



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:20 PM UTC

PDB ID : 1G21 / pdb_00001g21
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
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Deposited on : 2000-10-16
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

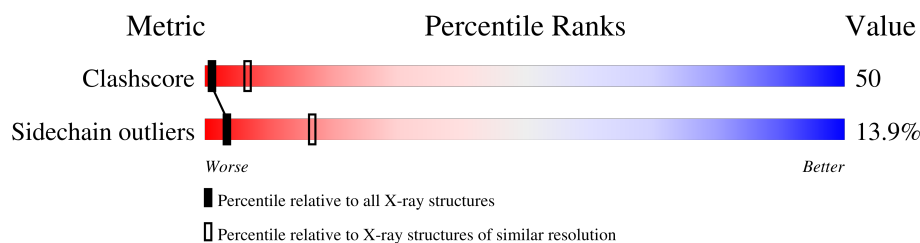
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	
3	E	289	
3	F	289	
3	G	289	
3	H	289	

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
5	CFM	A	1496	-	-	X	-
5	CFM	C	3496	-	-	X	-
9	ATP	G	7292	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24237 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 MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	268	Total	C	N	O	S	109	0	0
			2029	1265	347	397	20			
3	F	267	Total	C	N	O	S	71	0	0
			2020	1260	346	394	20			
3	G	268	Total	C	N	O	S	130	0	0
			2029	1265	347	397	20			
3	H	268	Total	C	N	O	S	116	0	0
			2029	1265	347	397	20			

There are 4 discrepancies between the modelled and reference sequences:

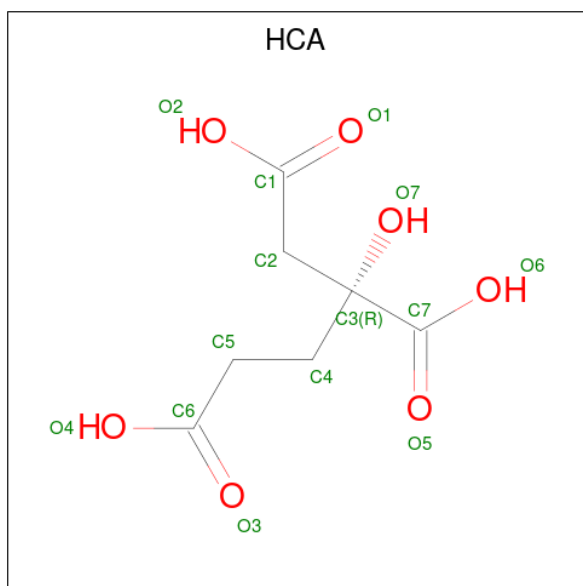
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P00459
F	?	-	LEU	deletion	UNP P00459
G	?	-	LEU	deletion	UNP P00459

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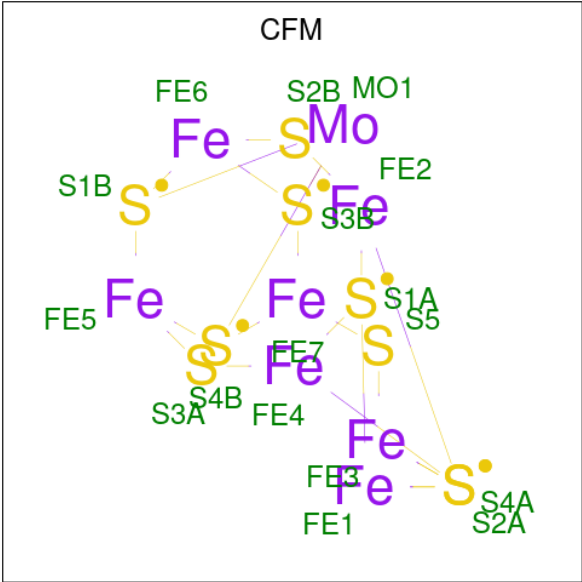
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P00459

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



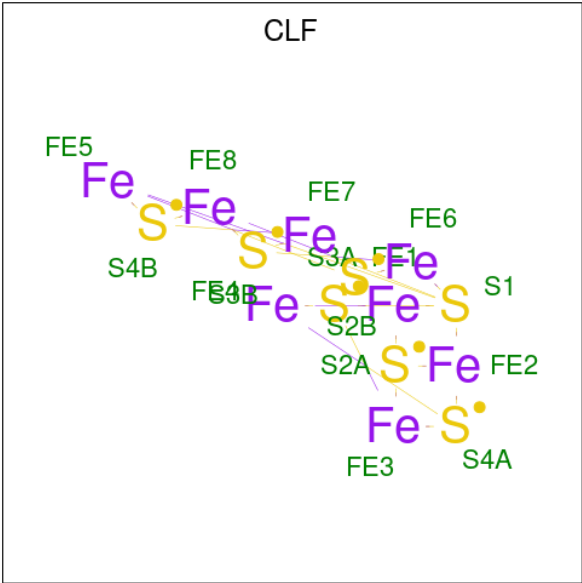
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		

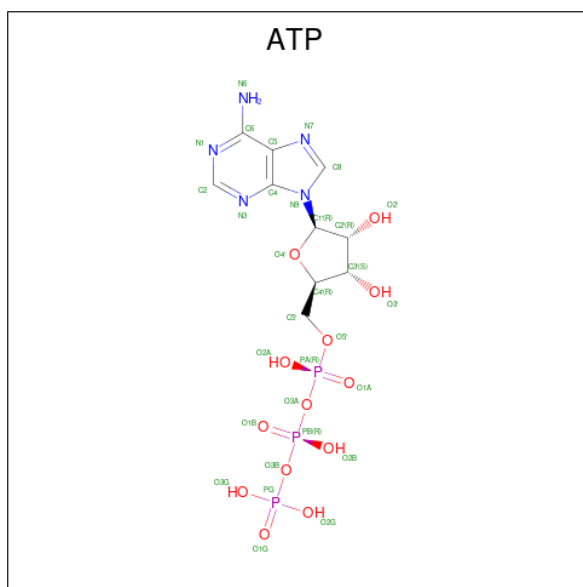
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	G	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



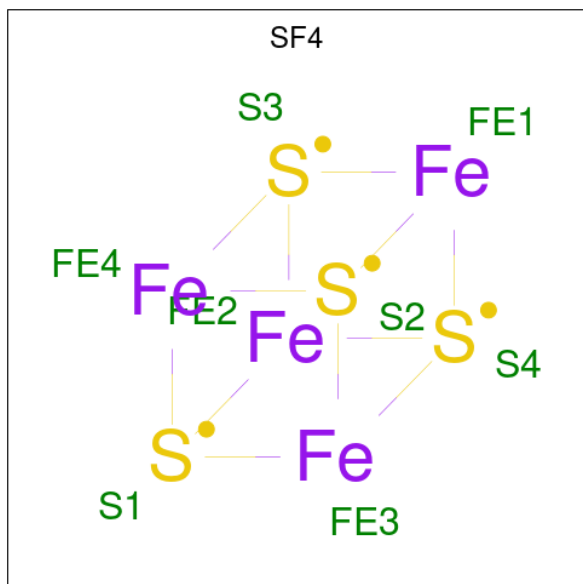
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
9	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



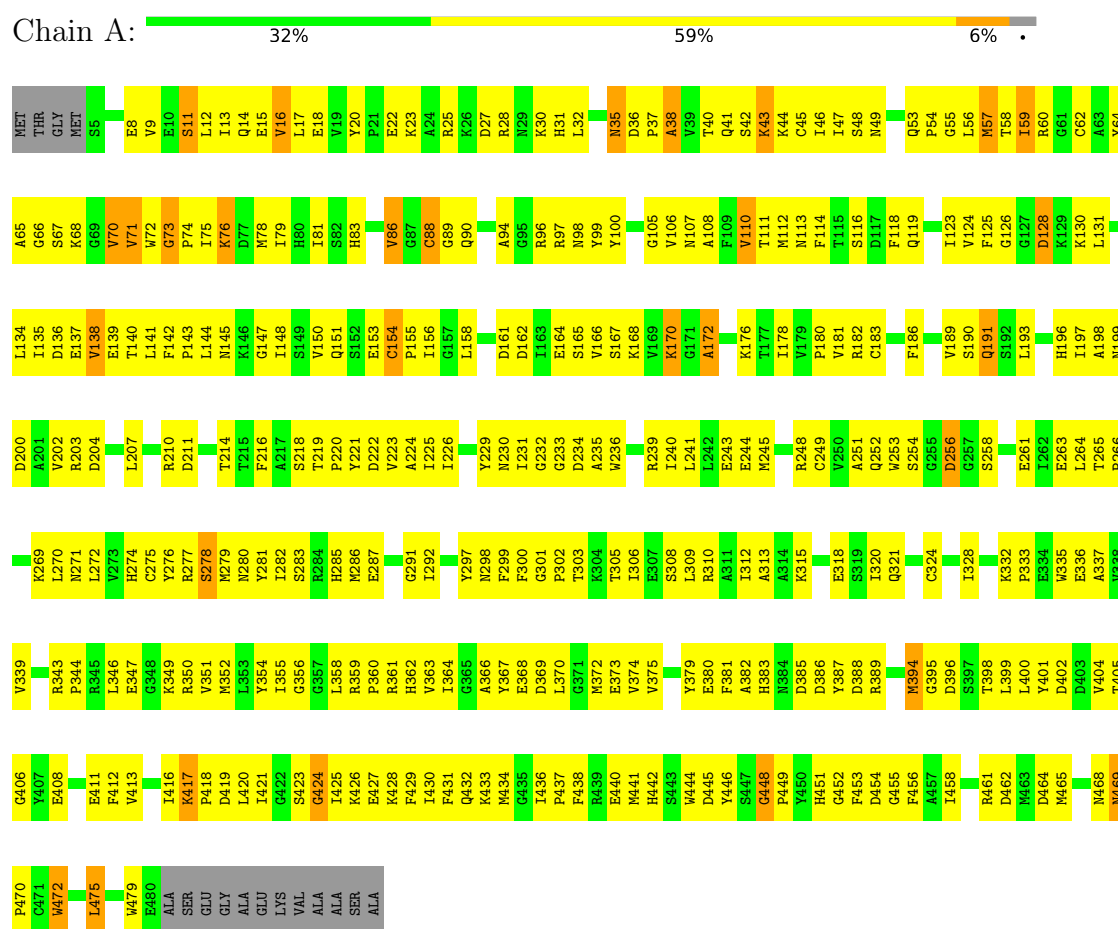
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total	Fe	S	0	0
			8	4	4		
10	G	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

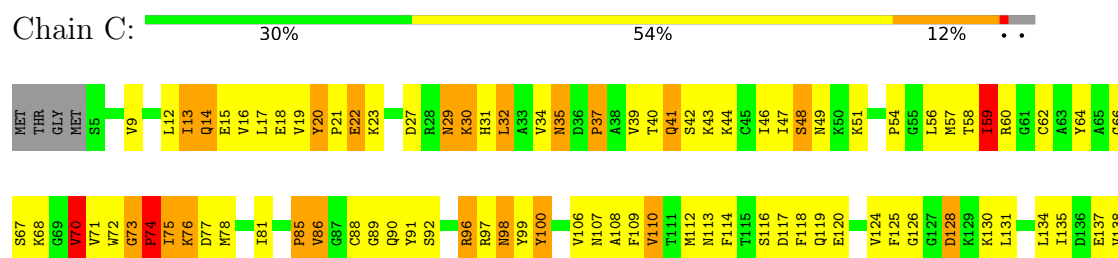
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

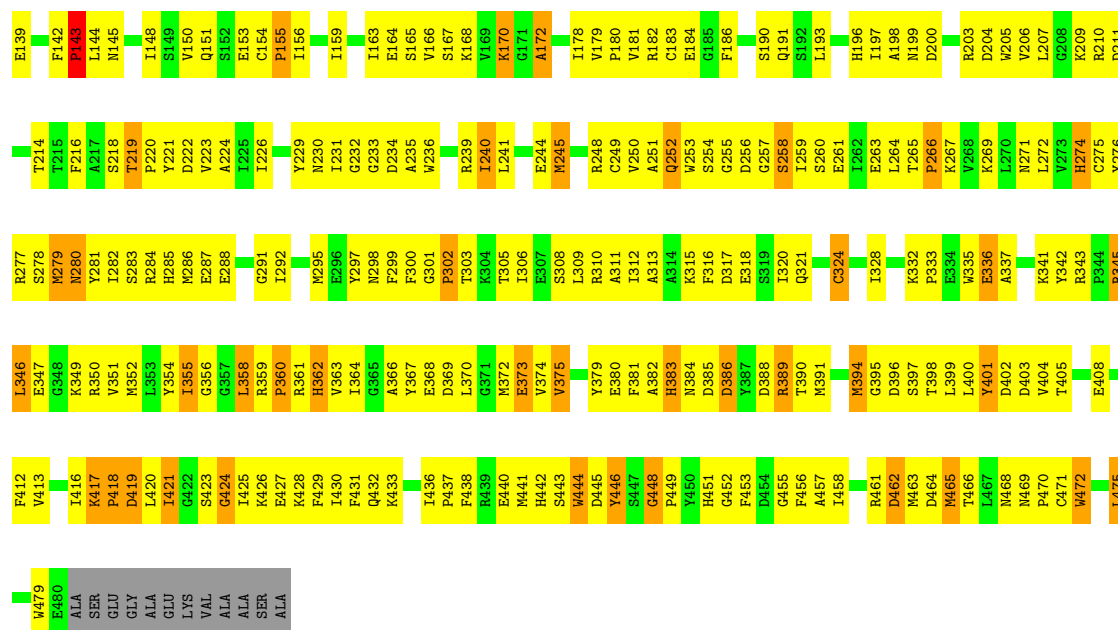
Note EDS was not executed.

• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



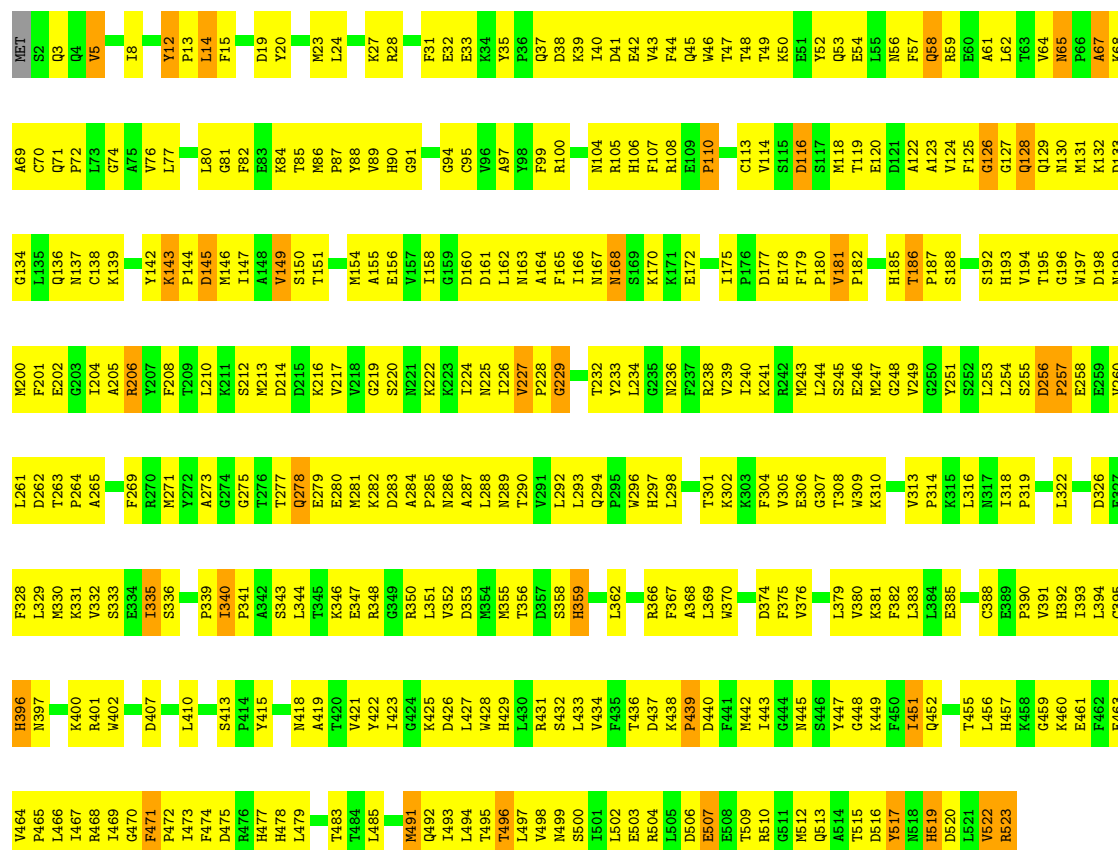
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



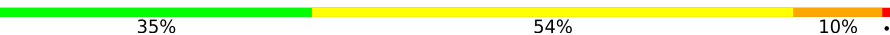


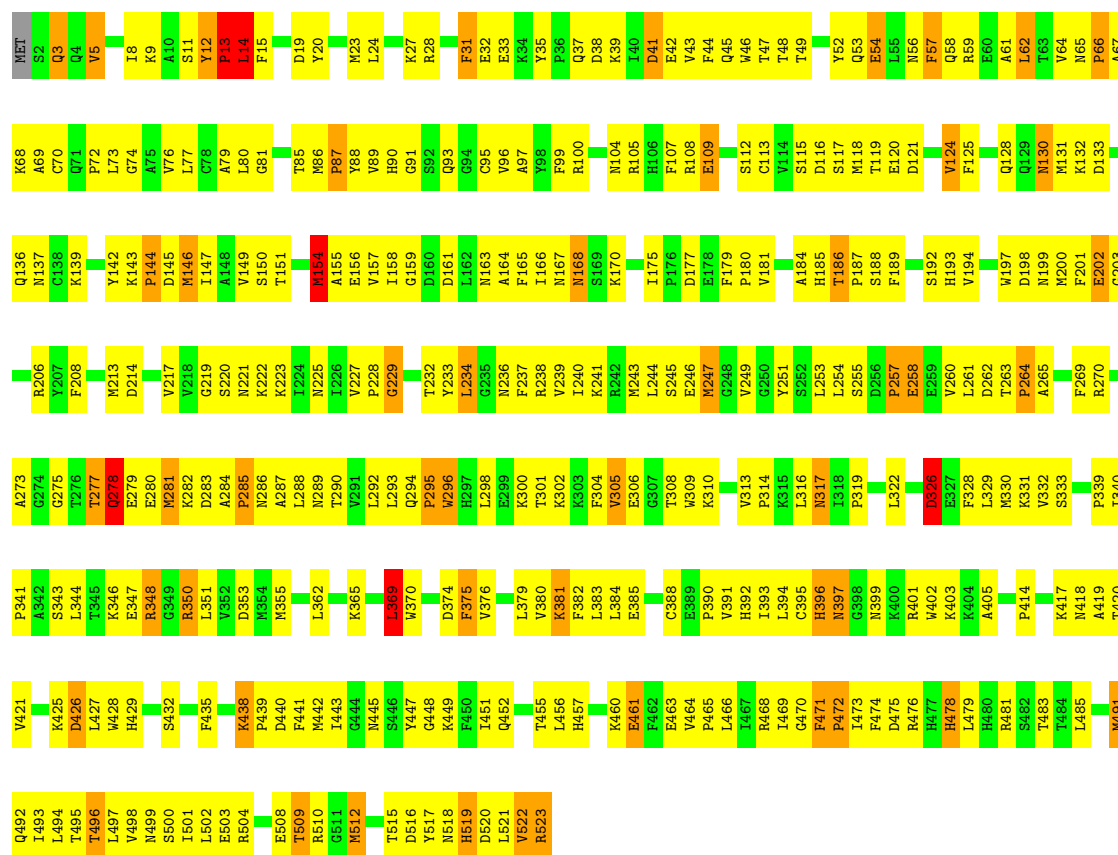
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain B: 31% 62% 7%

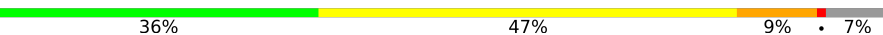


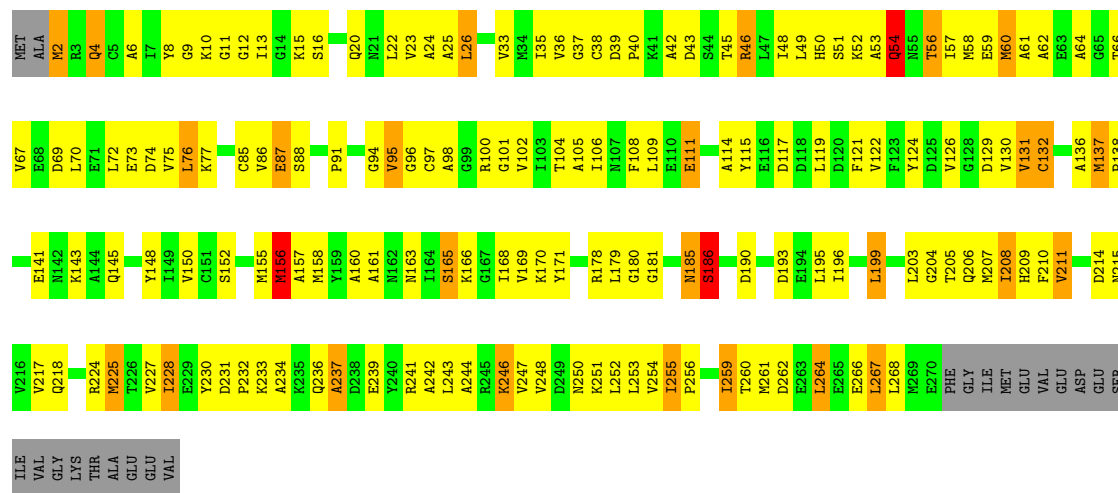
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D:  35% 54% 10%

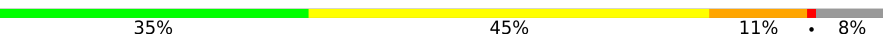


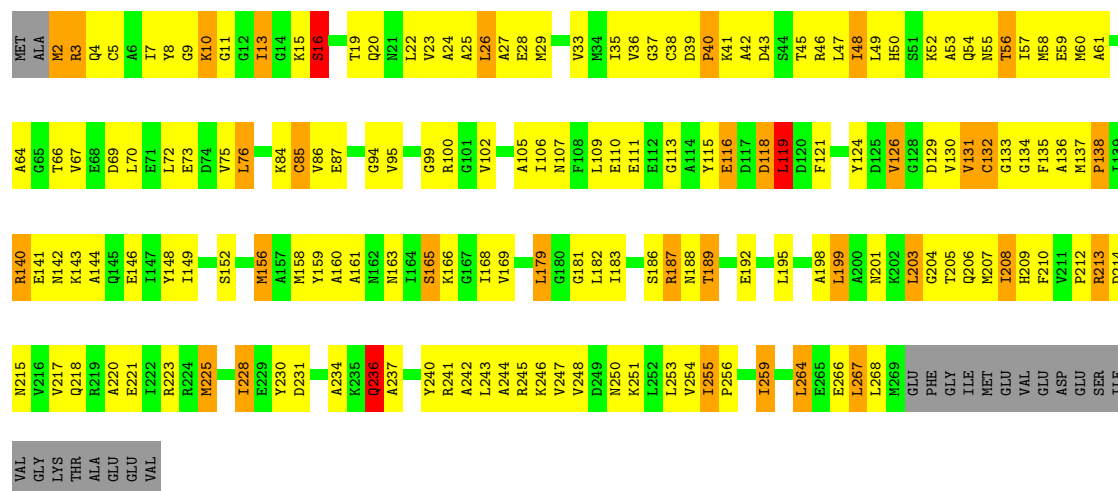
• Molecule 3: NITROGENASE IRON PROTEIN

Chain E:  36% 47% 9% 7%



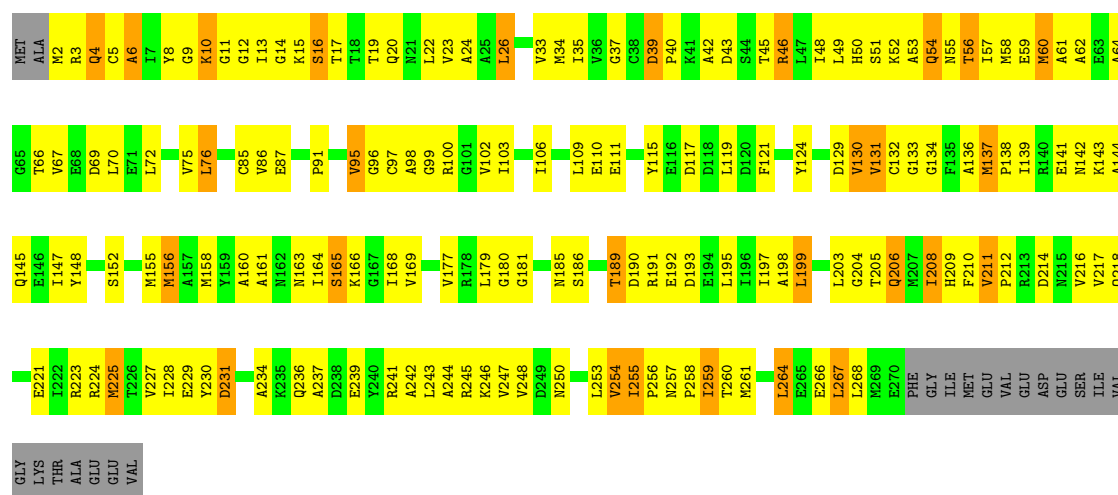
• Molecule 3: NITROGENASE IRON PROTEIN

Chain F:  35% 45% 11% 8%



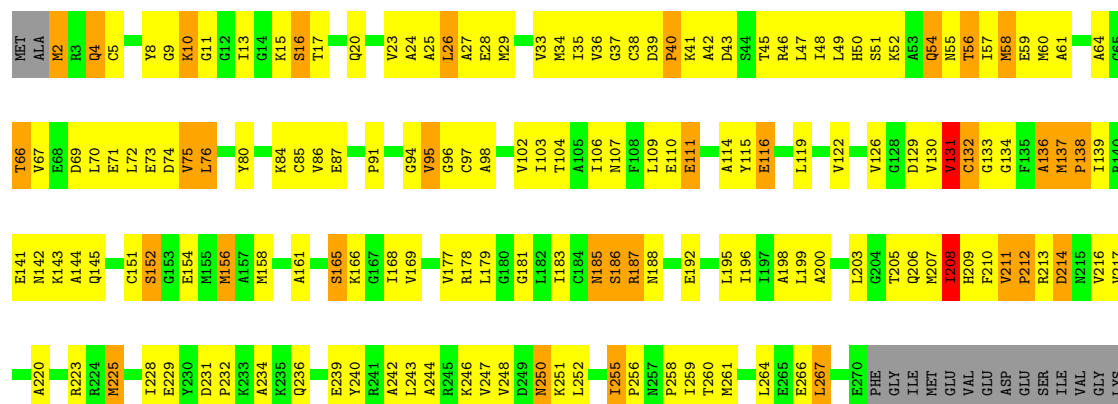
• Molecule 3: NITROGENASE IRON PROTEIN

Chain G: 35% 48% 10% 7%



• Molecule 3: NITROGENASE IRON PROTEIN

Chain H: 36% 45% 11% 7%



THR
ALA
GLU
GLU
VAL

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.50Å 121.50Å 264.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	71.6 (20.00-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24237	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HCA, MG, CFM, CA, ATP, SF4, CLF

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	0.67	1/3864 (0.0%)	1.16	38/5212 (0.7%)
1	C	0.60	0/3864	1.17	42/5212 (0.8%)
2	B	0.72	2/4276 (0.0%)	1.51	56/5782 (1.0%)
2	D	0.66	1/4276 (0.0%)	1.42	40/5782 (0.7%)
3	E	0.68	0/2052	1.25	22/2764 (0.8%)
3	F	0.73	1/2043 (0.0%)	1.27	16/2752 (0.6%)
3	G	0.64	0/2052	1.15	18/2764 (0.7%)
3	H	0.71	2/2052 (0.1%)	1.23	20/2764 (0.7%)
All	All	0.67	7/24479 (0.0%)	1.30	252/33032 (0.8%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	156	MET	SD-CE	-8.37	1.58	1.79
1	A	57	MET	SD-CE	-7.88	1.59	1.79
2	D	109	GLU	C-N	-6.80	1.24	1.33
2	B	13	PRO	CA-CB	-6.58	1.44	1.53
2	B	257	PRO	N-CA	5.62	1.54	1.47
3	H	40	PRO	N-CD	5.44	1.55	1.47
3	F	40	PRO	N-CD	5.38	1.55	1.47

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	TYR	CA-C-N	46.49	177.95	119.84
2	B	12	TYR	C-N-CA	46.49	177.95	119.84
2	D	12	TYR	CA-C-N	43.69	174.45	119.84
2	D	12	TYR	C-N-CA	43.69	174.45	119.84
2	D	12	TYR	C-N-CD	-12.75	72.71	125.00
2	B	12	TYR	C-N-CD	-12.02	75.71	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	119	LEU	N-CA-C	11.82	127.16	110.50
1	A	172	ALA	N-CA-C	-11.29	98.00	112.23
1	C	172	ALA	N-CA-C	-11.21	98.99	112.89
1	C	128	ASP	N-CA-C	-11.02	99.97	113.41
1	A	71	VAL	N-CA-C	11.00	120.75	110.74
1	A	38	ALA	N-CA-C	10.66	126.61	113.50
2	B	227	VAL	CA-C-N	10.65	133.16	119.84
2	B	227	VAL	C-N-CA	10.65	133.16	119.84
3	E	145	GLN	OE1-CD-NE2	-10.63	111.97	122.60
2	D	145	ASP	N-CA-C	-10.53	100.93	113.88
2	B	58	GLN	OE1-CD-NE2	-10.23	112.37	122.60
3	H	54	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	C	417	LYS	CA-C-N	9.93	129.86	120.03
1	C	417	LYS	C-N-CA	9.93	129.86	120.03
3	E	54	GLN	OE1-CD-NE2	-9.85	112.75	122.60
3	G	206	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	C	41	GLN	OE1-CD-NE2	-9.79	112.81	122.60
2	B	145	ASP	N-CA-C	-9.59	101.70	113.50
1	A	41	GLN	OE1-CD-NE2	-9.53	113.07	122.60
3	E	20	GLN	OE1-CD-NE2	-9.48	113.12	122.60
3	F	187	ARG	N-CA-C	-9.45	101.68	113.02
3	F	236	GLN	OE1-CD-NE2	-9.43	113.17	122.60
2	B	513	GLN	OE1-CD-NE2	-9.35	113.25	122.60
3	G	54	GLN	OE1-CD-NE2	-9.32	113.28	122.60
1	C	14	GLN	OE1-CD-NE2	-9.09	113.52	122.60
3	F	116	GLU	N-CA-C	9.08	130.14	110.80
2	B	116	ASP	N-CA-C	-8.79	95.78	109.76
2	B	313	VAL	CA-C-N	8.69	128.71	119.76
2	B	313	VAL	C-N-CA	8.69	128.71	119.76
1	A	88	CYS	CA-CB-SG	-8.65	94.51	114.40
1	A	76	LYS	N-CA-C	8.56	121.56	111.71
2	D	95	CYS	CA-CB-SG	-8.46	94.93	114.40
3	E	24	ALA	N-CA-C	-8.44	102.04	111.07
2	B	14	LEU	N-CA-C	8.40	121.19	111.11
2	D	313	VAL	CA-C-N	8.37	128.38	119.76
2	D	313	VAL	C-N-CA	8.37	128.38	119.76
1	A	128	ASP	N-CA-C	-8.24	102.10	112.90
1	C	475	LEU	N-CA-C	8.21	120.00	111.14
3	F	13	ILE	N-CA-C	-8.13	105.29	112.12
3	E	211	VAL	CA-C-N	8.10	128.59	119.92
3	E	211	VAL	C-N-CA	8.10	128.59	119.92
3	H	186	SER	N-CA-C	8.07	127.99	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	N-CA-C	-7.88	103.81	113.50
3	E	186	SER	N-CA-C	7.84	122.24	110.64
3	F	136	ALA	N-CA-C	-7.83	103.54	113.72
3	G	218	GLN	N-CA-C	-7.69	102.23	111.69
2	B	335	ILE	N-CA-C	7.69	118.60	111.45
3	H	131	VAL	N-CA-C	7.52	119.19	110.62
3	F	189	THR	N-CA-C	-7.51	99.70	110.59
2	D	491	MET	N-CA-C	-7.49	103.19	111.36
1	A	59	ILE	N-CA-C	-7.46	104.70	113.42
3	F	24	ALA	N-CA-C	-7.40	103.15	111.07
2	B	335	ILE	CB-CA-C	-7.39	102.24	111.92
3	H	16	SER	N-CA-C	7.37	119.31	111.28
3	H	136	ALA	N-CA-C	-7.31	104.38	113.38
2	B	181	VAL	CA-C-N	7.27	127.27	119.78
2	B	181	VAL	C-N-CA	7.27	127.27	119.78
1	A	70	VAL	N-CA-C	7.26	118.20	111.45
1	A	41	GLN	CG-CD-NE2	7.22	127.23	116.40
3	E	145	GLN	CG-CD-NE2	7.20	127.20	116.40
3	G	133	GLY	N-CA-C	7.19	120.84	112.50
2	D	13	PRO	CA-N-CD	-7.16	101.98	112.00
1	C	285	HIS	N-CA-C	-7.14	103.53	111.82
3	F	132	CYS	N-CA-C	7.12	117.67	108.34
1	A	73	GLY	CA-C-N	7.12	128.74	119.84
1	A	73	GLY	C-N-CA	7.12	128.74	119.84
3	F	16	SER	N-CA-C	7.00	118.56	111.07
1	C	22	GLU	N-CA-C	6.98	120.69	111.75
1	C	59	ILE	N-CA-C	-6.97	105.83	113.43
3	G	206	GLN	CG-CD-NE2	6.94	126.82	116.40
3	F	236	GLN	CG-CD-NE2	6.80	126.60	116.40
2	D	14	LEU	N-CA-C	6.79	119.30	111.02
2	B	513	GLN	CG-CD-NE2	6.78	126.57	116.40
2	D	471	PHE	C-N-CD	-6.77	105.71	120.60
1	A	211	ASP	N-CA-C	6.76	118.73	111.36
2	B	359	HIS	N-CA-C	6.74	119.48	111.33
1	C	110	VAL	N-CA-C	6.72	117.34	110.82
2	B	13	PRO	CA-N-CD	-6.71	102.61	112.00
2	B	368	ALA	N-CA-C	-6.69	98.07	109.24
2	D	438	LYS	N-CA-C	6.67	119.31	109.50
1	C	41	GLN	CG-CD-NE2	6.67	126.41	116.40
2	B	58	GLN	CG-CD-NE2	6.65	126.38	116.40
3	H	208	ILE	N-CA-C	6.65	118.20	110.62
3	G	54	GLN	CG-CD-NE2	6.65	126.37	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	PRO	CA-N-CD	-6.62	102.73	112.00
3	G	186	SER	N-CA-C	6.62	120.08	110.42
2	B	471	PHE	C-N-CD	-6.61	106.06	120.60
1	C	76	LYS	N-CA-C	6.60	120.60	112.54
3	G	24	ALA	N-CA-C	-6.60	104.01	111.07
1	C	73	GLY	CA-C-N	6.52	126.21	119.56
1	C	73	GLY	C-N-CA	6.52	126.21	119.56
1	C	14	GLN	CG-CD-NE2	6.50	126.14	116.40
2	D	405	ALA	N-CA-C	-6.49	103.42	112.45
2	B	440	ASP	N-CA-C	-6.49	104.05	112.68
1	A	475	LEU	N-CA-C	6.45	118.19	111.03
3	E	20	GLN	CG-CD-NE2	6.40	126.00	116.40
1	A	417	LYS	CA-C-N	6.39	126.76	119.92
1	A	417	LYS	C-N-CA	6.39	126.76	119.92
1	A	285	HIS	N-CA-C	-6.38	104.42	111.82
2	D	350	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	B	256	ASP	CA-C-N	6.36	126.28	119.28
2	B	256	ASP	C-N-CA	6.36	126.28	119.28
3	F	118	ASP	N-CA-C	6.31	124.24	110.80
3	H	54	GLN	CG-CD-NE2	6.30	125.86	116.40
2	D	214	ASP	N-CA-C	6.25	118.90	111.71
1	A	110	VAL	N-CA-C	6.25	117.26	111.45
2	B	214	ASP	N-CA-C	6.24	118.08	111.28
3	H	115	TYR	N-CA-C	-6.22	105.96	112.93
3	E	16	SER	N-CA-C	6.18	117.69	111.07
2	B	5	VAL	N-CA-C	6.16	122.14	109.34
2	B	206	ARG	N-CA-C	6.13	117.77	111.14
3	E	54	GLN	CG-CD-NE2	6.13	125.60	116.40
3	E	231	ASP	CA-C-N	6.12	127.49	119.84
3	E	231	ASP	C-N-CA	6.12	127.49	119.84
1	A	256	ASP	N-CA-C	-6.12	105.77	113.23
3	G	16	SER	N-CA-C	6.11	118.44	111.11
1	C	394	MET	N-CA-C	6.10	119.11	110.14
1	C	86	VAL	N-CA-C	6.09	120.94	112.35
2	D	109	GLU	CA-C-O	-6.08	111.83	120.16
2	B	67	ALA	N-CA-C	-6.08	103.17	111.56
3	E	42	ALA	N-CA-C	6.07	118.33	108.63
3	E	132	CYS	N-CA-C	6.03	116.24	108.34
2	B	438	LYS	N-CA-C	6.03	118.36	109.50
2	D	143	LYS	N-CA-C	5.99	123.05	109.81
1	A	434	MET	N-CA-C	-5.98	106.23	112.93
2	B	257	PRO	N-CA-C	5.98	121.72	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	PRO	CA-N-CD	-5.96	103.65	112.00
2	B	451	ILE	N-CA-C	-5.95	103.65	111.09
2	D	478	HIS	N-CA-C	5.94	119.84	112.24
1	C	386	ASP	N-CA-C	-5.93	106.17	113.41
3	H	211	VAL	O-C-N	5.93	126.74	121.41
2	B	65	ASN	CA-C-N	5.91	126.73	120.11
2	B	65	ASN	C-N-CA	5.91	126.73	120.11
1	C	13	ILE	N-CA-C	5.89	116.01	110.30
3	E	190	ASP	N-CA-C	-5.87	100.42	109.76
2	B	491	MET	N-CA-C	-5.87	104.96	111.36
1	C	13	ILE	CB-CA-C	-5.85	104.50	111.81
1	C	206	VAL	CB-CA-C	-5.84	106.75	111.71
2	B	186	THR	CA-C-N	5.83	127.13	119.84
2	B	186	THR	C-N-CA	5.83	127.13	119.84
1	C	70	VAL	N-CA-C	5.78	116.83	111.45
2	B	468	ARG	N-CA-C	5.78	118.16	107.99
3	G	189	THR	N-CA-C	-5.78	98.50	110.80
1	C	41	GLN	CA-C-N	-5.77	113.42	122.65
1	C	41	GLN	C-N-CA	-5.77	113.42	122.65
3	H	116	GLU	N-CA-C	5.76	117.37	111.14
3	H	75	VAL	CB-CA-C	-5.74	104.95	111.55
3	H	187	ARG	N-CA-C	-5.69	103.05	111.81
1	A	45	CYS	N-CA-C	5.68	120.21	112.04
3	H	132	CYS	N-CA-C	5.66	115.76	108.34
3	H	74	ASP	N-CA-C	5.63	117.49	111.36
1	C	14	GLN	CB-CA-C	5.62	121.64	110.17
1	A	16	VAL	N-CA-C	-5.62	105.24	110.53
1	C	336	GLU	N-CA-C	-5.62	105.06	111.07
3	E	237	ALA	N-CA-C	-5.61	105.55	112.90
3	G	39	ASP	CA-C-N	5.59	125.43	119.28
3	G	39	ASP	C-N-CA	5.59	125.43	119.28
1	A	35	ASN	N-CA-C	5.59	117.81	109.25
2	B	128	GLN	N-CA-C	5.59	118.22	111.40
1	A	469	ASN	CA-C-N	5.56	125.39	119.28
1	A	469	ASN	C-N-CA	5.56	125.39	119.28
2	D	186	THR	CA-C-N	5.56	126.79	119.84
2	D	186	THR	C-N-CA	5.56	126.79	119.84
2	B	126	GLY	N-CA-C	-5.56	104.58	112.81
2	D	5	VAL	N-CA-C	5.55	120.88	109.34
2	D	509	THR	N-CA-C	5.54	118.84	112.57
3	F	225	MET	N-CA-C	5.53	117.24	108.79
1	C	274	HIS	N-CA-C	-5.50	106.24	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	168	ASN	N-CA-C	-5.50	104.98	110.97
2	B	478	HIS	N-CA-C	5.49	119.14	111.90
2	D	154	MET	N-CA-C	5.48	117.96	111.33
2	B	400	LYS	N-CA-C	5.48	116.93	111.07
3	E	114	ALA	N-CA-C	-5.47	106.44	113.23
2	D	278	GLN	N-CA-C	-5.46	105.22	111.07
1	C	170	LYS	N-CA-C	-5.45	100.91	109.25
1	C	211	ASP	N-CA-C	5.45	117.30	111.36
1	A	278	SER	N-CA-C	5.44	118.04	111.40
3	F	237	ALA	N-CA-C	-5.44	105.00	111.69
2	D	396	HIS	N-CA-C	5.43	117.96	111.71
3	E	74	ASP	N-CA-C	5.42	117.27	111.36
1	C	49	ASN	N-CA-C	5.42	119.19	112.58
2	B	307	GLY	N-CA-C	5.40	119.03	112.49
3	F	27	ALA	N-CA-C	-5.38	105.33	111.14
1	A	424	GLY	N-CA-C	5.38	120.86	112.31
2	D	247	MET	N-CA-C	-5.38	106.88	113.50
1	A	472	TRP	N-CA-C	5.37	117.83	111.33
1	C	143	PRO	CA-N-CD	-5.37	104.48	112.00
3	F	126	VAL	N-CA-C	5.35	115.80	107.99
1	A	170	LYS	N-CA-C	-5.34	100.39	108.67
2	D	124	VAL	N-CA-C	5.34	116.11	110.72
2	D	296	TRP	N-CA-C	5.32	119.52	113.19
3	G	231	ASP	CA-C-N	5.32	126.49	119.84
3	G	231	ASP	C-N-CA	5.32	126.49	119.84
1	A	394	MET	N-CA-C	5.31	117.95	110.14
3	H	212	PRO	CA-N-CD	-5.31	104.57	112.00
2	D	509	THR	CA-C-N	-5.30	114.24	122.67
2	D	509	THR	C-N-CA	-5.30	114.24	122.67
2	B	278	GLN	N-CA-C	-5.29	105.41	111.07
2	B	396	HIS	N-CA-C	5.29	117.79	111.71
2	B	149	VAL	N-CA-C	5.29	116.40	109.58
1	C	448	GLY	CA-C-N	5.29	125.29	119.90
1	C	448	GLY	C-N-CA	5.29	125.29	119.90
3	G	211	VAL	N-CA-C	5.29	113.76	107.73
3	G	62	ALA	N-CA-C	-5.26	105.72	111.82
1	A	11	SER	N-CA-C	-5.25	106.38	112.89
3	E	262	ASP	N-CA-C	5.25	117.00	111.28
2	D	369	LEU	N-CA-C	5.23	116.75	108.96
1	C	245	MET	N-CA-C	-5.22	106.59	113.17
2	D	87	PRO	N-CA-C	-5.21	102.51	110.95
3	E	211	VAL	N-CA-C	5.21	113.66	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	GLU	N-CA-C	5.20	121.88	110.80
2	B	229	GLY	N-CA-C	-5.19	104.40	112.45
1	A	448	GLY	CA-C-N	5.17	125.17	119.90
1	A	448	GLY	C-N-CA	5.17	125.17	119.90
3	E	156	MET	CG-SD-CE	-5.17	89.53	100.90
1	A	154	CYS	CB-CA-C	-5.16	104.62	113.04
2	D	509	THR	CB-CA-C	-5.16	103.06	111.06
3	H	211	VAL	CA-C-N	5.14	125.42	119.92
3	H	211	VAL	C-N-CA	5.14	125.42	119.92
2	B	168	ASN	N-CA-C	-5.14	105.37	110.97
2	D	257	PRO	N-CA-C	5.12	120.56	113.65
1	C	20	TYR	N-CA-C	5.11	118.52	109.58
2	D	326	ASP	N-CA-C	-5.11	105.72	111.28
3	H	138	PRO	CB-CA-C	5.10	119.98	111.56
1	A	138	VAL	N-CA-C	-5.10	106.71	111.45
1	C	255	GLY	N-CA-C	-5.10	101.09	113.18
1	A	86	VAL	N-CA-C	5.10	119.94	109.34
1	C	472	TRP	N-CA-C	5.08	117.48	111.33
2	B	517	TYR	N-CA-C	-5.08	105.93	111.82
2	D	57	PHE	N-CA-C	5.08	117.55	111.71
2	B	143	LYS	N-CA-C	5.07	121.02	109.81
1	C	35	ASN	N-CA-C	5.07	117.02	108.96
1	A	43	LYS	N-CA-C	-5.06	105.27	111.75
1	C	375	VAL	N-CA-C	5.06	117.05	112.29
3	H	133	GLY	N-CA-C	5.06	118.80	112.73
2	B	40	ILE	N-CA-C	-5.05	105.58	110.42
1	C	424	GLY	N-CA-C	5.04	119.48	112.57
2	D	348	ARG	NE-CZ-NH2	5.04	123.74	119.20
3	H	24	ALA	N-CA-C	-5.04	105.79	111.28
1	C	74	PRO	N-CA-C	5.02	120.37	113.84
2	B	340	ILE	N-CA-C	-5.01	98.05	108.88
2	B	248	GLY	N-CA-C	-5.01	106.24	114.76
3	G	6	ALA	N-CA-C	-5.01	101.98	109.95
3	G	211	VAL	O-C-N	5.01	125.78	121.12
2	B	110	PRO	N-CA-C	5.01	118.74	111.03
2	D	229	GLY	N-CA-C	-5.00	105.17	112.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3776	0	3709	469	0
1	C	3776	0	3709	507	0
2	B	4170	0	4076	458	0
2	D	4170	0	4076	485	0
3	E	2029	0	2040	158	0
3	F	2020	0	2034	172	0
3	G	2029	0	2041	166	0
3	H	2029	0	2041	162	0
4	A	14	0	6	1	0
4	C	14	0	6	2	0
5	A	17	0	0	4	0
5	C	17	0	0	7	0
6	A	15	0	0	1	0
6	D	15	0	0	3	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	E	31	0	12	4	0
9	F	31	0	12	6	0
9	G	31	0	12	11	0
9	H	31	0	12	6	0
10	F	8	0	0	0	0
10	G	8	0	0	0	0
All	All	24237	0	23786	2341	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (2341) 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)
3:F:39:ASP:OD1	3:F:40:PRO:HD2	1.28	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:GLY:HA2	2:D:118:MET:CE	1.62	1.28
1:C:124:VAL:HG21	3:H:58:MET:CE	1.70	1.21
1:A:355:ILE:HG23	1:A:356:GLY:H	0.99	1.15
1:A:75:ILE:HG21	1:A:78:MET:HE3	1.27	1.14
3:F:39:ASP:OD1	3:F:40:PRO:CD	1.95	1.13
2:B:471:PHE:CD2	2:B:472:PRO:HD3	1.83	1.12
2:B:85:THR:HG21	2:B:146:MET:HE2	1.28	1.12
1:C:433:LYS:NZ	2:D:263:THR:HG23	1.66	1.10
3:F:106:ILE:CD1	3:F:138:PRO:HD3	1.82	1.09
1:C:355:ILE:CG2	1:C:356:GLY:H	1.63	1.08
1:C:124:VAL:HG21	3:H:58:MET:HE2	1.12	1.07
1:C:426:LYS:HZ1	2:D:97:ALA:HB1	1.18	1.07
2:B:128:GLN:HG3	2:B:132:LYS:HE3	1.09	1.06
1:A:105:GLY:HA2	1:A:112:MET:HE1	1.35	1.06
1:A:355:ILE:CG2	1:A:360:PRO:CD	2.33	1.06
1:A:86:VAL:HG11	2:B:68:LYS:HE3	1.36	1.06
1:C:355:ILE:HG22	1:C:356:GLY:N	1.62	1.04
1:C:167:SER:CB	1:C:180:PRO:HG3	1.86	1.04
1:C:167:SER:HB2	1:C:180:PRO:HG3	1.40	1.04
2:D:91:GLY:CA	2:D:118:MET:HE3	1.88	1.03
3:G:56:THR:HG23	3:G:59:GLU:HB2	1.40	1.03
2:B:128:GLN:CG	2:B:132:LYS:HE3	1.88	1.03
3:E:156:MET:SD	9:F:6292:ATP:H4'	1.99	1.02
1:A:355:ILE:HG22	1:A:360:PRO:CD	1.89	1.01
1:C:58:THR:HG22	1:C:60:ARG:H	1.25	1.01
3:H:56:THR:HG23	3:H:59:GLU:HB2	1.41	1.01
1:C:346:LEU:HD12	1:C:372:MET:SD	2.00	1.01
3:H:225:MET:HE3	3:H:229:GLU:OE2	1.61	1.00
2:B:212:SER:O	2:B:216:LYS:HE3	1.61	1.00
3:H:23:VAL:HG21	3:H:35:ILE:HD11	1.43	1.00
2:D:86:MET:CE	2:D:87:PRO:HD2	1.92	1.00
2:B:124:VAL:HG21	3:E:58:MET:HE2	1.41	0.99
2:B:289:ASN:HD21	2:B:314:PRO:HD3	1.27	0.99
2:D:124:VAL:HG21	3:G:58:MET:HE2	1.41	0.99
3:F:242:ALA:O	3:F:246:LYS:HG2	1.62	0.98
1:A:97:ARG:NH2	1:A:99:TYR:OH	1.95	0.98
9:G:7292:ATP:H5'2	3:H:156:MET:SD	2.02	0.98
1:A:124:VAL:HG21	3:F:58:MET:HE2	1.43	0.98
1:C:75:ILE:HG21	1:C:78:MET:HE3	1.46	0.97
1:C:253:TRP:CZ3	1:C:282:ILE:HD13	1.99	0.97
1:C:253:TRP:HZ3	1:C:282:ILE:HD13	1.25	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:CG2	1:A:360:PRO:HD3	1.93	0.97
2:B:220:SER:HB2	2:B:286:ASN:HB3	1.41	0.97
3:E:4:GLN:NE2	3:E:143:LYS:O	1.98	0.97
2:B:260:VAL:HG22	2:B:273:ALA:O	1.64	0.96
1:A:167:SER:HB2	1:A:180:PRO:HG3	1.46	0.96
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.48	0.96
3:E:56:THR:HG23	3:E:59:GLU:HB3	1.46	0.96
1:A:355:ILE:HG23	1:A:356:GLY:N	1.74	0.95
1:C:389:ARG:HH11	1:C:389:ARG:HG3	1.30	0.95
1:A:229:TYR:HA	1:A:254:SER:O	1.68	0.94
1:C:355:ILE:HG22	1:C:356:GLY:H	0.79	0.94
1:A:27:ASP:O	1:A:30:LYS:HG2	1.67	0.94
1:A:346:LEU:HD12	1:A:370:LEU:HD12	1.47	0.94
1:C:59:ILE:HG23	1:C:426:LYS:HD2	1.48	0.94
3:G:217:VAL:HG21	9:G:7292:ATP:H2	1.32	0.94
2:B:206:ARG:HG3	2:B:304:PHE:CZ	2.02	0.93
3:F:56:THR:O	3:F:60:MET:HB2	1.67	0.93
1:C:433:LYS:NZ	2:D:263:THR:CG2	2.31	0.93
1:A:355:ILE:CG2	1:A:356:GLY:N	2.31	0.93
3:E:35:ILE:CD1	3:E:48:ILE:HD12	1.98	0.93
1:C:209:LYS:HE2	1:C:263:GLU:OE1	1.69	0.93
3:G:189:THR:HG22	3:G:190:ASP:H	1.33	0.92
2:B:85:THR:CG2	2:B:146:MET:HE2	1.98	0.92
1:A:355:ILE:CG2	1:A:356:GLY:H	1.78	0.92
2:B:118:MET:HE3	2:B:127:GLY:HA3	1.51	0.92
3:F:13:ILE:O	3:F:187:ARG:NH2	2.03	0.92
3:F:186:SER:HB3	3:F:210:PHE:CZ	2.04	0.91
1:C:426:LYS:NZ	2:D:97:ALA:HB1	1.84	0.91
1:C:342:TYR:O	1:C:345:ARG:HG3	1.70	0.91
2:D:91:GLY:HA2	2:D:118:MET:HE3	0.91	0.91
2:D:220:SER:HB2	2:D:286:ASN:HB3	1.49	0.91
2:B:85:THR:HG22	2:B:146:MET:HB3	1.53	0.91
1:A:218:SER:OG	1:A:269:LYS:HE2	1.72	0.90
2:B:238:ARG:HE	2:B:258:GLU:CG	1.85	0.90
2:B:142:TYR:O	2:B:144:PRO:HD3	1.70	0.90
3:F:42:ALA:HA	3:F:87:GLU:OE1	1.72	0.90
2:D:471:PHE:CD2	2:D:472:PRO:HD3	2.07	0.89
1:C:355:ILE:HD12	1:C:359:ARG:HB2	1.52	0.89
2:D:3:GLN:HA	2:D:3:GLN:HE21	1.38	0.89
3:E:158:MET:HE1	3:E:195:LEU:HG	1.55	0.89
2:B:3:GLN:HE21	2:B:3:GLN:HA	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TYR:OH	1:C:408:GLU:HG2	1.72	0.88
1:C:433:LYS:HZ1	2:D:263:THR:HG23	1.37	0.88
1:A:405:THR:OG1	1:A:408:GLU:HG3	1.74	0.88
1:C:138:VAL:HG13	2:D:62:LEU:HD13	1.53	0.88
2:B:457:HIS:HD2	2:D:512:MET:HB3	1.39	0.87
1:A:182:ARG:O	1:A:197:ILE:HG21	1.74	0.87
2:B:77:LEU:HA	2:B:80:LEU:HD12	1.56	0.87
1:A:167:SER:CB	1:A:180:PRO:HG3	2.04	0.87
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.56	0.87
1:A:355:ILE:HG21	1:A:360:PRO:HD3	1.55	0.87
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.57	0.87
2:B:512:MET:HB3	2:D:457:HIS:HD2	1.38	0.86
1:A:20:TYR:OH	1:A:408:GLU:HG2	1.74	0.86
2:B:517:TYR:O	1:C:99:TYR:CE1	2.28	0.86
2:B:90:HIS:N	2:B:150:SER:O	2.07	0.86
2:B:90:HIS:HA	2:B:116:ASP:OD1	1.74	0.86
2:D:64:VAL:O	2:D:426:ASP:OD1	1.94	0.86
2:D:85:THR:HG22	2:D:146:MET:HB3	1.55	0.86
3:F:241:ARG:O	3:F:245:ARG:HG3	1.76	0.86
2:B:130:ASN:ND2	2:B:130:ASN:H	1.70	0.85
1:C:57:MET:HE1	2:D:100:ARG:CZ	2.06	0.85
1:C:71:VAL:HG11	1:C:198:ALA:HB1	1.58	0.85
3:G:243:LEU:O	3:G:247:VAL:HG23	1.77	0.85
2:B:350:ARG:HG2	2:D:264:PRO:HG3	1.59	0.85
3:F:13:ILE:HA	3:F:187:ARG:HH21	1.42	0.85
2:D:496:THR:O	2:D:500:SER:OG	1.95	0.84
1:A:277:ARG:CZ	1:A:383:HIS:CD2	2.60	0.84
2:D:260:VAL:HG23	2:D:273:ALA:O	1.77	0.84
1:A:58:THR:HG22	1:A:60:ARG:H	1.42	0.84
3:F:158:MET:HE1	3:F:195:LEU:HG	1.59	0.84
3:H:26:LEU:HD12	3:H:29:MET:HE3	1.59	0.84
1:A:388:ASP:OD1	1:A:389:ARG:HG3	1.78	0.84
2:B:206:ARG:HG3	2:B:304:PHE:CE1	2.13	0.84
2:B:161:ASP:O	2:B:165:PHE:CD1	2.31	0.84
2:B:397:ASN:H	2:B:397:ASN:HD22	1.24	0.84
1:A:219:THR:HG22	1:A:221:TYR:H	1.42	0.84
1:C:27:ASP:O	1:C:30:LYS:HG3	1.77	0.84
2:D:238:ARG:HE	2:D:258:GLU:CG	1.90	0.84
2:D:362:LEU:HD11	2:D:498:VAL:HG22	1.59	0.84
3:H:54:GLN:HG3	3:H:55:ASN:H	1.43	0.83
3:G:217:VAL:HG22	3:G:227:VAL:HG21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:CG2	3:H:58:MET:HE2	2.04	0.83
2:D:397:ASN:H	2:D:397:ASN:HD22	1.26	0.83
1:A:97:ARG:HH21	2:D:520:ASP:CG	1.86	0.83
3:G:42:ALA:HA	3:G:87:GLU:OE1	1.78	0.83
2:D:86:MET:HE3	2:D:87:PRO:CD	2.09	0.83
3:E:37:GLY:HA3	3:E:87:GLU:OE2	1.78	0.83
2:B:289:ASN:ND2	2:B:314:PRO:HD3	1.93	0.83
2:B:331:LYS:O	2:B:335:ILE:HG12	1.79	0.83
1:C:182:ARG:O	1:C:197:ILE:HG21	1.78	0.83
1:C:449:PRO:HG2	2:D:15:PHE:HZ	1.43	0.83
2:B:220:SER:N	2:B:286:ASN:O	2.11	0.83
1:C:234:ASP:HB3	1:C:451:HIS:CG	2.14	0.83
2:D:86:MET:HE3	2:D:87:PRO:HD2	1.58	0.83
3:G:241:ARG:O	3:G:245:ARG:HG3	1.79	0.83
1:A:385:ASP:O	1:A:388:ASP:OD1	1.96	0.82
2:D:452:GLN:NE2	2:D:465:PRO:HA	1.94	0.82
1:A:343:ARG:O	1:A:347:GLU:HG3	1.80	0.82
3:F:106:ILE:HD11	3:F:138:PRO:HD3	1.61	0.82
1:C:219:THR:HG22	1:C:221:TYR:H	1.42	0.82
2:B:142:TYR:C	2:B:144:PRO:HD3	2.05	0.82
1:C:167:SER:HB2	1:C:180:PRO:CG	2.08	0.82
3:E:12:GLY:HA2	3:F:156:MET:CE	2.09	0.82
1:C:405:THR:OG1	1:C:408:GLU:HG3	1.79	0.82
2:B:452:GLN:NE2	2:B:465:PRO:HA	1.95	0.82
1:C:298:ASN:HB2	1:C:362:HIS:HE2	1.43	0.82
1:C:57:MET:CE	2:D:100:ARG:NH2	2.44	0.81
2:D:326:ASP:OD2	2:D:348:ARG:HD2	1.81	0.81
3:G:37:GLY:HA3	3:G:87:GLU:OE2	1.80	0.81
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.43	0.81
2:D:161:ASP:O	2:D:165:PHE:CD1	2.34	0.81
2:D:130:ASN:H	2:D:130:ASN:ND2	1.79	0.81
2:B:197:TRP:CE3	2:B:229:GLY:HA2	2.15	0.80
3:H:56:THR:O	3:H:60:MET:HB2	1.81	0.80
2:B:59:ARG:NH2	2:B:429:HIS:CE1	2.50	0.80
1:C:210:ARG:HH11	1:C:264:LEU:HD21	1.46	0.80
1:A:355:ILE:HG22	1:A:360:PRO:CG	2.11	0.80
2:B:59:ARG:HH22	2:B:429:HIS:CE1	2.00	0.80
3:H:137:MET:HB3	3:H:138:PRO:HD3	1.63	0.80
1:A:234:ASP:HB3	1:A:451:HIS:CG	2.17	0.80
1:C:186:PHE:HE1	3:G:100:ARG:HH21	1.29	0.80
2:D:238:ARG:HD3	2:D:258:GLU:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:CG2	2:D:186:THR:H	1.94	0.80
3:H:231:ASP:OD2	3:H:234:ALA:HB2	1.81	0.80
3:H:244:ALA:O	3:H:248:VAL:HG23	1.82	0.80
1:A:355:ILE:HG21	1:A:360:PRO:CD	2.09	0.79
2:B:158:ILE:O	3:F:133:GLY:HA3	1.81	0.79
3:H:106:ILE:CD1	3:H:138:PRO:HD3	2.12	0.79
1:C:97:ARG:NH1	1:C:446:TYR:HA	1.96	0.79
3:G:49:LEU:O	3:G:50:HIS:HB2	1.80	0.79
1:C:59:ILE:HD13	1:C:427:GLU:OE2	1.82	0.79
1:A:31:HIS:O	1:A:46:ILE:HD11	1.83	0.79
1:C:170:LYS:O	1:C:178:ILE:HD12	1.82	0.79
3:F:43:ASP:HB2	3:F:46:ARG:HD3	1.62	0.79
2:D:305:VAL:HG13	2:D:309:TRP:CE3	2.17	0.79
3:F:204:GLY:O	3:F:254:VAL:HG21	1.83	0.79
2:B:151:THR:OG1	2:B:155:ALA:HB3	1.82	0.78
2:D:369:LEU:HD21	2:D:393:ILE:HG12	1.65	0.78
2:D:238:ARG:CD	2:D:258:GLU:HG3	2.13	0.78
3:E:35:ILE:HD11	3:E:48:ILE:HD12	1.65	0.78
2:D:238:ARG:NE	2:D:258:GLU:HG3	1.98	0.78
3:E:61:ALA:HB2	3:E:70:LEU:HD12	1.64	0.78
2:B:65:ASN:O	2:B:427:LEU:HB2	1.82	0.78
2:B:496:THR:O	2:B:500:SER:OG	2.00	0.78
2:D:77:LEU:HA	2:D:80:LEU:HD12	1.66	0.78
2:D:131:MET:HE1	2:D:149:VAL:HG11	1.64	0.78
1:C:167:SER:CB	1:C:180:PRO:CG	2.61	0.78
1:C:389:ARG:HH11	1:C:389:ARG:CG	1.97	0.78
1:C:58:THR:HG22	1:C:60:ARG:N	1.97	0.78
1:C:298:ASN:HD22	1:C:299:PHE:N	1.81	0.78
1:C:433:LYS:HZ3	2:D:263:THR:CG2	1.95	0.78
3:H:49:LEU:O	3:H:50:HIS:HB2	1.84	0.78
1:C:57:MET:HE1	2:D:100:ARG:NH2	1.99	0.78
2:B:279:GLU:OE1	2:B:282:LYS:HD2	1.83	0.78
2:D:128:GLN:HE22	2:D:168:ASN:HD22	1.31	0.78
2:D:233:TYR:HB2	2:D:236:ASN:HD22	1.50	0.77
2:D:91:GLY:CA	2:D:118:MET:CE	2.52	0.77
1:A:433:LYS:NZ	2:B:263:THR:O	2.17	0.77
1:C:71:VAL:HG22	1:C:279:MET:HE1	1.65	0.77
1:A:59:ILE:HG23	1:A:426:LYS:HD2	1.65	0.77
1:A:355:ILE:CG2	1:A:360:PRO:HD2	2.14	0.77
1:C:355:ILE:HD11	1:C:441:MET:HB3	1.67	0.77
1:A:199:ASN:HD21	1:A:279:MET:HE3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:94:GLY:O	3:E:95:VAL:HG23	1.85	0.77
1:A:429:PHE:CB	2:B:110:PRO:HD3	2.15	0.77
1:A:465:MET:O	1:A:469:ASN:HB2	1.85	0.77
1:C:75:ILE:HG21	1:C:78:MET:CE	2.15	0.77
1:C:355:ILE:HB	1:C:360:PRO:CD	2.14	0.77
1:C:355:ILE:HB	1:C:360:PRO:HG3	1.65	0.77
2:B:329:LEU:HD13	2:B:344:LEU:HD13	1.65	0.76
1:C:40:THR:HG22	1:C:40:THR:O	1.86	0.76
2:D:217:VAL:HB	2:D:220:SER:OG	1.84	0.76
1:C:193:LEU:O	1:C:197:ILE:HG13	1.84	0.76
2:D:397:ASN:H	2:D:397:ASN:ND2	1.79	0.76
1:C:385:ASP:HA	1:C:388:ASP:OD2	1.85	0.76
1:A:251:ALA:HA	1:A:261:GLU:HG2	1.65	0.76
1:C:131:LEU:O	1:C:135:ILE:HG13	1.86	0.76
1:C:433:LYS:HZ1	2:D:263:THR:CG2	1.95	0.76
1:A:71:VAL:HG11	1:A:198:ALA:HB1	1.68	0.76
2:D:86:MET:HE2	2:D:87:PRO:HD2	1.66	0.76
2:D:262:ASP:O	2:D:264:PRO:HD3	1.85	0.76
1:A:75:ILE:CG2	1:A:78:MET:HE3	2.14	0.76
2:B:369:LEU:HD12	2:B:379:LEU:HD23	1.67	0.76
2:D:116:ASP:HB2	2:D:130:ASN:HB2	1.68	0.75
2:D:329:LEU:HD13	2:D:344:LEU:HD13	1.68	0.75
1:A:355:ILE:HG22	1:A:360:PRO:HD2	1.67	0.75
3:H:186:SER:HB3	3:H:210:PHE:CZ	2.22	0.75
1:C:30:LYS:NZ	1:C:47:ILE:HD13	2.02	0.75
3:H:166:LYS:O	3:H:169:VAL:HG12	1.86	0.75
2:B:197:TRP:CZ3	2:B:229:GLY:HA2	2.22	0.75
2:D:46:TRP:O	2:D:49:THR:HG22	1.86	0.75
2:B:170:LYS:HD2	2:B:177:ASP:HA	1.69	0.75
2:D:49:THR:HG23	2:D:52:TYR:H	1.52	0.75
3:G:56:THR:O	3:G:60:MET:HB2	1.87	0.75
1:A:429:PHE:HB3	2:B:110:PRO:HD3	1.69	0.74
1:A:388:ASP:OD1	1:A:389:ARG:N	2.20	0.74
1:C:355:ILE:HB	1:C:360:PRO:CG	2.17	0.74
1:A:359:ARG:HH11	1:A:359:ARG:HG3	1.50	0.74
2:B:131:MET:HE1	2:B:149:VAL:HG11	1.69	0.74
2:B:397:ASN:H	2:B:397:ASN:ND2	1.79	0.74
2:B:512:MET:HE2	2:D:457:HIS:CB	2.16	0.74
3:G:56:THR:HG23	3:G:59:GLU:CB	2.17	0.74
3:H:141:GLU:O	3:H:142:ASN:HB2	1.86	0.74
3:G:181:GLY:HA2	3:G:205:THR:OG1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:GLN:NE2	2:B:132:LYS:HD2	2.03	0.74
1:C:57:MET:CE	2:D:100:ARG:CZ	2.65	0.74
2:D:68:LYS:HG2	2:D:396:HIS:HD2	1.52	0.74
2:B:217:VAL:HB	2:B:220:SER:OG	1.87	0.74
1:C:251:ALA:HA	1:C:261:GLU:HG2	1.70	0.74
3:F:206:GLN:NE2	3:F:250:ASN:OD1	2.21	0.74
3:H:55:ASN:HB3	3:H:60:MET:SD	2.27	0.74
2:B:233:TYR:HB2	2:B:236:ASN:HD22	1.52	0.74
2:D:170:LYS:HD2	2:D:177:ASP:HA	1.70	0.74
3:F:56:THR:HG23	3:F:59:GLU:HB2	1.70	0.74
1:C:31:HIS:O	1:C:46:ILE:HD11	1.88	0.73
1:A:276:TYR:HB3	1:A:361:ARG:HH22	1.53	0.73
2:B:128:GLN:O	2:B:132:LYS:HG3	1.88	0.73
2:D:28:ARG:HA	2:D:32:GLU:HG3	1.69	0.73
2:D:65:ASN:O	2:D:427:LEU:HB2	1.89	0.73
3:H:106:ILE:HD13	3:H:138:PRO:HD3	1.71	0.73
1:A:131:LEU:O	1:A:135:ILE:HG13	1.88	0.73
3:H:60:MET:HB3	3:H:70:LEU:HD11	1.69	0.73
1:A:360:PRO:HB2	1:A:379:TYR:CE2	2.24	0.73
2:B:151:THR:CG2	2:B:186:THR:H	2.01	0.73
1:C:56:LEU:O	1:C:57:MET:HB2	1.87	0.73
1:A:210:ARG:HH11	1:A:264:LEU:HD21	1.52	0.73
1:A:280:ASN:HD22	1:A:280:ASN:N	1.86	0.73
3:F:183:ILE:HD13	3:F:243:LEU:HD11	1.70	0.73
2:B:178:GLU:O	2:B:180:PRO:HD3	1.89	0.73
1:C:116:SER:O	1:C:130:LYS:HE2	1.86	0.73
1:C:355:ILE:HD12	1:C:359:ARG:CB	2.18	0.73
2:B:238:ARG:HE	2:B:258:GLU:HG2	1.53	0.73
3:F:110:GLU:OE2	3:F:143:LYS:NZ	2.22	0.73
3:G:23:VAL:HG21	3:G:35:ILE:HD11	1.70	0.73
1:C:86:VAL:HG21	2:D:68:LYS:HE3	1.71	0.73
3:E:57:ILE:HG12	3:E:75:VAL:HG21	1.71	0.73
2:B:124:VAL:CG2	3:E:58:MET:HE2	2.19	0.72
3:F:49:LEU:O	3:F:50:HIS:HB2	1.89	0.72
3:F:207:MET:CE	3:F:210:PHE:HB2	2.20	0.72
3:G:106:ILE:HD12	3:G:137:MET:HB3	1.71	0.72
2:B:305:VAL:HG13	2:B:309:TRP:CE3	2.23	0.72
2:D:238:ARG:HE	2:D:258:GLU:HG3	1.50	0.72
3:F:23:VAL:HG21	3:F:35:ILE:HD11	1.71	0.72
2:B:422:TYR:HD2	2:B:425:LYS:HZ2	1.36	0.72
1:C:209:LYS:HE2	1:C:263:GLU:CD	2.12	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:GLN:HG3	3:F:55:ASN:H	1.54	0.72
3:H:39:ASP:OD1	3:H:40:PRO:HD2	1.88	0.72
3:E:57:ILE:HG13	3:E:75:VAL:HG11	1.71	0.72
3:G:22:LEU:HD11	3:G:247:VAL:HG21	1.72	0.72
2:B:512:MET:CB	2:D:457:HIS:HD2	2.02	0.72
1:C:280:ASN:HD22	1:C:280:ASN:N	1.87	0.72
1:C:433:LYS:HZ3	2:D:263:THR:HG23	1.53	0.72
2:D:260:VAL:CG2	2:D:273:ALA:O	2.36	0.72
2:B:362:LEU:HD11	2:B:498:VAL:HG22	1.72	0.72
2:D:124:VAL:HG11	3:G:58:MET:HG3	1.71	0.72
2:D:146:MET:CG	2:D:180:PRO:HB2	2.19	0.72
2:B:14:LEU:HD12	2:B:14:LEU:O	1.90	0.72
2:B:139:LYS:HG3	2:B:179:PHE:CE1	2.25	0.72
1:A:193:LEU:O	1:A:197:ILE:HG13	1.89	0.72
2:D:12:TYR:CD2	2:D:13:PRO:HD3	2.25	0.72
3:F:13:ILE:CA	3:F:187:ARG:HH21	2.03	0.72
1:A:151:GLN:NE2	1:A:181:VAL:HG11	2.04	0.71
2:B:49:THR:HG23	2:B:52:TYR:H	1.53	0.71
2:B:238:ARG:NE	2:B:258:GLU:HG3	2.05	0.71
1:C:15:GLU:O	1:C:18:GLU:HB2	1.90	0.71
2:D:301:THR:O	2:D:305:VAL:HG23	1.89	0.71
1:C:280:ASN:ND2	1:C:281:TYR:H	1.88	0.71
1:A:277:ARG:NE	1:A:383:HIS:CD2	2.58	0.71
2:B:301:THR:O	2:B:305:VAL:HG23	1.89	0.71
2:D:283:ASP:OD1	2:D:283:ASP:O	2.08	0.71
3:E:56:THR:O	3:E:60:MET:HB2	1.91	0.71
1:A:128:ASP:HB3	1:A:166:VAL:HG21	1.70	0.71
1:A:138:VAL:HG21	1:A:148:ILE:CD1	2.20	0.71
1:A:258:SER:HB2	1:A:261:GLU:HB2	1.72	0.71
1:A:479:TRP:HZ3	2:D:326:ASP:HB3	1.53	0.71
3:E:204:GLY:O	3:E:254:VAL:HG21	1.89	0.71
2:B:302:LYS:HE2	2:B:306:GLU:OE2	1.91	0.71
1:A:58:THR:HG22	1:A:60:ARG:N	2.03	0.71
1:A:98:ASN:ND2	1:A:98:ASN:H	1.89	0.71
2:D:124:VAL:CG2	3:G:58:MET:HE2	2.20	0.71
3:G:115:TYR:C	3:G:117:ASP:H	1.97	0.71
3:G:141:GLU:O	3:G:142:ASN:HB2	1.90	0.71
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.72	0.71
2:B:346:LYS:HG3	2:D:264:PRO:HG2	1.73	0.71
1:C:98:ASN:ND2	1:C:98:ASN:H	1.87	0.71
3:G:217:VAL:CG2	9:G:7292:ATP:H2	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ASP:OD2	2:D:350:ARG:NE	2.24	0.71
3:F:60:MET:HB3	3:F:70:LEU:HD11	1.72	0.71
3:G:56:THR:CG2	3:G:59:GLU:HB2	2.19	0.71
2:D:130:ASN:ND2	2:D:130:ASN:N	2.39	0.70
3:F:55:ASN:HB3	3:F:60:MET:SD	2.31	0.70
1:C:360:PRO:HB2	1:C:379:TYR:CE2	2.26	0.70
1:C:430:ILE:HG12	2:D:269:PHE:CE1	2.26	0.70
2:D:146:MET:CE	2:D:208:PHE:CZ	2.73	0.70
3:F:195:LEU:HD21	3:F:268:LEU:HD23	1.73	0.70
1:C:138:VAL:HG21	1:C:148:ILE:CD1	2.21	0.70
1:A:75:ILE:HG21	1:A:78:MET:CE	2.14	0.70
2:B:45:GLN:O	2:B:48:THR:HG22	1.91	0.70
2:D:86:MET:HE3	2:D:86:MET:HA	1.74	0.70
1:C:159:ILE:HD12	3:H:97:CYS:HB2	1.72	0.70
2:D:292:LEU:O	2:D:295:PRO:HD3	1.90	0.70
3:G:259:ILE:HD12	3:G:264:LEU:HD23	1.72	0.70
1:A:298:ASN:HB2	1:A:362:HIS:NE2	2.07	0.70
1:A:352:MET:HB3	1:A:421:ILE:HG23	1.74	0.70
1:C:346:LEU:CD1	1:C:372:MET:SD	2.79	0.70
3:F:244:ALA:O	3:F:248:VAL:HG23	1.92	0.70
2:B:46:TRP:O	2:B:49:THR:HG22	1.92	0.70
1:C:68:LYS:C	1:C:68:LYS:HD3	2.17	0.70
1:C:355:ILE:CG2	5:C:3496:CFM:S3A	2.80	0.70
1:C:425:ILE:HG22	4:C:3494:HCA:C6	2.21	0.70
1:C:465:MET:O	1:C:469:ASN:HB2	1.92	0.70
2:B:238:ARG:CD	2:B:258:GLU:HG3	2.22	0.70
2:D:96:VAL:HG13	2:D:113:CYS:SG	2.32	0.70
3:E:23:VAL:HG12	3:E:33:VAL:HG11	1.73	0.70
2:B:512:MET:HE2	2:D:457:HIS:CG	2.26	0.70
2:D:142:TYR:O	2:D:144:PRO:HD3	1.90	0.70
3:E:35:ILE:HD12	3:E:48:ILE:HD12	1.73	0.70
3:G:224:ARG:O	3:G:225:MET:HG2	1.92	0.70
1:A:35:ASN:HB2	1:A:400:LEU:HD11	1.74	0.69
1:A:350:ARG:HH11	1:A:375:VAL:HG11	1.56	0.69
1:C:30:LYS:HZ2	1:C:47:ILE:HD13	1.55	0.69
1:C:75:ILE:CG2	1:C:78:MET:HE3	2.20	0.69
3:H:223:ARG:O	3:H:223:ARG:HG2	1.91	0.69
2:B:238:ARG:NE	2:B:258:GLU:CG	2.55	0.69
1:C:355:ILE:HG22	5:C:3496:CFM:S3A	2.31	0.69
2:D:128:GLN:HE22	2:D:168:ASN:ND2	1.89	0.69
1:C:298:ASN:HB2	1:C:362:HIS:NE2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:GLN:O	2:D:48:THR:HG22	1.92	0.69
2:D:403:LYS:NZ	2:D:421:VAL:HB	2.07	0.69
2:D:142:TYR:C	2:D:144:PRO:HD3	2.18	0.69
3:E:11:GLY:HA2	9:E:5292:ATP:O1G	1.93	0.69
3:F:207:MET:HE1	3:F:210:PHE:HB2	1.74	0.69
1:A:86:VAL:CG1	2:B:68:LYS:HE3	2.19	0.69
1:C:134:LEU:HD12	2:D:61:ALA:O	1.92	0.69
2:D:394:LEU:HD23	2:D:395:CYS:N	2.07	0.69
3:G:156:MET:SD	9:H:8292:ATP:H4'	2.32	0.69
1:A:116:SER:O	1:A:130:LYS:HE2	1.93	0.69
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.27	0.69
2:B:124:VAL:HG11	3:E:58:MET:HG3	1.74	0.69
3:G:224:ARG:C	3:G:225:MET:HG2	2.16	0.69
3:H:56:THR:HG23	3:H:59:GLU:CB	2.22	0.69
2:D:146:MET:HG3	2:D:180:PRO:CB	2.21	0.69
1:A:64:TYR:CE2	1:A:88:CYS:HB3	2.28	0.69
1:A:421:ILE:HD11	1:A:436:ILE:HG21	1.75	0.69
1:A:446:TYR:CE2	2:D:522:VAL:HG23	2.28	0.68
2:B:59:ARG:NH2	2:B:426:ASP:OD2	2.26	0.68
3:H:250:ASN:C	3:H:250:ASN:HD22	2.00	0.68
1:A:99:TYR:CE1	2:D:517:TYR:O	2.47	0.68
1:C:274:HIS:O	1:C:358:LEU:HD11	1.93	0.68
3:E:12:GLY:HA2	3:F:156:MET:HE1	1.74	0.68
2:B:130:ASN:H	2:B:130:ASN:HD22	1.41	0.68
3:H:50:HIS:O	3:H:51:SER:HB3	1.94	0.68
1:C:62:CYS:O	1:C:191:GLN:HA	1.94	0.68
1:C:154:CYS:HB2	1:C:155:PRO:CD	2.23	0.68
1:C:449:PRO:HG2	2:D:15:PHE:CZ	2.28	0.68
2:D:322:LEU:O	2:D:326:ASP:OD1	2.12	0.68
3:E:181:GLY:HA2	3:E:205:THR:OG1	1.93	0.68
3:G:192:GLU:HB3	3:G:210:PHE:HE2	1.58	0.68
3:F:26:LEU:HD12	3:F:29:MET:CE	2.23	0.68
3:H:57:ILE:HG12	3:H:75:VAL:HG21	1.75	0.68
1:A:189:VAL:HG23	1:A:190:SER:N	2.08	0.68
1:C:48:SER:HB3	1:C:402:ASP:OD2	1.94	0.68
2:B:238:ARG:HE	2:B:258:GLU:HG3	1.59	0.68
1:C:287:GLU:O	1:C:291:GLY:HA2	1.93	0.68
3:E:23:VAL:HG21	3:E:35:ILE:HD11	1.76	0.68
1:C:359:ARG:HH11	1:C:359:ARG:HG3	1.58	0.68
2:B:118:MET:HB3	2:B:154:MET:HE3	1.76	0.68
2:B:517:TYR:O	1:C:99:TYR:CD1	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LYS:HD3	1:C:68:LYS:O	1.94	0.68
1:C:74:PRO:HG3	1:C:98:ASN:OD1	1.94	0.68
1:C:343:ARG:O	1:C:347:GLU:HG3	1.94	0.68
1:A:74:PRO:HG3	1:A:98:ASN:OD1	1.94	0.67
1:A:280:ASN:ND2	1:A:281:TYR:H	1.92	0.67
1:C:355:ILE:CB	1:C:360:PRO:HD3	2.24	0.67
1:A:449:PRO:HG2	2:B:15:PHE:HZ	1.58	0.67
2:D:222:LYS:HA	2:D:288:LEU:HD21	1.77	0.67
1:A:367:TYR:CD2	1:A:372:MET:HE3	2.30	0.67
1:C:137:GLU:OE1	2:D:59:ARG:HG3	1.94	0.67
1:C:404:VAL:HG23	1:C:408:GLU:HB2	1.77	0.67
1:A:346:LEU:HD12	1:A:370:LEU:CD1	2.21	0.67
1:A:441:MET:SD	1:A:444:TRP:HZ3	2.17	0.67
2:B:91:GLY:HA2	2:B:118:MET:SD	2.34	0.67
2:B:326:ASP:HB3	1:C:479:TRP:HZ3	1.58	0.67
1:C:253:TRP:CZ3	1:C:282:ILE:CD1	2.76	0.67
2:D:375:PHE:HE2	2:D:470:GLY:HA2	1.59	0.67
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.29	0.67
3:E:10:LYS:H	3:E:13:ILE:CD1	2.08	0.67
3:E:171:TYR:OH	3:F:94:GLY:O	2.10	0.67
3:E:195:LEU:HD21	3:E:268:LEU:HD23	1.77	0.67
1:A:124:VAL:CG2	3:F:58:MET:HE2	2.23	0.67
2:B:314:PRO:HB3	2:B:316:LEU:HD13	1.75	0.67
2:D:146:MET:HE2	2:D:208:PHE:CZ	2.29	0.67
3:E:54:GLN:HG2	3:E:77:LYS:HZ2	1.59	0.67
1:C:275:CYS:HA	1:C:358:LEU:HD13	1.75	0.67
1:C:332:LYS:O	1:C:336:GLU:HG3	1.94	0.67
1:C:352:MET:HB3	1:C:421:ILE:HG23	1.77	0.67
2:D:225:ASN:HB2	2:D:290:THR:HA	1.77	0.67
3:E:185:ASN:HA	3:E:211:VAL:HB	1.76	0.67
2:B:130:ASN:ND2	2:B:130:ASN:N	2.40	0.67
1:A:168:LYS:O	1:A:172:ALA:HB2	1.94	0.67
1:C:186:PHE:CB	2:D:154:MET:HE1	2.25	0.67
1:C:229:TYR:HA	1:C:254:SER:O	1.93	0.67
1:A:178:ILE:O	1:A:180:PRO:HD3	1.95	0.67
3:E:13:ILE:O	3:E:185:ASN:ND2	2.28	0.67
1:C:271:ASN:OD1	1:C:286:MET:HE2	1.95	0.66
2:D:294:GLN:HB3	2:D:374:ASP:OD2	1.94	0.66
3:F:37:GLY:HA3	3:F:87:GLU:OE2	1.95	0.66
1:A:97:ARG:NH2	2:D:520:ASP:OD2	2.28	0.66
1:C:144:LEU:CG	2:D:43:VAL:HG21	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:THR:HB	1:C:266:PRO:HD3	1.78	0.66
3:E:35:ILE:HD11	3:E:48:ILE:CD1	2.24	0.66
1:A:14:GLN:O	1:A:18:GLU:HG3	1.95	0.66
1:A:359:ARG:HG3	1:A:359:ARG:NH1	2.08	0.66
1:A:444:TRP:HA	1:A:444:TRP:CE3	2.28	0.66
2:D:88:TYR:HB2	2:D:147:ILE:HG22	1.77	0.66
2:B:213:MET:HE2	2:B:308:THR:O	1.96	0.66
1:C:298:ASN:CG	1:C:362:HIS:CD2	2.74	0.66
3:F:26:LEU:HD12	3:F:29:MET:HE3	1.77	0.66
1:A:97:ARG:NH1	1:A:446:TYR:HA	2.10	0.66
1:A:239:ARG:HG3	1:A:249:CYS:SG	2.36	0.66
2:D:81:GLY:HA2	2:D:257:PRO:HD3	1.78	0.66
2:B:37:GLN:HG3	2:B:41:ASP:OD1	1.95	0.66
1:C:433:LYS:NZ	2:D:263:THR:O	2.28	0.66
2:D:37:GLN:HG3	2:D:41:ASP:OD1	1.95	0.66
2:D:220:SER:N	2:D:286:ASN:O	2.28	0.66
2:D:107:PHE:CE2	2:D:261:LEU:HD23	2.31	0.66
1:C:230:ASN:HB2	1:C:235:ALA:CB	2.25	0.66
1:C:235:ALA:HB1	1:C:252:GLN:HE21	1.61	0.66
2:D:146:MET:CE	2:D:208:PHE:CE1	2.79	0.66
3:H:45:THR:HG21	3:H:85:CYS:HB3	1.77	0.66
1:A:303:THR:HG22	1:A:369:ASP:OD1	1.95	0.66
1:C:99:TYR:CE2	1:C:232:GLY:HA2	2.31	0.66
1:C:210:ARG:NH1	1:C:264:LEU:HD21	2.10	0.66
1:C:302:PRO:HD3	1:C:456:PHE:CG	2.30	0.66
1:C:303:THR:HG22	1:C:369:ASP:OD1	1.95	0.66
3:G:179:LEU:HD12	3:G:256:PRO:HG3	1.78	0.66
1:A:425:ILE:HD11	2:B:105:ARG:HG2	1.78	0.66
2:B:107:PHE:CE2	2:B:261:LEU:HD23	2.31	0.66
1:C:85:PRO:HG3	2:D:189:PHE:HB3	1.77	0.66
2:D:91:GLY:HA2	2:D:118:MET:HE2	1.75	0.66
3:G:231:ASP:OD2	3:G:234:ALA:HB2	1.95	0.66
3:H:86:VAL:HG21	3:H:109:LEU:HD11	1.78	0.66
1:C:138:VAL:HG21	1:C:148:ILE:HD11	1.78	0.65
3:E:2:MET:HB2	3:E:119:LEU:O	1.95	0.65
3:G:57:ILE:CG1	3:G:75:VAL:HG11	2.26	0.65
1:A:138:VAL:HG21	1:A:148:ILE:HD11	1.78	0.65
1:A:401:TYR:HB2	1:A:404:VAL:HB	1.77	0.65
3:F:106:ILE:HD12	3:F:138:PRO:HD3	1.78	0.65
3:H:137:MET:HB3	3:H:138:PRO:CD	2.25	0.65
2:B:89:VAL:HG22	2:B:150:SER:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ALA:O	2:B:168:ASN:ND2	2.28	0.65
3:G:61:ALA:HB2	3:G:70:LEU:HD12	1.78	0.65
2:D:213:MET:HE2	2:D:308:THR:O	1.97	0.65
2:D:302:LYS:HE2	2:D:306:GLU:OE2	1.97	0.65
3:F:189:THR:OG1	3:F:192:GLU:HB2	1.95	0.65
1:A:76:LYS:O	1:A:108:ALA:HA	1.95	0.65
1:A:417:LYS:N	1:A:418:PRO:HD3	2.12	0.65
2:B:47:THR:HA	2:B:52:TYR:CG	2.32	0.65
1:A:58:THR:HG21	1:A:60:ARG:HB2	1.77	0.65
3:F:57:ILE:HG12	3:F:75:VAL:HG21	1.78	0.65
3:G:87:GLU:OE2	3:G:87:GLU:HA	1.97	0.65
1:C:35:ASN:HB2	1:C:400:LEU:HD11	1.79	0.65
2:D:146:MET:HA	2:D:179:PHE:HE2	1.61	0.65
2:D:260:VAL:HG22	2:D:273:ALA:H	1.60	0.65
2:D:284:ALA:HB3	2:D:285:PRO:HD3	1.79	0.65
2:B:130:ASN:HD22	2:B:130:ASN:N	1.94	0.65
1:C:350:ARG:HH11	1:C:375:VAL:HG11	1.61	0.65
2:D:56:ASN:O	2:D:59:ARG:HB2	1.97	0.65
3:F:2:MET:HB2	3:F:119:LEU:O	1.97	0.65
1:C:404:VAL:CG2	1:C:408:GLU:HB2	2.27	0.64
3:E:207:MET:CE	3:E:210:PHE:HB2	2.25	0.64
3:G:189:THR:HG22	3:G:190:ASP:N	2.10	0.64
2:D:81:GLY:CA	2:D:257:PRO:HD3	2.28	0.64
3:E:54:GLN:HG2	3:E:77:LYS:NZ	2.13	0.64
3:H:15:LYS:N	9:H:8292:ATP:O1B	2.29	0.64
1:C:332:LYS:HG2	1:C:336:GLU:OE2	1.98	0.64
2:D:448:GLY:C	2:D:466:LEU:HD22	2.22	0.64
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.30	0.64
1:C:17:LEU:HD11	1:C:29:ASN:HA	1.78	0.64
1:C:37:PRO:HD3	1:C:396:ASP:HA	1.79	0.64
1:C:355:ILE:O	1:C:380:GLU:HG2	1.97	0.64
2:D:57:PHE:CD2	2:D:425:LYS:NZ	2.66	0.64
3:E:10:LYS:HZ3	3:E:156:MET:HG3	1.63	0.64
1:A:444:TRP:HA	1:A:444:TRP:HE3	1.61	0.64
2:B:397:ASN:ND2	2:B:397:ASN:N	2.45	0.64
2:D:239:VAL:HG11	2:D:483:THR:HG21	1.79	0.64
2:D:394:LEU:HD23	2:D:394:LEU:C	2.23	0.64
1:A:352:MET:HE1	1:A:413:VAL:HA	1.80	0.64
2:D:362:LEU:HD11	2:D:498:VAL:CG2	2.26	0.64
3:E:52:LYS:O	3:E:53:ALA:HB2	1.98	0.64
1:A:275:CYS:SG	1:A:278:SER:HB2	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:206:GLN:NE2	3:G:250:ASN:OD1	2.30	0.64
3:H:187:ARG:NH2	3:H:195:LEU:CD2	2.61	0.64
1:A:99:TYR:CE2	1:A:232:GLY:HA2	2.33	0.64
2:B:142:TYR:C	2:B:144:PRO:CD	2.69	0.64
2:B:146:MET:HA	2:B:179:PHE:HE2	1.61	0.64
2:D:206:ARG:HG2	2:D:304:PHE:CE1	2.33	0.64
3:F:220:ALA:HB1	3:F:225:MET:O	1.97	0.64
1:A:332:LYS:O	1:A:336:GLU:HG3	1.98	0.64
1:A:405:THR:OG1	1:A:408:GLU:CG	2.46	0.64
2:B:119:THR:HG22	2:B:120:GLU:H	1.63	0.64
1:C:76:LYS:O	1:C:108:ALA:HA	1.98	0.64
3:G:34:MET:HB2	3:G:119:LEU:CD1	2.27	0.64
3:H:37:GLY:HA3	3:H:87:GLU:OE2	1.97	0.64
1:A:35:ASN:CB	1:A:400:LEU:HD11	2.28	0.64
1:A:71:VAL:HG22	1:A:279:MET:HE1	1.79	0.63
1:C:138:VAL:HG13	2:D:62:LEU:CD1	2.28	0.63
1:C:209:LYS:CE	1:C:263:GLU:OE1	2.45	0.63
1:C:458:ILE:HG23	1:C:461:ARG:NH2	2.14	0.63
2:D:47:THR:HA	2:D:52:TYR:CG	2.32	0.63
1:A:207:LEU:HD11	1:A:266:PRO:CG	2.28	0.63
1:C:144:LEU:HD11	2:D:43:VAL:HG21	1.80	0.63
1:A:302:PRO:HD3	1:A:456:PHE:CG	2.34	0.63
2:B:64:VAL:O	2:B:426:ASP:OD1	2.16	0.63
2:B:247:MET:HE3	2:B:340:ILE:HA	1.79	0.63
1:C:276:TYR:O	1:C:280:ASN:HB3	1.99	0.63
1:C:359:ARG:HG3	1:C:359:ARG:NH1	2.12	0.63
1:C:423:SER:HB3	1:C:427:GLU:HG3	1.80	0.63
1:A:230:ASN:HB2	1:A:235:ALA:CB	2.28	0.63
1:C:9:VAL:O	1:C:13:ILE:HG13	1.98	0.63
1:C:58:THR:CG2	1:C:60:ARG:H	2.08	0.63
2:D:128:GLN:NE2	2:D:168:ASN:ND2	2.46	0.63
1:A:35:ASN:HB2	1:A:400:LEU:CD1	2.29	0.63
1:A:276:TYR:O	1:A:280:ASN:HB3	1.99	0.63
2:B:3:GLN:HE21	2:B:3:GLN:CA	2.09	0.63
1:C:12:LEU:O	1:C:16:VAL:HG23	1.98	0.63
1:C:178:ILE:O	1:C:180:PRO:HD2	1.99	0.63
1:C:433:LYS:CE	2:D:263:THR:HG23	2.28	0.63
2:B:238:ARG:HD3	2:B:258:GLU:HG3	1.79	0.63
2:D:3:GLN:HE21	2:D:3:GLN:CA	2.09	0.63
3:E:98:ALA:O	3:E:102:VAL:HG23	1.98	0.63
2:B:460:LYS:HE3	2:B:507:GLU:OE2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:LEU:HD22	2:D:523:ARG:HD3	1.80	0.63
3:E:129:ASP:HB3	3:E:131:VAL:HG12	1.80	0.63
3:G:45:THR:HG21	3:G:85:CYS:HB3	1.81	0.63
1:A:23:LYS:NZ	2:B:133:ASP:OD2	2.15	0.63
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.81	0.63
3:G:13:ILE:O	3:G:185:ASN:ND2	2.32	0.63
2:B:47:THR:OG1	2:B:431:ARG:NH1	2.31	0.63
1:C:167:SER:OG	1:C:180:PRO:HG3	1.98	0.63
1:C:423:SER:CB	1:C:427:GLU:HG3	2.29	0.63
1:A:419:ASP:O	1:A:437:PRO:HD2	1.99	0.62
2:B:225:ASN:HB2	2:B:290:THR:HA	1.81	0.62
2:B:375:PHE:C	2:B:375:PHE:HD1	2.06	0.62
1:C:253:TRP:HZ3	1:C:282:ILE:CD1	2.06	0.62
1:C:298:ASN:HD22	1:C:298:ASN:C	2.03	0.62
1:C:400:LEU:HD12	1:C:400:LEU:N	2.13	0.62
2:B:254:LEU:HB3	2:B:281:MET:HE2	1.81	0.62
1:C:309:LEU:HD11	1:C:453:PHE:HE1	1.64	0.62
2:D:90:HIS:ND1	2:D:116:ASP:OD2	2.32	0.62
3:F:13:ILE:C	3:F:187:ARG:NH2	2.57	0.62
1:A:58:THR:CG2	1:A:60:ARG:HB2	2.28	0.62
2:B:239:VAL:HG11	2:B:483:THR:HG21	1.80	0.62
3:G:23:VAL:HA	3:G:26:LEU:HB2	1.81	0.62
3:H:134:GLY:O	3:H:137:MET:HB2	1.99	0.62
2:D:222:LYS:O	2:D:222:LYS:HG2	1.97	0.62
2:D:375:PHE:HD1	2:D:375:PHE:C	2.06	0.62
3:F:7:ILE:HD12	3:F:19:THR:OG1	2.00	0.62
3:F:13:ILE:HA	3:F:187:ARG:NH2	2.12	0.62
1:A:302:PRO:HD3	1:A:456:PHE:CD1	2.34	0.62
1:C:144:LEU:HD11	2:D:43:VAL:CG2	2.29	0.62
2:D:279:GLU:OE2	2:D:282:LYS:HD2	1.99	0.62
2:D:375:PHE:C	2:D:375:PHE:CD1	2.77	0.62
3:E:91:PRO:HD2	3:E:98:ALA:HB2	1.81	0.62
3:E:166:LYS:O	3:E:169:VAL:HG12	2.00	0.62
3:G:57:ILE:HG12	3:G:75:VAL:HG21	1.82	0.62
3:H:42:ALA:HA	3:H:87:GLU:OE1	1.99	0.62
1:A:170:LYS:O	1:A:178:ILE:HD12	1.99	0.62
2:D:284:ALA:HB3	2:D:285:PRO:CD	2.30	0.62
3:E:87:GLU:OE2	3:E:87:GLU:HA	1.99	0.62
2:B:499:ASN:O	2:B:503:GLU:HG3	2.00	0.62
3:H:16:SER:O	3:H:20:GLN:HG3	2.00	0.62
1:A:189:VAL:HG23	1:A:190:SER:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:HD22	1:A:280:ASN:H	1.45	0.62
2:B:375:PHE:C	2:B:375:PHE:CD1	2.77	0.62
2:B:392:HIS:ND1	2:B:433:LEU:HD12	2.15	0.62
2:B:509:THR:HA	2:B:515:THR:HB	1.82	0.62
2:B:520:ASP:O	2:D:449:LYS:NZ	2.33	0.62
3:E:215:ASN:HA	3:E:218:GLN:OE1	2.00	0.62
3:G:212:PRO:HB2	3:G:236:GLN:HE21	1.65	0.62
2:B:322:LEU:O	2:B:326:ASP:OD1	2.18	0.61
3:F:57:ILE:HD12	3:F:105:ALA:HB1	1.81	0.61
2:D:369:LEU:HD23	2:D:393:ILE:HA	1.82	0.61
3:F:86:VAL:HG21	3:F:109:LEU:HD11	1.82	0.61
3:F:195:LEU:O	3:F:198:ALA:HB3	2.00	0.61
3:G:129:ASP:HB3	3:G:131:VAL:HG12	1.82	0.61
2:B:375:PHE:HE2	2:B:470:GLY:HA2	1.65	0.61
2:B:471:PHE:CD2	2:B:472:PRO:CD	2.74	0.61
1:C:218:SER:OG	1:C:269:LYS:HE2	2.00	0.61
2:D:238:ARG:HE	2:D:258:GLU:HG2	1.63	0.61
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.31	0.61
3:H:250:ASN:C	3:H:250:ASN:ND2	2.58	0.61
1:C:300:PHE:HB3	1:C:366:ALA:HB2	1.82	0.61
1:C:444:TRP:CE3	1:C:444:TRP:HA	2.36	0.61
3:G:204:GLY:O	3:G:254:VAL:HG21	2.00	0.61
3:H:87:GLU:OE2	3:H:87:GLU:HA	2.01	0.61
2:D:254:LEU:HD22	2:D:281:MET:HE2	1.83	0.61
3:E:115:TYR:C	3:E:117:ASP:H	2.08	0.61
3:E:131:VAL:HG22	3:E:132:CYS:N	2.15	0.61
1:A:219:THR:HG23	1:A:220:PRO:HD2	1.83	0.61
1:A:225:ILE:HD11	1:A:249:CYS:SG	2.39	0.61
2:B:238:ARG:HD3	2:B:258:GLU:CD	2.26	0.61
1:C:274:HIS:O	1:C:358:LEU:CD1	2.48	0.61
2:D:70:CYS:O	2:D:193:HIS:HA	2.01	0.61
3:E:23:VAL:CG1	3:E:33:VAL:HG11	2.31	0.61
3:E:217:VAL:HB	9:E:5292:ATP:C2	2.36	0.61
3:G:9:GLY:O	3:G:15:LYS:HE2	2.00	0.61
1:A:141:LEU:HD23	2:B:59:ARG:HD2	1.81	0.61
1:A:332:LYS:HG2	1:A:336:GLU:OE2	2.00	0.61
2:B:56:ASN:O	2:B:59:ARG:HB2	2.01	0.61
2:B:328:PHE:O	2:B:332:VAL:HG23	2.01	0.61
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.66	0.61
2:D:146:MET:CE	2:D:208:PHE:HZ	2.13	0.61
2:D:222:LYS:HA	2:D:288:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NH2	2:D:520:ASP:CG	2.58	0.61
2:B:302:LYS:O	2:B:306:GLU:HG3	2.01	0.61
1:C:124:VAL:HG21	3:H:58:MET:HE3	1.73	0.61
2:D:317:ASN:ND2	2:D:317:ASN:H	1.98	0.61
3:G:223:ARG:O	3:G:224:ARG:HB2	2.01	0.61
3:G:106:ILE:CD1	3:G:137:MET:HB3	2.31	0.61
3:H:64:ALA:HB1	3:H:69:ASP:HB3	1.82	0.61
3:F:242:ALA:O	3:F:246:LYS:CG	2.43	0.60
3:H:38:CYS:HB3	3:H:102:VAL:HG13	1.83	0.60
1:A:277:ARG:CZ	1:A:383:HIS:HD2	2.12	0.60
2:B:105:ARG:HB2	2:B:474:PHE:CE2	2.36	0.60
2:D:72:PRO:HB2	2:D:99:PHE:CZ	2.35	0.60
1:C:389:ARG:CG	1:C:389:ARG:NH1	2.61	0.60
3:E:237:ALA:O	3:E:241:ARG:HG3	2.01	0.60
2:D:86:MET:CE	2:D:87:PRO:CD	2.71	0.60
2:D:370:TRP:HH2	2:D:448:GLY:HA3	1.66	0.60
1:A:309:LEU:HD11	1:A:453:PHE:HE1	1.66	0.60
1:A:355:ILE:O	1:A:380:GLU:HG2	2.01	0.60
2:B:422:TYR:HD2	2:B:425:LYS:HD2	1.64	0.60
1:C:112:MET:HE1	2:D:428:TRP:CZ3	2.36	0.60
1:C:178:ILE:HG22	1:C:180:PRO:HD3	1.83	0.60
1:C:222:ASP:OD1	1:C:248:ARG:NH1	2.34	0.60
2:B:131:MET:HG2	2:B:165:PHE:HB3	1.83	0.60
1:A:222:ASP:OD1	1:A:248:ARG:NH1	2.35	0.60
1:A:404:VAL:HG23	1:A:408:GLU:HB2	1.83	0.60
1:C:341:LYS:HD2	2:D:5:VAL:CG1	2.31	0.60
3:G:212:PRO:HB2	3:G:236:GLN:NE2	2.16	0.60
1:C:421:ILE:HD11	1:C:436:ILE:HG21	1.83	0.60
1:C:426:LYS:HZ1	2:D:97:ALA:CB	2.06	0.60
2:D:499:ASN:O	2:D:503:GLU:HG3	2.01	0.60
3:E:179:LEU:HD12	3:E:256:PRO:HG3	1.82	0.60
3:G:22:LEU:O	3:G:22:LEU:HD23	2.02	0.60
2:B:129:GLN:NE2	2:B:129:GLN:HA	2.17	0.60
2:B:236:ASN:HA	2:B:239:VAL:HG12	1.84	0.60
1:C:35:ASN:CB	1:C:400:LEU:HD11	2.32	0.60
2:D:328:PHE:O	2:D:332:VAL:HG23	2.02	0.60
3:E:243:LEU:O	3:E:247:VAL:HG23	2.02	0.60
1:C:186:PHE:HB3	2:D:154:MET:CE	2.31	0.60
1:C:433:LYS:HE3	2:D:263:THR:O	2.01	0.60
1:A:9:VAL:O	1:A:13:ILE:HG13	2.01	0.59
1:A:352:MET:HE2	1:A:418:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:GLU:HG2	2:D:476:ARG:HH11	1.66	0.59
1:C:32:LEU:N	1:C:32:LEU:HD23	2.18	0.59
1:C:417:LYS:N	1:C:418:PRO:HD3	2.17	0.59
2:D:119:THR:HG22	2:D:120:GLU:H	1.67	0.59
3:F:13:ILE:C	3:F:187:ARG:HH21	2.09	0.59
3:H:243:LEU:O	3:H:247:VAL:HG23	2.01	0.59
3:F:146:GLU:HG2	3:F:253:LEU:HD22	1.83	0.59
3:G:40:PRO:HG3	3:G:98:ALA:HB1	1.84	0.59
2:D:131:MET:HG2	2:D:165:PHE:HB3	1.83	0.59
3:E:10:LYS:O	3:E:13:ILE:HG12	2.02	0.59
1:A:207:LEU:HD11	1:A:266:PRO:HG3	1.84	0.59
1:A:355:ILE:HG21	1:A:359:ARG:HB2	1.83	0.59
2:B:81:GLY:CA	2:B:257:PRO:HD3	2.32	0.59
1:C:230:ASN:HB2	1:C:235:ALA:HB3	1.82	0.59
2:D:59:ARG:NH1	2:D:429:HIS:CE1	2.71	0.59
3:F:20:GLN:NE2	3:F:47:LEU:HD12	2.18	0.59
3:G:12:GLY:HA2	3:H:156:MET:HE1	1.84	0.59
3:G:217:VAL:HG22	3:G:227:VAL:CG2	2.31	0.59
1:C:42:SER:HB3	1:C:46:ILE:HG22	1.83	0.59
1:C:280:ASN:HD22	1:C:280:ASN:H	1.49	0.59
1:A:128:ASP:OD1	1:A:161:ASP:HB3	2.02	0.59
1:A:287:GLU:O	1:A:291:GLY:HA2	2.01	0.59
2:B:212:SER:O	2:B:216:LYS:CE	2.45	0.59
2:D:236:ASN:HA	2:D:239:VAL:HG12	1.85	0.59
1:A:423:SER:OG	1:A:427:GLU:HG3	2.03	0.59
1:A:479:TRP:CZ3	2:D:326:ASP:HB3	2.36	0.59
1:C:96:ARG:HG2	1:C:96:ARG:NH1	2.18	0.59
3:F:45:THR:HG21	3:F:85:CYS:HB3	1.84	0.59
1:C:405:THR:OG1	1:C:408:GLU:CG	2.50	0.59
1:C:424:GLY:CA	1:C:442:HIS:HD2	2.16	0.59
2:D:362:LEU:CD1	2:D:498:VAL:HG22	2.30	0.59
2:D:494:LEU:O	2:D:498:VAL:HG23	2.02	0.59
3:F:106:ILE:HD12	3:F:137:MET:CG	2.32	0.59
1:A:425:ILE:CD1	2:B:105:ARG:HG2	2.33	0.59
3:E:88:SER:HA	3:E:105:ALA:CB	2.33	0.59
3:F:198:ALA:HB1	3:F:267:LEU:HD21	1.84	0.59
2:B:494:LEU:O	2:B:498:VAL:HG23	2.03	0.59
1:C:230:ASN:OD1	1:C:233:GLY:CA	2.51	0.59
1:C:433:LYS:CE	2:D:263:THR:O	2.50	0.59
3:G:191:ARG:O	3:G:195:LEU:HB2	2.03	0.59
1:A:350:ARG:HD2	1:A:375:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ASN:HD22	2:B:397:ASN:N	1.88	0.58
1:C:128:ASP:HB3	1:C:166:VAL:HG21	1.85	0.58
1:C:230:ASN:OD1	1:C:233:GLY:HA2	2.03	0.58
3:E:255:ILE:O	3:E:255:ILE:HG22	2.02	0.58
3:H:55:ASN:HD22	3:H:55:ASN:N	1.99	0.58
1:A:32:LEU:N	1:A:32:LEU:HD23	2.18	0.58
1:A:280:ASN:HD22	1:A:281:TYR:H	1.50	0.58
1:A:479:TRP:CD2	2:D:340:ILE:HD12	2.38	0.58
2:B:72:PRO:HB2	2:B:99:PHE:CZ	2.38	0.58
2:B:91:GLY:O	2:B:116:ASP:O	2.20	0.58
2:B:162:LEU:HD12	2:B:185:HIS:HD2	1.68	0.58
2:B:394:LEU:HD23	2:B:395:CYS:N	2.18	0.58
1:C:253:TRP:NE1	1:C:265:THR:OG1	2.34	0.58
1:A:404:VAL:CG2	1:A:408:GLU:HB2	2.33	0.58
3:F:72:LEU:HD11	3:F:76:LEU:HD12	1.86	0.58
2:B:56:ASN:OD1	2:B:59:ARG:NH1	2.36	0.58
2:B:449:LYS:NZ	2:D:520:ASP:O	2.35	0.58
3:H:49:LEU:HD11	3:H:85:CYS:HB2	1.85	0.58
1:A:298:ASN:HD22	1:A:298:ASN:C	2.11	0.58
1:C:299:PHE:HB3	1:C:452:GLY:H	1.69	0.58
1:C:352:MET:HE1	1:C:413:VAL:HA	1.84	0.58
3:E:91:PRO:HB2	3:E:95:VAL:O	2.03	0.58
3:F:148:TYR:CE2	3:F:208:ILE:HD12	2.39	0.58
2:B:246:GLU:OE2	2:B:343:SER:HB2	2.03	0.58
2:B:283:ASP:OD1	2:B:283:ASP:O	2.22	0.58
1:C:37:PRO:HD2	1:C:396:ASP:CG	2.29	0.58
2:D:128:GLN:O	2:D:132:LYS:HG3	2.03	0.58
2:D:130:ASN:N	2:D:130:ASN:HD22	2.00	0.58
3:F:57:ILE:HG13	3:F:75:VAL:HG11	1.86	0.58
3:F:215:ASN:HA	3:F:218:GLN:OE1	2.04	0.58
1:A:426:LYS:HE3	2:B:97:ALA:O	2.04	0.58
1:C:277:ARG:NH2	1:C:280:ASN:OD1	2.35	0.58
2:D:151:THR:OG1	2:D:155:ALA:HB3	2.03	0.58
3:F:115:TYR:OH	3:F:124:TYR:OH	2.22	0.58
1:A:300:PHE:HB3	1:A:366:ALA:HB2	1.85	0.58
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.84	0.58
2:B:129:GLN:HA	2:B:129:GLN:HE21	1.69	0.58
2:B:394:LEU:HD23	2:B:394:LEU:C	2.28	0.58
2:B:523:ARG:HG3	2:D:475:ASP:HA	1.85	0.58
1:C:298:ASN:C	1:C:298:ASN:ND2	2.57	0.58
1:C:419:ASP:O	1:C:437:PRO:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLU:HB2	1:C:445:ASP:HB2	1.85	0.58
2:D:131:MET:HE3	2:D:166:ILE:HG13	1.85	0.58
3:E:136:ALA:HB2	3:F:94:GLY:CA	2.34	0.58
1:A:150:VAL:O	1:A:181:VAL:HG12	2.04	0.58
1:A:224:ALA:CB	1:A:251:ALA:HB3	2.34	0.58
2:B:3:GLN:HA	2:B:3:GLN:NE2	2.17	0.58
2:B:70:CYS:HB2	2:B:188:SER:HB3	1.85	0.58
2:B:314:PRO:CB	2:B:316:LEU:HD13	2.34	0.58
2:B:457:HIS:HD2	2:D:512:MET:CB	2.15	0.58
3:E:115:TYR:O	3:E:117:ASP:N	2.30	0.58
1:A:116:SER:O	1:A:130:LYS:CE	2.52	0.57
2:B:370:TRP:HH2	2:B:448:GLY:HA3	1.68	0.57
1:C:444:TRP:HA	1:C:444:TRP:HE3	1.68	0.57
2:D:158:ILE:HG22	3:G:97:CYS:HB2	1.85	0.57
3:F:8:TYR:CE1	3:F:126:VAL:HG21	2.38	0.57
1:A:210:ARG:NH1	1:A:264:LEU:HD21	2.19	0.57
2:B:57:PHE:HE2	2:B:425:LYS:NZ	2.01	0.57
1:C:35:ASN:HB2	1:C:400:LEU:CD1	2.34	0.57
1:C:66:GLY:O	1:C:70:VAL:HG22	2.04	0.57
1:C:124:VAL:CG2	3:H:58:MET:CE	2.64	0.57
1:C:360:PRO:HB2	1:C:379:TYR:CZ	2.39	0.57
1:C:401:TYR:HB2	1:C:404:VAL:HB	1.85	0.57
1:A:231:ILE:O	1:A:234:ASP:OD2	2.23	0.57
1:A:400:LEU:N	1:A:400:LEU:HD12	2.19	0.57
2:B:467:ILE:HD13	2:B:497:LEU:HD23	1.87	0.57
1:C:151:GLN:NE2	1:C:181:VAL:HG11	2.19	0.57
2:D:197:TRP:CE3	2:D:229:GLY:HA2	2.39	0.57
2:D:317:ASN:H	2:D:317:ASN:HD22	1.51	0.57
3:F:49:LEU:O	3:F:50:HIS:CB	2.52	0.57
3:G:166:LYS:O	3:G:169:VAL:HG12	2.04	0.57
2:B:471:PHE:HD2	2:B:472:PRO:HD3	1.62	0.57
2:D:390:PRO:O	2:D:419:ALA:HB1	2.04	0.57
3:F:141:GLU:O	3:F:142:ASN:HB2	2.02	0.57
1:A:36:ASP:OD1	1:A:38:ALA:HB3	2.04	0.57
1:A:167:SER:HB2	1:A:180:PRO:CG	2.28	0.57
1:A:271:ASN:OD1	1:A:286:MET:HE2	2.04	0.57
1:C:58:THR:HG22	1:C:59:ILE:N	2.19	0.57
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.86	0.57
2:D:118:MET:HE1	2:D:155:ALA:HB2	1.85	0.57
3:F:199:LEU:O	3:F:203:LEU:HB2	2.04	0.57
3:G:91:PRO:HB2	3:G:95:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:4:GLN:HB3	3:H:122:VAL:HB	1.87	0.57
3:H:45:THR:OG1	3:H:49:LEU:HD12	2.04	0.57
2:B:375:PHE:CZ	2:B:469:ILE:HG22	2.39	0.57
2:B:502:LEU:HD22	2:B:523:ARG:HD3	1.84	0.57
1:C:17:LEU:CD1	1:C:29:ASN:HA	2.35	0.57
1:C:299:PHE:CD2	1:C:305:THR:HG23	2.40	0.57
1:C:355:ILE:HD11	1:C:441:MET:CB	2.33	0.57
2:D:397:ASN:HD22	2:D:397:ASN:N	1.89	0.57
3:E:4:GLN:CD	3:E:143:LYS:O	2.48	0.57
3:H:26:LEU:HD12	3:H:29:MET:CE	2.32	0.57
2:B:473:ILE:HG21	2:B:479:LEU:HD22	1.87	0.57
2:D:128:GLN:NE2	2:D:165:PHE:HA	2.15	0.57
2:D:154:MET:O	2:D:158:ILE:HG12	2.04	0.57
3:F:23:VAL:HA	3:F:26:LEU:HB2	1.86	0.57
1:C:34:VAL:CG1	1:C:397:SER:HA	2.35	0.57
1:C:280:ASN:HD22	1:C:281:TYR:H	1.53	0.57
1:C:298:ASN:ND2	1:C:299:PHE:N	2.53	0.57
1:C:429:PHE:O	1:C:433:LYS:HG2	2.05	0.57
2:D:3:GLN:HA	2:D:3:GLN:NE2	2.17	0.57
2:D:238:ARG:NE	2:D:258:GLU:CG	2.60	0.57
3:H:35:ILE:CD1	3:H:48:ILE:HD12	2.35	0.57
1:A:287:GLU:HA	1:A:292:ILE:H	1.69	0.57
1:A:446:TYR:CE2	2:D:522:VAL:CG2	2.87	0.57
1:A:446:TYR:HE2	2:D:522:VAL:CG2	2.18	0.57
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.19	0.57
1:C:280:ASN:ND2	1:C:281:TYR:N	2.52	0.57
3:E:56:THR:HG23	3:E:59:GLU:CB	2.30	0.57
3:E:208:ILE:O	3:E:246:LYS:HE3	2.05	0.57
3:G:57:ILE:HG13	3:G:75:VAL:HG11	1.87	0.57
3:H:94:GLY:O	3:H:95:VAL:HG23	2.04	0.57
1:A:230:ASN:OD1	1:A:233:GLY:HA2	2.04	0.57
1:A:251:ALA:HA	1:A:261:GLU:CG	2.34	0.57
2:B:206:ARG:CG	2:B:304:PHE:CE1	2.88	0.57
2:B:459:GLY:HA3	2:B:461:GLU:OE1	2.04	0.57
1:C:207:LEU:HD11	1:C:266:PRO:HD3	1.86	0.57
1:C:425:ILE:HG22	4:C:3494:HCA:O3	2.05	0.57
2:D:62:LEU:HD21	2:D:64:VAL:CG2	2.34	0.57
3:E:100:ARG:HD2	3:E:100:ARG:O	2.04	0.57
3:F:106:ILE:HD11	3:F:138:PRO:CD	2.35	0.57
3:G:16:SER:O	3:G:20:GLN:HG3	2.05	0.57
1:A:421:ILE:HD11	1:A:436:ILE:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:GLN:CD	2:D:510:ARG:NH1	2.63	0.56
1:C:396:ASP:O	1:C:397:SER:HB2	2.05	0.56
1:C:423:SER:OG	1:C:427:GLU:HG3	2.05	0.56
2:D:456:LEU:HD13	2:D:463:GLU:OE2	2.05	0.56
3:F:107:ASN:O	3:F:111:GLU:HB2	2.05	0.56
3:F:186:SER:HA	3:F:192:GLU:CD	2.30	0.56
1:A:68:LYS:O	1:A:68:LYS:HD3	2.06	0.56
3:F:56:THR:HG23	3:F:59:GLU:CB	2.35	0.56
1:A:90:GLN:NE2	2:B:447:TYR:CZ	2.73	0.56
1:A:380:GLU:HG3	1:A:381:PHE:CD2	2.41	0.56
1:A:429:PHE:HB2	2:B:110:PRO:HD3	1.86	0.56
2:B:448:GLY:C	2:B:466:LEU:HD22	2.30	0.56
1:C:144:LEU:CD1	2:D:43:VAL:HG21	2.35	0.56
1:C:351:VAL:HG11	1:C:367:TYR:CE2	2.40	0.56
2:D:67:ALA:HB3	2:D:396:HIS:HB2	1.87	0.56
2:D:246:GLU:OE2	2:D:343:SER:HB2	2.05	0.56
2:D:403:LYS:HZ1	2:D:421:VAL:HB	1.68	0.56
2:D:442:MET:HG3	2:D:464:VAL:HG12	1.86	0.56
3:F:45:THR:CG2	3:F:85:CYS:HB3	2.35	0.56
3:G:57:ILE:HG12	3:G:75:VAL:HG11	1.88	0.56
3:G:72:LEU:HD11	3:G:76:LEU:HD12	1.87	0.56
3:G:86:VAL:HG21	3:G:109:LEU:HD11	1.87	0.56
3:G:141:GLU:O	3:G:142:ASN:CB	2.52	0.56
3:H:45:THR:CG2	3:H:85:CYS:HB3	2.34	0.56
3:H:141:GLU:O	3:H:142:ASN:CB	2.51	0.56
1:A:277:ARG:HE	1:A:383:HIS:HE2	1.52	0.56
2:B:309:TRP:O	2:B:310:LYS:HB2	2.04	0.56
2:B:375:PHE:HZ	2:B:469:ILE:HG22	1.69	0.56
2:B:503:GLU:HG2	2:D:476:ARG:NH1	2.21	0.56
1:C:97:ARG:CZ	1:C:446:TYR:HA	2.34	0.56
2:D:314:PRO:CB	2:D:316:LEU:HD13	2.35	0.56
3:H:55:ASN:N	3:H:55:ASN:ND2	2.50	0.56
1:A:97:ARG:NH2	2:D:520:ASP:OD1	2.36	0.56
2:B:122:ALA:HB3	2:B:154:MET:HE1	1.86	0.56
2:B:456:LEU:HD13	2:B:463:GLU:OE2	2.05	0.56
1:C:385:ASP:C	1:C:385:ASP:OD2	2.48	0.56
3:G:217:VAL:HG21	9:G:7292:ATP:C2	2.28	0.56
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.21	0.56
1:A:449:PRO:HG2	2:B:15:PHE:CZ	2.40	0.56
1:C:239:ARG:NH1	1:C:252:GLN:OE1	2.38	0.56
1:C:351:VAL:HG23	1:C:420:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HG23	1:A:461:ARG:NH2	2.20	0.56
1:C:57:MET:HE3	2:D:100:ARG:NH1	2.20	0.56
2:D:390:PRO:O	2:D:419:ALA:CB	2.54	0.56
1:C:72:TRP:O	1:C:73:GLY:C	2.49	0.56
1:C:199:ASN:HD21	1:C:279:MET:HE3	1.71	0.56
2:D:442:MET:HG3	2:D:464:VAL:CG1	2.35	0.56
3:H:57:ILE:HG13	3:H:75:VAL:HG11	1.88	0.56
1:C:118:PHE:CZ	1:C:156:ILE:HD11	2.41	0.56
1:A:423:SER:CB	1:A:427:GLU:HG3	2.36	0.56
2:B:239:VAL:HG11	2:B:483:THR:CG2	2.36	0.56
1:C:287:GLU:HA	1:C:292:ILE:H	1.69	0.56
1:C:426:LYS:NZ	2:D:97:ALA:CB	2.66	0.55
2:D:239:VAL:HG11	2:D:483:THR:CG2	2.36	0.55
2:D:289:ASN:ND2	2:D:314:PRO:HD3	2.21	0.55
3:G:131:VAL:HG22	3:G:132:CYS:N	2.19	0.55
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.70	0.55
2:B:50:LYS:HG3	2:B:436:THR:HG22	1.87	0.55
2:D:67:ALA:HB3	2:D:396:HIS:CB	2.37	0.55
3:E:12:GLY:HA2	3:F:156:MET:HE3	1.85	0.55
3:F:137:MET:HB3	3:F:138:PRO:CD	2.36	0.55
3:F:243:LEU:O	3:F:247:VAL:HG23	2.06	0.55
1:A:280:ASN:ND2	1:A:281:TYR:N	2.54	0.55
2:B:517:TYR:O	1:C:99:TYR:HE1	1.85	0.55
1:C:186:PHE:HB3	2:D:154:MET:HE1	1.88	0.55
1:C:210:ARG:HH11	1:C:264:LEU:CD2	2.17	0.55
2:D:59:ARG:HH12	2:D:429:HIS:CE1	2.25	0.55
1:A:17:LEU:HD21	1:A:28:ARG:HB2	1.88	0.55
1:A:70:VAL:CG2	1:A:71:VAL:N	2.69	0.55
2:B:125:PHE:CZ	3:E:58:MET:O	2.58	0.55
1:C:235:ALA:HB1	1:C:252:GLN:NE2	2.20	0.55
1:C:358:LEU:O	1:C:362:HIS:HB2	2.06	0.55
2:D:88:TYR:HB2	2:D:147:ILE:CG2	2.37	0.55
3:F:43:ASP:CB	3:F:46:ARG:HD3	2.34	0.55
1:A:37:PRO:HD3	1:A:396:ASP:HA	1.87	0.55
1:C:119:GLN:OE1	1:C:119:GLN:HA	2.05	0.55
1:C:358:LEU:HD22	5:C:3496:CFM:S4A	2.47	0.55
3:E:8:TYR:CE1	3:E:126:VAL:HG21	2.42	0.55
3:E:15:LYS:N	9:E:5292:ATP:O1B	2.40	0.55
1:A:136:ASP:O	1:A:140:THR:HG22	2.07	0.55
1:A:144:LEU:CG	2:B:43:VAL:HG21	2.37	0.55
1:A:151:GLN:CD	1:A:181:VAL:HG11	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG11	1:A:367:TYR:CE2	2.41	0.55
2:B:228:PRO:O	2:B:294:GLN:HG3	2.07	0.55
2:B:238:ARG:HD3	2:B:258:GLU:CG	2.36	0.55
2:B:422:TYR:CD2	2:B:425:LYS:HD2	2.42	0.55
1:C:346:LEU:HG	1:C:370:LEU:HD12	1.89	0.55
1:C:351:VAL:CG1	1:C:374:VAL:HG22	2.36	0.55
2:D:260:VAL:HG22	2:D:273:ALA:N	2.21	0.55
3:G:61:ALA:HB2	3:G:70:LEU:CD1	2.36	0.55
1:A:277:ARG:NE	1:A:383:HIS:NE2	2.53	0.55
1:A:355:ILE:CB	1:A:360:PRO:HD3	2.37	0.55
1:C:433:LYS:NZ	2:D:263:THR:HG22	2.22	0.55
2:D:90:HIS:O	2:D:151:THR:HA	2.05	0.55
3:F:201:ASN:C	3:F:203:LEU:H	2.15	0.55
3:G:14:GLY:HA3	3:G:185:ASN:HD22	1.70	0.55
3:H:20:GLN:OE1	3:H:47:LEU:HB2	2.06	0.55
1:C:98:ASN:ND2	1:C:98:ASN:N	2.52	0.55
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.89	0.55
1:A:138:VAL:HG23	1:A:139:GLU:H	1.72	0.55
1:A:151:GLN:HA	1:A:181:VAL:HG13	1.89	0.55
1:A:332:LYS:N	1:A:333:PRO:HD2	2.21	0.55
3:E:208:ILE:HG22	3:E:209:HIS:N	2.22	0.55
1:A:138:VAL:HG13	2:B:62:LEU:HD22	1.88	0.55
2:D:128:GLN:NE2	2:D:168:ASN:HD22	2.01	0.55
3:E:23:VAL:HA	3:E:26:LEU:HB2	1.88	0.55
3:G:239:GLU:O	3:G:242:ALA:HB3	2.07	0.55
3:H:138:PRO:O	3:H:143:LYS:CB	2.55	0.55
1:A:275:CYS:HA	1:A:358:LEU:HD13	1.87	0.54
1:C:342:TYR:O	1:C:343:ARG:C	2.50	0.54
1:C:380:GLU:HG3	1:C:381:PHE:CD2	2.42	0.54
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.07	0.54
1:A:99:TYR:CD1	2:D:517:TYR:O	2.61	0.54
2:B:70:CYS:O	2:B:193:HIS:HA	2.06	0.54
2:B:434:VAL:HG12	2:B:439:PRO:HG2	1.88	0.54
2:B:512:MET:HB3	2:D:457:HIS:CD2	2.30	0.54
1:C:224:ALA:CB	1:C:251:ALA:HB3	2.38	0.54
1:C:346:LEU:HD11	1:C:463:MET:HB2	1.88	0.54
2:D:219:GLY:N	2:D:287:ALA:O	2.40	0.54
1:A:225:ILE:CD1	1:A:249:CYS:SG	2.95	0.54
1:A:239:ARG:NH1	1:A:252:GLN:OE1	2.40	0.54
1:A:385:ASP:O	1:A:388:ASP:CG	2.51	0.54
1:C:332:LYS:N	1:C:333:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ILE:CG2	1:C:360:PRO:HD3	2.37	0.54
3:E:61:ALA:HB1	3:E:67:VAL:HA	1.89	0.54
3:H:2:MET:HB2	3:H:119:LEU:O	2.07	0.54
3:H:39:ASP:OD1	3:H:40:PRO:CD	2.56	0.54
3:H:144:ALA:O	3:H:177:VAL:HG23	2.08	0.54
1:A:134:LEU:HD12	2:B:61:ALA:O	2.08	0.54
2:B:457:HIS:CD2	2:D:512:MET:HB3	2.31	0.54
1:C:41:GLN:HE21	1:C:43:LYS:HG3	1.73	0.54
1:C:324:CYS:SG	1:C:328:ILE:HD11	2.48	0.54
3:F:213:ARG:HG2	9:F:6292:ATP:H2	1.72	0.54
1:A:131:LEU:HD12	1:A:166:VAL:HG11	1.89	0.54
2:B:227:VAL:HG12	2:B:298:LEU:HD13	1.90	0.54
1:A:298:ASN:C	1:A:298:ASN:ND2	2.65	0.54
2:B:156:GLU:CD	2:B:187:PRO:HG3	2.33	0.54
2:B:217:VAL:O	2:B:286:ASN:HA	2.07	0.54
2:B:413:SER:OG	2:B:415:TYR:HD1	1.90	0.54
1:C:358:LEU:CD2	5:C:3496:CFM:S4A	2.96	0.54
2:D:251:TYR:CD1	2:D:251:TYR:C	2.85	0.54
2:D:401:ARG:HB2	2:D:401:ARG:HH11	1.73	0.54
3:G:244:ALA:O	3:G:248:VAL:HG23	2.07	0.54
3:H:198:ALA:HB1	3:H:267:LEU:HD21	1.89	0.54
1:A:35:ASN:HD21	1:A:394:MET:HB2	1.73	0.54
1:A:81:ILE:HD13	1:A:134:LEU:CD2	2.37	0.54
1:A:298:ASN:ND2	1:A:300:PHE:H	2.06	0.54
2:B:146:MET:HA	2:B:179:PHE:CE2	2.41	0.54
2:D:375:PHE:HZ	2:D:469:ILE:HG22	1.72	0.54
3:E:43:ASP:HB2	3:E:46:ARG:HH11	1.73	0.54
3:E:165:SER:HB2	3:E:256:PRO:HB3	1.89	0.54
3:E:195:LEU:HD21	3:E:268:LEU:CD2	2.38	0.54
3:F:25:ALA:HB2	3:F:228:ILE:CD1	2.38	0.54
1:A:265:THR:HB	1:A:266:PRO:HD3	1.88	0.54
1:A:356:GLY:O	1:A:379:TYR:HD2	1.91	0.54
2:B:81:GLY:O	2:B:275:GLY:HA2	2.07	0.54
2:B:356:THR:HG22	1:C:471:CYS:SG	2.48	0.54
1:C:81:ILE:HD13	1:C:134:LEU:CD2	2.37	0.54
1:C:239:ARG:HG3	1:C:249:CYS:SG	2.48	0.54
2:D:91:GLY:N	2:D:116:ASP:OD1	2.34	0.54
2:D:188:SER:HB3	6:D:3498:CLF:S3B	2.48	0.54
2:D:314:PRO:HB2	2:D:316:LEU:HD13	1.88	0.54
2:D:473:ILE:HG21	2:D:479:LEU:HD22	1.90	0.54
3:H:187:ARG:NH2	3:H:195:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HB2	1:A:235:ALA:HB3	1.87	0.54
2:B:81:GLY:HA2	2:B:257:PRO:HD3	1.90	0.54
1:C:430:ILE:HG23	2:D:269:PHE:CD1	2.43	0.54
3:E:10:LYS:O	3:E:11:GLY:C	2.49	0.54
3:F:179:LEU:HB2	3:F:256:PRO:HG3	1.90	0.54
3:G:193:ASP:O	3:G:197:ILE:HG13	2.07	0.54
3:H:242:ALA:O	3:H:246:LYS:HG2	2.08	0.54
1:A:106:VAL:HG21	2:B:44:PHE:HB2	1.90	0.54
1:A:423:SER:HB3	1:A:427:GLU:HG3	1.90	0.54
2:B:39:LYS:O	2:B:43:VAL:HG23	2.08	0.54
2:B:442:MET:HG3	2:B:464:VAL:HG12	1.90	0.54
1:C:240:ILE:HG23	1:C:241:LEU:N	2.23	0.54
2:D:161:ASP:O	2:D:165:PHE:HD1	1.86	0.54
2:D:236:ASN:HB3	2:D:485:LEU:HD22	1.89	0.54
3:F:166:LYS:O	3:F:169:VAL:HG12	2.07	0.54
3:H:23:VAL:HA	3:H:26:LEU:HB2	1.88	0.54
2:D:39:LYS:HA	2:D:42:GLU:HB2	1.90	0.53
2:D:238:ARG:HD3	2:D:258:GLU:CG	2.36	0.53
3:E:186:SER:N	3:E:211:VAL:O	2.26	0.53
3:F:15:LYS:N	9:F:6292:ATP:O1B	2.41	0.53
3:F:25:ALA:O	3:F:28:GLU:HB3	2.08	0.53
3:G:189:THR:HB	3:G:192:GLU:HG2	1.90	0.53
9:G:7292:ATP:C5'	3:H:156:MET:SD	2.89	0.53
2:B:418:ASN:O	2:B:418:ASN:ND2	2.41	0.53
1:C:70:VAL:CG2	1:C:71:VAL:N	2.71	0.53
1:C:458:ILE:HG22	1:C:462:ASP:OD2	2.08	0.53
2:D:44:PHE:C	2:D:44:PHE:CD2	2.86	0.53
3:E:57:ILE:CG1	3:E:75:VAL:HG11	2.38	0.53
3:F:3:ARG:HH11	3:F:3:ARG:HG3	1.73	0.53
1:A:99:TYR:HE2	1:A:232:GLY:HA2	1.73	0.53
1:C:57:MET:HB2	2:D:142:TYR:OH	2.09	0.53
1:C:230:ASN:OD1	1:C:230:ASN:O	2.26	0.53
1:C:350:ARG:HD2	1:C:375:VAL:HG11	1.91	0.53
3:F:186:SER:HB2	3:F:192:GLU:OE1	2.07	0.53
1:A:105:GLY:HA2	1:A:112:MET:CE	2.23	0.53
1:A:224:ALA:HB1	1:A:251:ALA:HB3	1.90	0.53
1:C:60:ARG:HD3	1:C:190:SER:HB3	1.89	0.53
1:C:417:LYS:N	1:C:418:PRO:CD	2.72	0.53
2:D:91:GLY:O	2:D:116:ASP:O	2.27	0.53
3:G:95:VAL:O	3:G:95:VAL:HG12	2.09	0.53
1:A:35:ASN:ND2	1:A:394:MET:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:C	1:A:112:MET:H	2.15	0.53
1:A:299:PHE:CD2	1:A:305:THR:HG23	2.43	0.53
1:C:30:LYS:NZ	1:C:47:ILE:CD1	2.71	0.53
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.49	0.53
1:C:186:PHE:HE1	3:G:100:ARG:NH2	2.02	0.53
2:D:369:LEU:CD2	2:D:393:ILE:HA	2.38	0.53
3:F:186:SER:C	3:F:188:ASN:H	2.17	0.53
3:G:131:VAL:CG2	3:G:132:CYS:N	2.71	0.53
1:A:15:GLU:O	1:A:18:GLU:HB2	2.09	0.53
1:A:59:ILE:HD13	1:A:427:GLU:OE2	2.09	0.53
2:B:85:THR:HG21	2:B:146:MET:CE	2.20	0.53
2:B:241:LYS:O	2:B:245:SER:HB2	2.08	0.53
1:C:14:GLN:O	1:C:18:GLU:HG3	2.08	0.53
1:C:306:ILE:HD11	1:C:335:TRP:NE1	2.23	0.53
2:D:156:GLU:HG3	2:D:187:PRO:HA	1.91	0.53
2:D:375:PHE:CZ	2:D:469:ILE:HG22	2.42	0.53
3:G:255:ILE:HG22	3:G:255:ILE:O	2.07	0.53
3:H:138:PRO:O	3:H:143:LYS:HB2	2.08	0.53
1:A:416:ILE:C	1:A:418:PRO:HD3	2.34	0.53
1:C:90:GLN:HG3	1:C:90:GLN:O	2.09	0.53
3:E:35:ILE:CD1	3:E:48:ILE:CD1	2.79	0.53
3:F:39:ASP:OD1	3:F:40:PRO:N	2.42	0.53
3:F:259:ILE:HD12	3:F:264:LEU:HD23	1.89	0.53
2:B:129:GLN:HE21	2:B:129:GLN:CA	2.22	0.53
1:C:99:TYR:HE2	1:C:232:GLY:HA2	1.74	0.53
1:C:277:ARG:NE	1:C:277:ARG:HA	2.23	0.53
1:C:302:PRO:HD3	1:C:456:PHE:CD1	2.44	0.53
2:D:139:LYS:HG3	2:D:179:PHE:CE1	2.43	0.53
2:D:322:LEU:HD11	2:D:348:ARG:HH21	1.73	0.53
3:E:61:ALA:N	3:E:70:LEU:HD11	2.24	0.53
1:A:68:LYS:HD3	1:A:68:LYS:C	2.34	0.53
1:A:72:TRP:O	1:A:73:GLY:C	2.51	0.53
2:D:76:VAL:HG13	2:D:87:PRO:HB3	1.90	0.53
2:D:451:ILE:O	2:D:455:THR:HG23	2.09	0.53
3:G:224:ARG:C	3:G:225:MET:CG	2.82	0.53
3:G:237:ALA:O	3:G:241:ARG:HG3	2.09	0.53
3:H:61:ALA:HB1	3:H:67:VAL:HA	1.91	0.53
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.44	0.53
2:B:38:ASP:O	2:B:42:GLU:HG3	2.08	0.53
2:B:44:PHE:C	2:B:44:PHE:CD2	2.86	0.53
2:B:351:LEU:O	2:B:355:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASP:O	1:C:203:ARG:HG3	2.09	0.53
1:C:298:ASN:ND2	1:C:300:PHE:H	2.07	0.53
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.90	0.53
1:C:428:LYS:HD2	1:C:440:GLU:HG3	1.91	0.53
2:D:289:ASN:HD21	2:D:314:PRO:HD3	1.74	0.53
3:H:217:VAL:HG11	9:H:8292:ATP:C8	2.44	0.53
1:A:219:THR:C	1:A:221:TYR:H	2.17	0.52
1:A:355:ILE:HD13	1:A:359:ARG:HB2	1.91	0.52
1:A:424:GLY:HA2	1:A:442:HIS:HD2	1.73	0.52
2:B:131:MET:HE3	2:B:166:ILE:HG13	1.91	0.52
2:B:512:MET:HE2	2:D:457:HIS:HB2	1.91	0.52
1:C:125:PHE:C	1:C:126:GLY:O	2.49	0.52
3:G:33:VAL:HG22	3:G:121:PHE:HB2	1.91	0.52
3:H:137:MET:CB	3:H:138:PRO:CD	2.87	0.52
1:C:428:LYS:HD2	1:C:440:GLU:CG	2.39	0.52
2:D:43:VAL:O	2:D:47:THR:HG23	2.10	0.52
2:D:81:GLY:O	2:D:275:GLY:HA2	2.08	0.52
2:D:516:ASP:O	2:D:519:HIS:HB2	2.09	0.52
3:G:4:GLN:NE2	3:G:124:TYR:OH	2.41	0.52
3:H:217:VAL:HG11	9:H:8292:ATP:N7	2.24	0.52
1:A:413:VAL:HG21	1:A:431:PHE:CE2	2.44	0.52
2:B:219:GLY:N	2:B:287:ALA:O	2.42	0.52
1:C:13:ILE:O	1:C:17:LEU:HG	2.08	0.52
1:C:138:VAL:CG1	2:D:62:LEU:HD13	2.34	0.52
1:C:144:LEU:HG	2:D:43:VAL:HG21	1.90	0.52
1:C:224:ALA:HB1	1:C:251:ALA:HB3	1.91	0.52
2:D:184:ALA:O	2:D:186:THR:HG23	2.10	0.52
3:F:64:ALA:HB1	3:F:69:ASP:HB3	1.90	0.52
3:G:64:ALA:HB1	3:G:69:ASP:HB3	1.90	0.52
1:A:67:SER:OG	1:A:183:CYS:HB3	2.10	0.52
1:A:387:TYR:OH	1:A:402:ASP:HB2	2.10	0.52
2:B:510:ARG:O	2:B:510:ARG:HG2	2.08	0.52
1:C:207:LEU:HD11	1:C:266:PRO:CD	2.40	0.52
1:C:440:GLU:HB2	1:C:445:ASP:CB	2.39	0.52
2:D:494:LEU:HD23	2:D:494:LEU:C	2.35	0.52
2:B:57:PHE:CE2	2:B:425:LYS:NZ	2.77	0.52
2:B:116:ASP:OD1	2:B:116:ASP:N	2.29	0.52
1:C:58:THR:HG21	1:C:60:ARG:HB2	1.90	0.52
1:C:216:PHE:CE1	1:C:264:LEU:HD13	2.45	0.52
1:C:355:ILE:CG2	1:C:356:GLY:N	2.36	0.52
2:D:68:LYS:HG2	2:D:396:HIS:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:87:GLU:OE2	3:F:87:GLU:HA	2.10	0.52
3:H:154:GLU:O	3:H:158:MET:HG3	2.10	0.52
1:A:355:ILE:HG21	1:A:360:PRO:HD2	1.87	0.52
2:B:340:ILE:HD12	1:C:479:TRP:CD2	2.44	0.52
2:D:510:ARG:HB2	2:D:519:HIS:NE2	2.24	0.52
3:E:10:LYS:H	3:E:13:ILE:HD11	1.74	0.52
3:E:33:VAL:HG22	3:E:121:PHE:HB2	1.91	0.52
3:F:195:LEU:HD12	3:F:267:LEU:HD22	1.91	0.52
3:F:201:ASN:C	3:F:203:LEU:N	2.66	0.52
1:A:382:ALA:HB1	1:A:386:ASP:CB	2.40	0.52
2:B:59:ARG:NH2	2:B:429:HIS:HE1	2.07	0.52
2:B:118:MET:CB	2:B:154:MET:HE3	2.40	0.52
3:E:131:VAL:CG2	3:E:132:CYS:N	2.71	0.52
3:F:106:ILE:HD13	3:F:138:PRO:HD3	1.86	0.52
1:A:298:ASN:CG	1:A:362:HIS:CD2	2.88	0.52
2:B:151:THR:HG23	2:B:186:THR:H	1.74	0.52
2:B:451:ILE:O	2:B:455:THR:HG23	2.09	0.52
3:E:61:ALA:HB2	3:E:70:LEU:CD1	2.35	0.52
3:H:212:PRO:HG2	3:H:239:GLU:OE2	2.09	0.52
1:A:42:SER:C	1:A:44:LYS:N	2.65	0.52
1:A:199:ASN:ND2	1:A:279:MET:HE3	2.23	0.52
2:B:442:MET:HG3	2:B:464:VAL:CG1	2.39	0.52
2:D:88:TYR:CB	2:D:147:ILE:HG22	2.40	0.52
2:D:391:VAL:HG12	2:D:392:HIS:CE1	2.45	0.52
2:D:397:ASN:ND2	2:D:397:ASN:N	2.45	0.52
1:A:72:TRP:CZ2	1:A:202:VAL:HG22	2.45	0.52
2:B:118:MET:HE2	2:B:122:ALA:HB1	1.92	0.52
1:C:159:ILE:CD1	3:H:97:CYS:HB2	2.39	0.52
1:C:424:GLY:HA2	1:C:442:HIS:HD2	1.75	0.52
2:D:241:LYS:O	2:D:245:SER:HB2	2.10	0.52
2:D:302:LYS:O	2:D:306:GLU:HG3	2.10	0.52
1:A:136:ASP:OD1	1:A:170:LYS:NZ	2.28	0.51
1:C:245:MET:HE3	1:C:309:LEU:HD22	1.92	0.51
1:C:421:ILE:HD11	1:C:436:ILE:CG2	2.38	0.51
3:F:57:ILE:CG1	3:F:75:VAL:HG11	2.40	0.51
3:F:106:ILE:HD12	3:F:137:MET:HG2	1.93	0.51
3:G:185:ASN:HA	3:G:211:VAL:HB	1.92	0.51
1:A:131:LEU:HD11	1:A:135:ILE:HD11	1.93	0.51
1:A:355:ILE:CD1	1:A:359:ARG:HB2	2.40	0.51
2:B:391:VAL:HG12	2:B:392:HIS:CE1	2.45	0.51
1:C:40:THR:O	1:C:40:THR:CG2	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:TRP:HZ2	2:D:255:SER:HG	1.55	0.51
1:A:55:GLY:HA2	2:B:114:VAL:HB	1.92	0.51
1:A:299:PHE:HB3	1:A:452:GLY:H	1.75	0.51
1:C:250:VAL:HG13	2:D:31:PHE:CD2	2.45	0.51
2:D:317:ASN:ND2	2:D:317:ASN:N	2.57	0.51
2:D:456:LEU:HD11	2:D:460:LYS:HD2	1.92	0.51
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.40	0.51
1:A:116:SER:HA	1:A:134:LEU:CD1	2.40	0.51
1:A:245:MET:HE1	1:A:309:LEU:O	2.10	0.51
2:B:82:PHE:CZ	2:B:255:SER:HB2	2.46	0.51
2:B:156:GLU:HG3	2:B:187:PRO:HA	1.93	0.51
1:C:385:ASP:OD2	1:C:386:ASP:OD1	2.29	0.51
2:D:293:LEU:HD22	2:D:319:PRO:HG2	1.91	0.51
2:D:309:TRP:O	2:D:310:LYS:HB2	2.10	0.51
3:G:148:TYR:CE2	3:G:208:ILE:HD12	2.45	0.51
2:B:289:ASN:ND2	2:B:314:PRO:CD	2.71	0.51
2:B:434:VAL:HA	2:B:439:PRO:HD2	1.92	0.51
1:C:35:ASN:ND2	1:C:395:GLY:O	2.44	0.51
2:D:351:LEU:O	2:D:355:MET:HG3	2.09	0.51
3:G:22:LEU:HD23	3:G:22:LEU:C	2.34	0.51
2:B:76:VAL:HG13	2:B:87:PRO:HB3	1.92	0.51
1:C:42:SER:O	1:C:46:ILE:O	2.28	0.51
1:C:116:SER:HA	1:C:134:LEU:CD1	2.41	0.51
1:C:221:TYR:O	1:C:223:VAL:HG13	2.10	0.51
1:C:449:PRO:CG	2:D:15:PHE:HZ	2.18	0.51
2:D:254:LEU:HB3	2:D:281:MET:HE2	1.92	0.51
2:D:509:THR:HG21	2:D:518:ASN:HD22	1.76	0.51
3:G:160:ALA:HA	3:G:163:ASN:HB3	1.93	0.51
1:A:337:ALA:HB1	2:B:5:VAL:HG21	1.93	0.51
1:C:275:CYS:SG	1:C:278:SER:HB2	2.51	0.51
1:C:364:ILE:O	1:C:367:TYR:HB2	2.11	0.51
2:D:206:ARG:HG2	2:D:304:PHE:CZ	2.45	0.51
2:D:263:THR:OG1	2:D:270:ARG:HD2	2.11	0.51
3:E:22:LEU:HD23	3:E:22:LEU:C	2.36	0.51
3:F:186:SER:HB3	3:F:210:PHE:HZ	1.65	0.51
3:G:208:ILE:O	3:G:246:LYS:HD3	2.11	0.51
1:A:89:GLY:C	1:A:113:ASN:ND2	2.69	0.51
2:B:445:ASN:OD1	2:B:447:TYR:HB2	2.11	0.51
3:E:73:GLU:OE1	3:E:73:GLU:N	2.44	0.51
3:E:206:GLN:NE2	3:E:250:ASN:OD1	2.44	0.51
3:E:217:VAL:HG22	3:E:227:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:158:MET:HE1	3:G:195:LEU:HG	1.93	0.51
3:H:40:PRO:HG3	3:H:98:ALA:HB1	1.93	0.51
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.91	0.51
2:B:181:VAL:N	2:B:182:PRO:HD3	2.26	0.51
2:B:422:TYR:HB3	2:B:425:LYS:HD2	1.91	0.51
1:C:277:ARG:HA	1:C:277:ARG:HE	1.76	0.51
3:F:10:LYS:O	3:F:13:ILE:HG12	2.11	0.51
3:G:98:ALA:O	3:G:102:VAL:HG23	2.10	0.51
1:A:16:VAL:HG11	1:A:408:GLU:HA	1.92	0.51
1:A:277:ARG:NE	1:A:383:HIS:HE2	2.08	0.51
1:A:280:ASN:N	1:A:280:ASN:ND2	2.58	0.51
1:A:355:ILE:HG22	1:A:360:PRO:HG2	1.92	0.51
2:B:523:ARG:CG	2:D:475:ASP:HA	2.40	0.51
1:C:134:LEU:HG	2:D:62:LEU:HB2	1.92	0.51
1:C:200:ASP:HA	1:C:203:ARG:HG2	1.92	0.51
1:C:258:SER:HB2	1:C:261:GLU:HB2	1.93	0.51
1:C:399:LEU:C	1:C:400:LEU:HD12	2.35	0.51
2:D:125:PHE:HA	3:G:91:PRO:HB3	1.93	0.51
2:D:185:HIS:C	2:D:187:PRO:HD3	2.36	0.51
3:E:10:LYS:H	3:E:13:ILE:HD13	1.75	0.51
3:F:16:SER:OG	9:F:6292:ATP:O2A	2.29	0.51
3:F:236:GLN:HG2	3:F:240:TYR:CE2	2.45	0.51
3:H:72:LEU:HD11	3:H:76:LEU:CD1	2.41	0.51
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.26	0.50
1:A:355:ILE:HG23	5:A:1496:CFM:S3A	2.51	0.50
2:B:88:TYR:HB2	2:B:147:ILE:HG23	1.92	0.50
1:C:351:VAL:HG12	1:C:374:VAL:HG22	1.94	0.50
2:D:247:MET:HE3	2:D:340:ILE:HA	1.91	0.50
3:E:52:LYS:O	3:E:53:ALA:CB	2.60	0.50
3:G:34:MET:HE1	3:G:115:TYR:CE1	2.46	0.50
3:H:49:LEU:O	3:H:50:HIS:CB	2.57	0.50
3:H:131:VAL:HG22	3:H:132:CYS:SG	2.51	0.50
1:A:141:LEU:CD2	2:B:59:ARG:HD2	2.41	0.50
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.12	0.50
2:B:222:LYS:HD3	2:B:288:LEU:HD21	1.93	0.50
2:B:390:PRO:O	2:B:419:ALA:HB1	2.11	0.50
1:C:34:VAL:HG13	1:C:397:SER:HA	1.94	0.50
1:C:230:ASN:HB2	1:C:235:ALA:HB2	1.92	0.50
1:C:241:LEU:HD21	1:C:453:PHE:HD1	1.75	0.50
1:C:266:PRO:O	1:C:292:ILE:HD11	2.11	0.50
1:C:471:CYS:SG	1:C:472:TRP:N	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:52:LYS:O	3:F:53:ALA:HB2	2.11	0.50
3:G:223:ARG:O	3:G:223:ARG:HG2	2.11	0.50
3:H:107:ASN:O	3:H:111:GLU:HB2	2.10	0.50
3:H:207:MET:CE	3:H:210:PHE:HB2	2.41	0.50
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.26	0.50
2:B:70:CYS:CB	2:B:188:SER:HB3	2.41	0.50
2:B:118:MET:HB3	2:B:154:MET:CE	2.41	0.50
2:B:369:LEU:HD21	2:B:393:ILE:HG12	1.93	0.50
1:C:405:THR:H	1:C:408:GLU:HG3	1.76	0.50
2:D:146:MET:HA	2:D:179:PHE:CE2	2.45	0.50
2:D:157:VAL:C	2:D:159:GLY:H	2.19	0.50
3:G:96:GLY:O	3:H:132:CYS:HB2	2.12	0.50
3:H:179:LEU:HB2	3:H:256:PRO:HG3	1.94	0.50
1:A:144:LEU:HD22	2:B:35:TYR:CD1	2.46	0.50
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.46	0.50
2:B:206:ARG:CG	2:B:304:PHE:CZ	2.88	0.50
2:B:284:ALA:HB3	2:B:285:PRO:CD	2.41	0.50
1:C:226:ILE:HG23	1:C:279:MET:HG2	1.93	0.50
1:C:343:ARG:HG3	1:C:370:LEU:O	2.11	0.50
1:C:416:ILE:C	1:C:418:PRO:HD3	2.37	0.50
1:C:429:PHE:CZ	2:D:108:ARG:HA	2.46	0.50
3:H:73:GLU:OE1	3:H:73:GLU:N	2.44	0.50
1:A:46:ILE:HG12	1:A:47:ILE:N	2.25	0.50
2:B:422:TYR:HD2	2:B:425:LYS:CD	2.23	0.50
1:C:106:VAL:HG21	2:D:44:PHE:HB2	1.93	0.50
1:C:277:ARG:NH1	1:C:383:HIS:CG	2.79	0.50
2:D:234:LEU:O	2:D:238:ARG:HG2	2.12	0.50
3:F:165:SER:HA	3:F:168:ILE:HD12	1.91	0.50
3:G:52:LYS:O	3:G:53:ALA:HB2	2.12	0.50
3:G:264:LEU:O	3:G:267:LEU:HB2	2.11	0.50
1:A:245:MET:HE3	1:A:309:LEU:HD22	1.92	0.50
2:B:522:VAL:HG23	1:C:446:TYR:CE2	2.46	0.50
1:C:164:GLU:HA	1:C:180:PRO:HB3	1.93	0.50
2:D:39:LYS:O	2:D:43:VAL:HG23	2.12	0.50
3:E:148:TYR:CD2	3:E:208:ILE:HD12	2.46	0.50
3:G:225:MET:CE	3:G:230:TYR:HA	2.41	0.50
3:H:54:GLN:HG3	3:H:55:ASN:N	2.21	0.50
1:A:57:MET:CG	2:B:142:TYR:CZ	2.94	0.50
1:A:125:PHE:C	1:A:126:GLY:O	2.54	0.50
1:A:430:ILE:HG12	2:B:269:PHE:CE1	2.47	0.50
1:C:151:GLN:HA	1:C:181:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:GLN:HB3	3:E:122:VAL:HB	1.94	0.50
3:G:100:ARG:O	3:G:100:ARG:HD2	2.10	0.50
3:G:137:MET:CB	3:G:138:PRO:HD3	2.42	0.50
1:A:230:ASN:HB2	1:A:235:ALA:HB2	1.92	0.50
1:A:359:ARG:HB2	1:A:360:PRO:HD3	1.93	0.50
1:C:230:ASN:O	1:C:230:ASN:CG	2.54	0.50
1:A:354:TYR:CE1	1:A:404:VAL:HG12	2.46	0.50
2:B:494:LEU:HD23	2:B:494:LEU:C	2.37	0.50
1:C:231:ILE:O	1:C:234:ASP:OD2	2.30	0.50
2:D:180:PRO:HG2	2:D:278:GLN:OE1	2.12	0.50
2:D:382:PHE:HD1	2:D:385:GLU:OE2	1.95	0.50
2:D:445:ASN:OD1	2:D:447:TYR:HB2	2.12	0.50
3:F:131:VAL:HG22	3:F:132:CYS:SG	2.51	0.50
3:F:231:ASP:OD2	3:F:234:ALA:HB2	2.11	0.50
3:H:103:ILE:HG12	3:H:137:MET:HG2	1.93	0.50
3:H:141:GLU:HA	3:H:141:GLU:OE1	2.12	0.50
2:B:326:ASP:HB3	1:C:479:TRP:CZ3	2.43	0.49
2:B:326:ASP:OD2	2:B:348:ARG:NE	2.43	0.49
1:C:210:ARG:HH22	2:D:33:GLU:CD	2.20	0.49
1:C:349:LYS:O	1:C:372:MET:HA	2.12	0.49
2:D:510:ARG:CG	2:D:510:ARG:O	2.60	0.49
1:A:40:THR:O	1:A:40:THR:HG22	2.13	0.49
1:A:62:CYS:O	1:A:191:GLN:HA	2.12	0.49
1:A:151:GLN:HA	1:A:181:VAL:CG1	2.42	0.49
1:A:351:VAL:CG1	1:A:374:VAL:HG22	2.42	0.49
1:C:107:ASN:ND2	1:C:107:ASN:O	2.45	0.49
1:C:138:VAL:HG23	1:C:139:GLU:H	1.77	0.49
3:G:55:ASN:HB3	3:G:60:MET:SD	2.52	0.49
3:H:161:ALA:O	3:H:165:SER:OG	2.30	0.49
1:A:106:VAL:HG12	1:A:144:LEU:HD12	1.94	0.49
1:A:221:TYR:CE2	1:A:320:ILE:HD11	2.47	0.49
1:A:469:ASN:CG	1:A:470:PRO:HD2	2.37	0.49
2:B:53:GLN:OE1	2:B:432:SER:HB3	2.12	0.49
2:B:236:ASN:HB3	2:B:485:LEU:HD22	1.93	0.49
1:C:37:PRO:HG2	1:C:396:ASP:HB2	1.93	0.49
3:E:155:MET:CE	3:E:261:MET:HE3	2.42	0.49
3:G:43:ASP:HB2	3:G:46:ARG:HD3	1.93	0.49
2:B:212:SER:C	2:B:216:LYS:HE3	2.36	0.49
2:B:224:ILE:HD12	2:B:249:VAL:CG1	2.42	0.49
2:B:247:MET:HB3	2:B:249:VAL:HG23	1.93	0.49
2:D:495:THR:HG22	2:D:499:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:141:GLU:HA	3:E:141:GLU:OE1	2.13	0.49
3:G:34:MET:HB2	3:G:119:LEU:HD11	1.92	0.49
1:A:35:ASN:ND2	1:A:395:GLY:O	2.46	0.49
2:B:43:VAL:O	2:B:47:THR:HG23	2.12	0.49
2:B:59:ARG:CZ	2:B:429:HIS:CE1	2.96	0.49
1:C:125:PHE:O	1:C:126:GLY:O	2.30	0.49
2:D:93:GLN:HB3	2:D:117:SER:OG	2.13	0.49
2:D:403:LYS:HZ2	2:D:421:VAL:HB	1.77	0.49
3:F:72:LEU:HD11	3:F:76:LEU:CD1	2.42	0.49
3:G:102:VAL:O	3:G:106:ILE:HG13	2.13	0.49
1:A:83:HIS:O	1:A:153:GLU:HG3	2.12	0.49
1:A:196:HIS:HA	1:A:281:TYR:CD1	2.47	0.49
1:A:203:ARG:HA	1:A:207:LEU:HB3	1.93	0.49
1:A:359:ARG:HG2	5:A:1496:CFM:S3A	2.52	0.49
1:A:405:THR:H	1:A:408:GLU:HG3	1.77	0.49
2:B:222:LYS:HA	2:B:288:LEU:HD21	1.95	0.49
3:F:195:LEU:HD21	3:F:268:LEU:CD2	2.40	0.49
3:G:192:GLU:HB3	3:G:210:PHE:CE2	2.44	0.49
1:C:272:LEU:HD13	1:C:312:ILE:HD13	1.93	0.49
2:D:19:ASP:OD2	2:D:20:TYR:N	2.45	0.49
3:E:180:GLY:HA2	3:E:253:LEU:HD23	1.93	0.49
3:G:110:GLU:OE2	3:G:143:LYS:NZ	2.45	0.49
2:B:249:VAL:HG13	2:B:336:SER:HB2	1.94	0.49
1:C:78:MET:HE2	1:C:259:ILE:HB	1.93	0.49
1:C:399:LEU:HD21	1:C:412:PHE:CD2	2.47	0.49
3:G:50:HIS:NE2	3:G:229:GLU:OE2	2.40	0.49
1:A:203:ARG:HG3	1:A:204:ASP:OD2	2.12	0.49
1:A:210:ARG:HG3	1:A:263:GLU:HB3	1.95	0.49
2:B:125:PHE:HE2	3:E:62:ALA:HB2	1.78	0.49
2:B:206:ARG:HH11	2:B:210:LEU:HD22	1.78	0.49
2:B:296:TRP:CZ3	2:B:402:TRP:HA	2.47	0.49
1:C:107:ASN:ND2	1:C:107:ASN:C	2.67	0.49
1:C:144:LEU:HD21	2:D:43:VAL:HG21	1.94	0.49
1:C:196:HIS:HA	1:C:281:TYR:CD1	2.47	0.49
1:C:280:ASN:O	1:C:284:ARG:HG3	2.13	0.49
1:A:399:LEU:HD21	1:A:412:PHE:CD2	2.47	0.49
2:B:39:LYS:HA	2:B:42:GLU:HB2	1.95	0.49
2:B:198:ASP:CG	2:B:298:LEU:HA	2.38	0.49
1:C:41:GLN:HG3	1:C:43:LYS:H	1.76	0.49
1:C:76:LYS:HD3	1:C:256:ASP:OD2	2.13	0.49
1:C:342:TYR:OH	2:D:8:ILE:HD11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:VAL:HB	2:D:428:TRP:CB	2.43	0.49
2:D:197:TRP:CZ3	2:D:229:GLY:HA2	2.48	0.49
1:A:138:VAL:HG23	1:A:139:GLU:N	2.27	0.48
2:B:107:PHE:CZ	2:B:232:THR:HB	2.48	0.48
2:B:133:ASP:O	2:B:136:GLN:N	2.46	0.48
2:B:227:VAL:CG1	2:B:298:LEU:HD13	2.43	0.48
1:C:110:VAL:C	1:C:112:MET:H	2.20	0.48
1:C:219:THR:C	1:C:221:TYR:H	2.19	0.48
1:C:342:TYR:HA	1:C:345:ARG:HD2	1.94	0.48
2:D:254:LEU:O	2:D:255:SER:CB	2.61	0.48
3:E:43:ASP:HB2	3:E:46:ARG:HD3	1.93	0.48
3:E:264:LEU:O	3:E:267:LEU:HB2	2.13	0.48
3:F:61:ALA:HB1	3:F:67:VAL:HA	1.95	0.48
3:G:39:ASP:OD1	3:G:40:PRO:HD2	2.13	0.48
3:H:231:ASP:OD2	3:H:234:ALA:CB	2.56	0.48
1:A:298:ASN:HD22	1:A:299:PHE:N	2.10	0.48
1:A:349:LYS:O	1:A:372:MET:HA	2.13	0.48
1:A:449:PRO:CG	2:B:15:PHE:HZ	2.25	0.48
2:B:161:ASP:O	2:B:165:PHE:HD1	1.89	0.48
2:B:241:LYS:NZ	2:B:256:ASP:OD2	2.45	0.48
1:C:98:ASN:N	1:C:98:ASN:HD22	2.09	0.48
1:C:167:SER:HB3	1:C:180:PRO:HD3	1.95	0.48
2:D:146:MET:CE	2:D:208:PHE:HE1	2.26	0.48
2:D:495:THR:HG22	2:D:499:ASN:HD22	1.78	0.48
3:E:38:CYS:HB3	3:E:102:VAL:HG13	1.95	0.48
3:F:255:ILE:O	3:F:255:ILE:HG22	2.12	0.48
3:G:2:MET:HB2	3:G:119:LEU:O	2.13	0.48
2:B:422:TYR:OH	2:B:433:LEU:HD11	2.13	0.48
2:D:12:TYR:CD2	2:D:12:TYR:O	2.66	0.48
2:D:199:ASN:HD22	2:D:199:ASN:N	2.10	0.48
3:E:9:GLY:C	3:E:15:LYS:HE3	2.39	0.48
1:A:58:THR:HG22	1:A:59:ILE:N	2.28	0.48
2:B:278:GLN:H	2:B:278:GLN:HG2	1.50	0.48
1:C:66:GLY:HA2	1:C:70:VAL:HG13	1.95	0.48
3:G:115:TYR:O	3:G:117:ASP:N	2.38	0.48
3:H:23:VAL:HG21	3:H:35:ILE:CD1	2.28	0.48
1:A:167:SER:HB3	1:A:178:ILE:HG22	1.94	0.48
2:B:186:THR:N	2:B:187:PRO:HD3	2.29	0.48
1:C:251:ALA:HA	1:C:261:GLU:CG	2.41	0.48
1:C:430:ILE:HG12	2:D:269:PHE:HE1	1.75	0.48
1:C:469:ASN:CG	1:C:470:PRO:HD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:165:SER:HA	3:H:168:ILE:HD12	1.96	0.48
1:C:245:MET:CE	1:C:309:LEU:HD22	2.43	0.48
2:B:471:PHE:CE2	2:B:472:PRO:HD3	2.41	0.48
2:D:238:ARG:NH1	2:D:262:ASP:OD2	2.46	0.48
3:E:156:MET:HG2	3:E:157:ALA:N	2.29	0.48
2:B:388:CYS:O	2:B:390:PRO:HD3	2.14	0.48
1:C:389:ARG:HG3	1:C:389:ARG:NH1	2.11	0.48
2:D:146:MET:HE3	2:D:208:PHE:CZ	2.48	0.48
2:D:479:LEU:N	2:D:479:LEU:HD12	2.28	0.48
3:G:14:GLY:HA3	3:G:185:ASN:ND2	2.29	0.48
3:G:260:THR:O	3:G:261:MET:C	2.56	0.48
1:A:81:ILE:HD12	1:A:148:ILE:HG21	1.95	0.48
1:A:324:CYS:SG	1:A:328:ILE:HD11	2.53	0.48
1:A:351:VAL:HG23	1:A:420:LEU:HB3	1.95	0.48
1:A:373:GLU:O	1:A:373:GLU:HG3	2.12	0.48
2:B:81:GLY:HA3	2:B:257:PRO:HD3	1.96	0.48
2:B:192:SER:OG	2:B:194:VAL:HG22	2.14	0.48
2:B:247:MET:HA	2:B:341:PRO:HG3	1.96	0.48
2:B:362:LEU:HD11	2:B:498:VAL:CG2	2.42	0.48
2:D:20:TYR:O	2:D:24:LEU:HG	2.13	0.48
3:E:72:LEU:HD11	3:E:76:LEU:CD1	2.44	0.48
3:E:160:ALA:HA	3:E:163:ASN:HB3	1.96	0.48
1:A:119:GLN:OE1	1:A:119:GLN:HA	2.12	0.48
2:B:247:MET:CE	2:B:340:ILE:HA	2.44	0.48
2:B:475:ASP:HA	2:D:523:ARG:HG3	1.95	0.48
1:C:355:ILE:HG21	1:C:359:ARG:HB2	1.96	0.48
2:D:14:LEU:C	2:D:14:LEU:HD12	2.38	0.48
2:D:146:MET:HG2	2:D:180:PRO:O	2.13	0.48
3:G:72:LEU:HD11	3:G:76:LEU:CD1	2.43	0.48
3:H:151:CYS:SG	3:H:196:ILE:HD12	2.54	0.48
2:B:108:ARG:NH2	2:B:477:HIS:CD2	2.82	0.47
2:B:181:VAL:O	2:B:181:VAL:HG12	2.12	0.47
1:C:428:LYS:O	1:C:432:GLN:HG3	2.14	0.47
1:C:457:ALA:CB	2:D:3:GLN:HG2	2.44	0.47
3:F:16:SER:O	3:F:20:GLN:HG3	2.13	0.47
3:G:132:CYS:HB2	3:H:96:GLY:O	2.14	0.47
1:A:240:ILE:HG23	1:A:241:LEU:N	2.29	0.47
1:A:280:ASN:ND2	1:A:280:ASN:H	2.10	0.47
1:A:399:LEU:C	1:A:400:LEU:HD12	2.40	0.47
2:B:86:MET:HG2	2:B:138:CYS:SG	2.55	0.47
1:C:138:VAL:O	1:C:142:PHE:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ALA:HB1	2:D:5:VAL:HG21	1.96	0.47
2:D:89:VAL:HG22	2:D:150:SER:HB2	1.96	0.47
2:D:238:ARG:HH21	2:D:238:ARG:HG3	1.78	0.47
3:E:22:LEU:HD23	3:E:22:LEU:O	2.14	0.47
3:F:213:ARG:HG2	9:F:6292:ATP:C2	2.49	0.47
3:H:56:THR:CG2	3:H:59:GLU:HB2	2.28	0.47
1:A:89:GLY:C	1:A:113:ASN:HD21	2.22	0.47
1:A:301:GLY:HA2	1:A:456:PHE:CD1	2.48	0.47
2:B:142:TYR:CD2	2:B:271:MET:HE1	2.49	0.47
2:B:179:PHE:C	2:B:179:PHE:CD2	2.93	0.47
2:B:180:PRO:HG2	2:B:278:GLN:OE1	2.14	0.47
2:B:254:LEU:O	2:B:255:SER:HB3	2.14	0.47
2:B:475:ASP:HA	2:D:523:ARG:CG	2.44	0.47
1:C:142:PHE:O	1:C:145:ASN:ND2	2.47	0.47
1:C:277:ARG:HD2	1:C:386:ASP:OD2	2.14	0.47
2:D:192:SER:OG	2:D:194:VAL:HG22	2.14	0.47
2:D:379:LEU:HD21	2:D:443:ILE:HG21	1.95	0.47
3:E:106:ILE:HD12	3:E:137:MET:HB3	1.95	0.47
3:G:212:PRO:C	3:G:236:GLN:HE22	2.22	0.47
3:H:179:LEU:HD23	3:H:181:GLY:H	1.79	0.47
1:A:16:VAL:HG21	1:A:412:PHE:CE1	2.48	0.47
1:A:64:TYR:C	1:A:66:GLY:N	2.71	0.47
1:A:355:ILE:CG2	5:A:1496:CFM:S3A	3.02	0.47
1:A:449:PRO:O	1:A:455:GLY:HA2	2.13	0.47
2:B:71:GLN:HG2	2:B:192:SER:O	2.15	0.47
2:B:139:LYS:CG	2:B:179:PHE:CE1	2.97	0.47
1:C:219:THR:HG23	1:C:220:PRO:HD2	1.96	0.47
1:C:302:PRO:O	1:C:306:ILE:HG13	2.15	0.47
2:D:198:ASP:CG	2:D:298:LEU:HA	2.40	0.47
2:D:217:VAL:O	2:D:286:ASN:HA	2.14	0.47
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.95	0.47
2:D:509:THR:HA	2:D:515:THR:HB	1.96	0.47
1:C:90:GLN:HE22	2:D:66:PRO:C	2.21	0.47
1:C:361:ARG:HB3	1:C:379:TYR:OH	2.13	0.47
3:E:236:GLN:CG	3:E:236:GLN:O	2.62	0.47
3:H:179:LEU:HD12	3:H:256:PRO:HG3	1.96	0.47
1:A:118:PHE:CZ	1:A:156:ILE:HD11	2.49	0.47
1:A:399:LEU:HD23	1:A:416:ILE:HD11	1.97	0.47
1:A:424:GLY:CA	1:A:442:HIS:HD2	2.27	0.47
1:A:427:GLU:HB2	1:A:431:PHE:HE1	1.78	0.47
2:B:382:PHE:HD1	2:B:385:GLU:OE2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:HIS:CG	2:B:433:LEU:HD12	2.49	0.47
2:B:522:VAL:HB	2:D:474:PHE:HB3	1.96	0.47
1:C:203:ARG:HG3	1:C:204:ASP:OD2	2.15	0.47
2:D:369:LEU:HD23	2:D:369:LEU:O	2.14	0.47
2:D:509:THR:O	2:D:516:ASP:HA	2.15	0.47
3:E:155:MET:HE1	3:E:261:MET:HE3	1.95	0.47
3:F:3:ARG:NH2	3:F:146:GLU:OE1	2.43	0.47
3:G:34:MET:HB2	3:G:119:LEU:HD13	1.96	0.47
1:A:57:MET:SD	2:B:113:CYS:O	2.73	0.47
1:A:58:THR:CG2	1:A:60:ARG:H	2.20	0.47
1:A:100:TYR:CD2	1:A:100:TYR:N	2.83	0.47
1:A:144:LEU:HG	2:B:43:VAL:HG21	1.96	0.47
1:A:168:LYS:O	1:A:172:ALA:CB	2.61	0.47
1:A:210:ARG:HH11	1:A:264:LEU:CD2	2.26	0.47
1:A:303:THR:HG22	1:A:369:ASP:CG	2.39	0.47
2:B:71:GLN:O	2:B:196:GLY:HA3	2.15	0.47
2:B:367:PHE:CD2	2:B:443:ILE:HD11	2.49	0.47
2:B:492:GLN:O	2:B:493:ILE:C	2.58	0.47
2:B:512:MET:CB	2:D:457:HIS:CD2	2.92	0.47
1:C:60:ARG:HG2	1:C:380:GLU:O	2.14	0.47
1:C:138:VAL:HG23	1:C:139:GLU:N	2.30	0.47
1:C:168:LYS:O	1:C:172:ALA:HB2	2.15	0.47
1:C:346:LEU:HB3	1:C:372:MET:CG	2.45	0.47
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.50	0.47
2:D:254:LEU:O	2:D:255:SER:HB3	2.14	0.47
3:E:57:ILE:HD12	3:E:105:ALA:HB1	1.96	0.47
3:E:207:MET:HE3	3:E:210:PHE:HB2	1.95	0.47
3:F:26:LEU:CD1	3:F:244:ALA:HB1	2.43	0.47
3:F:223:ARG:O	3:F:223:ARG:HG2	2.14	0.47
3:G:50:HIS:O	3:G:51:SER:HB3	2.14	0.47
3:G:137:MET:O	3:G:143:LYS:HG3	2.15	0.47
3:G:147:ILE:HD11	3:G:177:VAL:HG21	1.97	0.47
3:G:180:GLY:HA2	3:G:253:LEU:HD23	1.96	0.47
1:A:359:ARG:O	1:A:363:VAL:HG13	2.15	0.47
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.96	0.47
2:B:495:THR:HG22	2:B:499:ASN:ND2	2.30	0.47
1:C:373:GLU:O	1:C:373:GLU:HG3	2.15	0.47
1:C:442:HIS:HA	5:C:3496:CFM:S4B	2.55	0.47
2:D:96:VAL:CG1	2:D:113:CYS:SG	3.03	0.47
2:D:426:ASP:OD1	2:D:426:ASP:C	2.57	0.47
3:E:39:ASP:OD1	3:E:40:PRO:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:GLU:HG2	3:F:253:LEU:CD2	2.45	0.47
3:G:199:LEU:CD1	3:G:259:ILE:HD11	2.45	0.47
1:A:145:ASN:ND2	1:A:147:GLY:H	2.13	0.47
1:A:158:LEU:HD21	2:B:123:ALA:HB1	1.96	0.47
1:A:253:TRP:CZ3	1:A:282:ILE:HG12	2.49	0.47
1:A:426:LYS:HA	2:B:104:ASN:HD21	1.79	0.47
1:C:20:TYR:OH	1:C:408:GLU:CG	2.56	0.47
1:C:97:ARG:NH1	1:C:446:TYR:CA	2.74	0.47
1:C:413:VAL:HG21	1:C:431:PHE:CE2	2.49	0.47
1:C:464:ASP:OD1	1:C:468:ASN:ND2	2.48	0.47
2:D:90:HIS:HA	2:D:116:ASP:OD1	2.15	0.47
2:D:284:ALA:CB	2:D:285:PRO:CD	2.92	0.47
3:F:43:ASP:N	3:F:43:ASP:OD1	2.47	0.47
3:G:115:TYR:C	3:G:117:ASP:N	2.64	0.47
3:G:195:LEU:HD21	3:G:268:LEU:CD2	2.45	0.47
3:G:223:ARG:HD2	3:G:230:TYR:CE1	2.50	0.47
1:A:428:LYS:HG2	1:A:438:PHE:CD2	2.50	0.47
2:B:106:HIS:CE1	2:B:471:PHE:HD1	2.32	0.47
2:B:163:ASN:OD1	2:B:167:ASN:ND2	2.48	0.47
1:C:207:LEU:HD11	1:C:266:PRO:CG	2.45	0.47
2:D:456:LEU:CD1	2:D:460:LYS:HD2	2.44	0.47
3:H:57:ILE:CG1	3:H:75:VAL:HG11	2.45	0.47
1:C:236:TRP:O	2:D:23:MET:HE1	2.15	0.46
3:F:29:MET:HE2	3:F:244:ALA:HB1	1.97	0.46
3:F:46:ARG:NH2	3:F:221:GLU:HG3	2.30	0.46
3:G:216:VAL:O	3:G:216:VAL:HG12	2.15	0.46
3:H:207:MET:HE3	3:H:210:PHE:HB2	1.97	0.46
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.55	0.46
2:B:57:PHE:C	2:B:59:ARG:H	2.22	0.46
2:B:380:VAL:O	2:B:383:LEU:HB2	2.15	0.46
2:B:506:ASP:O	2:B:510:ARG:HB2	2.15	0.46
2:D:86:MET:HE1	2:D:112:SER:HB2	1.97	0.46
2:D:105:ARG:HB2	2:D:474:PHE:CE2	2.50	0.46
2:D:370:TRP:HA	2:D:394:LEU:O	2.15	0.46
3:E:250:ASN:ND2	3:E:252:LEU:H	2.14	0.46
3:G:148:TYR:CE2	3:G:208:ILE:CD1	2.99	0.46
1:A:86:VAL:HG21	2:B:68:LYS:HE2	1.97	0.46
1:A:245:MET:HG3	1:A:324:CYS:HA	1.97	0.46
1:A:352:MET:CE	1:A:418:PRO:HG2	2.45	0.46
2:B:238:ARG:CD	2:B:258:GLU:CG	2.90	0.46
2:B:256:ASP:C	2:B:256:ASP:OD1	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:VAL:O	2:B:380:VAL:HG23	2.14	0.46
1:C:91:TYR:OH	2:D:73:LEU:HB2	2.15	0.46
1:C:428:LYS:HG3	1:C:438:PHE:CD2	2.51	0.46
2:D:163:ASN:OD1	2:D:167:ASN:ND2	2.49	0.46
2:D:493:ILE:O	2:D:497:LEU:HG	2.14	0.46
3:E:260:THR:O	3:E:261:MET:C	2.58	0.46
3:G:19:THR:O	3:G:23:VAL:HG22	2.16	0.46
1:C:64:TYR:HB2	6:D:3498:CLF:S3A	2.56	0.46
1:C:150:VAL:O	1:C:181:VAL:HG12	2.15	0.46
1:C:203:ARG:NE	1:C:204:ASP:OD2	2.48	0.46
2:D:62:LEU:CD2	2:D:64:VAL:HG23	2.46	0.46
3:F:225:MET:HE2	3:F:230:TYR:HA	1.97	0.46
1:A:48:SER:HB3	1:A:387:TYR:CE1	2.51	0.46
2:B:226:ILE:O	2:B:228:PRO:HD3	2.15	0.46
2:B:318:ILE:O	2:B:318:ILE:HG23	2.15	0.46
2:B:401:ARG:HB2	2:B:401:ARG:HH11	1.81	0.46
3:H:41:LYS:O	3:H:42:ALA:HB3	2.15	0.46
3:H:187:ARG:O	3:H:188:ASN:HB3	2.16	0.46
3:H:208:ILE:HG22	3:H:209:HIS:N	2.30	0.46
1:A:142:PHE:N	1:A:143:PRO:HD3	2.31	0.46
1:A:358:LEU:HD12	1:A:361:ARG:HH21	1.80	0.46
1:A:385:ASP:OD1	1:A:386:ASP:OD1	2.33	0.46
2:B:326:ASP:O	2:B:330:MET:HG3	2.15	0.46
1:C:229:TYR:N	1:C:229:TYR:CD1	2.83	0.46
1:C:276:TYR:O	1:C:276:TYR:CG	2.68	0.46
2:D:369:LEU:HD12	2:D:379:LEU:HD23	1.97	0.46
2:D:492:GLN:O	2:D:493:ILE:C	2.56	0.46
3:E:100:ARG:HD2	3:E:100:ARG:C	2.40	0.46
3:E:148:TYR:CE2	3:E:208:ILE:CD1	2.99	0.46
3:E:207:MET:HE1	3:E:210:PHE:HB2	1.96	0.46
3:F:73:GLU:OE1	3:F:73:GLU:N	2.45	0.46
3:H:61:ALA:HB2	3:H:70:LEU:HD12	1.96	0.46
3:H:66:THR:O	3:H:69:ASP:HB2	2.15	0.46
1:A:98:ASN:H	1:A:98:ASN:HD22	1.61	0.46
1:A:131:LEU:HD13	1:A:131:LEU:C	2.40	0.46
2:B:474:PHE:HB3	2:D:522:VAL:HB	1.96	0.46
3:G:39:ASP:OD1	3:G:40:PRO:N	2.49	0.46
3:H:39:ASP:OD2	3:H:41:LYS:HB2	2.16	0.46
3:H:76:LEU:HD21	3:H:84:LYS:HD3	1.97	0.46
3:H:187:ARG:HH21	3:H:195:LEU:HD22	1.80	0.46
1:A:90:GLN:NE2	2:B:447:TYR:CE1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:HB3	1:A:166:VAL:CG2	2.41	0.46
1:A:131:LEU:CD1	1:A:166:VAL:HG11	2.45	0.46
1:A:405:THR:O	1:A:406:GLY:C	2.57	0.46
1:A:425:ILE:HG22	4:A:1494:HCA:C6	2.46	0.46
2:B:84:LYS:HD3	2:B:145:ASP:CG	2.41	0.46
1:C:51:LYS:HE3	2:D:119:THR:OG1	2.15	0.46
2:D:90:HIS:HB3	2:D:150:SER:O	2.15	0.46
2:D:448:GLY:O	2:D:466:LEU:HD22	2.15	0.46
3:F:57:ILE:HG13	3:F:87:GLU:O	2.16	0.46
3:G:212:PRO:O	9:G:7292:ATP:N6	2.44	0.46
3:H:183:ILE:HD13	3:H:243:LEU:HD11	1.98	0.46
1:A:458:ILE:HG22	1:A:462:ASP:OD2	2.16	0.46
2:B:222:LYS:HA	2:B:288:LEU:CD2	2.46	0.46
2:B:227:VAL:HG12	2:B:298:LEU:CD1	2.45	0.46
2:B:257:PRO:HB3	2:B:261:LEU:HD22	1.98	0.46
1:C:58:THR:CG2	1:C:60:ARG:HB2	2.45	0.46
3:G:179:LEU:CD1	3:G:256:PRO:HG3	2.46	0.46
3:H:129:ASP:HB3	3:H:131:VAL:HG12	1.98	0.46
3:H:181:GLY:HA2	3:H:205:THR:OG1	2.16	0.46
1:A:22:GLU:HA	1:A:25:ARG:HB3	1.98	0.46
2:B:318:ILE:HD12	2:B:374:ASP:HB3	1.98	0.46
1:C:144:LEU:CD2	2:D:43:VAL:HG21	2.46	0.46
1:C:168:LYS:O	1:C:172:ALA:CB	2.64	0.46
1:C:186:PHE:CE1	3:G:100:ARG:NH2	2.81	0.46
1:C:302:PRO:HG3	1:C:335:TRP:HB2	1.98	0.46
1:C:449:PRO:O	1:C:455:GLY:HA2	2.16	0.46
2:D:418:ASN:O	2:D:418:ASN:ND2	2.49	0.46
3:E:58:MET:SD	3:E:104:THR:HG21	2.56	0.46
2:B:147:ILE:O	2:B:181:VAL:HA	2.15	0.45
2:B:390:PRO:O	2:B:419:ALA:CB	2.64	0.45
2:D:38:ASP:O	2:D:42:GLU:HG3	2.16	0.45
2:D:142:TYR:C	2:D:144:PRO:CD	2.88	0.45
2:D:146:MET:HE2	2:D:208:PHE:HZ	1.75	0.45
2:D:179:PHE:C	2:D:179:PHE:CD2	2.94	0.45
3:E:50:HIS:O	3:E:51:SER:HB3	2.15	0.45
3:E:72:LEU:HD11	3:E:76:LEU:HD12	1.98	0.45
3:H:72:LEU:HD11	3:H:76:LEU:HD12	1.98	0.45
1:A:297:TYR:HB2	1:A:308:SER:OG	2.16	0.45
2:B:227:VAL:HB	2:B:292:LEU:HD23	1.97	0.45
1:C:165:SER:O	1:C:168:LYS:HB2	2.16	0.45
1:C:380:GLU:HG3	1:C:381:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:VAL:O	2:D:383:LEU:HB2	2.17	0.45
2:D:399:ASN:OD1	2:D:399:ASN:C	2.60	0.45
1:A:272:LEU:HD13	1:A:312:ILE:HD13	1.98	0.45
2:B:329:LEU:CD1	2:B:344:LEU:HD13	2.41	0.45
2:B:512:MET:HE2	2:D:457:HIS:CD2	2.51	0.45
2:B:512:MET:HE1	2:D:44:PHE:HE1	1.80	0.45
1:C:144:LEU:HD22	2:D:35:TYR:CD1	2.51	0.45
1:C:239:ARG:HD3	2:D:23:MET:SD	2.55	0.45
2:D:257:PRO:HB3	2:D:261:LEU:HD22	1.98	0.45
3:H:192:GLU:HA	3:H:195:LEU:HB3	1.98	0.45
1:A:56:LEU:O	1:A:405:THR:HB	2.16	0.45
1:A:219:THR:HG22	1:A:221:TYR:N	2.21	0.45
1:A:245:MET:CE	1:A:309:LEU:HD22	2.47	0.45
2:B:67:ALA:HB3	2:B:396:HIS:HB2	1.98	0.45
1:C:46:ILE:HG12	1:C:47:ILE:N	2.31	0.45
1:C:359:ARG:O	1:C:363:VAL:HG13	2.16	0.45
2:D:221:ASN:CG	2:D:223:LYS:HD3	2.41	0.45
3:G:8:TYR:HD2	3:G:130:VAL:HG22	1.82	0.45
1:A:42:SER:O	1:A:43:LYS:C	2.60	0.45
1:A:239:ARG:HD3	2:B:23:MET:SD	2.57	0.45
1:C:298:ASN:CB	1:C:362:HIS:NE2	2.79	0.45
2:D:56:ASN:O	2:D:59:ARG:CB	2.64	0.45
3:E:136:ALA:HB2	3:F:94:GLY:HA2	1.98	0.45
3:F:23:VAL:HG12	3:F:33:VAL:HG11	1.99	0.45
3:H:8:TYR:CE1	3:H:126:VAL:HG21	2.52	0.45
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.84	0.45
1:A:189:VAL:CG2	1:A:190:SER:N	2.76	0.45
1:A:367:TYR:O	1:A:368:GLU:C	2.59	0.45
2:B:32:GLU:O	2:B:33:GLU:C	2.59	0.45
2:B:90:HIS:O	2:B:151:THR:HA	2.16	0.45
2:B:119:THR:HG22	2:B:120:GLU:N	2.31	0.45
2:B:472:PRO:HB3	2:B:474:PHE:CE2	2.51	0.45
1:C:58:THR:CG2	1:C:59:ILE:N	2.79	0.45
1:C:239:ARG:HD3	2:D:23:MET:CG	2.47	0.45
2:D:79:ALA:O	2:D:80:LEU:C	2.58	0.45
2:D:330:MET:O	2:D:333:SER:HB3	2.16	0.45
3:F:38:CYS:HB3	3:F:102:VAL:HG13	1.98	0.45
3:F:113:GLY:HA2	3:F:116:GLU:OE1	2.17	0.45
3:G:4:GLN:HE21	3:G:124:TYR:HE2	1.65	0.45
3:H:43:ASP:OD1	3:H:43:ASP:N	2.49	0.45
3:H:103:ILE:HA	3:H:137:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TYR:O	1:A:280:ASN:CB	2.64	0.45
1:A:360:PRO:HB2	1:A:379:TYR:CZ	2.52	0.45
1:A:448:GLY:HA3	1:A:458:ILE:HD13	1.98	0.45
2:B:14:LEU:HD12	2:B:14:LEU:C	2.41	0.45
2:B:56:ASN:O	2:B:59:ARG:HD3	2.17	0.45
2:B:85:THR:HA	2:B:146:MET:O	2.17	0.45
2:B:234:LEU:O	2:B:238:ARG:HG2	2.17	0.45
1:C:81:ILE:HD12	1:C:148:ILE:HG21	1.98	0.45
2:D:233:TYR:CB	2:D:236:ASN:HD22	2.25	0.45
3:E:25:ALA:HB2	3:E:228:ILE:CD1	2.47	0.45
3:E:233:LYS:O	3:E:234:ALA:C	2.59	0.45
3:F:3:ARG:HG3	3:F:3:ARG:NH1	2.31	0.45
1:A:35:ASN:ND2	1:A:394:MET:CB	2.80	0.45
1:A:36:ASP:O	1:A:38:ALA:N	2.50	0.45
1:A:98:ASN:ND2	1:A:98:ASN:N	2.57	0.45
1:A:343:ARG:N	1:A:344:PRO:CD	2.80	0.45
1:A:350:ARG:O	1:A:419:ASP:OD1	2.35	0.45
1:A:381:PHE:CZ	5:A:1496:CFM:S2B	3.10	0.45
2:B:122:ALA:O	2:B:126:GLY:N	2.48	0.45
1:C:457:ALA:HB3	2:D:3:GLN:HG2	1.99	0.45
2:D:91:GLY:CA	2:D:118:MET:HE2	2.40	0.45
2:D:146:MET:HE3	2:D:208:PHE:HZ	1.79	0.45
2:D:146:MET:HE1	2:D:208:PHE:HE1	1.82	0.45
3:F:3:ARG:NH1	3:F:121:PHE:CZ	2.84	0.45
3:F:217:VAL:HG11	9:F:6292:ATP:N7	2.32	0.45
3:H:9:GLY:C	3:H:15:LYS:HE3	2.41	0.45
1:A:90:GLN:N	1:A:113:ASN:HD21	2.15	0.45
1:A:190:SER:HB2	1:A:381:PHE:HB3	1.99	0.45
1:C:167:SER:HB3	1:C:178:ILE:HG22	1.98	0.45
1:C:337:ALA:CB	2:D:5:VAL:HG21	2.46	0.45
1:C:448:GLY:HA3	1:C:458:ILE:HD13	1.99	0.45
2:D:137:ASN:HD22	2:D:137:ASN:N	2.14	0.45
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.50	0.45
2:D:284:ALA:CB	2:D:285:PRO:HD3	2.45	0.45
3:E:244:ALA:O	3:E:248:VAL:HG23	2.17	0.45
1:A:236:TRP:O	2:B:23:MET:HE1	2.16	0.45
2:B:70:CYS:HB2	2:B:72:PRO:HD2	1.99	0.45
1:C:37:PRO:HD2	1:C:396:ASP:OD1	2.17	0.45
1:C:221:TYR:CE2	1:C:320:ILE:HD11	2.52	0.45
1:C:295:MET:HE1	1:C:311:ALA:HB1	1.99	0.45
1:C:297:TYR:HB2	1:C:308:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:HIS:CE1	2:D:116:ASP:OD2	2.70	0.45
2:D:277:THR:O	2:D:280:GLU:HB3	2.16	0.45
2:D:497:LEU:O	2:D:500:SER:N	2.50	0.45
3:H:231:ASP:OD2	3:H:234:ALA:N	2.50	0.45
1:C:260:SER:HB2	2:D:33:GLU:OE1	2.17	0.44
2:D:147:ILE:O	2:D:181:VAL:HA	2.16	0.44
3:F:149:ILE:O	3:F:182:LEU:HA	2.16	0.44
3:G:160:ALA:O	3:G:164:ILE:HG13	2.17	0.44
3:G:257:ASN:O	3:G:258:PRO:C	2.60	0.44
3:H:51:SER:O	3:H:52:LYS:C	2.59	0.44
1:A:9:VAL:O	1:A:12:LEU:HB3	2.16	0.44
1:A:35:ASN:HB3	1:A:398:THR:OG1	2.16	0.44
1:A:219:THR:C	1:A:221:TYR:N	2.75	0.44
1:A:253:TRP:CH2	1:A:282:ILE:HG12	2.52	0.44
1:A:310:ARG:O	1:A:313:ALA:HB3	2.17	0.44
2:B:512:MET:HG2	2:D:457:HIS:CD2	2.52	0.44
1:C:124:VAL:O	3:H:97:CYS:N	2.42	0.44
1:C:232:GLY:O	1:C:449:PRO:HG3	2.17	0.44
2:D:426:ASP:OD1	2:D:428:TRP:N	2.49	0.44
3:E:136:ALA:HB2	3:F:94:GLY:HA3	1.99	0.44
3:E:225:MET:CE	3:E:230:TYR:HA	2.47	0.44
3:H:220:ALA:HB1	3:H:225:MET:O	2.17	0.44
1:A:306:ILE:HD11	1:A:335:TRP:NE1	2.33	0.44
2:B:179:PHE:C	2:B:179:PHE:HD2	2.25	0.44
2:B:284:ALA:HB3	2:B:285:PRO:HD3	2.00	0.44
2:D:81:GLY:HA3	2:D:257:PRO:HD3	2.00	0.44
3:E:129:ASP:CB	3:E:131:VAL:HG12	2.47	0.44
3:G:43:ASP:OD1	3:G:43:ASP:N	2.50	0.44
9:G:7292:ATP:H4'	3:H:156:MET:SD	2.57	0.44
3:H:236:GLN:HE22	9:H:8292:ATP:N6	2.15	0.44
1:A:144:LEU:HD21	2:B:43:VAL:HG21	1.99	0.44
2:B:67:ALA:HB3	2:B:396:HIS:CB	2.46	0.44
2:B:278:GLN:O	2:B:279:GLU:C	2.60	0.44
2:B:353:ASP:OD2	2:D:109:GLU:OE2	2.35	0.44
2:D:14:LEU:HD12	2:D:14:LEU:O	2.17	0.44
2:D:133:ASP:O	2:D:136:GLN:N	2.50	0.44
2:D:369:LEU:CD2	2:D:369:LEU:N	2.80	0.44
2:D:426:ASP:H	2:D:429:HIS:CE1	2.36	0.44
3:E:49:LEU:O	3:E:50:HIS:HB2	2.17	0.44
3:E:148:TYR:CE2	3:E:208:ILE:HD12	2.52	0.44
3:G:10:LYS:O	3:G:11:GLY:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:A:383:HIS:CD2	2.84	0.44
1:A:417:LYS:N	1:A:418:PRO:CD	2.78	0.44
2:B:12:TYR:OH	2:D:508:GLU:HB3	2.17	0.44
2:B:168:ASN:O	2:B:172:GLU:HB2	2.17	0.44
2:B:314:PRO:HB3	2:B:316:LEU:CD1	2.46	0.44
1:C:198:ALA:O	1:C:199:ASN:C	2.60	0.44
1:C:265:THR:HG22	1:C:286:MET:CE	2.48	0.44
1:C:280:ASN:ND2	1:C:280:ASN:H	2.14	0.44
2:D:285:PRO:HG3	2:D:309:TRP:CD1	2.53	0.44
3:E:10:LYS:NZ	3:E:156:MET:HG3	2.29	0.44
3:G:98:ALA:C	3:G:100:ARG:N	2.75	0.44
3:H:138:PRO:O	3:H:143:LYS:HB3	2.17	0.44
3:H:152:SER:C	3:H:196:ILE:HD11	2.43	0.44
3:H:213:ARG:HG3	9:H:8292:ATP:H2	1.83	0.44
1:A:57:MET:HG2	2:B:142:TYR:CE1	2.53	0.44
1:A:100:TYR:OH	1:A:111:THR:HG23	2.16	0.44
2:B:88:TYR:O	2:B:150:SER:N	2.50	0.44
1:C:35:ASN:HD21	1:C:394:MET:HB2	1.83	0.44
1:C:59:ILE:CD1	1:C:427:GLU:OE2	2.58	0.44
1:C:219:THR:C	1:C:221:TYR:N	2.76	0.44
3:E:64:ALA:HB1	3:E:69:ASP:HB3	1.99	0.44
3:E:165:SER:HA	3:E:168:ILE:HD12	2.00	0.44
3:F:102:VAL:HG21	3:F:135:PHE:CE1	2.53	0.44
3:H:110:GLU:OE2	3:H:143:LYS:NZ	2.51	0.44
1:A:475:LEU:HD13	2:B:265:ALA:O	2.17	0.44
2:B:143:LYS:N	2:B:144:PRO:CD	2.80	0.44
2:B:251:TYR:CD1	2:B:251:TYR:C	2.95	0.44
1:C:193:LEU:HG	1:C:197:ILE:HD11	1.98	0.44
2:D:365:LYS:HG3	2:D:501:ILE:CD1	2.47	0.44
3:E:6:ALA:HA	3:E:124:TYR:HB2	1.99	0.44
3:E:115:TYR:C	3:E:117:ASP:N	2.72	0.44
3:F:195:LEU:CD1	3:F:267:LEU:HD22	2.48	0.44
3:G:189:THR:CG2	3:G:190:ASP:H	2.15	0.44
3:G:225:MET:HE2	3:G:230:TYR:HA	2.00	0.44
1:A:36:ASP:C	1:A:38:ALA:H	2.26	0.44
1:A:57:MET:HG3	2:B:142:TYR:CZ	2.53	0.44
1:A:107:ASN:ND2	1:A:107:ASN:C	2.74	0.44
1:A:274:HIS:HB2	1:A:297:TYR:CE2	2.52	0.44
2:B:158:ILE:HG22	3:E:97:CYS:HB2	2.00	0.44
1:C:70:VAL:CG2	1:C:71:VAL:HG23	2.47	0.44
2:D:79:ALA:C	2:D:81:GLY:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:VAL:HG22	3:G:100:ARG:HG3	2.00	0.44
3:E:86:VAL:HG21	3:E:109:LEU:HD11	2.00	0.44
3:F:4:GLN:HB2	3:F:144:ALA:HA	2.00	0.44
3:F:159:TYR:HA	3:F:264:LEU:HD11	2.00	0.44
3:G:33:VAL:HG12	3:G:34:MET:N	2.33	0.44
3:G:198:ALA:HB1	3:G:267:LEU:HD21	2.00	0.44
3:H:25:ALA:O	3:H:28:GLU:HB3	2.17	0.44
3:H:50:HIS:HE1	3:H:225:MET:HB3	1.81	0.44
2:B:41:ASP:O	2:B:45:GLN:HG2	2.18	0.44
2:B:204:ILE:O	2:B:205:ALA:C	2.61	0.44
1:C:151:GLN:CD	1:C:181:VAL:HG11	2.43	0.44
2:D:219:GLY:HA2	2:D:287:ALA:C	2.43	0.44
2:D:278:GLN:H	2:D:278:GLN:HG2	1.51	0.44
2:D:456:LEU:HD13	2:D:463:GLU:CD	2.43	0.44
2:D:479:LEU:N	2:D:479:LEU:CD1	2.81	0.44
3:F:76:LEU:HD21	3:F:84:LYS:HB3	1.99	0.44
3:G:39:ASP:OD1	3:G:40:PRO:CD	2.66	0.44
3:H:23:VAL:O	3:H:27:ALA:N	2.47	0.44
1:A:181:VAL:HG13	1:A:181:VAL:O	2.18	0.43
1:A:229:TYR:N	1:A:229:TYR:CD1	2.86	0.43
1:A:283:SER:HA	1:A:286:MET:HB2	2.00	0.43
2:B:118:MET:CE	2:B:127:GLY:HA3	2.37	0.43
1:C:168:LYS:HE3	1:C:205:TRP:HH2	1.82	0.43
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.32	0.43
1:C:345:ARG:HD3	1:C:464:ASP:CG	2.42	0.43
1:C:443:SER:C	1:C:445:ASP:N	2.75	0.43
3:F:22:LEU:HD23	3:F:22:LEU:C	2.43	0.43
3:F:46:ARG:HH21	3:F:221:GLU:HG3	1.83	0.43
3:G:86:VAL:HG21	3:G:109:LEU:CD1	2.49	0.43
3:G:91:PRO:HD2	3:G:98:ALA:HB2	1.99	0.43
3:G:165:SER:HA	3:G:168:ILE:HD12	2.00	0.43
1:A:364:ILE:O	1:A:367:TYR:HB2	2.18	0.43
2:B:208:PHE:HB3	2:B:282:LYS:HA	1.98	0.43
2:B:247:MET:HE2	2:B:339:PRO:O	2.18	0.43
2:B:426:ASP:OD1	2:B:428:TRP:N	2.50	0.43
2:B:437:ASP:O	2:B:439:PRO:HD3	2.18	0.43
1:C:90:GLN:NE2	2:D:66:PRO:C	2.75	0.43
1:C:359:ARG:CZ	1:C:444:TRP:CZ2	3.01	0.43
1:C:427:GLU:HB2	1:C:431:PHE:HE1	1.83	0.43
2:D:179:PHE:C	2:D:179:PHE:HD2	2.27	0.43
2:D:375:PHE:CE2	2:D:470:GLY:HA2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:ALA:HB2	3:F:70:LEU:HD12	2.00	0.43
3:F:152:SER:HB2	3:F:187:ARG:HG2	2.00	0.43
3:G:15:LYS:N	9:G:7292:ATP:O1B	2.51	0.43
3:G:61:ALA:HB1	3:G:67:VAL:HA	2.00	0.43
1:A:305:THR:O	1:A:309:LEU:HG	2.17	0.43
2:B:293:LEU:HD22	2:B:319:PRO:HG2	2.00	0.43
1:C:179:VAL:O	1:C:181:VAL:N	2.49	0.43
1:C:283:SER:HA	1:C:286:MET:HB2	2.01	0.43
2:D:49:THR:CG2	2:D:52:TYR:H	2.28	0.43
9:E:5292:ATP:H4'	3:F:156:MET:SD	2.58	0.43
3:H:158:MET:HE1	3:H:195:LEU:HG	1.99	0.43
3:H:206:GLN:NE2	3:H:250:ASN:OD1	2.50	0.43
3:H:255:ILE:O	3:H:255:ILE:HG22	2.16	0.43
1:A:125:PHE:O	1:A:126:GLY:O	2.35	0.43
1:A:433:LYS:HE2	2:D:353:ASP:OD2	2.19	0.43
2:B:175:ILE:O	2:B:175:ILE:HG13	2.18	0.43
2:B:228:PRO:HG3	2:B:253:LEU:HD11	2.00	0.43
2:B:352:VAL:HG11	1:C:475:LEU:HD22	2.01	0.43
1:C:35:ASN:ND2	1:C:394:MET:HB2	2.33	0.43
1:C:138:VAL:CG1	2:D:62:LEU:CD1	2.94	0.43
2:D:53:GLN:OE1	2:D:432:SER:HB3	2.18	0.43
2:D:104:ASN:O	2:D:108:ARG:N	2.44	0.43
2:D:472:PRO:HB3	2:D:474:PHE:CE2	2.54	0.43
3:F:42:ALA:CA	3:F:87:GLU:OE1	2.55	0.43
3:H:48:ILE:HG23	3:H:80:TYR:HB3	2.00	0.43
1:A:57:MET:HG2	2:B:142:TYR:CZ	2.53	0.43
1:A:70:VAL:CG2	1:A:71:VAL:HG23	2.48	0.43
1:A:388:ASP:OD1	1:A:388:ASP:C	2.61	0.43
1:A:431:PHE:CD1	1:A:431:PHE:N	2.87	0.43
2:B:71:GLN:OE1	2:B:195:THR:HG22	2.19	0.43
1:C:97:ARG:NH2	1:C:99:TYR:OH	2.44	0.43
1:C:100:TYR:CD2	1:C:100:TYR:N	2.87	0.43
1:C:219:THR:HG22	1:C:221:TYR:N	2.22	0.43
1:C:312:ILE:O	1:C:316:PHE:CD1	2.71	0.43
2:D:41:ASP:O	2:D:45:GLN:HG2	2.19	0.43
2:D:69:ALA:HB3	2:D:193:HIS:HB3	2.00	0.43
3:E:9:GLY:C	3:E:15:LYS:CE	2.91	0.43
1:A:20:TYR:OH	1:A:408:GLU:CG	2.58	0.43
1:A:240:ILE:O	1:A:244:GLU:HG3	2.18	0.43
1:A:361:ARG:HG2	1:A:362:HIS:N	2.34	0.43
2:B:475:ASP:O	2:D:502:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:THR:O	1:C:391:MET:C	2.61	0.43
2:D:91:GLY:N	2:D:118:MET:HE2	2.34	0.43
2:D:208:PHE:HB3	2:D:282:LYS:HA	2.01	0.43
2:D:227:VAL:HG12	2:D:298:LEU:HD13	2.00	0.43
3:G:208:ILE:HG22	3:G:209:HIS:N	2.33	0.43
1:A:8:GLU:O	1:A:12:LEU:N	2.49	0.43
1:A:76:LYS:HA	1:A:110:VAL:HG23	2.01	0.43
1:A:148:ILE:O	1:A:178:ILE:HA	2.18	0.43
1:A:276:TYR:CD1	1:A:280:ASN:HB3	2.53	0.43
1:A:337:ALA:CB	2:B:5:VAL:HG21	2.49	0.43
2:B:346:LYS:HG3	2:D:264:PRO:CG	2.47	0.43
2:B:369:LEU:N	2:B:369:LEU:HD23	2.33	0.43
1:C:89:GLY:C	1:C:113:ASN:ND2	2.77	0.43
1:C:142:PHE:N	1:C:143:PRO:CD	2.81	0.43
1:C:298:ASN:HD21	1:C:300:PHE:HD1	1.64	0.43
1:C:315:LYS:HD3	1:C:315:LYS:HA	1.72	0.43
1:C:413:VAL:HG11	1:C:431:PHE:HD2	1.84	0.43
3:G:195:LEU:HD11	3:G:268:LEU:HD23	2.01	0.43
3:H:236:GLN:HG2	3:H:240:TYR:CE2	2.53	0.43
1:A:65:ALA:O	1:A:70:VAL:HG13	2.19	0.43
1:A:158:LEU:CD2	2:B:123:ALA:HB1	2.48	0.43
1:A:230:ASN:CG	1:A:230:ASN:O	2.61	0.43
2:B:243:MET:O	2:B:244:LEU:C	2.61	0.43
2:B:381:LYS:C	2:B:381:LYS:CD	2.92	0.43
1:C:57:MET:CG	2:D:142:TYR:CZ	3.01	0.43
1:C:98:ASN:HB3	1:C:229:TYR:O	2.19	0.43
2:D:329:LEU:CD1	2:D:344:LEU:HD13	2.44	0.43
2:D:379:LEU:O	2:D:380:VAL:C	2.61	0.43
3:E:39:ASP:OD1	3:E:39:ASP:C	2.61	0.43
3:E:199:LEU:CD1	3:E:259:ILE:HD11	2.47	0.43
3:F:141:GLU:O	3:F:142:ASN:CB	2.67	0.43
1:A:54:PRO:HB2	2:B:134:GLY:CA	2.48	0.43
2:B:137:ASN:HD22	2:B:137:ASN:N	2.17	0.43
2:B:199:ASN:HD22	2:B:199:ASN:N	2.16	0.43
1:C:107:ASN:C	1:C:107:ASN:HD22	2.27	0.43
1:C:199:ASN:ND2	1:C:279:MET:HE3	2.34	0.43
2:D:238:ARG:HG3	2:D:238:ARG:NH2	2.34	0.43
3:F:19:THR:O	3:F:23:VAL:HG22	2.17	0.43
3:G:6:ALA:HA	3:G:124:TYR:HB2	2.01	0.43
1:A:134:LEU:HG	2:B:62:LEU:HD13	2.00	0.43
1:A:265:THR:HG22	1:A:286:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:LYS:O	2:B:347:GLU:C	2.61	0.43
1:C:88:CYS:HB2	1:C:153:GLU:OE1	2.19	0.43
2:D:124:VAL:HG11	3:G:58:MET:CG	2.46	0.43
2:D:228:PRO:HD2	2:D:254:LEU:O	2.18	0.43
2:D:498:VAL:O	2:D:502:LEU:HG	2.19	0.43
3:F:11:GLY:HA2	3:F:15:LYS:HE3	2.01	0.43
3:G:217:VAL:CG2	9:G:7292:ATP:C2	2.96	0.43
1:A:223:VAL:HG12	1:A:270:LEU:HB3	2.00	0.42
1:A:363:VAL:HG11	1:A:441:MET:HE3	2.01	0.42
1:A:440:GLU:HB2	1:A:445:ASP:HB2	2.00	0.42
2:B:71:GLN:N	2:B:72:PRO:CD	2.81	0.42
2:B:94:GLY:O	2:B:97:ALA:HB3	2.19	0.42
2:B:322:LEU:HD11	2:B:348:ARG:NE	2.34	0.42
2:B:362:LEU:CD1	2:B:498:VAL:HG22	2.47	0.42
1:C:71:VAL:CG1	1:C:198:ALA:HB1	2.40	0.42
1:C:310:ARG:O	1:C:313:ALA:HB3	2.19	0.42
1:C:359:ARG:HH11	1:C:359:ARG:CG	2.27	0.42
1:C:431:PHE:CD1	1:C:431:PHE:N	2.86	0.42
2:D:8:ILE:H	2:D:8:ILE:HG13	1.66	0.42
2:D:64:VAL:O	2:D:426:ASP:CG	2.60	0.42
3:G:139:ILE:HG21	3:G:147:ILE:HD11	2.02	0.42
3:G:160:ALA:O	3:G:161:ALA:C	2.62	0.42
3:G:217:VAL:O	3:G:221:GLU:HB3	2.19	0.42
3:H:33:VAL:HG12	3:H:34:MET:N	2.34	0.42
3:H:67:VAL:HG21	3:H:104:THR:HG21	2.00	0.42
1:A:231:ILE:O	1:A:234:ASP:CG	2.62	0.42
1:A:282:ILE:HD12	1:A:282:ILE:O	2.19	0.42
1:A:363:VAL:O	1:A:367:TYR:HD1	2.02	0.42
2:B:197:TRP:CE3	2:B:298:LEU:HD21	2.53	0.42
2:B:456:LEU:HD13	2:B:463:GLU:CD	2.43	0.42
2:B:498:VAL:O	2:B:502:LEU:HG	2.19	0.42
2:B:502:LEU:HD13	2:D:475:ASP:O	2.18	0.42
1:C:210:ARG:NH2	2:D:33:GLU:OE1	2.47	0.42
1:C:356:GLY:CA	1:C:381:PHE:CE2	3.02	0.42
1:C:383:HIS:N	1:C:383:HIS:ND1	2.67	0.42
2:D:64:VAL:HG12	2:D:428:TRP:HB2	2.01	0.42
1:A:49:ASN:ND2	1:A:189:VAL:HG21	2.34	0.42
1:A:176:LYS:HB2	1:A:176:LYS:HE3	1.84	0.42
1:A:214:THR:C	1:A:216:PHE:H	2.26	0.42
1:A:226:ILE:HG23	1:A:279:MET:HG2	2.01	0.42
1:A:464:ASP:OD1	1:A:468:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:MET:O	2:B:200:MET:HE3	2.19	0.42
2:B:233:TYR:CB	2:B:236:ASN:HD22	2.28	0.42
2:B:443:ILE:HA	2:B:467:ILE:O	2.19	0.42
2:D:201:PHE:O	2:D:202:GLU:C	2.61	0.42
2:D:394:LEU:C	2:D:394:LEU:CD2	2.92	0.42
1:A:302:PRO:HG3	1:A:335:TRP:HB2	2.01	0.42
2:B:19:ASP:OD2	2:B:20:TYR:N	2.51	0.42
2:B:181:VAL:N	2:B:182:PRO:CD	2.83	0.42
1:C:77:ASP:OD2	1:C:77:ASP:N	2.52	0.42
1:C:303:THR:HG22	1:C:369:ASP:CG	2.43	0.42
2:D:200:MET:O	2:D:200:MET:HE3	2.20	0.42
3:E:108:PHE:O	3:E:111:GLU:N	2.52	0.42
3:F:9:GLY:O	3:F:15:LYS:HE2	2.20	0.42
3:F:160:ALA:O	3:F:161:ALA:C	2.63	0.42
3:G:138:PRO:O	3:G:144:ALA:HB3	2.18	0.42
3:H:10:LYS:H	3:H:13:ILE:HD13	1.84	0.42
3:H:145:GLN:HA	3:H:177:VAL:HA	2.01	0.42
3:H:217:VAL:CG2	3:H:236:GLN:HE21	2.32	0.42
1:A:54:PRO:HB3	2:B:116:ASP:HA	2.01	0.42
1:A:114:PHE:HE2	1:A:142:PHE:CE1	2.37	0.42
1:A:193:LEU:HG	1:A:197:ILE:HD11	2.01	0.42
1:A:222:ASP:OD1	1:A:248:ARG:HG2	2.20	0.42
2:B:149:VAL:HG21	2:B:166:ILE:HD11	2.01	0.42
2:B:407:ASP:O	2:B:410:LEU:HB2	2.19	0.42
2:B:510:ARG:NH1	2:D:452:GLN:CD	2.77	0.42
1:C:108:ALA:C	1:C:109:PHE:CD1	2.98	0.42
1:C:274:HIS:HE2	1:C:300:PHE:HE1	1.65	0.42
1:C:363:VAL:O	1:C:367:TYR:HD1	2.01	0.42
1:C:442:HIS:CE1	5:C:3496:CFM:S1B	3.12	0.42
1:C:469:ASN:CG	1:C:470:PRO:CD	2.92	0.42
2:D:3:GLN:OE1	2:D:9:LYS:O	2.37	0.42
2:D:12:TYR:CD2	2:D:12:TYR:C	2.97	0.42
2:D:199:ASN:N	2:D:199:ASN:ND2	2.67	0.42
3:E:101:GLY:O	3:E:102:VAL:C	2.63	0.42
3:F:2:MET:HE3	3:F:4:GLN:HG2	2.02	0.42
3:F:137:MET:HB3	3:F:138:PRO:HD3	2.02	0.42
3:G:99:GLY:O	3:G:134:GLY:HA3	2.19	0.42
1:A:57:MET:SD	2:B:114:VAL:HG12	2.59	0.42
1:A:86:VAL:HG21	2:B:68:LYS:CE	2.49	0.42
1:A:440:GLU:HB2	1:A:445:ASP:CB	2.49	0.42
2:B:201:PHE:O	2:B:202:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:PRO:O	2:B:341:PRO:HD3	2.19	0.42
1:C:109:PHE:CD1	1:C:109:PHE:N	2.87	0.42
1:C:167:SER:HB3	1:C:180:PRO:CD	2.50	0.42
1:C:382:ALA:HB1	1:C:386:ASP:CB	2.49	0.42
1:C:384:ASN:O	1:C:388:ASP:CG	2.62	0.42
3:F:158:MET:O	3:F:159:TYR:C	2.63	0.42
3:F:179:LEU:CB	3:F:256:PRO:HG3	2.49	0.42
3:H:29:MET:HE1	3:H:248:VAL:HG21	2.01	0.42
1:A:219:THR:HG23	1:A:220:PRO:CD	2.49	0.42
1:A:239:ARG:NH2	2:B:27:LYS:HG3	2.35	0.42
1:A:274:HIS:HE1	1:A:299:PHE:H	1.68	0.42
1:A:389:ARG:HG3	1:A:389:ARG:HH11	1.84	0.42
2:B:379:LEU:O	2:B:380:VAL:C	2.63	0.42
2:B:522:VAL:CG2	1:C:446:TYR:CE2	3.03	0.42
1:C:356:GLY:HA2	1:C:381:PHE:CE2	2.55	0.42
1:C:405:THR:CB	1:C:408:GLU:HG3	2.49	0.42
2:D:202:GLU:O	2:D:203:GLY:C	2.63	0.42
2:D:240:ILE:HD13	2:D:240:ILE:HA	1.94	0.42
3:E:36:VAL:HA	3:E:86:VAL:HG23	2.01	0.42
3:E:40:PRO:HG3	3:E:98:ALA:HB1	2.02	0.42
3:E:45:THR:OG1	3:E:49:LEU:HD12	2.18	0.42
3:E:137:MET:CB	3:E:138:PRO:HD3	2.49	0.42
3:F:20:GLN:O	3:F:48:ILE:HD11	2.18	0.42
3:F:179:LEU:HB2	3:F:256:PRO:CG	2.50	0.42
3:G:14:GLY:CA	9:G:7292:ATP:O1B	2.68	0.42
3:H:114:ALA:C	3:H:116:GLU:H	2.27	0.42
1:A:12:LEU:O	1:A:16:VAL:HG23	2.19	0.42
1:A:138:VAL:CG1	2:B:62:LEU:HD22	2.48	0.42
1:A:189:VAL:CG2	1:A:190:SER:H	2.30	0.42
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.85	0.42
2:B:28:ARG:HA	2:B:32:GLU:HG3	2.02	0.42
2:D:74:GLY:HA3	2:D:193:HIS:O	2.19	0.42
3:G:9:GLY:C	3:G:15:LYS:HE2	2.44	0.42
3:H:185:ASN:HD21	3:H:211:VAL:CG1	2.33	0.42
1:A:48:SER:CB	1:A:402:ASP:OD2	2.68	0.42
1:A:144:LEU:HD11	2:B:43:VAL:HG21	2.02	0.42
1:A:239:ARG:NH1	2:B:27:LYS:HD2	2.35	0.42
1:A:298:ASN:HD21	1:A:300:PHE:HB2	1.85	0.42
1:A:445:ASP:C	1:A:446:TYR:CD1	2.98	0.42
2:B:118:MET:HE1	2:B:160:ASP:OD2	2.19	0.42
2:B:236:ASN:OD1	2:B:485:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ILE:HD13	2:B:493:ILE:CD1	2.50	0.42
1:C:57:MET:CE	2:D:100:ARG:NH1	2.82	0.42
1:C:86:VAL:CG2	2:D:68:LYS:HE3	2.47	0.42
1:C:114:PHE:CD1	1:C:114:PHE:N	2.88	0.42
2:D:165:PHE:HD1	2:D:165:PHE:H	1.67	0.42
2:D:322:LEU:HD11	2:D:348:ARG:NH2	2.34	0.42
2:D:339:PRO:O	2:D:341:PRO:HD3	2.19	0.42
2:D:438:LYS:HA	2:D:439:PRO:HD2	1.95	0.42
3:G:23:VAL:HG12	3:G:33:VAL:HG11	2.02	0.42
3:H:250:ASN:ND2	3:H:251:LYS:N	2.67	0.42
1:C:128:ASP:HB3	1:C:166:VAL:CG2	2.49	0.42
1:C:355:ILE:HG21	5:C:3496:CFM:S3A	2.59	0.42
3:E:224:ARG:C	3:E:225:MET:HG2	2.45	0.42
3:G:136:ALA:HB2	3:H:94:GLY:HA2	2.01	0.42
1:A:98:ASN:HD22	1:A:98:ASN:N	2.16	0.41
1:A:141:LEU:HD21	2:B:56:ASN:HA	2.02	0.41
1:A:318:GLU:HA	1:A:321:GLN:OE1	2.20	0.41
1:A:425:ILE:HG23	1:A:426:LYS:N	2.35	0.41
2:B:204:ILE:HG23	2:B:208:PHE:HE1	1.85	0.41
2:B:219:GLY:HA2	2:B:287:ALA:C	2.45	0.41
1:C:39:VAL:O	1:C:39:VAL:HG23	2.19	0.41
1:C:239:ARG:NH1	2:D:27:LYS:HD2	2.35	0.41
1:C:302:PRO:CD	1:C:456:PHE:CD1	3.03	0.41
1:C:318:GLU:HA	1:C:321:GLN:OE1	2.20	0.41
2:D:206:ARG:CG	2:D:304:PHE:CZ	3.03	0.41
2:D:365:LYS:O	2:D:388:CYS:HB3	2.19	0.41
2:D:375:PHE:HE2	2:D:470:GLY:CA	2.31	0.41
3:E:160:ALA:O	3:E:161:ALA:C	2.63	0.41
3:F:4:GLN:HB2	3:F:143:LYS:O	2.20	0.41
3:H:136:ALA:O	3:H:139:ILE:HG12	2.20	0.41
3:H:185:ASN:HD21	3:H:211:VAL:HG12	1.85	0.41
1:A:96:ARG:NH1	1:A:98:ASN:OD1	2.53	0.41
1:A:134:LEU:HG	2:B:62:LEU:CD1	2.50	0.41
1:A:136:ASP:CG	1:A:170:LYS:HZ1	2.19	0.41
1:A:277:ARG:HD3	1:A:386:ASP:OD2	2.21	0.41
1:A:355:ILE:HB	1:A:360:PRO:HD3	2.02	0.41
2:B:330:MET:O	2:B:333:SER:HB3	2.19	0.41
1:C:76:LYS:HG2	1:C:257:GLY:O	2.20	0.41
1:C:427:GLU:O	1:C:431:PHE:CD1	2.73	0.41
2:D:221:ASN:O	2:D:223:LYS:HG3	2.20	0.41
3:E:2:MET:HE3	3:E:4:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:96:GLY:O	3:F:132:CYS:HB2	2.19	0.41
3:F:4:GLN:CD	3:F:143:LYS:O	2.63	0.41
3:G:103:ILE:HG12	3:G:137:MET:HG2	2.02	0.41
3:H:98:ALA:O	3:H:102:VAL:HG23	2.20	0.41
3:H:166:LYS:HA	3:H:258:PRO:HG3	2.02	0.41
3:H:185:ASN:HD22	3:H:185:ASN:HA	1.40	0.41
1:A:239:ARG:O	1:A:243:GLU:HG3	2.20	0.41
1:A:286:MET:HE3	1:A:292:ILE:HD12	2.01	0.41
2:B:393:ILE:HD12	2:B:410:LEU:HD11	2.03	0.41
2:B:395:CYS:O	2:B:423:ILE:HA	2.21	0.41
1:C:210:ARG:HG3	1:C:263:GLU:HB3	2.01	0.41
1:C:226:ILE:O	1:C:226:ILE:HG22	2.20	0.41
2:D:54:GLU:CD	2:D:58:GLN:HE21	2.28	0.41
2:D:381:LYS:CD	2:D:381:LYS:C	2.93	0.41
2:D:388:CYS:O	2:D:390:PRO:HD3	2.21	0.41
3:F:36:VAL:HA	3:F:86:VAL:HG23	2.02	0.41
3:H:165:SER:HB3	3:H:179:LEU:HD12	2.02	0.41
1:A:198:ALA:O	1:A:199:ASN:C	2.63	0.41
1:A:221:TYR:O	1:A:223:VAL:HG13	2.20	0.41
1:A:454:ASP:HB3	2:B:14:LEU:HD21	2.01	0.41
6:A:1498:CLF:S3B	2:B:72:PRO:HG2	2.60	0.41
2:B:277:THR:O	2:B:280:GLU:HB3	2.20	0.41
2:B:294:GLN:HB2	2:B:297:HIS:CE1	2.55	0.41
1:C:358:LEU:HD11	1:C:362:HIS:ND1	2.36	0.41
1:C:364:ILE:O	1:C:368:GLU:HG2	2.21	0.41
2:D:237:PHE:O	2:D:241:LYS:HG3	2.21	0.41
2:D:369:LEU:HD11	2:D:380:VAL:CG2	2.50	0.41
2:D:375:PHE:HD1	2:D:375:PHE:O	2.03	0.41
2:D:414:PRO:HA	2:D:417:LYS:HG3	2.02	0.41
3:F:163:ASN:O	3:F:166:LYS:HB3	2.21	0.41
3:F:186:SER:HA	3:F:192:GLU:OE2	2.20	0.41
3:F:198:ALA:CB	3:F:267:LEU:HD21	2.50	0.41
3:G:185:ASN:OD1	9:G:7292:ATP:N6	2.54	0.41
3:H:214:ASP:OD2	3:H:216:VAL:HG23	2.20	0.41
3:H:260:THR:O	3:H:261:MET:C	2.63	0.41
1:A:144:LEU:HD22	2:B:35:TYR:CE1	2.56	0.41
1:A:230:ASN:OD1	1:A:233:GLY:CA	2.68	0.41
1:A:339:VAL:HG13	1:A:343:ARG:HB2	2.01	0.41
1:A:349:LYS:HD3	1:A:419:ASP:OD2	2.20	0.41
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.19	0.41
2:B:39:LYS:HD2	2:B:42:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ARG:HB3	2:B:391:VAL:HG21	2.01	0.41
1:C:37:PRO:HD2	1:C:396:ASP:CB	2.51	0.41
1:C:346:LEU:HB3	1:C:372:MET:HG3	2.02	0.41
1:C:349:LYS:HD3	1:C:419:ASP:OD2	2.20	0.41
2:D:57:PHE:C	2:D:59:ARG:H	2.27	0.41
2:D:170:LYS:HD3	2:D:175:ILE:HG13	2.02	0.41
2:D:427:LEU:HD23	2:D:427:LEU:HA	1.91	0.41
3:F:207:MET:O	3:F:208:ILE:C	2.63	0.41
3:H:36:VAL:HA	3:H:86:VAL:HG23	2.02	0.41
3:H:200:ALA:O	3:H:205:THR:O	2.39	0.41
1:A:67:SER:HB3	1:A:151:GLN:NE2	2.35	0.41
1:A:141:LEU:HD12	2:B:52:TYR:CE1	2.56	0.41
2:B:74:GLY:HA3	2:B:193:HIS:O	2.19	0.41
2:B:125:PHE:CE2	3:E:62:ALA:HB2	2.55	0.41
2:B:262:ASP:O	2:B:264:PRO:HD3	2.21	0.41
1:C:16:VAL:HG21	1:C:412:PHE:CE1	2.55	0.41
1:C:30:LYS:HZ1	1:C:47:ILE:CD1	2.33	0.41
1:C:404:VAL:HG22	1:C:408:GLU:HB2	2.02	0.41
2:D:278:GLN:C	2:D:280:GLU:N	2.77	0.41
3:E:106:ILE:CD1	3:E:137:MET:HB3	2.50	0.41
3:E:158:MET:HE3	3:E:196:ILE:HD13	2.01	0.41
3:F:100:ARG:HD2	3:F:100:ARG:O	2.20	0.41
1:A:36:ASP:C	1:A:38:ALA:N	2.78	0.41
1:A:164:GLU:HA	1:A:180:PRO:HB3	2.03	0.41
1:A:364:ILE:O	1:A:368:GLU:HG2	2.20	0.41
2:D:227:VAL:HB	2:D:292:LEU:HD23	2.02	0.41
2:D:362:LEU:HD21	2:D:497:LEU:HB2	2.03	0.41
2:D:440:ASP:HB3	2:D:441:PHE:CE1	2.56	0.41
2:D:481:ARG:CZ	2:D:481:ARG:HB3	2.50	0.41
3:E:242:ALA:O	3:E:246:LYS:HG2	2.21	0.41
3:F:23:VAL:CG1	3:F:33:VAL:HG11	2.51	0.41
3:F:102:VAL:HG21	3:F:135:PHE:CD1	2.56	0.41
3:H:91:PRO:HB2	3:H:95:VAL:O	2.20	0.41
3:H:195:LEU:O	3:H:198:ALA:HB3	2.21	0.41
1:A:59:ILE:HD13	1:A:427:GLU:CD	2.46	0.41
1:A:186:PHE:CD1	1:A:186:PHE:C	2.99	0.41
2:B:31:PHE:CD1	2:B:31:PHE:N	2.89	0.41
2:B:76:VAL:O	2:B:80:LEU:HG	2.20	0.41
2:B:125:PHE:HZ	3:E:58:MET:O	2.03	0.41
2:B:309:TRP:N	2:B:309:TRP:CD1	2.85	0.41
2:B:358:SER:OG	2:D:478:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:SER:HB3	1:C:183:CYS:HB3	2.02	0.41
1:C:106:VAL:HG12	1:C:144:LEU:HD12	2.02	0.41
1:C:214:THR:C	1:C:216:PHE:H	2.27	0.41
1:C:277:ARG:HE	1:C:277:ARG:CA	2.33	0.41
1:C:359:ARG:N	1:C:360:PRO:CD	2.83	0.41
1:C:402:ASP:O	1:C:403:ASP:HB3	2.21	0.41
1:C:475:LEU:HD13	2:D:265:ALA:O	2.21	0.41
2:D:186:THR:N	2:D:187:PRO:HD3	2.36	0.41
2:D:445:ASN:HB2	2:D:472:PRO:O	2.20	0.41
2:D:510:ARG:O	2:D:510:ARG:HG2	2.21	0.41
3:F:99:GLY:O	3:F:134:GLY:HA3	2.20	0.41
3:F:208:ILE:HG22	3:F:209:HIS:N	2.35	0.41
3:G:26:LEU:CD1	3:G:244:ALA:HB1	2.51	0.41
1:A:207:LEU:HD11	1:A:266:PRO:HD3	2.03	0.41
1:A:224:ALA:HB2	1:A:251:ALA:HB3	2.01	0.41
1:A:428:LYS:O	1:A:432:GLN:HG3	2.20	0.41
1:A:461:ARG:HG3	2:B:8:ILE:HD12	2.03	0.41
2:B:20:TYR:O	2:B:24:LEU:HG	2.21	0.41
2:B:170:LYS:HD3	2:B:175:ILE:HG13	2.03	0.41
2:B:421:VAL:HG12	2:B:422:TYR:N	2.35	0.41
2:B:495:THR:HG22	2:B:499:ASN:HD22	1.86	0.41
2:B:512:MET:CE	2:D:457:HIS:CD2	3.04	0.41
1:C:86:VAL:HB	1:C:117:ASP:OD2	2.19	0.41
1:C:346:LEU:HB3	1:C:372:MET:SD	2.61	0.41
1:C:403:ASP:CG	1:C:403:ASP:O	2.63	0.41
2:D:70:CYS:O	2:D:193:HIS:CA	2.69	0.41
2:D:146:MET:HE2	2:D:208:PHE:CE1	2.50	0.41
2:D:188:SER:HB2	6:D:3498:CLF:S2B	2.61	0.41
2:D:296:TRP:CZ3	2:D:402:TRP:HA	2.55	0.41
2:D:346:LYS:O	2:D:347:GLU:C	2.62	0.41
2:D:365:LYS:HG3	2:D:501:ILE:HD11	2.02	0.41
2:D:461:GLU:HG3	2:D:461:GLU:O	2.21	0.41
3:E:4:GLN:NE2	3:E:124:TYR:OH	2.54	0.41
3:E:108:PHE:O	3:E:109:LEU:C	2.64	0.41
3:E:168:ILE:C	3:E:170:LYS:N	2.79	0.41
3:F:85:CYS:C	3:F:86:VAL:HG13	2.46	0.41
3:F:161:ALA:O	3:F:165:SER:OG	2.39	0.41
3:G:95:VAL:O	3:G:95:VAL:CG1	2.62	0.41
3:H:10:LYS:O	3:H:11:GLY:C	2.62	0.41
3:H:23:VAL:HG12	3:H:33:VAL:HG11	2.03	0.41
3:H:70:LEU:HA	3:H:70:LEU:HD23	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:214:ASP:O	3:H:217:VAL:HG23	2.21	0.41
1:A:57:MET:CE	2:B:100:ARG:CZ	2.99	0.41
1:A:79:ILE:HG13	1:A:145:ASN:HB2	2.02	0.41
1:A:241:LEU:HD11	1:A:453:PHE:CD1	2.56	0.41
2:B:125:PHE:HZ	3:E:59:GLU:HA	1.86	0.41
1:C:222:ASP:OD1	1:C:248:ARG:HG2	2.20	0.41
1:C:301:GLY:HA2	1:C:456:PHE:CD1	2.56	0.41
2:D:456:LEU:HD11	2:D:460:LYS:CD	2.51	0.41
3:F:41:LYS:HB3	3:F:43:ASP:OD1	2.21	0.41
3:F:129:ASP:HB3	3:F:131:VAL:HG12	2.03	0.41
3:F:179:LEU:HD12	3:F:256:PRO:HG3	2.02	0.41
3:G:100:ARG:NH1	3:G:103:ILE:CG2	2.84	0.41
3:G:199:LEU:HD11	3:G:259:ILE:HD11	2.03	0.41
1:A:48:SER:HB2	1:A:402:ASP:OD2	2.21	0.40
1:A:90:GLN:N	1:A:113:ASN:ND2	2.68	0.40
1:A:107:ASN:ND2	1:A:107:ASN:O	2.53	0.40
1:A:413:VAL:HG11	1:A:431:PHE:HD2	1.85	0.40
2:B:54:GLU:O	2:B:58:GLN:HG3	2.22	0.40
2:B:69:ALA:HB3	2:B:193:HIS:HB3	2.03	0.40
2:B:457:HIS:CG	2:D:512:MET:HE2	2.56	0.40
2:B:510:ARG:O	2:B:510:ARG:CG	2.70	0.40
1:C:96:ARG:HH11	1:C:96:ARG:CG	2.33	0.40
1:C:148:ILE:O	1:C:178:ILE:HA	2.21	0.40
1:C:240:ILE:O	1:C:244:GLU:HG3	2.21	0.40
1:C:372:MET:HE1	1:C:420:LEU:HD23	2.02	0.40
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.27	0.40
2:D:243:MET:O	2:D:244:LEU:C	2.64	0.40
2:D:518:ASN:O	2:D:518:ASN:CG	2.63	0.40
3:E:61:ALA:HA	3:E:70:LEU:HG	2.03	0.40
3:F:13:ILE:CA	3:F:187:ARG:NH2	2.73	0.40
1:A:94:ALA:HB3	2:D:521:LEU:HD22	2.03	0.40
1:A:207:LEU:HD11	1:A:266:PRO:CD	2.52	0.40
1:A:218:SER:OG	1:A:269:LYS:CE	2.57	0.40
1:A:258:SER:HB2	1:A:261:GLU:H	1.86	0.40
2:B:185:HIS:CE1	3:F:140:ARG:HH12	2.39	0.40
2:B:457:HIS:CB	2:D:512:MET:HE2	2.51	0.40
1:C:204:ASP:HB2	1:C:205:TRP:CD1	2.57	0.40
2:D:62:LEU:HD23	2:D:64:VAL:HG23	2.02	0.40
2:D:247:MET:CE	2:D:340:ILE:HA	2.51	0.40
3:E:13:ILE:HD12	3:E:150:VAL:O	2.20	0.40
3:G:223:ARG:O	3:G:224:ARG:CB	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:HIS:O	3:H:51:SER:CB	2.61	0.40
3:H:186:SER:CB	3:H:210:PHE:CZ	3.00	0.40
1:A:200:ASP:HA	1:A:203:ARG:HG2	2.03	0.40
1:A:427:GLU:HB2	1:A:431:PHE:CE1	2.56	0.40
2:B:224:ILE:HD12	2:B:249:VAL:HG11	2.03	0.40
1:C:16:VAL:O	1:C:19:VAL:HG22	2.21	0.40
1:C:43:LYS:HE2	1:C:384:ASN:ND2	2.36	0.40
1:C:245:MET:HE1	1:C:309:LEU:O	2.22	0.40
2:D:157:VAL:C	2:D:159:GLY:N	2.79	0.40
3:E:131:VAL:HG22	3:E:132:CYS:SG	2.61	0.40
3:E:179:LEU:HB2	3:E:256:PRO:HG3	2.02	0.40
1:A:8:GLU:O	1:A:11:SER:N	2.55	0.40
1:A:31:HIS:C	1:A:32:LEU:HD23	2.46	0.40
1:A:67:SER:HB2	1:A:183:CYS:CB	2.52	0.40
1:A:118:PHE:HD1	1:A:123:ILE:HD13	1.86	0.40
1:A:315:LYS:HD3	1:A:315:LYS:HA	1.79	0.40
2:B:293:LEU:O	2:B:318:ILE:HA	2.20	0.40
2:B:415:TYR:CD1	2:B:415:TYR:N	2.90	0.40
1:C:9:VAL:HB	1:C:34:VAL:HG22	2.04	0.40
1:C:245:MET:HG3	1:C:324:CYS:HA	2.04	0.40
1:C:250:VAL:HA	2:D:31:PHE:CE2	2.55	0.40
2:D:247:MET:CB	2:D:249:VAL:HG23	2.50	0.40
3:E:94:GLY:O	3:E:95:VAL:CG2	2.64	0.40
3:E:239:GLU:OE1	3:E:239:GLU:HA	2.22	0.40
3:G:106:ILE:HD12	3:G:137:MET:CB	2.46	0.40
3:H:185:ASN:ND2	3:H:211:VAL:CG1	2.84	0.40
1:A:76:LYS:NZ	1:A:256:ASP:OD2	2.55	0.40
1:A:137:GLU:O	1:A:141:LEU:HB2	2.21	0.40
1:A:162:ASP:CG	1:A:165:SER:HB3	2.47	0.40
1:A:229:TYR:O	1:A:230:ASN:HB3	2.21	0.40
2:B:43:VAL:O	2:B:46:TRP:HB3	2.21	0.40
2:B:161:ASP:OD2	2:B:164:ALA:HB2	2.21	0.40
2:B:227:VAL:HA	2:B:228:PRO:HD2	1.95	0.40
2:B:240:ILE:HD13	2:B:240:ILE:HA	1.96	0.40
2:B:359:HIS:NE2	1:C:466:THR:HG23	2.36	0.40
2:B:516:ASP:O	2:B:519:HIS:HB2	2.21	0.40
1:C:106:VAL:HG21	2:D:44:PHE:HD1	1.87	0.40
1:C:236:TRP:HA	2:D:23:MET:HE1	2.04	0.40
1:C:437:PRO:HA	1:C:472:TRP:CH2	2.55	0.40
2:D:161:ASP:OD2	2:D:164:ALA:HB2	2.21	0.40
2:D:376:VAL:O	2:D:380:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:LEU:HD12	3:F:244:ALA:HB1	2.03	0.40
3:F:187:ARG:HA	3:F:187:ARG:HD3	1.90	0.40
3:H:250:ASN:ND2	3:H:252:LEU:N	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	C	405/415 (98%)	351 (87%)	54 (13%)	4	18
2	B	46/455 (10%)	39 (85%)	7 (15%)	3	14
2	D	453/455 (100%)	407 (90%)	46 (10%)	7	29
3	E	216/233 (93%)	181 (84%)	35 (16%)	2	12
3	F	215/233 (92%)	180 (84%)	35 (16%)	2	12
3	G	216/233 (93%)	181 (84%)	35 (16%)	2	12
3	H	216/233 (93%)	182 (84%)	34 (16%)	2	13
All	All	1767/2257 (78%)	1521 (86%)	246 (14%)	3	17

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	491	MET
2	B	496	THR
2	B	504	ARG
2	B	507	GLU

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Mol	Chain	Res	Type
2	B	519	HIS
2	B	522	VAL
2	B	523	ARG
1	C	21	PRO
1	C	22	GLU
1	C	23	LYS
1	C	29	ASN
1	C	30	LYS
1	C	32	LEU
1	C	37	PRO
1	C	44	LYS
1	C	48	SER
1	C	54	PRO
1	C	59	ILE
1	C	70	VAL
1	C	74	PRO
1	C	75	ILE
1	C	85	PRO
1	C	92	SER
1	C	96	ARG
1	C	98	ASN
1	C	100	TYR
1	C	120	GLU
1	C	143	PRO
1	C	155	PRO
1	C	163	ILE
1	C	184	GLU
1	C	219	THR
1	C	240	ILE
1	C	252	GLN
1	C	258	SER
1	C	266	PRO
1	C	267	LYS
1	C	279	MET
1	C	280	ASN
1	C	288	GLU
1	C	302	PRO
1	C	317	ASP
1	C	324	CYS
1	C	345	ARG
1	C	346	LEU
1	C	355	ILE

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Mol	Chain	Res	Type
1	C	358	LEU
1	C	360	PRO
1	C	362	HIS
1	C	373	GLU
1	C	383	HIS
1	C	389	ARG
1	C	398	THR
1	C	401	TYR
1	C	418	PRO
1	C	419	ASP
1	C	421	ILE
1	C	444	TRP
1	C	446	TYR
1	C	462	ASP
1	C	465	MET
2	D	3	GLN
2	D	11	SER
2	D	13	PRO
2	D	14	LEU
2	D	31	PHE
2	D	41	ASP
2	D	54	GLU
2	D	62	LEU
2	D	66	PRO
2	D	121	ASP
2	D	130	ASN
2	D	144	PRO
2	D	146	MET
2	D	154	MET
2	D	202	GLU
2	D	234	LEU
2	D	253	LEU
2	D	264	PRO
2	D	277	THR
2	D	278	GLN
2	D	281	MET
2	D	285	PRO
2	D	295	PRO
2	D	300	LYS
2	D	305	VAL
2	D	317	ASN
2	D	326	ASP

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Mol	Chain	Res	Type
2	D	331	LYS
2	D	369	LEU
2	D	375	PHE
2	D	381	LYS
2	D	384	LEU
2	D	397	ASN
2	D	420	THR
2	D	426	ASP
2	D	435	PHE
2	D	461	GLU
2	D	468	ARG
2	D	472	PRO
2	D	491	MET
2	D	496	THR
2	D	504	ARG
2	D	512	MET
2	D	519	HIS
2	D	522	VAL
2	D	523	ARG
3	E	2	MET
3	E	4	GLN
3	E	26	LEU
3	E	46	ARG
3	E	54	GLN
3	E	56	THR
3	E	60	MET
3	E	66	THR
3	E	76	LEU
3	E	87	GLU
3	E	95	VAL
3	E	111	GLU
3	E	130	VAL
3	E	131	VAL
3	E	137	MET
3	E	152	SER
3	E	156	MET
3	E	165	SER
3	E	185	ASN
3	E	186	SER
3	E	193	ASP
3	E	199	LEU
3	E	203	LEU

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Mol	Chain	Res	Type
3	E	208	ILE
3	E	214	ASP
3	E	225	MET
3	E	228	ILE
3	E	232	PRO
3	E	246	LYS
3	E	251	LYS
3	E	255	ILE
3	E	259	ILE
3	E	264	LEU
3	E	266	GLU
3	E	267	LEU
3	F	2	MET
3	F	3	ARG
3	F	5	CYS
3	F	10	LYS
3	F	16	SER
3	F	26	LEU
3	F	48	ILE
3	F	56	THR
3	F	66	THR
3	F	76	LEU
3	F	85	CYS
3	F	95	VAL
3	F	118	ASP
3	F	119	LEU
3	F	130	VAL
3	F	131	VAL
3	F	138	PRO
3	F	140	ARG
3	F	156	MET
3	F	165	SER
3	F	179	LEU
3	F	199	LEU
3	F	203	LEU
3	F	208	ILE
3	F	212	PRO
3	F	213	ARG
3	F	214	ASP
3	F	228	ILE
3	F	236	GLN
3	F	251	LYS

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Mol	Chain	Res	Type
3	F	255	ILE
3	F	259	ILE
3	F	264	LEU
3	F	266	GLU
3	F	267	LEU
3	G	3	ARG
3	G	4	GLN
3	G	5	CYS
3	G	10	LYS
3	G	17	THR
3	G	26	LEU
3	G	46	ARG
3	G	48	ILE
3	G	54	GLN
3	G	56	THR
3	G	60	MET
3	G	66	THR
3	G	76	LEU
3	G	95	VAL
3	G	111	GLU
3	G	130	VAL
3	G	131	VAL
3	G	137	MET
3	G	145	GLN
3	G	152	SER
3	G	155	MET
3	G	156	MET
3	G	165	SER
3	G	199	LEU
3	G	203	LEU
3	G	208	ILE
3	G	214	ASP
3	G	225	MET
3	G	228	ILE
3	G	254	VAL
3	G	255	ILE
3	G	259	ILE
3	G	264	LEU
3	G	266	GLU
3	G	267	LEU
3	H	2	MET
3	H	4	GLN

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Mol	Chain	Res	Type
3	H	5	CYS
3	H	10	LYS
3	H	17	THR
3	H	26	LEU
3	H	46	ARG
3	H	56	THR
3	H	58	MET
3	H	66	THR
3	H	71	GLU
3	H	76	LEU
3	H	95	VAL
3	H	111	GLU
3	H	130	VAL
3	H	131	VAL
3	H	137	MET
3	H	152	SER
3	H	165	SER
3	H	178	ARG
3	H	185	ASN
3	H	199	LEU
3	H	203	LEU
3	H	208	ILE
3	H	214	ASP
3	H	225	MET
3	H	228	ILE
3	H	232	PRO
3	H	250	ASN
3	H	255	ILE
3	H	259	ILE
3	H	264	LEU
3	H	266	GLU
3	H	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	480	HIS
2	B	518	ASN
1	C	14	GLN
1	C	35	ASN
1	C	41	GLN
1	C	49	ASN

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Mol	Chain	Res	Type
1	C	90	GLN
1	C	151	GLN
1	C	280	ASN
1	C	285	HIS
1	C	298	ASN
1	C	362	HIS
1	C	384	ASN
1	C	432	GLN
1	C	442	HIS
1	C	476	GLN
2	D	3	GLN
2	D	58	GLN
2	D	104	ASN
2	D	128	GLN
2	D	129	GLN
2	D	130	ASN
2	D	136	GLN
2	D	137	ASN
2	D	167	ASN
2	D	168	ASN
2	D	199	ASN
2	D	225	ASN
2	D	268	GLN
2	D	289	ASN
2	D	294	GLN
2	D	311	HIS
2	D	317	ASN
2	D	363	HIS
2	D	396	HIS
2	D	397	ASN
2	D	452	GLN
2	D	457	HIS
2	D	518	ASN
3	E	4	GLN
3	E	55	ASN
3	E	107	ASN
3	E	206	GLN
3	E	215	ASN
3	E	236	GLN
3	E	250	ASN
3	F	4	GLN
3	F	50	HIS

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Mol	Chain	Res	Type
3	F	107	ASN
3	F	201	ASN
3	F	206	GLN
3	F	236	GLN
3	F	250	ASN
3	G	4	GLN
3	G	54	GLN
3	G	206	GLN
3	G	236	GLN
3	G	250	ASN
3	H	4	GLN
3	H	54	GLN
3	H	55	ASN
3	H	163	ASN
3	H	185	ASN
3	H	206	GLN
3	H	236	GLN
3	H	250	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CLF	A	1498	1,2	0,24,24	-	-	-		
9	ATP	G	7292	8	32,33,33	1.82	6 (18%)	48,52,52	1.11	3 (6%)
9	ATP	H	8292	8	32,33,33	1.51	4 (12%)	48,52,52	1.05	4 (8%)
6	CLF	D	3498	1,2	0,24,24	-	-	-		
9	ATP	F	6292	8	32,33,33	1.57	3 (9%)	48,52,52	1.18	4 (8%)
10	SF4	F	5290	3	0,12,12	-	-	-		
5	CFM	A	1496	1	0,24,24	-	-	-		
9	ATP	E	5292	8	32,33,33	1.58	4 (12%)	48,52,52	1.07	2 (4%)
4	HCA	C	3494	-	13,13,13	2.35	4 (30%)	15,18,18	2.55	7 (46%)
4	HCA	A	1494	-	13,13,13	2.52	5 (38%)	15,18,18	2.03	4 (26%)
5	CFM	C	3496	1	0,24,24	-	-	-		
10	SF4	G	7290	3	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
6	CLF	A	1498	1,2	-	-	0/12/10/10
9	ATP	G	7292	8	-	9/22/38/38	0/3/3/3
9	ATP	H	8292	8	-	3/22/38/38	0/3/3/3
9	ATP	F	6292	8	-	7/22/38/38	0/3/3/3
6	CLF	D	3498	1,2	-	-	0/12/10/10
10	SF4	F	5290	3	-	-	0/6/5/5
9	ATP	E	5292	8	-	5/22/38/38	0/3/3/3
4	HCA	C	3494	-	-	5/17/17/17	-
4	HCA	A	1494	-	-	8/17/17/17	-
10	SF4	G	7290	3	-	-	0/6/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1494	HCA	O5-C7	6.99	1.44	1.22
4	C	3494	HCA	O5-C7	6.73	1.43	1.22
9	E	5292	ATP	PB-O3A	-6.22	1.52	1.59
9	H	8292	ATP	PB-O3A	-5.46	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	7292	ATP	PB-O3A	-5.32	1.53	1.59
9	F	6292	ATP	PB-O3A	-5.30	1.53	1.59
9	G	7292	ATP	C4-N3	4.58	1.43	1.34
9	F	6292	ATP	PB-O3B	4.55	1.64	1.59
9	G	7292	ATP	PB-O3B	3.67	1.63	1.59
9	E	5292	ATP	PB-O3B	3.48	1.63	1.59
4	C	3494	HCA	O3-C6	2.97	1.31	1.22
9	H	8292	ATP	PB-O3B	2.94	1.62	1.59
4	A	1494	HCA	O3-C6	2.92	1.31	1.22
9	E	5292	ATP	C4-N3	2.88	1.39	1.34
4	A	1494	HCA	O1-C1	2.76	1.31	1.22
4	A	1494	HCA	O6-C7	-2.76	1.20	1.30
4	C	3494	HCA	O6-C7	-2.33	1.22	1.30
9	H	8292	ATP	C4-N3	2.24	1.38	1.34
4	C	3494	HCA	O1-C1	2.21	1.29	1.22
9	H	8292	ATP	PB-O2B	-2.18	1.45	1.55
9	G	7292	ATP	O4'-C1'	2.15	1.47	1.42
9	G	7292	ATP	PG-O2G	-2.13	1.46	1.54
4	A	1494	HCA	C3-C7	-2.11	1.51	1.53
9	F	6292	ATP	C4-N3	2.08	1.38	1.34
9	G	7292	ATP	PB-O2B	-2.04	1.45	1.55
9	E	5292	ATP	PG-O2G	-2.04	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	O6-C7-C3	5.46	123.62	113.14
4	A	1494	HCA	O6-C7-C3	4.55	121.86	113.14
4	C	3494	HCA	O7-C3-C4	-3.79	102.81	108.88
4	C	3494	HCA	O2-C1-C2	3.50	125.44	114.35
4	A	1494	HCA	O5-C7-C3	-3.43	115.44	122.09
4	C	3494	HCA	O2-C1-O1	-3.43	114.52	123.33
9	G	7292	ATP	O3'-C3'-C4'	-3.35	101.46	111.08
9	E	5292	ATP	O4'-C1'-C2'	-3.09	99.99	106.62
9	H	8292	ATP	O4'-C1'-C2'	-2.96	100.27	106.62
9	F	6292	ATP	C3'-C2'-C1'	2.89	106.93	101.46
9	G	7292	ATP	O4'-C1'-C2'	-2.87	100.47	106.62
9	F	6292	ATP	O4'-C1'-C2'	-2.80	100.62	106.62
9	F	6292	ATP	O3'-C3'-C4'	-2.78	103.11	111.08
4	C	3494	HCA	O4-C6-C5	2.73	122.62	114.00
4	C	3494	HCA	O5-C7-C3	-2.70	116.87	122.09
9	E	5292	ATP	O3G-PG-O2G	2.63	117.68	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	8292	ATP	O3G-PG-O2G	2.56	117.41	107.80
4	C	3494	HCA	O4-C6-O3	-2.54	116.79	123.33
4	A	1494	HCA	O2-C1-O1	-2.54	116.81	123.33
4	A	1494	HCA	O2-C1-C2	2.39	121.91	114.35
9	H	8292	ATP	C3'-C2'-C1'	2.26	105.73	101.46
9	H	8292	ATP	O3'-C3'-C4'	-2.26	104.60	111.08
9	F	6292	ATP	O3G-PG-O2G	2.10	115.68	107.80
9	G	7292	ATP	C4-N9-C8	-2.07	103.56	105.74

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1494	HCA	C2-C3-C4-C5
4	A	1494	HCA	C7-C3-C4-C5
4	A	1494	HCA	O7-C3-C4-C5
4	C	3494	HCA	C2-C3-C4-C5
4	C	3494	HCA	C7-C3-C4-C5
4	C	3494	HCA	O7-C3-C4-C5
9	E	5292	ATP	PB-O3B-PG-O2G
9	E	5292	ATP	C5'-O5'-PA-O3A
9	F	6292	ATP	PB-O3B-PG-O2G
9	F	6292	ATP	C5'-O5'-PA-O2A
9	G	7292	ATP	C5'-O5'-PA-O1A
9	G	7292	ATP	C5'-O5'-PA-O2A
9	H	8292	ATP	C5'-O5'-PA-O3A
9	G	7292	ATP	C3'-C4'-C5'-O5'
4	A	1494	HCA	C1-C2-C3-C4
9	G	7292	ATP	O4'-C4'-C5'-O5'
4	A	1494	HCA	C1-C2-C3-C7
9	E	5292	ATP	PA-O3A-PB-O1B
9	F	6292	ATP	PA-O3A-PB-O1B
9	G	7292	ATP	C2'-C1'-N9-C4
9	F	6292	ATP	C5'-O5'-PA-O1A
9	F	6292	ATP	C5'-O5'-PA-O3A
9	G	7292	ATP	C5'-O5'-PA-O3A
9	G	7292	ATP	C2'-C1'-N9-C8
9	F	6292	ATP	O4'-C4'-C5'-O5'
4	A	1494	HCA	C4-C5-C6-O4
4	A	1494	HCA	C4-C5-C6-O3
9	G	7292	ATP	PB-O3B-PG-O2G
9	E	5292	ATP	PA-O3A-PB-O2B

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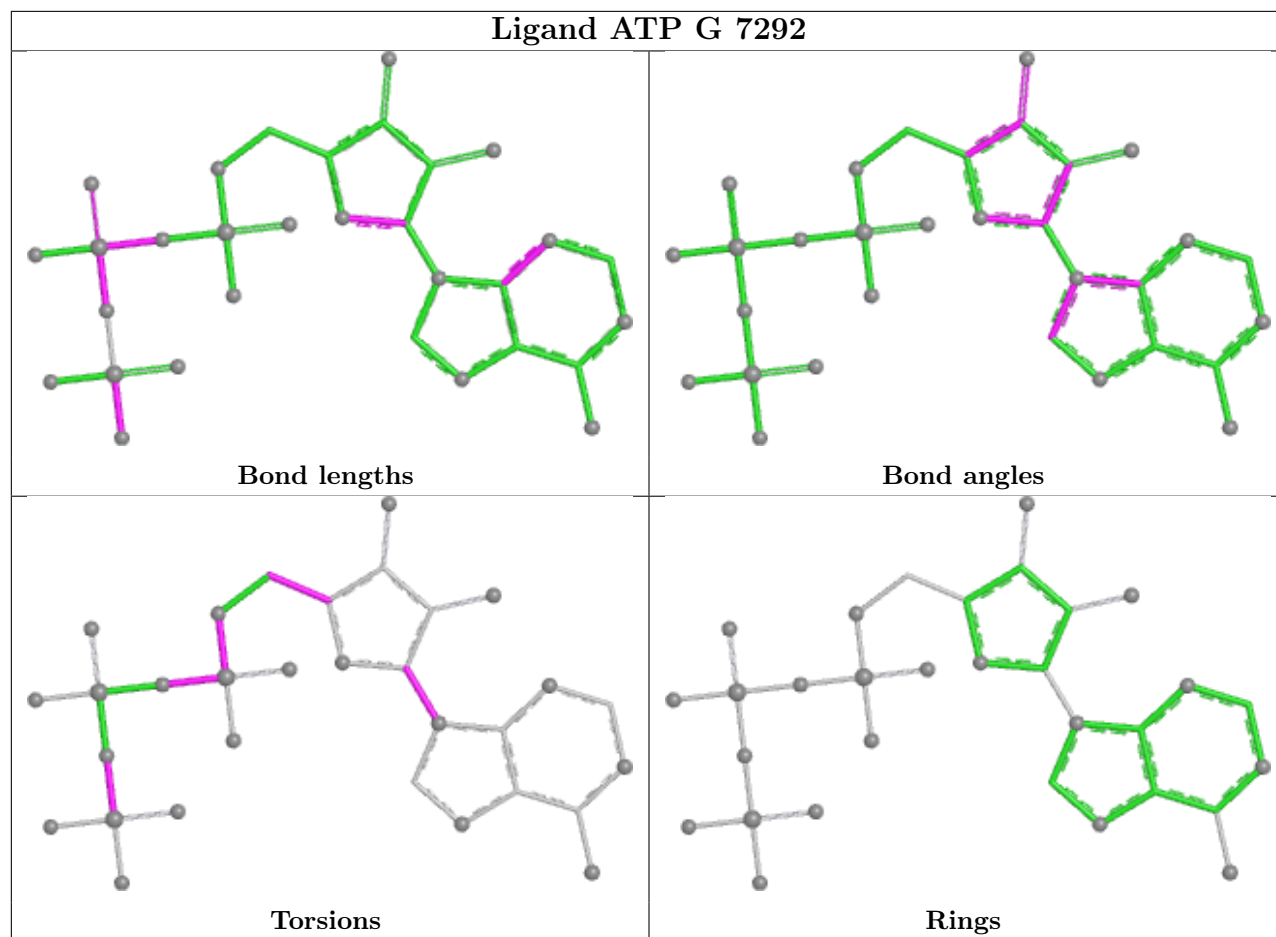
Mol	Chain	Res	Type	Atoms
9	F	6292	ATP	PA-O3A-PB-O2B
9	H	8292	ATP	PA-O3A-PB-O1B
4	C	3494	HCA	C3-C4-C5-C6
4	C	3494	HCA	C4-C5-C6-O4
4	A	1494	HCA	C1-C2-C3-O7
9	E	5292	ATP	PB-O3A-PA-O2A
9	G	7292	ATP	PB-O3A-PA-O2A
9	H	8292	ATP	PA-O3A-PB-O2B

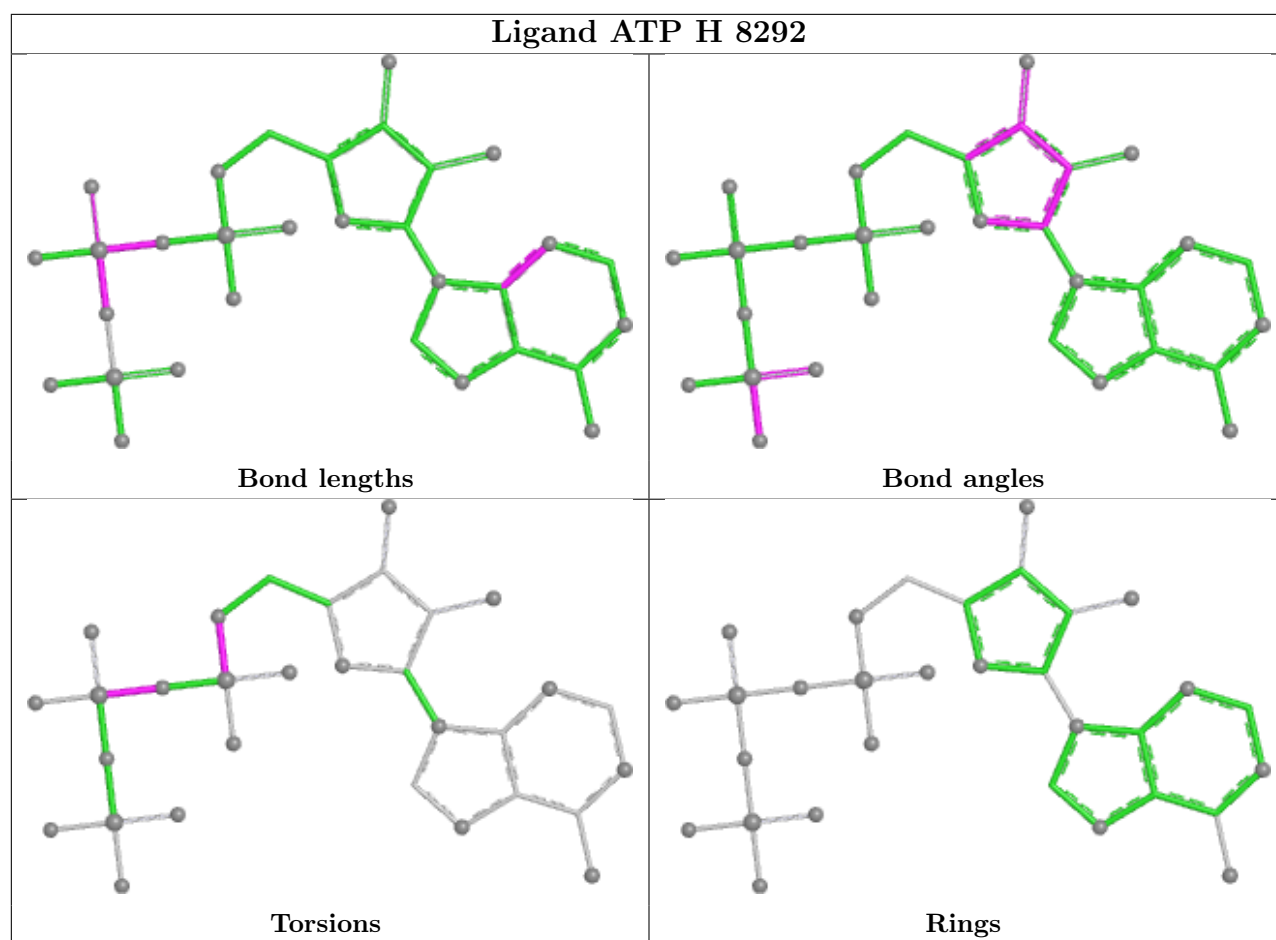
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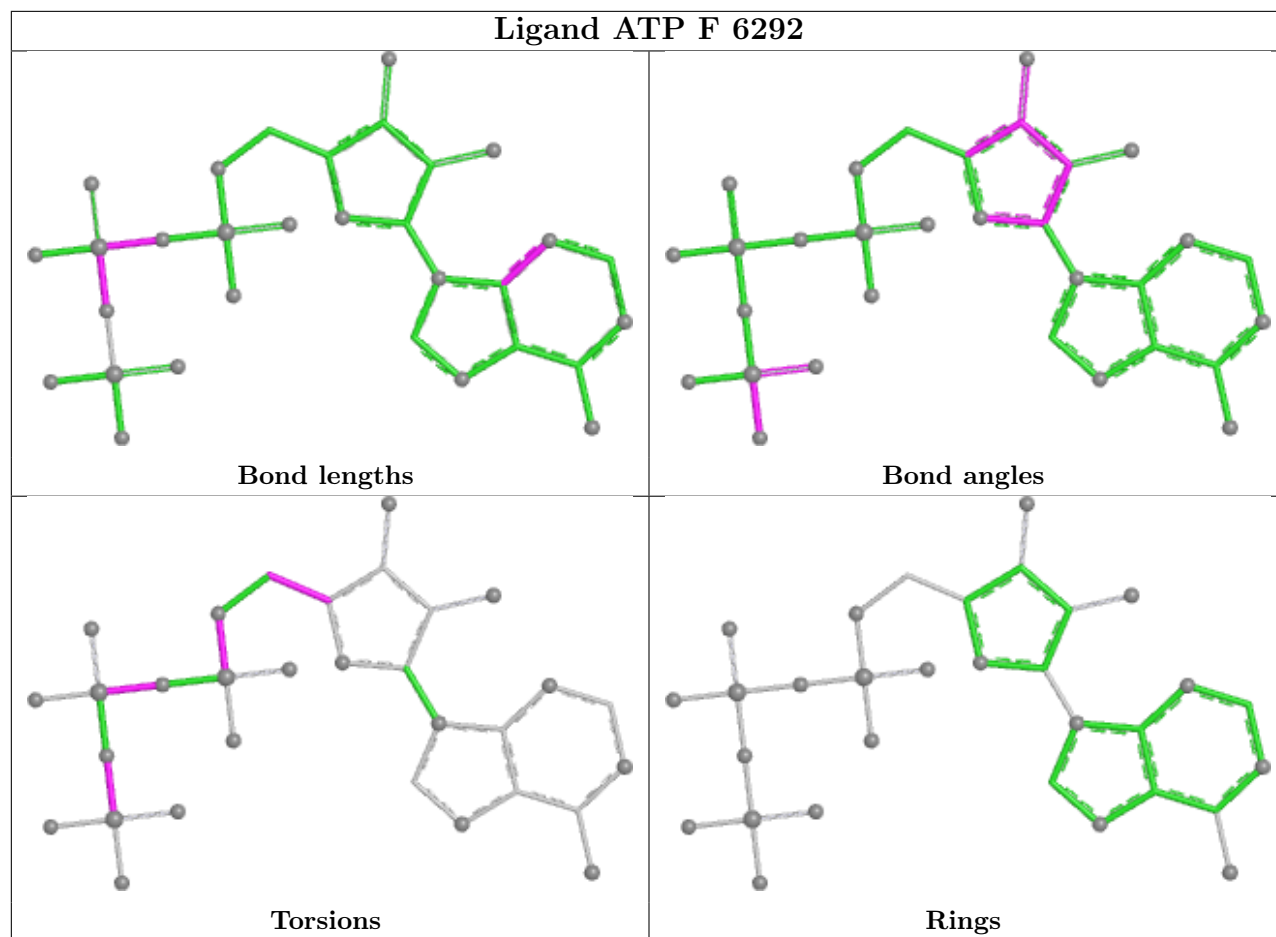
10 monomers are involved in 45 short contacts:

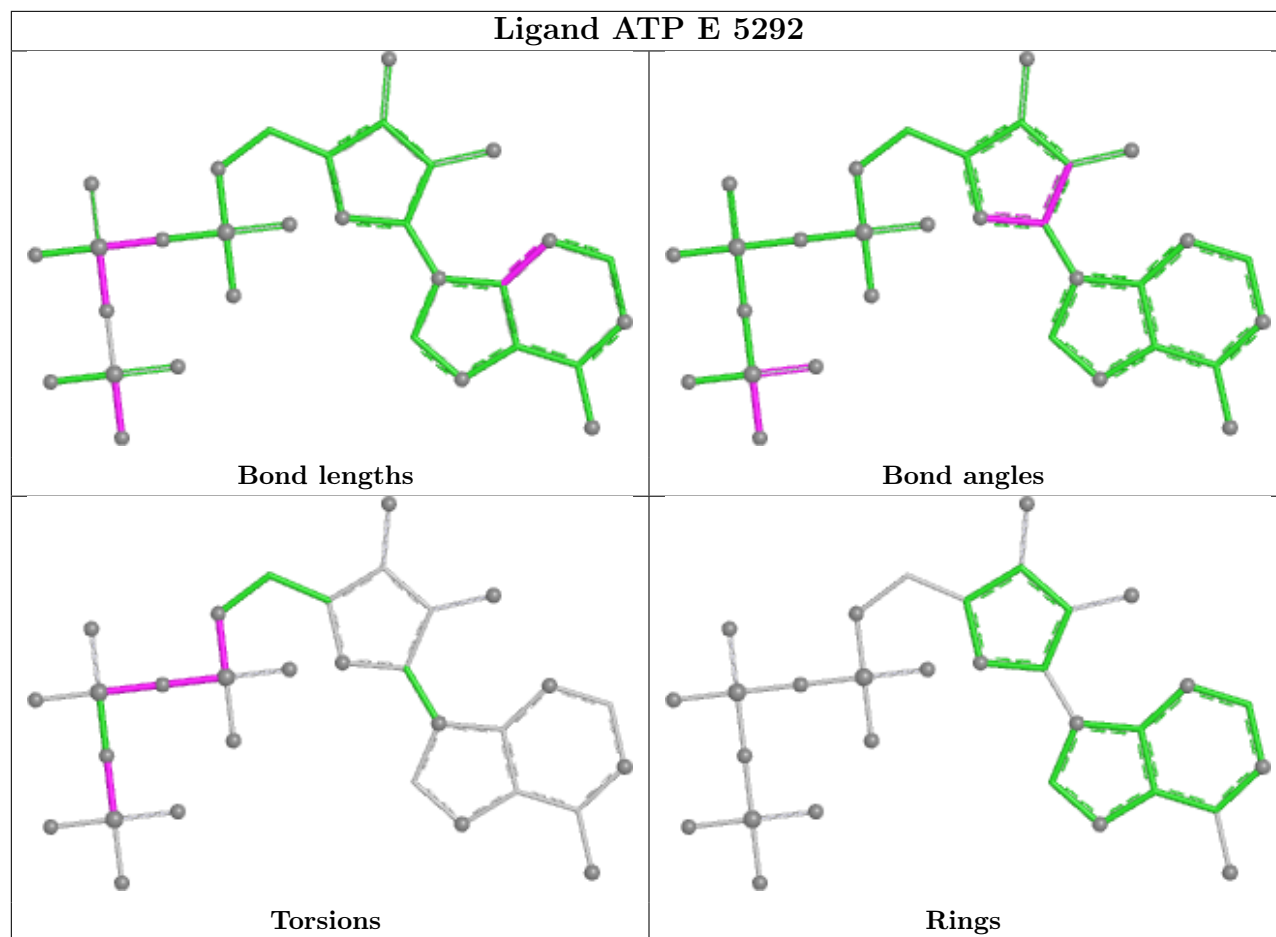
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1498	CLF	1	0
9	G	7292	ATP	11	0
9	H	8292	ATP	6	0
6	D	3498	CLF	3	0
9	F	6292	ATP	6	0
5	A	1496	CFM	4	0
9	E	5292	ATP	4	0
4	C	3494	HCA	2	0
4	A	1494	HCA	1	0
5	C	3496	CFM	7	0

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









5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.