG	2.03	0.69
2:F:119:ARG:C	2:F:122:TYR:CE2	2.65	0.69
1:G:57:HIS:HA	1:G:86:THR:HG22	1.73	0.69
2:H:159:PRO:HB2	2:H:257:ARG:HB2	1.72	0.69
2:H:363:ASP:OD2	2:H:363:ASP:N	2.25	0.69
1:A:314:ALA:HB2	1:E:191:PRO:CB	2.22	0.69
2:H:42:GLN:HA	2:H:64:THR:HG21	1.73	0.69
1:A:37:CYS:HB2	1:A:155:GLY:HA2	1.74	0.69
1:A:206:ILE:CG1	1:A:419:GLN:HB3	2.21	0.69
2:B:159:PRO:HB3	2:B:257:ARG:HD3	1.75	0.69
1:C:359:THR:HG22	4:C:502:CZL:S2A	2.33	0.69
1:E:177:GLY:HA2	1:E:241:HIS:CE1	2.28	0.69
1:E:403:ASN:OD1	1:E:403:ASN:N	2.26	0.69
1:E:421:ARG:CZ	1:E:422:GLU:H	2.06	0.69
2:F:326:LEU:HD11	2:F:350:ALA:HB1	1.74	0.69
1:G:48:PRO:HG2	1:G:229:ALA:HB1	1.75	0.69
1:G:66:SER:HB3	2:H:47:PHE:CE1	2.28	0.69
2:H:67:MET:CE	2:H:71:SER:HB2	2.22	0.69
2:H:289:VAL:HG23	2:H:294:LYS:HD3	1.74	0.69
1:C:206:ILE:C	1:C:419:GLN:O	2.32	0.69
2:D:168:ARG:CB	2:D:169:PRO:HD3	2.22	0.69
2:F:344:VAL:HG22	2:F:345:PRO:HD2	1.74	0.69
1:A:220:LEU:HG	1:A:300:THR:HG22	1.75	0.69
1:C:197:ASP:OD2	1:C:223:ARG:HD3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:417:ILE:O	1:G:417:ILE:HG22	1.93	0.69
2:H:107:GLN:N	2:H:107:GLN:NE2	2.39	0.69
2:B:220:ALA:O	2:B:221:LEU:HB3	1.91	0.68
2:D:93:PRO:HG3	2:D:96:ILE:HD11	1.75	0.68
1:G:71:GLY:HA2	1:G:420:GLU:O	1.92	0.68
2:H:168:ARG:CB	2:H:169:PRO:HD3	2.24	0.68
1:A:209:GLU:HG2	1:A:210:PHE:N	2.07	0.68
1:E:332:GLY:H	1:E:334:VAL:HG22	1.57	0.68
2:B:159:PRO:HB2	2:B:257:ARG:CB	2.24	0.68
2:D:20:GLN:HG3	2:D:145:GLY:CA	2.22	0.68
1:E:190:ARG:O	1:E:192:GLY:N	2.21	0.68
1:E:206:ILE:HG13	1:E:419:GLN:CG	2.24	0.68
1:E:381:ASN:HD22	1:E:381:ASN:N	1.91	0.68
2:H:34:SER:H	2:H:221:LEU:CD2	2.03	0.68
2:D:344:VAL:HG22	2:D:345:PRO:HD2	1.74	0.68
2:F:100:THR:CG2	2:F:135:THR:H	2.05	0.68
2:F:333:ARG:HB2	2:F:333:ARG:HH11	1.58	0.68
1:C:339:VAL:O	1:C:343:LEU:HD23	1.94	0.68
2:F:117:GLU:C	2:F:122:TYR:OH	2.32	0.68
2:F:191:SER:HB3	2:F:277:TRP:HZ3	1.58	0.68
2:F:218:PHE:N	2:F:218:PHE:CD2	2.61	0.68
1:G:206:ILE:C	1:G:419:GLN:O	2.32	0.68
2:D:159:PRO:HB2	2:D:257:ARG:CB	2.24	0.68
2:D:159:PRO:HB3	2:D:257:ARG:HD3	1.75	0.68
1:E:404:MET:HB2	1:E:414:PHE:CE1	2.29	0.68
1:G:220:LEU:HG	1:G:300:THR:HG22	1.74	0.68
1:A:207:ALA:HB2	1:A:421:ARG:O	1.94	0.68
1:C:27:LYS:HD2	1:C:27:LYS:O	1.93	0.68
1:C:252:LYS:HB2	1:C:361:GLU:OE2	1.94	0.68
1:C:381:ASN:H	1:C:381:ASN:HD22	1.40	0.68
1:G:359:THR:HG22	4:G:502:CZL:S2A	2.34	0.68
1:A:381:ASN:H	1:A:381:ASN:HD22	1.40	0.68
2:D:67:MET:CE	2:D:71:SER:HB2	2.24	0.68
1:E:383:ARG:HG2	1:E:384:VAL:H	1.58	0.68
1:E:409:LYS:HB3	2:F:218:PHE:CZ	2.28	0.68
1:G:381:ASN:HD22	1:G:381:ASN:N	1.92	0.68
1:C:383:ARG:H	2:D:217:ARG:HH22	1.42	0.68
2:F:383:SER:OG	2:F:403:GLN:HA	1.94	0.68
1:G:37:CYS:CB	1:G:155:GLY:CA	2.67	0.68
2:H:188:ILE:HD11	2:H:268:LEU:HD12	1.74	0.68
2:B:106:THR:C	2:B:107:GLN:HE21	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLY:HA2	2:D:43:GLY:HA2	1.76	0.67
2:D:258:THR:OG1	2:D:260:VAL:HG23	1.94	0.67
2:D:382:ASN:HB2	2:D:402:PRO:O	1.93	0.67
1:A:36:GLY:HA2	2:B:43:GLY:HA2	1.76	0.67
1:A:332:GLY:H	1:A:334:VAL:HG22	1.58	0.67
1:E:410:GLY:O	1:E:412:VAL:HG23	1.94	0.67
1:G:206:ILE:HG13	1:G:419:GLN:CG	2.23	0.67
1:E:450:VAL:HG12	2:H:301:GLN:NE2	2.05	0.67
2:F:333:ARG:HB2	2:F:333:ARG:NH1	2.10	0.67
2:H:126:LYS:O	2:H:127:ASP:HB2	1.94	0.67
1:A:29:LYS:HZ1	1:A:29:LYS:N	1.87	0.67
1:A:382:ALA:HB3	2:B:217:ARG:HG3	1.75	0.67
2:B:207:GLY:O	2:B:223:THR:O	2.12	0.67
1:C:123:THR:O	1:C:126:PRO:HD2	1.93	0.67
2:F:289:VAL:HG23	2:F:294:LYS:HD3	1.76	0.67
2:F:315:ARG:HG2	2:F:340:VAL:HG21	1.75	0.67
2:H:159:PRO:HB3	2:H:257:ARG:HD3	1.75	0.67
2:H:315:ARG:HG2	2:H:340:VAL:HG21	1.76	0.67
2:B:16:LEU:N	2:B:363:ASP:HB3	2.05	0.67
2:B:191:SER:HB3	2:B:277:TRP:HZ3	1.59	0.67
2:F:159:PRO:HB2	2:F:257:ARG:CB	2.24	0.67
1:G:174:TYR:CE1	1:G:237:VAL:HB	2.30	0.67
2:H:119:ARG:C	2:H:122:TYR:CE2	2.67	0.67
2:H:213:LEU:HD13	2:H:218:PHE:HB3	1.77	0.67
1:E:37:CYS:HB2	1:E:155:GLY:HA2	1.76	0.67
1:G:339:VAL:O	1:G:343:LEU:HD23	1.95	0.67
1:A:174:TYR:CE1	1:A:237:VAL:HB	2.30	0.67
1:A:411:ARG:HH22	2:B:214:ASP:HA	1.59	0.67
2:D:158:VAL:HG13	2:D:158:VAL:O	1.92	0.67
2:H:382:ASN:HB2	2:H:402:PRO:O	1.94	0.67
2:B:270:GLY:O	2:B:274:VAL:HG23	1.95	0.67
1:C:62:CYS:SG	1:C:123:THR:HG21	2.34	0.67
2:F:93:PRO:HG3	2:F:96:ILE:HD11	1.77	0.67
2:F:258:THR:OG1	2:F:260:VAL:HG23	1.94	0.67
2:H:16:LEU:N	2:H:363:ASP:HB3	2.06	0.67
2:H:220:ALA:O	2:H:221:LEU:HB3	1.95	0.67
2:D:104:SER:O	2:D:109:CYS:HB3	1.94	0.67
2:B:93:PRO:HG3	2:B:96:ILE:CG1	2.25	0.67
2:B:149:ALA:O	2:B:153:ILE:HG13	1.95	0.67
1:C:48:PRO:HB3	1:C:72:THR:HG21	1.77	0.67
2:F:119:ARG:N	2:F:122:TYR:CZ	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:302:ASP:CB	2:H:211:GLY:HA3	2.25	0.67
2:H:326:LEU:HD11	2:H:350:ALA:HB1	1.75	0.67
1:C:71:GLY:HA2	1:C:420:GLU:O	1.95	0.66
1:A:450:VAL:HG12	2:D:301:GLN:NE2	2.06	0.66
2:B:176:CYS:O	2:B:247:LEU:HD11	1.95	0.66
1:C:403:ASN:OD1	1:C:403:ASN:N	2.28	0.66
2:H:93:PRO:HG3	2:H:96:ILE:HD11	1.77	0.66
2:D:252:ASP:O	2:D:256:GLU:HG2	1.95	0.66
2:F:67:MET:CE	2:F:71:SER:HB2	2.25	0.66
2:F:93:PRO:HG3	2:F:96:ILE:CG1	2.26	0.66
1:C:177:GLY:HA3	1:C:241:HIS:CE1	2.30	0.66
2:H:39:HIS:HD2	2:H:65:THR:CG2	2.08	0.66
1:E:197:ASP:OD2	1:E:223:ARG:HD3	1.95	0.66
1:G:68:ASP:HA	1:G:81:ARG:HH22	1.59	0.66
1:G:398:ILE:HG23	1:G:417:ILE:HG12	1.78	0.66
1:A:30:PRO:HD3	2:B:64:THR:O	1.95	0.66
1:A:94:ILE:HD12	1:A:94:ILE:O	1.96	0.66
1:C:37:CYS:HB3	1:C:155:GLY:HA3	1.77	0.66
2:F:297:ARG:HD2	2:F:417:TYR:OH	1.95	0.66
1:A:397:LEU:HD22	1:A:398:ILE:N	2.11	0.66
1:A:67:TRP:CZ3	2:B:15:PRO:O	2.48	0.66
2:B:301:GLN:NE2	1:C:450:VAL:HG12	2.03	0.66
1:C:68:ASP:HA	1:C:81:ARG:HH22	1.60	0.66
1:C:106:ILE:O	1:C:110:VAL:HG22	1.94	0.66
1:C:310:LYS:NZ	1:G:191:PRO:HG2	2.11	0.66
1:E:27:LYS:O	1:E:27:LYS:HD2	1.96	0.66
1:E:346:LEU:O	1:E:346:LEU:HD23	1.96	0.66
1:G:174:TYR:HE2	1:G:238:GLN:HG2	1.57	0.66
2:H:124:GLU:CD	2:H:126:LYS:H	2.00	0.66
2:H:258:THR:OG1	2:H:260:VAL:HG23	1.96	0.66
1:A:380:GLY:HA3	1:A:384:VAL:HG23	1.78	0.66
2:B:168:ARG:HB2	2:B:169:PRO:HD3	1.78	0.66
1:C:301:GLU:O	1:C:304:ILE:HG13	1.96	0.66
2:F:212:HIS:HB3	2:F:223:THR:HG21	1.78	0.66
1:A:38:SER:OG	1:A:162:LEU:HD12	1.95	0.65
1:A:71:GLY:HA2	1:A:420:GLU:O	1.96	0.65
1:A:322:LEU:CD2	1:A:439:CYS:SG	2.82	0.65
1:C:332:GLY:H	1:C:334:VAL:HG22	1.60	0.65
1:E:199:ASN:HB2	1:E:246:ASN:ND2	2.12	0.65
2:F:104:SER:O	2:F:109:CYS:HB3	1.96	0.65
1:A:381:ASN:HD22	1:A:381:ASN:N	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:HIS:HD2	2:B:65:THR:CG2	2.09	0.65
2:D:119:ARG:N	2:D:122:TYR:CZ	2.64	0.65
2:F:16:LEU:N	2:F:363:ASP:HB3	2.08	0.65
2:F:198:ARG:HG3	2:F:198:ARG:O	1.95	0.65
1:C:417:ILE:HG22	1:C:417:ILE:O	1.97	0.65
2:D:289:VAL:HG23	2:D:294:LYS:HD3	1.77	0.65
2:D:379:VAL:O	2:D:396:LEU:HD23	1.96	0.65
2:B:93:PRO:HG3	2:B:96:ILE:HD11	1.77	0.65
2:B:315:ARG:HG2	2:B:340:VAL:HG21	1.76	0.65
2:F:149:ALA:O	2:F:153:ILE:HG13	1.97	0.65
1:G:245:VAL:CG1	1:G:290:LEU:HD23	2.26	0.65
1:G:380:GLY:HA3	1:G:384:VAL:HG23	1.76	0.65
2:H:126:LYS:HZ3	2:H:127:ASP:H	1.45	0.65
2:B:118:PHE:C	2:B:122:TYR:OH	2.35	0.65
1:E:108:GLN:HE22	2:F:11:LEU:N	1.89	0.65
2:H:118:PHE:N	2:H:122:TYR:OH	2.28	0.65
2:H:217:ARG:C	2:H:218:PHE:HD2	2.00	0.65
1:A:108:GLN:NE2	2:B:11:LEU:HB3	2.11	0.65
2:B:289:VAL:HG23	2:B:294:LYS:HD3	1.77	0.65
1:C:262:GLN:HG3	1:C:263:GLU:N	2.12	0.65
1:C:380:GLY:HA3	1:C:384:VAL:HG23	1.78	0.65
1:E:436:ARG:O	1:E:440:ILE:HG23	1.96	0.65
1:G:346:LEU:HD23	1:G:346:LEU:O	1.97	0.65
1:G:421:ARG:CZ	1:G:422:GLU:H	2.09	0.65
2:H:39:HIS:HA	2:H:65:THR:OG1	1.96	0.65
1:A:206:ILE:HB	1:A:420:GLU:N	2.11	0.65
2:B:126:LYS:O	2:B:127:ASP:HB2	1.97	0.65
2:H:20:GLN:HG2	2:H:135:THR:HB	1.78	0.65
1:A:330:TYR:HB3	1:A:399:ALA:HB2	1.78	0.65
1:C:206:ILE:CG2	1:C:420:GLU:HA	2.27	0.65
2:D:126:LYS:O	2:D:127:ASP:HB2	1.96	0.65
2:F:126:LYS:O	2:F:127:ASP:HB2	1.96	0.65
2:F:382:ASN:HB2	2:F:402:PRO:O	1.96	0.65
1:A:413:PRO:HA	1:A:447:TRP:CZ2	2.32	0.65
2:F:121:GLN:C	2:F:122:TYR:CD1	2.69	0.65
2:H:118:PHE:C	2:H:122:TYR:OH	2.35	0.65
2:H:160:GLU:CG	2:H:161:ARG:H	2.10	0.65
2:D:159:PRO:HB2	2:D:257:ARG:CG	2.27	0.65
2:D:168:ARG:NE	2:D:169:PRO:HD3	2.11	0.65
1:E:27:LYS:HD3	2:F:66:ALA:HB1	1.79	0.65
1:E:206:ILE:HB	1:E:420:GLU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:CYS:HB3	1:G:155:GLY:HA3	1.79	0.65
1:G:397:LEU:HD22	1:G:398:ILE:N	2.12	0.65
2:H:82:GLU:O	2:H:86:THR:OG1	2.10	0.65
1:C:209:GLU:HG2	1:C:210:PHE:N	2.07	0.64
2:D:326:LEU:HD11	2:D:350:ALA:HB1	1.79	0.64
1:G:436:ARG:O	1:G:440:ILE:HG23	1.97	0.64
2:H:159:PRO:HB2	2:H:257:ARG:CB	2.28	0.64
1:A:174:TYR:CZ	1:A:234:TYR:CE2	2.86	0.64
2:D:26:LEU:HA	2:D:29:LEU:HB2	1.80	0.64
2:F:28:ILE:HD12	2:F:34:SER:OG	1.97	0.64
1:G:245:VAL:HG13	1:G:290:LEU:HD23	1.76	0.64
2:B:382:ASN:HB2	2:B:402:PRO:O	1.96	0.64
1:C:329:LEU:HD13	1:C:340:VAL:HG22	1.79	0.64
1:G:403:ASN:N	1:G:403:ASN:OD1	2.30	0.64
2:H:168:ARG:NE	2:H:169:PRO:HD3	2.12	0.64
2:F:160:GLU:CG	2:F:161:ARG:H	2.09	0.64
2:F:302:ASP:HB2	2:H:211:GLY:HA3	1.79	0.64
2:F:340:VAL:O	2:F:340:VAL:HG12	1.97	0.64
2:D:198:ARG:HG3	2:D:198:ARG:O	1.98	0.64
1:E:71:GLY:HA2	1:E:420:GLU:O	1.98	0.64
1:E:206:ILE:HB	1:E:420:GLU:HA	1.80	0.64
1:G:174:TYR:CZ	1:G:238:GLN:HG2	2.32	0.64
2:H:67:MET:HE2	2:H:71:SER:HB2	1.78	0.64
1:A:37:CYS:HB3	1:A:155:GLY:HA3	1.76	0.64
2:D:315:ARG:HG2	2:D:340:VAL:HG21	1.79	0.64
1:E:123:THR:O	1:E:126:PRO:HD2	1.96	0.64
1:E:369:LEU:HD23	1:E:370:MET:HB3	1.79	0.64
2:F:420:SER:O	2:F:424:LEU:HD12	1.97	0.64
1:G:329:LEU:HD13	1:G:340:VAL:HG22	1.80	0.64
1:A:417:ILE:O	1:A:417:ILE:HG22	1.96	0.64
2:B:217:ARG:C	2:B:218:PHE:HD2	2.01	0.64
1:C:191:PRO:CG	1:G:314:ALA:HB2	2.27	0.64
1:C:381:ASN:HD22	1:C:381:ASN:N	1.95	0.64
2:D:100:THR:CG2	2:D:135:THR:H	2.10	0.64
2:D:149:ALA:O	2:D:153:ILE:HG13	1.97	0.64
2:D:160:GLU:CG	2:D:161:ARG:H	2.11	0.64
2:D:270:GLY:O	2:D:274:VAL:HG23	1.97	0.64
1:E:125:VAL:HB	1:E:126:PRO:HD3	1.80	0.64
2:F:378:LEU:HD13	2:F:379:VAL:N	2.11	0.64
1:G:177:GLY:HA3	1:G:241:HIS:CE1	2.32	0.64
1:A:128:LEU:HD23	2:B:106:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD23	1:A:370:MET:HB3	1.78	0.64
2:B:160:GLU:CG	2:B:161:ARG:H	2.10	0.64
1:C:287:PHE:O	1:C:291:LEU:HD23	1.97	0.64
1:C:369:LEU:HD23	1:C:370:MET:HB3	1.79	0.64
1:G:421:ARG:NH2	1:G:422:GLU:HB3	2.12	0.64
2:B:378:LEU:HD13	2:B:379:VAL:N	2.13	0.64
1:C:346:LEU:O	1:C:346:LEU:HD23	1.98	0.64
1:E:68:ASP:HA	1:E:81:ARG:HH22	1.62	0.64
1:A:432:LEU:O	1:A:436:ARG:HD2	1.98	0.63
2:D:106:THR:C	2:D:107:GLN:HE21	2.01	0.63
1:E:123:THR:CG2	3:E:501:SF4:S4	2.85	0.63
1:E:174:TYR:CZ	1:E:234:TYR:CE2	2.86	0.63
1:A:193:ILE:HD12	1:A:193:ILE:N	2.14	0.63
1:A:398:ILE:HG23	1:A:417:ILE:HG12	1.80	0.63
1:C:38:SER:OG	1:C:162:LEU:HD12	1.98	0.63
1:C:398:ILE:HG23	1:C:417:ILE:HG12	1.80	0.63
1:C:420:GLU:HG2	1:C:421:ARG:N	2.13	0.63
2:D:121:GLN:C	2:D:122:TYR:CD1	2.72	0.63
1:A:68:ASP:HA	1:A:81:ARG:HH22	1.62	0.63
1:A:403:ASN:N	1:A:403:ASN:OD1	2.31	0.63
1:C:37:CYS:HB2	1:C:155:GLY:HA2	1.80	0.63
2:F:207:GLY:O	2:F:223:THR:O	2.16	0.63
2:F:220:ALA:O	2:F:221:LEU:HB3	1.97	0.63
1:A:206:ILE:CG2	1:A:420:GLU:HA	2.29	0.63
2:B:168:ARG:CB	2:B:169:PRO:HD3	2.29	0.63
1:C:206:ILE:HB	1:C:420:GLU:N	2.13	0.63
2:D:176:CYS:O	2:D:247:LEU:HD11	1.98	0.63
1:E:411:ARG:HH22	2:F:214:ASP:HA	1.63	0.63
1:G:206:ILE:CG2	1:G:420:GLU:HA	2.27	0.63
1:A:206:ILE:HG13	1:A:419:GLN:HG3	1.80	0.63
2:B:57:ARG:O	2:B:58:GLU:CD	2.37	0.63
2:B:246:SER:HB3	2:B:323:ASP:OD2	1.98	0.63
1:C:30:PRO:HD3	2:D:64:THR:O	1.97	0.63
1:E:174:TYR:CZ	1:E:238:GLN:HG2	2.32	0.63
1:A:191:PRO:HG2	1:E:310:LYS:HZ3	1.60	0.63
1:A:420:GLU:HG2	1:A:421:ARG:N	2.14	0.63
1:C:123:THR:HG22	3:C:501:SF4:S4	2.38	0.63
2:F:168:ARG:HB2	2:F:169:PRO:HD3	1.81	0.63
2:H:168:ARG:HH21	2:H:169:PRO:HG3	1.63	0.63
2:D:31:LEU:O	2:D:221:LEU:HD21	1.99	0.63
2:F:379:VAL:O	2:F:396:LEU:HD23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:LEU:HA	2:H:29:LEU:HB2	1.80	0.63
2:H:93:PRO:HG3	2:H:96:ILE:CG1	2.29	0.63
2:B:242:VAL:CB	2:B:264:ARG:HB3	2.21	0.63
1:E:206:ILE:CG2	1:E:420:GLU:HA	2.28	0.63
2:F:38:PHE:HB2	2:F:45:THR:CG2	2.29	0.63
2:H:31:LEU:O	2:H:221:LEU:HD21	1.99	0.63
2:H:106:THR:C	2:H:107:GLN:HE21	2.02	0.63
1:A:389:VAL:HG13	1:A:394:ALA:HB3	1.80	0.63
1:A:37:CYS:SG	2:B:43:GLY:HA3	2.39	0.62
1:C:102:LEU:CD2	1:C:106:ILE:HD11	2.29	0.62
2:F:126:LYS:HZ3	2:F:127:ASP:H	1.45	0.62
2:H:382:ASN:C	2:H:382:ASN:HD22	2.02	0.62
1:A:262:GLN:HG3	1:A:263:GLU:N	2.13	0.62
2:B:124:GLU:CD	2:B:126:LYS:H	2.02	0.62
1:C:72:THR:HG23	1:C:204:TYR:O	1.99	0.62
2:D:168:ARG:HH21	2:D:169:PRO:HG3	1.64	0.62
1:E:355:THR:HB	1:E:377:LEU:HD11	1.80	0.62
1:G:66:SER:O	1:G:69:ASN:ND2	2.32	0.62
1:G:355:THR:HB	1:G:377:LEU:HD11	1.79	0.62
1:G:404:MET:HB2	1:G:414:PHE:CE1	2.33	0.62
1:A:346:LEU:HD23	1:A:346:LEU:O	2.00	0.62
1:C:125:VAL:HB	1:C:126:PRO:HD3	1.80	0.62
1:E:48:PRO:HG2	1:E:229:ALA:HB1	1.81	0.62
1:E:380:GLY:HA3	1:E:384:VAL:HG23	1.80	0.62
1:G:193:ILE:H	1:G:193:ILE:CD1	2.11	0.62
1:G:206:ILE:HB	1:G:420:GLU:N	2.13	0.62
2:H:121:GLN:C	2:H:122:TYR:CD1	2.72	0.62
1:A:421:ARG:CZ	1:A:422:GLU:H	2.12	0.62
2:B:379:VAL:O	2:B:396:LEU:HD23	1.98	0.62
1:C:404:MET:HB2	1:C:414:PHE:CE1	2.34	0.62
1:E:48:PRO:HB3	1:E:72:THR:HG21	1.81	0.62
2:H:191:SER:HB3	2:H:277:TRP:HZ3	1.64	0.62
1:E:382:ALA:HB2	1:E:406:THR:HB	1.82	0.62
2:F:100:THR:HG22	2:F:135:THR:N	2.11	0.62
2:H:164:GLN:O	2:H:167:LYS:HG2	2.00	0.62
1:A:421:ARG:NH2	1:A:422:GLU:HB3	2.14	0.62
2:B:104:SER:O	2:B:109:CYS:HB3	1.98	0.62
2:B:121:GLN:C	2:B:122:TYR:CD1	2.72	0.62
1:C:174:TYR:CZ	1:C:238:GLN:HG2	2.34	0.62
2:F:126:LYS:HG3	2:F:127:ASP:N	2.15	0.62
2:F:242:VAL:CB	2:F:264:ARG:HB3	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:O	1:G:95:MET:O	2.18	0.62
1:C:421:ARG:CZ	1:C:422:GLU:H	2.12	0.62
2:D:164:GLN:O	2:D:167:LYS:HG2	2.00	0.62
2:D:213:LEU:HG	2:D:223:THR:HG23	1.81	0.62
2:D:246:SER:HB3	2:D:323:ASP:OD2	1.99	0.62
2:F:388:SER:O	2:F:392:LEU:HD22	1.99	0.62
1:G:36:GLY:HA2	2:H:43:GLY:HA2	1.82	0.62
1:G:92:ASP:HA	1:G:97:ARG:HB3	1.81	0.62
2:B:8:ASN:O	2:B:9:LYS:CB	2.46	0.62
1:C:330:TYR:HB3	1:C:399:ALA:HB2	1.81	0.62
2:F:158:VAL:HG13	2:F:158:VAL:O	2.00	0.62
2:F:168:ARG:CB	2:F:169:PRO:HD3	2.29	0.62
2:H:4:ILE:N	2:H:353:ASP:OD2	2.33	0.62
1:A:383:ARG:H	2:B:217:ARG:NH2	1.97	0.62
2:B:348:ALA:O	2:B:349:ALA:O	2.18	0.62
2:D:124:GLU:CD	2:D:126:LYS:H	2.03	0.62
2:H:213:LEU:CD2	2:H:214:ASP:H	2.13	0.62
1:A:410:GLY:O	1:A:412:VAL:HG23	2.00	0.62
2:B:31:LEU:O	2:B:221:LEU:HD21	2.00	0.62
2:B:38:PHE:HB2	2:B:45:THR:CG2	2.30	0.62
1:C:206:ILE:HG13	1:C:419:GLN:HG3	1.81	0.62
2:B:118:PHE:N	2:B:122:TYR:OH	2.33	0.61
1:E:383:ARG:CA	2:F:217:ARG:HH12	2.13	0.61
2:F:164:GLN:O	2:F:167:LYS:HG2	2.00	0.61
1:G:92:ASP:OD2	1:G:97:ARG:HG2	1.98	0.61
2:H:388:SER:O	2:H:392:LEU:HD22	2.00	0.61
1:C:193:ILE:H	1:C:193:ILE:CD1	2.10	0.61
1:C:245:VAL:CG1	1:C:290:LEU:HD23	2.31	0.61
1:E:94:ILE:O	1:E:95:MET:O	2.19	0.61
1:G:125:VAL:HB	1:G:126:PRO:HD3	1.80	0.61
2:H:158:VAL:O	2:H:158:VAL:HG13	2.00	0.61
1:A:27:LYS:CD	2:B:66:ALA:HB1	2.30	0.61
1:C:421:ARG:NH2	1:C:422:GLU:HB3	2.16	0.61
1:G:94:ILE:O	1:G:94:ILE:HD12	2.00	0.61
2:H:126:LYS:HG3	2:H:127:ASP:N	2.15	0.61
1:A:172:LEU:HD12	1:A:173:LYS:CA	2.30	0.61
2:D:34:SER:H	2:D:221:LEU:CD2	2.09	0.61
2:F:382:ASN:ND2	2:F:384:HIS:HB2	2.14	0.61
1:G:389:VAL:HG13	1:G:394:ALA:HB3	1.83	0.61
2:B:388:SER:O	2:B:392:LEU:HD22	2.01	0.61
2:D:191:SER:HB3	2:D:277:TRP:HZ3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:LEU:HD12	1:E:172:LEU:C	2.20	0.61
2:F:168:ARG:NE	2:F:169:PRO:HD3	2.15	0.61
1:G:67:TRP:CH2	2:H:15:PRO:O	2.53	0.61
1:G:155:GLY:N	3:G:501:SF4:S4	2.72	0.61
2:H:349:ALA:O	2:H:350:ALA:C	2.39	0.61
1:C:174:TYR:CZ	1:C:234:TYR:CE2	2.88	0.61
2:D:42:GLN:CA	2:D:64:THR:HG21	2.30	0.61
2:D:93:PRO:HG3	2:D:96:ILE:CG1	2.30	0.61
1:E:172:LEU:HD12	1:E:173:LYS:CA	2.30	0.61
1:E:174:TYR:CE1	1:E:237:VAL:HB	2.35	0.61
1:E:432:LEU:O	1:E:436:ARG:HD2	2.01	0.61
1:G:37:CYS:SG	2:H:43:GLY:HA3	2.41	0.61
1:G:262:GLN:HG3	1:G:263:GLU:N	2.14	0.61
1:A:176:ILE:O	1:A:177:GLY:C	2.39	0.61
1:A:329:LEU:HD13	1:A:340:VAL:HG22	1.82	0.61
1:E:154:ALA:O	1:E:157:TYR:CD1	2.53	0.61
2:H:75:GLY:O	2:H:76:ALA:HB2	2.01	0.61
1:A:174:TYR:CZ	1:A:238:GLN:HG2	2.36	0.61
1:A:310:LYS:NZ	1:E:191:PRO:HG2	2.16	0.61
1:E:339:VAL:O	1:E:343:LEU:HD23	2.00	0.61
1:G:48:PRO:HB3	1:G:72:THR:HG21	1.81	0.61
2:H:17:LYS:HG3	2:H:345:PRO:CB	2.28	0.61
2:H:333:ARG:NH1	2:H:333:ARG:HB2	2.15	0.61
1:A:404:MET:HB2	1:A:414:PHE:CE1	2.36	0.61
2:F:382:ASN:HD22	2:F:382:ASN:C	2.04	0.61
2:D:317:ALA:HB3	2:D:379:VAL:HG22	1.81	0.61
2:F:217:ARG:C	2:F:218:PHE:HD2	2.04	0.61
1:C:67:TRP:CH2	2:D:15:PRO:O	2.54	0.60
1:C:314:ALA:HB2	1:G:191:PRO:CB	2.31	0.60
1:E:421:ARG:NH2	1:E:422:GLU:HB3	2.16	0.60
2:H:33:ARG:N	2:H:221:LEU:HD23	2.15	0.60
1:A:355:THR:HB	1:A:377:LEU:HD11	1.82	0.60
2:B:340:VAL:O	2:B:340:VAL:HG12	2.01	0.60
1:C:410:GLY:O	1:C:412:VAL:HG23	2.01	0.60
2:D:8:ASN:O	2:D:9:LYS:CB	2.48	0.60
1:E:398:ILE:HG23	1:E:417:ILE:HG12	1.83	0.60
1:G:306:ARG:NH2	1:G:307:GLU:OE1	2.35	0.60
1:G:369:LEU:HD23	1:G:370:MET:HB3	1.83	0.60
2:H:100:THR:CG2	2:H:135:THR:H	2.12	0.60
1:C:432:LEU:O	1:C:436:ARG:HD2	2.01	0.60
2:F:93:PRO:HG3	2:F:96:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HB	1:A:126:PRO:HD3	1.82	0.60
2:F:331:LEU:O	2:F:331:LEU:HD22	2.01	0.60
1:G:382:ALA:HB2	1:G:406:THR:HB	1.84	0.60
2:H:28:ILE:HG13	2:H:29:LEU:N	2.15	0.60
1:A:48:PRO:HB3	1:A:72:THR:HG21	1.84	0.60
1:A:339:VAL:O	1:A:343:LEU:HD23	2.02	0.60
2:B:27:ALA:HB2	2:B:146:PHE:CD1	2.36	0.60
1:C:172:LEU:HD12	1:C:173:LYS:CA	2.32	0.60
1:E:68:ASP:HB3	2:F:384:HIS:HE1	1.67	0.60
2:F:118:PHE:C	2:F:122:TYR:OH	2.40	0.60
2:B:158:VAL:O	2:B:158:VAL:HG13	2.00	0.60
1:C:108:GLN:NE2	2:D:11:LEU:HB3	2.16	0.60
2:D:118:PHE:N	2:D:122:TYR:OH	2.35	0.60
2:F:159:PRO:HG3	2:F:257:ARG:NH1	2.16	0.60
1:G:432:LEU:O	1:G:436:ARG:HD2	2.02	0.60
1:A:356:LYS:HG2	1:A:376:MET:SD	2.42	0.60
2:B:168:ARG:HH21	2:B:169:PRO:HG3	1.66	0.60
2:B:186:GLU:O	2:B:190:GLU:HG2	2.02	0.60
2:D:388:SER:O	2:D:392:LEU:HD22	2.01	0.60
1:E:176:ILE:O	1:E:177:GLY:C	2.40	0.60
1:E:177:GLY:HA3	1:E:241:HIS:CE1	2.35	0.60
1:G:108:GLN:NE2	2:H:11:LEU:H	1.95	0.60
2:B:213:LEU:CD2	2:B:214:ASP:H	2.15	0.60
1:G:54:HIS:HD2	1:G:121:TYR:OH	1.85	0.60
2:H:38:PHE:HB2	2:H:45:THR:CG2	2.32	0.60
2:F:176:CYS:O	2:F:247:LEU:HD11	2.01	0.60
1:G:420:GLU:HG2	1:G:421:ARG:N	2.15	0.60
2:H:104:SER:O	2:H:109:CYS:HB3	2.02	0.60
1:C:128:LEU:HD23	2:D:106:THR:HG21	1.84	0.60
1:C:207:ALA:HB2	1:C:421:ARG:O	2.02	0.60
1:C:310:LYS:HZ3	1:G:191:PRO:HG2	1.67	0.60
1:E:209:GLU:HG2	1:E:210:PHE:N	2.13	0.60
1:E:397:LEU:HD22	1:E:398:ILE:H	1.67	0.60
1:G:106:ILE:O	1:G:110:VAL:HG22	2.02	0.60
1:C:436:ARG:O	1:C:440:ILE:HG23	2.01	0.59
1:E:420:GLU:HG2	1:E:421:ARG:N	2.16	0.59
1:A:92:ASP:HA	1:A:97:ARG:HB3	1.84	0.59
1:C:245:VAL:HG13	1:C:290:LEU:HD23	1.83	0.59
2:F:186:GLU:O	2:F:190:GLU:HG2	2.02	0.59
1:G:359:THR:CG2	4:G:502:CZL:S2A	2.90	0.59
1:A:94:ILE:O	1:A:95:MET:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:HZ2	2:B:127:ASP:H	1.48	0.59
2:B:168:ARG:NE	2:B:169:PRO:HD3	2.16	0.59
2:B:213:LEU:HD13	2:B:218:PHE:HB3	1.83	0.59
2:D:126:LYS:HZ3	2:D:127:ASP:H	1.49	0.59
2:D:217:ARG:C	2:D:218:PHE:CD2	2.76	0.59
1:A:419:GLN:HE22	1:A:424:GLY:H	1.50	0.59
2:B:38:PHE:HB2	2:B:45:THR:HG22	1.85	0.59
1:C:355:THR:HB	1:C:377:LEU:HD11	1.84	0.59
2:D:331:LEU:O	2:D:331:LEU:HD22	2.02	0.59
2:F:75:GLY:O	2:F:76:ALA:HB2	2.02	0.59
1:A:67:TRP:O	1:A:81:ARG:NH2	2.36	0.59
2:B:212:HIS:HB3	2:B:223:THR:HG21	1.84	0.59
2:B:382:ASN:ND2	2:B:384:HIS:H	2.01	0.59
1:C:383:ARG:H	2:D:217:ARG:NH2	2.00	0.59
1:E:245:VAL:HG13	1:E:290:LEU:HD23	1.83	0.59
1:G:176:ILE:O	1:G:177:GLY:C	2.41	0.59
1:G:232:ALA:HA	1:G:236:GLU:OE1	2.03	0.59
1:C:149:ILE:HD12	1:C:149:ILE:N	2.17	0.59
2:D:156:THR:HG22	2:D:157:LEU:HD13	1.83	0.59
1:E:174:TYR:HE2	1:E:238:GLN:HG2	1.60	0.59
1:E:389:VAL:HG13	1:E:394:ALA:HB3	1.84	0.59
1:A:92:ASP:OD2	1:A:97:ARG:HG2	2.02	0.59
1:A:193:ILE:C	1:A:195:VAL:H	2.06	0.59
2:B:20:GLN:HG2	2:B:135:THR:HB	1.85	0.59
2:B:349:ALA:O	2:B:350:ALA:C	2.41	0.59
1:G:172:LEU:HD12	1:G:172:LEU:C	2.22	0.59
1:G:172:LEU:HD12	1:G:173:LYS:CA	2.32	0.59
1:C:389:VAL:HG13	1:C:394:ALA:HB3	1.85	0.59
2:D:300:LEU:O	2:D:300:LEU:HD12	2.02	0.59
2:F:433:GLU:HG3	2:F:434:HIS:CD2	2.37	0.59
2:H:212:HIS:HB3	2:H:223:THR:HG21	1.83	0.59
1:C:199:ASN:ND2	1:C:225:LEU:HB2	2.14	0.59
1:C:382:ALA:HB2	1:C:406:THR:HB	1.85	0.59
2:D:213:LEU:HD13	2:D:218:PHE:HB3	1.84	0.59
2:D:297:ARG:HD2	2:D:417:TYR:OH	2.03	0.59
1:E:245:VAL:CG1	1:E:290:LEU:HD23	2.33	0.59
1:A:172:LEU:HD12	1:A:172:LEU:C	2.23	0.59
2:D:410:PHE:CE2	2:D:411:GLN:HB2	2.38	0.59
1:E:421:ARG:NH2	1:E:422:GLU:H	2.00	0.59
1:G:108:GLN:NE2	2:H:11:LEU:HB3	2.17	0.59
2:H:100:THR:HG22	2:H:135:THR:N	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:HIS:HB3	1:A:291:LEU:HD11	1.85	0.58
1:C:337:TRP:O	1:C:337:TRP:CE3	2.56	0.58
1:E:36:GLY:HA2	2:F:43:GLY:HA2	1.84	0.58
2:H:93:PRO:HG3	2:H:96:ILE:CD1	2.33	0.58
1:A:27:LYS:HD2	1:A:27:LYS:O	2.02	0.58
1:A:382:ALA:HB2	1:A:406:THR:HB	1.85	0.58
2:B:76:ALA:O	2:B:77:ASP:C	2.42	0.58
2:B:173:ASN:HB2	2:B:240:THR:CG2	2.20	0.58
1:C:92:ASP:OD2	1:C:97:ARG:HG2	2.04	0.58
1:C:154:ALA:O	1:C:157:TYR:CD1	2.56	0.58
1:E:27:LYS:HD3	2:F:66:ALA:CB	2.33	0.58
1:E:206:ILE:HB	1:E:420:GLU:CA	2.33	0.58
1:E:330:TYR:HB3	1:E:399:ALA:HB2	1.86	0.58
2:F:159:PRO:CG	2:F:257:ARG:NH1	2.65	0.58
2:H:252:ASP:O	2:H:256:GLU:HG2	2.04	0.58
1:A:359:THR:HG22	4:A:502:CZL:S2A	2.43	0.58
2:B:100:THR:CG2	2:B:135:THR:H	2.16	0.58
1:C:94:ILE:O	1:C:95:MET:O	2.22	0.58
1:C:108:GLN:CD	2:D:11:LEU:HB3	2.23	0.58
2:D:348:ALA:O	2:D:349:ALA:O	2.21	0.58
1:E:29:LYS:CB	1:E:30:PRO:HD2	2.30	0.58
1:E:327:VAL:HG21	1:E:343:LEU:CD1	2.34	0.58
2:F:106:THR:C	2:F:107:GLN:HE21	2.05	0.58
2:F:246:SER:HB3	2:F:323:ASP:OD2	2.03	0.58
2:H:213:LEU:HG	2:H:223:THR:HG23	1.86	0.58
2:B:67:MET:HE3	2:B:71:SER:HB2	1.85	0.58
2:D:382:ASN:C	2:D:382:ASN:HD22	2.06	0.58
2:F:118:PHE:N	2:F:122:TYR:OH	2.36	0.58
2:F:124:GLU:CD	2:F:126:LYS:H	2.06	0.58
2:B:297:ARG:HD2	2:B:417:TYR:OH	2.03	0.58
1:C:232:ALA:HA	1:C:236:GLU:OE1	2.04	0.58
2:F:38:PHE:CD2	2:F:45:THR:HG22	2.38	0.58
2:F:213:LEU:HD13	2:F:218:PHE:HB3	1.85	0.58
1:G:29:LYS:HG3	2:H:66:ALA:HB3	1.85	0.58
1:E:92:ASP:OD2	1:E:97:ARG:HG2	2.03	0.58
2:B:117:GLU:C	2:B:122:TYR:HH	2.07	0.58
2:B:211:GLY:HA3	2:D:302:ASP:CB	2.34	0.58
1:C:174:TYR:CE1	1:C:237:VAL:HB	2.39	0.58
1:E:193:ILE:C	1:E:195:VAL:H	2.06	0.58
2:F:38:PHE:HB2	2:F:45:THR:HG22	1.86	0.58
1:C:27:LYS:CD	2:D:66:ALA:HB1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:HB3	1:C:191:PRO:HD2	0.73	0.58
1:C:409:LYS:HB3	2:D:218:PHE:HZ	1.65	0.58
1:E:92:ASP:HA	1:E:97:ARG:HB3	1.85	0.58
2:F:188:ILE:HD11	2:F:268:LEU:HD12	1.86	0.58
1:G:30:PRO:HD3	2:H:64:THR:O	2.03	0.58
1:A:204:TYR:CE1	1:A:229:ALA:HB3	2.39	0.57
1:C:176:ILE:O	1:C:177:GLY:C	2.43	0.57
2:D:17:LYS:HG3	2:D:345:PRO:CB	2.32	0.57
1:G:199:ASN:ND2	1:G:225:LEU:HB2	2.17	0.57
2:H:8:ASN:O	2:H:9:LYS:CB	2.51	0.57
2:H:156:THR:HG22	2:H:157:LEU:HD13	1.86	0.57
2:H:397:LEU:CD2	2:H:427:LEU:HD21	2.33	0.57
1:G:373:ASP:CG	1:G:374:VAL:H	2.08	0.57
2:H:410:PHE:CE2	2:H:411:GLN:HB2	2.39	0.57
2:D:38:PHE:HB2	2:D:45:THR:CG2	2.33	0.57
1:E:54:HIS:HD2	1:E:121:TYR:OH	1.87	0.57
1:E:86:THR:O	1:E:86:THR:HG23	2.04	0.57
2:H:126:LYS:HG3	2:H:127:ASP:H	1.68	0.57
1:A:37:CYS:CB	1:A:155:GLY:CA	2.72	0.57
1:A:370:MET:HG2	1:A:370:MET:O	2.02	0.57
1:C:27:LYS:HD2	1:C:27:LYS:C	2.25	0.57
2:D:20:GLN:HG2	2:D:135:THR:CB	2.35	0.57
2:B:42:GLN:CA	2:B:64:THR:HG21	2.35	0.57
2:B:191:SER:CB	2:B:277:TRP:HZ3	2.16	0.57
2:D:168:ARG:HB2	2:D:169:PRO:CD	2.34	0.57
2:D:382:ASN:ND2	2:D:384:HIS:H	2.02	0.57
1:G:287:PHE:O	1:G:291:LEU:HD23	2.04	0.57
1:A:206:ILE:HB	1:A:420:GLU:HA	1.87	0.57
1:C:68:ASP:O	1:C:81:ARG:NH2	2.38	0.57
1:C:193:ILE:C	1:C:195:VAL:H	2.08	0.57
1:C:206:ILE:HB	1:C:420:GLU:HA	1.87	0.57
2:D:118:PHE:C	2:D:122:TYR:OH	2.40	0.57
2:F:49:LYS:O	2:F:53:VAL:HG13	2.03	0.57
2:B:39:HIS:HA	2:B:65:THR:OG1	2.05	0.57
1:E:206:ILE:CB	1:E:420:GLU:HA	2.35	0.57
1:G:27:LYS:HD3	2:H:66:ALA:CB	2.33	0.57
2:H:317:ALA:HB3	2:H:379:VAL:HG22	1.85	0.57
1:C:37:CYS:CB	1:C:155:GLY:CA	2.72	0.57
1:C:181:PRO:HD3	1:C:242:ARG:HG3	1.86	0.57
1:C:204:TYR:HA	1:C:229:ALA:O	2.05	0.57
2:F:8:ASN:O	2:F:9:LYS:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:VAL:O	2:F:340:VAL:CG1	2.51	0.57
2:F:349:ALA:O	2:F:350:ALA:C	2.43	0.57
2:F:382:ASN:ND2	2:F:384:HIS:H	2.03	0.57
1:G:108:GLN:CD	2:H:11:LEU:HB3	2.24	0.57
2:H:176:CYS:O	2:H:247:LEU:HD11	2.04	0.57
1:A:29:LYS:HZ2	1:A:29:LYS:N	1.93	0.57
2:B:213:LEU:HG	2:B:223:THR:HG23	1.86	0.57
2:B:340:VAL:O	2:B:340:VAL:CG1	2.53	0.57
1:C:172:LEU:HD12	1:C:172:LEU:C	2.24	0.57
1:C:204:TYR:CE1	1:C:229:ALA:HB3	2.40	0.57
2:D:95:VAL:HG22	2:D:228:VAL:CG1	2.34	0.57
2:D:212:HIS:HB3	2:D:223:THR:HG21	1.85	0.57
2:D:340:VAL:O	2:D:340:VAL:HG12	2.04	0.57
1:E:118:VAL:C	1:E:119:PHE:HD1	2.08	0.57
1:E:301:GLU:O	1:E:304:ILE:HG13	2.05	0.57
1:G:193:ILE:C	1:G:195:VAL:H	2.07	0.57
2:B:27:ALA:HB2	2:B:146:PHE:CE1	2.40	0.57
2:B:93:PRO:HG3	2:B:96:ILE:CD1	2.34	0.57
2:D:75:GLY:O	2:D:76:ALA:HB2	2.05	0.57
2:D:85:LYS:O	2:D:89:GLU:HG2	2.05	0.57
2:D:213:LEU:HD12	2:D:223:THR:OG1	2.05	0.57
1:E:199:ASN:ND2	1:E:225:LEU:HB2	2.14	0.57
2:H:173:ASN:HB2	2:H:240:THR:CG2	2.23	0.57
1:A:102:LEU:CD2	1:A:106:ILE:HD11	2.35	0.56
1:A:337:TRP:CE3	1:A:337:TRP:O	2.58	0.56
1:C:397:LEU:HD22	1:C:398:ILE:H	1.70	0.56
2:D:433:GLU:HG3	2:D:434:HIS:HD2	1.69	0.56
2:H:331:LEU:O	2:H:331:LEU:HD22	2.05	0.56
1:A:245:VAL:HG13	1:A:290:LEU:HD23	1.87	0.56
2:D:33:ARG:N	2:D:221:LEU:HD23	2.20	0.56
1:E:370:MET:O	1:E:370:MET:HG2	2.04	0.56
1:G:102:LEU:CD2	1:G:106:ILE:HD11	2.36	0.56
1:G:353:THR:HG22	1:G:377:LEU:HD23	1.85	0.56
2:H:397:LEU:CD2	2:H:427:LEU:CD2	2.83	0.56
1:A:48:PRO:HG2	1:A:229:ALA:HB1	1.87	0.56
1:A:68:ASP:HB3	2:B:384:HIS:HE1	1.71	0.56
2:B:34:SER:H	2:B:221:LEU:CD2	2.09	0.56
2:D:93:PRO:HG3	2:D:96:ILE:CD1	2.34	0.56
2:D:191:SER:CB	2:D:277:TRP:HZ3	2.16	0.56
2:D:433:GLU:HG3	2:D:434:HIS:CD2	2.39	0.56
1:E:207:ALA:HB2	1:E:421:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:LEU:O	2:F:221:LEU:HD21	2.05	0.56
2:F:34:SER:H	2:F:221:LEU:CD2	2.13	0.56
2:F:82:GLU:O	2:F:86:THR:OG1	2.16	0.56
1:G:67:TRP:HZ3	2:H:15:PRO:O	1.87	0.56
1:G:421:ARG:HH22	1:G:422:GLU:HB3	1.71	0.56
1:G:425:TYR:HD1	1:G:433:GLU:OE1	1.89	0.56
2:H:117:GLU:C	2:H:122:TYR:HH	2.04	0.56
2:H:159:PRO:CG	2:H:257:ARG:NH1	2.67	0.56
2:H:160:GLU:CD	2:H:161:ARG:H	2.08	0.56
2:H:383:SER:OG	2:H:403:GLN:HA	2.04	0.56
1:E:181:PRO:CD	1:E:242:ARG:HG3	2.36	0.56
2:F:118:PHE:O	2:F:119:ARG:HD3	2.04	0.56
1:A:29:LYS:CB	1:A:30:PRO:HD2	2.28	0.56
2:B:433:GLU:HG3	2:B:434:HIS:CD2	2.41	0.56
2:D:126:LYS:HG3	2:D:127:ASP:N	2.20	0.56
1:G:356:LYS:HG2	1:G:376:MET:SD	2.45	0.56
2:H:213:LEU:HD12	2:H:223:THR:OG1	2.05	0.56
2:B:28:ILE:HG13	2:B:29:LEU:N	2.21	0.56
2:B:100:THR:HG22	2:B:134:ASN:HA	1.88	0.56
2:D:38:PHE:CD2	2:D:45:THR:HG22	2.41	0.56
2:D:173:ASN:HD22	2:D:240:THR:HG22	1.70	0.56
1:E:226:CYS:HB3	1:E:240:MET:HE2	1.88	0.56
2:F:17:LYS:HG3	2:F:345:PRO:CB	2.33	0.56
1:G:27:LYS:HD2	1:G:27:LYS:O	2.04	0.56
1:G:67:TRP:O	1:G:81:ARG:NH2	2.39	0.56
2:B:158:VAL:N	2:B:159:PRO:CD	2.69	0.56
2:D:158:VAL:N	2:D:159:PRO:CD	2.69	0.56
2:D:213:LEU:CD2	2:D:214:ASP:H	2.16	0.56
1:E:287:PHE:O	1:E:291:LEU:HD23	2.05	0.56
2:F:100:THR:HG22	2:F:134:ASN:HA	1.88	0.56
1:G:337:TRP:CE3	1:G:337:TRP:O	2.58	0.56
1:A:193:ILE:HD13	1:A:293:ASP:OD1	2.06	0.56
1:A:204:TYR:HB2	1:A:206:ILE:HD13	1.88	0.56
1:A:306:ARG:NH2	1:A:307:GLU:OE1	2.39	0.56
1:A:373:ASP:CG	1:A:374:VAL:H	2.09	0.56
1:A:409:LYS:HB3	2:B:218:PHE:HZ	1.71	0.56
1:E:173:LYS:HG3	1:E:173:LYS:O	2.04	0.56
1:E:176:ILE:HG13	1:E:178:THR:HG23	1.88	0.56
2:H:185:LEU:HB2	2:H:206:SER:OG	2.06	0.56
2:B:397:LEU:HD23	2:B:427:LEU:HD21	1.86	0.56
1:E:337:TRP:O	1:E:337:TRP:CE3	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:ASN:HB2	2:D:240:THR:CG2	2.23	0.56
2:F:68:ASP:CB	2:F:70:VAL:HG22	2.24	0.56
1:A:67:TRP:CD1	1:A:67:TRP:C	2.79	0.55
2:B:269:TYR:O	2:B:273:ALA:HB3	2.06	0.55
2:D:28:ILE:HD12	2:D:34:SER:OG	2.06	0.55
2:F:126:LYS:HG3	2:F:127:ASP:H	1.69	0.55
1:G:330:TYR:HB3	1:G:399:ALA:HB2	1.88	0.55
2:H:158:VAL:N	2:H:159:PRO:CD	2.69	0.55
1:A:67:TRP:CH2	2:B:15:PRO:O	2.60	0.55
1:A:197:ASP:OD2	1:A:223:ARG:HD3	2.06	0.55
1:C:275:TYR:CD2	1:C:338:SER:HB2	2.41	0.55
2:D:207:GLY:O	2:D:223:THR:O	2.25	0.55
1:E:174:TYR:CZ	1:E:234:TYR:CZ	2.94	0.55
1:E:421:ARG:NE	1:E:422:GLU:H	2.03	0.55
1:G:67:TRP:C	1:G:67:TRP:CD1	2.79	0.55
1:G:370:MET:O	1:G:370:MET:HG2	2.04	0.55
1:G:421:ARG:NH2	1:G:422:GLU:H	2.03	0.55
2:H:124:GLU:OE1	2:H:126:LYS:N	2.38	0.55
1:A:108:GLN:CD	2:B:11:LEU:HB3	2.26	0.55
1:A:123:THR:O	1:A:126:PRO:HD2	2.06	0.55
1:A:287:PHE:O	1:A:291:LEU:HD23	2.06	0.55
2:B:67:MET:HE2	2:B:71:SER:HB2	1.88	0.55
2:B:75:GLY:O	2:B:76:ALA:HB2	2.06	0.55
1:C:370:MET:O	1:C:370:MET:HG2	2.05	0.55
2:D:67:MET:HE2	2:D:71:SER:HB2	1.88	0.55
2:D:185:LEU:HB2	2:D:206:SER:OG	2.06	0.55
1:E:232:ALA:HA	1:E:236:GLU:OE1	2.05	0.55
2:F:26:LEU:HD21	2:F:401:PHE:CZ	2.42	0.55
2:F:95:VAL:HG22	2:F:228:VAL:CG1	2.37	0.55
2:F:213:LEU:CD2	2:F:214:ASP:H	2.16	0.55
2:H:160:GLU:O	2:H:161:ARG:C	2.45	0.55
2:H:191:SER:CB	2:H:277:TRP:HZ3	2.19	0.55
2:B:110:ASP:HB2	2:B:113:THR:HB	1.89	0.55
2:B:159:PRO:HB2	2:B:257:ARG:CG	2.37	0.55
2:B:433:GLU:HG3	2:B:434:HIS:HD2	1.71	0.55
1:C:92:ASP:HA	1:C:97:ARG:HB3	1.87	0.55
1:C:356:LYS:HG2	1:C:376:MET:SD	2.46	0.55
1:C:383:ARG:HE	2:D:90:ARG:HH12	1.54	0.55
2:D:188:ILE:HD11	2:D:268:LEU:HD12	1.87	0.55
1:E:204:TYR:CE1	1:E:229:ALA:HB3	2.41	0.55
2:F:20:GLN:HG2	2:F:135:THR:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:PRO:HG3	2:F:96:ILE:HG13	1.87	0.55
2:F:158:VAL:N	2:F:159:PRO:CD	2.70	0.55
1:G:169:GLU:O	1:G:172:LEU:HG	2.05	0.55
2:H:93:PRO:HG3	2:H:96:ILE:HG13	1.88	0.55
2:B:185:LEU:HB2	2:B:206:SER:OG	2.06	0.55
2:B:212:HIS:NE2	2:D:295:ARG:NE	2.54	0.55
2:B:401:PHE:HD2	2:B:401:PHE:O	1.89	0.55
1:C:383:ARG:N	2:D:217:ARG:HH12	2.05	0.55
1:E:383:ARG:HD2	2:F:217:ARG:HH22	1.72	0.55
1:G:190:ARG:HB3	1:G:191:PRO:HD2	0.74	0.55
1:G:362:ASP:C	1:G:366:ILE:HG13	2.27	0.55
2:H:118:PHE:O	2:H:119:ARG:HD3	2.06	0.55
2:B:164:GLN:O	2:B:167:LYS:HG2	2.06	0.55
2:D:349:ALA:O	2:D:350:ALA:C	2.45	0.55
1:G:137:CYS:SG	1:G:150:PRO:HB3	2.47	0.55
1:G:174:TYR:CZ	1:G:234:TYR:CE2	2.94	0.55
2:H:340:VAL:O	2:H:340:VAL:HG12	2.06	0.55
1:A:275:TYR:CD2	1:A:338:SER:HB2	2.41	0.55
2:D:396:LEU:HD22	2:D:397:LEU:N	2.21	0.55
1:E:137:CYS:SG	1:E:150:PRO:HB3	2.47	0.55
2:H:246:SER:HB3	2:H:323:ASP:OD2	2.07	0.55
1:A:199:ASN:ND2	1:A:225:LEU:HB2	2.13	0.55
2:B:285:SER:HB3	2:B:287:ASN:HD21	1.72	0.55
2:B:395:PRO:HG3	2:B:434:HIS:CG	2.42	0.55
1:C:169:GLU:O	1:C:172:LEU:HG	2.07	0.55
1:E:206:ILE:HG13	1:E:419:GLN:HG3	1.88	0.55
1:E:275:TYR:CD2	1:E:338:SER:HB2	2.41	0.55
1:E:356:LYS:HG2	1:E:376:MET:SD	2.47	0.55
1:A:199:ASN:HB2	1:A:246:ASN:ND2	2.21	0.55
1:A:314:ALA:HB2	1:E:191:PRO:CG	2.37	0.55
1:A:383:ARG:HE	2:B:90:ARG:HH12	1.55	0.55
1:C:306:ARG:NH2	1:C:307:GLU:OE1	2.40	0.55
1:C:383:ARG:HD2	2:D:217:ARG:HH22	1.72	0.55
2:F:185:LEU:HB2	2:F:206:SER:OG	2.06	0.55
1:G:123:THR:O	1:G:126:PRO:HD2	2.06	0.55
1:G:173:LYS:HG3	1:G:173:LYS:O	2.05	0.55
1:G:302:ALA:O	1:G:305:ALA:HB3	2.07	0.55
1:C:40:ASP:O	1:C:44:ILE:HG12	2.06	0.55
1:C:199:ASN:HB2	1:C:246:ASN:ND2	2.22	0.55
2:F:213:LEU:HD12	2:F:223:THR:OG1	2.06	0.55
1:G:409:LYS:HB3	2:H:218:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:THR:O	1:A:357:LYS:N	2.37	0.54
1:C:67:TRP:O	1:C:81:ARG:NH2	2.39	0.54
1:C:133:VAL:HG23	1:C:134:ASP:OD1	2.07	0.54
1:E:27:LYS:HD2	1:E:27:LYS:C	2.27	0.54
1:E:424:GLY:O	1:E:433:GLU:OE2	2.23	0.54
2:F:191:SER:CB	2:F:277:TRP:HZ3	2.20	0.54
1:G:386:LEU:HD21	2:H:216:ASN:HB3	1.87	0.54
1:G:419:GLN:HE22	1:G:424:GLY:H	1.55	0.54
2:H:401:PHE:HD2	2:H:401:PHE:O	1.90	0.54
1:A:54:HIS:HD2	1:A:121:TYR:OH	1.90	0.54
1:C:48:PRO:HG2	1:C:229:ALA:HB1	1.89	0.54
2:D:228:VAL:HG23	2:D:229:ALA:N	2.21	0.54
1:E:68:ASP:HB3	2:F:384:HIS:CE1	2.43	0.54
2:F:4:ILE:N	2:F:353:ASP:OD2	2.41	0.54
1:G:165:ARG:NH1	4:G:502:CZL:S4B	2.77	0.54
1:G:204:TYR:HA	1:G:229:ALA:O	2.06	0.54
1:A:424:GLY:O	1:A:433:GLU:OE2	2.25	0.54
2:B:160:GLU:CD	2:B:161:ARG:H	2.10	0.54
2:D:55:HIS:CE1	2:D:403:GLN:HG2	2.43	0.54
1:E:132:ASP:O	1:E:136:VAL:HG23	2.07	0.54
1:E:190:ARG:CB	1:E:191:PRO:CD	2.48	0.54
2:F:42:GLN:CA	2:F:64:THR:HG21	2.35	0.54
1:G:440:ILE:HG13	1:G:441:THR:N	2.22	0.54
2:H:20:GLN:HG2	2:H:135:THR:CB	2.37	0.54
1:E:190:ARG:HB3	1:E:191:PRO:HD2	0.72	0.54
2:F:29:LEU:O	2:F:221:LEU:HD11	2.06	0.54
1:G:433:GLU:O	1:G:437:GLN:HG2	2.07	0.54
1:A:421:ARG:NH2	1:A:422:GLU:H	2.06	0.54
2:D:354:SER:HB2	2:D:355:PRO:HD2	1.89	0.54
1:G:68:ASP:HB3	2:H:384:HIS:HE1	1.72	0.54
1:G:181:PRO:HD3	1:G:242:ARG:HG3	1.87	0.54
2:H:76:ALA:O	2:H:77:ASP:C	2.44	0.54
1:C:86:THR:HG23	1:C:86:THR:O	2.07	0.54
2:D:126:LYS:HG3	2:D:127:ASP:H	1.72	0.54
2:D:159:PRO:HG3	2:D:257:ARG:NH1	2.18	0.54
1:E:71:GLY:HA2	1:E:420:GLU:CA	2.37	0.54
2:H:397:LEU:HD22	2:H:427:LEU:HD23	1.89	0.54
2:B:420:SER:O	2:B:424:LEU:HD12	2.07	0.54
1:C:68:ASP:CA	1:C:81:ARG:HH22	2.21	0.54
1:E:57:HIS:O	1:E:126:PRO:HG2	2.08	0.54
1:G:68:ASP:O	1:G:81:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ILE:HB	1:G:420:GLU:HA	1.88	0.54
1:G:209:GLU:HG2	1:G:210:PHE:N	2.15	0.54
2:H:64:THR:HG22	2:H:66:ALA:N	2.22	0.54
2:H:175:LEU:HB3	2:H:247:LEU:HD13	1.89	0.54
2:H:374:GLY:O	2:H:375:GLN:HB2	2.07	0.54
1:A:193:ILE:H	1:A:193:ILE:CD1	2.16	0.54
2:B:173:ASN:HD22	2:B:240:THR:HG22	1.73	0.54
2:B:382:ASN:C	2:B:382:ASN:HD22	2.10	0.54
1:E:373:ASP:CG	1:E:374:VAL:H	2.11	0.54
2:F:67:MET:HE2	2:F:71:SER:HB2	1.89	0.54
2:F:160:GLU:CD	2:F:161:ARG:H	2.11	0.54
1:G:196:HIS:HB3	1:G:291:LEU:HD11	1.88	0.54
1:G:397:LEU:HD22	1:G:398:ILE:H	1.72	0.54
1:G:444:CYS:SG	1:G:446:VAL:HG23	2.47	0.54
1:A:206:ILE:HB	1:A:420:GLU:CA	2.37	0.54
1:C:359:THR:CG2	4:C:502:CZL:S2A	2.96	0.54
1:E:94:ILE:O	1:E:94:ILE:CD1	2.56	0.54
1:G:37:CYS:HB2	1:G:39:PHE:H	1.72	0.54
1:G:228:LEU:O	1:G:229:ALA:HB3	2.08	0.54
1:A:154:ALA:O	1:A:157:TYR:CD1	2.61	0.54
2:B:17:LYS:HG3	2:B:345:PRO:CB	2.35	0.54
2:B:89:GLU:OE2	2:B:124:GLU:HB2	2.07	0.54
1:C:29:LYS:CB	1:C:30:PRO:HD2	2.33	0.54
1:C:355:THR:O	1:C:357:LYS:N	2.37	0.54
2:D:331:LEU:HD22	2:D:331:LEU:C	2.28	0.54
1:E:193:ILE:C	1:E:195:VAL:N	2.62	0.54
2:F:24:ALA:HB1	2:F:149:ALA:HB2	1.90	0.54
1:G:199:ASN:HB2	1:G:246:ASN:ND2	2.22	0.54
1:A:353:THR:HG22	1:A:377:LEU:HD23	1.90	0.53
2:D:26:LEU:HD21	2:D:401:PHE:CZ	2.43	0.53
2:D:160:GLU:CD	2:D:161:ARG:H	2.12	0.53
2:F:76:ALA:O	2:F:77:ASP:C	2.45	0.53
1:A:196:HIS:ND1	1:A:291:LEU:HD12	2.23	0.53
2:D:76:ALA:O	2:D:77:ASP:C	2.47	0.53
1:E:362:ASP:C	1:E:366:ILE:HG13	2.28	0.53
2:F:125:TYR:O	2:F:126:LYS:CB	2.56	0.53
1:G:206:ILE:HG13	1:G:419:GLN:HG3	1.89	0.53
1:G:421:ARG:NE	1:G:422:GLU:H	2.05	0.53
2:H:95:VAL:HG22	2:H:228:VAL:CG1	2.38	0.53
2:B:354:SER:CB	2:B:355:PRO:HD2	2.38	0.53
2:D:256:GLU:HA	2:D:256:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:CYS:HA	3:E:501:SF4:S3	2.49	0.53
1:E:421:ARG:HH22	1:E:422:GLU:HB3	1.73	0.53
2:H:49:LYS:O	2:H:53:VAL:HG13	2.08	0.53
2:H:186:GLU:O	2:H:190:GLU:HG2	2.08	0.53
2:H:420:SER:O	2:H:424:LEU:HD12	2.07	0.53
1:A:433:GLU:O	1:A:437:GLN:HG2	2.07	0.53
2:B:126:LYS:HG3	2:B:127:ASP:N	2.23	0.53
1:C:206:ILE:HB	1:C:420:GLU:CA	2.38	0.53
2:D:344:VAL:O	2:D:361:VAL:HA	2.08	0.53
2:F:173:ASN:HD22	2:F:240:THR:HG22	1.73	0.53
2:F:269:TYR:O	2:F:273:ALA:HB3	2.08	0.53
1:G:29:LYS:HG2	2:H:65:THR:O	2.09	0.53
1:G:380:GLY:HA2	1:G:383:ARG:HD3	1.90	0.53
1:G:383:ARG:H	2:H:217:ARG:HH22	1.56	0.53
2:H:110:ASP:HB2	2:H:113:THR:HB	1.89	0.53
2:H:315:ARG:HG3	2:H:340:VAL:HG21	1.89	0.53
1:A:241:HIS:ND1	1:A:241:HIS:N	2.52	0.53
2:B:33:ARG:N	2:B:221:LEU:HD23	2.22	0.53
1:C:54:HIS:HD2	1:C:121:TYR:OH	1.92	0.53
1:C:123:THR:CG2	3:C:501:SF4:S4	2.97	0.53
1:C:353:THR:HG22	1:C:377:LEU:HD23	1.89	0.53
2:D:333:ARG:NH1	2:D:333:ARG:HB2	2.23	0.53
2:H:85:LYS:O	2:H:89:GLU:HG2	2.08	0.53
2:H:275:ASP:OD1	2:H:297:ARG:NE	2.29	0.53
2:H:333:ARG:HB2	2:H:333:ARG:HH11	1.72	0.53
1:A:68:ASP:HB3	2:B:384:HIS:CE1	2.43	0.53
1:A:397:LEU:HD22	1:A:398:ILE:H	1.74	0.53
2:B:4:ILE:N	2:B:353:ASP:OD2	2.42	0.53
2:B:95:VAL:HG22	2:B:228:VAL:CG1	2.38	0.53
2:D:385:ALA:O	2:D:386:LEU:C	2.46	0.53
2:H:38:PHE:CD2	2:H:45:THR:HG22	2.44	0.53
1:A:307:GLU:O	1:A:311:VAL:CG2	2.54	0.53
2:B:85:LYS:O	2:B:89:GLU:HG2	2.09	0.53
1:C:337:TRP:CD1	1:C:365:ARG:HG2	2.44	0.53
2:D:28:ILE:HD11	2:D:36:PRO:N	2.23	0.53
2:D:351:LEU:O	2:D:353:ASP:N	2.42	0.53
1:E:102:LEU:HD23	1:E:102:LEU:O	2.09	0.53
1:G:193:ILE:C	1:G:195:VAL:N	2.62	0.53
1:G:327:VAL:HG23	1:G:327:VAL:O	2.09	0.53
1:A:335:LYS:O	1:A:338:SER:OG	2.27	0.53
1:A:380:GLY:HA2	1:A:383:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:C	1:C:195:VAL:N	2.62	0.53
2:D:38:PHE:HB2	2:D:45:THR:HG22	1.91	0.53
2:D:353:ASP:O	2:D:354:SER:OG	2.21	0.53
1:E:133:VAL:HG23	1:E:134:ASP:OD1	2.09	0.53
1:E:228:LEU:O	1:E:229:ALA:HB3	2.09	0.53
2:F:252:ASP:O	2:F:256:GLU:HG2	2.09	0.53
2:F:333:ARG:HH11	2:F:333:ARG:CB	2.20	0.53
1:G:128:LEU:HD23	2:H:106:THR:HG21	1.90	0.53
2:H:75:GLY:O	2:H:76:ALA:CB	2.57	0.53
1:A:327:VAL:HG21	1:A:343:LEU:CD1	2.39	0.53
2:B:333:ARG:NH1	2:B:333:ARG:HB2	2.24	0.53
1:C:380:GLY:HA2	1:C:383:ARG:HD3	1.91	0.53
2:D:57:ARG:O	2:D:58:GLU:CD	2.47	0.53
2:D:401:PHE:O	2:D:401:PHE:HD2	1.92	0.53
1:G:181:PRO:CD	1:G:242:ARG:HG3	2.39	0.53
1:G:300:THR:O	1:G:304:ILE:HG23	2.09	0.53
2:H:118:PHE:O	2:H:122:TYR:CE2	2.61	0.53
2:H:256:GLU:HA	2:H:256:GLU:OE2	2.09	0.53
1:A:57:HIS:HE1	1:A:131:ASP:OD1	1.92	0.53
1:A:191:PRO:HG2	1:E:310:LYS:HZ2	1.74	0.53
1:G:68:ASP:CA	1:G:81:ARG:HH22	2.22	0.53
1:G:440:ILE:HG13	1:G:441:THR:H	1.74	0.53
1:A:362:ASP:C	1:A:366:ILE:HG13	2.28	0.52
2:B:159:PRO:HG3	2:B:257:ARG:NH1	2.19	0.52
2:B:354:SER:HB2	2:B:355:PRO:HD2	1.92	0.52
1:C:241:HIS:ND1	1:C:241:HIS:N	2.49	0.52
1:C:337:TRP:CD1	1:C:365:ARG:HB3	2.43	0.52
2:D:110:ASP:HB2	2:D:113:THR:HB	1.91	0.52
1:E:40:ASP:O	1:E:44:ILE:HG12	2.10	0.52
2:F:105:GLU:HG2	2:F:136:PRO:HG3	1.91	0.52
2:F:433:GLU:HG3	2:F:434:HIS:HD2	1.74	0.52
1:G:67:TRP:CZ3	2:H:15:PRO:HG2	2.44	0.52
1:G:132:ASP:O	1:G:136:VAL:HG23	2.08	0.52
1:G:367:ARG:HH21	1:G:375:LYS:HD2	1.74	0.52
2:H:28:ILE:HD11	2:H:36:PRO:N	2.24	0.52
1:A:174:TYR:O	1:A:174:TYR:CD2	2.63	0.52
1:A:206:ILE:CB	1:A:420:GLU:HA	2.40	0.52
1:A:430:GLY:O	1:A:433:GLU:OE1	2.27	0.52
2:B:36:PRO:HB2	2:B:62:LEU:HD13	1.90	0.52
2:B:211:GLY:HA3	2:D:302:ASP:HB2	1.90	0.52
2:D:117:GLU:C	2:D:122:TYR:HH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:TRP:O	1:E:81:ARG:NH2	2.42	0.52
1:E:154:ALA:O	1:E:157:TYR:HD1	1.92	0.52
1:E:380:GLY:HA2	1:E:383:ARG:HD3	1.91	0.52
2:F:28:ILE:HG13	2:F:29:LEU:N	2.23	0.52
2:F:39:HIS:CD2	2:F:80:VAL:HG22	2.44	0.52
1:G:206:ILE:HG22	1:G:420:GLU:HA	1.90	0.52
2:H:31:LEU:HD12	2:H:226:LEU:HB2	1.91	0.52
2:H:354:SER:CB	2:H:355:PRO:HD2	2.39	0.52
2:H:396:LEU:HD22	2:H:397:LEU:N	2.24	0.52
1:A:199:ASN:OD1	1:A:240:MET:HG2	2.09	0.52
2:B:118:PHE:O	2:B:122:TYR:CE2	2.62	0.52
1:C:287:PHE:O	1:C:291:LEU:CD2	2.57	0.52
1:C:419:GLN:HE22	1:C:424:GLY:H	1.57	0.52
1:C:421:ARG:NH2	1:C:422:GLU:H	2.07	0.52
1:E:102:LEU:CD2	1:E:106:ILE:HD11	2.40	0.52
1:G:68:ASP:HB3	2:H:384:HIS:CE1	2.44	0.52
1:G:176:ILE:HG13	1:G:178:THR:HG23	1.91	0.52
2:H:348:ALA:O	2:H:349:ALA:O	2.27	0.52
1:A:172:LEU:CD1	1:A:173:LYS:N	2.64	0.52
1:C:108:GLN:NE2	2:D:11:LEU:H	2.07	0.52
1:C:327:VAL:HG21	1:C:343:LEU:CD1	2.39	0.52
2:D:159:PRO:CG	2:D:257:ARG:NH1	2.70	0.52
1:E:67:TRP:C	1:E:67:TRP:CD1	2.82	0.52
1:E:241:HIS:ND1	1:E:241:HIS:N	2.45	0.52
1:E:337:TRP:CD1	1:E:365:ARG:HB3	2.44	0.52
2:F:75:GLY:O	2:F:76:ALA:CB	2.57	0.52
1:G:253:ALA:HA	4:G:502:CZL:S5A	2.49	0.52
2:H:27:ALA:HB2	2:H:146:PHE:CD1	2.44	0.52
1:A:337:TRP:CD1	1:A:365:ARG:HB3	2.45	0.52
2:B:82:GLU:O	2:B:86:THR:OG1	2.20	0.52
1:C:228:LEU:O	1:C:229:ALA:HB3	2.09	0.52
1:C:323:GLU:HA	1:C:323:GLU:OE2	2.09	0.52
2:H:397:LEU:HD23	2:H:427:LEU:CD2	2.35	0.52
1:C:71:GLY:HA2	1:C:420:GLU:CA	2.40	0.52
1:C:206:ILE:CB	1:C:420:GLU:HA	2.40	0.52
1:C:373:ASP:CG	1:C:374:VAL:H	2.13	0.52
1:E:307:GLU:O	1:E:311:VAL:CG2	2.55	0.52
2:H:264:ARG:O	2:H:265:PHE:CB	2.54	0.52
2:B:20:GLN:HG2	2:B:135:THR:CB	2.39	0.52
1:C:206:ILE:HG22	1:C:420:GLU:HA	1.90	0.52
1:E:30:PRO:HD3	2:F:64:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:LEU:HD22	1:G:322:LEU:N	2.25	0.52
1:G:336:SER:O	1:G:339:VAL:HG23	2.09	0.52
1:A:327:VAL:HG23	1:A:327:VAL:O	2.10	0.52
2:B:331:LEU:O	2:B:331:LEU:HD22	2.10	0.52
1:C:174:TYR:CZ	1:C:234:TYR:CZ	2.98	0.52
2:F:67:MET:HE3	2:F:71:SER:HB2	1.90	0.52
2:F:159:PRO:HB2	2:F:257:ARG:CG	2.39	0.52
2:F:228:VAL:HG23	2:F:229:ALA:N	2.25	0.52
1:G:383:ARG:CA	2:H:217:ARG:HH12	2.22	0.52
2:H:118:PHE:HA	2:H:122:TYR:CE1	2.44	0.52
2:B:93:PRO:HG3	2:B:96:ILE:HG13	1.90	0.52
1:C:65:SER:O	1:C:68:ASP:OD1	2.28	0.52
1:C:206:ILE:CD1	1:C:419:GLN:HB3	2.40	0.52
1:G:174:TYR:CD2	1:G:174:TYR:O	2.63	0.52
1:A:444:CYS:SG	1:A:446:VAL:HG23	2.50	0.52
2:B:51:PHE:CE1	2:B:402:PRO:HB3	2.46	0.52
1:C:421:ARG:NE	1:C:422:GLU:H	2.07	0.52
2:F:156:THR:HG22	2:F:157:LEU:HD13	1.92	0.52
2:F:317:ALA:HB3	2:F:379:VAL:HG22	1.91	0.52
1:G:143:ARG:HB3	1:G:143:ARG:NH1	2.25	0.52
1:A:48:PRO:HG2	1:A:204:TYR:HD1	1.75	0.51
1:A:337:TRP:CD1	1:A:365:ARG:HG2	2.45	0.51
1:A:421:ARG:NE	1:A:422:GLU:H	2.07	0.51
2:D:126:LYS:HZ2	2:D:127:ASP:H	1.52	0.51
2:F:348:ALA:O	2:F:349:ALA:O	2.27	0.51
1:G:337:TRP:CD1	1:G:365:ARG:HB3	2.44	0.51
1:A:86:THR:HG23	1:A:86:THR:O	2.09	0.51
1:A:252:LYS:CB	1:A:361:GLU:OE2	2.56	0.51
1:A:373:ASP:CG	1:A:374:VAL:N	2.64	0.51
2:B:26:LEU:HD21	2:B:401:PHE:CZ	2.45	0.51
1:C:362:ASP:C	1:C:366:ILE:HG13	2.31	0.51
1:E:169:GLU:O	1:E:172:LEU:HG	2.10	0.51
1:E:181:PRO:HD3	1:E:242:ARG:HG3	1.91	0.51
1:E:353:THR:HG22	1:E:377:LEU:HD23	1.91	0.51
1:G:38:SER:O	1:G:163:GLY:HA3	2.10	0.51
1:G:179:ARG:NH2	1:G:239:THR:CG2	2.73	0.51
1:G:206:ILE:HB	1:G:420:GLU:CA	2.40	0.51
1:G:328:LEU:HD22	1:G:389:VAL:HG22	1.92	0.51
1:A:206:ILE:HG22	1:A:420:GLU:HA	1.91	0.51
1:A:245:VAL:CG1	1:A:290:LEU:HD23	2.39	0.51
1:C:30:PRO:HB3	2:D:63:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:PHE:O	2:D:119:ARG:HD3	2.10	0.51
2:D:228:VAL:CG2	2:D:229:ALA:N	2.73	0.51
2:D:325:LEU:HD11	2:D:342:ALA:HB1	1.92	0.51
1:E:306:ARG:NH2	1:E:307:GLU:OE1	2.43	0.51
2:F:85:LYS:O	2:F:89:GLU:HG2	2.10	0.51
2:F:110:ASP:HB2	2:F:113:THR:HB	1.92	0.51
1:G:40:ASP:O	1:G:44:ILE:HG12	2.10	0.51
2:H:57:ARG:O	2:H:58:GLU:CD	2.49	0.51
1:C:196:HIS:ND1	1:C:291:LEU:HD12	2.26	0.51
1:E:227:THR:O	1:E:229:ALA:N	2.43	0.51
2:F:256:GLU:OE2	2:F:256:GLU:HA	2.10	0.51
1:G:355:THR:C	1:G:357:LYS:H	2.14	0.51
2:H:354:SER:HB2	2:H:355:PRO:HD2	1.92	0.51
2:H:382:ASN:ND2	2:H:384:HIS:H	2.07	0.51
1:A:179:ARG:NH2	1:A:239:THR:CG2	2.73	0.51
1:A:204:TYR:CE1	1:A:229:ALA:CB	2.93	0.51
2:B:74:MET:O	2:B:76:ALA:N	2.44	0.51
2:B:228:VAL:HG23	2:B:229:ALA:N	2.24	0.51
1:C:67:TRP:HZ3	2:D:15:PRO:O	1.91	0.51
1:C:94:ILE:O	1:C:94:ILE:CD1	2.56	0.51
2:D:124:GLU:OE1	2:D:126:LYS:N	2.42	0.51
2:D:340:VAL:O	2:D:340:VAL:CG1	2.59	0.51
1:E:68:ASP:O	1:E:81:ARG:NH2	2.43	0.51
2:F:89:GLU:OE2	2:F:124:GLU:HB2	2.11	0.51
2:F:213:LEU:HG	2:F:223:THR:HG23	1.93	0.51
1:A:421:ARG:HH22	1:A:422:GLU:HB3	1.74	0.51
2:B:191:SER:HB3	2:B:277:TRP:CZ3	2.43	0.51
1:E:57:HIS:HE1	1:E:131:ASP:OD1	1.94	0.51
1:E:357:LYS:N	1:E:357:LYS:HD2	2.25	0.51
2:F:396:LEU:HD22	2:F:397:LEU:N	2.25	0.51
1:G:323:GLU:HA	1:G:323:GLU:OE2	2.09	0.51
2:H:160:GLU:CG	2:H:161:ARG:N	2.72	0.51
1:A:38:SER:O	1:A:163:GLY:HA3	2.10	0.51
1:A:193:ILE:C	1:A:195:VAL:N	2.61	0.51
1:A:339:VAL:O	1:A:342:ALA:HB3	2.11	0.51
2:B:125:TYR:O	2:B:126:LYS:CB	2.57	0.51
1:C:421:ARG:HH22	1:C:422:GLU:HB3	1.76	0.51
1:E:327:VAL:HG21	1:E:343:LEU:HD11	1.92	0.51
2:F:175:LEU:HB3	2:F:247:LEU:HD13	1.92	0.51
1:G:252:LYS:CB	1:G:361:GLU:OE2	2.57	0.51
2:H:173:ASN:HD22	2:H:240:THR:HG22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:SER:O	1:A:339:VAL:HG23	2.10	0.51
2:B:160:GLU:CG	2:B:161:ARG:N	2.74	0.51
1:C:336:SER:O	1:C:339:VAL:HG23	2.11	0.51
1:E:47:LEU:N	1:E:48:PRO:HD3	2.26	0.51
1:E:204:TYR:HB2	1:E:206:ILE:HD13	1.92	0.51
1:E:355:THR:C	1:E:357:LYS:H	2.15	0.51
1:E:367:ARG:HH21	1:E:375:LYS:HD2	1.76	0.51
1:G:198:VAL:HG22	1:G:223:ARG:O	2.11	0.51
1:G:327:VAL:HG21	1:G:343:LEU:CD1	2.40	0.51
2:H:204:ASP:OD1	2:H:206:SER:HB2	2.11	0.51
2:H:269:TYR:O	2:H:273:ALA:HB3	2.10	0.51
1:A:169:GLU:O	1:A:172:LEU:HG	2.10	0.51
2:B:156:THR:HG22	2:B:157:LEU:HD13	1.92	0.51
2:B:354:SER:CB	2:B:355:PRO:CD	2.89	0.51
1:C:173:LYS:HG3	1:C:173:LYS:O	2.10	0.51
1:C:174:TYR:OH	1:C:238:GLN:CG	2.59	0.51
1:C:433:GLU:O	1:C:437:GLN:HG2	2.11	0.51
2:D:100:THR:HG22	2:D:135:THR:N	2.15	0.51
2:D:160:GLU:CG	2:D:161:ARG:N	2.73	0.51
1:E:204:TYR:CE1	1:E:229:ALA:CB	2.93	0.51
1:G:133:VAL:HG23	1:G:134:ASP:OD1	2.10	0.51
1:G:355:THR:O	1:G:357:LYS:N	2.39	0.51
1:A:296:LEU:O	1:A:300:THR:HG23	2.11	0.51
1:A:330:TYR:HB3	1:A:399:ALA:CB	2.41	0.51
2:B:36:PRO:HB2	2:B:62:LEU:CD1	2.41	0.51
2:B:38:PHE:CD2	2:B:45:THR:HG22	2.46	0.51
1:C:38:SER:O	1:C:163:GLY:HA3	2.11	0.51
1:C:204:TYR:CE1	1:C:229:ALA:CB	2.94	0.51
1:C:339:VAL:O	1:C:342:ALA:HB3	2.11	0.51
1:C:439:CYS:O	1:C:440:ILE:C	2.49	0.51
2:D:75:GLY:O	2:D:76:ALA:CB	2.59	0.51
1:E:204:TYR:HA	1:E:229:ALA:O	2.11	0.51
1:E:383:ARG:H	2:F:217:ARG:HH22	1.59	0.51
1:E:388:THR:O	1:E:392:TYR:HD2	1.94	0.51
2:F:55:HIS:CE1	2:F:403:GLN:HG2	2.46	0.51
2:F:160:GLU:CG	2:F:161:ARG:N	2.73	0.51
1:G:71:GLY:HA2	1:G:420:GLU:CA	2.41	0.51
1:G:206:ILE:CB	1:G:420:GLU:HA	2.40	0.51
1:A:132:ASP:O	1:A:136:VAL:HG23	2.10	0.50
1:A:143:ARG:NH1	1:A:143:ARG:HB3	2.25	0.50
1:A:174:TYR:CZ	1:A:234:TYR:CZ	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:NZ	1:C:142:GLU:OE1	2.36	0.50
2:D:118:PHE:O	2:D:118:PHE:CD2	2.64	0.50
1:G:171:MET:O	1:G:175:VAL:HB	2.11	0.50
1:A:323:GLU:OE2	1:A:347:GLY:O	2.30	0.50
2:B:39:HIS:CD2	2:B:80:VAL:HG22	2.46	0.50
2:B:124:GLU:OE1	2:B:126:LYS:N	2.43	0.50
2:B:126:LYS:HZ3	2:B:127:ASP:H	1.56	0.50
1:C:29:LYS:CG	2:D:65:THR:O	2.60	0.50
1:C:327:VAL:HG23	1:C:327:VAL:O	2.11	0.50
2:D:126:LYS:NZ	2:D:127:ASP:N	2.55	0.50
1:E:381:ASN:N	1:E:381:ASN:ND2	2.59	0.50
2:F:117:GLU:C	2:F:122:TYR:HH	2.14	0.50
2:H:28:ILE:HD12	2:H:34:SER:OG	2.11	0.50
2:H:85:LYS:CD	2:H:118:PHE:HE1	2.22	0.50
1:A:68:ASP:CA	1:A:81:ARG:HH22	2.24	0.50
1:A:367:ARG:HH21	1:A:375:LYS:HD2	1.76	0.50
2:B:118:PHE:O	2:B:118:PHE:CD2	2.64	0.50
2:B:126:LYS:HG3	2:B:127:ASP:H	1.75	0.50
2:B:264:ARG:O	2:B:265:PHE:CB	2.55	0.50
1:C:355:THR:C	1:C:357:LYS:H	2.14	0.50
2:F:385:ALA:O	2:F:386:LEU:C	2.50	0.50
1:G:154:ALA:O	1:G:157:TYR:CD1	2.64	0.50
1:A:67:TRP:HZ3	2:B:15:PRO:O	1.93	0.50
2:B:213:LEU:HD22	2:B:215:GLU:H	1.76	0.50
2:B:351:LEU:O	2:B:353:ASP:N	2.44	0.50
1:C:149:ILE:N	1:C:149:ILE:CD1	2.75	0.50
1:C:357:LYS:N	1:C:357:LYS:HD2	2.25	0.50
2:D:264:ARG:O	2:D:265:PHE:CB	2.55	0.50
1:E:143:ARG:HB3	1:E:143:ARG:NH1	2.27	0.50
1:E:355:THR:O	1:E:357:LYS:N	2.40	0.50
1:E:377:LEU:HD12	1:E:378:ASP:O	2.12	0.50
2:F:36:PRO:HB2	2:F:62:LEU:CD1	2.42	0.50
2:F:118:PHE:O	2:F:118:PHE:CD2	2.64	0.50
2:F:275:ASP:OD1	2:F:297:ARG:NE	2.33	0.50
2:F:401:PHE:HD2	2:F:401:PHE:O	1.94	0.50
1:G:190:ARG:CB	1:G:191:PRO:CD	2.49	0.50
1:A:37:CYS:HB2	1:A:39:PHE:H	1.76	0.50
1:A:57:HIS:O	1:A:126:PRO:HG2	2.11	0.50
1:A:322:LEU:HD22	1:A:322:LEU:N	2.26	0.50
1:E:37:CYS:CB	1:E:155:GLY:CA	2.73	0.50
1:E:65:SER:O	1:E:68:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:SER:HB3	1:E:166:ILE:HG21	1.93	0.50
1:E:383:ARG:HE	2:F:90:ARG:HH12	1.58	0.50
2:F:31:LEU:HD23	2:F:95:VAL:HG11	1.92	0.50
1:G:57:HIS:O	1:G:126:PRO:HG2	2.12	0.50
1:G:66:SER:HB3	2:H:47:PHE:CZ	2.47	0.50
1:G:275:TYR:CD2	1:G:338:SER:HB2	2.45	0.50
2:H:311:LEU:HD23	2:H:431:LEU:HD12	1.93	0.50
1:A:27:LYS:HD2	1:A:27:LYS:C	2.32	0.50
1:A:357:LYS:N	1:A:357:LYS:HD2	2.26	0.50
2:B:252:ASP:O	2:B:256:GLU:HG2	2.11	0.50
1:C:94:ILE:O	1:C:94:ILE:CG1	2.60	0.50
1:C:367:ARG:HH21	1:C:375:LYS:HD2	1.75	0.50
2:D:374:GLY:O	2:D:375:GLN:HB2	2.11	0.50
1:E:37:CYS:HB3	1:E:155:GLY:HA3	1.86	0.50
1:E:52:VAL:O	1:E:79:LEU:HD23	2.12	0.50
1:E:199:ASN:OD1	1:E:240:MET:HG2	2.12	0.50
1:E:322:LEU:HD22	1:E:322:LEU:N	2.27	0.50
1:E:433:GLU:O	1:E:437:GLN:HG2	2.10	0.50
2:F:285:SER:HB3	2:F:287:ASN:HD21	1.75	0.50
2:F:410:PHE:CE2	2:F:411:GLN:HB2	2.47	0.50
1:G:204:TYR:CE1	1:G:229:ALA:HB3	2.47	0.50
1:G:382:ALA:HB3	2:H:217:ARG:HG3	1.93	0.50
2:H:207:GLY:O	2:H:223:THR:O	2.29	0.50
2:H:213:LEU:HD22	2:H:215:GLU:H	1.76	0.50
1:C:29:LYS:HG2	2:D:65:THR:O	2.11	0.50
1:C:206:ILE:O	1:C:207:ALA:HB3	2.12	0.50
2:D:353:ASP:O	2:D:354:SER:CB	2.59	0.50
1:E:28:PRO:HD3	1:E:357:LYS:NZ	2.27	0.50
1:E:52:VAL:C	1:E:79:LEU:HD23	2.32	0.50
2:F:160:GLU:HG2	2:F:161:ARG:H	1.75	0.50
2:F:304:MET:O	2:F:308:HIS:HB3	2.12	0.50
1:G:339:VAL:O	1:G:342:ALA:HB3	2.11	0.50
2:H:228:VAL:HG23	2:H:229:ALA:N	2.27	0.50
2:H:340:VAL:O	2:H:340:VAL:CG1	2.58	0.50
1:A:227:THR:O	1:A:229:ALA:N	2.44	0.50
2:B:100:THR:HG22	2:B:135:THR:N	2.20	0.50
2:D:354:SER:CB	2:D:355:PRO:HD2	2.42	0.50
1:E:38:SER:O	1:E:163:GLY:HA3	2.11	0.50
1:E:296:LEU:O	1:E:300:THR:HG23	2.11	0.50
1:E:404:MET:CB	1:E:414:PHE:CE1	2.95	0.50
1:G:335:LYS:O	1:G:338:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:HIS:CD2	2:H:80:VAL:HG22	2.47	0.50
1:A:174:TYR:OH	1:A:238:GLN:HG3	2.11	0.50
1:C:67:TRP:CD1	1:C:67:TRP:C	2.84	0.50
1:C:179:ARG:NH2	1:C:239:THR:CG2	2.75	0.50
1:C:312:ARG:HH11	1:C:312:ARG:HB2	1.77	0.50
2:D:26:LEU:CD1	2:D:146:PHE:CD1	2.94	0.50
2:D:93:PRO:HG3	2:D:96:ILE:HG13	1.94	0.50
1:E:409:LYS:HB3	2:F:218:PHE:HZ	1.73	0.50
2:F:124:GLU:O	2:F:125:TYR:C	2.50	0.50
1:G:373:ASP:CG	1:G:374:VAL:N	2.64	0.50
1:G:411:ARG:HH22	2:H:214:ASP:HA	1.77	0.50
1:A:440:ILE:HG13	1:A:441:THR:N	2.27	0.49
2:B:118:PHE:HA	2:B:122:TYR:CE1	2.46	0.49
1:C:181:PRO:CD	1:C:242:ARG:HG3	2.42	0.49
1:C:383:ARG:N	2:D:217:ARG:NH1	2.59	0.49
2:F:121:GLN:CA	2:F:122:TYR:CD1	2.95	0.49
1:G:424:GLY:O	1:G:433:GLU:OE2	2.29	0.49
1:A:65:SER:O	1:A:68:ASP:OD1	2.30	0.49
1:A:133:VAL:HG23	1:A:134:ASP:OD1	2.12	0.49
1:A:149:ILE:N	1:A:149:ILE:HD12	2.27	0.49
1:A:177:GLY:HA3	1:A:241:HIS:CE1	2.41	0.49
1:E:383:ARG:HA	2:F:217:ARG:HH12	1.78	0.49
2:F:354:SER:CB	2:F:355:PRO:HD2	2.41	0.49
1:G:196:HIS:ND1	1:G:291:LEU:HD12	2.27	0.49
2:H:213:LEU:HD13	2:H:218:PHE:CG	2.47	0.49
1:C:57:HIS:HE1	1:C:131:ASP:OD1	1.96	0.49
1:C:190:ARG:CB	1:C:191:PRO:CD	2.48	0.49
2:F:27:ALA:HB2	2:F:146:PHE:CD1	2.46	0.49
1:G:367:ARG:HD2	1:G:372:ASP:HA	1.94	0.49
1:A:226:CYS:HB3	1:A:240:MET:HE2	1.94	0.49
1:A:355:THR:C	1:A:357:LYS:H	2.14	0.49
2:B:126:LYS:NZ	2:B:127:ASP:N	2.55	0.49
2:B:159:PRO:CG	2:B:257:ARG:NH1	2.71	0.49
1:C:29:LYS:HG3	2:D:66:ALA:HB3	1.94	0.49
2:D:28:ILE:HG13	2:D:29:LEU:N	2.27	0.49
2:F:118:PHE:HA	2:F:122:TYR:CE1	2.48	0.49
2:F:183:GLY:O	2:F:413:CYS:HB2	2.12	0.49
1:G:204:TYR:HB2	1:G:206:ILE:HD13	1.94	0.49
1:G:337:TRP:CD1	1:G:365:ARG:HG2	2.48	0.49
1:G:380:GLY:HA3	1:G:384:VAL:CG2	2.42	0.49
1:C:220:LEU:CD2	1:C:303:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:VAL:O	1:C:238:GLN:C	2.50	0.49
2:D:4:ILE:N	2:D:353:ASP:OD2	2.46	0.49
2:D:118:PHE:O	2:D:122:TYR:CE2	2.66	0.49
2:D:125:TYR:O	2:D:126:LYS:CB	2.58	0.49
1:E:68:ASP:CA	1:E:81:ARG:HH22	2.25	0.49
1:G:381:ASN:N	1:G:381:ASN:ND2	2.60	0.49
2:H:333:ARG:HH11	2:H:333:ARG:CB	2.25	0.49
1:A:204:TYR:HA	1:A:229:ALA:O	2.12	0.49
2:B:105:GLU:HG2	2:B:136:PRO:HG3	1.93	0.49
1:C:307:GLU:O	1:C:311:VAL:CG2	2.55	0.49
2:D:31:LEU:HD12	2:D:226:LEU:HB2	1.95	0.49
2:D:49:LYS:O	2:D:53:VAL:HG13	2.11	0.49
2:F:297:ARG:HG3	2:F:417:TYR:CE2	2.47	0.49
2:H:126:LYS:HZ3	2:H:127:ASP:N	2.09	0.49
1:A:209:GLU:CD	1:A:419:GLN:OE1	2.50	0.49
2:B:85:LYS:CD	2:B:118:PHE:HE1	2.20	0.49
1:C:381:ASN:HB2	2:D:217:ARG:HH21	1.77	0.49
1:E:206:ILE:CD1	1:E:419:GLN:HB3	2.42	0.49
1:E:206:ILE:HG22	1:E:420:GLU:HA	1.95	0.49
1:E:425:TYR:HD1	1:E:433:GLU:OE1	1.96	0.49
2:F:74:MET:O	2:F:76:ALA:N	2.45	0.49
2:F:107:GLN:HE21	2:F:107:GLN:H	1.55	0.49
2:F:351:LEU:O	2:F:353:ASP:N	2.46	0.49
2:F:387:ALA:O	2:F:391:ARG:HB2	2.13	0.49
1:G:207:ALA:HB2	1:G:421:ARG:O	2.12	0.49
1:G:209:GLU:HG3	1:G:426:ALA:HB3	1.94	0.49
1:G:423:PHE:HD2	1:G:423:PHE:O	1.95	0.49
2:H:38:PHE:HB2	2:H:45:THR:HG22	1.93	0.49
2:H:74:MET:O	2:H:75:GLY:C	2.51	0.49
2:H:297:ARG:HG3	2:H:417:TYR:CE2	2.47	0.49
1:A:302:ALA:O	1:A:305:ALA:HB3	2.12	0.49
2:B:188:ILE:HD11	2:B:268:LEU:HD12	1.94	0.49
1:C:383:ARG:CD	2:D:217:ARG:HH22	2.26	0.49
2:D:109:CYS:O	2:D:109:CYS:SG	2.70	0.49
1:A:126:PRO:O	1:A:131:ASP:HB2	2.12	0.49
1:A:252:LYS:HD2	1:A:361:GLU:HG2	1.94	0.49
2:B:401:PHE:O	2:B:401:PHE:CD2	2.65	0.49
1:C:48:PRO:HB3	1:C:72:THR:CG2	2.43	0.49
1:C:204:TYR:HB2	1:C:206:ILE:HD13	1.95	0.49
2:D:160:GLU:HG2	2:D:161:ARG:H	1.77	0.49
2:D:168:ARG:CB	2:D:169:PRO:CD	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ARG:NH2	1:E:239:THR:CG2	2.76	0.49
1:E:336:SER:O	1:E:339:VAL:HG23	2.12	0.49
2:F:344:VAL:HG13	2:F:346:ALA:H	1.78	0.49
1:G:61:ALA:HB2	2:H:137:ASP:CG	2.32	0.49
1:G:108:GLN:HE22	2:H:11:LEU:N	2.00	0.49
1:A:214:LEU:N	1:A:215:PRO:CD	2.76	0.49
1:A:409:LYS:C	1:A:411:ARG:H	2.16	0.49
2:B:49:LYS:O	2:B:53:VAL:HG13	2.13	0.49
2:B:311:LEU:HD23	2:B:431:LEU:HD12	1.94	0.49
2:B:385:ALA:O	2:B:386:LEU:C	2.50	0.49
2:D:118:PHE:HA	2:D:122:TYR:CE1	2.48	0.49
2:D:333:ARG:CB	2:D:333:ARG:HH11	2.26	0.49
1:E:444:CYS:SG	1:E:446:VAL:HG23	2.52	0.49
2:F:122:TYR:O	2:F:123:GLU:C	2.50	0.49
1:G:28:PRO:HD3	1:G:357:LYS:NZ	2.28	0.49
1:G:48:PRO:HG2	1:G:204:TYR:HD1	1.77	0.49
1:A:327:VAL:HG21	1:A:343:LEU:HD11	1.95	0.48
2:B:74:MET:O	2:B:75:GLY:C	2.50	0.48
2:B:160:GLU:O	2:B:161:ARG:C	2.52	0.48
2:B:160:GLU:HG2	2:B:161:ARG:H	1.78	0.48
1:C:171:MET:O	1:C:175:VAL:HB	2.13	0.48
2:D:420:SER:O	2:D:424:LEU:HD12	2.12	0.48
1:E:149:ILE:HD12	1:E:149:ILE:N	2.28	0.48
2:F:126:LYS:HZ3	2:F:127:ASP:N	2.11	0.48
1:G:252:LYS:HD2	1:G:361:GLU:HG2	1.95	0.48
2:H:125:TYR:O	2:H:126:LYS:CB	2.57	0.48
1:C:425:TYR:HD1	1:C:433:GLU:OE1	1.96	0.48
2:D:105:GLU:HG2	2:D:136:PRO:HG3	1.95	0.48
2:D:378:LEU:HD13	2:D:379:VAL:N	2.28	0.48
1:E:337:TRP:CD1	1:E:365:ARG:HG2	2.48	0.48
1:E:373:ASP:CG	1:E:374:VAL:N	2.66	0.48
2:H:126:LYS:CG	2:H:127:ASP:H	2.26	0.48
1:A:27:LYS:CG	2:B:66:ALA:HB1	2.44	0.48
1:A:40:ASP:O	1:A:44:ILE:HG12	2.12	0.48
1:A:67:TRP:CZ3	2:B:15:PRO:HG2	2.47	0.48
1:A:228:LEU:O	1:A:229:ALA:HB3	2.14	0.48
1:C:68:ASP:HB3	2:D:384:HIS:CE1	2.48	0.48
1:C:174:TYR:OH	1:C:238:GLN:HG3	2.12	0.48
2:D:115:LEU:O	2:D:119:ARG:N	2.47	0.48
1:E:359:THR:HG22	4:E:502:CZL:S2A	2.53	0.48
2:F:126:LYS:CG	2:F:127:ASP:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ARG:NE	2:F:162:ARG:HA	2.28	0.48
2:F:374:GLY:O	2:F:375:GLN:HB2	2.12	0.48
1:G:209:GLU:CD	1:G:419:GLN:OE1	2.51	0.48
2:H:159:PRO:HB2	2:H:257:ARG:CG	2.43	0.48
2:H:385:ALA:O	2:H:386:LEU:C	2.51	0.48
2:B:256:GLU:HA	2:B:256:GLU:OE2	2.13	0.48
2:B:315:ARG:HG3	2:B:340:VAL:HG21	1.94	0.48
1:C:148:VAL:C	1:C:149:ILE:HD12	2.34	0.48
1:G:343:LEU:HD23	1:G:343:LEU:H	1.77	0.48
2:H:74:MET:O	2:H:76:ALA:N	2.45	0.48
1:C:64:GLY:O	1:C:67:TRP:HE3	1.95	0.48
1:C:330:TYR:HB3	1:C:399:ALA:CB	2.43	0.48
2:D:121:GLN:CA	2:D:122:TYR:CD1	2.97	0.48
2:D:397:LEU:CD2	2:D:427:LEU:HD21	2.43	0.48
1:E:67:TRP:HZ3	2:F:15:PRO:O	1.92	0.48
1:E:323:GLU:HA	1:E:323:GLU:OE2	2.13	0.48
1:G:65:SER:O	1:G:68:ASP:OD1	2.30	0.48
1:G:362:ASP:O	1:G:366:ILE:CG1	2.58	0.48
1:G:383:ARG:HA	2:H:217:ARG:HH12	1.79	0.48
1:G:423:PHE:O	1:G:423:PHE:CD2	2.67	0.48
2:B:206:SER:O	2:D:295:ARG:NH2	2.47	0.48
2:B:228:VAL:CG2	2:B:229:ALA:N	2.76	0.48
1:C:354:GLY:N	1:C:366:ILE:CD1	2.75	0.48
2:D:39:HIS:CD2	2:D:80:VAL:HG22	2.49	0.48
1:E:209:GLU:HG3	1:E:426:ALA:HB3	1.96	0.48
1:G:166:ILE:O	1:G:166:ILE:HG22	2.14	0.48
2:H:124:GLU:O	2:H:125:TYR:C	2.51	0.48
2:H:354:SER:CB	2:H:355:PRO:CD	2.91	0.48
1:A:187:GLY:O	1:A:188:SER:HB3	2.12	0.48
1:A:310:LYS:HZ2	1:E:191:PRO:HG2	1.78	0.48
2:B:31:LEU:HD12	2:B:226:LEU:HB2	1.96	0.48
2:B:160:GLU:O	2:B:162:ARG:O	2.32	0.48
1:C:57:HIS:O	1:C:126:PRO:HG2	2.14	0.48
1:C:296:LEU:O	1:C:300:THR:HG23	2.13	0.48
2:D:304:MET:O	2:D:308:HIS:HB3	2.13	0.48
1:E:304:ILE:HD12	1:E:305:ALA:N	2.28	0.48
1:E:367:ARG:HD2	1:E:372:ASP:HA	1.96	0.48
2:H:401:PHE:O	2:H:401:PHE:CD2	2.67	0.48
2:B:333:ARG:HB2	2:B:333:ARG:HH11	1.78	0.48
1:C:300:THR:O	1:C:304:ILE:HG23	2.13	0.48
1:C:328:LEU:HD22	1:C:389:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LYS:C	1:C:411:ARG:H	2.17	0.48
1:A:171:MET:O	1:A:175:VAL:HB	2.14	0.48
1:A:323:GLU:OE2	1:A:323:GLU:HA	2.14	0.48
1:A:429:ASP:O	1:A:432:LEU:HB2	2.13	0.48
2:B:28:ILE:HD12	2:B:34:SER:OG	2.14	0.48
2:B:75:GLY:O	2:B:76:ALA:CB	2.61	0.48
2:B:217:ARG:C	2:B:218:PHE:CD2	2.84	0.48
1:C:191:PRO:HG2	1:G:310:LYS:NZ	2.29	0.48
1:C:388:THR:O	1:C:392:TYR:HD2	1.96	0.48
2:D:237:SER:O	2:D:260:VAL:HG13	2.13	0.48
2:D:335:MET:SD	2:D:424:LEU:CD2	3.01	0.48
2:D:410:PHE:CD2	2:D:411:GLN:HB2	2.49	0.48
2:F:126:LYS:CG	2:F:127:ASP:N	2.76	0.48
2:F:191:SER:HB3	2:F:277:TRP:CZ3	2.43	0.48
1:G:214:LEU:N	1:G:215:PRO:CD	2.77	0.48
1:A:166:ILE:O	1:A:166:ILE:HG22	2.14	0.48
2:B:213:LEU:HD12	2:B:223:THR:OG1	2.13	0.48
1:C:52:VAL:C	1:C:79:LEU:HD23	2.35	0.48
2:D:67:MET:HE3	2:D:71:SER:HB2	1.92	0.48
2:D:175:LEU:HB3	2:D:247:LEU:HD13	1.95	0.48
1:E:196:HIS:HB3	1:E:291:LEU:HD11	1.95	0.48
2:F:16:LEU:HD12	2:F:16:LEU:O	2.13	0.48
2:F:354:SER:CB	2:F:355:PRO:CD	2.91	0.48
1:G:220:LEU:CD2	1:G:303:LEU:HD13	2.44	0.48
1:G:353:THR:CG2	1:G:377:LEU:HD23	2.44	0.48
1:A:63:ALA:O	1:A:65:SER:N	2.47	0.47
1:A:66:SER:HB3	2:B:47:PHE:CZ	2.49	0.47
2:B:409:GLY:C	2:B:411:GLN:H	2.17	0.47
1:C:335:LYS:O	1:C:338:SER:OG	2.32	0.47
2:D:85:LYS:CD	2:D:118:PHE:HE1	2.23	0.47
2:D:95:VAL:CG2	2:D:228:VAL:CG1	2.92	0.47
2:D:397:LEU:CD2	2:D:427:LEU:CD2	2.92	0.47
1:E:174:TYR:OH	1:E:238:GLN:CG	2.62	0.47
1:E:248:MET:SD	1:E:258:ALA:HB2	2.53	0.47
2:F:20:GLN:HG2	2:F:135:THR:CB	2.44	0.47
2:F:93:PRO:CG	2:F:96:ILE:HG13	2.44	0.47
2:F:124:GLU:OE1	2:F:126:LYS:N	2.44	0.47
2:H:105:GLU:HG2	2:H:136:PRO:HG3	1.96	0.47
1:A:68:ASP:O	1:A:81:ARG:NH2	2.47	0.47
2:B:42:GLN:HA	2:B:64:THR:CG2	2.39	0.47
2:B:121:GLN:CA	2:B:122:TYR:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ASN:HD22	2:B:240:THR:CG2	2.27	0.47
2:B:382:ASN:HD22	2:B:384:HIS:N	2.12	0.47
2:D:42:GLN:HA	2:D:64:THR:CG2	2.38	0.47
2:D:74:MET:O	2:D:76:ALA:N	2.47	0.47
2:D:160:GLU:O	2:D:161:ARG:C	2.52	0.47
2:F:211:GLY:HA3	2:H:302:ASP:CB	2.44	0.47
2:F:397:LEU:CD2	2:F:427:LEU:CD2	2.92	0.47
1:G:172:LEU:CD1	1:G:173:LYS:N	2.65	0.47
1:G:383:ARG:HE	2:H:90:ARG:HH12	1.61	0.47
2:H:349:ALA:O	2:H:351:LEU:N	2.47	0.47
2:H:351:LEU:O	2:H:353:ASP:N	2.47	0.47
2:H:412:ARG:HB3	2:H:414:TRP:CZ3	2.49	0.47
1:A:137:CYS:SG	1:A:150:PRO:HB3	2.54	0.47
1:A:193:ILE:CD1	1:A:293:ASP:OD1	2.63	0.47
1:A:206:ILE:O	1:A:419:GLN:O	2.31	0.47
1:A:383:ARG:N	2:B:217:ARG:HH22	2.10	0.47
2:B:116:HIS:C	2:B:119:ARG:H	2.17	0.47
2:B:124:GLU:O	2:B:125:TYR:C	2.52	0.47
2:B:410:PHE:CE2	2:B:411:GLN:HB2	2.49	0.47
1:C:48:PRO:HG2	1:C:204:TYR:HD1	1.79	0.47
1:C:322:LEU:N	1:C:322:LEU:HD22	2.29	0.47
1:C:430:GLY:O	1:C:433:GLU:OE1	2.32	0.47
2:D:74:MET:O	2:D:75:GLY:C	2.52	0.47
2:D:383:SER:OG	2:D:403:GLN:HA	2.15	0.47
2:D:397:LEU:HD23	2:D:427:LEU:CD2	2.43	0.47
2:F:38:PHE:CG	2:F:45:THR:HG22	2.48	0.47
1:G:138:LYS:NZ	1:G:142:GLU:OE1	2.37	0.47
1:G:204:TYR:CE1	1:G:229:ALA:CB	2.97	0.47
2:H:36:PRO:HB2	2:H:62:LEU:CD1	2.45	0.47
2:H:331:LEU:HD22	2:H:331:LEU:C	2.33	0.47
1:A:380:GLY:HA3	1:A:384:VAL:CG2	2.44	0.47
1:C:383:ARG:HD2	2:D:217:ARG:NH2	2.29	0.47
2:D:21:THR:HG21	2:D:137:ASP:OD1	2.15	0.47
2:D:89:GLU:OE2	2:D:124:GLU:HB2	2.14	0.47
2:D:173:ASN:HD22	2:D:240:THR:CG2	2.26	0.47
2:D:186:GLU:O	2:D:190:GLU:HG2	2.14	0.47
1:E:343:LEU:HD23	1:E:343:LEU:H	1.79	0.47
2:F:213:LEU:HD22	2:F:215:GLU:H	1.79	0.47
2:F:397:LEU:HD23	2:F:427:LEU:CD2	2.40	0.47
1:G:118:VAL:C	1:G:119:PHE:HD1	2.17	0.47
1:G:174:TYR:CZ	1:G:234:TYR:CZ	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:357:LYS:N	1:G:357:LYS:HD2	2.29	0.47
2:H:285:SER:CB	2:H:287:ASN:HD21	2.27	0.47
2:H:310:MET:N	2:H:310:MET:HE3	2.30	0.47
1:A:383:ARG:HD2	2:B:217:ARG:HH22	1.79	0.47
2:B:213:LEU:HD13	2:B:218:PHE:CG	2.50	0.47
1:E:47:LEU:N	1:E:48:PRO:CD	2.78	0.47
1:E:61:ALA:HB2	2:F:137:ASP:CG	2.35	0.47
1:E:66:SER:HB3	2:F:47:PHE:CZ	2.50	0.47
2:F:325:LEU:HD11	2:F:342:ALA:HB1	1.97	0.47
1:G:27:LYS:HD2	1:G:27:LYS:C	2.34	0.47
2:H:126:LYS:CG	2:H:127:ASP:N	2.77	0.47
1:A:28:PRO:HD3	1:A:357:LYS:NZ	2.29	0.47
2:B:16:LEU:HD12	2:B:16:LEU:O	2.15	0.47
1:C:322:LEU:CD2	1:C:439:CYS:SG	2.95	0.47
2:D:34:SER:N	2:D:221:LEU:HD22	2.11	0.47
2:D:116:HIS:C	2:D:119:ARG:H	2.18	0.47
2:D:168:ARG:HE	2:D:168:ARG:HB2	1.54	0.47
2:D:191:SER:HG	2:D:277:TRP:HZ3	1.62	0.47
1:G:328:LEU:HD23	1:G:397:LEU:HD23	1.95	0.47
1:G:377:LEU:HD12	1:G:378:ASP:O	2.15	0.47
2:H:121:GLN:HB2	2:H:122:TYR:CE1	2.50	0.47
2:H:160:GLU:HG2	2:H:161:ARG:H	1.78	0.47
1:A:181:PRO:HD3	1:A:242:ARG:HG3	1.94	0.47
1:A:207:ALA:CB	1:A:421:ARG:O	2.63	0.47
1:C:28:PRO:HD3	1:C:357:LYS:NZ	2.30	0.47
1:E:358:SER:HB2	1:E:363:LYS:HE3	1.97	0.47
2:F:74:MET:O	2:F:75:GLY:C	2.53	0.47
2:F:168:ARG:HB2	2:F:169:PRO:CD	2.45	0.47
2:F:349:ALA:O	2:F:351:LEU:N	2.48	0.47
1:G:64:GLY:O	1:G:67:TRP:HE3	1.97	0.47
1:G:206:ILE:O	1:G:207:ALA:HB3	2.13	0.47
1:G:322:LEU:CD2	1:G:439:CYS:SG	2.95	0.47
2:H:100:THR:HG22	2:H:134:ASN:HA	1.97	0.47
2:H:121:GLN:CA	2:H:122:TYR:CD1	2.97	0.47
2:H:159:PRO:HG3	2:H:257:ARG:NH1	2.21	0.47
2:H:236:GLN:O	2:H:236:GLN:HG2	2.14	0.47
2:H:428:ALA:O	2:H:432:VAL:HG23	2.15	0.47
1:A:27:LYS:HG3	2:B:66:ALA:HB1	1.97	0.47
1:A:29:LYS:CG	2:B:65:THR:O	2.62	0.47
1:A:71:GLY:HA2	1:A:420:GLU:CA	2.44	0.47
1:A:94:ILE:O	1:A:94:ILE:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE1	1:A:426:ALA:HB3	2.10	0.47
1:A:232:ALA:HA	1:A:236:GLU:OE1	2.14	0.47
1:A:304:ILE:HD12	1:A:305:ALA:N	2.30	0.47
2:B:412:ARG:HB3	2:B:414:TRP:CZ3	2.50	0.47
1:C:327:VAL:HG21	1:C:343:LEU:HD11	1.95	0.47
1:C:367:ARG:HD3	1:C:367:ARG:HA	1.40	0.47
1:C:396:ILE:HD11	1:C:442:LEU:HD23	1.95	0.47
2:D:159:PRO:HB2	2:D:257:ARG:CD	2.44	0.47
1:E:206:ILE:CB	1:E:419:GLN:O	2.58	0.47
1:G:421:ARG:NH2	1:G:422:GLU:CB	2.77	0.47
1:A:62:CYS:HA	3:A:501:SF4:S3	2.55	0.47
2:B:310:MET:HG3	2:B:428:ALA:HB1	1.97	0.47
1:C:373:ASP:CG	1:C:374:VAL:N	2.68	0.47
2:D:401:PHE:O	2:D:401:PHE:CD2	2.68	0.47
1:E:37:CYS:HB2	1:E:39:PHE:H	1.80	0.47
1:E:323:GLU:OE2	1:E:347:GLY:O	2.33	0.47
1:E:335:LYS:O	1:E:338:SER:OG	2.32	0.47
2:F:217:ARG:C	2:F:218:PHE:CD2	2.85	0.47
1:G:323:GLU:OE2	1:G:347:GLY:O	2.33	0.47
1:G:404:MET:CB	1:G:414:PHE:CE1	2.97	0.47
1:A:191:PRO:CG	1:E:314:ALA:HB2	2.44	0.47
2:B:29:LEU:O	2:B:221:LEU:HD11	2.14	0.47
2:B:55:HIS:CE1	2:B:403:GLN:HG2	2.50	0.47
2:D:269:TYR:O	2:D:273:ALA:HB3	2.15	0.47
1:A:48:PRO:HG2	1:A:204:TYR:CD1	2.50	0.46
1:C:31:GLY:N	1:C:33:THR:OG1	2.48	0.46
1:E:118:VAL:O	1:E:119:PHE:HD1	1.98	0.46
1:E:328:LEU:HD22	1:E:389:VAL:HG22	1.97	0.46
2:F:113:THR:O	2:F:116:HIS:N	2.47	0.46
1:G:29:LYS:NZ	1:G:29:LYS:N	2.37	0.46
1:G:304:ILE:HD12	1:G:305:ALA:N	2.30	0.46
1:G:354:GLY:N	1:G:366:ILE:CD1	2.78	0.46
2:H:42:GLN:CA	2:H:64:THR:HG21	2.41	0.46
2:H:410:PHE:CD2	2:H:411:GLN:HB2	2.50	0.46
1:A:206:ILE:CB	1:A:419:GLN:O	2.59	0.46
1:C:367:ARG:HD2	1:C:372:ASP:HA	1.97	0.46
2:D:29:LEU:O	2:D:221:LEU:HD11	2.15	0.46
1:E:123:THR:C	1:E:126:PRO:HD2	2.36	0.46
1:E:171:MET:O	1:E:175:VAL:HB	2.16	0.46
2:F:121:GLN:HB2	2:F:122:TYR:CE1	2.49	0.46
1:G:27:LYS:CD	2:H:66:ALA:HB1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLY:O	1:G:86:THR:O	2.33	0.46
1:G:307:GLU:O	1:G:311:VAL:CG2	2.60	0.46
2:H:171:GLN:O	2:H:237:SER:HB2	2.16	0.46
2:H:285:SER:HB3	2:H:287:ASN:HD21	1.79	0.46
1:A:209:GLU:HG3	1:A:426:ALA:HB3	1.96	0.46
1:A:343:LEU:HD23	1:A:343:LEU:H	1.80	0.46
1:A:367:ARG:HD2	1:A:372:ASP:HA	1.98	0.46
1:A:439:CYS:O	1:A:440:ILE:C	2.53	0.46
2:B:295:ARG:NE	2:D:212:HIS:NE2	2.63	0.46
1:C:214:LEU:N	1:C:215:PRO:CD	2.78	0.46
2:D:159:PRO:CB	2:D:257:ARG:CD	2.90	0.46
1:E:409:LYS:C	1:E:411:ARG:H	2.18	0.46
2:F:311:LEU:HD23	2:F:431:LEU:HD12	1.97	0.46
1:G:388:THR:O	1:G:392:TYR:HD2	1.97	0.46
1:G:424:GLY:C	1:G:433:GLU:OE2	2.54	0.46
2:H:89:GLU:OE2	2:H:124:GLU:HB2	2.14	0.46
2:H:93:PRO:CG	2:H:96:ILE:HG13	2.46	0.46
2:H:168:ARG:CB	2:H:169:PRO:CD	2.92	0.46
1:A:381:ASN:HB2	2:B:217:ARG:HH21	1.80	0.46
2:B:168:ARG:HB2	2:B:169:PRO:CD	2.44	0.46
2:B:212:HIS:CE1	2:D:295:ARG:NE	2.83	0.46
2:D:213:LEU:HD22	2:D:215:GLU:H	1.80	0.46
2:D:311:LEU:HD23	2:D:431:LEU:HD12	1.97	0.46
1:E:48:PRO:HG2	1:E:204:TYR:HD1	1.81	0.46
2:F:33:ARG:N	2:F:221:LEU:HD23	2.30	0.46
1:G:409:LYS:HD2	2:H:218:PHE:CZ	2.50	0.46
2:H:27:ALA:HB2	2:H:146:PHE:CE1	2.50	0.46
2:H:228:VAL:CG2	2:H:229:ALA:N	2.78	0.46
1:A:24:GLY:O	1:A:25:CYS:HB3	2.16	0.46
1:A:206:ILE:H	1:A:206:ILE:HG12	1.33	0.46
1:A:404:MET:CB	1:A:414:PHE:CE1	2.99	0.46
2:B:36:PRO:HD2	2:B:61:PRO:O	2.16	0.46
2:B:218:PHE:O	2:B:220:ALA:N	2.49	0.46
1:G:52:VAL:O	1:G:79:LEU:HD23	2.16	0.46
2:H:378:LEU:HD13	2:H:379:VAL:N	2.30	0.46
1:A:78:ASP:O	1:A:81:ARG:HB2	2.16	0.46
1:A:214:LEU:HB3	1:A:215:PRO:HD3	1.97	0.46
2:B:95:VAL:HG22	2:B:228:VAL:HG11	1.97	0.46
1:E:174:TYR:CD2	1:E:174:TYR:O	2.68	0.46
1:E:328:LEU:HD23	1:E:397:LEU:HD23	1.98	0.46
1:E:440:ILE:HG13	1:E:441:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:354:SER:HB2	2:F:355:PRO:HD2	1.97	0.46
1:G:206:ILE:CD1	1:G:419:GLN:HB3	2.45	0.46
1:A:61:ALA:HB2	2:B:137:ASP:CG	2.36	0.46
2:B:221:LEU:C	2:B:223:THR:N	2.68	0.46
2:B:269:TYR:O	2:B:273:ALA:CB	2.64	0.46
2:B:383:SER:OG	2:B:403:GLN:HA	2.16	0.46
1:C:68:ASP:HB3	2:D:384:HIS:HE1	1.81	0.46
1:C:252:LYS:HD2	1:C:361:GLU:HG2	1.97	0.46
1:C:440:ILE:HG13	1:C:441:THR:N	2.30	0.46
2:D:285:SER:HB3	2:D:287:ASN:HD21	1.81	0.46
1:E:354:GLY:N	1:E:366:ILE:CD1	2.78	0.46
1:E:383:ARG:CD	2:F:217:ARG:HH22	2.29	0.46
1:E:421:ARG:CZ	1:E:422:GLU:N	2.75	0.46
2:F:116:HIS:HA	2:F:119:ARG:HB2	1.98	0.46
1:G:179:ARG:HB3	1:G:238:GLN:CB	2.46	0.46
2:H:36:PRO:HB2	2:H:62:LEU:HD13	1.98	0.46
2:H:156:THR:C	2:H:157:LEU:HD13	2.36	0.46
2:H:226:LEU:HD22	2:H:226:LEU:HA	1.67	0.46
1:A:382:ALA:O	1:A:386:LEU:N	2.48	0.46
2:B:179:ASN:HB3	2:B:324:LEU:HD11	1.98	0.46
2:B:212:HIS:CE1	2:D:295:ARG:HG3	2.51	0.46
1:C:196:HIS:HB3	1:C:291:LEU:HD11	1.97	0.46
2:D:38:PHE:CG	2:D:45:THR:HG22	2.51	0.46
2:F:36:PRO:HB2	2:F:62:LEU:HD13	1.98	0.46
2:F:401:PHE:O	2:F:401:PHE:CD2	2.69	0.46
1:G:155:GLY:HA3	3:G:501:SF4:S4	2.56	0.46
1:G:286:ASP:O	1:G:290:LEU:HB2	2.15	0.46
2:H:55:HIS:CE1	2:H:403:GLN:HG2	2.51	0.46
2:B:167:LYS:O	2:B:167:LYS:HG3	2.15	0.46
2:B:175:LEU:HB3	2:B:247:LEU:HD13	1.98	0.46
1:C:339:VAL:HG11	1:C:417:ILE:HD11	1.98	0.46
1:C:343:LEU:HD23	1:C:343:LEU:H	1.81	0.46
2:D:100:THR:HG22	2:D:134:ASN:HA	1.98	0.46
2:D:159:PRO:CB	2:D:257:ARG:CG	2.93	0.46
1:E:339:VAL:O	1:E:342:ALA:HB3	2.16	0.46
2:F:42:GLN:HA	2:F:64:THR:CG2	2.41	0.46
2:H:162:ARG:NE	2:H:162:ARG:HA	2.31	0.46
2:H:257:ARG:CZ	2:H:257:ARG:HB3	2.45	0.46
1:A:328:LEU:HD22	1:A:389:VAL:HG22	1.96	0.46
1:A:377:LEU:HD12	1:A:378:ASP:O	2.15	0.46
2:B:121:GLN:HB2	2:B:122:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:GLN:HE21	2:D:91:GLN:HB2	1.63	0.46
1:G:174:TYR:OH	1:G:238:GLN:CG	2.64	0.46
2:H:33:ARG:N	2:H:221:LEU:CD2	2.79	0.46
2:H:160:GLU:O	2:H:162:ARG:O	2.34	0.46
1:A:310:LYS:HZ3	1:E:191:PRO:HG2	1.81	0.45
1:A:362:ASP:O	1:A:366:ILE:CG1	2.61	0.45
1:A:383:ARG:N	2:B:217:ARG:NH2	2.63	0.45
2:B:300:LEU:HD12	2:B:300:LEU:O	2.16	0.45
1:C:174:TYR:CD2	1:C:174:TYR:O	2.68	0.45
1:C:323:GLU:OE2	1:C:347:GLY:O	2.34	0.45
1:C:404:MET:CB	1:C:414:PHE:CE1	2.99	0.45
1:E:24:GLY:O	1:E:25:CYS:HB3	2.16	0.45
1:E:29:LYS:HG3	2:F:66:ALA:HB3	1.98	0.45
1:E:341:SER:HA	1:E:344:GLN:HE21	1.80	0.45
1:G:316:GLU:HA	1:G:319:ARG:HG3	1.98	0.45
2:H:29:LEU:O	2:H:221:LEU:HD11	2.16	0.45
2:B:302:ASP:OD2	2:D:58:GLU:CD	2.55	0.45
1:C:46:LEU:HB2	1:C:121:TYR:OH	2.16	0.45
1:C:179:ARG:HB3	1:C:238:GLN:CB	2.46	0.45
2:D:126:LYS:C	2:D:128:VAL:H	2.20	0.45
1:E:189:GLU:O	1:E:190:ARG:O	2.34	0.45
1:E:196:HIS:ND1	1:E:291:LEU:HD12	2.31	0.45
2:F:57:ARG:O	2:F:58:GLU:CD	2.55	0.45
2:H:213:LEU:HD13	2:H:218:PHE:CB	2.45	0.45
1:A:94:ILE:O	1:A:94:ILE:CD1	2.62	0.45
1:A:181:PRO:CD	1:A:242:ARG:HG3	2.47	0.45
1:C:118:VAL:C	1:C:119:PHE:HD1	2.20	0.45
2:D:160:GLU:O	2:D:162:ARG:O	2.34	0.45
2:H:33:ARG:H	2:H:221:LEU:HD23	1.80	0.45
2:H:188:ILE:HD11	2:H:268:LEU:CD1	2.44	0.45
1:A:341:SER:HA	1:A:344:GLN:HE21	1.81	0.45
2:B:91:GLN:HE21	2:B:91:GLN:HB2	1.56	0.45
1:C:190:ARG:CG	1:C:191:PRO:HD2	2.42	0.45
1:C:383:ARG:HG2	1:C:384:VAL:N	2.28	0.45
2:D:16:LEU:HB2	2:D:363:ASP:HA	1.98	0.45
2:F:26:LEU:CD1	2:F:146:PHE:CD1	2.99	0.45
2:F:113:THR:O	2:F:117:GLU:N	2.47	0.45
1:G:62:CYS:HA	3:G:501:SF4:S3	2.56	0.45
1:G:126:PRO:O	1:G:131:ASP:HB2	2.16	0.45
1:G:328:LEU:HD22	1:G:389:VAL:CG2	2.46	0.45
2:H:116:HIS:C	2:H:119:ARG:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:299:GLN:OE1	2:H:418:ARG:NH2	2.45	0.45
1:C:295:ASP:O	1:C:299:ARG:HG3	2.17	0.45
1:C:337:TRP:O	1:C:337:TRP:HE3	1.98	0.45
2:D:122:TYR:O	2:D:123:GLU:C	2.55	0.45
2:D:159:PRO:HB2	2:D:257:ARG:HD3	1.97	0.45
1:E:382:ALA:CB	2:F:217:ARG:HG3	2.45	0.45
2:F:102:GLY:HA2	2:F:138:PHE:CE1	2.52	0.45
2:F:315:ARG:HG3	2:F:340:VAL:HG21	1.94	0.45
1:G:421:ARG:HE	1:G:421:ARG:HB3	1.15	0.45
1:A:174:TYR:OH	1:A:238:GLN:CG	2.64	0.45
1:A:328:LEU:HD22	1:A:389:VAL:CG2	2.47	0.45
2:B:197:LEU:HD12	2:B:281:LEU:HD22	1.98	0.45
2:D:126:LYS:HZ3	2:D:127:ASP:N	2.14	0.45
1:E:396:ILE:HG23	1:E:413:PRO:HB2	1.98	0.45
2:F:160:GLU:O	2:F:161:ARG:C	2.54	0.45
1:G:52:VAL:C	1:G:79:LEU:HD23	2.37	0.45
1:A:191:PRO:HB2	1:E:310:LYS:HG2	1.98	0.45
1:A:220:LEU:CD2	1:A:303:LEU:HD13	2.46	0.45
1:A:381:ASN:N	1:A:381:ASN:ND2	2.60	0.45
1:A:425:TYR:HD1	1:A:433:GLU:OE1	1.99	0.45
2:B:317:ALA:HB3	2:B:379:VAL:HG22	1.97	0.45
1:C:203:GLU:HB3	1:C:227:THR:HG23	1.99	0.45
1:C:316:GLU:HA	1:C:319:ARG:HG3	1.99	0.45
1:C:444:CYS:SG	1:C:446:VAL:HG23	2.57	0.45
2:D:382:ASN:HD22	2:D:384:HIS:N	2.14	0.45
1:E:78:ASP:O	1:E:81:ARG:HB2	2.17	0.45
1:E:94:ILE:O	1:E:94:ILE:CG1	2.65	0.45
1:E:417:ILE:HD13	1:E:417:ILE:HA	1.63	0.45
1:E:419:GLN:HE22	1:E:424:GLY:H	1.65	0.45
1:G:340:VAL:O	1:G:344:GLN:HB3	2.17	0.45
1:A:27:LYS:HD3	2:B:66:ALA:HB3	1.95	0.45
1:A:30:PRO:HA	1:A:33:THR:HG1	1.82	0.45
1:A:190:ARG:CB	1:A:191:PRO:CD	2.41	0.45
1:A:312:ARG:HB2	1:A:312:ARG:HH11	1.81	0.45
2:B:64:THR:HG22	2:B:66:ALA:N	2.26	0.45
1:C:123:THR:C	1:C:126:PRO:HD2	2.37	0.45
1:C:314:ALA:HB2	1:G:191:PRO:CG	2.46	0.45
2:D:382:ASN:ND2	2:D:384:HIS:N	2.64	0.45
1:E:172:LEU:C	1:E:172:LEU:CD1	2.84	0.45
1:G:203:GLU:HB3	1:G:227:THR:HG23	1.99	0.45
1:G:419:GLN:NE2	1:G:424:GLY:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:LEU:HD12	2:H:16:LEU:O	2.17	0.45
2:H:113:THR:O	2:H:117:GLU:N	2.48	0.45
2:H:316:THR:OG1	2:H:339:THR:HA	2.17	0.45
2:H:433:GLU:HG3	2:H:434:HIS:CD2	2.51	0.45
1:A:60:ILE:H	1:A:60:ILE:HG12	1.44	0.45
2:B:38:PHE:CG	2:B:45:THR:HG22	2.51	0.45
2:B:76:ALA:HA	2:B:79:ASN:OD1	2.17	0.45
2:B:156:THR:C	2:B:157:LEU:HD13	2.36	0.45
2:B:295:ARG:HG3	2:D:212:HIS:CE1	2.52	0.45
2:B:435:HIS:CD2	1:C:422:GLU:HG2	2.51	0.45
1:C:132:ASP:O	1:C:136:VAL:HG23	2.15	0.45
1:C:209:GLU:HG3	1:C:426:ALA:HB3	1.98	0.45
2:D:382:ASN:HD22	2:D:384:HIS:H	1.65	0.45
1:E:126:PRO:O	1:E:131:ASP:HB2	2.17	0.45
1:E:252:LYS:HD2	1:E:361:GLU:HG2	1.99	0.45
1:E:341:SER:HA	1:E:344:GLN:NE2	2.32	0.45
1:E:381:ASN:HB2	2:F:217:ARG:HH21	1.81	0.45
2:F:204:ASP:OD1	2:F:206:SER:HB2	2.17	0.45
1:A:209:GLU:HG3	1:A:209:GLU:O	2.16	0.45
1:A:423:PHE:O	1:A:423:PHE:HD2	1.99	0.45
1:E:164:ASN:O	1:E:254:MET:HE2	2.17	0.45
2:F:121:GLN:HB2	2:F:122:TYR:HE1	1.82	0.45
1:G:354:GLY:O	1:G:375:LYS:O	2.35	0.45
1:A:249:VAL:O	1:A:251:SER:N	2.50	0.44
1:A:423:PHE:O	1:A:423:PHE:CD2	2.70	0.44
2:B:160:GLU:CD	2:B:160:GLU:H	2.21	0.44
2:D:315:ARG:HG3	2:D:340:VAL:HG21	1.96	0.44
2:F:363:ASP:O	2:F:366:ASP:HB2	2.17	0.44
1:G:209:GLU:OE1	1:G:426:ALA:HB3	2.13	0.44
1:G:245:VAL:HG11	1:G:290:LEU:HD23	1.99	0.44
2:H:304:MET:O	2:H:308:HIS:HB3	2.17	0.44
2:B:113:THR:O	2:B:116:HIS:N	2.47	0.44
2:B:126:LYS:CG	2:B:127:ASP:H	2.31	0.44
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.81	0.44
2:D:168:ARG:CG	2:D:169:PRO:HD3	2.47	0.44
2:D:265:PHE:HB3	2:D:266:GLY:H	1.56	0.44
1:E:108:GLN:NE2	2:F:11:LEU:N	2.55	0.44
1:E:187:GLY:O	1:E:188:SER:HB3	2.16	0.44
2:F:228:VAL:CG2	2:F:229:ALA:N	2.80	0.44
1:G:94:ILE:O	1:G:94:ILE:CG1	2.66	0.44
2:H:26:LEU:HD21	2:H:401:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HG13	1:A:178:THR:HG23	2.00	0.44
1:A:316:GLU:HA	1:A:319:ARG:HG3	2.00	0.44
1:A:421:ARG:CZ	1:A:422:GLU:N	2.80	0.44
2:B:168:ARG:HE	2:B:168:ARG:HB2	1.64	0.44
2:B:316:THR:OG1	2:B:339:THR:HA	2.17	0.44
2:B:344:VAL:HG13	2:B:346:ALA:H	1.83	0.44
2:B:382:ASN:HD22	2:B:384:HIS:H	1.63	0.44
1:C:60:ILE:H	1:C:60:ILE:HG12	1.50	0.44
1:C:187:GLY:O	1:C:188:SER:HB3	2.16	0.44
1:C:286:ASP:O	1:C:290:LEU:HB2	2.17	0.44
1:C:377:LEU:HD12	1:C:378:ASP:O	2.16	0.44
2:D:95:VAL:HG22	2:D:228:VAL:HG11	1.98	0.44
2:D:162:ARG:HA	2:D:162:ARG:NE	2.31	0.44
2:D:344:VAL:HG13	2:D:346:ALA:H	1.83	0.44
1:E:404:MET:HB2	1:E:414:PHE:HE1	1.77	0.44
1:E:421:ARG:NH2	1:E:422:GLU:CB	2.80	0.44
2:F:117:GLU:O	2:F:122:TYR:OH	2.35	0.44
2:F:257:ARG:CZ	2:F:257:ARG:HB3	2.47	0.44
1:G:190:ARG:CG	1:G:191:PRO:HD2	2.41	0.44
1:G:383:ARG:H	2:H:217:ARG:NH2	2.14	0.44
2:H:18:ALA:HB1	2:H:22:MET:CE	2.47	0.44
2:H:67:MET:HE3	2:H:71:SER:HB2	1.96	0.44
1:A:179:ARG:NH2	1:A:235:ARG:O	2.50	0.44
1:A:388:THR:O	1:A:392:TYR:HD2	2.00	0.44
2:B:349:ALA:O	2:B:351:LEU:N	2.51	0.44
2:D:124:GLU:O	2:D:125:TYR:C	2.55	0.44
1:E:64:GLY:O	1:E:67:TRP:HE3	1.99	0.44
1:E:190:ARG:CG	1:E:191:PRO:HD2	2.41	0.44
2:F:218:PHE:O	2:F:220:ALA:N	2.50	0.44
1:G:379:GLU:H	1:G:379:GLU:HG2	1.53	0.44
2:H:168:ARG:HB2	2:H:169:PRO:CD	2.37	0.44
2:H:353:ASP:O	2:H:354:SER:CB	2.64	0.44
2:B:20:GLN:HG2	2:B:135:THR:CG2	2.47	0.44
2:B:362:GLY:HA3	2:B:366:ASP:OD1	2.16	0.44
1:C:316:GLU:N	1:C:317:PRO:CD	2.80	0.44
2:D:271:LEU:HD23	2:D:271:LEU:HA	1.83	0.44
1:E:175:VAL:O	1:E:177:GLY:N	2.50	0.44
2:F:94:SER:O	2:F:129:PRO:HD2	2.17	0.44
1:G:417:ILE:O	1:G:417:ILE:CG2	2.65	0.44
1:A:103:PHE:HZ	1:A:143:ARG:HD3	1.83	0.44
1:A:118:VAL:C	1:A:119:PHE:HD1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG22	1:A:223:ARG:O	2.18	0.44
2:B:176:CYS:C	2:B:247:LEU:HD11	2.38	0.44
2:D:121:GLN:HB2	2:D:122:TYR:CE1	2.52	0.44
2:D:354:SER:CB	2:D:355:PRO:CD	2.96	0.44
1:E:184:LEU:H	1:E:184:LEU:HG	1.67	0.44
1:E:439:CYS:O	1:E:440:ILE:C	2.54	0.44
2:F:271:LEU:HD23	2:F:271:LEU:HA	1.83	0.44
1:G:322:LEU:O	1:G:325:LYS:HG2	2.17	0.44
1:A:174:TYR:CE2	1:A:234:TYR:CE2	3.05	0.44
1:A:340:VAL:O	1:A:344:GLN:HB3	2.17	0.44
2:B:382:ASN:ND2	2:B:384:HIS:N	2.64	0.44
1:C:302:ALA:O	1:C:305:ALA:HB3	2.17	0.44
2:D:191:SER:HB3	2:D:277:TRP:CZ3	2.48	0.44
1:E:166:ILE:O	1:E:166:ILE:HG22	2.18	0.44
1:E:220:LEU:CD2	1:E:303:LEU:HD13	2.47	0.44
1:E:383:ARG:NE	2:F:90:ARG:HH12	2.16	0.44
2:F:23:GLY:HA3	2:F:142:PHE:O	2.18	0.44
2:F:28:ILE:HD11	2:F:36:PRO:N	2.33	0.44
2:F:395:PRO:HG3	2:F:434:HIS:CG	2.53	0.44
1:G:179:ARG:NH2	1:G:235:ARG:O	2.50	0.44
1:G:231:ASP:OD1	1:G:233:ARG:NH2	2.50	0.44
2:H:185:LEU:CB	2:H:206:SER:OG	2.66	0.44
2:H:191:SER:HG	2:H:277:TRP:HZ3	1.66	0.44
1:A:29:LYS:HG2	2:B:65:THR:O	2.18	0.44
2:B:89:GLU:OE2	2:B:124:GLU:CB	2.66	0.44
2:B:102:GLY:HA2	2:B:138:PHE:CE1	2.53	0.44
1:C:24:GLY:O	1:C:25:CYS:HB3	2.17	0.44
1:C:380:GLY:HA3	1:C:384:VAL:CG2	2.46	0.44
2:D:126:LYS:CG	2:D:127:ASP:H	2.31	0.44
1:E:249:VAL:O	1:E:251:SER:N	2.49	0.44
2:F:226:LEU:HD22	2:F:226:LEU:HA	1.67	0.44
2:F:255:ALA:O	2:F:258:THR:O	2.36	0.44
2:F:295:ARG:NE	2:H:212:HIS:NE2	2.66	0.44
1:G:68:ASP:OD1	1:G:68:ASP:N	2.51	0.44
2:H:118:PHE:O	2:H:118:PHE:CD2	2.71	0.44
2:H:191:SER:HB3	2:H:277:TRP:CZ3	2.47	0.44
1:A:64:GLY:O	1:A:67:TRP:HE3	2.00	0.44
1:A:155:GLY:N	3:A:501:SF4:S4	2.90	0.44
2:B:113:THR:O	2:B:117:GLU:N	2.50	0.44
2:B:122:TYR:O	2:B:123:GLU:C	2.55	0.44
1:E:149:ILE:N	1:E:149:ILE:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ASP:O	1:E:166:ILE:HG21	2.18	0.44
1:G:285:ARG:O	1:G:288:ALA:HB3	2.18	0.44
1:G:287:PHE:O	1:G:291:LEU:CD2	2.65	0.44
1:G:307:GLU:HG2	1:G:428:TYR:CG	2.52	0.44
1:G:429:ASP:O	1:G:432:LEU:HB2	2.17	0.44
2:H:23:GLY:HA3	2:H:142:PHE:O	2.18	0.44
2:H:38:PHE:CG	2:H:45:THR:HG22	2.52	0.44
1:A:108:GLN:NE2	2:B:11:LEU:H	2.12	0.43
1:A:310:LYS:HG2	1:E:191:PRO:HB2	2.00	0.43
1:A:353:THR:CG2	1:A:377:LEU:HD23	2.48	0.43
2:B:93:PRO:CG	2:B:96:ILE:HG13	2.47	0.43
2:B:95:VAL:CG2	2:B:228:VAL:CG1	2.96	0.43
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.73	0.43
1:C:193:ILE:HD13	1:C:293:ASP:OD1	2.18	0.43
1:C:231:ASP:OD1	1:C:233:ARG:NH2	2.51	0.43
2:D:99:LEU:HD23	2:D:133:VAL:HB	2.00	0.43
2:D:105:GLU:HG3	2:D:105:GLU:O	2.18	0.43
2:D:351:LEU:H	2:D:351:LEU:HG	1.54	0.43
1:E:27:LYS:CD	2:F:66:ALA:HB1	2.48	0.43
1:E:125:VAL:CB	1:E:126:PRO:HD3	2.47	0.43
1:E:275:TYR:HD2	1:E:338:SER:HB2	1.81	0.43
1:E:424:GLY:C	1:E:433:GLU:OE2	2.56	0.43
2:F:116:HIS:C	2:F:119:ARG:H	2.21	0.43
1:G:327:VAL:HG21	1:G:343:LEU:HD11	1.98	0.43
1:G:404:MET:HB2	1:G:414:PHE:HE1	1.81	0.43
2:H:175:LEU:HD23	2:H:175:LEU:HA	1.88	0.43
2:H:315:ARG:HG3	2:H:340:VAL:CG2	2.48	0.43
1:A:396:ILE:HG23	1:A:413:PRO:HB2	2.00	0.43
2:B:226:LEU:HD22	2:B:226:LEU:HA	1.69	0.43
2:D:218:PHE:O	2:D:220:ALA:N	2.51	0.43
1:E:397:LEU:O	1:E:414:PHE:HD2	2.01	0.43
2:F:125:TYR:N	2:F:125:TYR:CD1	2.84	0.43
2:F:173:ASN:HD22	2:F:240:THR:CG2	2.30	0.43
1:G:54:HIS:CD2	1:G:121:TYR:OH	2.69	0.43
1:G:102:LEU:HD23	1:G:102:LEU:O	2.17	0.43
1:G:355:THR:N	1:G:358:SER:OG	2.45	0.43
2:H:329:ASP:OD2	2:H:333:ARG:NH1	2.41	0.43
1:A:102:LEU:O	1:A:102:LEU:HD23	2.17	0.43
1:A:189:GLU:O	1:A:190:ARG:O	2.35	0.43
1:A:383:ARG:N	2:B:217:ARG:HH12	2.17	0.43
2:B:95:VAL:HG12	2:B:96:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:GLN:HB3	1:C:450:VAL:HG11	1.99	0.43
1:C:189:GLU:O	1:C:190:ARG:O	2.36	0.43
1:C:307:GLU:HG2	1:C:428:TYR:CG	2.53	0.43
1:C:358:SER:HB2	1:C:363:LYS:HE3	1.99	0.43
2:D:76:ALA:HA	2:D:79:ASN:OD1	2.18	0.43
1:E:330:TYR:HB3	1:E:399:ALA:CB	2.47	0.43
2:F:76:ALA:HA	2:F:79:ASN:OD1	2.19	0.43
2:F:200:LEU:HD22	2:F:200:LEU:C	2.38	0.43
2:F:315:ARG:HG3	2:F:340:VAL:CG2	2.49	0.43
1:G:377:LEU:O	1:G:384:VAL:HG11	2.17	0.43
2:H:126:LYS:NZ	2:H:127:ASP:N	2.56	0.43
1:A:286:ASP:O	1:A:290:LEU:HB2	2.18	0.43
1:A:287:PHE:O	1:A:291:LEU:CD2	2.66	0.43
2:B:20:GLN:HG2	2:B:135:THR:HG22	2.01	0.43
2:B:24:ALA:HB1	2:B:149:ALA:HB2	1.99	0.43
2:B:26:LEU:CD1	2:B:146:PHE:CD1	3.01	0.43
2:B:168:ARG:CB	2:B:169:PRO:CD	2.97	0.43
2:B:314:ALA:HA	2:B:377:GLN:OE1	2.17	0.43
1:C:409:LYS:HD2	2:D:218:PHE:CZ	2.52	0.43
2:F:70:VAL:C	2:F:72:SER:H	2.22	0.43
2:F:118:PHE:O	2:F:122:TYR:CE2	2.70	0.43
1:G:48:PRO:HG2	1:G:204:TYR:CD1	2.52	0.43
1:G:312:ARG:HB2	1:G:312:ARG:HH11	1.84	0.43
2:H:26:LEU:CD1	2:H:146:PHE:CD1	3.01	0.43
1:A:382:ALA:CB	2:B:217:ARG:HG3	2.46	0.43
2:B:94:SER:O	2:B:129:PRO:HD2	2.19	0.43
1:C:126:PRO:O	1:C:131:ASP:HB2	2.19	0.43
1:C:137:CYS:SG	1:C:150:PRO:HB3	2.58	0.43
1:C:204:TYR:CD1	1:C:229:ALA:O	2.71	0.43
1:C:340:VAL:O	1:C:344:GLN:HB3	2.18	0.43
1:C:382:ALA:O	1:C:386:LEU:N	2.50	0.43
1:E:157:TYR:HD1	1:E:157:TYR:H	1.67	0.43
1:E:362:ASP:O	1:E:366:ILE:CG1	2.63	0.43
2:F:168:ARG:H	2:F:236:GLN:HB2	1.84	0.43
2:F:312:SER:O	2:F:313:SER:CB	2.67	0.43
2:F:347:ARG:O	2:F:348:ALA:O	2.36	0.43
1:G:94:ILE:O	1:G:94:ILE:CD1	2.66	0.43
2:H:16:LEU:HB2	2:H:363:ASP:HA	2.01	0.43
2:H:213:LEU:CD1	2:H:218:PHE:HB3	2.46	0.43
1:A:322:LEU:O	1:A:325:LYS:HG2	2.18	0.43
1:A:341:SER:HA	1:A:344:GLN:NE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLY:O	2:B:413:CYS:HB2	2.19	0.43
2:B:236:GLN:O	2:B:236:GLN:HG2	2.18	0.43
2:B:395:PRO:HG3	2:B:434:HIS:ND1	2.33	0.43
1:C:179:ARG:NH2	1:C:235:ARG:O	2.51	0.43
1:C:328:LEU:HD22	1:C:389:VAL:CG2	2.49	0.43
1:C:440:ILE:HG13	1:C:441:THR:H	1.83	0.43
2:D:116:HIS:HA	2:D:119:ARG:HB2	2.00	0.43
2:F:331:LEU:HD22	2:F:331:LEU:C	2.38	0.43
1:G:155:GLY:CA	3:G:501:SF4:S4	3.05	0.43
1:G:187:GLY:O	1:G:188:SER:HB3	2.19	0.43
2:H:105:GLU:HG3	2:H:105:GLU:O	2.19	0.43
1:A:71:GLY:O	1:A:72:THR:O	2.36	0.43
1:A:204:TYR:CD1	1:A:229:ALA:O	2.72	0.43
1:C:47:LEU:N	1:C:48:PRO:HD3	2.34	0.43
1:C:304:ILE:HD12	1:C:305:ALA:N	2.34	0.43
1:C:304:ILE:O	1:C:308:GLU:HG3	2.18	0.43
2:D:26:LEU:HD13	2:D:146:PHE:CE1	2.54	0.43
2:D:260:VAL:HA	2:D:261:PRO:HD3	1.88	0.43
1:E:286:ASP:O	1:E:290:LEU:HB2	2.18	0.43
2:F:91:GLN:HE21	2:F:91:GLN:HB2	1.61	0.43
2:H:21:THR:HG21	2:H:137:ASP:OD1	2.18	0.43
2:H:39:HIS:HD2	2:H:65:THR:OG1	2.01	0.43
2:H:299:GLN:OE1	2:H:418:ARG:NE	2.48	0.43
1:A:345:ASP:OD1	1:A:346:LEU:N	2.52	0.43
1:A:383:ARG:CG	1:A:384:VAL:H	2.30	0.43
1:A:383:ARG:CD	2:B:217:ARG:HH22	2.32	0.43
2:B:221:LEU:O	2:B:221:LEU:HG	2.19	0.43
2:B:299:GLN:OE1	2:B:418:ARG:NH2	2.49	0.43
2:B:329:ASP:OD2	2:B:333:ARG:NH1	2.47	0.43
1:C:382:ALA:CB	2:D:217:ARG:HG3	2.42	0.43
1:E:99:GLU:O	1:E:100:LYS:C	2.57	0.43
1:E:179:ARG:HB3	1:E:238:GLN:CB	2.49	0.43
1:E:409:LYS:HD2	2:F:218:PHE:CZ	2.53	0.43
2:F:122:TYR:C	2:F:124:GLU:N	2.72	0.43
2:F:185:LEU:CB	2:F:206:SER:OG	2.67	0.43
1:G:103:PHE:HZ	1:G:143:ARG:HD3	1.84	0.43
1:G:152:ASP:O	1:G:166:ILE:HG21	2.18	0.43
1:G:172:LEU:C	1:G:172:LEU:CD1	2.86	0.43
2:H:173:ASN:HD22	2:H:240:THR:CG2	2.31	0.43
2:B:39:HIS:HD2	2:B:65:THR:CB	2.32	0.43
2:B:100:THR:CG2	2:B:134:ASN:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:CD	1:C:27:LYS:C	2.87	0.43
1:C:252:LYS:CB	1:C:361:GLU:OE2	2.64	0.43
1:C:304:ILE:HD12	1:C:304:ILE:C	2.40	0.43
1:C:353:THR:CG2	1:C:377:LEU:HD23	2.48	0.43
2:D:158:VAL:N	2:D:159:PRO:HD2	2.34	0.43
1:E:58:GLY:O	1:E:86:THR:O	2.36	0.43
1:E:383:ARG:H	2:F:217:ARG:NH2	2.16	0.43
1:G:47:LEU:N	1:G:48:PRO:HD3	2.34	0.43
1:G:149:ILE:N	1:G:149:ILE:HD12	2.34	0.43
1:G:293:ASP:OD2	1:G:294:PRO:HD2	2.19	0.43
2:H:109:CYS:O	2:H:110:ASP:C	2.57	0.43
2:H:329:ASP:OD1	2:H:356:LEU:HD22	2.19	0.43
2:H:352:VAL:CG1	2:H:354:SER:H	2.32	0.43
1:A:206:ILE:CD1	1:A:419:GLN:HB3	2.48	0.43
1:C:166:ILE:O	1:C:166:ILE:HG22	2.19	0.43
1:E:68:ASP:OD1	1:E:68:ASP:N	2.51	0.43
1:E:340:VAL:O	1:E:344:GLN:HB3	2.19	0.43
2:F:126:LYS:O	2:F:127:ASP:CB	2.65	0.43
2:F:344:VAL:O	2:F:361:VAL:HA	2.18	0.43
1:G:384:VAL:O	1:G:387:LYS:HG2	2.19	0.43
2:H:91:GLN:HE21	2:H:91:GLN:HB2	1.58	0.43
2:H:126:LYS:HZ2	2:H:127:ASP:H	1.61	0.43
2:H:160:GLU:CD	2:H:160:GLU:H	2.22	0.43
2:H:325:LEU:HD11	2:H:342:ALA:HB1	2.00	0.43
1:A:304:ILE:O	1:A:308:GLU:HG3	2.19	0.42
1:C:47:LEU:N	1:C:48:PRO:CD	2.82	0.42
1:C:154:ALA:O	1:C:157:TYR:HD1	2.01	0.42
1:C:198:VAL:HG22	1:C:223:ARG:O	2.19	0.42
1:C:289:ARG:HE	1:C:289:ARG:HB3	1.70	0.42
1:C:322:LEU:O	1:C:325:LYS:HG2	2.19	0.42
2:D:126:LYS:CG	2:D:127:ASP:N	2.82	0.42
2:D:173:ASN:ND2	2:D:240:THR:HG22	2.34	0.42
1:E:46:LEU:HB2	1:E:121:TYR:OH	2.19	0.42
1:E:128:LEU:HD23	2:F:106:THR:HG21	2.00	0.42
2:F:173:ASN:HB2	2:F:240:THR:CG2	2.24	0.42
2:F:221:LEU:O	2:F:221:LEU:HG	2.19	0.42
1:G:78:ASP:O	1:G:81:ARG:HB2	2.18	0.42
2:H:125:TYR:HB2	2:H:126:LYS:O	2.18	0.42
2:H:217:ARG:C	2:H:218:PHE:CD2	2.82	0.42
1:A:337:TRP:O	1:A:337:TRP:HE3	2.01	0.42
1:A:421:ARG:NH2	1:A:422:GLU:CB	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:ARG:HE	2:B:391:ARG:HB2	1.61	0.42
1:C:65:SER:C	1:C:67:TRP:H	2.22	0.42
1:E:379:GLU:H	1:E:379:GLU:HG2	1.56	0.42
1:E:383:ARG:N	2:F:217:ARG:HH12	2.17	0.42
2:F:168:ARG:CB	2:F:169:PRO:CD	2.97	0.42
2:F:213:LEU:HD13	2:F:218:PHE:CG	2.54	0.42
2:F:285:SER:CB	2:F:287:ASN:HD21	2.31	0.42
1:G:179:ARG:HB3	1:G:238:GLN:HB2	2.00	0.42
2:H:113:THR:O	2:H:116:HIS:N	2.49	0.42
2:H:347:ARG:O	2:H:348:ALA:O	2.37	0.42
1:A:383:ARG:HD2	2:B:217:ARG:NH2	2.34	0.42
2:B:304:MET:O	2:B:308:HIS:HB3	2.19	0.42
2:D:117:GLU:O	2:D:122:TYR:OH	2.32	0.42
2:D:126:LYS:O	2:D:127:ASP:CB	2.63	0.42
2:D:291:ASP:HA	2:D:294:LYS:HG3	2.01	0.42
1:E:48:PRO:HG2	1:E:204:TYR:CD1	2.55	0.42
2:F:159:PRO:CB	2:F:257:ARG:CD	2.93	0.42
1:G:248:MET:SD	1:G:258:ALA:HB2	2.59	0.42
2:H:149:ALA:O	2:H:153:ILE:CG1	2.62	0.42
2:H:386:LEU:HD23	2:H:386:LEU:HA	1.91	0.42
1:A:172:LEU:C	1:A:172:LEU:CD1	2.87	0.42
2:B:126:LYS:CG	2:B:127:ASP:N	2.82	0.42
1:C:179:ARG:HB3	1:C:238:GLN:HB3	2.01	0.42
1:C:207:ALA:CB	1:C:421:ARG:O	2.67	0.42
2:D:16:LEU:O	2:D:16:LEU:HD12	2.18	0.42
1:E:174:TYR:CE2	1:E:234:TYR:CE2	3.07	0.42
1:E:287:PHE:O	1:E:291:LEU:CD2	2.66	0.42
1:E:308:GLU:O	1:E:312:ARG:HD3	2.18	0.42
1:E:440:ILE:HG13	1:E:441:THR:H	1.85	0.42
2:F:221:LEU:C	2:F:223:THR:N	2.73	0.42
2:F:265:PHE:HB3	2:F:266:GLY:H	1.56	0.42
1:G:31:GLY:N	1:G:33:THR:OG1	2.52	0.42
1:G:184:LEU:HA	1:G:185:PRO:HD3	1.82	0.42
1:G:316:GLU:CD	1:G:316:GLU:C	2.77	0.42
2:B:167:LYS:HA	2:B:237:SER:H	1.84	0.42
2:B:295:ARG:NE	2:D:212:HIS:CE1	2.87	0.42
1:C:341:SER:HA	1:C:344:GLN:HE21	1.84	0.42
2:D:26:LEU:HD12	2:D:146:PHE:CD1	2.55	0.42
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.86	0.42
2:D:322:PRO:HG2	2:D:348:ALA:CB	2.49	0.42
2:D:335:MET:SD	2:D:424:LEU:HD21	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LYS:C	1:E:27:LYS:CD	2.87	0.42
1:E:220:LEU:HD21	1:E:303:LEU:HD13	2.01	0.42
2:F:89:GLU:OE2	2:F:124:GLU:CB	2.67	0.42
2:F:100:THR:CG2	2:F:134:ASN:HA	2.49	0.42
2:F:105:GLU:HG2	2:F:136:PRO:CG	2.50	0.42
1:G:433:GLU:HA	1:G:436:ARG:HD2	2.01	0.42
2:H:200:LEU:C	2:H:200:LEU:HD22	2.39	0.42
1:A:26:ALA:O	1:A:27:LYS:CB	2.63	0.42
1:A:174:TYR:CZ	1:A:234:TYR:CD2	3.08	0.42
1:C:71:GLY:HA2	1:C:420:GLU:C	2.40	0.42
1:C:312:ARG:HB2	1:C:312:ARG:NH1	2.35	0.42
1:C:383:ARG:NE	2:D:90:ARG:HH12	2.16	0.42
1:C:397:LEU:O	1:C:414:PHE:HD2	2.02	0.42
2:D:213:LEU:HD13	2:D:218:PHE:CG	2.55	0.42
2:D:352:VAL:CG1	2:D:354:SER:H	2.33	0.42
1:E:103:PHE:HZ	1:E:143:ARG:HD3	1.84	0.42
1:E:327:VAL:O	1:E:327:VAL:HG23	2.20	0.42
2:H:50:VAL:O	2:H:51:PHE:C	2.57	0.42
1:A:193:ILE:O	1:A:195:VAL:N	2.52	0.42
1:A:346:LEU:HD23	1:A:346:LEU:C	2.40	0.42
2:B:168:ARG:HG3	2:B:236:GLN:CB	2.44	0.42
2:B:335:MET:SD	2:B:424:LEU:CD2	3.08	0.42
1:C:30:PRO:HA	2:D:63:GLN:CD	2.38	0.42
1:C:172:LEU:C	1:C:172:LEU:CD1	2.87	0.42
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.80	0.42
1:C:220:LEU:HD21	1:C:303:LEU:HD13	2.00	0.42
2:D:22:MET:SD	2:D:48:ALA:HA	2.60	0.42
2:D:55:HIS:HE1	2:D:403:GLN:HG2	1.83	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG2	2.20	0.42
1:E:174:TYR:OH	1:E:238:GLN:HG3	2.20	0.42
1:E:312:ARG:HB2	1:E:312:ARG:HH11	1.85	0.42
2:F:158:VAL:N	2:F:159:PRO:HD2	2.34	0.42
1:G:193:ILE:O	1:G:195:VAL:N	2.53	0.42
2:H:39:HIS:HD2	2:H:65:THR:CB	2.32	0.42
2:H:398:ARG:NH1	2:H:405:ASP:OD1	2.52	0.42
2:B:116:HIS:HA	2:B:119:ARG:HB2	2.02	0.42
2:B:117:GLU:O	2:B:122:TYR:OH	2.32	0.42
2:B:162:ARG:NE	2:B:162:ARG:HA	2.34	0.42
1:C:68:ASP:OD1	1:C:68:ASP:N	2.53	0.42
1:C:191:PRO:HG3	1:G:314:ALA:HB2	2.00	0.42
1:C:417:ILE:HD13	1:C:417:ILE:HA	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:CYS:SG	1:E:123:THR:HG21	2.60	0.42
1:E:246:ASN:HD22	1:E:246:ASN:HA	1.69	0.42
1:E:346:LEU:HD23	1:E:346:LEU:C	2.39	0.42
1:E:367:ARG:HD3	1:E:367:ARG:HA	1.43	0.42
2:F:310:MET:N	2:F:310:MET:HE3	2.35	0.42
1:G:304:ILE:HD12	1:G:304:ILE:C	2.40	0.42
1:G:417:ILE:HD13	1:G:417:ILE:HA	1.62	0.42
1:A:417:ILE:HD13	1:A:417:ILE:HA	1.66	0.42
2:B:121:GLN:HB2	2:B:122:TYR:HE1	1.85	0.42
2:B:213:LEU:CD1	2:B:218:PHE:HB3	2.48	0.42
2:B:329:ASP:OD1	2:B:356:LEU:HD22	2.19	0.42
1:C:66:SER:HB3	2:D:47:PHE:CZ	2.54	0.42
1:C:293:ASP:OD2	1:C:294:PRO:HD2	2.19	0.42
1:C:355:THR:N	1:C:358:SER:OG	2.46	0.42
2:D:185:LEU:CB	2:D:206:SER:OG	2.67	0.42
2:D:395:PRO:HG3	2:D:434:HIS:CG	2.55	0.42
1:E:201:ILE:HA	1:E:228:LEU:HB3	2.01	0.42
1:E:209:GLU:OE1	1:E:426:ALA:HB3	2.19	0.42
1:E:270:PHE:CD2	1:E:286:ASP:OD2	2.73	0.42
1:E:322:LEU:CD2	1:E:439:CYS:SG	2.95	0.42
2:F:99:LEU:HD23	2:F:133:VAL:HB	2.02	0.42
2:F:109:CYS:O	2:F:110:ASP:C	2.59	0.42
2:F:409:GLY:C	2:F:411:GLN:H	2.23	0.42
1:G:29:LYS:CG	2:H:65:THR:O	2.68	0.42
2:H:131:VAL:HA	2:H:132:PRO:HD3	1.90	0.42
2:H:168:ARG:HE	2:H:168:ARG:HB2	1.58	0.42
1:A:201:ILE:HA	1:A:228:LEU:HB3	2.02	0.42
2:B:33:ARG:N	2:B:221:LEU:CD2	2.83	0.42
2:B:265:PHE:HB3	2:B:266:GLY:H	1.61	0.42
2:B:374:GLY:O	2:B:375:GLN:HB2	2.19	0.42
1:C:29:LYS:HZ2	1:C:29:LYS:HB2	1.84	0.42
1:C:206:ILE:O	1:C:419:GLN:O	2.38	0.42
1:C:323:GLU:OE2	1:C:324:GLY:N	2.53	0.42
1:C:377:LEU:O	1:C:384:VAL:HG11	2.19	0.42
2:D:200:LEU:HD22	2:D:200:LEU:C	2.40	0.42
2:D:236:GLN:HG2	2:D:236:GLN:O	2.19	0.42
2:D:333:ARG:HB2	2:D:333:ARG:HH11	1.83	0.42
2:D:362:GLY:HA3	2:D:366:ASP:OD1	2.20	0.42
1:E:353:THR:CG2	1:E:377:LEU:HD23	2.50	0.42
2:F:64:THR:HG22	2:F:66:ALA:N	2.25	0.42
2:F:397:LEU:HD22	2:F:427:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:VAL:HG11	1:G:417:ILE:HD11	2.02	0.42
2:H:68:ASP:CB	2:H:70:VAL:HG22	2.25	0.42
2:H:168:ARG:CG	2:H:169:PRO:HD3	2.50	0.42
1:A:47:LEU:C	1:A:49:VAL:H	2.23	0.41
1:A:203:GLU:HB3	1:A:227:THR:HG23	2.02	0.41
1:A:359:THR:CG2	4:A:502:CZL:S2A	3.07	0.41
1:A:440:ILE:HG13	1:A:441:THR:H	1.85	0.41
1:C:48:PRO:CB	1:C:72:THR:HG21	2.48	0.41
1:C:102:LEU:O	1:C:102:LEU:HD23	2.20	0.41
1:C:270:PHE:CD2	1:C:286:ASP:OD2	2.73	0.41
2:D:113:THR:O	2:D:117:GLU:N	2.52	0.41
2:D:349:ALA:O	2:D:351:LEU:N	2.53	0.41
2:F:159:PRO:CB	2:F:257:ARG:HH11	2.32	0.41
2:F:215:GLU:O	2:F:218:PHE:CE2	2.73	0.41
1:G:174:TYR:OH	1:G:238:GLN:HG2	2.19	0.41
1:G:341:SER:HA	1:G:344:GLN:HE21	1.85	0.41
1:G:421:ARG:CZ	1:G:422:GLU:N	2.78	0.41
2:H:122:TYR:O	2:H:123:GLU:C	2.57	0.41
2:H:160:GLU:HG2	2:H:161:ARG:N	2.35	0.41
1:A:248:MET:SD	1:A:258:ALA:HB2	2.59	0.41
1:A:383:ARG:N	2:B:217:ARG:NH1	2.68	0.41
1:A:419:GLN:NE2	1:A:424:GLY:H	2.15	0.41
2:B:33:ARG:H	2:B:221:LEU:HD23	1.85	0.41
2:B:105:GLU:HG2	2:B:136:PRO:CG	2.51	0.41
2:B:295:ARG:HH22	2:D:206:SER:HB3	1.85	0.41
1:C:63:ALA:O	1:C:65:SER:N	2.53	0.41
1:C:206:ILE:H	1:C:206:ILE:HG12	1.35	0.41
1:C:341:SER:HA	1:C:344:GLN:NE2	2.34	0.41
2:D:33:ARG:H	2:D:221:LEU:HD23	1.86	0.41
1:G:47:LEU:N	1:G:48:PRO:CD	2.83	0.41
1:G:175:VAL:O	1:G:177:GLY:N	2.52	0.41
2:H:183:GLY:O	2:H:413:CYS:HB2	2.20	0.41
2:H:382:ASN:CB	2:H:402:PRO:HD2	2.50	0.41
2:B:126:LYS:HZ2	2:B:127:ASP:N	2.16	0.41
2:B:340:VAL:CG1	2:B:374:GLY:HA3	2.50	0.41
2:B:344:VAL:O	2:B:361:VAL:HA	2.21	0.41
1:C:201:ILE:HA	1:C:228:LEU:HB3	2.01	0.41
1:C:246:ASN:O	1:C:269:TRP:HA	2.20	0.41
1:C:345:ASP:OD1	1:C:346:LEU:N	2.54	0.41
1:E:71:GLY:HA2	1:E:420:GLU:C	2.40	0.41
1:E:304:ILE:HD12	1:E:304:ILE:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:GLY:O	1:E:375:LYS:O	2.38	0.41
2:F:131:VAL:HA	2:F:132:PRO:HD3	1.86	0.41
2:F:171:GLN:O	2:F:237:SER:HB2	2.20	0.41
2:F:314:ALA:HA	2:F:377:GLN:OE1	2.19	0.41
1:G:346:LEU:HD23	1:G:346:LEU:C	2.40	0.41
1:G:356:LYS:HD3	1:G:378:ASP:HA	2.00	0.41
2:H:31:LEU:HD23	2:H:95:VAL:HG11	2.01	0.41
2:H:121:GLN:N	2:H:122:TYR:CD1	2.89	0.41
2:H:136:PRO:O	2:H:137:ASP:C	2.56	0.41
1:A:154:ALA:O	1:A:157:TYR:HD1	2.03	0.41
2:B:126:LYS:C	2:B:128:VAL:H	2.24	0.41
2:B:149:ALA:O	2:B:153:ILE:CG1	2.66	0.41
2:B:332:LEU:HB3	2:B:337:ALA:HB3	2.01	0.41
2:B:333:ARG:HH11	2:B:333:ARG:CB	2.32	0.41
1:C:48:PRO:HG2	1:C:204:TYR:CD1	2.55	0.41
1:C:293:ASP:OD2	1:C:294:PRO:CD	2.69	0.41
1:C:316:GLU:C	1:C:316:GLU:CD	2.78	0.41
1:C:346:LEU:HD23	1:C:346:LEU:C	2.41	0.41
1:C:433:GLU:HA	1:C:436:ARG:HD2	2.02	0.41
2:D:159:PRO:CB	2:D:257:ARG:HG3	2.51	0.41
2:D:397:LEU:HD22	2:D:427:LEU:HD23	2.02	0.41
2:F:38:PHE:CB	2:F:45:THR:HG22	2.50	0.41
2:F:107:GLN:NE2	2:F:107:GLN:H	2.16	0.41
2:F:125:TYR:HB2	2:F:126:LYS:O	2.20	0.41
2:F:291:ASP:HA	2:F:294:LYS:HG3	2.03	0.41
1:G:71:GLY:HA2	1:G:420:GLU:C	2.40	0.41
2:H:221:LEU:C	2:H:223:THR:N	2.74	0.41
2:H:291:ASP:HA	2:H:294:LYS:HG3	2.03	0.41
2:H:335:MET:SD	2:H:424:LEU:CD2	3.09	0.41
1:A:220:LEU:HD21	1:A:303:LEU:HD13	2.03	0.41
1:A:246:ASN:HD22	1:A:246:ASN:HA	1.70	0.41
1:C:31:GLY:C	1:C:33:THR:N	2.73	0.41
1:C:143:ARG:NH1	1:C:143:ARG:HB3	2.35	0.41
1:C:199:ASN:OD1	1:C:240:MET:HG2	2.21	0.41
1:C:249:VAL:O	1:C:251:SER:N	2.53	0.41
2:D:160:GLU:HG2	2:D:161:ARG:N	2.35	0.41
1:E:67:TRP:CZ3	2:F:15:PRO:HG2	2.56	0.41
1:E:380:GLY:HA3	1:E:384:VAL:CG2	2.47	0.41
1:E:381:ASN:HB2	2:F:217:ARG:NH2	2.36	0.41
1:E:421:ARG:HE	1:E:421:ARG:HB3	1.15	0.41
2:F:20:GLN:HA	2:F:141:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:PHE:CE1	2:F:402:PRO:HB3	2.54	0.41
2:F:55:HIS:HE1	2:F:403:GLN:HG2	1.85	0.41
2:F:329:ASP:OD1	2:F:356:LEU:HD22	2.21	0.41
2:H:95:VAL:HG22	2:H:228:VAL:HG11	2.02	0.41
1:A:50:ALA:HB3	1:A:77:PRO:HG2	2.01	0.41
2:B:125:TYR:N	2:B:125:TYR:CD1	2.83	0.41
2:B:396:LEU:HD22	2:B:397:LEU:N	2.36	0.41
2:D:93:PRO:CG	2:D:96:ILE:HG13	2.50	0.41
2:D:347:ARG:O	2:D:348:ALA:O	2.38	0.41
1:E:209:GLU:CD	1:E:419:GLN:OE1	2.56	0.41
1:E:304:ILE:O	1:E:308:GLU:HG3	2.20	0.41
2:F:156:THR:C	2:F:157:LEU:HD13	2.41	0.41
2:F:168:ARG:CG	2:F:169:PRO:HD3	2.50	0.41
2:F:351:LEU:H	2:F:351:LEU:HG	1.54	0.41
1:G:24:GLY:O	1:G:25:CYS:HB3	2.21	0.41
1:G:29:LYS:CB	1:G:30:PRO:HD2	2.32	0.41
1:G:182:ASP:HA	1:G:183:PRO:HD3	1.91	0.41
1:G:316:GLU:N	1:G:317:PRO:CD	2.84	0.41
1:G:322:LEU:N	1:G:322:LEU:CD2	2.83	0.41
1:G:439:CYS:O	1:G:440:ILE:C	2.57	0.41
2:H:344:VAL:HG13	2:H:346:ALA:H	1.86	0.41
2:H:395:PRO:HG3	2:H:434:HIS:CG	2.55	0.41
1:A:322:LEU:CD2	1:A:322:LEU:N	2.84	0.41
1:A:328:LEU:HD23	1:A:397:LEU:HD23	2.03	0.41
2:B:125:TYR:HB2	2:B:126:LYS:O	2.20	0.41
2:B:168:ARG:H	2:B:236:GLN:HB2	1.85	0.41
1:C:247:MET:HB2	1:C:270:PHE:CE1	2.55	0.41
1:E:383:ARG:HD2	2:F:217:ARG:NH2	2.34	0.41
2:F:53:VAL:O	2:F:57:ARG:HA	2.21	0.41
2:F:263:ARG:HE	2:F:263:ARG:HB2	1.60	0.41
1:G:47:LEU:C	1:G:49:VAL:H	2.24	0.41
1:G:128:LEU:C	1:G:130:GLY:H	2.23	0.41
1:G:304:ILE:O	1:G:308:GLU:HG3	2.20	0.41
1:G:358:SER:HB2	1:G:363:LYS:HE3	2.03	0.41
2:H:159:PRO:HB2	2:H:257:ARG:HD3	2.01	0.41
2:H:166:GLY:O	2:H:236:GLN:HA	2.21	0.41
2:H:256:GLU:OE2	2:H:256:GLU:CA	2.68	0.41
1:A:209:GLU:O	1:A:212:HIS:HB2	2.21	0.41
2:B:58:GLU:CD	2:D:302:ASP:OD2	2.59	0.41
2:B:100:THR:HG21	2:B:134:ASN:OD1	2.20	0.41
2:B:354:SER:HB2	2:B:355:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:THR:O	1:C:229:ALA:N	2.54	0.41
1:C:245:VAL:HG11	1:C:290:LEU:HD23	2.00	0.41
1:C:247:MET:HB2	1:C:270:PHE:CZ	2.56	0.41
1:C:429:ASP:O	1:C:432:LEU:HB2	2.20	0.41
2:D:102:GLY:HA2	2:D:138:PHE:CE1	2.55	0.41
1:E:174:TYR:CZ	1:E:234:TYR:CD2	3.08	0.41
1:E:193:ILE:O	1:E:195:VAL:N	2.53	0.41
1:E:328:LEU:HD22	1:E:389:VAL:CG2	2.50	0.41
2:F:302:ASP:OD2	2:H:58:GLU:CD	2.59	0.41
1:G:404:MET:HE2	1:G:405:TYR:CE2	2.56	0.41
1:A:29:LYS:HG3	2:B:66:ALA:HB3	2.02	0.41
1:A:148:VAL:C	1:A:149:ILE:HD12	2.40	0.41
1:A:149:ILE:N	1:A:149:ILE:CD1	2.84	0.41
2:B:28:ILE:HD11	2:B:36:PRO:N	2.36	0.41
2:B:191:SER:HG	2:B:277:TRP:HZ3	1.67	0.41
2:B:257:ARG:CZ	2:B:257:ARG:HB3	2.51	0.41
2:B:291:ASP:HA	2:B:294:LYS:HG3	2.03	0.41
2:B:352:VAL:CG1	2:B:354:SER:H	2.34	0.41
2:B:353:ASP:O	2:B:354:SER:CB	2.69	0.41
1:C:27:LYS:CG	2:D:66:ALA:HB1	2.50	0.41
1:C:61:ALA:HB2	2:D:137:ASP:CG	2.42	0.41
1:C:174:TYR:CZ	1:C:234:TYR:CD2	3.09	0.41
1:C:421:ARG:NH2	1:C:422:GLU:CB	2.81	0.41
1:C:424:GLY:O	1:C:433:GLU:OE2	2.39	0.41
2:D:51:PHE:CE1	2:D:402:PRO:HB3	2.56	0.41
2:D:176:CYS:C	2:D:247:LEU:HD11	2.41	0.41
2:D:329:ASP:OD1	2:D:356:LEU:HD22	2.20	0.41
2:D:409:GLY:C	2:D:411:GLN:H	2.23	0.41
1:E:63:ALA:O	1:E:65:SER:N	2.54	0.41
1:E:146:THR:O	1:E:148:VAL:HG23	2.21	0.41
1:E:322:LEU:N	1:E:322:LEU:CD2	2.84	0.41
1:E:417:ILE:O	1:E:417:ILE:CG2	2.59	0.41
2:F:16:LEU:HB2	2:F:363:ASP:HA	2.02	0.41
2:F:27:ALA:HB2	2:F:146:PHE:CE1	2.56	0.41
2:F:31:LEU:HD12	2:F:226:LEU:HB2	2.03	0.41
2:F:85:LYS:CD	2:F:118:PHE:HE1	2.23	0.41
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.87	0.41
2:F:211:GLY:HA3	2:H:302:ASP:HB2	2.03	0.41
2:F:269:TYR:O	2:F:273:ALA:CB	2.69	0.41
2:F:335:MET:SD	2:F:424:LEU:CD2	3.09	0.41
1:G:48:PRO:HB3	1:G:72:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:HIS:HE1	1:G:131:ASP:OD1	2.04	0.41
1:G:60:ILE:H	1:G:60:ILE:HG12	1.45	0.41
1:G:65:SER:C	1:G:67:TRP:H	2.22	0.41
1:G:193:ILE:HD13	1:G:293:ASP:OD1	2.20	0.41
1:G:249:VAL:O	1:G:251:SER:N	2.53	0.41
1:G:337:TRP:O	1:G:337:TRP:HE3	2.02	0.41
1:G:355:THR:CB	1:G:377:LEU:HD11	2.50	0.41
2:H:42:GLN:HA	2:H:64:THR:CG2	2.47	0.41
2:H:95:VAL:CG2	2:H:228:VAL:CG1	2.99	0.41
2:H:159:PRO:CB	2:H:257:ARG:HH11	2.31	0.41
2:H:382:ASN:ND2	2:H:384:HIS:N	2.69	0.41
2:B:326:LEU:HD23	2:B:326:LEU:N	2.35	0.41
1:C:99:GLU:O	1:C:100:LYS:C	2.58	0.41
1:C:356:LYS:HD3	1:C:378:ASP:HA	2.02	0.41
1:C:381:ASN:HB2	2:D:217:ARG:NH2	2.36	0.41
1:C:405:TYR:CE1	2:D:57:ARG:O	2.74	0.41
1:C:419:GLN:NE2	1:C:424:GLY:H	2.19	0.41
2:D:33:ARG:N	2:D:221:LEU:CD2	2.84	0.41
2:D:297:ARG:HG3	2:D:417:TYR:CE2	2.56	0.41
1:E:52:VAL:CG1	1:E:53:ALA:N	2.84	0.41
1:E:60:ILE:H	1:E:60:ILE:HG12	1.40	0.41
1:E:316:GLU:OE1	1:E:317:PRO:HD3	2.21	0.41
1:E:316:GLU:N	1:E:317:PRO:CD	2.84	0.41
1:E:335:LYS:H	1:E:335:LYS:HG3	1.64	0.41
1:E:381:ASN:H	1:E:381:ASN:ND2	2.10	0.41
1:E:384:VAL:O	1:E:387:LYS:HG2	2.21	0.41
1:E:430:GLY:O	1:E:433:GLU:OE1	2.39	0.41
2:F:119:ARG:HG2	2:F:119:ARG:HH11	1.86	0.41
2:H:76:ALA:HA	2:H:79:ASN:OD1	2.21	0.41
1:A:30:PRO:HB3	2:B:63:GLN:HG3	2.02	0.40
2:B:109:CYS:O	2:B:109:CYS:SG	2.80	0.40
2:B:118:PHE:O	2:B:119:ARG:HD3	2.15	0.40
1:C:125:VAL:CB	1:C:126:PRO:HD3	2.50	0.40
2:F:126:LYS:NZ	2:F:127:ASP:N	2.59	0.40
2:F:329:ASP:OD2	2:F:333:ARG:NH1	2.44	0.40
1:G:52:VAL:CG1	1:G:53:ALA:N	2.83	0.40
2:H:240:THR:HG23	2:H:260:VAL:HG11	2.03	0.40
2:B:159:PRO:CB	2:B:257:ARG:CD	2.94	0.40
2:D:125:TYR:HB2	2:D:126:LYS:O	2.22	0.40
1:E:134:ASP:OD1	1:E:134:ASP:N	2.54	0.40
1:E:316:GLU:CD	1:E:316:GLU:C	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ALA:O	1:E:386:LEU:N	2.48	0.40
2:F:352:VAL:CG1	2:F:354:SER:H	2.35	0.40
2:F:423:VAL:O	2:F:423:VAL:HG12	2.21	0.40
1:G:51:ASP:N	1:G:51:ASP:OD1	2.54	0.40
1:G:373:ASP:OD2	1:G:374:VAL:N	2.55	0.40
2:H:121:GLN:HB2	2:H:122:TYR:HE1	1.85	0.40
2:H:126:LYS:O	2:H:127:ASP:CB	2.63	0.40
1:A:354:GLY:N	1:A:366:ILE:CD1	2.83	0.40
1:A:424:GLY:C	1:A:433:GLU:OE2	2.60	0.40
2:B:271:LEU:O	2:B:272:ASP:C	2.57	0.40
1:C:310:LYS:HZ2	1:G:191:PRO:HG2	1.84	0.40
1:C:311:VAL:CG2	1:C:428:TYR:HB3	2.51	0.40
2:D:23:GLY:HA3	2:D:142:PHE:O	2.21	0.40
2:D:221:LEU:O	2:D:221:LEU:HG	2.22	0.40
2:D:226:LEU:HD22	2:D:226:LEU:HA	1.65	0.40
1:E:140:ALA:O	1:E:141:ALA:C	2.60	0.40
1:E:206:ILE:O	1:E:207:ALA:HB3	2.21	0.40
2:F:105:GLU:O	2:F:105:GLU:HG3	2.22	0.40
2:F:159:PRO:CB	2:F:257:ARG:CG	2.99	0.40
2:F:353:ASP:O	2:F:354:SER:CB	2.69	0.40
1:G:199:ASN:OD1	1:G:240:MET:HG2	2.21	0.40
1:G:322:LEU:HD11	1:G:439:CYS:SG	2.61	0.40
2:H:17:LYS:HB3	2:H:17:LYS:HE3	1.90	0.40
2:H:281:LEU:HD23	2:H:281:LEU:HA	1.92	0.40
1:A:383:ARG:HG2	1:A:384:VAL:N	2.31	0.40
2:B:159:PRO:HB2	2:B:257:ARG:CD	2.52	0.40
2:B:287:ASN:ND2	2:B:287:ASN:N	2.69	0.40
1:C:174:TYR:OH	1:C:238:GLN:HG2	2.21	0.40
1:C:174:TYR:OH	1:C:234:TYR:CD1	2.74	0.40
1:C:214:LEU:HD12	1:C:214:LEU:HA	1.83	0.40
1:C:375:LYS:O	1:C:375:LYS:HG2	2.21	0.40
2:D:39:HIS:HD2	2:D:65:THR:CB	2.34	0.40
2:D:121:GLN:N	2:D:122:TYR:CD1	2.88	0.40
2:D:122:TYR:C	2:D:124:GLU:N	2.72	0.40
2:D:256:GLU:OE2	2:D:256:GLU:CA	2.68	0.40
2:D:386:LEU:HD23	2:D:386:LEU:HA	1.86	0.40
2:D:428:ALA:O	2:D:432:VAL:HG23	2.21	0.40
2:F:117:GLU:O	2:F:121:GLN:OE1	2.39	0.40
2:F:167:LYS:HA	2:F:237:SER:H	1.85	0.40
2:F:200:LEU:HA	2:F:200:LEU:HD23	1.78	0.40
2:F:295:ARG:NE	2:H:212:HIS:CE1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:SER:HB3	1:G:166:ILE:HG21	2.04	0.40
2:H:202:ILE:HA	2:H:203:PRO:HA	1.70	0.40
2:H:271:LEU:HD23	2:H:271:LEU:HA	1.70	0.40
2:D:121:GLN:HB2	2:D:122:TYR:HE1	1.86	0.40
2:D:213:LEU:CG	2:D:223:THR:HG23	2.51	0.40
2:D:275:ASP:OD1	2:D:297:ARG:NE	2.37	0.40
2:D:363:ASP:O	2:D:366:ASP:HB2	2.21	0.40
1:E:119:PHE:N	1:E:119:PHE:CD1	2.89	0.40
1:E:206:ILE:O	1:E:419:GLN:O	2.39	0.40
2:F:168:ARG:HE	2:F:168:ARG:HB2	1.61	0.40
2:F:285:SER:HB3	2:F:287:ASN:ND2	2.37	0.40
1:G:206:ILE:H	1:G:206:ILE:HG12	1.33	0.40
1:G:382:ALA:O	1:G:386:LEU:N	2.51	0.40
2:H:32:ALA:N	2:H:226:LEU:O	2.44	0.40
2:H:159:PRO:CB	2:H:257:ARG:CD	2.96	0.40
2:H:221:LEU:O	2:H:221:LEU:HG	2.22	0.40
2:H:351:LEU:O	2:H:352:VAL:CG1	2.60	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ARG:NH1	2:H:161:ARG:NH1[1_455]	1.89	0.31
2:B:170:ARG:NH1	2:H:161:ARG:O[1_455]	2.03	0.17
2:B:170:ARG:CZ	2:H:161:ARG:CZ[1_455]	2.04	0.16
2:D:169:PRO:CA	2:H:170:ARG:NH1[1_455]	2.09	0.11
2:B:170:ARG:NE	2:H:161:ARG:NE[1_455]	2.10	0.10
2:D:169:PRO:C	2:H:170:ARG:NH1[1_455]	2.11	0.09
2:B:170:ARG:NH1	2:H:161:ARG:CZ[1_455]	2.18	0.02

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	425/483 (88%)	348 (82%)	54 (13%)	23 (5%)	2 1
1	C	425/483 (88%)	350 (82%)	50 (12%)	25 (6%)	1 0
1	E	425/483 (88%)	355 (84%)	47 (11%)	23 (5%)	2 1
1	G	425/483 (88%)	347 (82%)	53 (12%)	25 (6%)	1 0
2	B	430/458 (94%)	361 (84%)	46 (11%)	23 (5%)	2 1
2	D	430/458 (94%)	359 (84%)	48 (11%)	23 (5%)	2 1
2	F	430/458 (94%)	359 (84%)	47 (11%)	24 (6%)	2 1
2	H	430/458 (94%)	356 (83%)	49 (11%)	25 (6%)	1 0
All	All	3420/3764 (91%)	2835 (83%)	394 (12%)	191 (6%)	2 1

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	64	GLY
1	A	95	MET
1	A	177	GLY
1	A	190	ARG
1	A	191	PRO
1	A	381	ASN
2	B	9	LYS
2	B	76	ALA
2	B	121	GLN
2	B	158	VAL
2	B	164	GLN
2	B	169	PRO
2	B	219	ASN
2	B	222	THR
2	B	265	PHE
2	B	348	ALA
2	B	349	ALA
2	B	352	VAL
2	B	354	SER
1	C	30	PRO
1	C	64	GLY
1	C	95	MET
1	C	190	ARG
1	C	191	PRO
1	C	381	ASN
1	C	421	ARG

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Mol	Chain	Res	Type
2	D	9	LYS
2	D	73	VAL
2	D	76	ALA
2	D	121	GLN
2	D	158	VAL
2	D	164	GLN
2	D	169	PRO
2	D	219	ASN
2	D	222	THR
2	D	265	PHE
2	D	348	ALA
2	D	349	ALA
2	D	352	VAL
2	D	354	SER
1	E	30	PRO
1	E	64	GLY
1	E	95	MET
1	E	177	GLY
1	E	190	ARG
1	E	191	PRO
1	E	381	ASN
1	E	421	ARG
2	F	76	ALA
2	F	121	GLN
2	F	158	VAL
2	F	164	GLN
2	F	169	PRO
2	F	219	ASN
2	F	222	THR
2	F	265	PHE
2	F	348	ALA
2	F	349	ALA
2	F	352	VAL
2	F	354	SER
1	G	30	PRO
1	G	64	GLY
1	G	95	MET
1	G	177	GLY
1	G	190	ARG
1	G	191	PRO
1	G	381	ASN
2	H	73	VAL

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Mol	Chain	Res	Type
2	H	76	ALA
2	H	121	GLN
2	H	158	VAL
2	H	164	GLN
2	H	169	PRO
2	H	219	ASN
2	H	222	THR
2	H	265	PHE
2	H	348	ALA
2	H	349	ALA
2	H	352	VAL
2	H	354	SER
1	A	25	CYS
1	A	27	LYS
1	A	229	ALA
1	A	421	ARG
2	B	73	VAL
2	B	75	GLY
2	B	77	ASP
1	C	27	LYS
1	C	63	ALA
1	C	177	GLY
1	C	229	ALA
2	D	75	GLY
2	D	77	ASP
2	D	237	SER
1	E	25	CYS
1	E	27	LYS
1	E	63	ALA
1	E	211	TRP
1	E	229	ALA
2	F	9	LYS
2	F	73	VAL
2	F	75	GLY
2	F	77	ASP
1	G	25	CYS
1	G	27	LYS
1	G	63	ALA
1	G	176	ILE
1	G	211	TRP
1	G	342	ALA
1	G	421	ARG

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Mol	Chain	Res	Type
2	H	9	LYS
2	H	75	GLY
2	H	77	ASP
1	A	28	PRO
1	A	63	ALA
1	A	188	SER
1	A	211	TRP
1	A	342	ALA
2	B	111	LEU
2	B	237	SER
1	C	25	CYS
1	C	28	PRO
1	C	69	ASN
1	C	176	ILE
1	C	211	TRP
1	C	228	LEU
1	C	342	ALA
1	E	28	PRO
1	E	69	ASN
1	E	176	ILE
1	E	188	SER
1	E	342	ALA
1	E	371	GLY
2	F	111	LEU
1	G	28	PRO
1	G	69	ASN
1	G	229	ALA
2	H	111	LEU
2	H	237	SER
1	A	69	ASN
1	A	176	ILE
1	A	238	GLN
2	B	350	ALA
2	B	362	GLY
2	B	402	PRO
2	D	111	LEU
2	D	362	GLY
2	D	402	PRO
1	E	228	LEU
1	E	250	CYS
2	F	237	SER
2	F	350	ALA

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Mol	Chain	Res	Type
2	F	362	GLY
1	G	72	THR
1	G	188	SER
2	H	29	LEU
2	H	161	ARG
2	H	362	GLY
2	H	402	PRO
1	A	72	THR
1	A	228	LEU
1	A	371	GLY
2	B	168	ARG
1	C	188	SER
1	C	238	GLN
1	C	250	CYS
1	C	371	GLY
1	C	399	ALA
2	D	168	ARG
2	D	341	ALA
2	D	375	GLN
1	E	399	ALA
2	F	168	ARG
2	F	402	PRO
1	G	371	GLY
2	H	168	ARG
2	B	271	LEU
2	F	161	ARG
1	G	141	ALA
1	G	228	LEU
1	G	250	CYS
2	H	110	ASP
2	H	350	ALA
1	G	129	ILE
1	A	195	VAL
1	C	129	ILE
1	C	195	VAL
1	E	195	VAL
1	G	195	VAL
2	F	132	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	343/388 (88%)	260 (76%)	83 (24%)	0	0
1	C	343/388 (88%)	257 (75%)	86 (25%)	0	0
1	E	343/388 (88%)	257 (75%)	86 (25%)	0	0
1	G	343/388 (88%)	260 (76%)	83 (24%)	0	0
2	B	335/363 (92%)	266 (79%)	69 (21%)	1	1
2	D	335/363 (92%)	265 (79%)	70 (21%)	1	1
2	F	335/363 (92%)	265 (79%)	70 (21%)	1	1
2	H	335/363 (92%)	265 (79%)	70 (21%)	1	1
All	All	2712/3004 (90%)	2095 (77%)	617 (23%)	1	1

All (617) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	29	LYS
1	A	33	THR
1	A	34	ASP
1	A	37	CYS
1	A	48	PRO
1	A	60	ILE
1	A	62	CYS
1	A	67	TRP
1	A	69	ASN
1	A	70	ARG
1	A	72	THR
1	A	73	ARG
1	A	81	ARG
1	A	97	ARG
1	A	101	ARG
1	A	111	GLU
1	A	123	THR
1	A	134	ASP

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Mol	Chain	Res	Type
1	A	156	PHE
1	A	157	TYR
1	A	160	LYS
1	A	164	ASN
1	A	172	LEU
1	A	184	LEU
1	A	186	VAL
1	A	190	ARG
1	A	193	ILE
1	A	195	VAL
1	A	203	GLU
1	A	206	ILE
1	A	209	GLU
1	A	216	LEU
1	A	220	LEU
1	A	235	ARG
1	A	256	ASN
1	A	257	VAL
1	A	259	ARG
1	A	261	LEU
1	A	262	GLN
1	A	269	TRP
1	A	271	GLU
1	A	273	SER
1	A	279	ASP
1	A	285	ARG
1	A	287	PHE
1	A	292	ASP
1	A	307	GLU
1	A	311	VAL
1	A	315	LEU
1	A	322	LEU
1	A	323	GLU
1	A	329	LEU
1	A	335	LYS
1	A	337	TRP
1	A	338	SER
1	A	339	VAL
1	A	341	SER
1	A	343	LEU
1	A	344	GLN
1	A	353	THR

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Mol	Chain	Res	Type
1	A	359	THR
1	A	365	ARG
1	A	367	ARG
1	A	369	LEU
1	A	370	MET
1	A	375	LYS
1	A	376	MET
1	A	379	GLU
1	A	381	ASN
1	A	383	ARG
1	A	393	GLN
1	A	396	ILE
1	A	397	LEU
1	A	403	ASN
1	A	419	GLN
1	A	420	GLU
1	A	421	ARG
1	A	423	PHE
1	A	433	GLU
1	A	440	ILE
1	A	442	LEU
1	A	448	GLU
2	B	17	LYS
2	B	21	THR
2	B	26	LEU
2	B	28	ILE
2	B	31	LEU
2	B	41	SER
2	B	58	GLU
2	B	62	LEU
2	B	69	GLN
2	B	74	MET
2	B	77	ASP
2	B	85	LYS
2	B	90	ARG
2	B	91	GLN
2	B	94	SER
2	B	103	LEU
2	B	107	GLN
2	B	109	CYS
2	B	115	LEU
2	B	119	ARG

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Mol	Chain	Res	Type
2	B	122	TYR
2	B	123	GLU
2	B	137	ASP
2	B	157	LEU
2	B	158	VAL
2	B	160	GLU
2	B	161	ARG
2	B	168	ARG
2	B	170	ARG
2	B	172	VAL
2	B	180	LEU
2	B	190	GLU
2	B	194	SER
2	B	198	ARG
2	B	200	LEU
2	B	210	ASP
2	B	212	HIS
2	B	213	LEU
2	B	217	ARG
2	B	218	PHE
2	B	221	LEU
2	B	222	THR
2	B	223	THR
2	B	226	LEU
2	B	227	SER
2	B	257	ARG
2	B	262	ASP
2	B	263	ARG
2	B	264	ARG
2	B	265	PHE
2	B	277	TRP
2	B	287	ASN
2	B	308	HIS
2	B	310	MET
2	B	339	THR
2	B	344	VAL
2	B	351	LEU
2	B	352	VAL
2	B	356	LEU
2	B	359	VAL
2	B	361	VAL
2	B	363	ASP

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Mol	Chain	Res	Type
2	B	378	LEU
2	B	382	ASN
2	B	386	LEU
2	B	391	ARG
2	B	396	LEU
2	B	398	ARG
2	B	401	PHE
1	C	27	LYS
1	C	29	LYS
1	C	33	THR
1	C	34	ASP
1	C	37	CYS
1	C	60	ILE
1	C	62	CYS
1	C	67	TRP
1	C	68	ASP
1	C	69	ASN
1	C	70	ARG
1	C	72	THR
1	C	73	ARG
1	C	81	ARG
1	C	86	THR
1	C	97	ARG
1	C	101	ARG
1	C	102	LEU
1	C	111	GLU
1	C	123	THR
1	C	131	ASP
1	C	134	ASP
1	C	156	PHE
1	C	157	TYR
1	C	159	THR
1	C	160	LYS
1	C	164	ASN
1	C	172	LEU
1	C	184	LEU
1	C	186	VAL
1	C	190	ARG
1	C	193	ILE
1	C	195	VAL
1	C	203	GLU
1	C	206	ILE

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Mol	Chain	Res	Type
1	C	209	GLU
1	C	216	LEU
1	C	220	LEU
1	C	235	ARG
1	C	256	ASN
1	C	257	VAL
1	C	259	ARG
1	C	261	LEU
1	C	262	GLN
1	C	269	TRP
1	C	271	GLU
1	C	273	SER
1	C	279	ASP
1	C	285	ARG
1	C	287	PHE
1	C	292	ASP
1	C	307	GLU
1	C	311	VAL
1	C	315	LEU
1	C	322	LEU
1	C	323	GLU
1	C	329	LEU
1	C	335	LYS
1	C	337	TRP
1	C	338	SER
1	C	339	VAL
1	C	341	SER
1	C	343	LEU
1	C	344	GLN
1	C	353	THR
1	C	359	THR
1	C	365	ARG
1	C	367	ARG
1	C	369	LEU
1	C	370	MET
1	C	375	LYS
1	C	376	MET
1	C	379	GLU
1	C	381	ASN
1	C	383	ARG
1	C	393	GLN
1	C	396	ILE

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Mol	Chain	Res	Type
1	C	397	LEU
1	C	403	ASN
1	C	419	GLN
1	C	420	GLU
1	C	421	ARG
1	C	423	PHE
1	C	433	GLU
1	C	442	LEU
1	C	448	GLU
2	D	21	THR
2	D	26	LEU
2	D	28	ILE
2	D	31	LEU
2	D	58	GLU
2	D	62	LEU
2	D	69	GLN
2	D	74	MET
2	D	77	ASP
2	D	85	LYS
2	D	90	ARG
2	D	91	GLN
2	D	94	SER
2	D	103	LEU
2	D	107	GLN
2	D	109	CYS
2	D	115	LEU
2	D	119	ARG
2	D	122	TYR
2	D	127	ASP
2	D	137	ASP
2	D	157	LEU
2	D	158	VAL
2	D	160	GLU
2	D	161	ARG
2	D	163	ASP
2	D	168	ARG
2	D	170	ARG
2	D	172	VAL
2	D	180	LEU
2	D	190	GLU
2	D	198	ARG
2	D	200	LEU

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Mol	Chain	Res	Type
2	D	210	ASP
2	D	212	HIS
2	D	213	LEU
2	D	217	ARG
2	D	218	PHE
2	D	221	LEU
2	D	222	THR
2	D	223	THR
2	D	226	LEU
2	D	227	SER
2	D	257	ARG
2	D	262	ASP
2	D	263	ARG
2	D	264	ARG
2	D	265	PHE
2	D	277	TRP
2	D	287	ASN
2	D	308	HIS
2	D	310	MET
2	D	313	SER
2	D	331	LEU
2	D	339	THR
2	D	344	VAL
2	D	347	ARG
2	D	351	LEU
2	D	352	VAL
2	D	356	LEU
2	D	359	VAL
2	D	361	VAL
2	D	363	ASP
2	D	378	LEU
2	D	382	ASN
2	D	386	LEU
2	D	391	ARG
2	D	396	LEU
2	D	398	ARG
2	D	401	PHE
1	E	27	LYS
1	E	29	LYS
1	E	33	THR
1	E	34	ASP
1	E	37	CYS

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Mol	Chain	Res	Type
1	E	60	ILE
1	E	62	CYS
1	E	67	TRP
1	E	69	ASN
1	E	70	ARG
1	E	72	THR
1	E	73	ARG
1	E	78	ASP
1	E	81	ARG
1	E	86	THR
1	E	95	MET
1	E	97	ARG
1	E	101	ARG
1	E	111	GLU
1	E	123	THR
1	E	131	ASP
1	E	134	ASP
1	E	156	PHE
1	E	157	TYR
1	E	159	THR
1	E	160	LYS
1	E	164	ASN
1	E	172	LEU
1	E	184	LEU
1	E	190	ARG
1	E	193	ILE
1	E	195	VAL
1	E	203	GLU
1	E	206	ILE
1	E	209	GLU
1	E	216	LEU
1	E	220	LEU
1	E	235	ARG
1	E	256	ASN
1	E	257	VAL
1	E	259	ARG
1	E	261	LEU
1	E	262	GLN
1	E	269	TRP
1	E	271	GLU
1	E	273	SER
1	E	279	ASP

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Mol	Chain	Res	Type
1	E	285	ARG
1	E	287	PHE
1	E	292	ASP
1	E	307	GLU
1	E	311	VAL
1	E	315	LEU
1	E	322	LEU
1	E	323	GLU
1	E	329	LEU
1	E	337	TRP
1	E	338	SER
1	E	339	VAL
1	E	341	SER
1	E	343	LEU
1	E	344	GLN
1	E	353	THR
1	E	359	THR
1	E	365	ARG
1	E	367	ARG
1	E	369	LEU
1	E	370	MET
1	E	375	LYS
1	E	376	MET
1	E	379	GLU
1	E	381	ASN
1	E	383	ARG
1	E	393	GLN
1	E	396	ILE
1	E	397	LEU
1	E	402	ARG
1	E	403	ASN
1	E	419	GLN
1	E	420	GLU
1	E	421	ARG
1	E	423	PHE
1	E	433	GLU
1	E	440	ILE
1	E	442	LEU
1	E	448	GLU
2	F	14	SER
2	F	21	THR
2	F	26	LEU

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Mol	Chain	Res	Type
2	F	28	ILE
2	F	31	LEU
2	F	41	SER
2	F	58	GLU
2	F	62	LEU
2	F	69	GLN
2	F	74	MET
2	F	77	ASP
2	F	85	LYS
2	F	90	ARG
2	F	91	GLN
2	F	94	SER
2	F	103	LEU
2	F	107	GLN
2	F	109	CYS
2	F	115	LEU
2	F	119	ARG
2	F	122	TYR
2	F	157	LEU
2	F	158	VAL
2	F	160	GLU
2	F	161	ARG
2	F	168	ARG
2	F	170	ARG
2	F	172	VAL
2	F	180	LEU
2	F	190	GLU
2	F	194	SER
2	F	198	ARG
2	F	200	LEU
2	F	210	ASP
2	F	212	HIS
2	F	213	LEU
2	F	217	ARG
2	F	218	PHE
2	F	221	LEU
2	F	222	THR
2	F	223	THR
2	F	226	LEU
2	F	227	SER
2	F	257	ARG
2	F	262	ASP

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Mol	Chain	Res	Type
2	F	263	ARG
2	F	264	ARG
2	F	265	PHE
2	F	277	TRP
2	F	287	ASN
2	F	308	HIS
2	F	310	MET
2	F	313	SER
2	F	331	LEU
2	F	339	THR
2	F	344	VAL
2	F	347	ARG
2	F	351	LEU
2	F	352	VAL
2	F	356	LEU
2	F	359	VAL
2	F	361	VAL
2	F	363	ASP
2	F	378	LEU
2	F	382	ASN
2	F	386	LEU
2	F	391	ARG
2	F	396	LEU
2	F	398	ARG
2	F	401	PHE
1	G	27	LYS
1	G	29	LYS
1	G	33	THR
1	G	34	ASP
1	G	37	CYS
1	G	60	ILE
1	G	67	TRP
1	G	69	ASN
1	G	70	ARG
1	G	72	THR
1	G	73	ARG
1	G	81	ARG
1	G	86	THR
1	G	101	ARG
1	G	111	GLU
1	G	123	THR
1	G	131	ASP

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Mol	Chain	Res	Type
1	G	134	ASP
1	G	156	PHE
1	G	157	TYR
1	G	160	LYS
1	G	164	ASN
1	G	172	LEU
1	G	184	LEU
1	G	190	ARG
1	G	193	ILE
1	G	195	VAL
1	G	203	GLU
1	G	206	ILE
1	G	209	GLU
1	G	216	LEU
1	G	220	LEU
1	G	235	ARG
1	G	240	MET
1	G	256	ASN
1	G	257	VAL
1	G	259	ARG
1	G	261	LEU
1	G	262	GLN
1	G	269	TRP
1	G	271	GLU
1	G	273	SER
1	G	279	ASP
1	G	285	ARG
1	G	287	PHE
1	G	292	ASP
1	G	307	GLU
1	G	311	VAL
1	G	315	LEU
1	G	322	LEU
1	G	323	GLU
1	G	329	LEU
1	G	335	LYS
1	G	337	TRP
1	G	338	SER
1	G	339	VAL
1	G	341	SER
1	G	343	LEU
1	G	344	GLN

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Mol	Chain	Res	Type
1	G	353	THR
1	G	359	THR
1	G	365	ARG
1	G	367	ARG
1	G	369	LEU
1	G	370	MET
1	G	375	LYS
1	G	376	MET
1	G	379	GLU
1	G	381	ASN
1	G	383	ARG
1	G	393	GLN
1	G	396	ILE
1	G	397	LEU
1	G	402	ARG
1	G	403	ASN
1	G	419	GLN
1	G	420	GLU
1	G	421	ARG
1	G	423	PHE
1	G	433	GLU
1	G	440	ILE
1	G	442	LEU
1	G	448	GLU
2	H	21	THR
2	H	26	LEU
2	H	28	ILE
2	H	31	LEU
2	H	41	SER
2	H	58	GLU
2	H	62	LEU
2	H	69	GLN
2	H	74	MET
2	H	77	ASP
2	H	85	LYS
2	H	90	ARG
2	H	91	GLN
2	H	94	SER
2	H	103	LEU
2	H	107	GLN
2	H	109	CYS
2	H	115	LEU

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Mol	Chain	Res	Type
2	H	119	ARG
2	H	122	TYR
2	H	137	ASP
2	H	157	LEU
2	H	158	VAL
2	H	160	GLU
2	H	161	ARG
2	H	163	ASP
2	H	168	ARG
2	H	170	ARG
2	H	172	VAL
2	H	180	LEU
2	H	190	GLU
2	H	194	SER
2	H	198	ARG
2	H	200	LEU
2	H	210	ASP
2	H	212	HIS
2	H	213	LEU
2	H	217	ARG
2	H	218	PHE
2	H	221	LEU
2	H	222	THR
2	H	223	THR
2	H	226	LEU
2	H	227	SER
2	H	257	ARG
2	H	262	ASP
2	H	263	ARG
2	H	264	ARG
2	H	265	PHE
2	H	277	TRP
2	H	287	ASN
2	H	308	HIS
2	H	310	MET
2	H	315	ARG
2	H	331	LEU
2	H	339	THR
2	H	344	VAL
2	H	351	LEU
2	H	352	VAL
2	H	356	LEU

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Mol	Chain	Res	Type
2	H	359	VAL
2	H	361	VAL
2	H	363	ASP
2	H	378	LEU
2	H	382	ASN
2	H	386	LEU
2	H	391	ARG
2	H	396	LEU
2	H	398	ARG
2	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	57	HIS
1	A	69	ASN
1	A	108	GLN
1	A	199	ASN
1	A	246	ASN
1	A	344	GLN
1	A	381	ASN
1	A	419	GLN
2	B	39	HIS
2	B	91	GLN
2	B	107	GLN
2	B	112	HIS
2	B	173	ASN
2	B	287	ASN
2	B	301	GLN
2	B	308	HIS
2	B	382	ASN
2	B	384	HIS
2	B	434	HIS
2	B	435	HIS
1	C	54	HIS
1	C	57	HIS
1	C	69	ASN
1	C	108	GLN
1	C	199	ASN
1	C	246	ASN
1	C	256	ASN

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Mol	Chain	Res	Type
1	C	344	GLN
1	C	381	ASN
1	C	419	GLN
2	D	39	HIS
2	D	91	GLN
2	D	107	GLN
2	D	112	HIS
2	D	121	GLN
2	D	173	ASN
2	D	287	ASN
2	D	301	GLN
2	D	308	HIS
2	D	382	ASN
2	D	384	HIS
2	D	434	HIS
2	D	435	HIS
1	E	54	HIS
1	E	57	HIS
1	E	69	ASN
1	E	108	GLN
1	E	164	ASN
1	E	199	ASN
1	E	246	ASN
1	E	256	ASN
1	E	344	GLN
1	E	381	ASN
1	E	419	GLN
2	F	20	GLN
2	F	39	HIS
2	F	91	GLN
2	F	107	GLN
2	F	112	HIS
2	F	121	GLN
2	F	287	ASN
2	F	301	GLN
2	F	308	HIS
2	F	382	ASN
2	F	384	HIS
2	F	434	HIS
1	G	54	HIS
1	G	57	HIS
1	G	69	ASN

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Mol	Chain	Res	Type
1	G	108	GLN
1	G	199	ASN
1	G	246	ASN
1	G	256	ASN
1	G	344	GLN
1	G	381	ASN
1	G	393	GLN
1	G	419	GLN
2	H	39	HIS
2	H	91	GLN
2	H	107	GLN
2	H	121	GLN
2	H	287	ASN
2	H	301	GLN
2	H	308	HIS
2	H	382	ASN
2	H	384	HIS
2	H	434	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CZL	A	502	-	5,34,34	2.44	1 (20%)	-		
4	CZL	E	502	-	5,34,34	2.50	1 (20%)	-		
3	SF4	C	501	2,1	0,12,12	-	-	-		
4	CZL	G	502	-	5,34,34	2.37	1 (20%)	-		
3	SF4	E	501	2,1	0,12,12	-	-	-		
3	SF4	A	501	2,1	0,12,12	-	-	-		
4	CZL	C	502	-	5,34,34	1.95	1 (20%)	-		
3	SF4	G	501	2,1	0,12,12	-	-	-		

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	SF4	C	501	2,1	-	-	0/6/5/5
3	SF4	A	501	2,1	-	-	0/6/5/5
3	SF4	E	501	2,1	-	-	0/6/5/5
3	SF4	G	501	2,1	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	502	CZL	S5A-FE7	5.09	2.34	2.24
4	A	502	CZL	S5A-FE7	4.95	2.34	2.24
4	G	502	CZL	S5A-FE7	4.77	2.34	2.24
4	C	502	CZL	S5A-FE7	3.69	2.31	2.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	CZL	3	0

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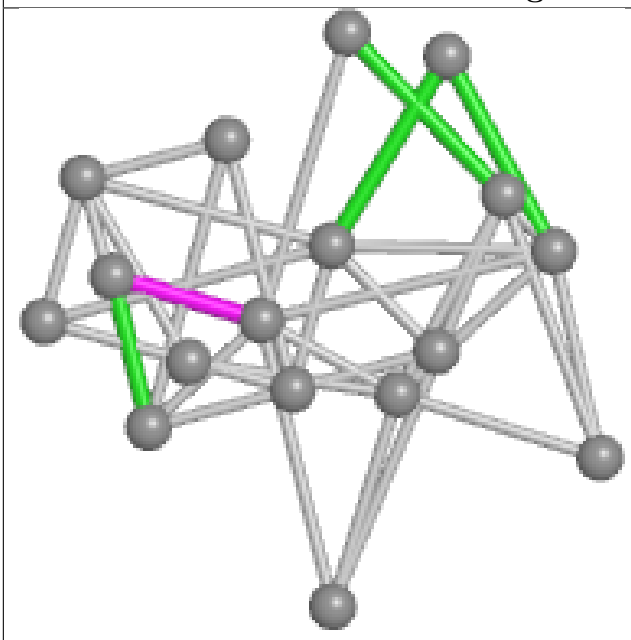
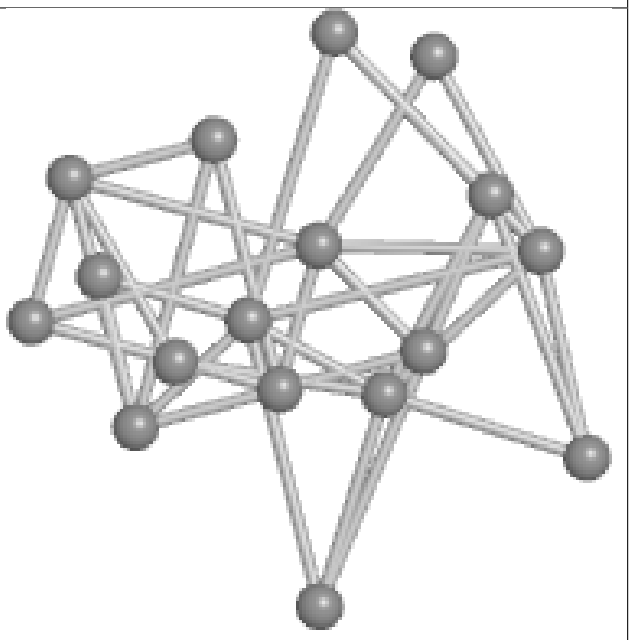
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	502	CZL	2	0
3	C	501	SF4	2	0
4	G	502	CZL	4	0
3	E	501	SF4	3	0
3	A	501	SF4	2	0
4	C	502	CZL	3	0
3	G	501	SF4	4	0

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

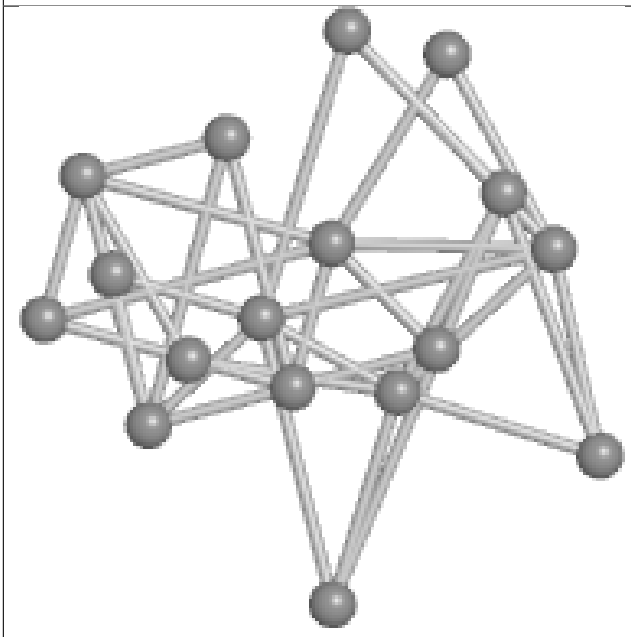
Ligand CZL A 502



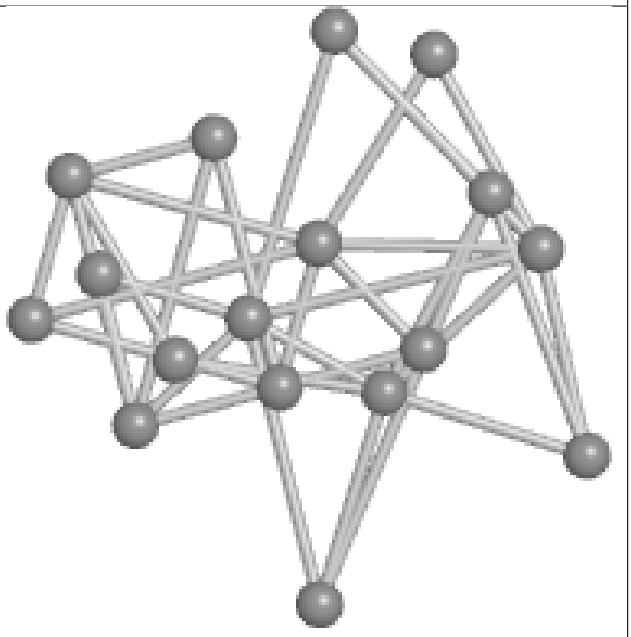
Bond lengths



Bond angles

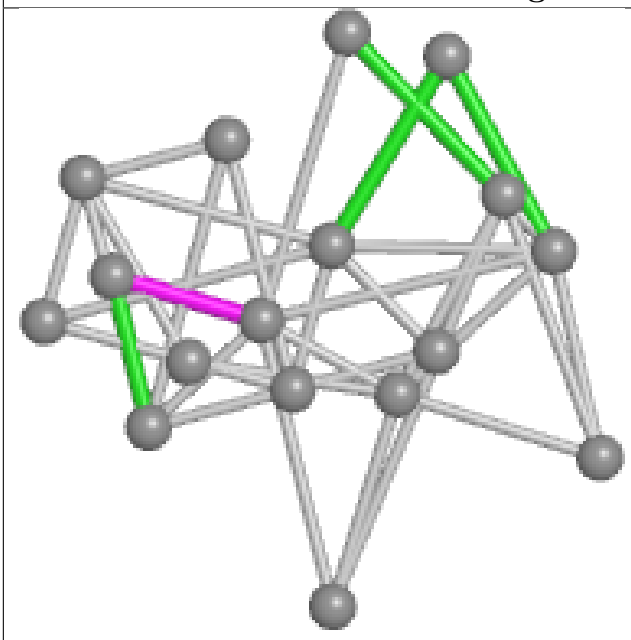


Torsions

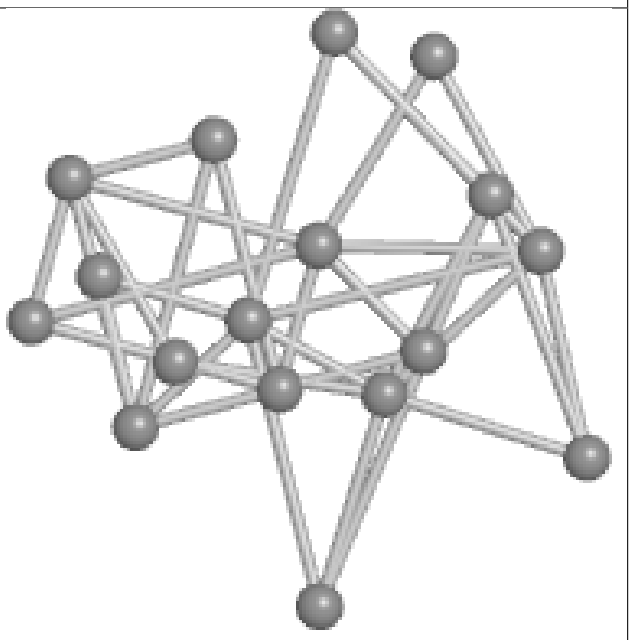


Rings

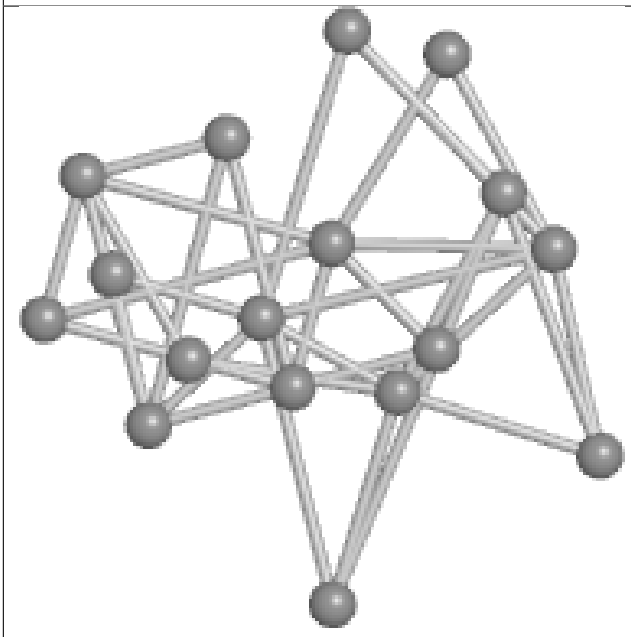
Ligand CZL E 502



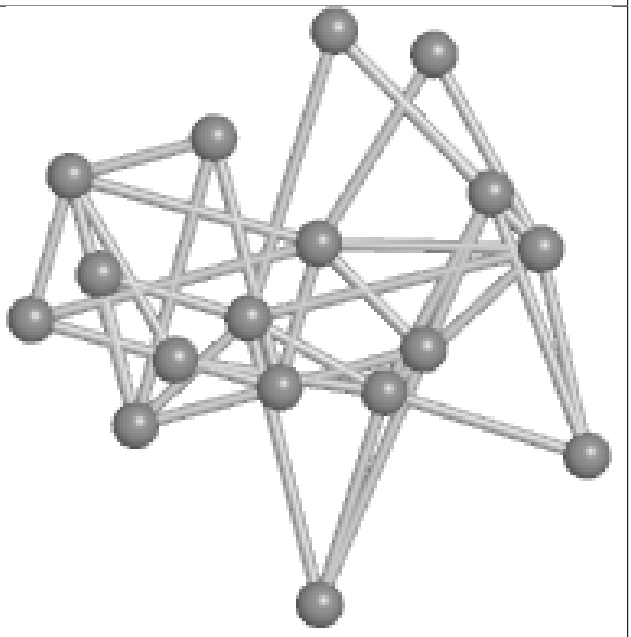
Bond lengths



Bond angles

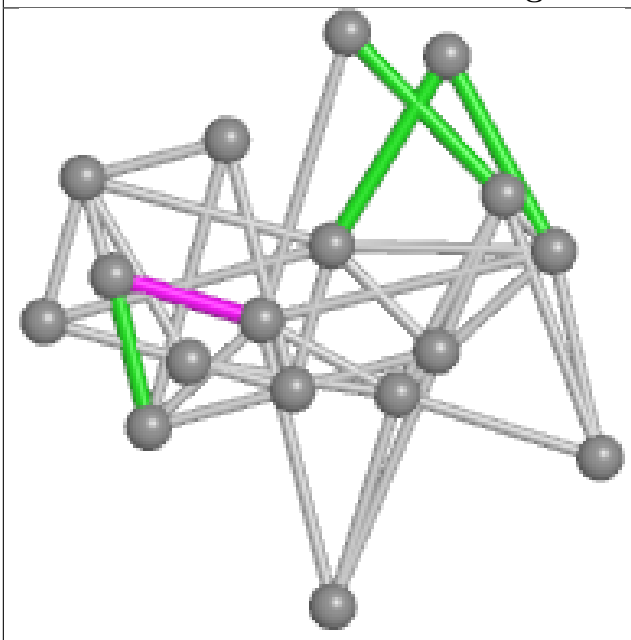


Torsions

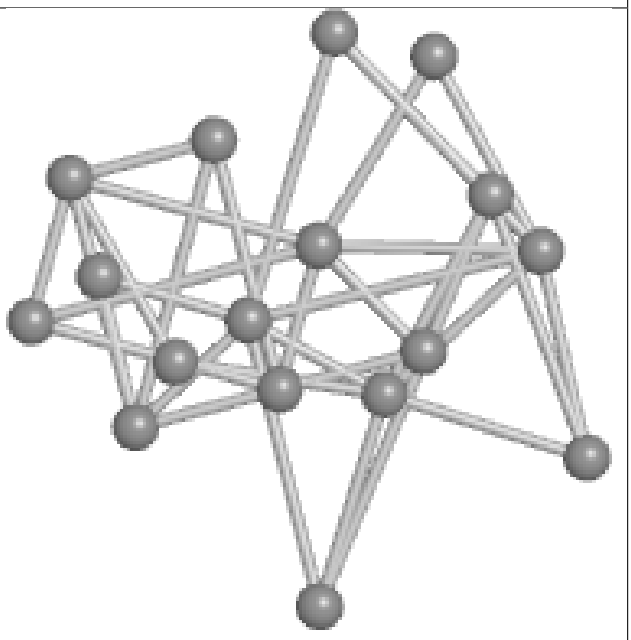


Rings

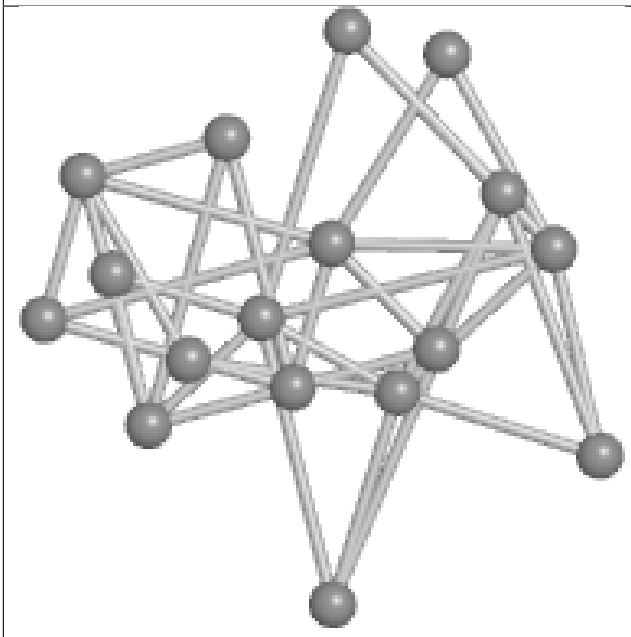
Ligand CZL G 502



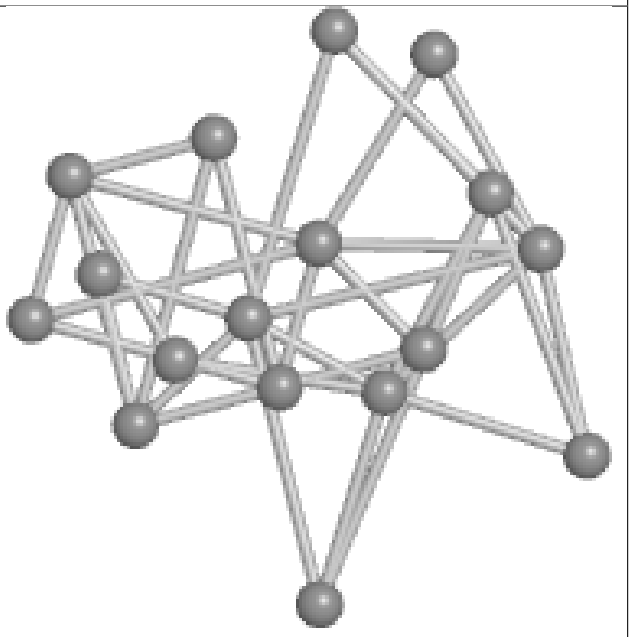
Bond lengths



Bond angles

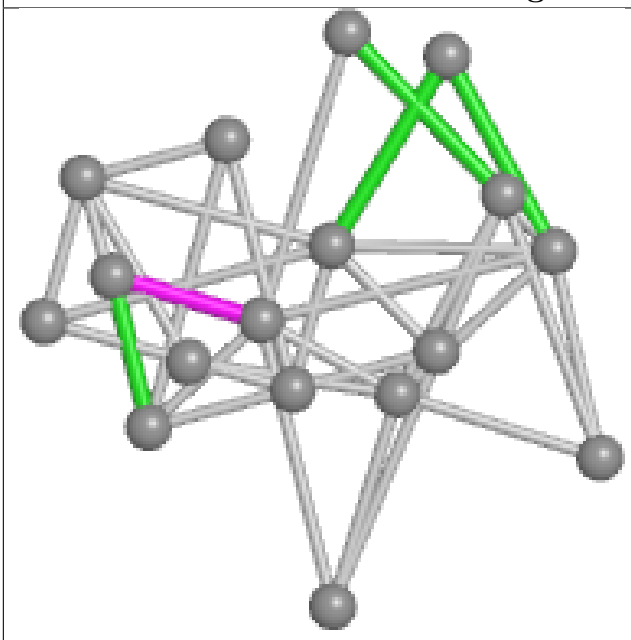


Torsions

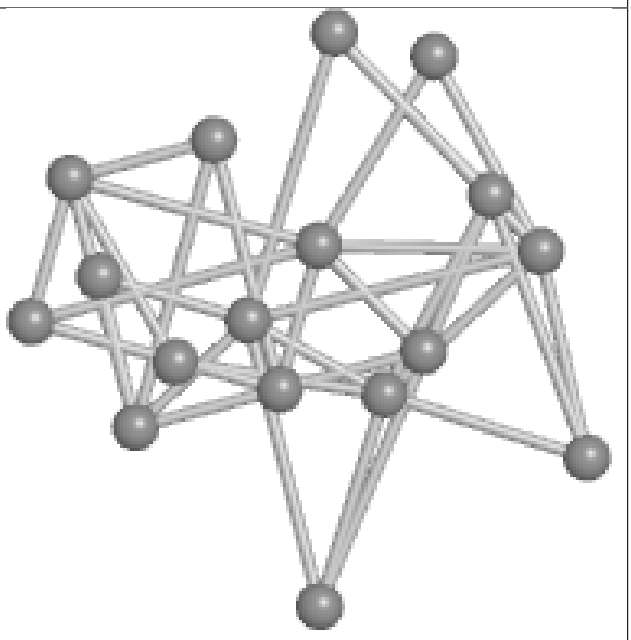


Rings

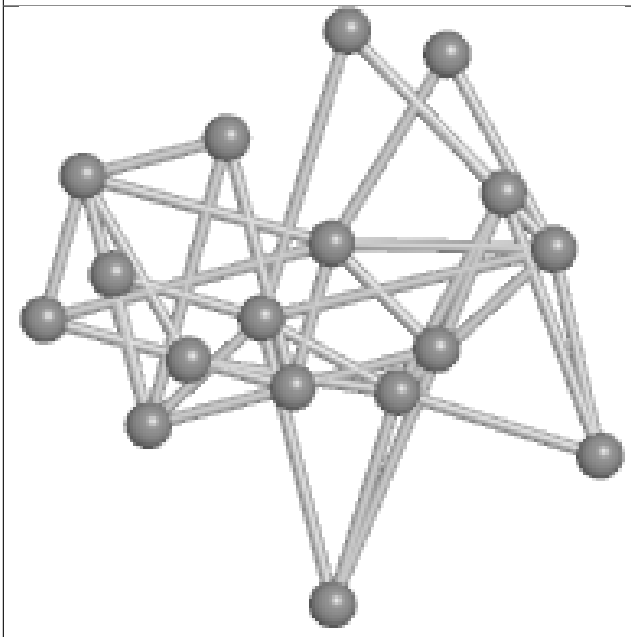
Ligand CZL C 502



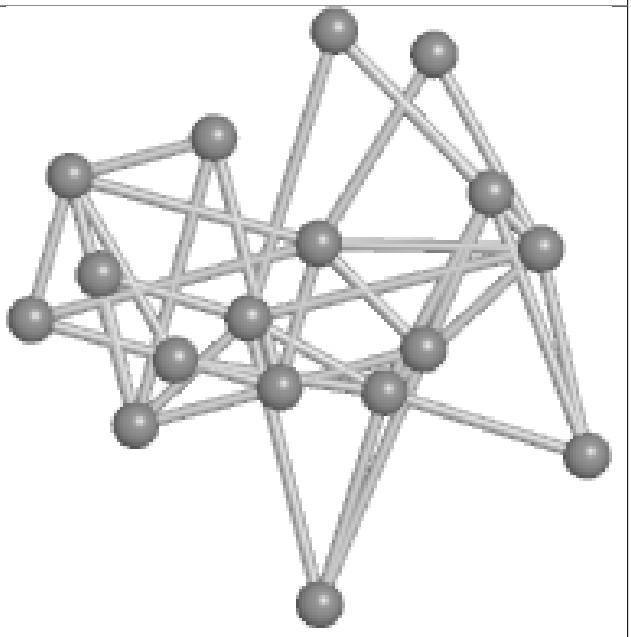
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	427/483 (88%)	0.80	55 (12%) 3 3	14, 42, 91, 112	0
1	C	427/483 (88%)	0.99	77 (18%) 1 1	17, 44, 91, 116	0
1	E	427/483 (88%)	0.96	65 (15%) 2 1	15, 43, 91, 117	0
1	G	427/483 (88%)	1.00	73 (17%) 1 1	17, 44, 93, 114	0
2	B	432/458 (94%)	0.51	23 (5%) 26 25	14, 35, 72, 89	0
2	D	432/458 (94%)	0.55	28 (6%) 18 17	12, 36, 75, 91	0
2	F	432/458 (94%)	0.70	39 (9%) 9 8	14, 37, 73, 90	0
2	H	432/458 (94%)	0.58	37 (8%) 10 9	13, 37, 74, 89	0
All	All	3436/3764 (91%)	0.76	397 (11%) 4 4	12, 40, 82, 117	0

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	376	MET	22.0
1	G	337	TRP	10.9
1	E	371	GLY	10.8
1	C	334	VAL	10.1
1	G	376	MET	9.5
1	G	32	ALA	9.1
2	D	165	VAL	8.7
1	G	366	ILE	8.2
1	E	376	MET	7.9
2	D	161	ARG	7.9
1	C	377	LEU	7.8
1	G	334	VAL	7.4
2	H	218	PHE	7.4
1	E	31	GLY	7.4
1	E	379	GLU	7.3
2	D	222	THR	7.3

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Mol	Chain	Res	Type	RSRZ
2	B	158	VAL	7.1
1	E	95	MET	6.7
1	E	419	GLN	6.6
1	E	420	GLU	6.5
1	G	419	GLN	6.5
2	H	74	MET	6.5
2	F	222	THR	6.3
2	F	104	SER	6.3
1	C	350	VAL	6.1
1	C	32	ALA	6.1
1	C	25	CYS	6.0
1	C	393	GLN	5.8
1	G	382	ALA	5.7
2	F	165	VAL	5.7
1	G	378	ASP	5.6
1	C	420	GLU	5.6
2	F	127	ASP	5.4
1	G	381	ASN	5.4
2	D	109	CYS	5.4
1	A	375	LYS	5.3
1	E	361	GLU	5.0
1	A	337	TRP	5.0
2	H	265	PHE	4.9
1	E	375	LYS	4.9
1	C	371	GLY	4.9
2	H	125	TYR	4.9
1	G	352	ALA	4.8
1	G	420	GLU	4.8
2	H	165	VAL	4.8
1	C	95	MET	4.8
1	G	338	SER	4.8
1	G	71	GLY	4.8
2	D	75	GLY	4.7
1	G	354	GLY	4.7
1	E	195	VAL	4.7
1	C	375	LYS	4.7
1	C	340	VAL	4.7
1	C	194	ARG	4.6
1	A	423	PHE	4.6
1	C	378	ASP	4.6
2	H	77	ASP	4.5
1	E	32	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	154	VAL	4.5
1	G	339	VAL	4.5
1	G	369	LEU	4.4
2	B	109	CYS	4.4
2	F	118	PHE	4.4
1	G	365	ARG	4.4
2	H	164	GLN	4.4
1	G	377	LEU	4.3
1	E	291	LEU	4.3
1	C	354	GLY	4.3
1	G	359	THR	4.3
1	C	336	SER	4.2
2	B	77	ASP	4.2
1	G	353	THR	4.2
1	A	32	ALA	4.2
2	D	69	GLN	4.1
1	C	355	THR	4.1
2	D	223	THR	4.1
1	C	402	ARG	4.1
1	E	338	SER	4.1
1	A	387	LYS	4.1
2	H	231	LEU	4.1
1	G	360	GLU	4.0
2	F	274	VAL	4.0
1	G	379	GLU	4.0
1	E	357	LYS	4.0
2	D	125	TYR	4.0
2	F	77	ASP	4.0
1	G	195	VAL	4.0
2	D	353	ASP	4.0
1	G	386	LEU	3.9
2	F	251	ALA	3.9
1	G	414	PHE	3.9
1	E	312	ARG	3.9
1	G	324	GLY	3.9
2	H	158	VAL	3.9
1	C	322	LEU	3.9
2	H	213	LEU	3.9
1	C	382	ALA	3.9
1	C	368	GLU	3.8
1	E	374	VAL	3.8
1	E	336	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	336	SER	3.8
1	G	333	GLY	3.7
1	G	340	VAL	3.7
2	H	212	HIS	3.7
1	A	348	MET	3.7
1	E	394	ALA	3.7
2	D	127	ASP	3.7
1	G	349	LYS	3.7
2	F	90	ARG	3.7
2	H	219	ASN	3.6
2	F	98	LEU	3.6
2	H	352	VAL	3.6
1	G	348	MET	3.6
1	G	345	ASP	3.6
1	E	65	SER	3.6
1	E	391	GLU	3.6
1	G	361	GLU	3.6
2	D	74	MET	3.6
1	A	420	GLU	3.6
1	G	387	LYS	3.5
1	A	374	VAL	3.5
1	C	370	MET	3.5
2	F	112	HIS	3.5
1	C	365	ARG	3.5
1	A	170	ALA	3.4
2	F	346	ALA	3.4
2	H	176	CYS	3.4
1	A	377	LEU	3.4
1	C	369	LEU	3.4
1	A	336	SER	3.4
1	C	290	LEU	3.3
2	F	241	LEU	3.3
1	A	63	ALA	3.3
1	E	337	TRP	3.3
1	A	373	ASP	3.3
1	C	229	ALA	3.3
1	A	393	GLN	3.3
2	B	165	VAL	3.3
2	F	111	LEU	3.3
1	C	360	GLU	3.2
1	C	296	LEU	3.2
1	G	380	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	202	ILE	3.2
1	C	353	THR	3.2
1	G	346	LEU	3.2
1	E	393	GLN	3.2
2	B	64	THR	3.2
1	G	350	VAL	3.2
1	C	361	GLU	3.2
1	A	322	LEU	3.2
1	E	423	PHE	3.2
1	C	338	SER	3.1
1	E	328	LEU	3.1
2	F	64	THR	3.1
1	C	379	GLU	3.1
1	A	334	VAL	3.1
1	E	33	THR	3.1
2	H	112	HIS	3.1
1	A	291	LEU	3.1
1	A	356	LYS	3.1
1	G	362	ASP	3.1
1	G	393	GLN	3.1
1	E	343	LEU	3.1
1	G	292	ASP	3.1
1	G	172	LEU	3.1
2	B	213	LEU	3.1
1	C	337	TRP	3.0
1	G	91	ASN	3.0
1	E	421	ARG	3.0
1	C	325	LYS	3.0
1	E	288	ALA	3.0
1	A	87	ASP	3.0
2	D	123	GLU	3.0
2	F	265	PHE	3.0
1	A	33	THR	3.0
1	A	176	ILE	3.0
2	F	188	ILE	3.0
1	A	341	SER	3.0
1	C	330	TYR	3.0
1	E	174	TYR	3.0
2	B	222	THR	3.0
2	B	74	MET	3.0
1	G	255	LEU	3.0
1	C	151	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	419	GLN	2.9
1	E	381	ASN	2.9
2	H	106	THR	2.9
2	H	235	GLY	2.9
1	C	384	VAL	2.9
1	E	355	THR	2.9
1	G	355	THR	2.9
1	C	419	GLN	2.9
1	C	352	ALA	2.9
1	E	290	LEU	2.9
1	G	314	ALA	2.9
1	G	315	LEU	2.9
2	D	213	LEU	2.9
2	B	212	HIS	2.9
1	G	290	LEU	2.8
1	A	378	ASP	2.8
1	E	25	CYS	2.8
1	C	97	ARG	2.8
2	B	112	HIS	2.8
1	A	174	TYR	2.8
1	C	255	LEU	2.8
1	C	367	ARG	2.8
1	E	70	ARG	2.8
2	F	66	ALA	2.8
1	C	326	ARG	2.8
2	F	154	VAL	2.8
1	A	371	GLY	2.8
2	F	158	VAL	2.7
2	H	228	VAL	2.7
1	E	364	ALA	2.7
2	B	111	LEU	2.7
1	A	338	SER	2.7
2	F	125	TYR	2.7
2	B	161	ARG	2.7
1	A	415	LEU	2.7
1	E	96	GLY	2.7
1	A	399	ALA	2.7
1	A	379	GLU	2.7
2	H	222	THR	2.7
1	C	421	ARG	2.7
2	B	118	PHE	2.7
1	C	389	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	335	LYS	2.6
2	B	169	PRO	2.6
1	C	390	ASP	2.6
1	C	358	SER	2.6
1	G	384	VAL	2.6
1	C	174	TYR	2.6
2	F	352	VAL	2.6
1	A	384	VAL	2.6
2	F	101	THR	2.6
1	C	160	LYS	2.6
1	C	435	VAL	2.6
1	A	172	LEU	2.6
1	E	176	ILE	2.6
2	H	353	ASP	2.6
2	D	220	ALA	2.5
2	F	100	THR	2.5
2	B	347	ARG	2.5
1	E	372	ASP	2.5
1	E	319	ARG	2.5
2	D	131	VAL	2.5
1	A	96	GLY	2.5
1	G	358	SER	2.5
1	G	95	MET	2.5
1	A	321	ARG	2.5
1	E	365	ARG	2.5
2	F	170	ARG	2.5
2	B	265	PHE	2.5
1	A	289	ARG	2.5
1	E	326	ARG	2.5
1	A	288	ALA	2.5
1	E	34	ASP	2.5
1	A	300	THR	2.5
2	H	351	LEU	2.5
1	E	194	ARG	2.5
2	D	401	PHE	2.5
1	C	87	ASP	2.5
1	G	343	LEU	2.4
2	H	115	LEU	2.4
1	E	44	ILE	2.4
1	C	155	GLY	2.4
1	G	168	GLY	2.4
1	C	187	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	161	ARG	2.4
2	F	254	LEU	2.4
1	E	358	SER	2.4
1	E	339	VAL	2.4
1	C	348	MET	2.4
1	G	266	GLY	2.4
2	D	135	THR	2.4
1	C	303	LEU	2.4
1	G	385	LEU	2.4
1	A	95	MET	2.4
2	D	130	ILE	2.4
2	H	133	VAL	2.4
1	G	70	ARG	2.4
1	G	372	ASP	2.4
2	D	295	ARG	2.4
1	C	33	THR	2.4
2	B	117	GLU	2.4
1	A	195	VAL	2.3
1	G	330	TYR	2.3
1	E	415	LEU	2.3
1	A	194	ARG	2.3
2	H	4	ILE	2.3
1	E	353	THR	2.3
1	C	211	TRP	2.3
2	D	81	VAL	2.3
1	C	167	ALA	2.3
1	C	394	ALA	2.3
1	E	35	GLY	2.3
2	F	166	GLY	2.3
2	D	162	ARG	2.3
2	F	161	ARG	2.3
2	H	38	PHE	2.3
1	A	313	ALA	2.3
1	C	383	ARG	2.3
2	H	75	GLY	2.3
2	H	120	THR	2.3
1	A	328	LEU	2.3
1	E	329	LEU	2.3
1	E	348	MET	2.3
1	E	370	MET	2.3
2	D	78	GLU	2.3
1	G	64	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	2.3
1	G	368	GLU	2.3
1	G	374	VAL	2.3
1	G	436	ARG	2.3
1	C	363	LYS	2.3
1	A	229	ALA	2.3
2	B	363	ASP	2.3
1	E	397	LEU	2.3
2	F	75	GLY	2.2
1	E	38	SER	2.2
1	C	387	LYS	2.2
1	G	357	LYS	2.2
2	H	131	VAL	2.2
1	C	103	PHE	2.2
2	D	258	THR	2.2
1	G	332	GLY	2.2
1	G	335	LYS	2.2
1	E	289	ARG	2.2
1	G	253	ALA	2.2
2	H	76	ALA	2.2
2	H	124	GLU	2.2
1	A	418	ASN	2.2
1	A	414	PHE	2.2
2	D	218	PHE	2.2
2	D	254	LEU	2.2
2	F	213	LEU	2.2
1	G	211	TRP	2.2
1	C	372	ASP	2.2
2	F	169	PRO	2.2
1	C	397	LEU	2.2
1	A	211	TRP	2.1
2	F	172	VAL	2.1
1	A	366	ILE	2.1
1	E	24	GLY	2.1
2	H	162	ARG	2.1
2	B	159	PRO	2.1
1	C	328	LEU	2.1
1	C	392	TYR	2.1
2	F	223	THR	2.1
1	C	357	LYS	2.1
1	E	131	ASP	2.1
1	A	69	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	GLY	2.1
1	A	94	ILE	2.1
1	E	346	LEU	2.1
1	E	369	LEU	2.1
1	G	284	LEU	2.1
2	B	291	ASP	2.1
2	D	117	GLU	2.1
1	C	100	LYS	2.1
1	C	195	VAL	2.1
1	C	339	VAL	2.1
1	E	340	VAL	2.1
1	C	422	GLU	2.1
1	E	97	ARG	2.1
2	F	401	PHE	2.1
2	H	251	ALA	2.1
1	A	70	ARG	2.1
1	G	331	THR	2.1
2	B	351	LEU	2.1
2	F	119	ARG	2.1
1	A	125	VAL	2.1
1	G	87	ASP	2.1
1	E	386	LEU	2.1
1	G	279	ASP	2.0
1	E	66	SER	2.0
2	D	94	SER	2.0
2	F	115	LEU	2.0
2	H	79	ASN	2.0
2	H	99	LEU	2.0
1	C	289	ARG	2.0
1	C	345	ASP	2.0
2	B	352	VAL	2.0
1	A	164	ASN	2.0
1	A	64	GLY	2.0
1	C	366	ILE	2.0
1	G	162	LEU	2.0
2	H	153	ILE	2.0
1	C	316	GLU	2.0
1	G	185	PRO	2.0
2	F	74	MET	2.0
1	E	407	ALA	2.0
1	G	351	VAL	2.0
1	E	436	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	103	LEU	2.0
2	D	265	PHE	2.0
2	H	204	ASP	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)

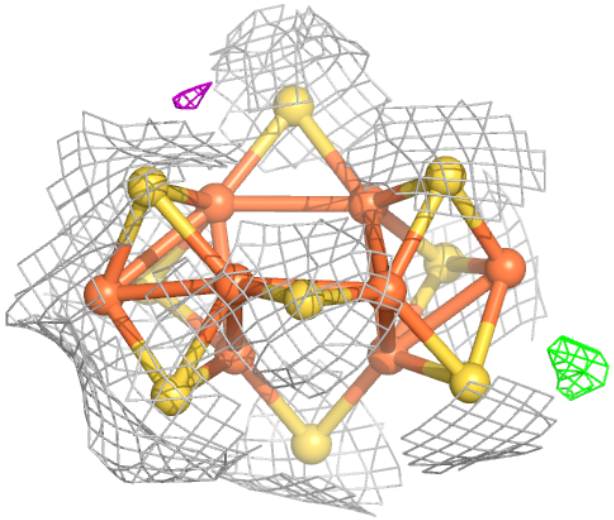
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

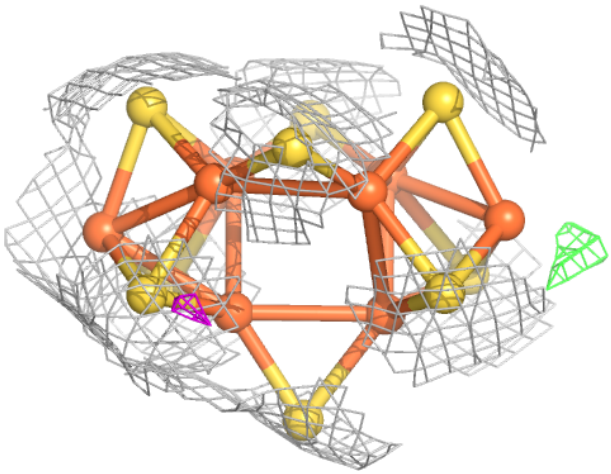
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SF4	G	501	8/8	0.95	0.16	25,29,31,44	0
4	CZL	G	502	17/17	0.95	0.11	55,87,123,129	0
3	SF4	E	501	8/8	0.96	0.13	14,32,40,43	0
3	SF4	A	501	8/8	0.96	0.15	17,21,23,28	0
4	CZL	A	502	17/17	0.96	0.14	26,47,58,62	0
4	CZL	C	502	17/17	0.96	0.09	59,81,108,114	0
4	CZL	E	502	17/17	0.96	0.12	74,89,128,134	0
3	SF4	C	501	8/8	0.96	0.16	16,26,34,53	0

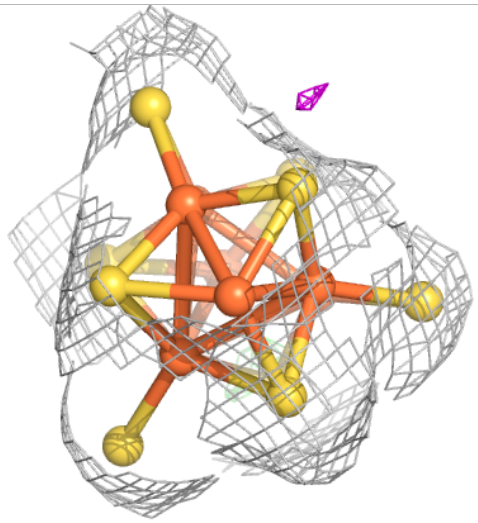
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CZL G 502:

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

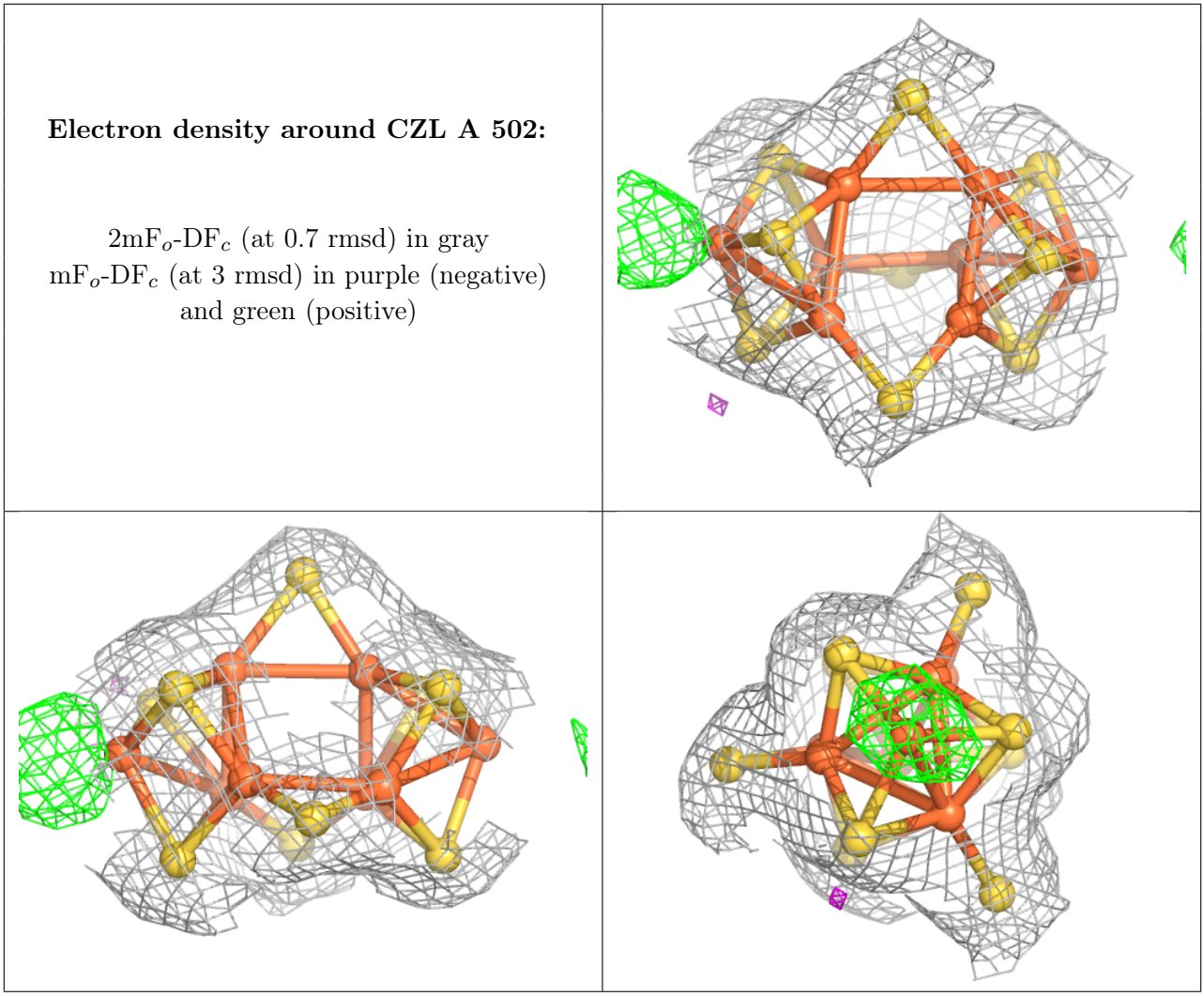






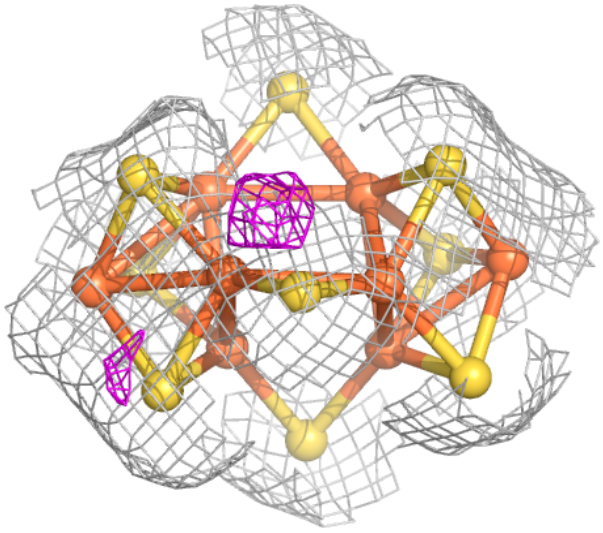
Electron density around CZL A 502:

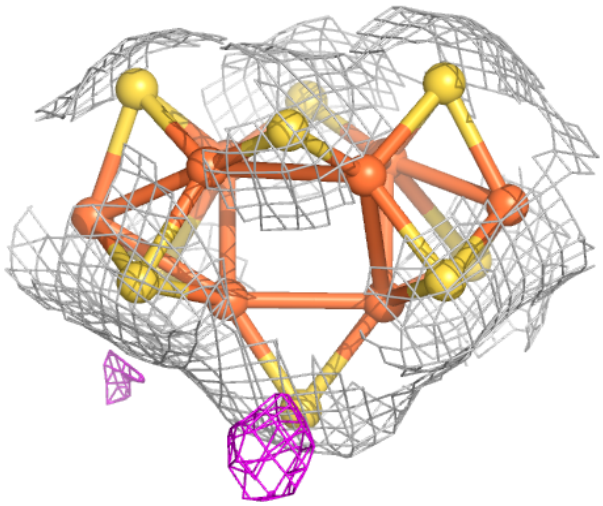
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

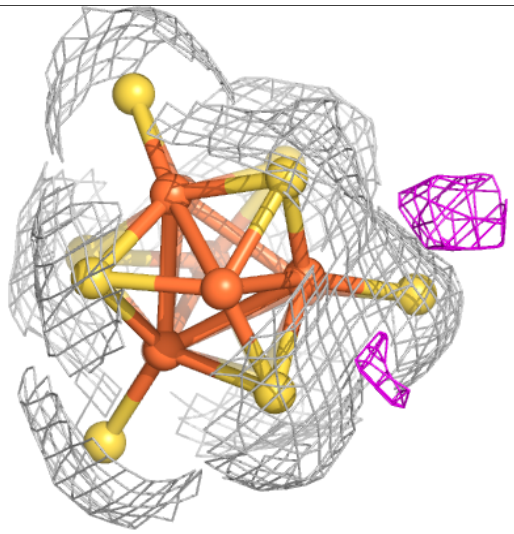


Electron density around CZL C 502:

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

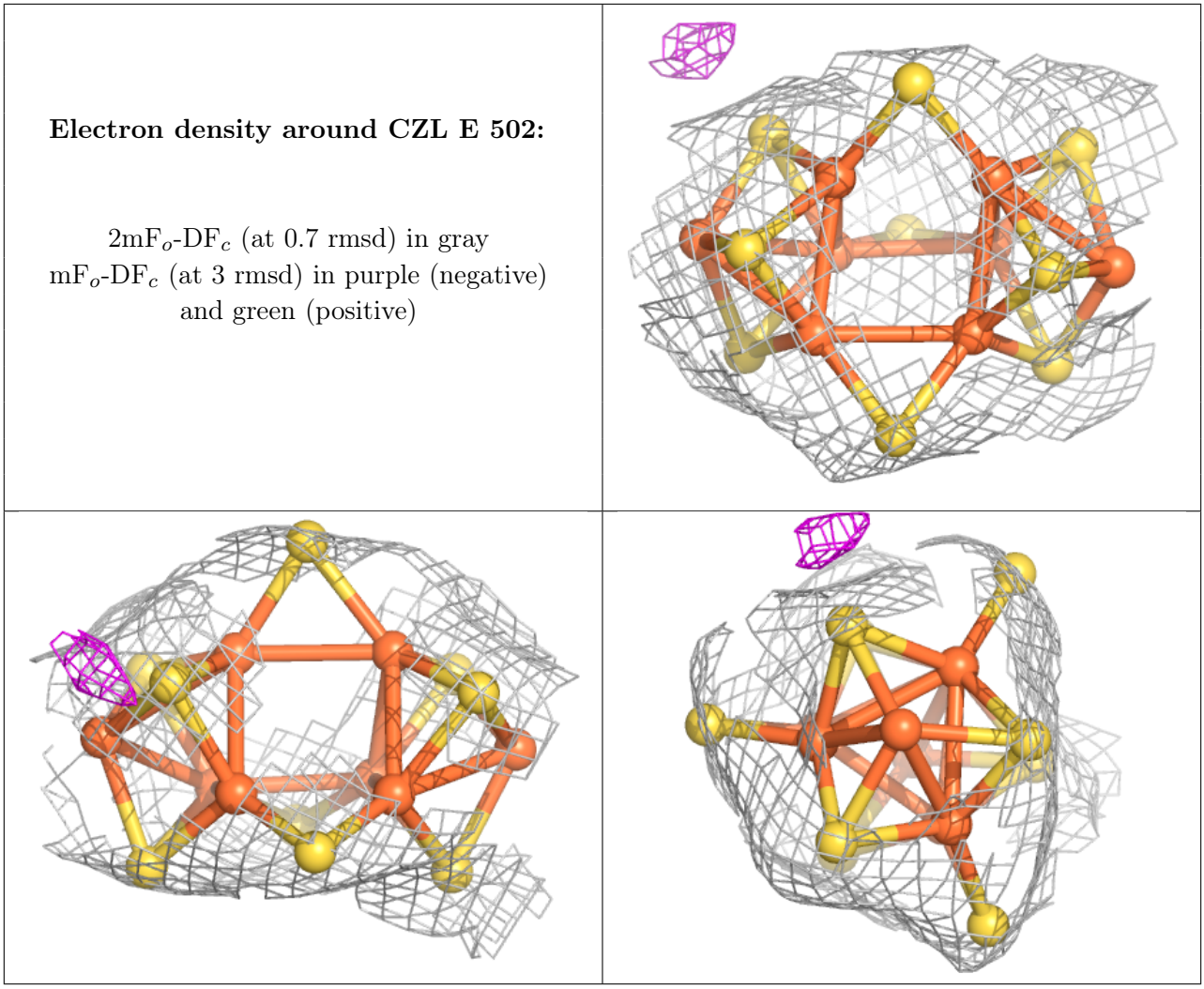






Electron density around CZL E 502:

$2mF_o$-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

There are no such residues in this entry.