Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1M1Y
Title	:	Chemical Crosslink of Nitrogenase MoFe Protein and Fe Protein
Authors	:	Schmid, B.; Einsle, O.; Chiu, H.J.; Willing, A.; Yoshida, M.; Howard, J.B.; Rees, D.C.
Deposited on	:	2002-06-20
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

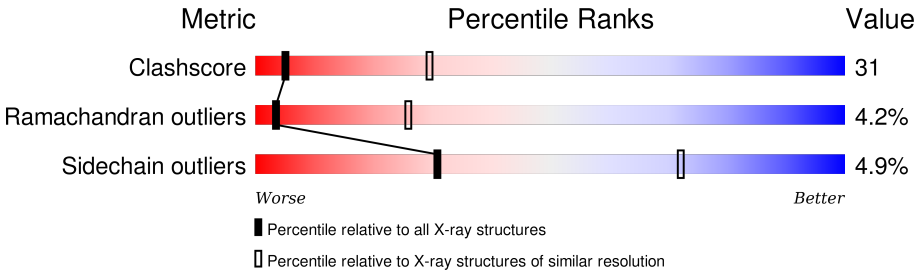
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	51% 42%
1	C	491	50% 43%
1	I	491	50% 43%
1	K	491	51% 43%
2	B	522	53% 44%
2	D	522	50% 47%
2	J	522	49% 47%

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Mol	Chain	Length	Quality of chain
2	L	522	51% 45%
3	E	289	31% 59% 8%
3	F	289	50% 43% 7%
3	G	289	31% 60% 8%
3	H	289	48% 45% 7%
3	M	289	35% 57% 7%
3	N	289	46% 47% 7%
3	O	289	34% 57% 8%
3	P	289	45% 48% 7%

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
6	CFM	A	6496	-	-	X	-
6	CFM	C	7496	-	-	X	-
7	CLF	A	6498	-	-	X	-
8	SF4	E	290	-	-	X	-
8	SF4	G	1290	-	-	X	-
8	SF4	N	2290	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49464 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	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	C	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	I	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	K	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			

- 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
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called nitrogenase IRON protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	F	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	G	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	H	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

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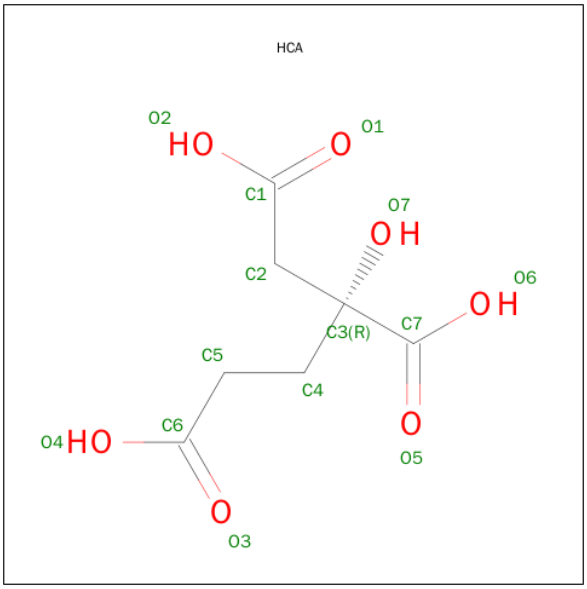
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	N	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	O	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	P	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



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

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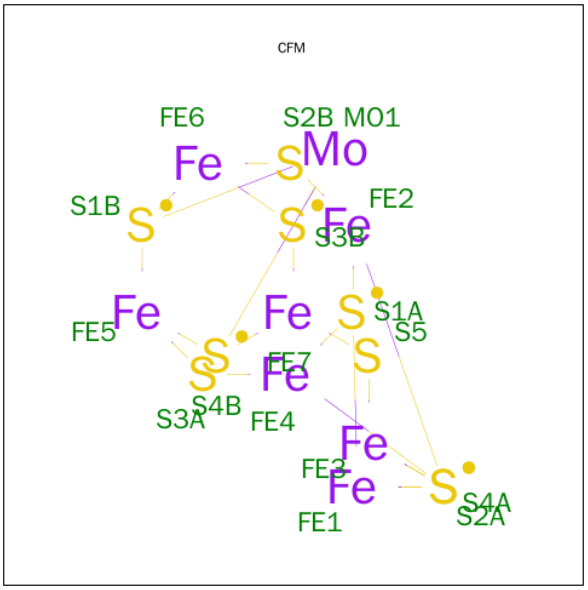
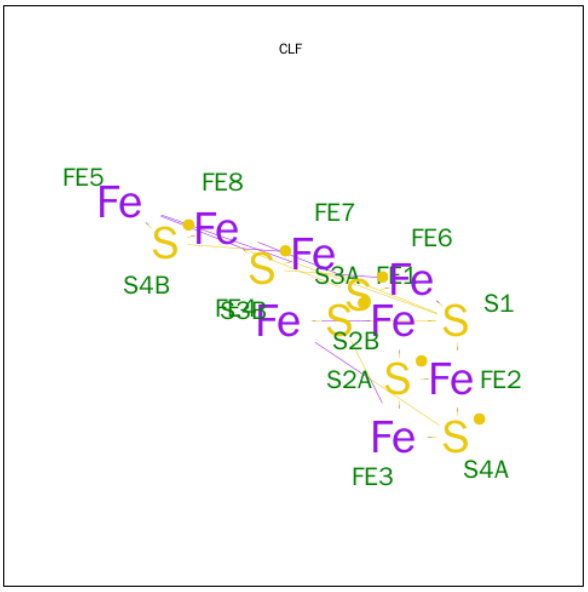
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 14 7 7	0	0
5	I	1	Total C O 14 7 7	0	0
5	K	1	Total C O 14 7 7	0	0

- Molecule 6 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



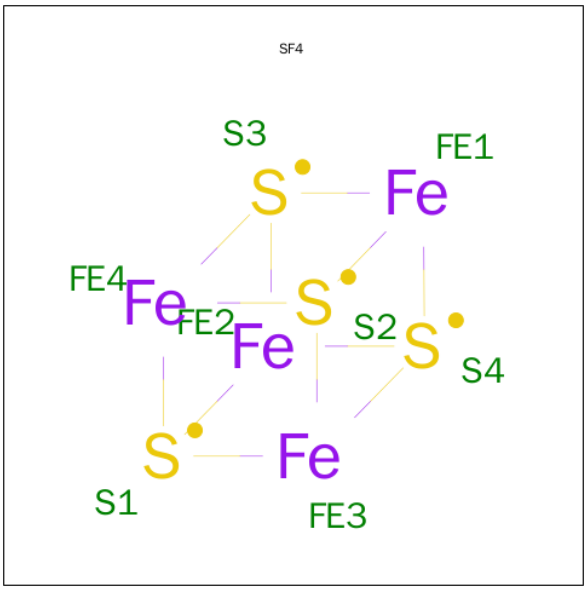
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe Mo S 17 7 1 9	0	0
6	C	1	Total Fe Mo S 17 7 1 9	0	0
6	I	1	Total Fe Mo S 17 7 1 9	0	0
6	K	1	Total Fe Mo S 17 7 1 9	0	0

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



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

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Fe S 8 4 4	0	0
8	G	1	Total Fe S 8 4 4	0	0
8	N	1	Total Fe S 8 4 4	0	0
8	P	1	Total Fe S 8 4 4	0	0

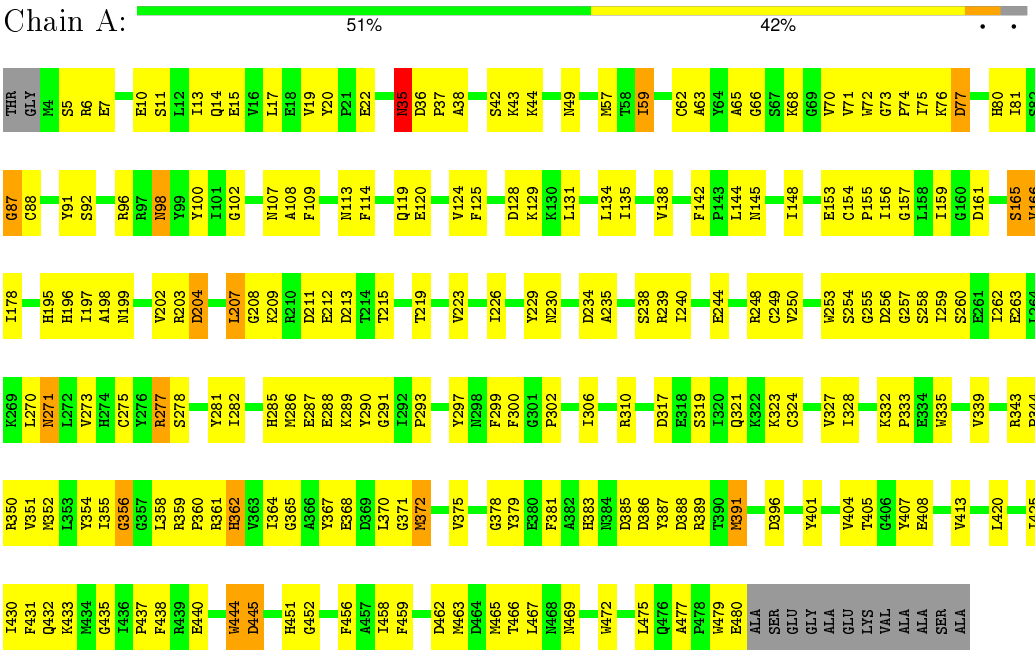
3 Residue-property plots (i)

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

Note EDS was not executed.

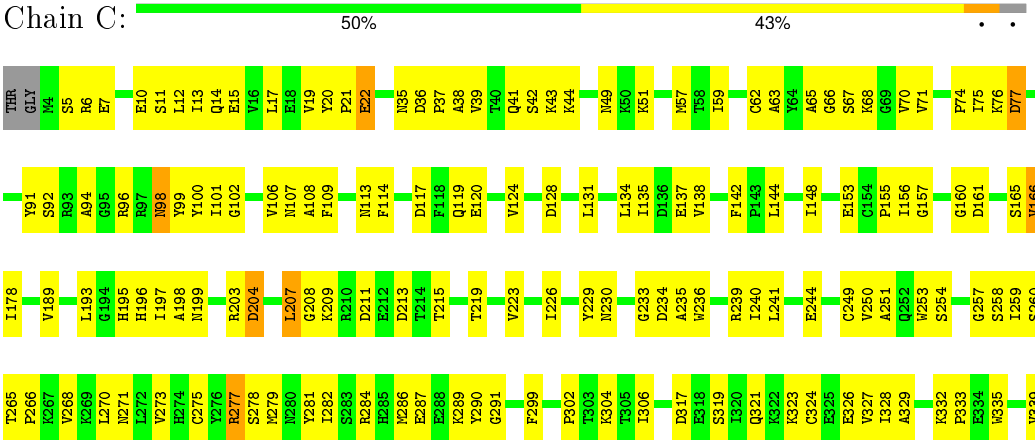
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

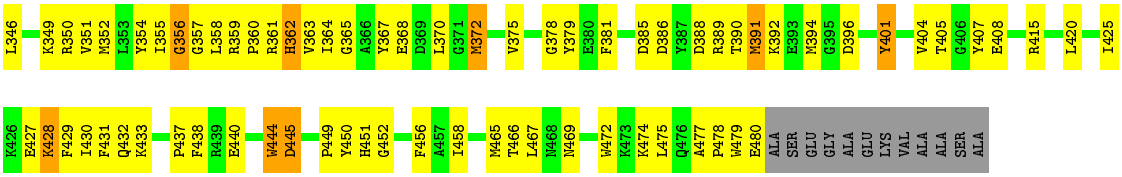
Chain A:



- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

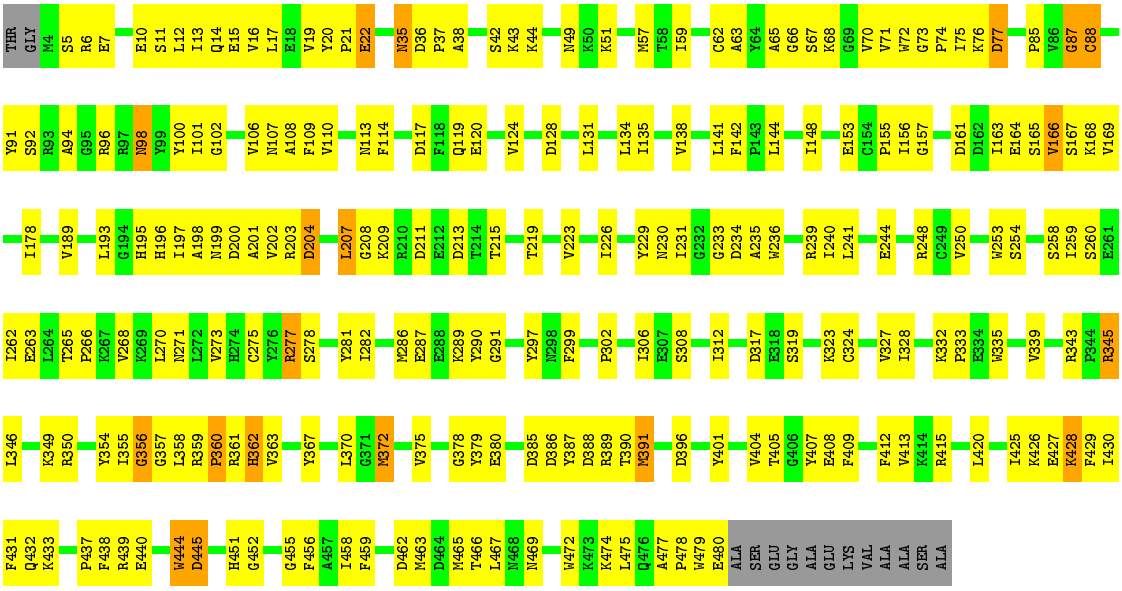
Chain C:





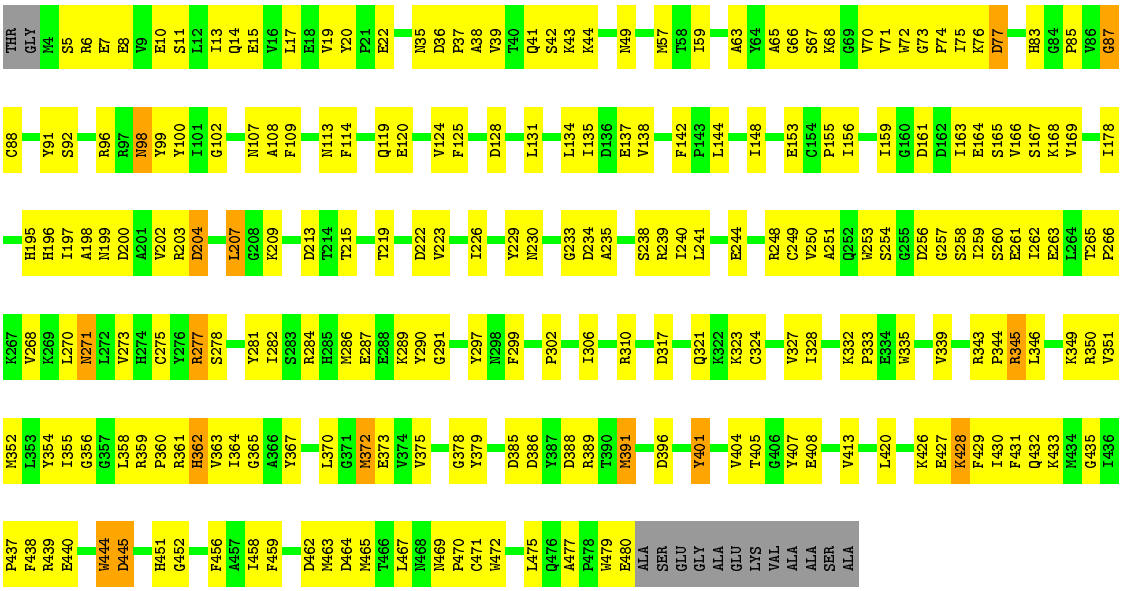
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain I:



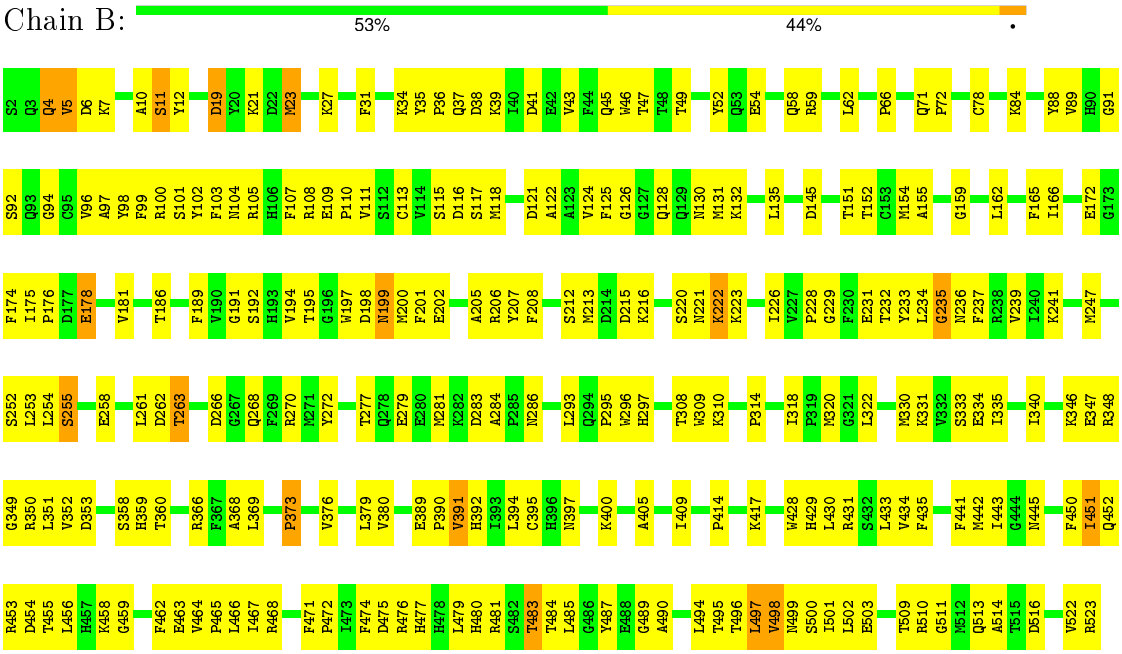
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain K:



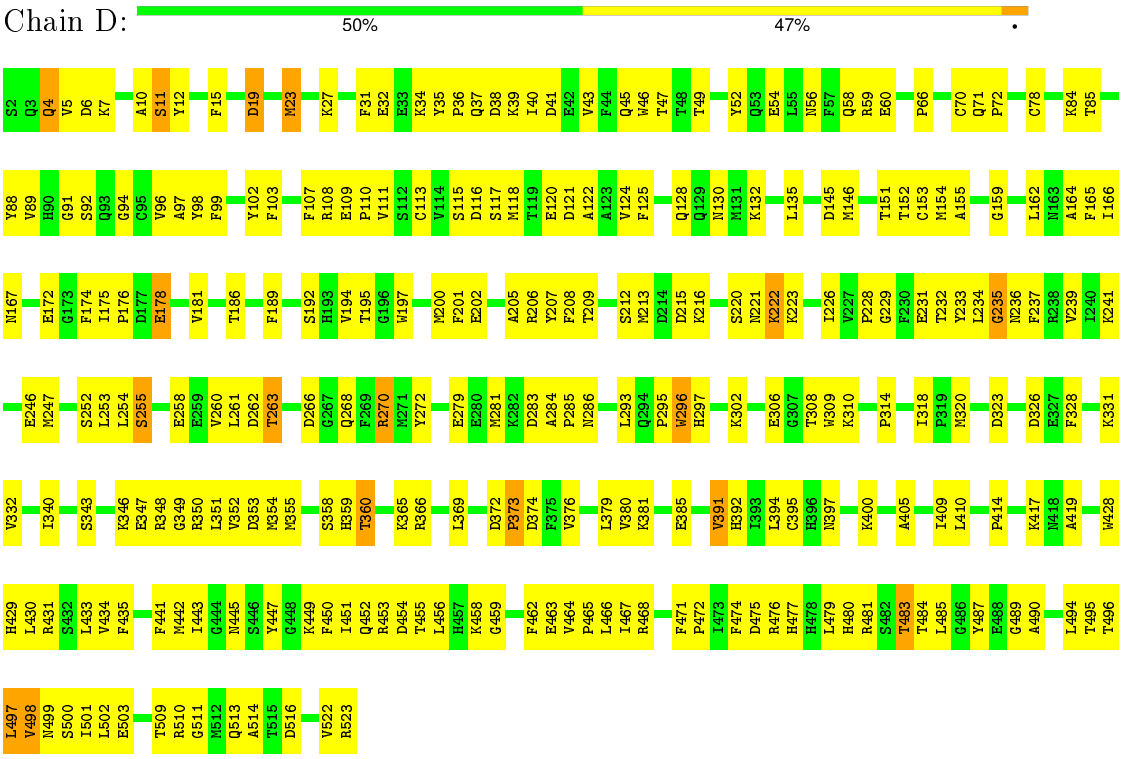
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B:



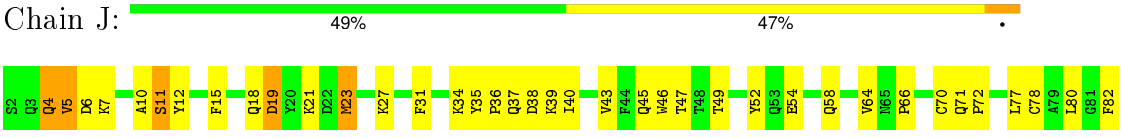
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

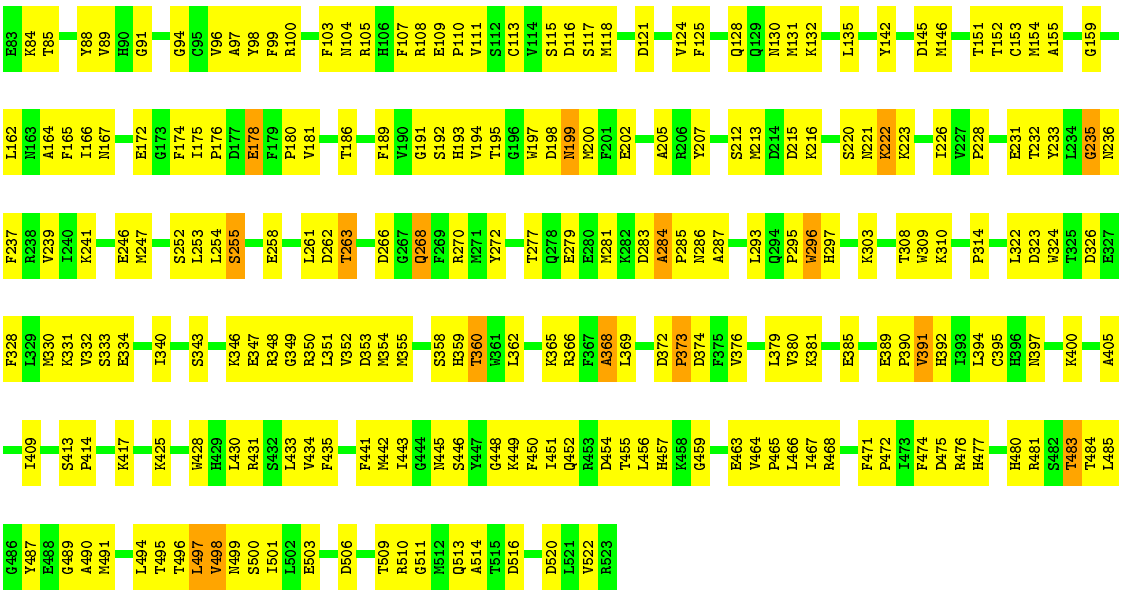
Chain D:



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

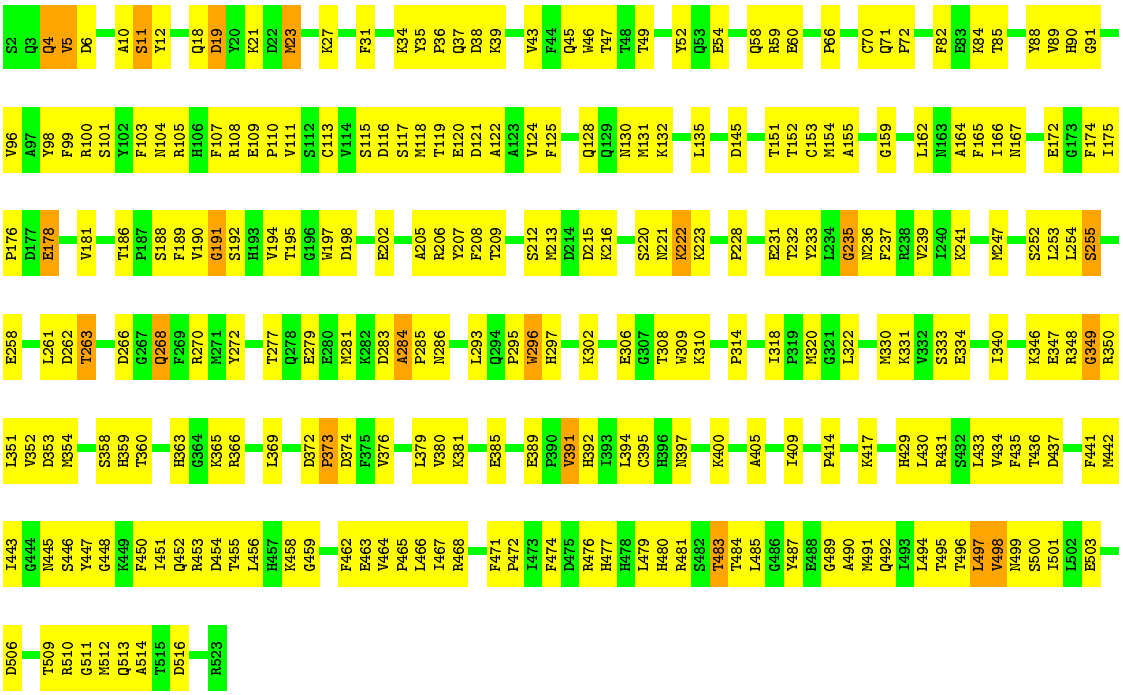
Chain J:





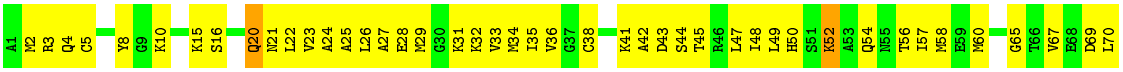
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

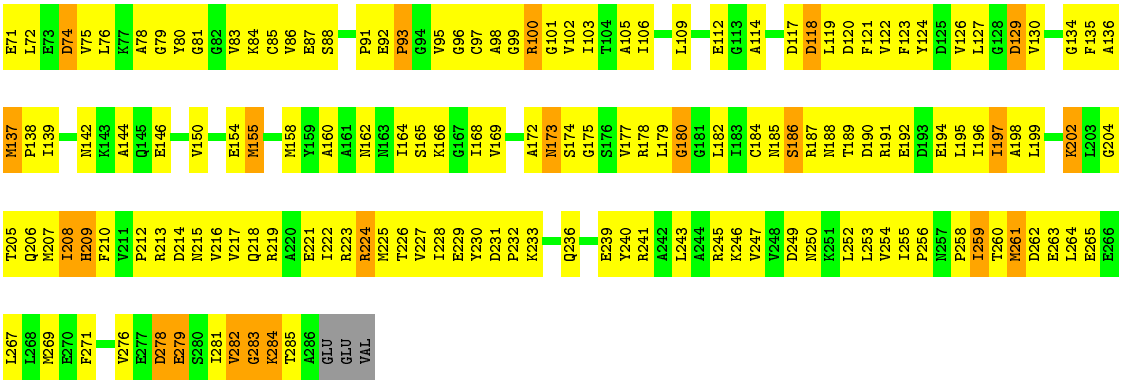
Chain L:



• Molecule 3: nitrogenase IRON protein 1

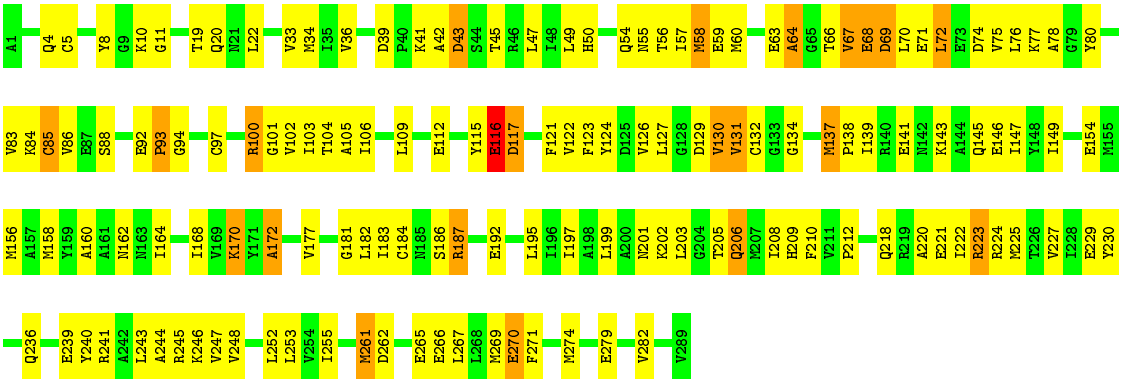
Chain E:





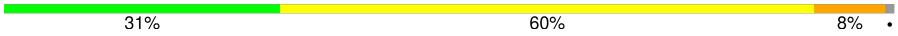
• Molecule 3: nitrogenase IRON protein 1

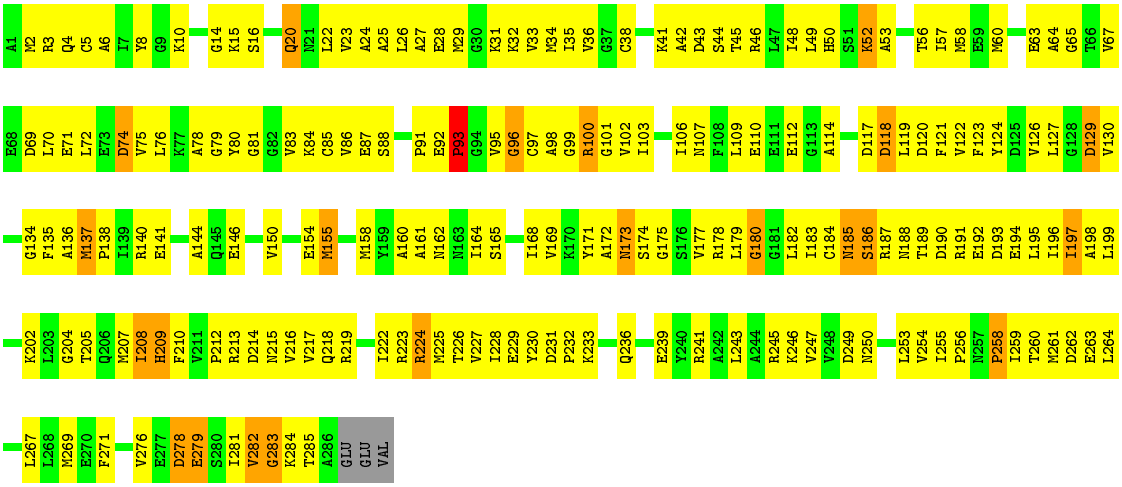
Chain F:



• Molecule 3: nitrogenase IRON protein 1

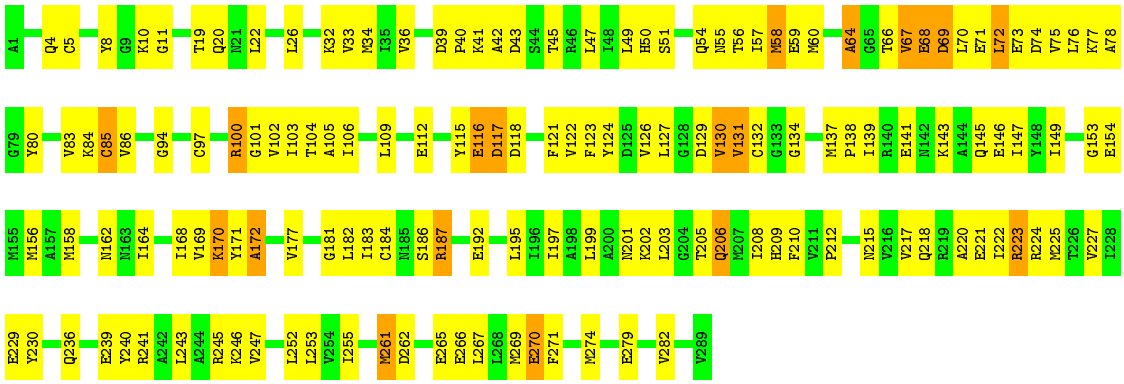
Chain G:





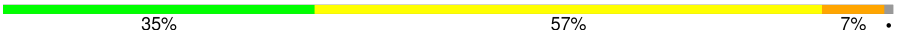
• Molecule 3: nitrogenase IRON protein 1

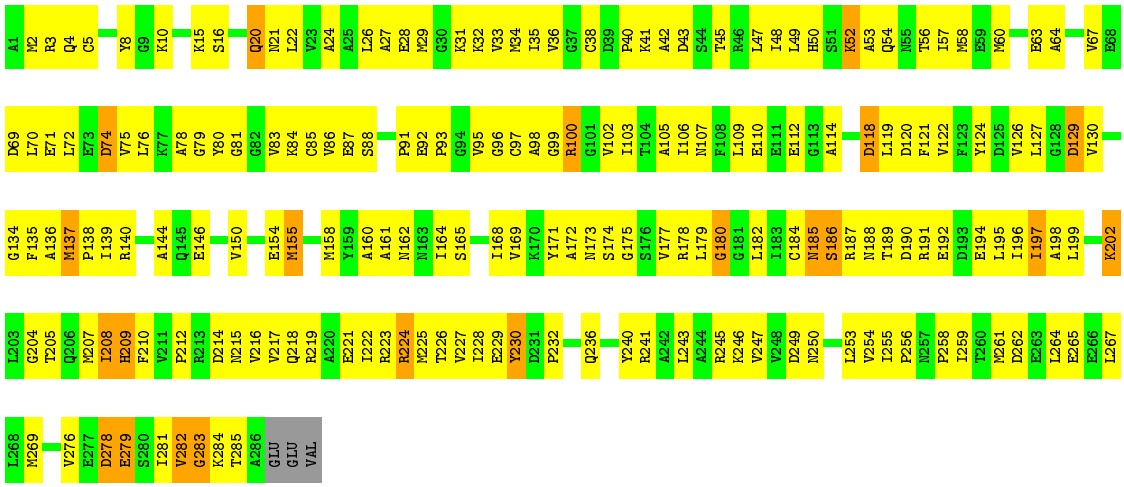
Chain H:



• Molecule 3: nitrogenase IRON protein 1

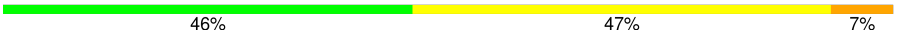
Chain M:

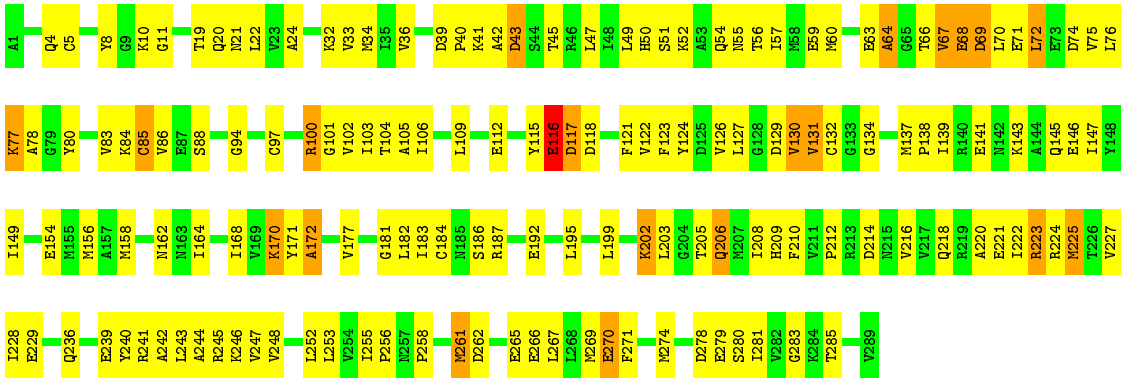




• Molecule 3: nitrogenase IRON protein 1

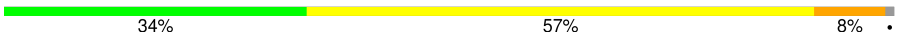
Chain N:

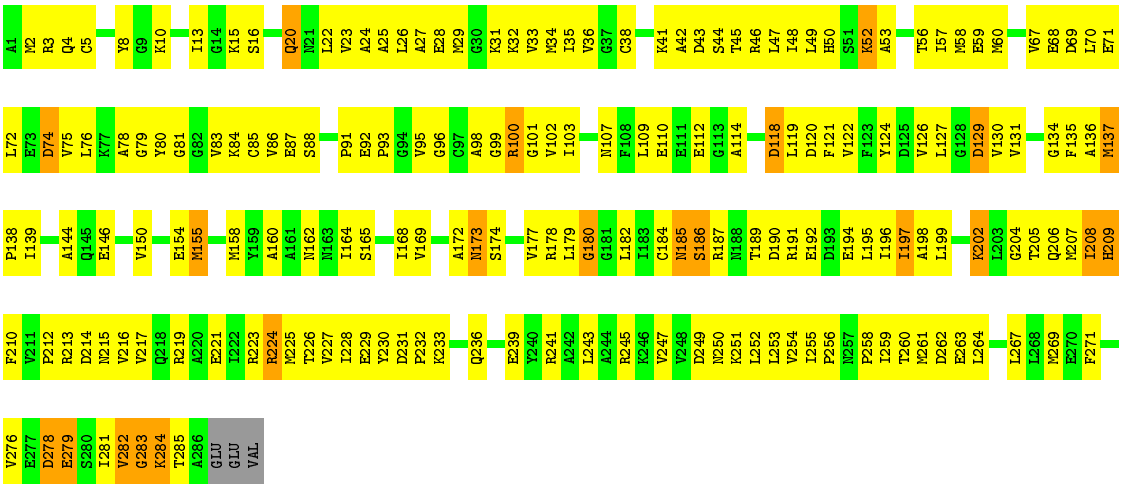




• Molecule 3: nitrogenase IRON protein 1

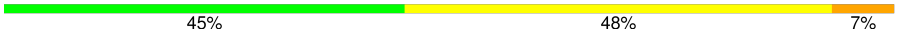
Chain O:

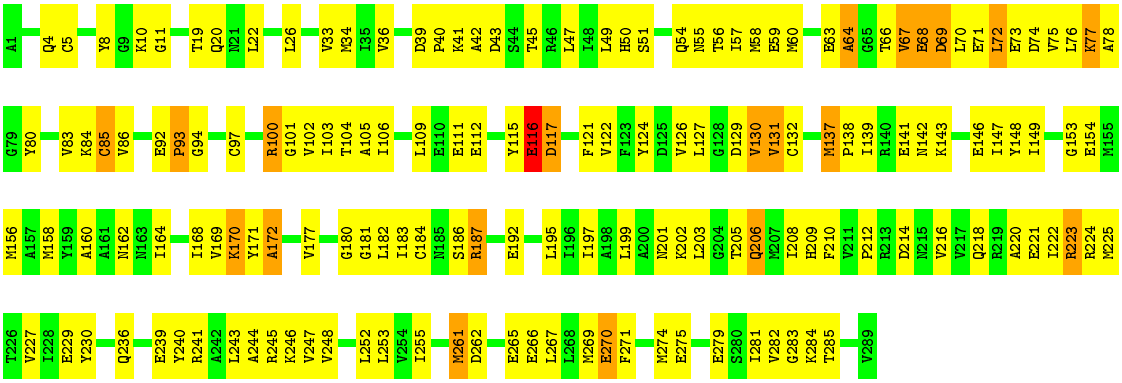




- Molecule 3: nitrogenase IRON protein 1

Chain P:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.27Å 214.94Å 320.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	4.1 (50.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49464	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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: SF4, HCA, CLF, CA, CFM

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	0.49	0/3878	0.68	0/5229
1	C	0.43	0/3878	0.65	0/5229
1	I	0.43	0/3878	0.66	0/5229
1	K	0.41	0/3878	0.65	0/5229
2	B	0.53	0/4280	0.68	0/5786
2	D	0.49	0/4280	0.67	0/5786
2	J	0.46	0/4280	0.67	1/5786 (0.0%)
2	L	0.49	0/4280	0.67	0/5786
3	E	0.42	0/2185	0.61	0/2943
3	F	0.45	0/2210	0.62	0/2975
3	G	0.43	0/2185	0.61	0/2943
3	H	0.42	0/2210	0.62	0/2975
3	M	0.47	0/2185	0.62	0/2943
3	N	0.46	0/2210	0.62	0/2975
3	O	0.42	0/2185	0.63	0/2943
3	P	0.44	0/2210	0.63	0/2975
All	All	0.46	0/50212	0.65	1/67732 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	368	ALA	N-CA-C	-5.13	97.16	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	3732	214	0
1	C	3790	0	3732	217	0
1	I	3790	0	3731	216	0
1	K	3790	0	3730	194	0
2	B	4174	0	4088	238	0
2	D	4174	0	4088	243	0
2	J	4174	0	4089	245	0
2	L	4174	0	4089	246	0
3	E	2161	0	2176	195	0
3	F	2186	0	2197	153	0
3	G	2161	0	2176	194	0
3	H	2186	0	2197	155	0
3	M	2161	0	2176	198	0
3	N	2186	0	2197	171	0
3	O	2161	0	2176	195	0
3	P	2186	0	2197	174	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	14	0	6	1	0
5	C	14	0	6	1	0
5	I	14	0	6	1	0
5	K	14	0	6	1	0
6	A	17	0	0	7	0
6	C	17	0	0	5	0
6	I	17	0	0	3	0
6	K	17	0	0	3	0
7	A	15	0	0	4	0
7	D	15	0	0	3	0
7	J	15	0	0	3	0
7	K	15	0	0	3	0
8	E	8	0	0	2	0
8	G	8	0	0	2	0
8	N	8	0	0	5	0
8	P	8	0	0	0	0
All	All	49464	0	48795	3018	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 31.

All (3018) 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)
2:B:400:LYS:NZ	3:F:112:GLU:CD	1.81	1.34
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.32	1.11
2:B:400:LYS:HZ3	3:F:112:GLU:CD	1.43	1.09
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.35	1.08
2:L:96:VAL:HG21	2:L:115:SER:HB2	1.34	1.08
3:O:52:LYS:H	3:O:52:LYS:HD3	1.20	1.06
2:J:96:VAL:HG21	2:J:115:SER:HB2	1.34	1.06
3:F:137:MET:HB3	3:F:138:PRO:HD3	1.37	1.06
3:G:52:LYS:HD3	3:G:52:LYS:H	1.19	1.05
3:E:52:LYS:HD3	3:E:52:LYS:H	1.20	1.02
3:G:189:THR:HB	3:G:192:GLU:HB2	1.37	1.02
3:M:52:LYS:HD3	3:M:52:LYS:H	1.22	1.01
2:J:477:HIS:H	2:L:499:ASN:HD21	1.03	1.01
3:H:137:MET:HB3	3:H:138:PRO:HD3	1.42	1.01
3:N:137:MET:HB3	3:N:138:PRO:HD3	1.42	1.00
3:E:189:THR:HB	3:E:192:GLU:HB2	1.44	0.99
3:P:137:MET:HB3	3:P:138:PRO:HD3	1.46	0.98
2:B:400:LYS:HZ2	3:F:112:GLU:CD	1.54	0.98
3:G:162:ASN:HD21	3:G:259:ILE:HG12	1.27	0.97
3:M:162:ASN:HD21	3:M:259:ILE:HG12	1.29	0.96
3:G:259:ILE:HD11	3:G:264:LEU:HG	1.49	0.94
3:M:189:THR:HB	3:M:192:GLU:HB2	1.49	0.94
1:A:88:CYS:HG	7:A:6498:CLF:FE4	0.69	0.94
3:H:50:HIS:O	3:H:224:ARG:HD3	1.68	0.94
3:O:189:THR:HB	3:O:192:GLU:HB2	1.50	0.94
3:N:76:LEU:HD11	3:N:84:LYS:HB3	1.49	0.93
3:M:91:PRO:HA	3:M:100:ARG:HH22	1.33	0.93
3:G:91:PRO:HA	3:G:100:ARG:HH22	1.31	0.93
1:K:88:CYS:HG	7:K:9498:CLF:FE4	0.68	0.93
3:M:281:ILE:HG22	3:N:223:ARG:HD2	1.51	0.93
3:O:91:PRO:HA	3:O:100:ARG:HH22	1.30	0.93
3:E:76:LEU:HD11	3:E:84:LYS:HB3	1.51	0.92
3:M:76:LEU:HD11	3:M:84:LYS:HB3	1.52	0.92
3:N:50:HIS:O	3:N:224:ARG:HD3	1.70	0.92
2:J:499:ASN:HD21	2:L:477:HIS:H	1.13	0.91
3:E:162:ASN:HD21	3:E:259:ILE:HG12	1.30	0.91
3:E:259:ILE:HD11	3:E:264:LEU:HG	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:91:PRO:HA	3:E:100:ARG:HH22	1.34	0.90
3:F:206:GLN:HG2	3:F:252:LEU:HD22	1.52	0.90
3:P:206:GLN:HG2	3:P:252:LEU:HD22	1.52	0.89
2:B:477:HIS:H	2:D:499:ASN:HD21	1.13	0.88
3:F:50:HIS:O	3:F:224:ARG:HD3	1.74	0.88
1:A:433:LYS:HE3	2:B:263:THR:HG23	1.54	0.88
3:O:259:ILE:HD11	3:O:264:LEU:HG	1.56	0.88
3:O:162:ASN:HD21	3:O:259:ILE:HG12	1.37	0.88
1:I:203:ARG:HD2	1:I:204:ASP:OD1	1.73	0.88
3:N:241:ARG:HB3	3:N:245:ARG:HH12	1.36	0.87
3:H:127:LEU:HD21	3:H:129:ASP:HB2	1.56	0.87
3:M:32:LYS:HB3	3:M:119:LEU:HD12	1.57	0.87
3:P:50:HIS:O	3:P:224:ARG:HD3	1.73	0.87
3:F:241:ARG:HB3	3:F:245:ARG:HH12	1.37	0.87
1:I:433:LYS:HE3	2:J:263:THR:HG23	1.56	0.86
3:P:127:LEU:HD21	3:P:129:ASP:HB2	1.56	0.86
3:N:206:GLN:HG2	3:N:252:LEU:HD22	1.58	0.86
3:H:206:GLN:HG2	3:H:252:LEU:HD22	1.58	0.86
3:N:127:LEU:HD21	3:N:129:ASP:HB2	1.55	0.86
1:K:203:ARG:HD2	1:K:204:ASP:OD1	1.75	0.86
3:M:259:ILE:HD11	3:M:264:LEU:HG	1.55	0.85
1:C:433:LYS:HE3	2:D:263:THR:HG23	1.56	0.85
3:F:127:LEU:HD21	3:F:129:ASP:HB2	1.59	0.85
3:O:32:LYS:HB3	3:O:119:LEU:HD12	1.59	0.85
3:E:32:LYS:HB3	3:E:119:LEU:HD12	1.58	0.85
3:P:76:LEU:HD11	3:P:84:LYS:HB3	1.58	0.85
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.42	0.85
2:J:128:GLN:HE22	2:J:165:PHE:HA	1.42	0.84
3:O:76:LEU:HD11	3:O:84:LYS:HB3	1.58	0.84
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.42	0.84
2:B:499:ASN:HD21	2:D:477:HIS:H	1.19	0.84
1:K:433:LYS:HE3	2:L:263:THR:HG23	1.59	0.83
2:B:213:MET:HE2	2:B:309:TRP:HA	1.57	0.83
2:D:400:LYS:NZ	3:H:112:GLU:CD	2.32	0.83
3:F:76:LEU:HD11	3:F:84:LYS:HB3	1.57	0.83
1:A:203:ARG:HD2	1:A:204:ASP:OD1	1.78	0.83
3:M:160:ALA:O	3:M:164:ILE:HG13	1.79	0.82
1:I:88:CYS:HG	7:J:8498:CLF:FE4	0.91	0.82
3:H:76:LEU:HD11	3:H:84:LYS:HB3	1.59	0.82
3:M:223:ARG:HG2	3:N:281:ILE:HD12	1.60	0.82
3:M:136:ALA:HB1	3:N:94:GLY:HA2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:ASN:ND2	3:G:259:ILE:HG12	1.94	0.81
3:G:32:LYS:HB3	3:G:119:LEU:HD12	1.60	0.81
3:H:241:ARG:HB3	3:H:245:ARG:HH12	1.45	0.81
1:C:203:ARG:HD2	1:C:204:ASP:OD1	1.81	0.81
2:L:466:LEU:HD12	2:L:467:ILE:N	1.96	0.81
3:E:197:ILE:HG23	3:E:207:MET:HB3	1.63	0.81
1:I:120:GLU:O	1:I:124:VAL:HG23	1.81	0.80
3:O:160:ALA:O	3:O:164:ILE:HG13	1.81	0.80
3:O:285:THR:HG21	3:P:230:TYR:CE1	2.15	0.80
3:P:241:ARG:HB3	3:P:245:ARG:HH12	1.45	0.80
3:G:267:LEU:O	3:G:267:LEU:HD23	1.82	0.80
1:I:74:PRO:HB2	1:I:254:SER:HB2	1.64	0.80
2:D:452:GLN:OE1	2:D:465:PRO:HA	1.82	0.80
3:E:267:LEU:HD23	3:E:267:LEU:O	1.82	0.80
3:G:76:LEU:HD11	3:G:84:LYS:HB3	1.64	0.80
2:B:394:LEU:HD23	2:B:395:CYS:N	1.97	0.79
1:K:74:PRO:HB2	1:K:254:SER:HB2	1.62	0.79
3:E:160:ALA:O	3:E:164:ILE:HG13	1.80	0.79
2:B:510:ARG:CZ	2:D:452:GLN:HE21	1.96	0.79
3:F:141:GLU:HB3	3:F:143:LYS:HE2	1.65	0.79
2:J:466:LEU:HD12	2:J:467:ILE:N	1.97	0.79
2:B:452:GLN:OE1	2:B:465:PRO:HA	1.83	0.79
2:D:466:LEU:HD12	2:D:467:ILE:N	1.98	0.79
1:A:250:VAL:HG13	2:B:31:PHE:CD1	2.18	0.79
1:I:389:ARG:HG3	1:I:389:ARG:HH11	1.48	0.79
3:G:197:ILE:HG23	3:G:207:MET:HB3	1.66	0.78
3:M:162:ASN:ND2	3:M:259:ILE:HG12	1.97	0.78
3:M:197:ILE:HG23	3:M:207:MET:HB3	1.62	0.78
2:D:376:VAL:O	2:D:380:VAL:HG23	1.83	0.78
1:A:120:GLU:O	1:A:124:VAL:HG23	1.83	0.78
2:L:128:GLN:HE22	2:L:165:PHE:HA	1.46	0.78
2:J:178:GLU:CD	2:J:178:GLU:H	1.87	0.78
3:O:197:ILE:HG23	3:O:207:MET:HB3	1.65	0.78
2:L:452:GLN:OE1	2:L:465:PRO:HA	1.84	0.77
1:A:74:PRO:HB2	1:A:254:SER:HB2	1.67	0.77
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.12	0.77
2:B:358:SER:HB3	2:D:477:HIS:ND1	2.00	0.77
3:O:223:ARG:HD3	3:P:281:ILE:O	1.85	0.77
3:E:162:ASN:ND2	3:E:259:ILE:HG12	1.99	0.77
2:B:376:VAL:O	2:B:380:VAL:HG23	1.85	0.77
1:K:120:GLU:O	1:K:124:VAL:HG23	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:182:LEU:O	3:F:208:ILE:HG22	1.86	0.76
2:D:394:LEU:HD23	2:D:395:CYS:N	2.00	0.76
3:G:160:ALA:O	3:G:164:ILE:HG13	1.86	0.76
3:G:52:LYS:N	3:G:52:LYS:HD3	2.00	0.76
2:B:178:GLU:H	2:B:178:GLU:CD	1.89	0.76
3:O:162:ASN:ND2	3:O:259:ILE:HG12	2.00	0.76
2:J:394:LEU:HD23	2:J:395:CYS:N	2.01	0.76
3:E:103:ILE:HG13	3:E:137:MET:HG3	1.68	0.76
1:I:239:ARG:HE	2:J:23:MET:HE3	1.49	0.75
3:F:137:MET:HB3	3:F:138:PRO:CD	2.15	0.75
2:J:452:GLN:OE1	2:J:465:PRO:HA	1.85	0.75
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.15	0.75
1:A:335:TRP:O	1:A:339:VAL:HG23	1.86	0.75
3:H:41:LYS:HD3	3:H:41:LYS:O	1.85	0.75
3:E:76:LEU:CD1	3:E:84:LYS:HB3	2.16	0.75
3:N:141:GLU:HB3	3:N:143:LYS:HE2	1.66	0.75
3:H:139:ILE:HG23	3:H:177:VAL:HG21	1.66	0.75
3:G:103:ILE:HG13	3:G:137:MET:HG3	1.67	0.75
3:M:76:LEU:CD1	3:M:84:LYS:HB3	2.17	0.75
3:M:136:ALA:CB	3:N:94:GLY:HA2	2.16	0.74
1:C:120:GLU:O	1:C:124:VAL:HG23	1.85	0.74
2:D:400:LYS:HZ2	3:H:112:GLU:CD	1.89	0.74
2:J:96:VAL:CG2	2:J:115:SER:HB2	2.15	0.74
1:C:250:VAL:HG13	2:D:31:PHE:CD1	2.21	0.74
3:H:182:LEU:O	3:H:208:ILE:HG22	1.86	0.74
2:L:394:LEU:HD23	2:L:395:CYS:N	2.03	0.74
3:O:52:LYS:N	3:O:52:LYS:HD3	2.01	0.74
1:A:88:CYS:HB2	1:A:153:GLU:OE2	1.88	0.74
3:G:127:LEU:HD11	3:G:129:ASP:HB2	1.68	0.74
2:D:178:GLU:H	2:D:178:GLU:CD	1.91	0.74
3:O:48:ILE:HG22	3:O:49:LEU:HD23	1.69	0.74
1:C:74:PRO:HB2	1:C:254:SER:HB2	1.68	0.74
3:M:103:ILE:HG13	3:M:137:MET:HG3	1.68	0.74
2:J:510:ARG:CZ	2:L:452:GLN:HE21	2.01	0.74
3:M:127:LEU:HD11	3:M:129:ASP:HB2	1.70	0.74
3:E:208:ILE:O	3:E:209:HIS:HB2	1.87	0.73
3:O:91:PRO:HA	3:O:100:ARG:NH2	2.03	0.73
3:M:267:LEU:O	3:M:267:LEU:HD23	1.87	0.73
3:M:4:GLN:HA	3:M:122:VAL:HB	1.69	0.73
3:O:267:LEU:HD23	3:O:267:LEU:O	1.88	0.73
3:N:139:ILE:HG23	3:N:177:VAL:HG21	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:335:TRP:O	1:K:339:VAL:HG23	1.88	0.73
2:J:192:SER:OG	2:J:194:VAL:HG22	1.88	0.73
3:G:136:ALA:CB	3:H:94:GLY:HA2	2.18	0.73
3:F:139:ILE:HG23	3:F:177:VAL:HG21	1.70	0.73
1:I:230:ASN:HA	1:I:235:ALA:H	1.53	0.73
1:C:335:TRP:O	1:C:339:VAL:HG23	1.89	0.73
3:P:139:ILE:HG23	3:P:177:VAL:HG21	1.70	0.73
1:A:19:VAL:HG11	1:A:407:TYR:CE2	2.23	0.73
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.19	0.73
3:O:136:ALA:CB	3:P:94:GLY:HA2	2.19	0.73
2:L:96:VAL:CG2	2:L:115:SER:HB2	2.13	0.73
3:N:41:LYS:O	3:N:41:LYS:HD3	1.88	0.73
1:C:57:MET:HE2	2:D:113:CYS:H	1.52	0.73
3:E:127:LEU:HD11	3:E:129:ASP:HB2	1.71	0.73
3:P:41:LYS:O	3:P:41:LYS:HD3	1.89	0.72
2:J:477:HIS:ND1	2:L:358:SER:HB3	2.03	0.72
1:K:59:ILE:H	1:K:59:ILE:HD12	1.54	0.72
1:K:275:CYS:HA	1:K:358:LEU:HD22	1.70	0.72
1:C:230:ASN:HA	1:C:235:ALA:H	1.54	0.72
1:I:88:CYS:HB2	1:I:153:GLU:OE2	1.90	0.72
3:N:147:ILE:HG21	3:N:168:ILE:HD11	1.71	0.72
3:H:141:GLU:HB3	3:H:143:LYS:HE2	1.70	0.72
3:M:91:PRO:HA	3:M:100:ARG:NH2	2.04	0.72
3:G:91:PRO:HA	3:G:100:ARG:NH2	2.05	0.72
2:J:213:MET:HE2	2:J:309:TRP:HA	1.71	0.72
1:I:335:TRP:O	1:I:339:VAL:HG23	1.90	0.72
1:K:59:ILE:N	1:K:59:ILE:HD12	2.04	0.72
2:J:452:GLN:HE21	2:L:510:ARG:CZ	2.02	0.72
3:O:186:SER:HB2	3:O:212:PRO:HA	1.71	0.72
1:C:226:ILE:O	1:C:273:VAL:HA	1.90	0.72
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.72	0.72
3:N:54:GLN:HE22	3:N:86:VAL:HA	1.55	0.72
2:B:466:LEU:HD12	2:B:467:ILE:N	2.05	0.72
3:M:135:PHE:HZ	3:N:130:VAL:HG11	1.53	0.71
1:C:339:VAL:O	1:C:343:ARG:HB3	1.90	0.71
3:N:208:ILE:HD11	3:N:246:LYS:HB3	1.70	0.71
3:N:208:ILE:O	3:N:246:LYS:HD3	1.89	0.71
3:G:4:GLN:HA	3:G:122:VAL:HB	1.71	0.71
1:K:19:VAL:HG11	1:K:407:TYR:CE2	2.25	0.71
2:L:466:LEU:HD12	2:L:467:ILE:H	1.53	0.71
3:O:49:LEU:HD11	3:O:85:CYS:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HA	1:A:235:ALA:H	1.55	0.71
3:O:127:LEU:HD11	3:O:129:ASP:HB2	1.71	0.71
3:M:49:LEU:HD21	3:M:85:CYS:SG	2.30	0.71
3:O:49:LEU:HD21	3:O:85:CYS:SG	2.29	0.71
3:O:103:ILE:HG13	3:O:137:MET:HG3	1.72	0.71
1:A:239:ARG:HE	2:B:23:MET:HE3	1.56	0.71
1:C:239:ARG:HE	2:D:23:MET:HE3	1.56	0.71
3:F:41:LYS:HD3	3:F:41:LYS:O	1.91	0.71
1:C:13:ILE:O	1:C:17:LEU:HG	1.90	0.71
2:J:376:VAL:O	2:J:380:VAL:HG23	1.90	0.71
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.74	0.70
1:C:346:LEU:O	1:C:349:LYS:HG2	1.91	0.70
3:G:48:ILE:HG22	3:G:49:LEU:HD23	1.71	0.70
3:G:2:MET:HA	3:G:120:ASP:O	1.91	0.70
1:K:226:ILE:O	1:K:273:VAL:HA	1.92	0.70
2:D:247:MET:HE2	2:D:340:ILE:HA	1.73	0.70
3:M:45:THR:CG2	3:M:85:CYS:HB3	2.21	0.70
1:A:389:ARG:HG3	1:A:389:ARG:HH11	1.55	0.70
1:I:250:VAL:HG13	2:J:31:PHE:CD1	2.26	0.70
3:E:91:PRO:HA	3:E:100:ARG:NH2	2.05	0.70
1:A:35:ASN:ND2	1:A:36:ASP:H	1.90	0.70
1:C:19:VAL:HG11	1:C:407:TYR:CE2	2.26	0.70
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.20	0.70
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.26	0.70
3:H:10:LYS:HG2	3:H:11:GLY:N	2.07	0.70
3:M:48:ILE:HG22	3:M:49:LEU:HD23	1.73	0.69
1:A:59:ILE:H	1:A:59:ILE:HD12	1.56	0.69
3:O:225:MET:HE3	3:O:229:GLU:OE1	1.92	0.69
2:J:494:LEU:O	2:J:498:VAL:HG12	1.92	0.69
3:E:71:GLU:HB3	3:E:74:ASP:OD1	1.92	0.69
1:A:275:CYS:HG	6:A:6496:CFM:FE1	1.05	0.69
3:O:15:LYS:NZ	3:O:127:LEU:HA	2.08	0.69
3:E:76:LEU:HD11	3:E:84:LYS:CB	2.23	0.69
1:A:289:LYS:HG2	1:A:289:LYS:O	1.91	0.69
3:H:8:TYR:HB3	3:H:164:ILE:HD13	1.74	0.69
1:I:19:VAL:HG11	1:I:407:TYR:CE2	2.28	0.69
3:G:208:ILE:O	3:G:209:HIS:HB2	1.92	0.69
3:M:165:SER:HB3	3:M:256:PRO:HB2	1.72	0.69
2:D:466:LEU:HD12	2:D:467:ILE:H	1.57	0.69
3:F:208:ILE:HD11	3:F:246:LYS:HB3	1.75	0.69
1:I:339:VAL:O	1:I:343:ARG:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.28	0.69
1:I:234:ASP:HB3	1:I:451:HIS:ND1	2.08	0.69
2:L:247:MET:HE1	2:L:340:ILE:HG12	1.75	0.69
3:E:4:GLN:HA	3:E:122:VAL:HB	1.75	0.69
2:B:205:ALA:HA	2:B:281:MET:CE	2.22	0.69
3:H:137:MET:HB3	3:H:138:PRO:CD	2.22	0.68
1:A:367:TYR:HD1	1:A:372:MET:HG2	1.58	0.68
3:M:49:LEU:HD11	3:M:85:CYS:HB2	1.75	0.68
3:O:76:LEU:CD1	3:O:84:LYS:HB3	2.23	0.68
2:B:477:HIS:ND1	2:D:358:SER:HB3	2.08	0.68
3:F:208:ILE:O	3:F:246:LYS:HD3	1.93	0.68
1:K:339:VAL:O	1:K:343:ARG:HB3	1.92	0.68
2:B:468:ARG:HG3	2:B:468:ARG:HH11	1.58	0.68
1:K:77:ASP:OD2	1:K:258:SER:HB2	1.93	0.68
2:J:247:MET:HE2	2:J:340:ILE:HA	1.75	0.68
3:E:99:GLY:HA3	3:E:134:GLY:HA2	1.76	0.68
3:H:33:VAL:HG12	3:H:34:MET:N	2.08	0.68
3:G:127:LEU:HD13	3:G:129:ASP:H	1.58	0.68
3:E:49:LEU:HD11	3:E:85:CYS:HB2	1.76	0.68
3:F:147:ILE:HG21	3:F:168:ILE:HD11	1.74	0.68
3:E:92:GLU:OE1	3:F:170:LYS:HE3	1.94	0.68
1:I:275:CYS:HA	1:I:358:LEU:HD22	1.75	0.68
3:N:8:TYR:HB3	3:N:164:ILE:HD13	1.76	0.68
3:E:48:ILE:HG22	3:E:49:LEU:HD23	1.74	0.68
1:K:354:TYR:CZ	1:K:404:VAL:HG12	2.29	0.68
3:N:60:MET:HE3	3:N:75:VAL:HG22	1.76	0.68
3:P:182:LEU:O	3:P:208:ILE:HG22	1.93	0.68
2:B:511:GLY:O	2:B:516:ASP:HB3	1.93	0.68
2:B:247:MET:HE2	2:B:340:ILE:HA	1.76	0.68
3:P:141:GLU:HB3	3:P:143:LYS:HE2	1.76	0.68
3:O:165:SER:HB3	3:O:256:PRO:HB2	1.76	0.68
3:P:184:CYS:HG	3:P:210:PHE:HE1	1.40	0.68
3:E:52:LYS:N	3:E:52:LYS:HD3	2.01	0.67
3:M:184:CYS:HG	3:M:210:PHE:HE1	1.39	0.67
3:G:49:LEU:HD11	3:G:85:CYS:HB2	1.74	0.67
1:A:35:ASN:HD22	1:A:36:ASP:H	1.41	0.67
2:L:247:MET:HE2	2:L:340:ILE:HA	1.75	0.67
3:E:96:GLY:HA3	3:E:100:ARG:NH1	2.08	0.67
3:F:225:MET:HE2	3:F:230:TYR:HA	1.76	0.67
2:B:452:GLN:HE21	2:D:510:ARG:CZ	2.07	0.67
2:B:220:SER:OG	2:B:286:ASN:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:205:ALA:HA	2:J:281:MET:CE	2.25	0.67
3:P:33:VAL:HG12	3:P:34:MET:N	2.08	0.67
3:H:184:CYS:HG	3:H:210:PHE:HE1	1.42	0.67
1:C:113:ASN:HD22	2:D:66:PRO:CD	2.07	0.67
3:H:223:ARG:HB3	3:H:225:MET:HG2	1.77	0.67
3:N:212:PRO:HG2	3:N:236:GLN:OE1	1.95	0.67
3:O:4:GLN:HA	3:O:122:VAL:HB	1.74	0.67
1:K:230:ASN:HA	1:K:235:ALA:H	1.57	0.67
3:G:225:MET:HE3	3:G:229:GLU:OE1	1.94	0.67
3:E:197:ILE:HG23	3:E:207:MET:CB	2.24	0.67
3:O:197:ILE:HG23	3:O:207:MET:CB	2.25	0.67
3:G:165:SER:HB3	3:G:256:PRO:HB2	1.77	0.67
3:N:102:VAL:HG12	3:N:106:ILE:HD11	1.76	0.67
3:O:45:THR:CG2	3:O:85:CYS:HB3	2.25	0.67
3:M:127:LEU:HD13	3:M:129:ASP:H	1.59	0.67
3:G:228:ILE:O	3:G:232:PRO:HG3	1.95	0.67
1:I:355:ILE:HG22	1:I:356:GLY:H	1.59	0.67
3:E:186:SER:HB2	3:E:212:PRO:HA	1.75	0.67
1:C:88:CYS:HB2	1:C:153:GLU:OE2	1.95	0.67
1:K:13:ILE:O	1:K:17:LEU:HG	1.95	0.67
1:I:253:TRP:CZ2	1:I:262:ILE:HG23	2.29	0.67
2:J:466:LEU:HD12	2:J:467:ILE:H	1.56	0.67
3:G:186:SER:HB2	3:G:212:PRO:HA	1.77	0.67
3:P:208:ILE:O	3:P:246:LYS:HD3	1.95	0.66
2:B:43:VAL:O	2:B:46:TRP:HB3	1.95	0.66
3:N:47:LEU:HD22	3:N:225:MET:O	1.96	0.66
3:F:33:VAL:HG12	3:F:34:MET:N	2.08	0.66
3:M:225:MET:HE1	3:M:230:TYR:HA	1.77	0.66
3:M:99:GLY:HA3	3:M:134:GLY:HA2	1.77	0.66
3:N:182:LEU:O	3:N:208:ILE:HG22	1.95	0.66
2:L:91:GLY:HA3	2:L:152:THR:OG1	1.95	0.66
3:O:127:LEU:HD13	3:O:129:ASP:H	1.61	0.66
3:M:186:SER:HB2	3:M:212:PRO:HA	1.75	0.66
1:K:66:GLY:O	1:K:70:VAL:HB	1.95	0.66
2:J:358:SER:HB3	2:L:477:HIS:ND1	2.10	0.66
1:A:59:ILE:HD12	1:A:59:ILE:N	2.11	0.66
1:K:367:TYR:HD1	1:K:372:MET:HG2	1.61	0.66
2:J:151:THR:HG23	2:J:162:LEU:HD11	1.77	0.66
3:M:197:ILE:HG23	3:M:207:MET:CB	2.25	0.66
3:M:208:ILE:O	3:M:209:HIS:HB2	1.94	0.66
1:I:367:TYR:HD1	1:I:372:MET:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:236:GLN:O	3:F:239:GLU:HB2	1.96	0.66
3:E:225:MET:HE1	3:E:230:TYR:HA	1.77	0.66
3:G:182:LEU:HD12	3:G:196:ILE:HG22	1.78	0.66
3:N:137:MET:HB3	3:N:138:PRO:CD	2.22	0.66
3:O:169:VAL:HG23	3:O:256:PRO:HG2	1.77	0.66
3:H:208:ILE:O	3:H:246:LYS:HD3	1.95	0.66
3:N:10:LYS:HG2	3:N:11:GLY:N	2.10	0.66
1:C:35:ASN:ND2	1:C:36:ASP:H	1.93	0.66
3:N:223:ARG:HB3	3:N:225:MET:HG2	1.77	0.66
3:M:223:ARG:HG2	3:N:281:ILE:CD1	2.24	0.66
3:E:169:VAL:HG23	3:E:256:PRO:HG2	1.77	0.66
3:G:76:LEU:CD1	3:G:84:LYS:HB3	2.26	0.66
1:C:35:ASN:HD22	1:C:36:ASP:H	1.43	0.66
2:J:373:PRO:HD3	2:J:397:ASN:OD1	1.96	0.66
2:B:295:PRO:O	2:B:297:HIS:N	2.29	0.66
3:M:86:VAL:HG21	3:M:109:LEU:HD11	1.78	0.65
3:E:165:SER:HB3	3:E:256:PRO:HB2	1.78	0.65
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.31	0.65
3:O:20:GLN:NE2	3:O:48:ILE:HG12	2.11	0.65
3:G:49:LEU:HD21	3:G:85:CYS:SG	2.35	0.65
1:I:226:ILE:O	1:I:273:VAL:HA	1.95	0.65
3:G:72:LEU:HD13	3:G:112:GLU:CB	2.26	0.65
1:K:389:ARG:HG3	1:K:389:ARG:HH11	1.61	0.65
3:M:52:LYS:HD3	3:M:52:LYS:N	2.05	0.65
3:H:54:GLN:HE22	3:H:86:VAL:HA	1.61	0.65
3:F:10:LYS:HG2	3:F:11:GLY:N	2.12	0.65
2:B:178:GLU:N	2:B:178:GLU:CD	2.50	0.65
3:H:147:ILE:HG21	3:H:168:ILE:HD11	1.78	0.65
1:I:275:CYS:HB3	1:I:278:SER:OG	1.97	0.65
1:A:68:LYS:C	1:A:68:LYS:HD3	2.17	0.65
3:G:197:ILE:HG23	3:G:207:MET:CB	2.27	0.65
3:P:137:MET:HB3	3:P:138:PRO:CD	2.24	0.65
3:N:127:LEU:CD2	3:N:129:ASP:HB2	2.27	0.65
1:K:35:ASN:ND2	1:K:36:ASP:H	1.94	0.65
3:P:147:ILE:HG21	3:P:168:ILE:HD11	1.79	0.65
3:E:228:ILE:O	3:E:232:PRO:HG3	1.96	0.65
3:E:20:GLN:NE2	3:E:48:ILE:HG12	2.11	0.65
1:A:87:GLY:HA3	7:A:6498:CLF:S2B	2.36	0.65
3:F:54:GLN:HE22	3:F:86:VAL:HA	1.62	0.65
1:C:59:ILE:HD12	1:C:59:ILE:N	2.11	0.65
2:J:91:GLY:HA3	2:J:152:THR:OG1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:92:GLU:OE1	3:N:170:LYS:HE3	1.97	0.65
3:G:52:LYS:CD	3:G:52:LYS:H	2.03	0.65
3:G:45:THR:HG21	3:G:85:CYS:HB3	1.80	0.64
1:C:275:CYS:HB3	1:C:278:SER:OG	1.97	0.64
2:J:70:CYS:SG	2:J:72:PRO:HG2	2.37	0.64
3:O:192:GLU:O	3:O:196:ILE:HG12	1.98	0.64
2:B:247:MET:HE1	2:B:340:ILE:HG12	1.78	0.64
2:J:236:ASN:HB3	2:J:485:LEU:HD12	1.80	0.64
1:K:57:MET:HE2	2:L:113:CYS:H	1.61	0.64
3:E:2:MET:HA	3:E:120:ASP:O	1.98	0.64
2:D:509:THR:O	2:D:516:ASP:HA	1.97	0.64
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.13	0.64
2:L:151:THR:HG23	2:L:162:LEU:HD11	1.79	0.64
1:I:66:GLY:O	1:I:70:VAL:HB	1.97	0.64
1:I:13:ILE:O	1:I:17:LEU:HG	1.96	0.64
3:P:72:LEU:C	3:P:72:LEU:HD22	2.17	0.64
3:O:52:LYS:H	3:O:52:LYS:CD	2.04	0.64
1:I:35:ASN:ND2	1:I:36:ASP:H	1.96	0.64
3:E:52:LYS:HB3	3:E:224:ARG:NH1	2.13	0.64
3:O:208:ILE:O	3:O:209:HIS:HB2	1.97	0.64
2:B:477:HIS:H	2:D:499:ASN:ND2	1.93	0.64
3:F:47:LEU:HD22	3:F:225:MET:O	1.97	0.64
2:J:231:GLU:CD	2:J:236:ASN:HD22	2.01	0.64
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.01	0.64
2:B:91:GLY:HA3	2:B:152:THR:OG1	1.98	0.64
3:O:33:VAL:HG22	3:O:121:PHE:HB2	1.80	0.64
1:A:19:VAL:HG13	1:A:20:TYR:N	2.12	0.64
1:I:68:LYS:HD3	1:I:68:LYS:C	2.18	0.64
2:L:178:GLU:CD	2:L:178:GLU:H	2.00	0.64
2:B:213:MET:CE	2:B:309:TRP:HA	2.28	0.64
1:K:275:CYS:HB3	1:K:278:SER:OG	1.98	0.64
3:E:241:ARG:HG2	3:E:245:ARG:NH1	2.12	0.64
1:C:389:ARG:HG3	1:C:389:ARG:HH11	1.63	0.64
3:M:182:LEU:HD12	3:M:196:ILE:HG22	1.80	0.64
1:C:289:LYS:O	1:C:289:LYS:HG2	1.97	0.64
3:P:10:LYS:HG2	3:P:11:GLY:N	2.12	0.64
3:M:215:ASN:O	3:M:219:ARG:HG3	1.97	0.63
2:D:494:LEU:O	2:D:498:VAL:HG12	1.98	0.63
2:B:247:MET:CE	2:B:340:ILE:HA	2.28	0.63
2:D:205:ALA:HA	2:D:281:MET:CE	2.28	0.63
1:A:199:ASN:OD1	1:A:281:TYR:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ILE:HG22	1:C:356:GLY:H	1.61	0.63
2:L:376:VAL:O	2:L:380:VAL:HG23	1.98	0.63
3:M:76:LEU:HD11	3:M:84:LYS:CB	2.25	0.63
3:E:278:ASP:CB	3:E:281:ILE:HD12	2.29	0.63
2:D:192:SER:OG	2:D:194:VAL:HG22	1.99	0.63
2:J:103:PHE:CB	2:J:111:VAL:HG21	2.28	0.63
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.81	0.63
3:P:100:ARG:HD3	3:P:101:GLY:N	2.14	0.63
3:M:192:GLU:O	3:M:196:ILE:HG12	1.99	0.63
3:G:278:ASP:CB	3:G:281:ILE:HD12	2.28	0.63
3:E:285:THR:HG21	3:F:230:TYR:CE1	2.34	0.63
3:E:15:LYS:NZ	3:E:127:LEU:HA	2.13	0.63
3:M:228:ILE:O	3:M:232:PRO:HG3	1.98	0.63
1:I:199:ASN:OD1	1:I:281:TYR:HB2	1.97	0.63
3:P:56:THR:OG1	3:P:59:GLU:HG3	1.98	0.63
1:K:250:VAL:HG13	2:L:31:PHE:CD1	2.33	0.63
3:E:136:ALA:CB	3:F:94:GLY:HA2	2.27	0.63
1:I:59:ILE:HD12	1:I:59:ILE:N	2.12	0.63
3:O:278:ASP:CB	3:O:281:ILE:HD12	2.28	0.63
2:J:178:GLU:CD	2:J:178:GLU:N	2.51	0.63
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.81	0.63
1:A:66:GLY:O	1:A:70:VAL:HB	1.98	0.63
1:C:68:LYS:HD3	1:C:68:LYS:C	2.19	0.63
3:N:33:VAL:HG12	3:N:34:MET:N	2.13	0.63
3:P:86:VAL:HG21	3:P:109:LEU:HD11	1.81	0.63
1:K:234:ASP:HB3	1:K:451:HIS:ND1	2.13	0.63
3:H:86:VAL:HG21	3:H:109:LEU:HD11	1.81	0.63
1:C:59:ILE:H	1:C:59:ILE:HD12	1.64	0.63
3:P:103:ILE:HG23	3:P:104:THR:N	2.13	0.63
2:D:178:GLU:CD	2:D:178:GLU:N	2.52	0.63
1:I:332:LYS:HA	1:I:335:TRP:NE1	2.13	0.63
3:O:185:ASN:N	3:O:185:ASN:HD22	1.96	0.63
2:L:205:ALA:HA	2:L:281:MET:CE	2.29	0.63
3:O:96:GLY:HA3	3:O:100:ARG:NH1	2.13	0.62
1:K:477:ALA:HB3	1:K:480:GLU:HG2	1.80	0.62
1:K:88:CYS:HB2	1:K:153:GLU:OE2	1.98	0.62
3:P:54:GLN:HE22	3:P:86:VAL:HA	1.64	0.62
2:D:400:LYS:HZ3	3:H:112:GLU:CD	2.00	0.62
2:B:466:LEU:HD12	2:B:467:ILE:H	1.64	0.62
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.15	0.62
3:F:115:TYR:O	3:F:117:ASP:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:ARG:HE	2:L:23:MET:HE3	1.63	0.62
1:K:289:LYS:HG2	1:K:289:LYS:O	1.97	0.62
2:J:477:HIS:H	2:L:499:ASN:ND2	1.86	0.62
3:O:217:VAL:HG22	3:O:227:VAL:HG21	1.80	0.62
1:C:75:ILE:H	1:C:75:ILE:HD12	1.63	0.62
3:E:225:MET:HE3	3:E:229:GLU:OE1	1.98	0.62
3:E:192:GLU:O	3:E:196:ILE:HG12	1.99	0.62
3:O:285:THR:HG21	3:P:230:TYR:HE1	1.61	0.62
3:M:15:LYS:NZ	3:M:127:LEU:HA	2.15	0.62
3:M:2:MET:HA	3:M:120:ASP:O	1.99	0.62
3:E:127:LEU:HD13	3:E:129:ASP:H	1.62	0.62
3:P:223:ARG:HB3	3:P:225:MET:HG2	1.80	0.62
2:D:233:TYR:HD1	2:D:484:THR:HG23	1.64	0.62
1:I:77:ASP:OD2	1:I:258:SER:HB2	2.00	0.62
3:G:225:MET:HE1	3:G:230:TYR:HA	1.80	0.62
3:E:194:GLU:HA	3:E:197:ILE:HG13	1.81	0.62
3:P:47:LEU:HD22	3:P:225:MET:O	1.99	0.62
3:M:225:MET:HE3	3:M:229:GLU:OE1	1.99	0.62
3:E:215:ASN:O	3:E:219:ARG:HG3	1.99	0.62
1:A:76:LYS:O	1:A:108:ALA:HA	2.00	0.62
1:C:76:LYS:O	1:C:108:ALA:HA	2.00	0.62
3:H:47:LEU:HD22	3:H:225:MET:O	1.99	0.62
1:K:355:ILE:HG22	1:K:356:GLY:H	1.64	0.62
1:A:306:ILE:HG23	1:A:328:ILE:HD13	1.81	0.62
1:I:286:MET:O	1:I:290:TYR:HB2	2.00	0.62
1:C:57:MET:CE	2:D:113:CYS:H	2.13	0.62
1:I:59:ILE:HD12	1:I:59:ILE:H	1.65	0.62
3:F:8:TYR:HB3	3:F:164:ILE:HD13	1.80	0.62
3:O:99:GLY:HA3	3:O:134:GLY:HA2	1.80	0.62
3:E:56:THR:HG22	3:E:87:GLU:HB3	1.82	0.62
2:L:494:LEU:O	2:L:498:VAL:HG12	2.00	0.62
3:M:278:ASP:CB	3:M:281:ILE:HD12	2.29	0.62
2:L:400:LYS:HG3	3:P:111:GLU:HG2	1.82	0.62
1:A:226:ILE:O	1:A:273:VAL:HA	2.00	0.62
1:A:91:TYR:HB2	2:B:98:TYR:CD1	2.35	0.62
2:J:295:PRO:O	2:J:297:HIS:N	2.32	0.62
1:A:277:ARG:NH1	1:A:386:ASP:OD2	2.31	0.62
3:F:223:ARG:HB3	3:F:225:MET:HG2	1.81	0.61
1:A:275:CYS:HB3	1:A:278:SER:OG	2.00	0.61
1:K:76:LYS:O	1:K:108:ALA:HA	2.00	0.61
1:A:339:VAL:O	1:A:343:ARG:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:136:ALA:HB1	3:H:94:GLY:HA2	1.82	0.61
1:C:367:TYR:HD1	1:C:372:MET:HG2	1.64	0.61
3:O:2:MET:HA	3:O:120:ASP:O	2.00	0.61
2:L:431:ARG:O	2:L:434:VAL:HG22	2.00	0.61
3:M:29:MET:O	3:M:29:MET:HG2	2.00	0.61
3:E:127:LEU:HD12	3:E:135:PHE:CE2	2.36	0.61
1:I:57:MET:HE2	2:J:113:CYS:H	1.65	0.61
3:P:218:GLN:O	3:P:222:ILE:HG13	2.01	0.61
3:M:5:CYS:SG	3:M:146:GLU:HG3	2.40	0.61
2:L:400:LYS:HZ2	3:P:112:GLU:CD	2.03	0.61
1:K:75:ILE:H	1:K:75:ILE:HD12	1.65	0.61
3:F:100:ARG:O	3:F:103:ILE:HG22	2.00	0.61
3:P:115:TYR:O	3:P:117:ASP:N	2.33	0.61
3:H:67:VAL:C	3:H:69:ASP:H	2.03	0.61
3:N:184:CYS:HG	3:N:210:PHE:HE1	1.49	0.61
2:D:91:GLY:HA3	2:D:152:THR:OG1	2.01	0.61
3:P:127:LEU:CD2	3:P:129:ASP:HB2	2.30	0.61
3:O:76:LEU:HD11	3:O:84:LYS:CB	2.30	0.61
1:K:332:LYS:HA	1:K:335:TRP:NE1	2.16	0.61
2:J:494:LEU:HD23	2:J:494:LEU:O	2.01	0.61
3:P:208:ILE:HG23	3:P:209:HIS:N	2.16	0.61
2:L:241:LYS:HE3	2:L:253:LEU:HD23	1.83	0.61
2:D:220:SER:OG	2:D:286:ASN:HB3	2.00	0.61
3:M:241:ARG:HG2	3:M:245:ARG:NH1	2.15	0.61
3:E:184:CYS:HB2	3:E:196:ILE:HG13	1.83	0.61
3:G:96:GLY:HA3	3:G:100:ARG:NH1	2.14	0.61
1:I:239:ARG:NE	2:J:23:MET:HE3	2.15	0.61
3:G:212:PRO:HG2	3:G:236:GLN:OE1	2.01	0.61
1:C:19:VAL:HG13	1:C:20:TYR:N	2.15	0.61
3:E:52:LYS:CD	3:E:52:LYS:H	2.04	0.61
1:C:332:LYS:N	1:C:333:PRO:HD2	2.15	0.61
1:A:355:ILE:HG22	1:A:356:GLY:H	1.65	0.61
1:I:277:ARG:NH1	1:I:386:ASP:OD2	2.33	0.61
3:P:67:VAL:C	3:P:69:ASP:H	2.04	0.61
3:F:60:MET:HE3	3:F:75:VAL:HG22	1.81	0.61
3:F:102:VAL:HG12	3:F:106:ILE:HD11	1.81	0.61
3:F:64:ALA:HB1	3:F:69:ASP:HB2	1.83	0.61
3:M:52:LYS:H	3:M:52:LYS:CD	2.07	0.61
3:G:15:LYS:NZ	3:G:127:LEU:HA	2.16	0.61
3:M:15:LYS:HG3	3:M:150:VAL:HG21	1.83	0.61
3:E:15:LYS:HG3	3:E:150:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:35:ASN:ND2	1:K:391:MET:HG2	2.16	0.61
3:O:5:CYS:SG	3:O:146:GLU:HG3	2.41	0.61
2:L:132:LYS:HD3	2:L:174:PHE:CE2	2.36	0.61
3:G:162:ASN:HD21	3:G:259:ILE:CG1	2.08	0.60
3:H:225:MET:HE2	3:H:230:TYR:HA	1.82	0.60
1:I:35:ASN:HD22	1:I:36:ASP:H	1.48	0.60
2:L:231:GLU:CD	2:L:236:ASN:HD22	2.05	0.60
3:F:195:LEU:HD13	3:F:271:PHE:CD2	2.36	0.60
2:D:213:MET:CE	2:D:309:TRP:HA	2.31	0.60
1:K:131:LEU:O	1:K:135:ILE:HG13	2.00	0.60
3:M:33:VAL:HG22	3:M:121:PHE:HB2	1.82	0.60
2:D:247:MET:CE	2:D:340:ILE:HA	2.30	0.60
3:F:100:ARG:HD3	3:F:101:GLY:N	2.15	0.60
3:E:182:LEU:HD12	3:E:196:ILE:HG22	1.83	0.60
3:O:182:LEU:HD12	3:O:196:ILE:HG22	1.82	0.60
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.16	0.60
1:I:332:LYS:N	1:I:333:PRO:HD2	2.15	0.60
1:K:20:TYR:OH	1:K:408:GLU:HG3	2.02	0.60
3:P:19:THR:O	3:P:22:LEU:HB3	2.02	0.60
3:G:184:CYS:HB2	3:G:196:ILE:HG13	1.83	0.60
3:H:127:LEU:HD23	3:H:129:ASP:H	1.66	0.60
3:H:236:GLN:O	3:H:239:GLU:HB2	2.01	0.60
2:D:468:ARG:HH11	2:D:468:ARG:HG3	1.66	0.60
1:A:13:ILE:O	1:A:17:LEU:HG	2.02	0.60
3:N:115:TYR:O	3:N:117:ASP:N	2.34	0.60
3:G:71:GLU:HB3	3:G:74:ASP:OD1	2.00	0.60
2:D:372:ASP:O	2:D:376:VAL:HG23	2.01	0.60
1:C:96:ARG:NH2	6:C:7496:CFM:S5	2.72	0.60
2:J:247:MET:CE	2:J:340:ILE:HA	2.31	0.60
2:B:330:MET:HE3	1:C:479:TRP:HE3	1.67	0.60
2:J:132:LYS:HD3	2:J:174:PHE:CE2	2.36	0.60
1:A:477:ALA:HB3	1:A:480:GLU:HG2	1.82	0.60
3:M:72:LEU:HD13	3:M:112:GLU:CB	2.32	0.60
3:E:29:MET:HG2	3:E:29:MET:O	2.02	0.60
3:H:102:VAL:HG12	3:H:106:ILE:HD11	1.84	0.60
3:O:225:MET:HE1	3:O:230:TYR:HA	1.81	0.60
2:L:118:MET:HA	2:L:130:ASN:ND2	2.16	0.60
3:G:192:GLU:O	3:G:196:ILE:HG12	2.02	0.60
1:K:253:TRP:CZ2	1:K:262:ILE:HG23	2.37	0.60
1:I:346:LEU:O	1:I:349:LYS:HG2	2.02	0.60
3:F:212:PRO:HG2	3:F:236:GLN:OE1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:356:GLY:HA3	6:K:9496:CFM:S1B	2.42	0.60
3:H:212:PRO:HG2	3:H:236:GLN:OE1	2.02	0.60
3:H:115:TYR:O	3:H:117:ASP:N	2.35	0.60
1:K:199:ASN:OD1	1:K:281:TYR:HB2	2.01	0.60
3:M:169:VAL:HG23	3:M:256:PRO:HG2	1.83	0.60
1:C:229:TYR:CE2	6:C:7496:CFM:S2A	2.94	0.60
3:M:20:GLN:NE2	3:M:48:ILE:HG12	2.17	0.60
1:A:35:ASN:ND2	1:A:36:ASP:N	2.49	0.60
1:C:286:MET:O	1:C:290:TYR:HB2	2.02	0.60
2:J:220:SER:OG	2:J:286:ASN:HB3	2.02	0.60
3:O:22:LEU:HD11	3:O:243:LEU:HG	1.83	0.60
3:E:33:VAL:HG22	3:E:121:PHE:HB2	1.84	0.60
3:H:127:LEU:CD2	3:H:129:ASP:HB2	2.30	0.60
1:C:477:ALA:HB3	1:C:480:GLU:HG2	1.83	0.60
2:L:441:PHE:CE2	2:L:501:ILE:HG12	2.37	0.60
1:A:266:PRO:HB3	1:A:290:TYR:CE1	2.37	0.60
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.17	0.60
2:B:468:ARG:HG3	2:B:468:ARG:NH1	2.16	0.60
3:F:103:ILE:HG23	3:F:104:THR:N	2.16	0.60
3:F:67:VAL:C	3:F:69:ASP:H	2.05	0.60
2:D:132:LYS:HD3	2:D:174:PHE:CE2	2.36	0.60
3:P:60:MET:HE3	3:P:75:VAL:HG22	1.83	0.60
1:K:324:CYS:O	1:K:328:ILE:HG13	2.01	0.60
3:N:86:VAL:HG21	3:N:109:LEU:HD11	1.82	0.59
3:E:199:LEU:HB2	3:E:267:LEU:HD11	1.84	0.59
3:M:45:THR:HG21	3:M:85:CYS:HB3	1.84	0.59
1:K:35:ASN:HD22	1:K:36:ASP:H	1.49	0.59
2:L:233:TYR:HD1	2:L:484:THR:HG23	1.65	0.59
2:D:118:MET:HA	2:D:130:ASN:ND2	2.17	0.59
3:O:223:ARG:O	3:O:225:MET:N	2.35	0.59
1:I:356:GLY:HA3	6:I:8496:CFM:S1B	2.41	0.59
1:A:131:LEU:O	1:A:135:ILE:HG13	2.02	0.59
3:M:265:GLU:OE1	3:N:52:LYS:HD3	2.02	0.59
3:N:19:THR:O	3:N:22:LEU:HB3	2.02	0.59
3:N:33:VAL:HG22	3:N:121:PHE:HB2	1.84	0.59
3:M:281:ILE:CG2	3:N:223:ARG:HD2	2.30	0.59
3:E:99:GLY:HA3	3:E:134:GLY:CA	2.32	0.59
1:A:350:ARG:HB3	1:A:375:VAL:CG1	2.32	0.59
3:P:267:LEU:O	3:P:270:GLU:HG3	2.02	0.59
2:B:270:ARG:HH11	2:B:270:ARG:HG3	1.67	0.59
2:D:347:GLU:OE1	2:D:487:TYR:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:ASN:N	3:E:185:ASN:HD22	2.00	0.59
1:C:356:GLY:HA3	6:C:7496:CFM:S1B	2.42	0.59
1:C:223:VAL:HG12	1:C:270:LEU:HB3	1.84	0.59
1:A:213:ASP:OD2	1:A:215:THR:HG23	2.02	0.59
3:N:267:LEU:O	3:N:270:GLU:HG3	2.02	0.59
3:G:41:LYS:HB3	3:G:43:ASP:OD1	2.03	0.59
3:E:284:LYS:C	3:E:284:LYS:HD3	2.22	0.59
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.85	0.59
3:O:72:LEU:HD13	3:O:112:GLU:CB	2.32	0.59
2:B:118:MET:HA	2:B:130:ASN:ND2	2.17	0.59
3:N:67:VAL:C	3:N:69:ASP:H	2.05	0.59
3:H:195:LEU:HD13	3:H:271:PHE:CD2	2.37	0.59
3:P:225:MET:HE2	3:P:230:TYR:HA	1.82	0.59
2:B:236:ASN:O	2:B:239:VAL:HG12	2.03	0.59
3:F:267:LEU:O	3:F:270:GLU:HG3	2.02	0.59
3:O:71:GLU:HB3	3:O:74:ASP:OD1	2.03	0.59
2:J:431:ARG:O	2:J:434:VAL:HG22	2.02	0.59
5:K:9494:HCA:O7	5:K:9494:HCA:O2	2.19	0.59
3:G:35:ILE:HD12	3:G:48:ILE:HG13	1.85	0.59
2:J:88:TYR:OH	2:J:116:ASP:HB3	2.02	0.59
1:K:346:LEU:O	1:K:349:LYS:HG2	2.03	0.59
3:M:202:LYS:HD3	3:M:267:LEU:HD12	1.84	0.59
1:K:35:ASN:ND2	1:K:36:ASP:N	2.51	0.59
1:I:35:ASN:ND2	1:I:391:MET:HG2	2.18	0.59
2:B:233:TYR:HD1	2:B:484:THR:HG23	1.68	0.59
1:I:354:TYR:CZ	1:I:404:VAL:HG12	2.38	0.59
1:K:223:VAL:HG12	1:K:270:LEU:HB3	1.83	0.59
2:L:499:ASN:O	2:L:503:GLU:HB2	2.02	0.59
3:P:76:LEU:HA	3:P:86:VAL:HG12	1.85	0.59
3:N:103:ILE:HG23	3:N:104:THR:N	2.18	0.59
1:C:35:ASN:ND2	1:C:36:ASP:N	2.51	0.59
1:C:131:LEU:O	1:C:135:ILE:HG13	2.03	0.59
2:J:270:ARG:HG3	2:J:270:ARG:NH1	2.18	0.59
3:P:105:ALA:O	3:P:109:LEU:HG	2.03	0.59
2:J:372:ASP:O	2:J:376:VAL:HG23	2.03	0.59
1:A:356:GLY:HA3	6:A:6496:CFM:S1B	2.42	0.59
1:I:19:VAL:HG13	1:I:20:TYR:N	2.16	0.59
2:L:220:SER:OG	2:L:286:ASN:HB3	2.03	0.59
3:E:284:LYS:HD3	3:E:285:THR:N	2.18	0.58
1:I:239:ARG:NH1	2:J:27:LYS:HD2	2.18	0.58
3:M:127:LEU:HD12	3:M:135:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:247:MET:CE	2:L:340:ILE:HA	2.33	0.58
1:A:77:ASP:OD2	1:A:258:SER:HB2	2.01	0.58
3:P:236:GLN:O	3:P:239:GLU:HB2	2.03	0.58
3:G:52:LYS:HB3	3:G:224:ARG:NH1	2.18	0.58
3:E:191:ARG:HE	3:E:194:GLU:CD	2.07	0.58
2:B:494:LEU:HD23	2:B:494:LEU:O	2.03	0.58
1:K:332:LYS:N	1:K:333:PRO:HD2	2.18	0.58
1:I:479:TRP:CZ2	2:L:340:ILE:HG21	2.37	0.58
1:K:65:ALA:O	1:K:70:VAL:HG23	2.04	0.58
2:J:235:GLY:C	2:J:483:THR:HG23	2.23	0.58
2:B:431:ARG:HG2	2:B:431:ARG:HH11	1.68	0.58
2:B:270:ARG:HG3	2:B:270:ARG:NH1	2.18	0.58
1:I:131:LEU:O	1:I:135:ILE:HG13	2.03	0.58
2:D:431:ARG:O	2:D:434:VAL:HG22	2.03	0.58
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.84	0.58
3:H:208:ILE:HD11	3:H:246:LYS:HB3	1.84	0.58
3:O:45:THR:HG21	3:O:85:CYS:HB3	1.84	0.58
1:A:405:THR:HG23	1:A:408:GLU:CD	2.23	0.58
2:D:373:PRO:HD3	2:D:397:ASN:OD1	2.03	0.58
1:I:195:HIS:O	1:I:198:ALA:HB3	2.04	0.58
3:O:86:VAL:HG21	3:O:109:LEU:HD11	1.86	0.58
3:N:56:THR:OG1	3:N:59:GLU:HG3	2.04	0.58
3:P:80:TYR:CD2	3:P:229:GLU:HG3	2.39	0.58
3:N:243:LEU:O	3:N:247:VAL:HG23	2.04	0.58
1:C:20:TYR:OH	1:C:408:GLU:HG3	2.04	0.58
1:I:479:TRP:HE3	2:L:330:MET:HE3	1.68	0.58
2:J:270:ARG:HG3	2:J:270:ARG:HH11	1.67	0.58
3:E:217:VAL:HG22	3:E:227:VAL:HG21	1.85	0.58
1:A:75:ILE:H	1:A:75:ILE:HD12	1.69	0.58
2:B:400:LYS:HD2	3:F:112:GLU:HG3	1.84	0.58
3:N:206:GLN:CG	3:N:252:LEU:HD22	2.31	0.58
1:C:66:GLY:O	1:C:70:VAL:HB	2.03	0.58
1:K:19:VAL:HG13	1:K:20:TYR:N	2.18	0.58
3:G:72:LEU:HD13	3:G:112:GLU:HB2	1.86	0.58
1:K:306:ILE:HG23	1:K:328:ILE:HD13	1.85	0.58
3:N:64:ALA:HB1	3:N:69:ASP:HB2	1.86	0.58
1:C:6:ARG:NH2	1:C:396:ASP:OD2	2.37	0.58
3:G:194:GLU:HA	3:G:197:ILE:HG13	1.85	0.58
3:N:76:LEU:HA	3:N:86:VAL:HG12	1.86	0.58
1:A:71:VAL:O	1:A:74:PRO:HD2	2.03	0.58
1:I:289:LYS:HG2	1:I:289:LYS:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ARG:O	2:B:434:VAL:HG22	2.03	0.58
3:G:29:MET:O	3:G:29:MET:HG2	2.04	0.58
2:B:132:LYS:HD3	2:B:174:PHE:CE2	2.38	0.58
2:D:70:CYS:SG	2:D:72:PRO:HG2	2.44	0.58
1:C:306:ILE:HG23	1:C:328:ILE:HD13	1.86	0.58
2:L:103:PHE:CB	2:L:111:VAL:HG21	2.33	0.58
3:F:184:CYS:HG	3:F:210:PHE:HE1	1.52	0.58
2:B:192:SER:OG	2:B:194:VAL:HG22	2.03	0.58
1:K:467:LEU:O	1:K:467:LEU:HD23	2.03	0.58
3:O:225:MET:SD	3:P:283:GLY:HA2	2.44	0.58
2:B:494:LEU:O	2:B:498:VAL:HG12	2.04	0.58
3:F:149:ILE:HB	3:F:182:LEU:HD22	1.85	0.58
3:G:217:VAL:HG22	3:G:227:VAL:HG21	1.83	0.58
2:D:511:GLY:O	2:D:516:ASP:HB3	2.04	0.58
2:J:4:GLN:O	2:J:6:ASP:N	2.37	0.58
3:O:52:LYS:HB3	3:O:224:ARG:NH1	2.18	0.58
3:M:165:SER:HB3	3:M:256:PRO:CB	2.33	0.58
3:M:217:VAL:HG22	3:M:227:VAL:HG21	1.86	0.58
1:K:266:PRO:HB3	1:K:290:TYR:CE1	2.39	0.58
2:L:373:PRO:HD3	2:L:397:ASN:OD1	2.04	0.58
3:E:86:VAL:HG21	3:E:109:LEU:HD11	1.86	0.58
3:P:208:ILE:HD11	3:P:246:LYS:HB3	1.85	0.58
3:G:243:LEU:O	3:G:247:VAL:HG23	2.03	0.58
3:M:199:LEU:HB2	3:M:267:LEU:HD11	1.86	0.57
3:F:206:GLN:CG	3:F:252:LEU:HD22	2.29	0.57
3:F:76:LEU:HA	3:F:86:VAL:HG12	1.85	0.57
1:C:239:ARG:NE	2:D:23:MET:HE3	2.18	0.57
2:D:468:ARG:NH1	2:D:468:ARG:HG3	2.19	0.57
1:K:68:LYS:C	1:K:68:LYS:HD3	2.25	0.57
3:M:185:ASN:HD22	3:M:185:ASN:N	2.01	0.57
1:C:465:MET:O	1:C:469:ASN:HB2	2.04	0.57
3:O:92:GLU:OE2	3:P:170:LYS:HE3	2.04	0.57
3:M:96:GLY:HA3	3:M:100:ARG:NH1	2.19	0.57
2:B:497:LEU:O	2:B:500:SER:N	2.36	0.57
1:A:65:ALA:O	1:A:70:VAL:HG23	2.04	0.57
2:D:43:VAL:O	2:D:46:TRP:HB3	2.02	0.57
3:E:224:ARG:HG3	3:F:282:VAL:HG13	1.86	0.57
3:E:182:LEU:O	3:E:208:ILE:HG22	2.03	0.57
3:G:199:LEU:HB2	3:G:267:LEU:HD11	1.86	0.57
2:D:128:GLN:NE2	2:D:165:PHE:HA	2.18	0.57
2:B:455:THR:OG1	2:B:463:GLU:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:236:GLN:O	3:N:239:GLU:HB2	2.03	0.57
1:A:467:LEU:O	1:A:467:LEU:HD23	2.03	0.57
3:H:103:ILE:HG23	3:H:104:THR:N	2.18	0.57
3:O:41:LYS:HB3	3:O:43:ASP:OD1	2.05	0.57
3:O:8:TYR:HB3	3:O:164:ILE:HD13	1.86	0.57
2:J:451:ILE:O	2:J:455:THR:HG23	2.04	0.57
3:P:195:LEU:HD13	3:P:271:PHE:CD2	2.39	0.57
2:J:46:TRP:O	2:J:49:THR:HG23	2.04	0.57
2:D:88:TYR:OH	2:D:116:ASP:HB3	2.04	0.57
3:H:60:MET:CE	3:H:75:VAL:HG13	2.34	0.57
3:H:56:THR:OG1	3:H:59:GLU:HG3	2.03	0.57
3:M:95:VAL:HG22	3:N:171:TYR:OH	2.05	0.57
3:G:33:VAL:HG22	3:G:121:PHE:HB2	1.86	0.57
3:G:33:VAL:O	3:G:83:VAL:HG13	2.04	0.57
3:M:135:PHE:CZ	3:N:130:VAL:HG11	2.37	0.57
2:D:236:ASN:HB3	2:D:485:LEU:HD12	1.86	0.57
3:F:60:MET:HE1	3:F:75:VAL:HG13	1.87	0.57
1:I:467:LEU:HD23	1:I:467:LEU:O	2.04	0.57
1:K:213:ASP:OD2	1:K:215:THR:HG23	2.04	0.57
2:J:153:CYS:SG	7:J:8498:CLF:S2B	3.03	0.57
3:O:35:ILE:HD12	3:O:48:ILE:HG13	1.87	0.57
2:L:494:LEU:O	2:L:494:LEU:HD23	2.04	0.57
3:H:102:VAL:O	3:H:106:ILE:HG13	2.05	0.57
3:O:215:ASN:O	3:O:219:ARG:HG3	2.05	0.57
2:L:235:GLY:O	2:L:483:THR:HG23	2.04	0.57
3:F:253:LEU:H	3:F:253:LEU:HD22	1.70	0.57
3:P:245:ARG:HH11	3:P:245:ARG:HG3	1.68	0.57
3:G:86:VAL:HG21	3:G:109:LEU:HD11	1.85	0.57
2:L:451:ILE:O	2:L:455:THR:HG23	2.03	0.57
2:B:235:GLY:C	2:B:483:THR:HG23	2.25	0.57
3:F:86:VAL:HG21	3:F:109:LEU:HD11	1.85	0.57
3:M:50:HIS:CE1	3:N:283:GLY:HA2	2.39	0.57
1:I:71:VAL:O	1:I:74:PRO:HD2	2.05	0.57
2:B:509:THR:O	2:B:516:ASP:HA	2.05	0.57
2:L:236:ASN:HB3	2:L:485:LEU:HD12	1.87	0.57
1:C:77:ASP:OD2	1:C:258:SER:HB2	2.05	0.57
3:M:202:LYS:HE3	3:M:259:ILE:HG21	1.86	0.57
3:E:164:ILE:O	3:E:168:ILE:HG13	2.03	0.57
3:G:20:GLN:NE2	3:G:48:ILE:HG12	2.20	0.57
1:A:57:MET:CE	2:B:113:CYS:H	2.18	0.57
1:A:57:MET:HE2	2:B:113:CYS:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:213:MET:CE	2:L:309:TRP:HA	2.35	0.57
3:G:15:LYS:HG3	3:G:150:VAL:HG21	1.86	0.57
3:H:60:MET:HE1	3:H:75:VAL:HG13	1.86	0.57
1:I:76:LYS:O	1:I:108:ALA:HA	2.05	0.57
1:K:7:GLU:HA	1:K:10:GLU:OE1	2.05	0.57
2:J:405:ALA:O	2:J:409:ILE:HG13	2.05	0.57
3:H:267:LEU:O	3:H:270:GLU:HG3	2.04	0.57
3:O:223:ARG:NE	3:P:281:ILE:HB	2.20	0.56
3:O:212:PRO:HG2	3:O:236:GLN:OE1	2.05	0.56
1:A:59:ILE:HD13	1:A:354:TYR:CE2	2.40	0.56
1:A:96:ARG:NH2	6:A:6496:CFM:S5	2.72	0.56
2:J:235:GLY:O	2:J:483:THR:HG23	2.04	0.56
2:J:43:VAL:O	2:J:46:TRP:HB3	2.04	0.56
3:M:49:LEU:HD23	3:M:79:GLY:HA3	1.86	0.56
3:P:183:ILE:HG12	3:P:208:ILE:CG2	2.35	0.56
2:L:178:GLU:CD	2:L:178:GLU:N	2.58	0.56
2:D:494:LEU:O	2:D:494:LEU:HD23	2.05	0.56
1:K:480:GLU:HA	1:K:480:GLU:OE2	2.05	0.56
1:A:480:GLU:OE2	1:A:480:GLU:HA	2.05	0.56
3:G:185:ASN:N	3:G:185:ASN:HD22	2.03	0.56
2:D:441:PHE:CE2	2:D:501:ILE:HG12	2.40	0.56
3:E:22:LEU:HD11	3:E:243:LEU:HG	1.87	0.56
2:B:96:VAL:HA	2:B:99:PHE:CD2	2.41	0.56
3:G:202:LYS:HD3	3:G:267:LEU:HD12	1.87	0.56
3:G:284:LYS:HD3	3:G:284:LYS:C	2.26	0.56
3:M:5:CYS:SG	3:M:146:GLU:HB2	2.45	0.56
3:O:284:LYS:C	3:O:284:LYS:HD3	2.26	0.56
3:P:80:TYR:HD2	3:P:229:GLU:HG3	1.70	0.56
3:G:256:PRO:C	3:G:258:PRO:HD3	2.26	0.56
1:A:144:LEU:HD22	2:B:35:TYR:CD1	2.40	0.56
3:F:56:THR:OG1	3:F:59:GLU:HG3	2.05	0.56
1:K:350:ARG:HB3	1:K:375:VAL:CG1	2.35	0.56
1:I:306:ILE:HG23	1:I:328:ILE:HD13	1.85	0.56
1:K:144:LEU:HD22	2:L:35:TYR:CD1	2.40	0.56
3:O:228:ILE:O	3:O:232:PRO:HG3	2.04	0.56
2:L:497:LEU:O	2:L:500:SER:N	2.38	0.56
2:B:445:ASN:HB2	2:B:472:PRO:O	2.05	0.56
3:M:194:GLU:HA	3:M:197:ILE:HG13	1.87	0.56
2:B:499:ASN:ND2	2:D:477:HIS:H	1.98	0.56
1:A:286:MET:O	1:A:290:TYR:HB2	2.06	0.56
3:E:49:LEU:HD21	3:E:85:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:99:GLY:HA3	3:G:134:GLY:HA2	1.86	0.56
1:C:35:ASN:ND2	1:C:391:MET:HG2	2.19	0.56
2:B:236:ASN:HB3	2:B:485:LEU:HD12	1.87	0.56
1:I:324:CYS:O	1:I:328:ILE:HG13	2.05	0.56
2:D:295:PRO:O	2:D:297:HIS:N	2.39	0.56
3:H:19:THR:O	3:H:22:LEU:HB3	2.05	0.56
1:A:7:GLU:HA	1:A:10:GLU:OE1	2.05	0.56
3:E:10:LYS:O	3:E:10:LYS:HG2	2.05	0.56
3:F:205:THR:OG1	3:F:206:GLN:N	2.37	0.56
2:L:452:GLN:OE1	2:L:466:LEU:N	2.39	0.56
3:N:183:ILE:HG12	3:N:208:ILE:CG2	2.36	0.56
3:H:100:ARG:HD3	3:H:100:ARG:C	2.26	0.56
1:C:7:GLU:HA	1:C:10:GLU:OE1	2.06	0.56
3:P:8:TYR:HB3	3:P:164:ILE:HD13	1.88	0.56
2:B:4:GLN:O	2:B:6:ASP:N	2.37	0.56
3:M:52:LYS:HB3	3:M:224:ARG:NH1	2.21	0.56
2:J:499:ASN:ND2	2:L:477:HIS:H	1.94	0.56
1:C:429:PHE:CZ	2:D:108:ARG:HA	2.39	0.56
3:M:164:ILE:O	3:M:168:ILE:HG13	2.06	0.56
3:G:169:VAL:HG23	3:G:256:PRO:HG2	1.86	0.56
3:O:127:LEU:HD12	3:O:135:PHE:CE2	2.41	0.56
2:B:23:MET:HE2	2:B:23:MET:O	2.05	0.56
3:G:218:GLN:O	3:G:222:ILE:HG13	2.06	0.56
1:I:477:ALA:HB3	1:I:480:GLU:HG2	1.87	0.56
1:K:428:LYS:O	1:K:432:GLN:HG3	2.06	0.56
3:N:105:ALA:O	3:N:109:LEU:HG	2.06	0.56
3:G:78:ALA:HA	3:G:83:VAL:O	2.06	0.56
3:M:35:ILE:HD12	3:M:48:ILE:HG13	1.87	0.56
1:C:354:TYR:CE1	1:C:404:VAL:HG12	2.41	0.56
3:N:57:ILE:HA	3:N:60:MET:CE	2.35	0.56
2:D:497:LEU:O	2:D:500:SER:N	2.39	0.56
3:P:100:ARG:O	3:P:103:ILE:HG22	2.06	0.56
2:B:431:ARG:NH1	2:B:435:PHE:HE2	2.03	0.56
3:H:57:ILE:HA	3:H:60:MET:CE	2.36	0.56
1:C:209:LYS:HD3	1:C:263:GLU:OE2	2.06	0.56
2:B:513:GLN:HE21	1:C:102:GLY:HA2	1.70	0.56
3:E:256:PRO:C	3:E:258:PRO:HD3	2.26	0.56
3:H:218:GLN:O	3:H:222:ILE:HG13	2.04	0.56
1:I:113:ASN:HD22	2:J:66:PRO:CD	2.19	0.56
1:C:213:ASP:OD2	1:C:215:THR:HG23	2.06	0.56
3:N:97:CYS:HA	8:N:2290:SF4:S4	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:NH1	1:A:444:TRP:CH2	2.74	0.56
3:N:60:MET:HE1	3:N:75:VAL:HG13	1.88	0.56
2:J:236:ASN:O	2:J:237:PHE:C	2.43	0.56
2:J:103:PHE:HB2	2:J:111:VAL:HG21	1.87	0.56
3:G:279:GLU:O	3:G:282:VAL:HG22	2.06	0.56
2:B:71:GLN:N	2:B:72:PRO:HD2	2.21	0.56
3:E:223:ARG:O	3:E:225:MET:N	2.39	0.56
3:M:184:CYS:HB2	3:M:196:ILE:HG13	1.87	0.56
3:M:99:GLY:HA3	3:M:134:GLY:CA	2.35	0.56
2:L:400:LYS:CG	3:P:111:GLU:HG2	2.36	0.56
1:A:323:LYS:O	1:A:327:VAL:HG23	2.07	0.56
1:I:265:THR:O	1:I:268:VAL:HG22	2.05	0.56
2:J:132:LYS:HD3	2:J:174:PHE:HE2	1.71	0.56
3:G:56:THR:HG22	3:G:87:GLU:HB3	1.87	0.56
2:B:59:ARG:HH22	2:B:429:HIS:CE1	2.24	0.56
2:L:391:VAL:HG23	2:L:392:HIS:CG	2.41	0.56
1:I:223:VAL:HG12	1:I:270:LEU:HB3	1.88	0.56
3:N:206:GLN:HG2	3:N:252:LEU:CD2	2.33	0.55
3:H:76:LEU:HA	3:H:86:VAL:HG12	1.87	0.55
3:O:165:SER:HB3	3:O:256:PRO:CB	2.35	0.55
1:K:71:VAL:O	1:K:74:PRO:HD2	2.07	0.55
3:M:127:LEU:HB3	3:M:135:PHE:CE1	2.41	0.55
3:M:212:PRO:HG2	3:M:236:GLN:OE1	2.06	0.55
3:P:212:PRO:HG2	3:P:236:GLN:OE1	2.06	0.55
1:C:106:VAL:HG11	2:D:40:ILE:HG23	1.88	0.55
3:N:45:THR:CG2	3:N:85:CYS:HB2	2.35	0.55
3:F:19:THR:O	3:F:22:LEU:HB3	2.07	0.55
1:A:428:LYS:O	1:A:432:GLN:HG3	2.06	0.55
2:J:118:MET:HA	2:J:130:ASN:ND2	2.21	0.55
3:M:71:GLU:HB3	3:M:74:ASP:OD1	2.06	0.55
1:K:14:GLN:HE21	1:K:14:GLN:HA	1.71	0.55
3:G:223:ARG:O	3:G:225:MET:N	2.40	0.55
3:O:194:GLU:HA	3:O:197:ILE:HG13	1.87	0.55
2:D:165:PHE:H	2:D:165:PHE:HD1	1.53	0.55
2:J:213:MET:CE	2:J:309:TRP:HA	2.34	0.55
2:B:46:TRP:O	2:B:49:THR:HG23	2.07	0.55
3:F:212:PRO:HG2	3:F:236:GLN:HE22	1.71	0.55
2:D:236:ASN:O	2:D:239:VAL:HG12	2.06	0.55
1:I:266:PRO:HB3	1:I:290:TYR:CE1	2.41	0.55
2:D:213:MET:HE2	2:D:309:TRP:HA	1.87	0.55
3:M:144:ALA:O	3:M:177:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:227:VAL:HG21	3:H:240:TYR:HE2	1.71	0.55
3:M:179:LEU:HD23	3:M:205:THR:HB	1.87	0.55
3:G:57:ILE:HG13	3:G:75:VAL:HG11	1.88	0.55
2:L:308:THR:O	2:L:310:LYS:HG2	2.07	0.55
1:A:14:GLN:HE21	1:A:14:GLN:HA	1.71	0.55
3:G:224:ARG:HG3	3:H:282:VAL:HG13	1.88	0.55
3:O:78:ALA:HB2	3:O:84:LYS:HD3	1.88	0.55
3:O:164:ILE:O	3:O:168:ILE:HG13	2.06	0.55
3:G:76:LEU:HD11	3:G:84:LYS:CB	2.34	0.55
1:C:87:GLY:HA3	7:D:7498:CLF:S2B	2.46	0.55
1:K:14:GLN:HA	1:K:14:GLN:NE2	2.20	0.55
1:C:265:THR:O	1:C:268:VAL:HG22	2.06	0.55
3:F:206:GLN:HG2	3:F:252:LEU:CD2	2.31	0.55
3:H:208:ILE:HG23	3:H:209:HIS:N	2.21	0.55
3:G:127:LEU:HD12	3:G:135:PHE:CE2	2.41	0.55
3:G:127:LEU:HB3	3:G:135:PHE:CE1	2.42	0.55
1:I:229:TYR:CE2	6:I:8496:CFM:S2A	3.00	0.55
3:P:57:ILE:HA	3:P:60:MET:CE	2.37	0.55
2:L:103:PHE:HB2	2:L:111:VAL:HG21	1.88	0.55
2:L:511:GLY:O	2:L:516:ASP:HB3	2.07	0.55
2:B:103:PHE:CB	2:B:111:VAL:HG21	2.36	0.55
2:D:235:GLY:C	2:D:483:THR:HG23	2.27	0.55
3:E:281:ILE:HG22	3:F:223:ARG:HD2	1.88	0.55
2:J:165:PHE:H	2:J:165:PHE:HD1	1.53	0.55
1:C:428:LYS:O	1:C:432:GLN:HG3	2.06	0.55
2:B:452:GLN:OE1	2:B:466:LEU:N	2.35	0.55
3:H:183:ILE:HG12	3:H:208:ILE:CG2	2.36	0.55
1:I:193:LEU:O	1:I:197:ILE:HG13	2.07	0.55
3:M:78:ALA:HB2	3:M:84:LYS:HD3	1.88	0.55
3:N:245:ARG:HH11	3:N:245:ARG:HG3	1.70	0.55
3:H:10:LYS:HG2	3:H:11:GLY:H	1.69	0.55
3:E:5:CYS:SG	3:E:146:GLU:HG3	2.47	0.55
2:L:43:VAL:O	2:L:46:TRP:HB3	2.06	0.55
1:A:223:VAL:HG12	1:A:270:LEU:HB3	1.88	0.55
3:P:71:GLU:HG3	3:P:72:LEU:HD13	1.88	0.55
1:I:35:ASN:ND2	1:I:36:ASP:N	2.55	0.55
1:C:480:GLU:HA	1:C:480:GLU:OE2	2.06	0.55
2:D:270:ARG:HH11	2:D:270:ARG:HG3	1.71	0.55
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.89	0.55
3:G:215:ASN:O	3:G:219:ARG:HG3	2.06	0.55
1:C:199:ASN:OD1	1:C:281:TYR:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:199:LEU:HD23	3:H:203:LEU:HD23	1.88	0.55
2:D:455:THR:OG1	2:D:463:GLU:HA	2.06	0.55
2:B:96:VAL:HA	2:B:99:PHE:HD2	1.72	0.55
3:N:205:THR:OG1	3:N:206:GLN:N	2.39	0.55
3:G:78:ALA:HB2	3:G:84:LYS:HD3	1.88	0.55
2:J:247:MET:HE1	2:J:340:ILE:HG12	1.89	0.55
1:C:282:ILE:O	1:C:286:MET:HG3	2.07	0.55
2:L:236:ASN:O	2:L:237:PHE:C	2.44	0.55
2:D:431:ARG:HG2	2:D:431:ARG:HH11	1.70	0.55
3:P:253:LEU:N	3:P:253:LEU:HD22	2.22	0.55
3:P:45:THR:CG2	3:P:85:CYS:HB2	2.36	0.55
3:M:243:LEU:O	3:M:247:VAL:HG23	2.07	0.55
3:P:102:VAL:HG12	3:P:106:ILE:HD11	1.89	0.55
3:E:72:LEU:HD13	3:E:112:GLU:CB	2.36	0.55
3:M:56:THR:HG22	3:M:87:GLU:HB3	1.89	0.55
3:P:36:VAL:HG22	3:P:86:VAL:HG22	1.88	0.55
1:I:389:ARG:NH1	1:I:389:ARG:HG3	2.21	0.55
2:L:165:PHE:HD1	2:L:165:PHE:H	1.54	0.55
1:A:266:PRO:HB3	1:A:290:TYR:CD1	2.42	0.55
3:E:35:ILE:HD12	3:E:48:ILE:HG13	1.88	0.55
1:I:355:ILE:HB	1:I:360:PRO:HD3	1.88	0.55
3:P:160:ALA:O	3:P:164:ILE:HG13	2.07	0.55
3:O:47:LEU:HD21	3:O:221:GLU:HG2	1.89	0.55
2:B:308:THR:O	2:B:310:LYS:HG2	2.07	0.55
3:F:78:ALA:HA	3:F:83:VAL:O	2.06	0.55
1:A:429:PHE:CZ	2:B:108:ARG:HA	2.42	0.55
3:F:127:LEU:CD2	3:F:129:ASP:HB2	2.34	0.55
3:F:127:LEU:HD23	3:F:129:ASP:H	1.71	0.55
2:L:430:LEU:HD12	2:L:433:LEU:HD12	1.89	0.55
3:N:209:HIS:HB3	3:N:243:LEU:HD13	1.88	0.55
2:D:456:LEU:O	2:D:459:GLY:N	2.40	0.55
3:N:244:ALA:O	3:N:248:VAL:HG23	2.07	0.55
3:P:154:GLU:OE1	3:P:156:MET:HB2	2.07	0.55
2:B:373:PRO:HD3	2:B:397:ASN:OD1	2.07	0.55
3:F:33:VAL:CG1	3:F:34:MET:N	2.69	0.54
3:E:214:ASP:HB3	3:E:216:VAL:HG12	1.88	0.54
1:C:266:PRO:HB3	1:C:290:TYR:CE1	2.42	0.54
2:B:235:GLY:O	2:B:483:THR:HG23	2.08	0.54
2:L:71:GLN:HB3	2:L:186:THR:HB	1.88	0.54
2:J:414:PRO:O	2:J:417:LYS:HG3	2.07	0.54
3:O:194:GLU:HA	3:O:197:ILE:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:164:ILE:O	3:G:168:ILE:HG13	2.07	0.54
1:A:332:LYS:N	1:A:333:PRO:HD2	2.22	0.54
3:M:16:SER:O	3:M:20:GLN:HG2	2.07	0.54
2:L:441:PHE:HE2	2:L:501:ILE:HG12	1.72	0.54
3:H:60:MET:HE3	3:H:75:VAL:HG22	1.87	0.54
2:D:451:ILE:O	2:D:455:THR:HG23	2.07	0.54
1:K:265:THR:O	1:K:268:VAL:HG22	2.07	0.54
1:K:91:TYR:HB2	2:L:98:TYR:CD1	2.42	0.54
2:D:10:ALA:O	2:D:11:SER:C	2.45	0.54
3:N:149:ILE:HB	3:N:182:LEU:HD22	1.88	0.54
1:K:355:ILE:HB	1:K:360:PRO:HD3	1.89	0.54
2:D:359:HIS:CG	2:D:360:THR:N	2.76	0.54
3:E:279:GLU:O	3:E:282:VAL:HG22	2.07	0.54
3:M:284:LYS:C	3:M:284:LYS:HD3	2.27	0.54
1:I:62:CYS:HB3	2:J:94:GLY:HA3	1.90	0.54
3:E:218:GLN:O	3:E:222:ILE:HG13	2.07	0.54
2:D:96:VAL:HA	2:D:99:PHE:CD2	2.42	0.54
3:M:279:GLU:O	3:M:282:VAL:HG22	2.07	0.54
3:H:71:GLU:OE2	3:H:112:GLU:HG2	2.08	0.54
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.89	0.54
1:I:359:ARG:O	1:I:363:VAL:HG22	2.07	0.54
3:H:212:PRO:HG2	3:H:236:GLN:HE22	1.72	0.54
1:K:350:ARG:HB3	1:K:375:VAL:HG13	1.88	0.54
1:A:14:GLN:NE2	1:A:14:GLN:HA	2.22	0.54
3:H:33:VAL:CG1	3:H:34:MET:N	2.70	0.54
3:M:40:PRO:HG2	3:N:130:VAL:CG1	2.37	0.54
2:J:497:LEU:O	2:J:500:SER:N	2.41	0.54
1:K:359:ARG:O	1:K:363:VAL:HG22	2.07	0.54
2:L:431:ARG:HH11	2:L:431:ARG:HG2	1.72	0.54
3:M:72:LEU:HD13	3:M:112:GLU:HB2	1.90	0.54
2:J:4:GLN:HB3	2:J:6:ASP:OD1	2.07	0.54
3:F:253:LEU:N	3:F:253:LEU:HD22	2.22	0.54
3:M:60:MET:HB3	3:M:70:LEU:HD21	1.89	0.54
2:B:366:ARG:HH11	2:B:366:ARG:HG2	1.72	0.54
1:I:427:GLU:O	1:I:430:ILE:N	2.38	0.54
3:O:182:LEU:O	3:O:208:ILE:HG22	2.08	0.54
3:O:162:ASN:HD21	3:O:259:ILE:CG1	2.15	0.54
2:J:128:GLN:NE2	2:J:165:PHE:HA	2.19	0.54
3:N:208:ILE:HG23	3:N:209:HIS:N	2.23	0.54
2:D:247:MET:HE1	2:D:340:ILE:HG12	1.90	0.54
1:A:354:TYR:CE1	1:A:404:VAL:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:60:MET:CE	3:N:75:VAL:HG13	2.38	0.54
3:M:186:SER:CB	3:M:212:PRO:HA	2.37	0.54
1:A:350:ARG:HB3	1:A:375:VAL:HG13	1.89	0.54
3:H:100:ARG:HD3	3:H:101:GLY:N	2.23	0.54
2:L:235:GLY:C	2:L:483:THR:HG23	2.28	0.54
2:D:235:GLY:O	2:D:483:THR:HG23	2.08	0.54
1:C:92:SER:HB3	2:D:98:TYR:CE1	2.43	0.54
3:N:195:LEU:HD13	3:N:271:PHE:CD2	2.43	0.54
3:G:202:LYS:HE3	3:G:259:ILE:HG21	1.89	0.54
3:G:8:TYR:HB3	3:G:164:ILE:HD13	1.88	0.54
3:E:103:ILE:HG13	3:E:137:MET:CG	2.36	0.54
3:H:172:ALA:HB1	3:H:255:ILE:HG12	1.89	0.54
3:G:50:HIS:HE1	3:G:229:GLU:OE1	1.90	0.54
2:B:128:GLN:NE2	2:B:165:PHE:HA	2.18	0.54
3:N:100:ARG:C	3:N:100:ARG:HD3	2.28	0.54
3:N:100:ARG:HH11	3:N:100:ARG:HG3	1.73	0.54
3:N:102:VAL:O	3:N:106:ILE:HG13	2.07	0.54
2:D:46:TRP:O	2:D:49:THR:HG23	2.06	0.54
2:B:59:ARG:NH2	2:B:429:HIS:CE1	2.76	0.54
2:L:346:LYS:O	2:L:347:GLU:C	2.45	0.54
3:G:5:CYS:SG	3:G:146:GLU:HG3	2.47	0.54
1:C:378:GLY:HA3	1:C:401:TYR:CD2	2.42	0.54
2:B:347:GLU:OE1	2:B:487:TYR:HB2	2.08	0.54
2:J:509:THR:O	2:J:516:ASP:HA	2.08	0.54
3:O:184:CYS:HB2	3:O:196:ILE:HG13	1.89	0.54
3:O:281:ILE:HG22	3:P:223:ARG:HD2	1.90	0.54
2:B:510:ARG:CZ	2:D:452:GLN:NE2	2.70	0.54
2:D:132:LYS:HD3	2:D:174:PHE:HE2	1.73	0.54
3:G:241:ARG:HG2	3:G:245:ARG:NH1	2.23	0.54
3:M:178:ARG:HB2	3:M:253:LEU:HB3	1.90	0.54
1:A:265:THR:O	1:A:268:VAL:HG22	2.08	0.54
2:L:124:VAL:HG23	2:L:125:PHE:N	2.23	0.54
3:E:50:HIS:HE1	3:E:229:GLU:OE1	1.91	0.54
3:E:194:GLU:HA	3:E:197:ILE:CG1	2.38	0.54
1:K:87:GLY:HA3	7:K:9498:CLF:S2B	2.48	0.54
7:K:9498:CLF:S2B	2:L:153:CYS:SG	3.05	0.54
3:O:202:LYS:HD3	3:O:267:LEU:HD12	1.88	0.54
2:B:128:GLN:HA	2:B:165:PHE:CD2	2.43	0.54
1:I:239:ARG:NH2	2:J:27:LYS:HB2	2.23	0.54
3:N:184:CYS:HB3	3:N:210:PHE:HD1	1.72	0.54
3:F:60:MET:CE	3:F:75:VAL:HG13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:MET:O	1:K:290:TYR:HB2	2.08	0.54
3:O:92:GLU:OE1	3:P:170:LYS:HE3	2.08	0.54
3:M:22:LEU:HD11	3:M:243:LEU:HG	1.90	0.54
2:B:100:ARG:O	2:B:104:ASN:ND2	2.41	0.54
2:D:103:PHE:CB	2:D:111:VAL:HG21	2.38	0.54
2:L:192:SER:OG	2:L:194:VAL:HG22	2.07	0.54
2:J:494:LEU:HD23	2:J:494:LEU:C	2.28	0.53
3:P:100:ARG:C	3:P:100:ARG:HD3	2.28	0.53
2:D:468:ARG:HD2	2:D:476:ARG:HG3	1.90	0.53
3:O:72:LEU:HD13	3:O:112:GLU:HB2	1.91	0.53
3:N:72:LEU:C	3:N:72:LEU:HD22	2.28	0.53
2:B:405:ALA:O	2:B:409:ILE:HG13	2.08	0.53
2:L:270:ARG:NH1	2:L:270:ARG:HG3	2.24	0.53
3:G:144:ALA:O	3:G:177:VAL:HG22	2.08	0.53
1:I:350:ARG:HB3	1:I:375:VAL:CG1	2.38	0.53
3:P:20:GLN:HE22	3:P:47:LEU:H	1.57	0.53
3:F:33:VAL:HG22	3:F:121:PHE:HB2	1.89	0.53
3:F:243:LEU:O	3:F:247:VAL:HG23	2.08	0.53
2:L:394:LEU:CD1	2:L:430:LEU:HB2	2.38	0.53
3:O:103:ILE:HG13	3:O:137:MET:CG	2.38	0.53
3:G:49:LEU:HD23	3:G:79:GLY:HA3	1.91	0.53
3:G:214:ASP:HB3	3:G:216:VAL:HG12	1.91	0.53
2:D:231:GLU:CD	2:D:236:ASN:HD22	2.12	0.53
1:A:92:SER:HB3	2:B:98:TYR:HE1	1.74	0.53
1:I:465:MET:O	1:I:469:ASN:HB2	2.08	0.53
3:H:154:GLU:OE1	3:H:156:MET:HB2	2.08	0.53
1:K:209:LYS:HD3	1:K:263:GLU:OE2	2.07	0.53
2:L:88:TYR:OH	2:L:116:ASP:HB3	2.08	0.53
3:F:199:LEU:C	3:F:199:LEU:HD23	2.28	0.53
3:O:95:VAL:HG12	3:O:96:GLY:N	2.22	0.53
3:P:33:VAL:CG1	3:P:34:MET:N	2.70	0.53
3:E:165:SER:HB3	3:E:256:PRO:CB	2.38	0.53
3:F:183:ILE:HG12	3:F:208:ILE:CG2	2.37	0.53
3:P:149:ILE:HB	3:P:182:LEU:CD2	2.38	0.53
3:P:100:ARG:HG3	3:P:100:ARG:HH11	1.74	0.53
1:C:75:ILE:HD12	1:C:75:ILE:N	2.22	0.53
2:L:236:ASN:O	2:L:239:VAL:HG12	2.08	0.53
3:N:71:GLU:OE2	3:N:112:GLU:HG2	2.08	0.53
1:C:277:ARG:NH1	1:C:386:ASP:OD2	2.39	0.53
2:J:233:TYR:HD1	2:J:484:THR:HG23	1.73	0.53
3:F:45:THR:CG2	3:F:85:CYS:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:256:PRO:C	3:M:258:PRO:HD3	2.29	0.53
1:C:239:ARG:NH2	2:D:27:LYS:HB2	2.23	0.53
2:B:431:ARG:NH1	2:B:435:PHE:CE2	2.77	0.53
1:K:266:PRO:HB3	1:K:290:TYR:CD1	2.43	0.53
3:P:199:LEU:C	3:P:199:LEU:HD23	2.28	0.53
1:C:350:ARG:HB3	1:C:375:VAL:CG1	2.38	0.53
3:P:36:VAL:HG22	3:P:86:VAL:CG2	2.38	0.53
3:O:256:PRO:C	3:O:258:PRO:HD3	2.29	0.53
3:O:186:SER:HB3	3:O:213:ARG:HG3	1.91	0.53
3:N:149:ILE:HB	3:N:182:LEU:CD2	2.38	0.53
2:J:132:LYS:HB3	2:J:174:PHE:CE2	2.43	0.53
1:C:350:ARG:HB3	1:C:375:VAL:HG13	1.90	0.53
1:I:7:GLU:HA	1:I:10:GLU:OE1	2.08	0.53
1:A:317:ASP:O	1:A:321:GLN:HG3	2.09	0.53
2:J:489:GLY:O	2:J:490:ALA:C	2.47	0.53
2:J:513:GLN:HE21	1:K:102:GLY:HA2	1.74	0.53
1:K:203:ARG:HA	1:K:207:LEU:HB2	1.90	0.53
1:C:359:ARG:NH1	1:C:444:TRP:CH2	2.77	0.53
2:B:340:ILE:HG21	1:C:479:TRP:CZ2	2.43	0.53
2:L:205:ALA:HA	2:L:281:MET:HE1	1.89	0.53
2:D:346:LYS:O	2:D:347:GLU:C	2.45	0.53
3:H:253:LEU:HD22	3:H:253:LEU:H	1.73	0.53
1:A:100:TYR:CD2	1:A:100:TYR:C	2.82	0.53
3:M:38:CYS:CB	3:M:126:VAL:HG22	2.39	0.53
3:M:8:TYR:HB3	3:M:164:ILE:HD13	1.91	0.53
1:A:239:ARG:NE	2:B:23:MET:HE3	2.21	0.53
2:B:468:ARG:HD2	2:B:476:ARG:HG3	1.89	0.53
1:K:66:GLY:HA2	1:K:70:VAL:HG21	1.90	0.53
3:O:99:GLY:HA3	3:O:134:GLY:CA	2.38	0.53
1:I:75:ILE:H	1:I:75:ILE:HD12	1.73	0.53
1:I:203:ARG:HA	1:I:207:LEU:HB2	1.90	0.53
3:H:205:THR:OG1	3:H:206:GLN:N	2.41	0.53
3:P:33:VAL:HG22	3:P:121:PHE:HB2	1.91	0.53
3:N:100:ARG:HD3	3:N:101:GLY:N	2.23	0.53
1:I:96:ARG:NH2	6:I:8496:CFM:S5	2.75	0.53
2:J:103:PHE:HB3	2:J:111:VAL:HG21	1.90	0.53
2:D:441:PHE:HE2	2:D:501:ILE:HG12	1.72	0.53
2:L:414:PRO:O	2:L:417:LYS:HG3	2.09	0.53
1:C:259:ILE:HG23	1:C:260:SER:N	2.23	0.53
3:G:194:GLU:HA	3:G:197:ILE:CG1	2.39	0.53
3:F:20:GLN:HE22	3:F:47:LEU:H	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:206:GLN:HG2	3:N:252:LEU:HD13	1.91	0.53
2:B:494:LEU:HD23	2:B:494:LEU:C	2.29	0.53
2:L:128:GLN:HA	2:L:165:PHE:CD2	2.43	0.53
3:N:100:ARG:O	3:N:103:ILE:HG22	2.09	0.53
3:N:134:GLY:N	8:N:2290:SF4:S2	2.81	0.53
2:B:205:ALA:HA	2:B:281:MET:HE1	1.91	0.53
2:J:236:ASN:O	2:J:239:VAL:HG12	2.08	0.53
3:P:10:LYS:HG2	3:P:11:GLY:H	1.72	0.53
2:L:270:ARG:HH11	2:L:270:ARG:HG3	1.74	0.53
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.91	0.53
2:B:88:TYR:OH	2:B:116:ASP:HB3	2.08	0.53
3:G:34:MET:HG3	3:G:84:LYS:O	2.09	0.53
3:O:186:SER:CB	3:O:212:PRO:HA	2.38	0.53
1:A:35:ASN:ND2	1:A:391:MET:HG2	2.24	0.53
2:B:236:ASN:O	2:B:237:PHE:C	2.47	0.53
2:L:494:LEU:C	2:L:494:LEU:HD23	2.28	0.53
3:N:124:TYR:O	3:N:126:VAL:HG23	2.09	0.53
2:D:96:VAL:HA	2:D:99:PHE:HD2	1.74	0.52
3:E:20:GLN:HE21	3:E:48:ILE:HG12	1.72	0.52
1:C:96:ARG:HD3	1:C:98:ASN:OD1	2.09	0.52
3:O:36:VAL:HA	3:O:86:VAL:HG23	1.91	0.52
3:P:253:LEU:H	3:P:253:LEU:HD22	1.74	0.52
1:I:91:TYR:HB2	2:J:98:TYR:CD1	2.44	0.52
2:B:241:LYS:HE3	2:B:253:LEU:HD23	1.91	0.52
3:M:194:GLU:HA	3:M:197:ILE:CG1	2.40	0.52
3:O:165:SER:HA	3:O:168:ILE:HD12	1.91	0.52
3:F:208:ILE:HG23	3:F:209:HIS:N	2.24	0.52
3:O:15:LYS:HG3	3:O:150:VAL:HG21	1.90	0.52
1:I:420:LEU:C	1:I:420:LEU:HD23	2.29	0.52
3:H:253:LEU:HD22	3:H:253:LEU:N	2.24	0.52
1:I:240:ILE:O	1:I:244:GLU:HG3	2.10	0.52
1:A:102:GLY:HA2	2:D:513:GLN:HE21	1.74	0.52
2:J:347:GLU:OE1	2:J:487:TYR:HB2	2.08	0.52
2:L:366:ARG:HG2	2:L:366:ARG:HH11	1.74	0.52
1:C:239:ARG:NH1	2:D:27:LYS:HD2	2.23	0.52
3:F:267:LEU:HD22	3:F:271:PHE:HE2	1.74	0.52
3:O:56:THR:HG22	3:O:87:GLU:HB3	1.91	0.52
3:H:199:LEU:C	3:H:199:LEU:HD23	2.30	0.52
3:F:199:LEU:HD23	3:F:203:LEU:HD23	1.91	0.52
1:K:125:PHE:CZ	3:P:142:ASN:ND2	2.77	0.52
1:K:239:ARG:NH1	2:L:27:LYS:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:ASN:O	2:D:237:PHE:C	2.48	0.52
3:H:100:ARG:O	3:H:103:ILE:HG22	2.10	0.52
3:E:72:LEU:HD13	3:E:112:GLU:HB2	1.91	0.52
3:M:41:LYS:HG3	3:N:156:MET:CE	2.40	0.52
1:I:87:GLY:HA3	7:J:8498:CLF:S2B	2.49	0.52
1:A:389:ARG:NH1	1:A:389:ARG:HG3	2.24	0.52
3:E:212:PRO:HG2	3:E:236:GLN:OE1	2.09	0.52
2:J:71:GLN:N	2:J:72:PRO:HD2	2.24	0.52
1:I:36:ASP:OD1	1:I:38:ALA:HB3	2.09	0.52
3:F:100:ARG:C	3:F:100:ARG:HD3	2.30	0.52
3:H:100:ARG:HH11	3:H:100:ARG:HG3	1.73	0.52
3:E:144:ALA:O	3:E:177:VAL:HG22	2.08	0.52
3:H:223:ARG:O	3:H:224:ARG:HB2	2.08	0.52
3:E:32:LYS:HG2	3:E:118:ASP:O	2.10	0.52
2:D:452:GLN:OE1	2:D:466:LEU:N	2.41	0.52
1:K:59:ILE:HD13	1:K:354:TYR:CE2	2.44	0.52
2:J:205:ALA:HA	2:J:281:MET:HE1	1.89	0.52
1:C:113:ASN:HD22	2:D:66:PRO:HD2	1.72	0.52
2:D:92:SER:OG	7:D:7498:CLF:S2A	2.62	0.52
1:A:324:CYS:O	1:A:328:ILE:HG13	2.10	0.52
3:E:36:VAL:HB	3:E:124:TYR:CD1	2.45	0.52
1:K:427:GLU:O	1:K:428:LYS:C	2.48	0.52
2:B:348:ARG:O	2:B:351:LEU:N	2.43	0.52
3:N:253:LEU:H	3:N:253:LEU:HD22	1.73	0.52
1:K:420:LEU:C	1:K:420:LEU:HD23	2.29	0.52
3:N:36:VAL:HG22	3:N:86:VAL:HG22	1.91	0.52
3:O:284:LYS:HD3	3:O:285:THR:N	2.25	0.52
3:P:127:LEU:HD23	3:P:129:ASP:H	1.75	0.52
1:A:59:ILE:HG23	1:A:426:LYS:HD2	1.92	0.52
1:A:92:SER:HB3	2:B:98:TYR:CE1	2.45	0.52
2:L:46:TRP:O	2:L:49:THR:HG23	2.09	0.52
2:L:71:GLN:N	2:L:72:PRO:HD2	2.25	0.52
1:K:277:ARG:NH1	1:K:386:ASP:OD2	2.42	0.52
1:A:148:ILE:O	1:A:178:ILE:HA	2.09	0.52
2:L:489:GLY:O	2:L:490:ALA:C	2.48	0.52
1:A:113:ASN:HD22	2:B:66:PRO:CD	2.23	0.52
3:M:214:ASP:HB3	3:M:216:VAL:HG12	1.91	0.52
3:F:57:ILE:HA	3:F:60:MET:CE	2.40	0.52
2:B:10:ALA:O	2:B:11:SER:C	2.48	0.52
2:J:441:PHE:CE2	2:J:501:ILE:HG12	2.45	0.52
2:D:241:LYS:HE3	2:D:253:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:198:ALA:O	3:M:202:LYS:HG3	2.09	0.52
3:H:71:GLU:HG3	3:H:72:LEU:HD13	1.92	0.52
3:H:245:ARG:HG3	3:H:245:ARG:HH11	1.75	0.52
3:O:214:ASP:HB3	3:O:216:VAL:HG12	1.92	0.52
1:K:405:THR:HG23	1:K:408:GLU:CD	2.30	0.52
2:D:71:GLN:N	2:D:72:PRO:HD2	2.25	0.52
2:L:213:MET:HE2	2:L:309:TRP:HA	1.91	0.52
1:I:92:SER:HB3	2:J:98:TYR:CE1	2.45	0.52
2:J:54:GLU:O	2:J:58:GLN:HG3	2.10	0.52
1:C:12:LEU:HD13	1:C:415:ARG:NH1	2.24	0.52
3:M:269:MET:SD	3:M:276:VAL:HA	2.50	0.52
2:B:391:VAL:HG23	2:B:392:HIS:CG	2.44	0.52
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.44	0.52
2:L:405:ALA:O	2:L:409:ILE:HG13	2.10	0.52
3:H:20:GLN:HE22	3:H:47:LEU:H	1.58	0.52
3:F:80:TYR:HD2	3:F:229:GLU:HG3	1.75	0.52
1:K:226:ILE:HB	1:K:273:VAL:HG22	1.91	0.52
1:K:57:MET:CE	2:L:113:CYS:H	2.23	0.52
3:H:64:ALA:HB1	3:H:69:ASP:HB2	1.91	0.52
2:L:445:ASN:HB2	2:L:472:PRO:O	2.10	0.52
3:F:172:ALA:HB1	3:F:255:ILE:HG12	1.92	0.52
2:J:314:PRO:HB3	2:J:331:LYS:HE2	1.92	0.52
1:C:137:GLU:OE2	2:D:59:ARG:HA	2.11	0.52
3:M:50:HIS:HE1	3:M:229:GLU:OE1	1.92	0.51
3:H:186:SER:HB2	3:H:212:PRO:HA	1.91	0.51
1:I:474:LYS:HB3	2:L:322:LEU:HD21	1.92	0.51
2:D:109:GLU:HG3	2:D:261:LEU:O	2.10	0.51
2:J:232:THR:HG21	2:J:471:PHE:CD1	2.45	0.51
2:J:96:VAL:HA	2:J:99:PHE:CD2	2.46	0.51
2:B:19:ASP:O	2:B:23:MET:HB2	2.11	0.51
2:D:247:MET:CE	2:D:340:ILE:HG12	2.40	0.51
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.92	0.51
3:M:60:MET:HE1	3:M:74:ASP:O	2.10	0.51
3:N:218:GLN:O	3:N:222:ILE:HG13	2.11	0.51
1:I:114:PHE:HE2	1:I:142:PHE:CE2	2.29	0.51
2:B:314:PRO:HB3	2:B:331:LYS:HE2	1.92	0.51
2:L:295:PRO:O	2:L:297:HIS:N	2.43	0.51
3:N:269:MET:HA	3:N:274:MET:O	2.11	0.51
1:C:467:LEU:HD23	1:C:467:LEU:O	2.11	0.51
3:N:145:GLN:NE2	3:N:145:GLN:HA	2.24	0.51
1:I:428:LYS:O	1:I:432:GLN:HG3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:TYR:CD2	3:F:229:GLU:HG3	2.45	0.51
2:B:450:PHE:O	2:B:453:ARG:N	2.44	0.51
2:D:430:LEU:HD12	2:D:433:LEU:HD12	1.92	0.51
1:K:367:TYR:O	1:K:372:MET:HB2	2.10	0.51
1:K:96:ARG:NH2	6:K:9496:CFM:S5	2.74	0.51
3:G:154:GLU:OE2	3:G:155:MET:HB3	2.10	0.51
2:L:4:GLN:O	2:L:6:ASP:N	2.44	0.51
1:I:107:ASN:HD21	2:J:34:LYS:HE2	1.76	0.51
3:F:72:LEU:C	3:F:72:LEU:HD22	2.30	0.51
2:B:441:PHE:CE2	2:B:501:ILE:HG12	2.45	0.51
1:I:478:PRO:HB2	2:L:330:MET:CE	2.40	0.51
1:C:36:ASP:OD1	1:C:38:ALA:HB3	2.10	0.51
1:K:75:ILE:N	1:K:75:ILE:HD12	2.25	0.51
2:D:89:VAL:HG12	2:D:152:THR:HG23	1.92	0.51
2:B:71:GLN:HB3	2:B:186:THR:HB	1.92	0.51
2:L:509:THR:O	2:L:516:ASP:HA	2.11	0.51
3:P:199:LEU:HD23	3:P:203:LEU:HD23	1.92	0.51
5:C:7494:HCA:O7	5:C:7494:HCA:O2	2.29	0.51
3:E:27:ALA:HB1	3:E:81:GLY:O	2.10	0.51
2:D:135:LEU:HB3	2:D:175:ILE:HD13	1.93	0.51
2:D:4:GLN:O	2:D:6:ASP:N	2.43	0.51
3:O:26:LEU:O	3:O:31:LYS:HB2	2.10	0.51
3:N:127:LEU:HD23	3:N:129:ASP:H	1.75	0.51
2:B:430:LEU:HD12	2:B:433:LEU:HD12	1.91	0.51
3:G:72:LEU:HD13	3:G:112:GLU:HB3	1.90	0.51
1:K:92:SER:HB3	2:L:98:TYR:CE1	2.45	0.51
1:K:465:MET:O	1:K:469:ASN:HB2	2.09	0.51
1:K:378:GLY:HA3	1:K:401:TYR:CD2	2.46	0.51
2:D:391:VAL:HG23	2:D:392:HIS:CG	2.45	0.51
3:O:130:VAL:HG23	3:O:130:VAL:O	2.11	0.51
3:F:71:GLU:OE2	3:F:112:GLU:HG2	2.10	0.51
2:B:165:PHE:HD1	2:B:165:PHE:H	1.58	0.51
3:E:49:LEU:HD23	3:E:79:GLY:HA3	1.91	0.51
3:N:208:ILE:CD1	3:N:246:LYS:HB3	2.37	0.51
3:N:10:LYS:HG2	3:N:11:GLY:H	1.72	0.51
2:D:308:THR:O	2:D:310:LYS:HG2	2.10	0.51
1:I:144:LEU:HG	2:J:43:VAL:HG21	1.93	0.51
2:L:84:LYS:HA	2:L:272:TYR:CD1	2.45	0.51
3:E:179:LEU:HG	3:E:180:GLY:H	1.76	0.51
3:E:179:LEU:HD23	3:E:205:THR:HB	1.92	0.51
2:B:197:TRP:O	2:B:198:ASP:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.46	0.51
3:M:32:LYS:HG2	3:M:118:ASP:O	2.10	0.51
1:C:203:ARG:HA	1:C:207:LEU:HB2	1.93	0.51
3:G:103:ILE:HG13	3:G:137:MET:CG	2.37	0.51
3:O:136:ALA:HB1	3:P:94:GLY:HA2	1.90	0.51
3:E:99:GLY:HA3	3:E:134:GLY:O	2.11	0.51
3:F:10:LYS:HG2	3:F:11:GLY:H	1.74	0.51
2:J:431:ARG:HG2	2:J:431:ARG:HH11	1.76	0.51
3:N:154:GLU:OE1	3:N:156:MET:HB2	2.10	0.51
2:J:47:THR:HA	2:J:52:TYR:CG	2.46	0.51
2:D:262:ASP:CG	2:D:481:ARG:HH12	2.14	0.51
1:K:107:ASN:HD21	2:L:34:LYS:HE2	1.75	0.51
1:A:440:GLU:HG3	1:A:445:ASP:OD2	2.11	0.51
2:L:468:ARG:HG3	2:L:468:ARG:HH11	1.76	0.51
3:O:223:ARG:HG2	3:P:281:ILE:HG13	1.92	0.51
2:J:452:GLN:OE1	2:J:466:LEU:N	2.42	0.51
1:C:57:MET:CE	2:D:113:CYS:N	2.73	0.51
1:C:359:ARG:O	1:C:363:VAL:HG22	2.11	0.51
3:P:209:HIS:HB3	3:P:243:LEU:HD13	1.92	0.51
2:L:400:LYS:NZ	3:P:112:GLU:CD	2.63	0.51
1:C:324:CYS:O	1:C:328:ILE:HG13	2.10	0.51
2:J:346:LYS:O	2:J:347:GLU:C	2.46	0.51
2:D:379:LEU:HD21	2:D:443:ILE:HG21	1.93	0.51
2:D:366:ARG:HH11	2:D:366:ARG:HG2	1.76	0.51
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.46	0.51
1:C:226:ILE:HB	1:C:273:VAL:HG22	1.93	0.51
1:C:239:ARG:CZ	2:D:27:LYS:HB2	2.41	0.51
1:K:359:ARG:NH1	1:K:444:TRP:CH2	2.79	0.51
2:B:103:PHE:HB2	2:B:111:VAL:HG21	1.91	0.51
2:L:90:HIS:ND1	2:L:116:ASP:OD2	2.28	0.51
3:E:27:ALA:HA	3:E:31:LYS:O	2.10	0.51
3:P:244:ALA:O	3:P:248:VAL:HG23	2.11	0.51
3:G:281:ILE:HG22	3:H:223:ARG:HD2	1.92	0.51
3:G:285:THR:HG21	3:H:230:TYR:CE1	2.46	0.51
3:E:198:ALA:O	3:E:202:LYS:HG3	2.11	0.51
3:M:223:ARG:O	3:M:225:MET:N	2.44	0.51
1:C:465:MET:HG3	1:C:466:THR:N	2.26	0.51
1:C:345:ARG:HG2	1:C:345:ARG:HH11	1.75	0.51
3:H:124:TYR:O	3:H:126:VAL:HG23	2.11	0.51
1:K:287:GLU:O	1:K:291:GLY:HA2	2.11	0.51
3:N:227:VAL:HG21	3:N:240:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:241:LYS:HE3	2:J:253:LEU:HD23	1.93	0.51
1:C:156:ILE:HG22	1:C:157:GLY:N	2.26	0.51
3:H:45:THR:CG2	3:H:85:CYS:HB2	2.40	0.51
3:M:204:GLY:O	3:M:254:VAL:HG21	2.11	0.51
2:L:96:VAL:HA	2:L:99:PHE:CD2	2.46	0.50
3:O:32:LYS:HG2	3:O:118:ASP:O	2.10	0.50
1:C:427:GLU:O	1:C:428:LYS:C	2.49	0.50
1:A:346:LEU:O	1:A:349:LYS:HG2	2.11	0.50
2:L:89:VAL:HG12	2:L:152:THR:HG23	1.93	0.50
1:K:36:ASP:OD1	1:K:38:ALA:HB3	2.11	0.50
3:N:158:MET:HE1	3:N:195:LEU:HD11	1.93	0.50
2:J:475:ASP:O	2:J:476:ARG:NH1	2.37	0.50
2:B:228:PRO:HA	2:B:293:LEU:HD12	1.92	0.50
3:M:26:LEU:O	3:M:31:LYS:HB2	2.11	0.50
3:F:50:HIS:CE1	3:F:229:GLU:OE1	2.64	0.50
3:F:50:HIS:HE1	3:F:229:GLU:OE1	1.94	0.50
3:F:149:ILE:HB	3:F:182:LEU:CD2	2.40	0.50
3:G:165:SER:HB3	3:G:256:PRO:CB	2.40	0.50
3:G:99:GLY:HA3	3:G:134:GLY:O	2.12	0.50
3:N:57:ILE:HA	3:N:60:MET:HE2	1.94	0.50
2:L:19:ASP:O	2:L:23:MET:HB2	2.12	0.50
2:D:270:ARG:NH1	2:D:270:ARG:HG3	2.23	0.50
3:G:178:ARG:HB2	3:G:253:LEU:HB3	1.93	0.50
3:E:57:ILE:HG13	3:E:75:VAL:HG11	1.92	0.50
3:N:33:VAL:CG1	3:N:34:MET:N	2.74	0.50
2:D:499:ASN:O	2:D:503:GLU:HB2	2.12	0.50
3:F:245:ARG:HH11	3:F:245:ARG:HG3	1.76	0.50
3:O:20:GLN:HE21	3:O:48:ILE:HG12	1.75	0.50
2:L:352:VAL:O	2:L:353:ASP:C	2.49	0.50
2:D:405:ALA:O	2:D:409:ILE:HG13	2.11	0.50
2:B:109:GLU:HG3	2:B:261:LEU:O	2.11	0.50
3:H:184:CYS:HB3	3:H:210:PHE:HD1	1.76	0.50
1:K:239:ARG:NE	2:L:23:MET:HE3	2.26	0.50
3:M:27:ALA:HB1	3:M:81:GLY:O	2.12	0.50
3:O:29:MET:O	3:O:29:MET:HG2	2.10	0.50
3:O:67:VAL:C	3:O:69:ASP:H	2.14	0.50
1:I:437:PRO:HA	1:I:472:TRP:CZ2	2.46	0.50
3:G:182:LEU:O	3:G:208:ILE:HG22	2.10	0.50
3:O:194:GLU:HA	3:O:197:ILE:HD11	1.92	0.50
3:E:202:LYS:HE3	3:E:259:ILE:HG21	1.94	0.50
1:A:433:LYS:HE2	2:B:110:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:479:TRP:CD2	2:L:340:ILE:HD12	2.46	0.50
1:A:367:TYR:CD1	1:A:372:MET:HG2	2.44	0.50
3:E:186:SER:CB	3:E:212:PRO:HA	2.41	0.50
1:K:66:GLY:HA2	1:K:70:VAL:CG2	2.41	0.50
3:E:136:ALA:HB1	3:F:94:GLY:HA2	1.92	0.50
3:F:266:GLU:O	3:F:270:GLU:HB3	2.12	0.50
3:N:71:GLU:HG3	3:N:72:LEU:HD13	1.93	0.50
2:B:215:ASP:OD2	2:B:216:LYS:HE3	2.12	0.50
1:C:42:SER:O	1:C:44:LYS:N	2.45	0.50
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.47	0.50
3:N:4:GLN:HA	3:N:122:VAL:HG13	1.94	0.50
3:G:191:ARG:HE	3:G:194:GLU:CD	2.14	0.50
3:H:72:LEU:HD22	3:H:72:LEU:C	2.32	0.50
3:H:33:VAL:HG22	3:H:121:PHE:HB2	1.92	0.50
1:K:354:TYR:CE1	1:K:404:VAL:HG12	2.46	0.50
3:F:39:ASP:OD2	3:F:41:LYS:HB3	2.12	0.50
1:I:20:TYR:OH	1:I:408:GLU:HG3	2.12	0.50
3:G:186:SER:CB	3:G:212:PRO:HA	2.42	0.50
1:I:367:TYR:O	1:I:372:MET:HB2	2.12	0.50
2:L:132:LYS:HD3	2:L:174:PHE:HE2	1.74	0.50
3:G:22:LEU:HD11	3:G:243:LEU:HG	1.93	0.50
2:L:347:GLU:OE1	2:L:487:TYR:HB2	2.11	0.50
1:K:385:ASP:HA	1:K:388:ASP:OD2	2.11	0.50
3:P:214:ASP:OD1	3:P:216:VAL:HG12	2.11	0.50
3:M:187:ARG:HB3	3:M:187:ARG:NH1	2.27	0.50
1:I:209:LYS:HD3	1:I:263:GLU:OE2	2.10	0.50
2:J:10:ALA:O	2:J:11:SER:C	2.49	0.50
2:J:128:GLN:HA	2:J:165:PHE:CD2	2.47	0.50
1:A:42:SER:O	1:A:44:LYS:N	2.44	0.50
1:C:317:ASP:O	1:C:321:GLN:HG3	2.11	0.50
1:A:427:GLU:O	1:A:428:LYS:C	2.49	0.50
3:P:45:THR:HG21	3:P:85:CYS:HB2	1.93	0.50
2:L:4:GLN:HB3	2:L:6:ASP:OD1	2.12	0.50
2:D:302:LYS:HE2	2:D:306:GLU:OE1	2.11	0.50
3:O:241:ARG:HG2	3:O:245:ARG:NH1	2.27	0.50
2:J:135:LEU:HB3	2:J:175:ILE:HD13	1.94	0.50
1:A:203:ARG:HA	1:A:207:LEU:HB2	1.94	0.50
3:E:127:LEU:HB3	3:E:135:PHE:CE1	2.47	0.50
3:G:16:SER:O	3:G:20:GLN:HG2	2.11	0.50
3:E:60:MET:HE1	3:E:74:ASP:O	2.11	0.50
3:P:186:SER:HB2	3:P:212:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLY:O	2:B:97:ALA:HB3	2.12	0.50
1:K:317:ASP:O	1:K:321:GLN:HG3	2.12	0.50
3:M:182:LEU:O	3:M:208:ILE:HG22	2.12	0.50
1:A:19:VAL:CG1	1:A:20:TYR:N	2.75	0.50
2:J:71:GLN:HB3	2:J:186:THR:HB	1.94	0.50
2:J:221:ASN:ND2	2:J:286:ASN:C	2.65	0.50
1:K:42:SER:O	1:K:44:LYS:N	2.45	0.50
1:A:167:SER:O	1:A:168:LYS:C	2.50	0.50
3:O:154:GLU:OE2	3:O:155:MET:HB3	2.11	0.50
2:L:206:ARG:O	2:L:208:PHE:N	2.45	0.50
1:K:345:ARG:HH11	1:K:345:ARG:HG2	1.77	0.50
1:K:85:PRO:CD	1:K:155:PRO:HG2	2.42	0.49
3:N:20:GLN:HE22	3:N:47:LEU:H	1.59	0.49
2:B:369:LEU:CD1	2:B:376:VAL:HG13	2.42	0.49
1:I:332:LYS:HA	1:I:335:TRP:CD1	2.47	0.49
2:B:221:ASN:OD1	2:B:223:LYS:HB2	2.12	0.49
2:D:10:ALA:O	2:D:12:TYR:N	2.45	0.49
2:J:78:CYS:HB2	2:J:197:TRP:CD1	2.47	0.49
3:P:122:VAL:HG13	3:P:122:VAL:O	2.12	0.49
3:P:5:CYS:SG	3:P:146:GLU:HB2	2.51	0.49
3:M:172:ALA:HB1	3:M:255:ILE:HD13	1.94	0.49
1:A:259:ILE:HG23	1:A:260:SER:N	2.26	0.49
2:D:489:GLY:O	2:D:490:ALA:C	2.50	0.49
1:A:458:ILE:O	1:A:459:PHE:C	2.50	0.49
2:B:499:ASN:O	2:B:503:GLU:HB2	2.12	0.49
2:B:213:MET:HE2	2:B:309:TRP:CA	2.35	0.49
1:C:59:ILE:HD13	1:C:354:TYR:CE2	2.47	0.49
2:D:233:TYR:CD1	2:D:484:THR:HG23	2.46	0.49
1:A:428:LYS:HA	1:A:438:PHE:CD1	2.47	0.49
3:F:244:ALA:O	3:F:248:VAL:HG23	2.13	0.49
3:N:78:ALA:HA	3:N:83:VAL:O	2.12	0.49
3:G:91:PRO:HB3	3:G:98:ALA:HA	1.94	0.49
3:N:47:LEU:HD21	3:N:221:GLU:HA	1.93	0.49
3:E:34:MET:HG3	3:E:84:LYS:O	2.12	0.49
1:I:239:ARG:CZ	2:J:27:LYS:HB2	2.42	0.49
1:C:405:THR:HG23	1:C:408:GLU:CD	2.33	0.49
3:O:92:GLU:CD	3:P:170:LYS:HE3	2.32	0.49
3:G:57:ILE:CG1	3:G:75:VAL:HG11	2.43	0.49
2:L:10:ALA:O	2:L:11:SER:C	2.50	0.49
2:D:54:GLU:O	2:D:58:GLN:HG3	2.12	0.49
3:G:95:VAL:HG12	3:G:96:GLY:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:GLN:HA	3:F:122:VAL:HG13	1.95	0.49
1:C:230:ASN:OD1	1:C:233:GLY:HA2	2.13	0.49
3:G:97:CYS:SG	3:G:134:GLY:HA2	2.52	0.49
1:I:354:TYR:CE1	1:I:404:VAL:HG12	2.47	0.49
3:F:103:ILE:HG23	3:F:104:THR:H	1.77	0.49
2:J:511:GLY:O	2:J:516:ASP:HB3	2.13	0.49
2:L:124:VAL:HG23	2:L:125:PHE:CD2	2.48	0.49
2:J:468:ARG:HD2	2:J:476:ARG:HG3	1.93	0.49
2:D:314:PRO:HB3	2:D:331:LYS:HE2	1.95	0.49
1:I:427:GLU:O	1:I:428:LYS:C	2.50	0.49
3:E:162:ASN:HD21	3:E:259:ILE:CG1	2.15	0.49
3:P:39:ASP:OD2	3:P:41:LYS:HB3	2.12	0.49
2:J:23:MET:HE2	2:J:23:MET:O	2.12	0.49
3:H:149:ILE:HB	3:H:182:LEU:HD22	1.93	0.49
2:D:494:LEU:HD23	2:D:494:LEU:C	2.33	0.49
2:L:297:HIS:O	2:L:297:HIS:CD2	2.65	0.49
3:O:27:ALA:HB1	3:O:81:GLY:O	2.13	0.49
2:L:458:LYS:HG2	2:L:462:PHE:CD2	2.48	0.49
2:L:47:THR:HA	2:L:52:TYR:CG	2.47	0.49
3:N:172:ALA:HB1	3:N:255:ILE:HG12	1.94	0.49
1:A:195:HIS:O	1:A:198:ALA:HB3	2.13	0.49
1:I:361:ARG:HG3	1:I:362:HIS:N	2.27	0.49
3:M:99:GLY:HA3	3:M:134:GLY:O	2.12	0.49
1:C:381:PHE:CZ	6:C:7496:CFM:S2B	3.05	0.49
1:C:266:PRO:HB3	1:C:290:TYR:CD1	2.47	0.49
2:L:431:ARG:NH1	2:L:435:PHE:HE2	2.11	0.49
3:N:45:THR:HG21	3:N:85:CYS:HB2	1.94	0.49
1:I:345:ARG:HG2	1:I:345:ARG:HH11	1.77	0.49
3:N:214:ASP:OD1	3:N:216:VAL:HG12	2.13	0.49
3:O:179:LEU:HG	3:O:180:GLY:H	1.76	0.49
2:D:124:VAL:HG23	2:D:125:PHE:CD2	2.47	0.49
3:O:199:LEU:HB2	3:O:267:LEU:HD11	1.94	0.49
2:L:128:GLN:NE2	2:L:165:PHE:HA	2.23	0.49
2:L:348:ARG:O	2:L:351:LEU:N	2.46	0.49
3:M:41:LYS:HB3	3:M:43:ASP:OD1	2.13	0.49
1:K:259:ILE:HG23	1:K:260:SER:N	2.28	0.49
2:L:59:ARG:NH2	2:L:429:HIS:CE1	2.81	0.49
1:K:240:ILE:O	1:K:244:GLU:HG3	2.13	0.49
2:J:352:VAL:O	2:J:353:ASP:C	2.51	0.49
3:O:191:ARG:HE	3:O:194:GLU:CD	2.15	0.49
3:P:206:GLN:CG	3:P:252:LEU:HD22	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:279:GLU:O	3:O:282:VAL:HG22	2.13	0.49
3:P:47:LEU:HD21	3:P:221:GLU:HA	1.94	0.49
2:J:452:GLN:NE2	2:L:510:ARG:CZ	2.74	0.49
2:J:430:LEU:HD12	2:J:433:LEU:HD12	1.93	0.49
3:P:184:CYS:HB3	3:P:210:PHE:HD1	1.77	0.49
1:I:96:ARG:HD3	1:I:98:ASN:OD1	2.12	0.49
2:L:23:MET:O	2:L:23:MET:HE2	2.13	0.49
3:E:26:LEU:O	3:E:31:LYS:HB2	2.13	0.49
3:O:57:ILE:HG13	3:O:75:VAL:HG11	1.93	0.49
2:B:262:ASP:OD2	2:D:350:ARG:HD3	2.13	0.49
3:M:88:SER:HB3	3:M:102:VAL:HG22	1.94	0.49
2:B:458:LYS:HG2	2:B:462:PHE:CD2	2.47	0.49
3:M:130:VAL:O	3:M:130:VAL:HG23	2.12	0.49
3:E:95:VAL:HG12	3:E:96:GLY:N	2.27	0.49
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.12	0.49
3:M:97:CYS:SG	3:M:134:GLY:HA2	2.53	0.49
3:F:212:PRO:HG2	3:F:236:GLN:NE2	2.27	0.49
2:D:194:VAL:HG23	2:D:195:THR:N	2.27	0.49
1:I:57:MET:CE	2:J:113:CYS:H	2.26	0.49
3:H:57:ILE:HA	3:H:60:MET:HE2	1.95	0.49
3:M:284:LYS:HD3	3:M:285:THR:N	2.27	0.49
2:J:94:GLY:O	2:J:97:ALA:HB3	2.13	0.49
2:B:348:ARG:HB2	2:B:487:TYR:CE2	2.48	0.49
3:M:27:ALA:HA	3:M:31:LYS:O	2.13	0.49
1:C:14:GLN:NE2	1:C:14:GLN:HA	2.28	0.49
1:I:6:ARG:NH2	1:I:396:ASP:OD2	2.46	0.49
3:F:197:ILE:O	3:F:201:ASN:ND2	2.46	0.49
3:E:208:ILE:O	3:E:208:ILE:HG12	2.12	0.49
3:O:208:ILE:O	3:O:208:ILE:HG12	2.13	0.49
3:E:202:LYS:HD3	3:E:267:LEU:HD12	1.95	0.49
2:L:222:LYS:HD2	2:L:222:LYS:N	2.28	0.49
2:B:489:GLY:O	2:B:490:ALA:C	2.51	0.49
3:O:204:GLY:O	3:O:254:VAL:HG21	2.13	0.49
3:F:124:TYR:O	3:F:126:VAL:HG23	2.13	0.49
3:F:71:GLU:HG3	3:F:72:LEU:HD13	1.94	0.48
3:G:184:CYS:HG	3:G:210:PHE:HE1	1.50	0.48
3:P:206:GLN:HG2	3:P:252:LEU:CD2	2.34	0.48
2:B:450:PHE:O	2:B:451:ILE:C	2.52	0.48
3:O:72:LEU:HD13	3:O:112:GLU:HB3	1.94	0.48
2:D:71:GLN:HB3	2:D:186:THR:HB	1.95	0.48
2:L:455:THR:OG1	2:L:463:GLU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:124:VAL:HG23	2:L:125:PHE:H	1.78	0.48
2:D:103:PHE:HB2	2:D:111:VAL:HG21	1.94	0.48
1:K:6:ARG:NH2	1:K:396:ASP:OD2	2.46	0.48
1:A:465:MET:HG3	1:A:466:THR:N	2.27	0.48
2:J:366:ARG:HH11	2:J:366:ARG:HG2	1.78	0.48
3:O:80:TYR:HE1	3:O:229:GLU:HG3	1.78	0.48
3:O:202:LYS:HE3	3:O:259:ILE:HG21	1.93	0.48
2:D:108:ARG:CZ	2:D:477:HIS:CD2	2.97	0.48
2:B:451:ILE:O	2:B:455:THR:HG23	2.13	0.48
1:C:381:PHE:HZ	6:C:7496:CFM:S2B	2.35	0.48
3:O:5:CYS:SG	3:O:146:GLU:HB2	2.52	0.48
3:O:56:THR:OG1	3:O:59:GLU:HG3	2.13	0.48
2:B:59:ARG:NH2	2:B:429:HIS:NE2	2.61	0.48
2:B:10:ALA:O	2:B:12:TYR:N	2.46	0.48
1:C:137:GLU:OE2	2:D:60:GLU:N	2.43	0.48
2:D:124:VAL:HG23	2:D:125:PHE:N	2.28	0.48
3:F:154:GLU:OE1	3:F:156:MET:HB2	2.13	0.48
2:L:228:PRO:HA	2:L:293:LEU:HD12	1.94	0.48
2:L:18:GLN:O	2:L:21:LYS:HB2	2.12	0.48
3:M:91:PRO:HB3	3:M:98:ALA:HA	1.94	0.48
3:P:55:ASN:HD22	3:P:77:LYS:NZ	2.11	0.48
2:D:27:LYS:NZ	2:D:32:GLU:OE2	2.47	0.48
2:B:297:HIS:CD2	2:B:297:HIS:O	2.66	0.48
2:B:89:VAL:HG12	2:B:152:THR:HG23	1.95	0.48
1:I:480:GLU:OE2	1:I:480:GLU:HA	2.13	0.48
3:E:72:LEU:HD11	3:E:114:ALA:HB2	1.94	0.48
1:C:91:TYR:HB2	2:D:98:TYR:CD1	2.48	0.48
3:G:5:CYS:SG	3:G:146:GLU:HB2	2.53	0.48
3:M:172:ALA:HB1	3:M:255:ILE:CD1	2.43	0.48
1:I:213:ASP:OD2	1:I:215:THR:HG23	2.13	0.48
2:B:107:PHE:HD1	2:B:480:HIS:CD2	2.32	0.48
3:G:269:MET:SD	3:G:276:VAL:HA	2.53	0.48
3:G:207:MET:O	3:G:209:HIS:N	2.46	0.48
3:F:4:GLN:HG2	3:F:122:VAL:HG11	1.95	0.48
2:D:394:LEU:CD1	2:D:430:LEU:HB2	2.43	0.48
2:L:135:LEU:HB3	2:L:175:ILE:HD13	1.95	0.48
3:P:78:ALA:HA	3:P:83:VAL:O	2.14	0.48
2:L:100:ARG:O	2:L:104:ASN:ND2	2.47	0.48
2:B:47:THR:HA	2:B:52:TYR:CG	2.48	0.48
3:G:80:TYR:HE1	3:G:229:GLU:HG3	1.77	0.48
3:M:184:CYS:SG	3:M:210:PHE:CE1	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:HIS:CE1	3:H:229:GLU:OE1	2.67	0.48
3:N:36:VAL:HG22	3:N:86:VAL:CG2	2.43	0.48
3:P:205:THR:OG1	3:P:206:GLN:N	2.38	0.48
3:H:206:GLN:HG2	3:H:252:LEU:CD2	2.39	0.48
3:H:71:GLU:HG3	3:H:72:LEU:CD1	2.44	0.48
3:H:39:ASP:OD2	3:H:41:LYS:HB3	2.13	0.48
3:M:135:PHE:O	3:M:138:PRO:HD2	2.12	0.48
1:C:444:TRP:CE3	1:C:444:TRP:HA	2.49	0.48
1:I:66:GLY:HA2	1:I:70:VAL:HG21	1.95	0.48
2:D:47:THR:HA	2:D:52:TYR:CG	2.48	0.48
3:H:261:MET:O	3:H:265:GLU:HG3	2.13	0.48
3:E:154:GLU:OE2	3:E:155:MET:HB3	2.13	0.48
3:E:267:LEU:C	3:E:267:LEU:HD23	2.33	0.48
3:M:223:ARG:CG	3:N:281:ILE:HD12	2.35	0.48
3:G:36:VAL:HB	3:G:124:TYR:CD1	2.48	0.48
2:J:455:THR:OG1	2:J:463:GLU:HA	2.13	0.48
3:H:209:HIS:HB3	3:H:243:LEU:HD13	1.94	0.48
1:A:370:LEU:O	1:A:372:MET:N	2.47	0.48
1:C:289:LYS:HE3	1:C:290:TYR:OH	2.13	0.48
1:K:323:LYS:O	1:K:327:VAL:HG23	2.14	0.48
1:C:92:SER:HB3	2:D:98:TYR:HE1	1.78	0.48
2:J:468:ARG:HH11	2:J:468:ARG:HG3	1.78	0.48
1:A:465:MET:O	1:A:469:ASN:HB2	2.14	0.48
1:I:14:GLN:HA	1:I:14:GLN:NE2	2.29	0.48
2:J:228:PRO:HA	2:J:293:LEU:HD12	1.96	0.48
3:M:95:VAL:HG12	3:M:96:GLY:N	2.29	0.48
3:M:36:VAL:HB	3:M:124:TYR:CD1	2.48	0.48
3:F:105:ALA:O	3:F:109:LEU:HG	2.13	0.48
2:B:369:LEU:HD11	2:B:376:VAL:HG13	1.95	0.48
3:O:49:LEU:HD23	3:O:79:GLY:HA3	1.96	0.48
2:D:23:MET:HE2	2:D:23:MET:O	2.12	0.48
3:F:186:SER:HA	3:F:192:GLU:OE1	2.14	0.48
2:B:233:TYR:CD1	2:B:484:THR:HG23	2.48	0.48
3:F:66:THR:H	3:F:69:ASP:CG	2.17	0.48
2:J:266:ASP:OD2	2:J:270:ARG:NH2	2.46	0.48
2:B:346:LYS:O	2:B:347:GLU:C	2.50	0.48
3:N:253:LEU:HD22	3:N:253:LEU:N	2.28	0.48
3:M:107:ASN:HA	3:M:110:GLU:OE1	2.13	0.48
1:A:425:ILE:HG13	1:A:425:ILE:O	2.13	0.48
3:G:208:ILE:HG12	3:G:208:ILE:O	2.13	0.48
3:P:49:LEU:C	3:P:51:SER:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:LYS:HG2	3:G:118:ASP:O	2.13	0.48
1:K:361:ARG:HG3	1:K:362:HIS:N	2.28	0.48
1:A:66:GLY:HA2	1:A:70:VAL:HG21	1.95	0.48
3:P:71:GLU:OE2	3:P:112:GLU:HG2	2.13	0.48
3:P:103:ILE:CG2	3:P:104:THR:N	2.75	0.48
3:P:59:GLU:O	3:P:63:GLU:HG3	2.13	0.48
3:F:100:ARG:HG3	3:F:100:ARG:HH11	1.79	0.48
1:K:428:LYS:HA	1:K:438:PHE:CD1	2.49	0.48
3:M:26:LEU:C	3:M:31:LYS:HB2	2.34	0.48
1:I:42:SER:O	1:I:44:LYS:N	2.46	0.48
2:J:100:ARG:O	2:J:104:ASN:ND2	2.46	0.48
3:O:178:ARG:HB2	3:O:253:LEU:HB3	1.95	0.48
3:M:57:ILE:HD12	3:M:105:ALA:CB	2.44	0.48
3:P:245:ARG:NH1	3:P:245:ARG:HG3	2.27	0.48
2:J:450:PHE:O	2:J:451:ILE:C	2.51	0.48
1:C:71:VAL:O	1:C:74:PRO:HD2	2.14	0.48
1:A:360:PRO:HB2	1:A:379:TYR:CE2	2.49	0.48
1:I:444:TRP:CE3	1:I:444:TRP:HA	2.49	0.48
2:L:431:ARG:NH1	2:L:435:PHE:CE2	2.82	0.48
3:H:212:PRO:HG2	3:H:236:GLN:NE2	2.29	0.48
2:D:37:GLN:HG3	2:D:41:ASP:OD1	2.14	0.48
2:B:472:PRO:HB2	2:B:474:PHE:CZ	2.49	0.48
1:I:350:ARG:HB3	1:I:375:VAL:HG13	1.96	0.48
2:D:445:ASN:HB2	2:D:472:PRO:O	2.13	0.48
3:F:269:MET:HA	3:F:274:MET:O	2.14	0.48
3:P:130:VAL:O	3:P:132:CYS:N	2.47	0.48
3:E:38:CYS:CB	3:E:126:VAL:HG22	2.43	0.48
3:N:199:LEU:C	3:N:199:LEU:HD23	2.34	0.48
3:E:207:MET:O	3:E:209:HIS:N	2.47	0.48
3:G:267:LEU:HD23	3:G:267:LEU:C	2.34	0.48
3:E:33:VAL:O	3:E:83:VAL:HG13	2.14	0.48
3:H:105:ALA:O	3:H:109:LEU:HG	2.14	0.48
1:A:20:TYR:OH	1:A:408:GLU:HG3	2.14	0.48
1:A:75:ILE:N	1:A:75:ILE:HD12	2.28	0.48
2:L:103:PHE:HB3	2:L:111:VAL:HG21	1.96	0.48
3:F:184:CYS:HB3	3:F:210:PHE:HD1	1.79	0.48
1:I:75:ILE:HD12	1:I:75:ILE:N	2.29	0.48
3:G:175:GLY:O	3:G:178:ARG:NH2	2.46	0.48
3:P:131:VAL:O	3:P:131:VAL:HG12	2.14	0.48
1:K:134:LEU:HD23	1:K:138:VAL:CG2	2.44	0.48
3:E:184:CYS:CB	3:E:196:ILE:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:220:ALA:HB1	3:P:225:MET:O	2.14	0.47
1:I:155:PRO:HG3	2:J:153:CYS:HB3	1.95	0.47
1:I:389:ARG:HH11	1:I:389:ARG:CG	2.20	0.47
1:C:360:PRO:HB2	1:C:379:TYR:CE2	2.49	0.47
1:C:65:ALA:O	1:C:70:VAL:HG23	2.14	0.47
3:M:20:GLN:HE21	3:M:48:ILE:HG12	1.77	0.47
3:P:243:LEU:O	3:P:247:VAL:HG23	2.14	0.47
3:G:72:LEU:HD11	3:G:114:ALA:HB2	1.96	0.47
3:F:97:CYS:O	3:F:100:ARG:HB3	2.13	0.47
3:M:72:LEU:HD13	3:M:112:GLU:HB3	1.95	0.47
3:G:42:ALA:HA	3:G:87:GLU:OE1	2.13	0.47
1:C:144:LEU:HG	2:D:43:VAL:HG21	1.95	0.47
2:L:468:ARG:NH1	2:L:468:ARG:HG3	2.28	0.47
2:D:107:PHE:HD1	2:D:480:HIS:CD2	2.32	0.47
1:K:113:ASN:HD22	2:L:66:PRO:CD	2.27	0.47
2:J:348:ARG:O	2:J:351:LEU:N	2.47	0.47
2:D:128:GLN:HA	2:D:165:PHE:CD2	2.49	0.47
3:F:34:MET:HA	3:F:84:LYS:O	2.13	0.47
2:J:297:HIS:CD2	2:J:297:HIS:O	2.67	0.47
3:O:243:LEU:O	3:O:247:VAL:HG23	2.14	0.47
3:E:36:VAL:HA	3:E:86:VAL:HG23	1.95	0.47
1:C:144:LEU:HD22	2:D:35:TYR:CD1	2.50	0.47
2:J:197:TRP:O	2:J:198:ASP:C	2.51	0.47
3:O:179:LEU:HD23	3:O:205:THR:HB	1.96	0.47
1:A:98:ASN:ND2	1:A:98:ASN:H	2.12	0.47
3:M:162:ASN:HD21	3:M:259:ILE:CG1	2.12	0.47
1:K:429:PHE:CZ	2:L:108:ARG:HA	2.49	0.47
1:C:19:VAL:CG1	1:C:20:TYR:N	2.77	0.47
2:L:247:MET:CE	2:L:340:ILE:HG12	2.41	0.47
2:B:475:ASP:O	2:B:476:ARG:NH1	2.40	0.47
1:I:66:GLY:HA2	1:I:70:VAL:CG2	2.45	0.47
1:I:102:GLY:HA2	2:L:513:GLN:HE21	1.79	0.47
3:G:38:CYS:HB2	3:G:126:VAL:HA	1.96	0.47
1:K:437:PRO:HA	1:K:472:TRP:CZ2	2.50	0.47
2:D:414:PRO:O	2:D:417:LYS:HG3	2.13	0.47
3:E:47:LEU:HD21	3:E:221:GLU:HG2	1.96	0.47
3:O:230:TYR:O	3:P:285:THR:HB	2.14	0.47
3:P:181:GLY:HA2	3:P:205:THR:OG1	2.14	0.47
3:P:127:LEU:HD23	3:P:127:LEU:C	2.35	0.47
3:G:86:VAL:HG11	3:G:109:LEU:HD21	1.97	0.47
3:H:149:ILE:HB	3:H:182:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LYS:HA	1:C:335:TRP:CD1	2.49	0.47
3:N:239:GLU:O	3:N:242:ALA:HB3	2.14	0.47
3:P:149:ILE:HB	3:P:182:LEU:HD22	1.96	0.47
2:D:221:ASN:ND2	2:D:286:ASN:C	2.68	0.47
2:J:132:LYS:HB3	2:J:174:PHE:CD2	2.50	0.47
2:L:391:VAL:HG23	2:L:392:HIS:CD2	2.49	0.47
2:J:262:ASP:CG	2:J:481:ARG:HH12	2.18	0.47
2:L:254:LEU:O	2:L:255:SER:CB	2.63	0.47
1:A:196:HIS:O	1:A:197:ILE:C	2.50	0.47
3:G:10:LYS:HG2	3:G:10:LYS:O	2.13	0.47
3:O:223:ARG:O	3:O:224:ARG:C	2.52	0.47
1:I:428:LYS:HA	1:I:438:PHE:CD1	2.50	0.47
3:P:49:LEU:O	3:P:50:HIS:HB2	2.14	0.47
1:C:433:LYS:HE2	2:D:110:PRO:HD3	1.96	0.47
3:F:36:VAL:HG22	3:F:86:VAL:HG22	1.96	0.47
1:K:339:VAL:HG12	1:K:343:ARG:HB2	1.97	0.47
1:A:405:THR:HG23	1:A:408:GLU:OE2	2.15	0.47
3:N:186:SER:HB2	3:N:212:PRO:HA	1.96	0.47
3:N:212:PRO:HG2	3:N:236:GLN:HE22	1.78	0.47
1:K:229:TYR:CE2	6:K:9496:CFM:S2A	3.07	0.47
3:M:57:ILE:HG13	3:M:75:VAL:HG11	1.95	0.47
2:D:283:ASP:O	2:D:284:ALA:C	2.52	0.47
3:E:187:ARG:HB3	3:E:187:ARG:NH1	2.29	0.47
2:J:391:VAL:HG23	2:J:392:HIS:CG	2.49	0.47
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.97	0.47
2:B:84:LYS:HA	2:B:272:TYR:CD1	2.49	0.47
1:C:101:ILE:HG12	1:C:236:TRP:CZ2	2.49	0.47
3:F:5:CYS:SG	3:F:146:GLU:HB2	2.54	0.47
1:C:351:VAL:HG13	1:C:420:LEU:HD23	1.97	0.47
3:H:197:ILE:O	3:H:201:ASN:ND2	2.48	0.47
2:L:96:VAL:HA	2:L:99:PHE:HD2	1.80	0.47
3:G:198:ALA:O	3:G:202:LYS:HG3	2.14	0.47
1:C:430:ILE:HG22	1:C:431:PHE:N	2.30	0.47
1:C:444:TRP:HE3	1:C:444:TRP:HA	1.80	0.47
3:G:216:VAL:HG22	3:G:227:VAL:HG13	1.97	0.47
2:L:233:TYR:CD1	2:L:484:THR:HG23	2.48	0.47
2:J:254:LEU:O	2:J:255:SER:CB	2.63	0.47
3:O:231:ASP:OD1	3:O:233:LYS:HB2	2.15	0.47
2:J:109:GLU:HG3	2:J:261:LEU:O	2.14	0.47
2:J:96:VAL:HA	2:J:99:PHE:HD2	1.79	0.47
1:C:427:GLU:O	1:C:430:ILE:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ALA:HA	2:B:281:MET:HE3	1.97	0.47
3:P:64:ALA:HB1	3:P:69:ASP:HB2	1.95	0.47
3:O:72:LEU:HD11	3:O:114:ALA:HB2	1.97	0.47
1:K:413:VAL:HG21	1:K:431:PHE:CE1	2.50	0.47
2:D:318:ILE:HG12	2:D:320:MET:HG3	1.96	0.47
1:C:14:GLN:HA	1:C:14:GLN:HE21	1.78	0.47
1:C:114:PHE:HE2	1:C:142:PHE:CE2	2.33	0.47
1:A:209:LYS:HD3	1:A:263:GLU:OE2	2.14	0.47
3:G:92:GLU:OE1	3:H:170:LYS:HE3	2.15	0.47
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.95	0.47
3:H:5:CYS:HB2	3:H:123:PHE:CE1	2.50	0.47
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.79	0.47
3:H:5:CYS:O	3:H:123:PHE:HA	2.15	0.47
3:G:187:ARG:NH1	3:G:187:ARG:HB3	2.29	0.47
3:F:131:VAL:O	3:F:131:VAL:HG12	2.15	0.47
3:G:249:ASP:O	3:G:250:ASN:C	2.52	0.47
3:G:179:LEU:HD23	3:G:205:THR:HB	1.96	0.47
2:L:54:GLU:O	2:L:58:GLN:HG3	2.15	0.47
2:B:277:THR:HB	2:B:279:GLU:OE2	2.15	0.47
3:N:245:ARG:NH1	3:N:245:ARG:HG3	2.30	0.47
2:B:368:ALA:O	2:B:442:MET:HA	2.15	0.47
1:A:361:ARG:HG3	1:A:362:HIS:N	2.30	0.47
2:B:295:PRO:C	2:B:297:HIS:H	2.18	0.47
1:K:444:TRP:HA	1:K:444:TRP:CE3	2.50	0.47
2:D:222:LYS:HD2	2:D:222:LYS:N	2.30	0.47
1:K:427:GLU:O	1:K:430:ILE:N	2.48	0.47
2:L:84:LYS:HB2	2:L:145:ASP:HB2	1.96	0.47
1:K:458:ILE:HD13	2:L:10:ALA:HA	1.96	0.47
3:F:261:MET:O	3:F:265:GLU:HG3	2.15	0.47
3:G:26:LEU:O	3:G:31:LYS:HB2	2.15	0.47
3:P:274:MET:HG2	3:P:275:GLU:N	2.29	0.47
1:I:259:ILE:HG23	1:I:260:SER:N	2.28	0.47
3:E:204:GLY:O	3:E:254:VAL:HG21	2.14	0.47
2:L:318:ILE:O	2:L:318:ILE:HG23	2.14	0.47
2:J:277:THR:HB	2:J:279:GLU:OE2	2.15	0.47
3:G:192:GLU:O	3:G:195:LEU:HB3	2.14	0.47
3:M:208:ILE:O	3:M:208:ILE:HG12	2.15	0.47
3:N:76:LEU:HD21	3:N:84:LYS:HD3	1.97	0.47
3:N:134:GLY:HA3	8:N:2290:SF4:S2	2.55	0.47
2:J:89:VAL:HG12	2:J:152:THR:HG23	1.96	0.47
3:F:102:VAL:O	3:F:106:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:GLN:HA	1:I:14:GLN:HE21	1.80	0.47
2:J:350:ARG:HD3	2:L:262:ASP:OD2	2.14	0.47
2:B:352:VAL:O	2:B:353:ASP:C	2.52	0.47
3:E:249:ASP:O	3:E:250:ASN:C	2.52	0.47
1:K:100:TYR:C	1:K:100:TYR:CD2	2.88	0.47
3:O:224:ARG:HG3	3:P:282:VAL:HG13	1.97	0.47
3:O:194:GLU:HA	3:O:197:ILE:CD1	2.45	0.47
3:N:50:HIS:CE1	3:N:229:GLU:OE1	2.68	0.47
3:P:34:MET:HA	3:P:84:LYS:O	2.14	0.47
1:C:428:LYS:HA	1:C:438:PHE:CD1	2.50	0.47
2:J:452:GLN:HE21	2:L:510:ARG:NH1	2.13	0.47
3:M:127:LEU:HD12	3:M:135:PHE:CZ	2.50	0.47
1:K:405:THR:HG1	1:K:408:GLU:HG3	1.79	0.47
1:I:19:VAL:CG1	1:I:20:TYR:N	2.78	0.47
2:J:340:ILE:HG21	1:K:479:TRP:CZ2	2.50	0.47
1:I:360:PRO:HB2	1:I:379:TYR:CE2	2.50	0.47
1:I:444:TRP:HE3	1:I:444:TRP:HA	1.79	0.47
1:A:144:LEU:HG	2:B:43:VAL:HG21	1.97	0.47
3:P:71:GLU:HG3	3:P:72:LEU:CD1	2.45	0.47
2:L:221:ASN:OD1	2:L:223:LYS:HB2	2.14	0.47
3:E:86:VAL:HG11	3:E:109:LEU:HD21	1.97	0.47
1:I:196:HIS:O	1:I:197:ILE:C	2.50	0.47
2:J:348:ARG:O	2:J:349:GLY:C	2.51	0.47
2:L:262:ASP:CG	2:L:481:ARG:HH12	2.18	0.47
2:J:268:GLN:HB2	2:J:268:GLN:HE21	1.49	0.47
3:E:172:ALA:HB1	3:E:255:ILE:HD13	1.97	0.47
2:D:442:MET:HG3	2:D:464:VAL:HG12	1.97	0.47
2:L:109:GLU:HG3	2:L:261:LEU:O	2.15	0.47
1:K:462:ASP:O	1:K:463:MET:C	2.53	0.47
3:F:218:GLN:O	3:F:222:ILE:HG13	2.14	0.47
3:M:283:GLY:O	3:N:225:MET:SD	2.73	0.46
3:O:285:THR:HG23	3:P:223:ARG:HH21	1.80	0.46
2:J:510:ARG:CZ	2:L:452:GLN:NE2	2.73	0.46
3:E:127:LEU:C	3:E:127:LEU:HD13	2.36	0.46
1:A:229:TYR:CE2	6:A:6496:CFM:S2A	3.08	0.46
1:I:478:PRO:HB2	2:L:330:MET:HE3	1.96	0.46
1:K:367:TYR:CD1	1:K:372:MET:HG2	2.47	0.46
2:L:365:LYS:HE2	2:L:501:ILE:HD13	1.97	0.46
3:O:60:MET:HB3	3:O:70:LEU:HD21	1.97	0.46
1:C:458:ILE:HD13	2:D:10:ALA:HA	1.97	0.46
2:J:468:ARG:NH1	2:J:468:ARG:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:ILE:HD13	2:D:181:VAL:HG12	1.96	0.46
3:F:92:GLU:O	3:F:93:PRO:C	2.53	0.46
1:C:196:HIS:O	1:C:197:ILE:C	2.53	0.46
2:J:18:GLN:O	2:J:21:LYS:HB2	2.16	0.46
3:G:130:VAL:O	3:G:130:VAL:HG23	2.15	0.46
1:I:429:PHE:CZ	2:J:108:ARG:HA	2.50	0.46
2:B:498:VAL:HG13	2:B:499:ASN:N	2.30	0.46
3:M:80:TYR:HE1	3:M:229:GLU:HG3	1.79	0.46
1:K:389:ARG:HG3	1:K:389:ARG:NH1	2.29	0.46
1:I:465:MET:HG3	1:I:466:THR:N	2.29	0.46
3:E:26:LEU:C	3:E:31:LYS:HB2	2.35	0.46
2:L:59:ARG:HH22	2:L:429:HIS:CE1	2.33	0.46
3:G:27:ALA:HB1	3:G:81:GLY:O	2.15	0.46
2:B:124:VAL:HG23	2:B:125:PHE:N	2.30	0.46
2:L:283:ASP:O	2:L:284:ALA:C	2.54	0.46
3:E:78:ALA:HB2	3:E:84:LYS:HD3	1.97	0.46
3:F:49:LEU:O	3:F:50:HIS:HB2	2.14	0.46
1:K:433:LYS:HE2	2:L:110:PRO:HD3	1.96	0.46
2:B:452:GLN:NE2	2:D:510:ARG:CZ	2.78	0.46
1:A:239:ARG:HG2	2:B:23:MET:SD	2.55	0.46
2:L:400:LYS:NZ	3:P:111:GLU:OE1	2.48	0.46
1:C:319:SER:O	1:C:323:LYS:HG3	2.15	0.46
3:E:5:CYS:SG	3:E:146:GLU:HB2	2.55	0.46
3:M:42:ALA:HA	3:M:87:GLU:OE1	2.15	0.46
2:B:124:VAL:HG23	2:B:125:PHE:H	1.80	0.46
1:A:114:PHE:HE2	1:A:142:PHE:CE2	2.33	0.46
1:I:134:LEU:HD23	1:I:138:VAL:HG23	1.97	0.46
2:D:254:LEU:O	2:D:255:SER:CB	2.63	0.46
3:P:172:ALA:HB1	3:P:255:ILE:HG12	1.95	0.46
2:J:445:ASN:HB2	2:J:472:PRO:O	2.15	0.46
1:C:100:TYR:C	1:C:100:TYR:CD2	2.89	0.46
3:E:223:ARG:O	3:E:224:ARG:C	2.53	0.46
3:P:76:LEU:HD13	3:P:86:VAL:HG13	1.96	0.46
2:J:19:ASP:O	2:J:23:MET:HB2	2.15	0.46
3:G:216:VAL:HG11	3:G:236:GLN:HB3	1.98	0.46
3:M:216:VAL:HG11	3:M:236:GLN:HB3	1.96	0.46
1:K:360:PRO:HB2	1:K:379:TYR:CE2	2.50	0.46
1:I:282:ILE:O	1:I:286:MET:HG3	2.15	0.46
3:E:243:LEU:O	3:E:247:VAL:HG23	2.16	0.46
2:J:262:ASP:OD2	2:L:350:ARG:HD3	2.14	0.46
2:L:381:LYS:O	2:L:385:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:CD	1:A:155:PRO:HG2	2.45	0.46
3:P:197:ILE:O	3:P:201:ASN:ND2	2.49	0.46
3:N:5:CYS:O	3:N:123:PHE:HA	2.16	0.46
3:N:5:CYS:HB2	3:N:123:PHE:CE1	2.51	0.46
3:F:130:VAL:O	3:F:132:CYS:N	2.48	0.46
3:F:227:VAL:HG21	3:F:240:TYR:HE2	1.81	0.46
5:I:8494:HCA:O2	5:I:8494:HCA:O7	2.32	0.46
1:K:155:PRO:O	1:K:159:ILE:HG12	2.15	0.46
3:O:136:ALA:HB2	3:P:94:GLY:HA2	1.97	0.46
1:A:381:PHE:HZ	6:A:6496:CFM:S2B	2.38	0.46
1:C:88:CYS:HG	7:D:7498:CLF:FE4	1.31	0.46
2:L:372:ASP:O	2:L:376:VAL:HG23	2.15	0.46
1:A:135:ILE:O	1:A:138:VAL:HB	2.15	0.46
3:P:266:GLU:O	3:P:270:GLU:HB3	2.16	0.46
2:L:348:ARG:O	2:L:349:GLY:C	2.54	0.46
3:N:71:GLU:HG3	3:N:72:LEU:CD1	2.45	0.46
1:I:134:LEU:HD23	1:I:134:LEU:C	2.35	0.46
1:I:148:ILE:O	1:I:178:ILE:HA	2.15	0.46
3:F:71:GLU:HG3	3:F:72:LEU:CD1	2.46	0.46
3:H:80:TYR:CD2	3:H:229:GLU:HG3	2.51	0.46
3:N:181:GLY:HA2	3:N:205:THR:OG1	2.16	0.46
3:E:16:SER:O	3:E:20:GLN:HG2	2.16	0.46
1:K:230:ASN:OD1	1:K:233:GLY:HA2	2.16	0.46
3:P:57:ILE:HA	3:P:60:MET:HE2	1.97	0.46
2:B:118:MET:HA	2:B:130:ASN:HD22	1.80	0.46
3:H:78:ALA:HA	3:H:83:VAL:O	2.16	0.46
2:D:381:LYS:O	2:D:385:GLU:HG3	2.16	0.46
2:B:254:LEU:O	2:B:255:SER:CB	2.63	0.46
1:K:167:SER:O	1:K:168:LYS:C	2.54	0.46
1:C:299:PHE:HB3	1:C:452:GLY:H	1.80	0.46
1:I:253:TRP:HA	1:I:254:SER:HA	1.67	0.46
1:A:479:TRP:CZ2	2:D:340:ILE:HG21	2.51	0.46
2:J:295:PRO:HG2	2:J:296:TRP:H	1.81	0.46
3:H:186:SER:CB	3:H:212:PRO:HA	2.46	0.46
3:P:60:MET:CE	3:P:75:VAL:HG13	2.46	0.46
2:L:266:ASP:OD2	2:L:270:ARG:NH2	2.48	0.46
2:L:314:PRO:HB3	2:L:331:LYS:HE2	1.97	0.46
1:I:100:TYR:CD2	1:I:100:TYR:C	2.88	0.46
3:M:154:GLU:OE2	3:M:155:MET:HB3	2.15	0.46
3:M:5:CYS:O	3:M:124:TYR:HD2	1.98	0.46
3:P:33:VAL:CG1	3:P:34:MET:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:LEU:CD1	2:B:430:LEU:HB2	2.46	0.46
2:J:330:MET:HE3	1:K:479:TRP:HE3	1.79	0.46
2:B:221:ASN:ND2	2:B:286:ASN:C	2.69	0.46
2:J:70:CYS:SG	2:J:72:PRO:CG	3.04	0.46
1:I:266:PRO:HB3	1:I:290:TYR:CD1	2.51	0.46
3:M:179:LEU:HG	3:M:180:GLY:H	1.79	0.46
3:G:231:ASP:OD1	3:G:233:LYS:HB2	2.16	0.46
3:M:218:GLN:O	3:M:222:ILE:HG13	2.15	0.46
3:E:194:GLU:HA	3:E:197:ILE:CD1	2.46	0.46
3:E:194:GLU:HA	3:E:197:ILE:HD11	1.97	0.46
3:G:284:LYS:HD3	3:G:285:THR:N	2.31	0.46
3:N:134:GLY:CA	8:N:2290:SF4:S2	3.04	0.46
3:N:266:GLU:O	3:N:270:GLU:HB3	2.16	0.46
2:B:431:ARG:HG2	2:B:431:ARG:NH1	2.31	0.46
2:L:450:PHE:O	2:L:453:ARG:N	2.48	0.46
3:F:45:THR:HG21	3:F:85:CYS:HB2	1.97	0.46
2:D:102:TYR:OH	2:D:472:PRO:HG3	2.16	0.46
2:D:284:ALA:HB3	2:D:285:PRO:HD3	1.98	0.46
3:G:188:ASN:HD22	3:G:188:ASN:N	2.13	0.46
2:J:215:ASP:OD2	2:J:216:LYS:HE3	2.16	0.46
1:C:11:SER:O	1:C:15:GLU:HG3	2.15	0.46
2:B:359:HIS:CG	2:B:360:THR:N	2.84	0.46
1:I:428:LYS:HA	1:I:438:PHE:CE1	2.51	0.46
3:M:194:GLU:HA	3:M:197:ILE:HD11	1.98	0.46
3:H:47:LEU:HD21	3:H:221:GLU:HA	1.98	0.46
3:N:80:TYR:CD2	3:N:229:GLU:HG3	2.51	0.46
3:N:39:ASP:OD1	3:N:127:LEU:HD12	2.16	0.46
2:B:452:GLN:HE21	2:D:510:ARG:NH1	2.14	0.46
1:C:66:GLY:HA2	1:C:70:VAL:HG21	1.97	0.46
3:G:186:SER:HB3	3:G:213:ARG:HG3	1.98	0.46
1:C:76:LYS:HG2	1:C:257:GLY:O	2.16	0.46
2:L:296:TRP:HB2	2:L:374:ASP:OD1	2.16	0.46
3:N:54:GLN:HG2	3:N:55:ASN:N	2.32	0.45
3:M:282:VAL:HA	3:N:223:ARG:HG3	1.98	0.45
3:M:86:VAL:HG11	3:M:109:LEU:HD21	1.98	0.45
3:F:47:LEU:HD21	3:F:221:GLU:HA	1.96	0.45
2:J:510:ARG:NH1	2:L:452:GLN:HE21	2.14	0.45
3:O:127:LEU:C	3:O:127:LEU:HD13	2.36	0.45
3:P:67:VAL:N	3:P:69:ASP:OD2	2.48	0.45
3:F:57:ILE:HA	3:F:60:MET:HE2	1.97	0.45
3:H:186:SER:HA	3:H:192:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:221:ASN:OD1	2:J:223:LYS:HB2	2.16	0.45
3:O:60:MET:HE1	3:O:74:ASP:O	2.16	0.45
3:H:97:CYS:O	3:H:100:ARG:HB3	2.15	0.45
3:E:269:MET:SD	3:E:276:VAL:HA	2.56	0.45
1:A:351:VAL:HG12	1:A:352:MET:N	2.31	0.45
1:K:114:PHE:HE2	1:K:142:PHE:CE2	2.34	0.45
3:G:67:VAL:C	3:G:69:ASP:H	2.20	0.45
2:B:222:LYS:N	2:B:222:LYS:HD2	2.30	0.45
3:O:207:MET:O	3:O:209:HIS:N	2.49	0.45
2:L:107:PHE:HD1	2:L:480:HIS:CD2	2.34	0.45
1:I:433:LYS:HE3	2:J:263:THR:CG2	2.39	0.45
3:P:33:VAL:HG12	3:P:34:MET:H	1.81	0.45
3:E:127:LEU:HD12	3:E:135:PHE:CZ	2.50	0.45
1:C:361:ARG:HG3	1:C:362:HIS:N	2.31	0.45
2:J:247:MET:CE	2:J:340:ILE:HG12	2.45	0.45
3:P:208:ILE:HG23	3:P:209:HIS:H	1.81	0.45
1:A:91:TYR:CB	2:B:98:TYR:HD1	2.29	0.45
2:J:233:TYR:CD1	2:J:484:THR:HG23	2.51	0.45
3:G:179:LEU:HG	3:G:180:GLY:H	1.81	0.45
2:L:442:MET:HG3	2:L:464:VAL:HG12	1.99	0.45
3:M:32:LYS:CB	3:M:119:LEU:HA	2.46	0.45
3:P:223:ARG:O	3:P:224:ARG:HB2	2.16	0.45
3:H:206:GLN:CG	3:H:252:LEU:HD22	2.38	0.45
1:C:66:GLY:HA2	1:C:70:VAL:CG2	2.46	0.45
3:E:42:ALA:HA	3:E:87:GLU:OE1	2.15	0.45
1:I:113:ASN:HD22	2:J:66:PRO:HD2	1.80	0.45
1:A:427:GLU:O	1:A:430:ILE:N	2.48	0.45
3:M:38:CYS:HB2	3:M:126:VAL:HG22	1.98	0.45
3:E:172:ALA:HB1	3:E:255:ILE:CD1	2.46	0.45
3:O:187:ARG:NH1	3:O:187:ARG:HB3	2.32	0.45
2:B:522:VAL:HA	2:D:474:PHE:HB3	1.98	0.45
1:A:107:ASN:HD21	2:B:34:LYS:HE2	1.81	0.45
1:C:148:ILE:O	1:C:178:ILE:HA	2.16	0.45
3:M:47:LEU:HD21	3:M:221:GLU:HG2	1.98	0.45
3:H:220:ALA:HB1	3:H:225:MET:O	2.16	0.45
2:L:153:CYS:SG	2:L:188:SER:CB	3.04	0.45
3:H:206:GLN:HG2	3:H:252:LEU:HD13	1.97	0.45
3:M:165:SER:HA	3:M:168:ILE:HD12	1.97	0.45
1:A:239:ARG:CZ	1:A:249:CYS:SG	3.05	0.45
1:A:444:TRP:HA	1:A:444:TRP:CE3	2.51	0.45
3:H:130:VAL:O	3:H:132:CYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:MET:CE	1:C:478:PRO:HB2	2.46	0.45
3:F:57:ILE:HG22	3:F:58:MET:N	2.31	0.45
2:L:221:ASN:ND2	2:L:286:ASN:C	2.70	0.45
3:P:4:GLN:HG2	3:P:122:VAL:HG11	1.98	0.45
1:K:195:HIS:O	1:K:198:ALA:HB3	2.17	0.45
2:B:456:LEU:O	2:B:459:GLY:N	2.50	0.45
2:J:166:ILE:HD13	2:J:181:VAL:HG12	1.97	0.45
3:E:195:LEU:HA	3:E:271:PHE:CE2	2.52	0.45
3:O:192:GLU:O	3:O:195:LEU:HB3	2.16	0.45
3:N:76:LEU:HD13	3:N:86:VAL:HG13	1.98	0.45
2:L:153:CYS:SG	2:L:188:SER:HB2	2.57	0.45
3:O:91:PRO:HB3	3:O:98:ALA:HA	1.98	0.45
3:F:208:ILE:CD1	3:F:246:LYS:HB3	2.44	0.45
3:M:40:PRO:HG2	3:N:130:VAL:HG12	1.97	0.45
1:K:332:LYS:HA	1:K:335:TRP:CD1	2.52	0.45
3:G:41:LYS:O	3:G:42:ALA:HB3	2.16	0.45
2:J:354:MET:SD	2:J:491:MET:HG2	2.56	0.45
1:I:134:LEU:HD23	1:I:138:VAL:CG2	2.46	0.45
2:B:479:LEU:HA	2:B:479:LEU:HD23	1.83	0.45
3:M:249:ASP:O	3:M:250:ASN:C	2.55	0.45
3:E:67:VAL:C	3:E:69:ASP:H	2.20	0.45
3:O:249:ASP:O	3:O:250:ASN:C	2.55	0.45
3:E:260:THR:OG1	3:E:263:GLU:HG3	2.17	0.45
1:C:339:VAL:HG12	1:C:343:ARG:HB2	1.99	0.45
2:B:340:ILE:HD12	1:C:479:TRP:CD2	2.51	0.45
1:A:68:LYS:C	1:A:68:LYS:CD	2.84	0.45
2:B:233:TYR:HB2	2:B:236:ASN:ND2	2.32	0.45
3:F:64:ALA:CB	3:F:69:ASP:HB2	2.46	0.45
1:K:310:ARG:HA	1:K:324:CYS:SG	2.56	0.45
1:C:144:LEU:HD11	2:D:43:VAL:HG21	1.97	0.45
3:H:103:ILE:HG23	3:H:104:THR:H	1.79	0.45
2:D:103:PHE:HB3	2:D:111:VAL:HG21	1.99	0.45
3:H:45:THR:HG21	3:H:85:CYS:HB2	1.99	0.45
2:D:78:CYS:HB2	2:D:197:TRP:CD1	2.51	0.45
2:J:107:PHE:HD1	2:J:480:HIS:CD2	2.35	0.45
2:L:197:TRP:O	2:L:198:ASP:C	2.55	0.45
1:I:413:VAL:HG21	1:I:431:PHE:CE1	2.51	0.45
2:J:82:PHE:HB2	2:J:85:THR:OG1	2.17	0.45
3:O:10:LYS:O	3:O:10:LYS:HG2	2.16	0.45
3:P:227:VAL:HG21	3:P:240:TYR:HE2	1.81	0.45
3:G:88:SER:HB3	3:G:102:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:191:ARG:HG2	3:E:194:GLU:OE2	2.17	0.45
3:M:191:ARG:HE	3:M:194:GLU:CD	2.20	0.45
3:M:192:GLU:O	3:M:195:LEU:HB3	2.16	0.45
3:O:33:VAL:O	3:O:83:VAL:HG13	2.17	0.45
2:B:497:LEU:O	2:B:498:VAL:C	2.55	0.45
1:A:239:ARG:NH1	2:B:27:LYS:HD2	2.32	0.45
1:I:231:ILE:HG13	1:I:359:ARG:HH22	1.82	0.45
1:A:144:LEU:HD22	2:B:35:TYR:CE1	2.52	0.45
2:L:19:ASP:N	2:L:19:ASP:OD1	2.42	0.45
2:D:450:PHE:O	2:D:451:ILE:C	2.55	0.45
1:I:439:ARG:HD3	1:I:466:THR:OG1	2.16	0.45
2:B:197:TRP:CZ3	2:B:229:GLY:HA2	2.52	0.45
3:M:102:VAL:O	3:M:106:ILE:HG13	2.16	0.45
1:I:440:GLU:HG3	1:I:445:ASP:OD2	2.16	0.45
2:D:279:GLU:H	2:D:279:GLU:CD	2.18	0.45
3:G:199:LEU:C	3:G:199:LEU:HD23	2.37	0.45
2:J:499:ASN:O	2:J:503:GLU:HB2	2.17	0.45
3:E:91:PRO:HB3	3:E:98:ALA:HA	1.99	0.45
2:J:394:LEU:CD1	2:J:430:LEU:HB2	2.47	0.45
3:O:185:ASN:ND2	3:O:185:ASN:N	2.64	0.45
1:K:444:TRP:HA	1:K:444:TRP:HE3	1.80	0.45
2:D:132:LYS:HB3	2:D:174:PHE:CE2	2.52	0.45
1:K:299:PHE:HB3	1:K:452:GLY:H	1.81	0.45
3:O:260:THR:OG1	3:O:263:GLU:HG3	2.17	0.45
1:A:6:ARG:NH2	1:A:396:ASP:OD2	2.50	0.45
2:J:379:LEU:HD21	2:J:443:ILE:HG21	1.99	0.45
2:B:54:GLU:O	2:B:58:GLN:HG3	2.17	0.45
7:A:6498:CLF:S2A	2:B:92:SER:OG	2.67	0.45
3:N:34:MET:HA	3:N:84:LYS:O	2.16	0.45
3:M:76:LEU:HD13	3:M:86:VAL:HG13	1.99	0.45
3:E:278:ASP:OD1	3:E:281:ILE:HB	2.16	0.45
1:C:433:LYS:HE3	2:D:263:THR:CG2	2.38	0.45
3:N:130:VAL:O	3:N:132:CYS:N	2.50	0.45
3:O:137:MET:O	3:O:137:MET:HE2	2.16	0.45
2:J:497:LEU:O	2:J:498:VAL:C	2.55	0.45
1:A:367:TYR:O	1:A:372:MET:HB2	2.17	0.45
2:D:221:ASN:OD1	2:D:223:LYS:HB2	2.16	0.45
3:P:186:SER:CB	3:P:212:PRO:HA	2.47	0.45
3:G:27:ALA:HA	3:G:31:LYS:O	2.17	0.45
2:B:206:ARG:O	2:B:208:PHE:N	2.50	0.45
1:K:440:GLU:HG3	1:K:445:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:O	1:A:166:VAL:C	2.54	0.45
2:L:119:THR:HB	2:L:120:GLU:H	1.68	0.45
1:K:148:ILE:O	1:K:178:ILE:HA	2.17	0.45
3:H:145:GLN:NE2	3:H:145:GLN:HA	2.31	0.45
3:N:220:ALA:HB1	3:N:225:MET:O	2.16	0.45
3:N:50:HIS:HE1	3:N:229:GLU:OE1	2.00	0.45
1:A:253:TRP:HA	1:A:254:SER:HA	1.69	0.45
1:I:226:ILE:HB	1:I:273:VAL:HG22	1.98	0.45
3:H:57:ILE:HG22	3:H:58:MET:N	2.32	0.45
1:K:430:ILE:HG22	1:K:431:PHE:N	2.32	0.45
1:A:428:LYS:HA	1:A:438:PHE:CE1	2.52	0.45
1:C:420:LEU:C	1:C:420:LEU:HD23	2.37	0.45
2:L:442:MET:HG3	2:L:464:VAL:CG1	2.47	0.45
5:A:6494:HCA:O2	5:A:6494:HCA:O7	2.32	0.45
2:B:414:PRO:O	2:B:417:LYS:HG3	2.16	0.45
3:E:88:SER:HB3	3:E:102:VAL:HG22	1.98	0.45
1:C:240:ILE:HG23	1:C:241:LEU:N	2.31	0.45
2:D:410:LEU:HD22	2:D:419:ALA:CB	2.47	0.45
1:A:299:PHE:HB3	1:A:452:GLY:H	1.81	0.45
3:H:49:LEU:C	3:H:51:SER:H	2.19	0.44
3:M:34:MET:HG3	3:M:84:LYS:O	2.18	0.44
1:A:332:LYS:HA	1:A:335:TRP:CD1	2.52	0.44
3:G:99:GLY:HA3	3:G:134:GLY:CA	2.47	0.44
1:I:231:ILE:HG13	1:I:359:ARG:NH2	2.32	0.44
3:M:33:VAL:O	3:M:83:VAL:HG13	2.17	0.44
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.99	0.44
1:A:317:ASP:OD1	1:A:319:SER:HB3	2.17	0.44
2:D:226:ILE:O	2:D:253:LEU:HD12	2.18	0.44
2:J:10:ALA:O	2:J:12:TYR:N	2.50	0.44
2:B:84:LYS:HB2	2:B:145:ASP:HB2	1.99	0.44
1:A:271:ASN:HA	1:A:271:ASN:HD22	1.63	0.44
2:J:359:HIS:CG	2:J:360:THR:N	2.85	0.44
3:O:267:LEU:HD23	3:O:267:LEU:C	2.38	0.44
3:F:127:LEU:C	3:F:127:LEU:HD23	2.37	0.44
3:F:122:VAL:O	3:F:122:VAL:HG13	2.16	0.44
3:H:33:VAL:CG1	3:H:34:MET:H	2.31	0.44
3:N:186:SER:CB	3:N:212:PRO:HA	2.47	0.44
1:A:239:ARG:NE	1:A:249:CYS:SG	2.90	0.44
3:O:36:VAL:HB	3:O:124:TYR:CD1	2.52	0.44
3:G:5:CYS:HB2	3:G:123:PHE:CD1	2.52	0.44
2:J:279:GLU:CD	2:J:279:GLU:H	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:379:LEU:HD21	2:L:443:ILE:HG21	1.98	0.44
3:E:41:LYS:HB3	3:E:43:ASP:OD1	2.17	0.44
3:H:169:VAL:O	3:H:171:TYR:N	2.51	0.44
2:L:495:THR:O	2:L:496:THR:C	2.55	0.44
2:B:283:ASP:O	2:B:284:ALA:C	2.56	0.44
3:E:80:TYR:HE1	3:E:229:GLU:HG3	1.82	0.44
3:G:184:CYS:CB	3:G:196:ILE:HG13	2.47	0.44
3:M:207:MET:O	3:M:209:HIS:N	2.51	0.44
3:H:181:GLY:HA2	3:H:205:THR:OG1	2.17	0.44
3:E:165:SER:HA	3:E:168:ILE:HD12	1.99	0.44
1:C:239:ARG:NE	1:C:249:CYS:SG	2.90	0.44
3:H:132:CYS:SG	3:H:134:GLY:N	2.88	0.44
2:L:132:LYS:HB3	2:L:174:PHE:CE2	2.52	0.44
1:C:327:VAL:O	1:C:328:ILE:C	2.56	0.44
1:K:144:LEU:HD22	2:L:35:TYR:CE1	2.51	0.44
2:B:391:VAL:HG23	2:B:392:HIS:CD2	2.52	0.44
2:D:262:ASP:OD1	2:D:481:ARG:NH1	2.49	0.44
1:A:98:ASN:N	1:A:98:ASN:ND2	2.65	0.44
2:B:21:LYS:HB3	2:B:21:LYS:HE2	1.83	0.44
3:E:130:VAL:HG23	3:E:130:VAL:O	2.17	0.44
2:D:352:VAL:O	2:D:353:ASP:C	2.53	0.44
3:G:172:ALA:HB1	3:G:255:ILE:CD1	2.47	0.44
2:J:308:THR:O	2:J:310:LYS:HG2	2.18	0.44
2:J:124:VAL:HG23	2:J:125:PHE:CD2	2.52	0.44
3:N:278:ASP:OD2	3:N:280:SER:OG	2.34	0.44
3:M:67:VAL:C	3:M:69:ASP:H	2.20	0.44
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.99	0.44
3:N:49:LEU:C	3:N:51:SER:H	2.19	0.44
3:G:60:MET:HB3	3:G:70:LEU:HD21	1.98	0.44
3:G:158:MET:HE2	3:G:199:LEU:HD13	1.99	0.44
3:E:283:GLY:O	3:F:225:MET:SD	2.75	0.44
1:A:119:GLN:O	1:A:120:GLU:C	2.55	0.44
3:N:132:CYS:SG	3:N:134:GLY:N	2.91	0.44
1:A:36:ASP:OD1	1:A:38:ALA:HB3	2.18	0.44
2:J:151:THR:CG2	2:J:162:LEU:HD11	2.47	0.44
2:L:369:LEU:HD12	2:L:369:LEU:C	2.38	0.44
1:A:57:MET:CE	2:B:113:CYS:N	2.80	0.44
3:H:266:GLU:O	3:H:270:GLU:HB3	2.17	0.44
1:K:144:LEU:HG	2:L:43:VAL:HG21	2.00	0.44
2:B:105:ARG:HD3	2:D:522:VAL:HG21	1.99	0.44
2:D:266:ASP:OD2	2:D:270:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ARG:O	2:B:349:GLY:C	2.56	0.44
3:E:139:ILE:HG23	3:E:177:VAL:HG11	1.98	0.44
2:D:4:GLN:HB3	2:D:6:ASP:OD1	2.17	0.44
1:K:297:TYR:HD2	1:K:299:PHE:CE1	2.36	0.44
1:C:240:ILE:O	1:C:244:GLU:HG3	2.17	0.44
1:I:387:TYR:O	1:I:390:THR:HB	2.18	0.44
2:B:495:THR:O	2:B:496:THR:C	2.53	0.44
2:B:318:ILE:HG12	2:B:320:MET:HG3	1.99	0.44
1:C:195:HIS:O	1:C:198:ALA:HB3	2.17	0.44
2:L:82:PHE:HB2	2:L:85:THR:OG1	2.18	0.44
3:N:202:LYS:N	3:N:202:LYS:HD2	2.33	0.44
2:J:108:ARG:CZ	2:J:477:HIS:CD2	3.00	0.44
3:O:78:ALA:HA	3:O:83:VAL:O	2.17	0.44
3:F:76:LEU:HD13	3:F:86:VAL:HG13	1.99	0.44
3:N:97:CYS:O	3:N:100:ARG:HB3	2.16	0.44
3:N:103:ILE:HG23	3:N:104:THR:H	1.83	0.44
2:J:194:VAL:HG23	2:J:195:THR:N	2.32	0.44
1:I:230:ASN:OD1	1:I:233:GLY:HA2	2.18	0.44
1:A:20:TYR:HH	1:A:405:THR:HG21	1.82	0.44
3:G:20:GLN:HE21	3:G:48:ILE:HG12	1.81	0.44
2:B:333:SER:O	2:B:334:GLU:C	2.55	0.44
1:I:59:ILE:HG23	1:I:426:LYS:HD2	1.99	0.44
3:O:43:ASP:HB3	3:O:46:ARG:CZ	2.47	0.44
2:L:37:GLN:O	2:L:39:LYS:N	2.50	0.44
2:J:365:LYS:HE2	2:J:501:ILE:HD13	2.00	0.44
1:C:437:PRO:HG3	1:C:472:TRP:CE2	2.53	0.44
2:L:472:PRO:HB2	2:L:474:PHE:CZ	2.52	0.44
3:P:4:GLN:HA	3:P:122:VAL:HG13	1.99	0.44
2:J:389:GLU:O	2:J:391:VAL:N	2.51	0.44
2:L:120:GLU:C	2:L:122:ALA:H	2.21	0.44
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.52	0.44
1:C:167:SER:O	1:C:168:LYS:C	2.55	0.44
1:C:440:GLU:HG3	1:C:445:ASP:OD2	2.16	0.44
1:A:72:TRP:CZ2	1:A:202:VAL:HG22	2.53	0.44
2:B:442:MET:SD	2:B:451:ILE:HG21	2.58	0.44
3:G:165:SER:HA	3:G:168:ILE:HD12	2.00	0.44
2:J:369:LEU:CD1	2:J:376:VAL:HG13	2.48	0.44
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.17	0.44
1:A:444:TRP:HA	1:A:444:TRP:HE3	1.81	0.44
3:N:131:VAL:CG2	3:N:164:ILE:HG12	2.48	0.44
1:C:389:ARG:NH1	1:C:389:ARG:HG3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:97:CYS:O	3:P:100:ARG:HB3	2.17	0.44
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.33	0.44
1:A:327:VAL:O	1:A:328:ILE:C	2.55	0.44
2:D:475:ASP:O	2:D:476:ARG:NH1	2.42	0.44
3:O:27:ALA:HA	3:O:31:LYS:O	2.17	0.44
3:N:5:CYS:SG	3:N:146:GLU:HB2	2.57	0.44
1:C:63:ALA:O	1:C:67:SER:N	2.51	0.44
1:A:302:PRO:HD3	1:A:456:PHE:CG	2.52	0.44
1:C:51:LYS:HA	1:C:189:VAL:HG11	1.99	0.44
1:K:85:PRO:HD3	1:K:155:PRO:HG2	1.98	0.44
3:F:245:ARG:HG3	3:F:245:ARG:NH1	2.33	0.44
3:N:212:PRO:HG2	3:N:236:GLN:NE2	2.32	0.44
3:H:131:VAL:HG21	3:H:164:ILE:HG12	1.99	0.44
2:B:247:MET:CE	2:B:340:ILE:HG12	2.47	0.44
1:A:226:ILE:HB	1:A:273:VAL:HG22	1.98	0.44
3:F:103:ILE:CG2	3:F:104:THR:N	2.80	0.44
1:C:323:LYS:O	1:C:327:VAL:HG23	2.17	0.44
1:C:144:LEU:CG	2:D:43:VAL:HG21	2.48	0.44
2:B:78:CYS:HB2	2:B:197:TRP:CD1	2.53	0.44
3:N:4:GLN:HG2	3:N:122:VAL:HG11	1.99	0.44
1:K:458:ILE:O	1:K:459:PHE:C	2.55	0.44
2:D:124:VAL:HG23	2:D:125:PHE:H	1.81	0.44
2:J:353:ASP:O	2:J:354:MET:C	2.56	0.44
3:G:38:CYS:CB	3:G:126:VAL:HG22	2.48	0.44
2:L:166:ILE:HD13	2:L:181:VAL:HG12	2.00	0.44
1:A:208:GLY:HA2	1:A:211:ASP:OD1	2.17	0.44
1:I:462:ASP:O	1:I:463:MET:C	2.55	0.44
3:O:24:ALA:HB2	3:O:226:THR:HG21	1.99	0.44
2:J:368:ALA:O	2:J:442:MET:HA	2.18	0.44
1:C:475:LEU:HD12	1:C:475:LEU:H	1.82	0.44
3:O:32:LYS:CB	3:O:119:LEU:HA	2.47	0.44
2:B:369:LEU:C	2:B:369:LEU:HD12	2.38	0.44
3:M:2:MET:HE3	3:M:122:VAL:HG21	2.00	0.44
3:N:186:SER:HA	3:N:192:GLU:OE1	2.18	0.44
3:E:60:MET:HB3	3:E:70:LEU:HD21	2.00	0.44
3:E:186:SER:HB3	3:E:213:ARG:HG3	2.00	0.44
3:P:103:ILE:HG23	3:P:104:THR:H	1.81	0.44
2:J:221:ASN:HD21	2:J:287:ALA:N	2.16	0.44
2:D:348:ARG:HB2	2:D:487:TYR:CE2	2.52	0.44
3:O:42:ALA:HA	3:O:87:GLU:OE1	2.17	0.44
2:B:135:LEU:HB3	2:B:175:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:26:LEU:C	3:O:31:LYS:HB2	2.37	0.44
2:D:94:GLY:O	2:D:97:ALA:HB3	2.17	0.44
2:D:442:MET:HG3	2:D:464:VAL:CG1	2.47	0.44
2:J:222:LYS:N	2:J:222:LYS:HD2	2.33	0.44
1:K:196:HIS:O	1:K:197:ILE:C	2.56	0.44
3:G:260:THR:OG1	3:G:263:GLU:HG3	2.18	0.44
1:C:326:GLU:O	1:C:329:ALA:HB3	2.17	0.44
3:O:223:ARG:NH1	3:P:284:LYS:O	2.46	0.44
3:M:158:MET:HE2	3:M:199:LEU:HD13	2.00	0.44
3:H:127:LEU:HD23	3:H:129:ASP:N	2.32	0.44
3:M:161:ALA:HA	3:M:164:ILE:HD12	2.00	0.44
1:I:339:VAL:HG12	1:I:343:ARG:HB2	1.99	0.44
3:H:130:VAL:O	3:H:131:VAL:C	2.56	0.44
2:B:35:TYR:O	2:B:36:PRO:C	2.55	0.44
3:M:216:VAL:HG22	3:M:227:VAL:HG13	1.99	0.44
3:F:186:SER:HB2	3:F:212:PRO:HA	2.00	0.44
1:I:59:ILE:HD13	1:I:354:TYR:CE2	2.52	0.44
2:L:70:CYS:SG	2:L:72:PRO:HG2	2.58	0.44
2:L:10:ALA:O	2:L:12:TYR:N	2.50	0.44
1:C:351:VAL:HG12	1:C:352:MET:N	2.32	0.44
3:H:5:CYS:SG	3:H:146:GLU:HB2	2.58	0.44
2:J:37:GLN:O	2:J:39:LYS:N	2.51	0.44
2:D:85:THR:HA	2:D:146:MET:O	2.18	0.44
3:P:169:VAL:O	3:P:171:TYR:N	2.51	0.44
3:O:269:MET:SD	3:O:276:VAL:HA	2.58	0.44
3:M:10:LYS:O	3:M:10:LYS:HG2	2.17	0.44
3:M:184:CYS:CB	3:M:196:ILE:HG13	2.48	0.43
3:H:50:HIS:HE1	3:H:229:GLU:OE1	2.01	0.43
3:P:50:HIS:CE1	3:P:229:GLU:OE1	2.71	0.43
3:P:40:PRO:HD2	3:P:127:LEU:HD13	1.99	0.43
3:O:131:VAL:HG12	3:P:94:GLY:H	1.82	0.43
3:N:60:MET:CE	3:N:75:VAL:HG22	2.47	0.43
1:I:289:LYS:HE3	1:I:290:TYR:OH	2.18	0.43
3:H:67:VAL:N	3:H:69:ASP:OD2	2.49	0.43
1:C:475:LEU:N	1:C:475:LEU:HD12	2.33	0.43
1:K:251:ALA:HB2	1:K:261:GLU:O	2.19	0.43
2:J:283:ASP:O	2:J:284:ALA:C	2.55	0.43
1:I:72:TRP:CZ2	1:I:202:VAL:HG22	2.53	0.43
3:G:23:VAL:C	3:G:25:ALA:N	2.72	0.43
1:A:287:GLU:O	1:A:291:GLY:HA2	2.18	0.43
2:J:446:SER:C	2:J:448:GLY:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:271:ASN:HA	1:K:271:ASN:HD22	1.56	0.43
3:G:91:PRO:O	3:G:93:PRO:HD3	2.18	0.43
3:O:34:MET:HG3	3:O:84:LYS:O	2.18	0.43
3:G:32:LYS:CB	3:G:119:LEU:HA	2.47	0.43
1:C:253:TRP:HA	1:C:254:SER:HA	1.63	0.43
1:A:275:CYS:SG	6:A:6496:CFM:S1A	3.16	0.43
2:B:330:MET:O	2:B:333:SER:HB3	2.18	0.43
1:K:359:ARG:N	1:K:360:PRO:CD	2.81	0.43
1:A:310:ARG:HA	1:A:324:CYS:SG	2.58	0.43
1:A:430:ILE:HG22	1:A:431:PHE:N	2.33	0.43
2:B:226:ILE:O	2:B:253:LEU:HD12	2.19	0.43
3:O:107:ASN:HA	3:O:110:GLU:OE1	2.18	0.43
1:A:156:ILE:HG22	1:A:157:GLY:N	2.33	0.43
3:O:144:ALA:O	3:O:177:VAL:HG22	2.18	0.43
3:E:173:ASN:N	3:E:173:ASN:HD22	2.16	0.43
1:C:98:ASN:H	1:C:98:ASN:ND2	2.16	0.43
1:K:19:VAL:CG1	1:K:20:TYR:N	2.81	0.43
1:C:239:ARG:HG2	2:D:23:MET:SD	2.58	0.43
1:A:359:ARG:N	1:A:360:PRO:CD	2.80	0.43
3:G:134:GLY:HA3	8:G:1290:SF4:S1	2.58	0.43
2:B:37:GLN:HG3	2:B:41:ASP:OD1	2.17	0.43
2:J:71:GLN:OE1	2:J:186:THR:HA	2.18	0.43
3:P:66:THR:N	3:P:69:ASP:OD1	2.51	0.43
2:B:132:LYS:HD3	2:B:174:PHE:HE2	1.83	0.43
2:J:456:LEU:O	2:J:459:GLY:N	2.51	0.43
1:I:427:GLU:O	1:I:429:PHE:N	2.52	0.43
1:A:154:CYS:SG	7:A:6498:CLF:S2A	3.16	0.43
3:H:33:VAL:HG12	3:H:34:MET:H	1.82	0.43
3:N:103:ILE:CG2	3:N:104:THR:N	2.81	0.43
3:G:48:ILE:HG22	3:G:79:GLY:HA3	1.99	0.43
3:G:212:PRO:HG3	3:G:239:GLU:HG3	2.01	0.43
2:B:36:PRO:O	2:B:37:GLN:C	2.56	0.43
2:J:295:PRO:C	2:J:297:HIS:H	2.21	0.43
2:D:215:ASP:OD2	2:D:216:LYS:HE3	2.18	0.43
3:H:187:ARG:HB2	3:H:192:GLU:OE2	2.18	0.43
1:C:144:LEU:CD1	2:D:43:VAL:HG21	2.49	0.43
2:B:4:GLN:C	2:B:6:ASP:N	2.72	0.43
3:G:57:ILE:HG12	3:G:75:VAL:HG21	1.99	0.43
1:I:474:LYS:HB3	2:L:322:LEU:CD2	2.49	0.43
3:G:26:LEU:C	3:G:31:LYS:HB2	2.39	0.43
1:A:85:PRO:HD3	1:A:155:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ILE:O	1:C:425:ILE:HG13	2.17	0.43
1:C:385:ASP:HA	1:C:388:ASP:OD2	2.17	0.43
3:G:204:GLY:O	3:G:254:VAL:HG21	2.19	0.43
3:H:269:MET:HA	3:H:274:MET:O	2.18	0.43
2:J:146:MET:HA	2:J:180:PRO:HG2	2.00	0.43
2:B:199:ASN:O	2:B:200:MET:C	2.57	0.43
3:P:261:MET:O	3:P:265:GLU:HG3	2.18	0.43
3:N:223:ARG:O	3:N:224:ARG:HB2	2.17	0.43
3:F:223:ARG:O	3:F:224:ARG:HB2	2.19	0.43
2:B:131:MET:HG2	2:B:165:PHE:HB3	2.01	0.43
3:H:34:MET:HA	3:H:84:LYS:O	2.17	0.43
1:I:73:GLY:N	1:I:74:PRO:CD	2.82	0.43
2:L:164:ALA:O	2:L:167:ASN:N	2.52	0.43
3:E:20:GLN:OE1	3:E:44:SER:C	2.57	0.43
1:C:361:ARG:HB3	1:C:379:TYR:OH	2.18	0.43
3:O:135:PHE:O	3:O:138:PRO:HD2	2.19	0.43
3:N:131:VAL:HG21	3:N:164:ILE:HG12	2.00	0.43
3:P:60:MET:HE1	3:P:75:VAL:HG13	2.00	0.43
2:B:266:ASP:OD2	2:B:270:ARG:NH2	2.51	0.43
1:C:317:ASP:OD1	1:C:319:SER:HB3	2.18	0.43
1:I:144:LEU:CG	2:J:43:VAL:HG21	2.48	0.43
2:B:102:TYR:OH	2:B:472:PRO:HG3	2.19	0.43
2:J:441:PHE:HE2	2:J:501:ILE:HG12	1.82	0.43
3:E:57:ILE:CG1	3:E:75:VAL:HG11	2.49	0.43
1:K:137:GLU:OE2	2:L:59:ARG:HA	2.18	0.43
2:L:261:LEU:HD23	2:L:261:LEU:HA	1.81	0.43
3:O:10:LYS:O	3:O:13:ILE:HG12	2.18	0.43
3:F:43:ASP:OD1	3:F:43:ASP:N	2.51	0.43
1:K:302:PRO:HD3	1:K:456:PHE:CG	2.54	0.43
1:I:208:GLY:HA2	1:I:211:ASP:OD1	2.19	0.43
3:G:24:ALA:HB2	3:G:226:THR:HG21	2.01	0.43
3:H:4:GLN:HA	3:H:122:VAL:HG13	1.99	0.43
3:H:4:GLN:HG2	3:H:122:VAL:HG11	2.00	0.43
3:M:278:ASP:HB2	3:M:281:ILE:HD12	1.99	0.43
2:L:164:ALA:O	2:L:165:PHE:C	2.56	0.43
3:N:100:ARG:NH1	3:N:100:ARG:HG3	2.33	0.43
1:K:20:TYR:HH	1:K:408:GLU:CD	2.21	0.43
1:A:379:TYR:HD1	1:A:387:TYR:CE1	2.36	0.43
3:E:99:GLY:HA3	3:E:134:GLY:C	2.39	0.43
3:E:214:ASP:CB	3:E:216:VAL:HG12	2.48	0.43
3:M:72:LEU:HD11	3:M:114:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:HB3	1:A:375:VAL:HG11	1.98	0.43
2:J:428:TRP:O	2:J:431:ARG:HB3	2.18	0.43
2:D:37:GLN:O	2:D:39:LYS:N	2.52	0.43
2:L:450:PHE:O	2:L:451:ILE:C	2.56	0.43
2:B:350:ARG:HD3	2:D:262:ASP:OD2	2.18	0.43
2:J:228:PRO:HD2	2:J:254:LEU:O	2.19	0.43
2:L:284:ALA:HB3	2:L:285:PRO:HD3	2.01	0.43
1:I:106:VAL:HG11	2:J:40:ILE:HG23	2.01	0.43
1:I:287:GLU:O	1:I:291:GLY:HA2	2.18	0.43
1:A:212:GLU:HB3	2:L:279:GLU:HB3	2.01	0.43
1:C:134:LEU:HD23	1:C:138:VAL:CG2	2.49	0.43
2:J:164:ALA:O	2:J:167:ASN:N	2.52	0.43
1:A:282:ILE:O	1:A:286:MET:HG3	2.18	0.43
1:C:339:VAL:O	1:C:343:ARG:CB	2.63	0.43
1:I:357:GLY:HA2	1:I:379:TYR:HD2	1.83	0.43
1:K:66:GLY:C	1:K:70:VAL:HB	2.38	0.43
3:P:71:GLU:C	3:P:73:GLU:N	2.72	0.43
2:D:216:LYS:HA	2:D:286:ASN:HD21	1.83	0.43
2:D:35:TYR:O	2:D:36:PRO:C	2.57	0.43
2:B:474:PHE:HB3	2:D:522:VAL:HA	1.99	0.43
2:L:389:GLU:O	2:L:391:VAL:N	2.51	0.43
2:J:354:MET:O	2:J:355:MET:C	2.56	0.43
1:C:193:LEU:O	1:C:197:ILE:HG13	2.19	0.43
2:D:296:TRP:HB2	2:D:374:ASP:OD1	2.18	0.43
2:J:84:LYS:HD2	2:J:145:ASP:OD2	2.19	0.43
1:I:11:SER:O	1:I:15:GLU:HG3	2.18	0.43
2:L:215:ASP:OD2	2:L:216:LYS:HE3	2.18	0.43
3:O:278:ASP:HB2	3:O:281:ILE:HD12	2.00	0.43
1:A:73:GLY:N	1:A:74:PRO:CD	2.81	0.43
3:G:137:MET:HB3	3:G:138:PRO:HD3	2.00	0.43
1:C:119:GLN:O	1:C:120:GLU:C	2.56	0.43
3:E:216:VAL:HG11	3:E:236:GLN:HB3	2.01	0.43
1:K:370:LEU:O	1:K:372:MET:N	2.52	0.43
2:B:4:GLN:O	2:B:7:LYS:N	2.48	0.43
2:B:101:SER:HA	2:B:104:ASN:HD22	1.84	0.43
1:A:80:HIS:O	1:A:114:PHE:HB2	2.18	0.43
2:D:197:TRP:CZ3	2:D:229:GLY:HA2	2.54	0.43
1:I:219:THR:HG23	1:I:248:ARG:NH2	2.33	0.43
3:N:21:ASN:O	3:N:24:ALA:HB3	2.19	0.43
1:I:21:PRO:O	1:I:22:GLU:C	2.57	0.43
3:E:225:MET:HE2	3:E:229:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:184:CYS:HG	3:E:210:PHE:HE1	1.62	0.43
1:A:433:LYS:HE3	2:B:263:THR:CG2	2.37	0.43
1:I:85:PRO:CD	1:I:155:PRO:HG2	2.49	0.43
3:G:127:LEU:HD12	3:G:135:PHE:CZ	2.54	0.43
1:A:235:ALA:O	1:A:238:SER:N	2.50	0.43
1:C:367:TYR:O	1:C:372:MET:HB2	2.18	0.43
1:A:35:ASN:HD22	1:A:36:ASP:N	2.09	0.43
1:C:405:THR:HG23	1:C:408:GLU:OE2	2.18	0.43
1:A:368:GLU:C	1:A:370:LEU:H	2.22	0.43
1:I:98:ASN:H	1:I:98:ASN:ND2	2.16	0.43
3:F:187:ARG:HB2	3:F:192:GLU:OE2	2.19	0.43
2:D:431:ARG:O	2:D:434:VAL:CG2	2.66	0.43
2:B:71:GLN:OE1	2:B:186:THR:HA	2.18	0.43
2:D:59:ARG:HH22	2:D:429:HIS:CE1	2.37	0.43
2:L:84:LYS:HD2	2:L:145:ASP:OD2	2.18	0.43
1:K:137:GLU:OE2	2:L:60:GLU:N	2.45	0.43
2:L:101:SER:HA	2:L:104:ASN:HD22	1.84	0.43
3:E:38:CYS:HB2	3:E:126:VAL:HG22	2.01	0.43
2:D:206:ARG:O	2:D:208:PHE:N	2.51	0.43
3:M:21:ASN:HB3	3:M:240:TYR:CD1	2.54	0.43
2:J:522:VAL:HG21	2:L:105:ARG:HD3	1.99	0.43
1:A:129:LYS:HE3	1:A:129:LYS:HB2	1.88	0.43
3:M:184:CYS:SG	3:M:210:PHE:HE1	2.37	0.43
3:F:33:VAL:CG1	3:F:34:MET:H	2.31	0.43
3:F:209:HIS:HB3	3:F:243:LEU:HD13	2.00	0.43
1:C:343:ARG:N	1:C:344:PRO:CD	2.82	0.43
3:P:208:ILE:CG2	3:P:209:HIS:N	2.81	0.43
2:D:205:ALA:HA	2:D:281:MET:HE1	1.99	0.43
1:C:68:LYS:CD	1:C:68:LYS:C	2.87	0.43
1:K:239:ARG:NE	1:K:249:CYS:SG	2.92	0.43
1:C:75:ILE:H	1:C:75:ILE:CD1	2.32	0.43
3:N:116:GLU:OE1	3:N:116:GLU:N	2.52	0.43
2:D:118:MET:HA	2:D:130:ASN:HD22	1.82	0.43
2:D:431:ARG:NH1	2:D:435:PHE:HE2	2.16	0.43
1:I:420:LEU:CD1	1:I:467:LEU:HD12	2.48	0.43
2:B:4:GLN:O	2:B:5:VAL:C	2.57	0.43
2:B:88:TYR:CE2	2:B:135:LEU:HD23	2.54	0.43
2:B:389:GLU:O	2:B:391:VAL:N	2.52	0.43
2:L:322:LEU:HB3	2:L:385:GLU:OE2	2.19	0.43
1:I:458:ILE:HD13	2:J:10:ALA:HA	2.00	0.43
1:K:134:LEU:HD23	1:K:138:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:LEU:O	2:J:80:LEU:HB2	2.19	0.43
2:L:491:MET:O	2:L:492:GLN:C	2.56	0.43
3:O:50:HIS:HE1	3:O:229:GLU:OE1	2.01	0.42
3:H:80:TYR:HD2	3:H:229:GLU:HG3	1.83	0.42
3:E:158:MET:HE2	3:E:199:LEU:HD13	2.00	0.42
2:B:108:ARG:CZ	2:B:477:HIS:CD2	3.02	0.42
3:F:220:ALA:HB1	3:F:225:MET:O	2.18	0.42
3:P:39:ASP:OD1	3:P:127:LEU:HD12	2.19	0.42
3:E:137:MET:HB3	3:E:138:PRO:HD3	2.01	0.42
2:L:394:LEU:HD23	2:L:394:LEU:C	2.40	0.42
1:C:346:LEU:HB3	1:C:372:MET:SD	2.59	0.42
1:A:66:GLY:HA2	1:A:70:VAL:CG2	2.49	0.42
1:K:235:ALA:O	1:K:238:SER:N	2.52	0.42
3:E:214:ASP:CG	3:E:216:VAL:HG12	2.40	0.42
2:B:4:GLN:HB3	2:B:6:ASP:OD1	2.18	0.42
1:I:62:CYS:O	1:I:63:ALA:C	2.56	0.42
2:D:4:GLN:O	2:D:7:LYS:N	2.50	0.42
3:G:246:LYS:O	3:G:250:ASN:HB2	2.19	0.42
2:J:283:ASP:C	2:J:285:PRO:HD2	2.39	0.42
3:F:116:GLU:OE1	3:F:116:GLU:N	2.52	0.42
1:K:351:VAL:HG12	1:K:352:MET:N	2.33	0.42
2:D:246:GLU:OE2	2:D:343:SER:HB2	2.19	0.42
1:C:284:ARG:HG2	1:C:284:ARG:HH11	1.84	0.42
1:I:475:LEU:H	1:I:475:LEU:HD12	1.84	0.42
3:F:206:GLN:HG2	3:F:252:LEU:HD13	2.02	0.42
3:O:202:LYS:HB3	3:O:202:LYS:HE3	1.94	0.42
2:J:131:MET:HG2	2:J:165:PHE:HB3	2.00	0.42
3:F:36:VAL:HG22	3:F:86:VAL:CG2	2.49	0.42
3:H:54:GLN:HG2	3:H:55:ASN:N	2.34	0.42
2:B:394:LEU:HD23	2:B:394:LEU:C	2.38	0.42
3:M:127:LEU:C	3:M:127:LEU:HD13	2.39	0.42
1:C:223:VAL:HG23	1:C:249:CYS:HA	2.00	0.42
8:E:290:SF4:S2	3:F:134:GLY:N	2.92	0.42
1:I:359:ARG:N	1:I:360:PRO:CD	2.81	0.42
2:L:369:LEU:HD11	2:L:376:VAL:HG13	2.01	0.42
3:P:100:ARG:HG3	3:P:100:ARG:NH1	2.33	0.42
2:D:348:ARG:O	2:D:351:LEU:N	2.53	0.42
2:D:59:ARG:NH2	2:D:429:HIS:CE1	2.87	0.42
1:K:98:ASN:ND2	1:K:98:ASN:H	2.17	0.42
2:J:495:THR:O	2:J:496:THR:C	2.57	0.42
2:D:120:GLU:C	2:D:122:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:SER:O	1:I:168:LYS:C	2.57	0.42
3:O:184:CYS:HG	3:O:210:PHE:HE1	1.62	0.42
3:F:80:TYR:CD1	3:F:80:TYR:C	2.92	0.42
3:H:36:VAL:HG22	3:H:86:VAL:CG2	2.49	0.42
3:H:245:ARG:NH1	3:H:245:ARG:HG3	2.33	0.42
2:B:221:ASN:OD1	2:B:223:LYS:N	2.51	0.42
1:K:76:LYS:HG2	1:K:257:GLY:O	2.18	0.42
1:I:57:MET:CE	2:J:113:CYS:N	2.82	0.42
3:P:116:GLU:N	3:P:116:GLU:OE1	2.53	0.42
2:D:431:ARG:HG2	2:D:431:ARG:NH1	2.35	0.42
3:E:54:GLN:NE2	3:E:75:VAL:O	2.52	0.42
1:A:420:LEU:C	1:A:420:LEU:HD23	2.40	0.42
1:I:475:LEU:N	1:I:475:LEU:HD12	2.35	0.42
3:N:256:PRO:O	3:N:258:PRO:HD3	2.19	0.42
1:A:285:HIS:O	1:A:288:GLU:N	2.52	0.42
1:K:11:SER:O	1:K:15:GLU:HG3	2.19	0.42
3:G:278:ASP:HB2	3:G:281:ILE:HD12	2.00	0.42
3:F:54:GLN:HG2	3:F:55:ASN:N	2.33	0.42
1:I:88:CYS:CB	1:I:153:GLU:OE2	2.64	0.42
1:A:71:VAL:C	1:A:74:PRO:HD2	2.38	0.42
3:O:16:SER:O	3:O:20:GLN:HG2	2.19	0.42
3:O:20:GLN:OE1	3:O:44:SER:C	2.58	0.42
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.84	0.42
3:H:131:VAL:CG2	3:H:164:ILE:HG12	2.49	0.42
2:B:37:GLN:O	2:B:39:LYS:N	2.53	0.42
1:I:354:TYR:OH	1:I:380:GLU:HA	2.19	0.42
3:P:115:TYR:O	3:P:116:GLU:C	2.57	0.42
2:D:445:ASN:OD1	2:D:447:TYR:HB2	2.19	0.42
2:B:200:MET:O	2:B:201:PHE:C	2.57	0.42
3:O:88:SER:HB3	3:O:102:VAL:HG22	2.01	0.42
2:B:502:LEU:HD22	2:B:523:ARG:HD2	2.00	0.42
1:K:163:ILE:O	1:K:164:GLU:C	2.58	0.42
3:O:195:LEU:HA	3:O:271:PHE:CE2	2.54	0.42
3:O:3:ARG:NH1	3:O:121:PHE:HZ	2.16	0.42
1:I:451:HIS:O	1:I:455:GLY:HA3	2.20	0.42
3:M:3:ARG:NH1	3:M:121:PHE:HZ	2.16	0.42
2:L:221:ASN:HD22	2:L:286:ASN:HB2	1.84	0.42
3:P:158:MET:HE1	3:P:195:LEU:HD11	2.01	0.42
3:M:60:MET:CB	3:M:70:LEU:HD21	2.50	0.42
2:J:413:SER:HA	2:J:414:PRO:HD3	1.92	0.42
2:L:194:VAL:HG23	2:L:195:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:445:ASN:OD1	2:L:447:TYR:HB2	2.20	0.42
2:L:59:ARG:NH2	2:L:429:HIS:NE2	2.67	0.42
3:M:54:GLN:NE2	3:M:75:VAL:O	2.52	0.42
2:J:36:PRO:O	2:J:37:GLN:C	2.58	0.42
1:C:287:GLU:O	1:C:291:GLY:HA2	2.20	0.42
1:I:12:LEU:HD13	1:I:415:ARG:NH1	2.34	0.42
3:G:100:ARG:HE	3:G:101:GLY:N	2.18	0.42
3:N:80:TYR:HD2	3:N:229:GLU:HG3	1.85	0.42
3:O:198:ALA:O	3:O:202:LYS:HG3	2.19	0.42
3:O:158:MET:HE2	3:O:199:LEU:HD13	2.01	0.42
3:H:71:GLU:C	3:H:73:GLU:N	2.73	0.42
1:C:359:ARG:N	1:C:360:PRO:CD	2.82	0.42
1:K:405:THR:OG1	1:K:408:GLU:HG3	2.19	0.42
1:C:239:ARG:CZ	1:C:249:CYS:SG	3.07	0.42
1:I:359:ARG:NH1	1:I:444:TRP:CH2	2.88	0.42
3:P:71:GLU:O	3:P:73:GLU:N	2.53	0.42
3:H:66:THR:H	3:H:69:ASP:CG	2.23	0.42
2:L:451:ILE:HD12	2:L:451:ILE:H	1.85	0.42
3:P:214:ASP:CG	3:P:216:VAL:HG12	2.39	0.42
2:J:84:LYS:HA	2:J:272:TYR:CD1	2.54	0.42
3:G:173:ASN:N	3:G:173:ASN:HD22	2.18	0.42
2:D:502:LEU:HD22	2:D:523:ARG:HD2	2.00	0.42
3:E:142:ASN:HD21	3:E:175:GLY:HA3	1.85	0.42
1:C:364:ILE:HD11	1:C:394:MET:SD	2.60	0.42
3:E:78:ALA:HA	3:E:83:VAL:O	2.20	0.42
3:O:283:GLY:O	3:P:225:MET:SD	2.77	0.42
3:P:54:GLN:HG2	3:P:55:ASN:N	2.34	0.42
2:B:450:PHE:O	2:B:452:GLN:N	2.53	0.42
1:C:358:LEU:HD11	1:C:362:HIS:CE1	2.55	0.42
2:J:333:SER:O	2:J:334:GLU:C	2.58	0.42
3:P:66:THR:H	3:P:69:ASP:CG	2.23	0.42
2:L:348:ARG:HB2	2:L:487:TYR:CE2	2.54	0.42
2:J:326:ASP:OD1	2:J:487:TYR:OH	2.34	0.42
1:I:156:ILE:HG22	1:I:157:GLY:N	2.34	0.42
2:J:324:TRP:CZ2	2:J:381:LYS:HD3	2.55	0.42
2:J:520:ASP:CG	1:K:99:TYR:HH	2.23	0.42
2:D:164:ALA:O	2:D:167:ASN:N	2.53	0.42
3:F:145:GLN:NE2	3:F:145:GLN:HA	2.34	0.42
2:L:268:GLN:HE21	2:L:268:GLN:HB2	1.53	0.42
3:G:223:ARG:O	3:G:224:ARG:C	2.57	0.42
2:L:108:ARG:CZ	2:L:477:HIS:CD2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:39:ASP:OD2	3:N:41:LYS:HB3	2.19	0.42
1:C:427:GLU:O	1:C:429:PHE:N	2.53	0.42
1:A:253:TRP:CZ3	1:A:282:ILE:HG12	2.55	0.42
3:O:49:LEU:N	3:O:49:LEU:HD23	2.34	0.42
3:P:67:VAL:C	3:P:69:ASP:N	2.73	0.42
2:D:213:MET:HE1	2:D:309:TRP:HA	2.00	0.42
3:N:64:ALA:CB	3:N:69:ASP:HB2	2.49	0.42
3:E:187:ARG:O	3:E:188:ASN:HB2	2.20	0.42
1:K:439:ARG:HG3	1:K:463:MET:CE	2.50	0.42
2:J:37:GLN:O	2:J:40:ILE:N	2.52	0.42
1:C:364:ILE:O	1:C:365:GLY:C	2.55	0.42
3:N:32:LYS:NZ	3:N:118:ASP:HB2	2.35	0.42
3:H:32:LYS:NZ	3:H:118:ASP:HB2	2.35	0.42
2:D:479:LEU:HA	2:D:479:LEU:HD23	1.77	0.42
3:O:184:CYS:CB	3:O:196:ILE:HG13	2.49	0.42
3:E:199:LEU:HD23	3:E:199:LEU:C	2.40	0.42
3:H:36:VAL:HG22	3:H:86:VAL:HG22	2.02	0.42
1:I:119:GLN:O	1:I:120:GLU:C	2.58	0.42
1:I:71:VAL:C	1:I:74:PRO:HD2	2.40	0.42
1:K:343:ARG:HB3	1:K:344:PRO:HD3	2.02	0.42
1:A:358:LEU:HD11	1:A:362:HIS:CE1	2.54	0.42
1:A:300:PHE:CD2	1:A:362:HIS:HB3	2.54	0.42
1:A:70:VAL:O	1:A:96:ARG:NH1	2.52	0.42
3:E:134:GLY:HA3	8:E:290:SF4:S1	2.60	0.42
1:A:68:LYS:HD3	1:A:68:LYS:O	2.20	0.42
2:J:296:TRP:HB2	2:J:374:ASP:OD1	2.20	0.42
3:H:66:THR:N	3:H:69:ASP:OD1	2.53	0.42
2:D:348:ARG:O	2:D:349:GLY:C	2.57	0.42
3:P:186:SER:HA	3:P:192:GLU:OE1	2.20	0.42
3:E:5:CYS:HB2	3:E:123:PHE:CD1	2.54	0.42
3:P:153:GLY:O	3:P:154:GLU:HB2	2.20	0.42
2:D:56:ASN:OD1	2:D:59:ARG:NH2	2.41	0.42
2:J:254:LEU:O	2:J:255:SER:HB3	2.20	0.42
2:D:353:ASP:O	2:D:354:MET:C	2.58	0.42
3:E:261:MET:O	3:E:265:GLU:HG3	2.20	0.42
2:L:436:THR:OG1	2:L:437:ASP:N	2.53	0.42
1:I:200:ASP:O	1:I:201:ALA:C	2.58	0.42
2:J:322:LEU:HB3	2:J:385:GLU:OE2	2.20	0.42
2:L:232:THR:HG21	2:L:471:PHE:CD1	2.55	0.42
1:A:134:LEU:C	1:A:134:LEU:HD23	2.40	0.42
3:G:184:CYS:SG	3:G:210:PHE:CE1	3.04	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:193:ASP:HB3	3:G:210:PHE:CE1	2.54	0.42
3:N:33:VAL:CG1	3:N:34:MET:H	2.33	0.42
2:B:441:PHE:HE2	2:B:501:ILE:HG12	1.85	0.42
1:I:239:ARG:NE	2:J:23:MET:CE	2.81	0.42
1:A:344:PRO:C	1:A:346:LEU:H	2.23	0.42
3:G:136:ALA:HB2	3:H:94:GLY:HA2	2.01	0.42
1:C:332:LYS:N	1:C:333:PRO:CD	2.82	0.42
3:G:20:GLN:OE1	3:G:44:SER:C	2.58	0.42
2:D:497:LEU:O	2:D:498:VAL:C	2.58	0.42
2:L:118:MET:HA	2:L:130:ASN:HD22	1.84	0.42
3:E:217:VAL:HA	3:E:227:VAL:CG2	2.50	0.42
1:A:270:LEU:CD1	1:A:293:PRO:HG2	2.50	0.42
3:M:38:CYS:HB2	3:M:126:VAL:HA	2.02	0.42
3:P:269:MET:HA	3:P:274:MET:O	2.20	0.42
1:I:425:ILE:HG13	1:I:425:ILE:O	2.20	0.42
2:B:166:ILE:HD13	2:B:181:VAL:HG12	2.02	0.42
3:P:92:GLU:O	3:P:93:PRO:C	2.57	0.42
3:G:184:CYS:SG	3:G:210:PHE:HE1	2.43	0.41
3:M:76:LEU:CD1	3:M:86:VAL:HG13	2.50	0.41
3:P:50:HIS:HE1	3:P:229:GLU:OE1	2.03	0.41
3:G:3:ARG:NH1	3:G:121:PHE:HZ	2.18	0.41
1:A:230:ASN:OD1	1:A:235:ALA:HB3	2.20	0.41
3:N:57:ILE:HG13	3:N:75:VAL:HG11	2.01	0.41
2:B:234:LEU:O	2:B:236:ASN:N	2.52	0.41
1:A:76:LYS:HG2	1:A:257:GLY:O	2.19	0.41
3:N:66:THR:H	3:N:69:ASP:CG	2.23	0.41
2:L:302:LYS:HE2	2:L:306:GLU:OE1	2.20	0.41
1:I:63:ALA:O	1:I:67:SER:N	2.52	0.41
2:J:391:VAL:HG23	2:J:392:HIS:CD2	2.54	0.41
2:J:84:LYS:HB2	2:J:145:ASP:HB2	2.01	0.41
1:I:51:LYS:HA	1:I:189:VAL:HG11	2.01	0.41
1:A:385:ASP:HA	1:A:388:ASP:OD2	2.19	0.41
3:G:107:ASN:HA	3:G:110:GLU:OE1	2.20	0.41
1:C:39:VAL:HG12	1:C:41:GLN:H	1.85	0.41
1:K:155:PRO:HG3	2:L:153:CYS:HB3	2.01	0.41
3:P:80:TYR:CD1	3:P:80:TYR:C	2.93	0.41
3:F:34:MET:O	3:F:122:VAL:HA	2.20	0.41
3:M:134:GLY:HA3	8:N:2290:SF4:S1	2.60	0.41
1:K:59:ILE:HG23	1:K:426:LYS:HD2	2.02	0.41
1:C:405:THR:OG1	1:C:408:GLU:HG3	2.20	0.41
1:A:381:PHE:CZ	6:A:6496:CFM:S2B	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:158:MET:HE1	3:F:195:LEU:HD11	2.02	0.41
3:H:100:ARG:NH1	3:H:100:ARG:HG3	2.34	0.41
1:I:350:ARG:HB3	1:I:375:VAL:HG11	2.00	0.41
1:C:259:ILE:CG2	1:C:260:SER:N	2.83	0.41
1:C:42:SER:C	1:C:44:LYS:N	2.74	0.41
3:E:38:CYS:HB2	3:E:126:VAL:HA	2.01	0.41
1:C:142:PHE:HE1	2:D:428:TRP:CZ2	2.38	0.41
3:M:246:LYS:O	3:M:250:ASN:HB2	2.20	0.41
3:G:172:ALA:HB1	3:G:255:ILE:HD13	2.01	0.41
2:J:442:MET:HG3	2:J:464:VAL:CG1	2.50	0.41
2:J:442:MET:HG3	2:J:464:VAL:HG12	2.01	0.41
3:O:139:ILE:HG23	3:O:177:VAL:HG11	2.01	0.41
1:A:378:GLY:HA3	1:A:401:TYR:CD2	2.54	0.41
2:D:458:LYS:HG2	2:D:462:PHE:CD2	2.55	0.41
3:E:23:VAL:C	3:E:25:ALA:N	2.73	0.41
1:A:240:ILE:O	1:A:244:GLU:HG3	2.20	0.41
3:H:49:LEU:O	3:H:50:HIS:HB2	2.20	0.41
3:H:40:PRO:HD2	3:H:127:LEU:HD13	2.03	0.41
3:H:127:LEU:HD23	3:H:127:LEU:C	2.41	0.41
3:M:32:LYS:HB2	3:M:119:LEU:HA	2.01	0.41
2:B:178:GLU:N	2:B:178:GLU:OE2	2.53	0.41
2:L:394:LEU:HD13	2:L:430:LEU:HB2	2.01	0.41
3:O:216:VAL:HG11	3:O:236:GLN:HB3	2.02	0.41
2:D:19:ASP:O	2:D:23:MET:HB2	2.19	0.41
1:A:42:SER:HB3	1:A:391:MET:CE	2.50	0.41
2:L:431:ARG:O	2:L:434:VAL:CG2	2.67	0.41
3:O:74:ASP:OD1	3:O:74:ASP:N	2.53	0.41
2:J:64:VAL:HG12	2:J:428:TRP:HB2	2.02	0.41
2:D:431:ARG:NH1	2:D:435:PHE:CE2	2.88	0.41
2:J:118:MET:HA	2:J:130:ASN:HD22	1.82	0.41
3:M:139:ILE:HG23	3:M:177:VAL:HG11	2.02	0.41
3:N:199:LEU:HD23	3:N:203:LEU:HD23	2.02	0.41
2:L:318:ILE:HG12	2:L:320:MET:HG3	2.01	0.41
2:L:279:GLU:H	2:L:279:GLU:CD	2.22	0.41
2:L:479:LEU:HA	2:L:479:LEU:HD23	1.85	0.41
3:E:24:ALA:HB2	3:E:226:THR:HG21	2.02	0.41
1:A:219:THR:HG23	1:A:248:ARG:NH2	2.36	0.41
3:G:140:ARG:HG3	3:G:171:TYR:CE1	2.56	0.41
3:O:23:VAL:C	3:O:25:ALA:N	2.73	0.41
2:D:260:VAL:HG22	2:D:260:VAL:O	2.19	0.41
3:G:195:LEU:HA	3:G:271:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:20:GLN:HE22	3:F:47:LEU:N	2.17	0.41
1:I:433:LYS:HE2	2:J:110:PRO:HD3	2.01	0.41
3:H:76:LEU:HD13	3:H:86:VAL:HG13	2.03	0.41
1:K:71:VAL:C	1:K:74:PRO:HD2	2.40	0.41
3:M:40:PRO:HG2	3:N:130:VAL:HG11	2.00	0.41
1:C:70:VAL:O	1:C:96:ARG:NH1	2.53	0.41
8:G:1290:SF4:S2	3:H:134:GLY:N	2.93	0.41
2:B:475:ASP:O	2:B:476:ARG:HG2	2.20	0.41
2:D:234:LEU:O	2:D:236:ASN:N	2.54	0.41
3:F:160:ALA:O	3:F:164:ILE:HG13	2.20	0.41
3:O:22:LEU:HD13	3:O:243:LEU:HD23	2.02	0.41
3:E:5:CYS:O	3:E:124:TYR:HD2	2.02	0.41
2:L:209:THR:O	2:L:213:MET:HG2	2.20	0.41
1:I:141:LEU:HB3	2:J:52:TYR:OH	2.19	0.41
1:I:458:ILE:O	1:I:459:PHE:C	2.58	0.41
2:B:262:ASP:CG	2:B:481:ARG:HH12	2.24	0.41
2:L:277:THR:HB	2:L:279:GLU:OE2	2.20	0.41
3:P:26:LEU:HA	3:P:26:LEU:HD12	1.82	0.41
1:I:297:TYR:HD2	1:I:299:PHE:CE1	2.38	0.41
1:I:302:PRO:HD3	1:I:456:PHE:CG	2.55	0.41
1:I:378:GLY:HA3	1:I:401:TYR:CD2	2.55	0.41
1:I:16:VAL:HG21	1:I:412:PHE:CE1	2.55	0.41
3:M:194:GLU:HA	3:M:197:ILE:CD1	2.50	0.41
3:O:191:ARG:HG2	3:O:194:GLU:OE2	2.20	0.41
3:O:194:GLU:O	3:O:197:ILE:HG13	2.21	0.41
3:E:117:ASP:O	3:E:118:ASP:C	2.59	0.41
2:B:441:PHE:CD1	2:B:465:PRO:HB2	2.55	0.41
1:C:239:ARG:NE	2:D:23:MET:CE	2.84	0.41
3:E:97:CYS:SG	3:E:134:GLY:HA2	2.61	0.41
1:I:370:LEU:O	1:I:372:MET:N	2.53	0.41
1:I:57:MET:HB3	2:J:142:TYR:OH	2.20	0.41
1:K:327:VAL:O	1:K:328:ILE:C	2.59	0.41
2:J:431:ARG:NH1	2:J:435:PHE:HE2	2.18	0.41
2:J:4:GLN:C	2:J:6:ASP:N	2.73	0.41
3:M:41:LYS:HD3	3:M:41:LYS:O	2.20	0.41
1:A:142:PHE:HE1	2:B:428:TRP:CZ2	2.39	0.41
2:D:354:MET:O	2:D:355:MET:C	2.58	0.41
2:L:456:LEU:O	2:L:459:GLY:N	2.52	0.41
3:P:124:TYR:O	3:P:126:VAL:HG23	2.21	0.41
1:C:21:PRO:O	1:C:22:GLU:C	2.58	0.41
3:E:231:ASP:OD1	3:E:233:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:192:GLU:O	3:E:195:LEU:HB3	2.20	0.41
2:J:450:PHE:O	2:J:452:GLN:N	2.53	0.41
3:G:14:GLY:O	3:G:15:LYS:C	2.58	0.41
3:E:15:LYS:HZ2	3:E:127:LEU:HA	1.84	0.41
1:C:370:LEU:O	1:C:372:MET:N	2.53	0.41
3:O:99:GLY:HA3	3:O:134:GLY:O	2.20	0.41
3:F:267:LEU:HD22	3:F:271:PHE:CE2	2.54	0.41
3:P:187:ARG:HB2	3:P:192:GLU:OE2	2.21	0.41
2:D:450:PHE:O	2:D:453:ARG:N	2.54	0.41
3:E:72:LEU:HD13	3:E:112:GLU:HB3	2.03	0.41
1:I:465:MET:HB2	2:L:363:HIS:CD2	2.56	0.41
3:H:153:GLY:O	3:H:154:GLU:HB2	2.19	0.41
2:D:379:LEU:HD21	2:D:443:ILE:CG2	2.51	0.41
2:B:122:ALA:HB1	2:B:126:GLY:O	2.21	0.41
1:C:302:PRO:HD3	1:C:456:PHE:CG	2.56	0.41
1:K:470:PRO:O	1:K:471:CYS:C	2.59	0.41
1:A:255:GLY:O	1:A:256:ASP:C	2.58	0.41
1:I:317:ASP:OD1	1:I:319:SER:HB3	2.20	0.41
1:A:462:ASP:O	1:A:463:MET:C	2.57	0.41
3:F:20:GLN:NE2	3:F:47:LEU:HB2	2.36	0.41
3:G:32:LYS:HB2	3:G:119:LEU:HA	2.01	0.41
3:G:76:LEU:HD13	3:G:86:VAL:HG13	2.02	0.41
3:E:166:LYS:HG2	3:E:258:PRO:HB3	2.02	0.41
2:D:369:LEU:HD11	2:D:376:VAL:HG13	2.02	0.41
1:I:239:ARG:HE	2:J:23:MET:CE	2.27	0.41
1:I:332:LYS:N	1:I:333:PRO:CD	2.82	0.41
2:J:330:MET:O	2:J:333:SER:N	2.54	0.41
1:K:57:MET:CE	2:L:113:CYS:N	2.84	0.41
3:P:103:ILE:CG2	3:P:104:THR:H	2.34	0.41
2:D:351:LEU:HD12	2:D:351:LEU:O	2.21	0.41
3:O:86:VAL:HG11	3:O:109:LEU:HD21	2.03	0.41
2:J:4:GLN:O	2:J:5:VAL:C	2.59	0.41
3:M:185:ASN:ND2	3:M:185:ASN:N	2.68	0.41
2:D:295:PRO:C	2:D:297:HIS:H	2.24	0.41
1:I:240:ILE:HG23	1:I:241:LEU:N	2.34	0.41
2:L:353:ASP:O	2:L:354:MET:C	2.57	0.41
1:K:240:ILE:HG23	1:K:241:LEU:N	2.34	0.41
3:E:246:LYS:O	3:E:250:ASN:HB2	2.21	0.41
1:A:81:ILE:HD13	1:A:114:PHE:HB3	2.03	0.41
1:A:155:PRO:O	1:A:159:ILE:HG12	2.20	0.41
1:A:351:VAL:HG13	1:A:420:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:409:PHE:O	1:I:413:VAL:HG23	2.21	0.41
1:A:297:TYR:HD2	1:A:299:PHE:CE1	2.38	0.41
3:H:122:VAL:HG13	3:H:122:VAL:O	2.21	0.41
2:J:303:LYS:HB2	2:J:303:LYS:NZ	2.35	0.41
1:A:435:GLY:HA3	1:A:475:LEU:HD22	2.03	0.41
1:I:164:GLU:CD	1:I:164:GLU:H	2.24	0.41
2:J:328:PHE:O	2:J:332:VAL:HG23	2.20	0.41
1:K:284:ARG:HG2	1:K:284:ARG:HH11	1.85	0.41
3:E:3:ARG:NH1	3:E:121:PHE:HZ	2.19	0.41
2:L:107:PHE:O	2:L:108:ARG:C	2.58	0.41
1:C:428:LYS:HA	1:C:438:PHE:CE1	2.55	0.41
2:D:369:LEU:CD1	2:D:376:VAL:HG13	2.51	0.41
1:A:124:VAL:HG12	1:A:125:PHE:CD1	2.56	0.41
1:A:289:LYS:HE3	1:A:290:TYR:OH	2.20	0.41
1:I:239:ARG:HG2	2:J:23:MET:SD	2.60	0.41
3:H:243:LEU:O	3:H:247:VAL:HG23	2.21	0.41
1:I:66:GLY:C	1:I:70:VAL:HB	2.39	0.41
3:H:67:VAL:C	3:H:69:ASP:N	2.72	0.41
3:F:67:VAL:N	3:F:69:ASP:OD2	2.52	0.41
2:L:233:TYR:HB2	2:L:236:ASN:ND2	2.36	0.41
2:J:64:VAL:CG1	2:J:428:TRP:HB2	2.51	0.41
1:I:144:LEU:HD11	2:J:43:VAL:HG21	2.02	0.41
2:D:365:LYS:HE2	2:D:501:ILE:HD13	2.03	0.41
1:K:428:LYS:HA	1:K:438:PHE:CE1	2.55	0.41
2:L:306:GLU:O	2:L:310:LYS:HA	2.21	0.41
3:M:175:GLY:O	3:M:178:ARG:NH2	2.48	0.41
2:J:323:ASP:O	2:J:326:ASP:HB2	2.20	0.41
2:B:331:LYS:O	2:B:335:ILE:HG13	2.21	0.41
3:E:102:VAL:O	3:E:106:ILE:HG13	2.20	0.41
2:J:124:VAL:HG23	2:J:125:PHE:N	2.36	0.41
1:I:299:PHE:HB3	1:I:452:GLY:H	1.85	0.41
1:K:364:ILE:O	1:K:365:GLY:C	2.58	0.41
1:A:11:SER:O	1:A:15:GLU:HG3	2.21	0.41
1:I:323:LYS:O	1:I:327:VAL:HG23	2.21	0.41
1:K:219:THR:HG23	1:K:248:ARG:NH2	2.36	0.41
3:P:148:TYR:CE1	3:P:180:GLY:HA3	2.56	0.41
1:I:165:SER:O	1:I:166:VAL:C	2.59	0.41
2:J:246:GLU:OE2	2:J:343:SER:HB2	2.20	0.41
3:N:33:VAL:HG12	3:N:34:MET:H	1.85	0.41
3:E:259:ILE:HG13	3:E:260:THR:N	2.35	0.41
3:F:127:LEU:HD23	3:F:129:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LYS:CB	3:E:119:LEU:HA	2.50	0.41
1:A:203:ARG:NH1	1:A:204:ASP:OD1	2.54	0.41
3:M:50:HIS:CE1	3:M:229:GLU:OE1	2.73	0.41
2:B:394:LEU:HD13	2:B:430:LEU:HB2	2.02	0.41
1:I:389:ARG:NH1	1:I:389:ARG:CG	2.78	0.41
1:C:253:TRP:HE3	1:C:279:MET:HE2	1.84	0.41
1:K:339:VAL:O	1:K:343:ARG:CB	2.65	0.41
1:I:339:VAL:O	1:I:343:ARG:CB	2.65	0.41
3:N:242:ALA:O	3:N:246:LYS:HG3	2.20	0.41
3:O:127:LEU:HB3	3:O:135:PHE:CE1	2.56	0.41
1:A:239:ARG:NH2	2:B:27:LYS:HB2	2.36	0.41
1:A:444:TRP:CE3	1:A:444:TRP:CA	3.04	0.41
1:A:66:GLY:C	1:A:70:VAL:HB	2.41	0.41
3:O:4:GLN:HG2	3:O:122:VAL:HG21	2.03	0.41
3:M:212:PRO:HG2	3:M:236:GLN:HE22	1.86	0.41
3:M:92:GLU:CD	3:N:170:LYS:HE3	2.40	0.41
2:L:369:LEU:CD1	2:L:376:VAL:HG13	2.51	0.41
3:F:66:THR:N	3:F:69:ASP:OD1	2.54	0.41
2:D:209:THR:O	2:D:213:MET:HG2	2.20	0.41
3:N:115:TYR:O	3:N:116:GLU:C	2.60	0.41
3:G:43:ASP:HB3	3:G:46:ARG:CZ	2.50	0.41
1:I:144:LEU:HD22	2:J:35:TYR:CD1	2.56	0.41
3:F:59:GLU:O	3:F:63:GLU:HG3	2.21	0.41
2:D:293:LEU:O	2:D:318:ILE:HA	2.21	0.41
2:D:359:HIS:CG	2:D:360:THR:H	2.38	0.41
1:I:92:SER:HB3	2:J:98:TYR:HE1	1.83	0.41
3:N:214:ASP:CG	3:N:216:VAL:HG12	2.40	0.41
3:O:57:ILE:CG1	3:O:75:VAL:HG11	2.50	0.41
2:L:228:PRO:HD2	2:L:254:LEU:O	2.21	0.41
1:C:155:PRO:HG3	2:D:153:CYS:HB3	2.01	0.41
3:O:172:ALA:HB1	3:O:255:ILE:HD13	2.02	0.41
1:A:62:CYS:O	1:A:63:ALA:C	2.57	0.41
3:O:173:ASN:HD22	3:O:173:ASN:N	2.18	0.41
3:E:21:ASN:HB3	3:E:240:TYR:CD1	2.55	0.41
2:D:200:MET:O	2:D:201:PHE:C	2.59	0.41
2:J:457:HIS:ND1	2:L:512:MET:HB3	2.35	0.41
3:O:100:ARG:HE	3:O:101:GLY:N	2.18	0.41
3:G:6:ALA:HB1	3:G:8:TYR:HE1	1.86	0.41
3:G:137:MET:HE2	3:G:141:GLU:CG	2.51	0.41
3:O:127:LEU:HD12	3:O:135:PHE:CZ	2.56	0.41
2:J:340:ILE:HD12	1:K:479:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:57:ILE:HG22	3:P:58:MET:N	2.36	0.41
3:H:103:ILE:CG2	3:H:104:THR:N	2.82	0.41
2:L:35:TYR:O	2:L:36:PRO:C	2.60	0.41
1:I:465:MET:CG	1:I:466:THR:N	2.84	0.41
2:B:389:GLU:O	2:B:391:VAL:HG13	2.21	0.41
3:F:5:CYS:O	3:F:123:PHE:HA	2.21	0.41
1:I:100:TYR:CE1	1:I:110:VAL:HB	2.56	0.41
1:A:351:VAL:HG22	1:A:420:LEU:HD22	2.03	0.41
2:J:283:ASP:O	2:J:285:PRO:N	2.54	0.41
1:C:134:LEU:HD23	1:C:134:LEU:C	2.41	0.41
1:C:85:PRO:CD	1:C:155:PRO:HG2	2.51	0.41
1:I:385:ASP:HA	1:I:388:ASP:OD2	2.20	0.41
1:K:39:VAL:HG12	1:K:41:GLN:H	1.86	0.41
3:O:38:CYS:CB	3:O:126:VAL:HG22	2.51	0.41
1:K:435:GLY:CA	1:K:475:LEU:HD22	2.51	0.41
1:K:83:HIS:CD2	1:K:156:ILE:HG12	2.56	0.41
3:N:228:ILE:HD13	3:N:228:ILE:HA	1.93	0.41
3:M:36:VAL:HA	3:M:86:VAL:HG23	2.02	0.40
3:F:49:LEU:O	3:F:50:HIS:CB	2.70	0.40
3:O:282:VAL:HG23	3:O:283:GLY:N	2.37	0.40
2:L:131:MET:HG2	2:L:165:PHE:HB3	2.03	0.40
3:H:208:ILE:HG23	3:H:209:HIS:H	1.86	0.40
1:C:71:VAL:C	1:C:74:PRO:HD2	2.41	0.40
3:O:212:PRO:HG3	3:O:239:GLU:HG3	2.02	0.40
1:I:265:THR:N	1:I:266:PRO:CD	2.84	0.40
1:A:383:HIS:O	1:A:386:ASP:HB2	2.20	0.40
2:D:36:PRO:O	2:D:37:GLN:C	2.58	0.40
2:D:297:HIS:O	2:D:297:HIS:CD2	2.74	0.40
1:A:83:HIS:CD2	1:A:156:ILE:HG12	2.55	0.40
1:I:101:ILE:HG12	1:I:236:TRP:CZ2	2.56	0.40
3:O:206:GLN:OE1	3:O:252:LEU:HD23	2.21	0.40
2:D:495:THR:O	2:D:496:THR:C	2.58	0.40
2:D:449:LYS:HB2	2:D:449:LYS:HE3	1.90	0.40
3:G:199:LEU:O	3:G:199:LEU:HD23	2.21	0.40
3:O:184:CYS:SG	3:O:210:PHE:CE1	3.11	0.40
3:N:55:ASN:HD22	3:N:77:LYS:NZ	2.19	0.40
3:P:76:LEU:CD1	3:P:86:VAL:HG13	2.51	0.40
1:K:253:TRP:HA	1:K:254:SER:HA	1.65	0.40
1:K:73:GLY:N	1:K:74:PRO:CD	2.83	0.40
1:A:59:ILE:CD1	1:A:59:ILE:N	2.80	0.40
1:I:65:ALA:O	1:I:70:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:TRP:O	2:D:310:LYS:HB2	2.22	0.40
1:K:350:ARG:HA	1:K:373:GLU:O	2.21	0.40
1:A:413:VAL:HG21	1:A:431:PHE:CE1	2.56	0.40
2:D:318:ILE:HG23	2:D:318:ILE:O	2.21	0.40
3:N:158:MET:CE	3:N:195:LEU:HD11	2.51	0.40
3:P:199:LEU:CD2	3:P:203:LEU:HD23	2.51	0.40
2:L:468:ARG:HD2	2:L:476:ARG:HG3	2.01	0.40
3:M:26:LEU:HB3	3:M:31:LYS:HB2	2.04	0.40
3:M:187:ARG:O	3:M:188:ASN:HB2	2.21	0.40
3:M:57:ILE:HG12	3:M:75:VAL:HG21	2.03	0.40
1:K:134:LEU:C	1:K:134:LEU:HD23	2.42	0.40
3:H:26:LEU:HD12	3:H:26:LEU:HA	1.84	0.40
3:O:251:LYS:HE3	3:O:251:LYS:HB3	1.92	0.40
2:D:84:LYS:HB2	2:D:145:ASP:HB2	2.03	0.40
2:D:84:LYS:HA	2:D:272:TYR:CD1	2.56	0.40
3:M:140:ARG:HG3	3:M:171:TYR:CE1	2.56	0.40
1:C:390:THR:O	1:C:392:LYS:N	2.54	0.40
2:J:105:ARG:HB3	2:J:474:PHE:CD1	2.56	0.40
1:A:364:ILE:O	1:A:365:GLY:C	2.59	0.40
3:N:261:MET:O	3:N:265:GLU:HG3	2.20	0.40
2:D:323:ASP:O	2:D:326:ASP:HB2	2.22	0.40
1:C:251:ALA:HB2	1:C:261:GLU:O	2.22	0.40
3:G:63:GLU:HB3	3:G:64:ALA:H	1.73	0.40
3:G:183:ILE:HG12	3:G:208:ILE:CG2	2.52	0.40
3:M:195:LEU:HD12	3:M:267:LEU:CD2	2.51	0.40
3:P:206:GLN:HG2	3:P:252:LEU:HD13	2.03	0.40
3:N:40:PRO:HD2	3:N:127:LEU:HD13	2.03	0.40
3:M:229:GLU:O	3:N:285:THR:HG22	2.22	0.40
2:B:442:MET:HG3	2:B:464:VAL:HG12	2.04	0.40
1:A:343:ARG:N	1:A:344:PRO:CD	2.85	0.40
1:K:339:VAL:CG1	1:K:343:ARG:HB2	2.50	0.40
1:K:358:LEU:HD11	1:K:362:HIS:CE1	2.56	0.40
1:C:368:GLU:C	1:C:370:LEU:H	2.24	0.40
2:J:71:GLN:HA	2:J:193:HIS:HA	2.04	0.40
3:H:158:MET:HE1	3:H:195:LEU:HD11	2.02	0.40
2:B:194:VAL:HG23	2:B:195:THR:N	2.36	0.40
2:B:59:ARG:HD3	2:B:62:LEU:HD23	2.03	0.40
2:B:351:LEU:O	2:B:351:LEU:HD12	2.21	0.40
3:F:199:LEU:O	3:F:203:LEU:HD23	2.20	0.40
2:J:226:ILE:O	2:J:253:LEU:HD12	2.21	0.40
3:E:57:ILE:HD12	3:E:105:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:130:VAL:O	3:P:131:VAL:C	2.59	0.40
2:J:21:LYS:HB3	2:J:21:LYS:HE2	1.87	0.40
1:K:222:ASP:HA	1:K:248:ARG:O	2.21	0.40
2:L:333:SER:O	2:L:334:GLU:C	2.60	0.40
1:C:107:ASN:HD21	2:D:34:LYS:HE2	1.86	0.40
1:I:308:SER:O	1:I:312:ILE:HG13	2.21	0.40
2:L:190:VAL:O	2:L:191:GLY:O	2.40	0.40
1:C:165:SER:O	1:C:166:VAL:C	2.60	0.40
3:M:63:GLU:HB3	3:M:64:ALA:H	1.75	0.40
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.95	0.40
3:G:278:ASP:OD1	3:G:281:ILE:HB	2.22	0.40
3:G:283:GLY:O	3:H:225:MET:SD	2.79	0.40
3:G:36:VAL:HA	3:G:86:VAL:HG23	2.02	0.40
1:K:253:TRP:CZ3	1:K:282:ILE:HG12	2.56	0.40
1:K:119:GLN:O	1:K:120:GLU:C	2.58	0.40
1:K:124:VAL:HG12	1:K:125:PHE:CD1	2.56	0.40
3:G:137:MET:HE1	3:G:138:PRO:HA	2.03	0.40
1:C:444:TRP:CE3	1:C:444:TRP:CA	3.04	0.40
3:E:212:PRO:HG3	3:E:239:GLU:HG3	2.04	0.40
3:F:60:MET:CE	3:F:75:VAL:HG22	2.48	0.40
3:N:59:GLU:O	3:N:63:GLU:HG3	2.21	0.40
2:D:70:CYS:SG	2:D:72:PRO:CG	3.09	0.40
3:O:41:LYS:O	3:O:42:ALA:HB3	2.21	0.40
3:H:199:LEU:CD2	3:H:203:LEU:HD23	2.50	0.40
2:J:400:LYS:HZ3	3:N:112:GLU:CD	2.25	0.40
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.91	0.40
2:L:4:GLN:O	2:L:5:VAL:C	2.60	0.40
2:L:21:LYS:HB3	2:L:21:LYS:HE2	1.92	0.40
2:B:279:GLU:CD	2:B:279:GLU:H	2.18	0.40
2:L:283:ASP:C	2:L:285:PRO:HD2	2.42	0.40
3:G:102:VAL:O	3:G:106:ILE:HG13	2.22	0.40
2:J:359:HIS:O	2:J:362:LEU:N	2.55	0.40
3:H:269:MET:HB3	3:H:274:MET:HE3	2.04	0.40
1:I:297:TYR:HD2	1:I:299:PHE:CD1	2.40	0.40
1:I:163:ILE:O	1:I:164:GLU:C	2.60	0.40
2:J:425:LYS:HA	2:J:425:LYS:HD3	1.96	0.40
3:H:215:ASN:C	3:H:217:VAL:N	2.74	0.40
1:K:63:ALA:O	1:K:67:SER:N	2.53	0.40
1:K:72:TRP:CZ2	1:K:202:VAL:HG22	2.57	0.40
2:D:328:PHE:O	2:D:332:VAL:HG23	2.21	0.40
3:E:206:GLN:OE1	3:E:252:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:256:ASP:CG	1:K:256:ASP:O	2.60	0.40
3:G:50:HIS:CE1	3:G:229:GLU:OE1	2.72	0.40
3:E:202:LYS:HE3	3:E:202:LYS:HB3	1.90	0.40
3:E:100:ARG:HE	3:E:101:GLY:N	2.20	0.40
3:E:278:ASP:CG	3:E:281:ILE:HD12	2.42	0.40
3:P:221:GLU:O	3:P:224:ARG:N	2.48	0.40
3:G:117:ASP:O	3:G:118:ASP:C	2.60	0.40
3:G:161:ALA:HA	3:G:164:ILE:HD12	2.03	0.40
3:M:99:GLY:HA3	3:M:134:GLY:C	2.42	0.40
3:O:216:VAL:HG22	3:O:227:VAL:HG13	2.03	0.40
1:I:405:THR:HG23	1:I:408:GLU:CD	2.41	0.40
1:I:346:LEU:HB3	1:I:372:MET:SD	2.61	0.40
2:D:221:ASN:O	2:D:222:LYS:HB2	2.22	0.40
1:K:199:ASN:O	1:K:200:ASP:C	2.59	0.40
2:J:4:GLN:O	2:J:7:LYS:N	2.51	0.40
3:E:22:LEU:HD13	3:E:243:LEU:HD23	2.03	0.40
2:L:36:PRO:O	2:L:37:GLN:C	2.58	0.40
2:L:71:GLN:OE1	2:L:186:THR:HA	2.22	0.40
2:L:348:ARG:O	2:L:350:ARG:N	2.54	0.40
1:A:113:ASN:HD22	2:B:66:PRO:HD2	1.86	0.40
1:K:8:GLU:O	1:K:11:SER:HB3	2.21	0.40
3:N:43:ASP:OD1	3:N:43:ASP:N	2.54	0.40
2:J:449:LYS:HB2	2:J:449:LYS:HE3	1.91	0.40
2:J:199:ASN:O	2:J:200:MET:C	2.57	0.40
1:C:208:GLY:HA2	1:C:211:ASP:OD1	2.21	0.40
2:L:446:SER:C	2:L:448:GLY:N	2.75	0.40
2:L:359:HIS:CG	2:L:360:THR:N	2.90	0.40
3:M:24:ALA:HB2	3:M:226:THR:HG21	2.02	0.40
1:C:449:PRO:O	1:C:450:TYR:HD1	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	475/491 (97%)	364 (77%)	96 (20%)	15 (3%)	5 33
1	C	475/491 (97%)	358 (75%)	102 (22%)	15 (3%)	5 33
1	I	475/491 (97%)	357 (75%)	104 (22%)	14 (3%)	6 36
1	K	475/491 (97%)	364 (77%)	99 (21%)	12 (2%)	7 41
2	B	520/522 (100%)	423 (81%)	74 (14%)	23 (4%)	3 24
2	D	520/522 (100%)	417 (80%)	82 (16%)	21 (4%)	4 27
2	J	520/522 (100%)	421 (81%)	74 (14%)	25 (5%)	3 22
2	L	520/522 (100%)	423 (81%)	75 (14%)	22 (4%)	3 26
3	E	284/289 (98%)	219 (77%)	50 (18%)	15 (5%)	2 19
3	F	287/289 (99%)	228 (79%)	43 (15%)	16 (6%)	2 18
3	G	284/289 (98%)	221 (78%)	47 (16%)	16 (6%)	2 18
3	H	287/289 (99%)	224 (78%)	50 (17%)	13 (4%)	3 24
3	M	284/289 (98%)	223 (78%)	47 (16%)	14 (5%)	3 22
3	N	287/289 (99%)	230 (80%)	44 (15%)	13 (4%)	3 24
3	O	284/289 (98%)	221 (78%)	48 (17%)	15 (5%)	2 19
3	P	287/289 (99%)	228 (79%)	45 (16%)	14 (5%)	3 22
All	All	6264/6364 (98%)	4921 (79%)	1080 (17%)	263 (4%)	3 26

All (263) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
2	B	296	TRP
1	C	22	GLU
3	E	118	ASP
3	E	208	ILE
3	E	224	ARG
3	E	282	VAL
3	F	131	VAL
3	G	118	ASP
3	G	208	ILE
3	G	224	ARG
3	G	282	VAL
3	H	131	VAL
1	I	22	GLU
2	J	296	TRP
1	K	22	GLU

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Mol	Chain	Res	Type
3	M	118	ASP
3	M	208	ILE
3	M	224	ARG
3	M	282	VAL
3	N	131	VAL
3	O	118	ASP
3	O	208	ILE
3	O	224	ARG
3	O	282	VAL
3	P	131	VAL
1	A	43	LYS
1	A	87	GLY
1	A	207	LEU
1	A	345	ARG
2	B	5	VAL
2	B	38	ASP
2	B	117	SER
2	B	159	GLY
2	B	207	TYR
1	C	43	LYS
1	C	87	GLY
1	C	391	MET
1	C	428	LYS
2	D	5	VAL
2	D	38	ASP
2	D	117	SER
2	D	159	GLY
2	D	207	TYR
2	D	212	SER
2	D	296	TRP
3	E	283	GLY
3	F	43	ASP
3	F	67	VAL
3	F	116	GLU
3	F	279	GLU
3	G	283	GLY
3	H	43	ASP
3	H	67	VAL
3	H	116	GLU
3	H	170	LYS
3	H	279	GLU
1	I	43	LYS

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Mol	Chain	Res	Type
1	I	87	GLY
1	I	345	ARG
1	I	428	LYS
2	J	5	VAL
2	J	38	ASP
2	J	117	SER
2	J	159	GLY
2	J	207	TYR
1	K	43	LYS
1	K	87	GLY
1	K	428	LYS
2	L	5	VAL
2	L	38	ASP
2	L	117	SER
2	L	121	ASP
2	L	159	GLY
2	L	207	TYR
2	L	296	TRP
3	N	43	ASP
3	N	67	VAL
3	N	116	GLU
3	N	117	ASP
3	N	279	GLU
3	O	155	MET
3	O	283	GLY
3	P	43	ASP
3	P	67	VAL
3	P	116	GLU
3	P	117	ASP
3	P	172	ALA
3	P	279	GLU
1	A	428	LYS
2	B	11	SER
2	B	121	ASP
2	B	212	SER
2	B	235	GLY
2	B	255	SER
2	B	497	LEU
1	C	207	LEU
1	C	345	ARG
2	D	11	SER
2	D	15	PHE

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Mol	Chain	Res	Type
2	D	121	ASP
2	D	235	GLY
2	D	255	SER
3	E	93	PRO
3	E	155	MET
3	E	209	HIS
3	E	284	LYS
3	F	88	SER
3	F	117	ASP
3	F	170	LYS
3	F	172	ALA
3	G	93	PRO
3	G	155	MET
3	G	180	GLY
3	G	186	SER
3	G	209	HIS
3	G	279	GLU
3	H	64	ALA
3	H	117	ASP
1	I	94	ALA
1	I	207	LEU
1	I	391	MET
2	J	11	SER
2	J	121	ASP
2	J	155	ALA
2	J	176	PRO
2	J	255	SER
2	J	497	LEU
1	K	207	LEU
1	K	345	ARG
1	K	391	MET
2	L	11	SER
2	L	189	PHE
2	L	191	GLY
2	L	212	SER
2	L	255	SER
3	M	93	PRO
3	M	155	MET
3	M	180	GLY
3	M	186	SER
3	M	209	HIS
3	M	279	GLU

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Mol	Chain	Res	Type
3	N	64	ALA
3	N	170	LYS
3	N	172	ALA
3	O	68	GLU
3	O	93	PRO
3	O	279	GLU
3	O	284	LYS
3	P	170	LYS
2	B	176	PRO
2	B	189	PHE
1	C	94	ALA
2	D	189	PHE
3	E	180	GLY
3	E	186	SER
3	E	279	GLU
3	G	174	SER
3	H	42	ALA
3	H	58	MET
3	H	68	GLU
3	H	172	ALA
1	I	117	ASP
2	J	15	PHE
2	J	154	MET
2	J	212	SER
2	J	235	GLY
2	J	498	VAL
2	J	514	ALA
1	K	165	SER
1	K	464	ASP
2	L	155	ALA
2	L	176	PRO
2	L	497	LEU
2	L	514	ALA
3	M	174	SER
3	N	42	ALA
3	N	68	GLU
3	N	88	SER
3	O	174	SER
3	O	180	GLY
3	O	186	SER
3	O	209	HIS
3	P	64	ALA

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Mol	Chain	Res	Type
1	A	35	ASN
1	A	165	SER
1	A	166	VAL
1	A	391	MET
2	B	154	MET
2	B	155	ALA
2	B	199	ASN
2	B	514	ALA
1	C	99	TYR
2	D	155	ALA
2	D	497	LEU
2	D	514	ALA
3	E	174	SER
3	F	58	MET
3	F	64	ALA
3	F	68	GLU
1	I	35	ASN
1	I	356	GLY
2	J	199	ASN
2	J	360	THR
2	L	154	MET
3	M	53	ALA
3	M	230	TYR
3	M	283	GLY
3	O	53	ALA
3	P	42	ALA
3	P	68	GLU
1	A	167	SER
1	A	169	VAL
2	B	191	GLY
2	B	373	PRO
2	B	498	VAL
1	C	117	ASP
2	D	154	MET
2	D	176	PRO
2	D	360	THR
3	F	42	ALA
3	G	53	ALA
2	J	189	PHE
2	J	373	PRO
1	K	169	VAL
2	L	373	PRO

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Mol	Chain	Res	Type
1	A	371	GLY
1	C	169	VAL
3	F	93	PRO
3	G	65	GLY
1	K	166	VAL
1	C	160	GLY
2	D	498	VAL
3	F	137	MET
2	J	284	ALA
2	J	390	PRO
1	K	37	PRO
3	P	93	PRO
1	A	37	PRO
1	A	356	GLY
1	C	37	PRO
1	C	166	VAL
2	D	373	PRO
3	E	259	ILE
3	G	258	PRO
3	H	130	VAL
2	L	349	GLY
2	L	498	VAL
3	P	137	MET
2	B	390	PRO
2	B	451	ILE
1	C	356	GLY
3	E	65	GLY
3	F	130	VAL
1	I	166	VAL
1	I	169	VAL
2	J	191	GLY
2	L	284	ALA
3	N	130	VAL
3	P	130	VAL
3	G	96	GLY
1	I	37	PRO
2	L	235	GLY

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/414 (98%)	390 (96%)	17 (4%)	36	75
1	C	407/414 (98%)	390 (96%)	17 (4%)	36	75
1	I	407/414 (98%)	391 (96%)	16 (4%)	39	78
1	K	407/414 (98%)	392 (96%)	15 (4%)	41	79
2	B	454/454 (100%)	439 (97%)	15 (3%)	45	81
2	D	454/454 (100%)	438 (96%)	16 (4%)	43	80
2	J	454/454 (100%)	438 (96%)	16 (4%)	43	80
2	L	454/454 (100%)	438 (96%)	16 (4%)	43	80
3	E	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	F	233/233 (100%)	216 (93%)	17 (7%)	17	57
3	G	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	H	233/233 (100%)	216 (93%)	17 (7%)	17	57
3	M	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	N	233/233 (100%)	215 (92%)	18 (8%)	16	54
3	O	230/233 (99%)	214 (93%)	16 (7%)	19	58
3	P	233/233 (100%)	216 (93%)	17 (7%)	17	57
All	All	5296/5336 (99%)	5035 (95%)	261 (5%)	31	72

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	35	ASN
1	A	49	ASN
1	A	59	ILE
1	A	77	ASP
1	A	98	ASN
1	A	109	PHE
1	A	128	ASP
1	A	145	ASN
1	A	161	ASP
1	A	204	ASP
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	362	HIS
1	A	372	MET
1	A	444	TRP
1	A	445	ASP
2	B	4	GLN
2	B	19	ASP
2	B	23	MET
2	B	45	GLN
2	B	172	GLU
2	B	178	GLU
2	B	202	GLU
2	B	222	LYS
2	B	252	SER
2	B	258	GLU
2	B	263	THR
2	B	268	GLN
2	B	391	VAL
2	B	454	ASP
2	B	483	THR
1	C	5	SER
1	C	49	ASN
1	C	77	ASP
1	C	88	CYS
1	C	98	ASN
1	C	109	PHE
1	C	128	ASP
1	C	161	ASP
1	C	204	ASP
1	C	219	THR
1	C	271	ASN
1	C	277	ARG
1	C	362	HIS
1	C	372	MET
1	C	401	TYR
1	C	444	TRP
1	C	445	ASP
2	D	4	GLN
2	D	19	ASP
2	D	23	MET
2	D	45	GLN
2	D	172	GLU

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Mol	Chain	Res	Type
2	D	178	GLU
2	D	202	GLU
2	D	222	LYS
2	D	252	SER
2	D	258	GLU
2	D	263	THR
2	D	268	GLN
2	D	270	ARG
2	D	391	VAL
2	D	454	ASP
2	D	483	THR
3	E	20	GLN
3	E	28	GLU
3	E	52	LYS
3	E	58	MET
3	E	74	ASP
3	E	93	PRO
3	E	100	ARG
3	E	129	ASP
3	E	137	MET
3	E	173	ASN
3	E	190	ASP
3	E	197	ILE
3	E	202	LYS
3	E	261	MET
3	E	262	ASP
3	E	278	ASP
3	F	68	GLU
3	F	69	ASP
3	F	70	LEU
3	F	72	LEU
3	F	74	ASP
3	F	77	LYS
3	F	85	CYS
3	F	100	ARG
3	F	116	GLU
3	F	162	ASN
3	F	187	ARG
3	F	202	LYS
3	F	206	GLN
3	F	223	ARG
3	F	261	MET

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Mol	Chain	Res	Type
3	F	262	ASP
3	F	270	GLU
3	G	20	GLN
3	G	28	GLU
3	G	52	LYS
3	G	58	MET
3	G	74	ASP
3	G	93	PRO
3	G	100	ARG
3	G	129	ASP
3	G	137	MET
3	G	173	ASN
3	G	185	ASN
3	G	190	ASP
3	G	197	ILE
3	G	261	MET
3	G	262	ASP
3	G	278	ASP
3	H	68	GLU
3	H	69	ASP
3	H	70	LEU
3	H	72	LEU
3	H	74	ASP
3	H	77	LYS
3	H	85	CYS
3	H	100	ARG
3	H	116	GLU
3	H	162	ASN
3	H	187	ARG
3	H	202	LYS
3	H	206	GLN
3	H	223	ARG
3	H	261	MET
3	H	262	ASP
3	H	270	GLU
1	I	5	SER
1	I	49	ASN
1	I	77	ASP
1	I	88	CYS
1	I	98	ASN
1	I	109	PHE
1	I	128	ASP

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Mol	Chain	Res	Type
1	I	161	ASP
1	I	204	ASP
1	I	271	ASN
1	I	277	ARG
1	I	360	PRO
1	I	362	HIS
1	I	372	MET
1	I	444	TRP
1	I	445	ASP
2	J	4	GLN
2	J	19	ASP
2	J	23	MET
2	J	45	GLN
2	J	172	GLU
2	J	178	GLU
2	J	202	GLU
2	J	222	LYS
2	J	252	SER
2	J	258	GLU
2	J	263	THR
2	J	268	GLN
2	J	391	VAL
2	J	454	ASP
2	J	483	THR
2	J	506	ASP
1	K	5	SER
1	K	49	ASN
1	K	77	ASP
1	K	98	ASN
1	K	109	PHE
1	K	128	ASP
1	K	161	ASP
1	K	204	ASP
1	K	271	ASN
1	K	277	ARG
1	K	362	HIS
1	K	372	MET
1	K	401	TYR
1	K	444	TRP
1	K	445	ASP
2	L	4	GLN
2	L	19	ASP

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Mol	Chain	Res	Type
2	L	23	MET
2	L	45	GLN
2	L	172	GLU
2	L	178	GLU
2	L	202	GLU
2	L	222	LYS
2	L	252	SER
2	L	258	GLU
2	L	263	THR
2	L	268	GLN
2	L	391	VAL
2	L	454	ASP
2	L	483	THR
2	L	506	ASP
3	M	20	GLN
3	M	28	GLU
3	M	52	LYS
3	M	58	MET
3	M	74	ASP
3	M	100	ARG
3	M	129	ASP
3	M	137	MET
3	M	173	ASN
3	M	185	ASN
3	M	190	ASP
3	M	197	ILE
3	M	202	LYS
3	M	261	MET
3	M	262	ASP
3	M	278	ASP
3	N	68	GLU
3	N	69	ASP
3	N	70	LEU
3	N	72	LEU
3	N	74	ASP
3	N	77	LYS
3	N	85	CYS
3	N	100	ARG
3	N	116	GLU
3	N	162	ASN
3	N	187	ARG
3	N	202	LYS

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Mol	Chain	Res	Type
3	N	206	GLN
3	N	223	ARG
3	N	225	MET
3	N	261	MET
3	N	262	ASP
3	N	270	GLU
3	O	20	GLN
3	O	28	GLU
3	O	52	LYS
3	O	58	MET
3	O	74	ASP
3	O	100	ARG
3	O	129	ASP
3	O	137	MET
3	O	173	ASN
3	O	185	ASN
3	O	190	ASP
3	O	197	ILE
3	O	202	LYS
3	O	261	MET
3	O	262	ASP
3	O	278	ASP
3	P	68	GLU
3	P	69	ASP
3	P	70	LEU
3	P	72	LEU
3	P	74	ASP
3	P	77	LYS
3	P	85	CYS
3	P	100	ARG
3	P	116	GLU
3	P	162	ASN
3	P	187	ARG
3	P	202	LYS
3	P	206	GLN
3	P	223	ARG
3	P	261	MET
3	P	262	ASP
3	P	270	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	35	ASN
1	A	49	ASN
1	A	83	HIS
1	A	113	ASN
1	A	274	HIS
1	A	432	GLN
2	B	37	GLN
2	B	45	GLN
2	B	104	ASN
2	B	128	GLN
2	B	137	ASN
2	B	168	ASN
2	B	268	GLN
2	B	278	GLN
2	B	286	ASN
2	B	499	ASN
2	B	513	GLN
2	B	518	ASN
1	C	14	GLN
1	C	35	ASN
1	C	49	ASN
1	C	113	ASN
1	C	271	ASN
1	C	274	HIS
1	C	432	GLN
2	D	37	GLN
2	D	45	GLN
2	D	104	ASN
2	D	128	GLN
2	D	137	ASN
2	D	268	GLN
2	D	278	GLN
2	D	286	ASN
2	D	478	HIS
2	D	499	ASN
2	D	513	GLN
2	D	519	HIS
3	E	50	HIS
3	E	107	ASN
3	E	162	ASN
3	E	173	ASN
3	E	185	ASN

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Mol	Chain	Res	Type
3	E	188	ASN
3	F	20	GLN
3	F	50	HIS
3	F	54	GLN
3	F	55	ASN
3	F	142	ASN
3	F	145	GLN
3	F	162	ASN
3	F	163	ASN
3	F	185	ASN
3	F	201	ASN
3	G	50	HIS
3	G	107	ASN
3	G	162	ASN
3	G	173	ASN
3	G	185	ASN
3	G	188	ASN
3	H	20	GLN
3	H	50	HIS
3	H	55	ASN
3	H	142	ASN
3	H	145	GLN
3	H	162	ASN
3	H	163	ASN
3	H	185	ASN
3	H	201	ASN
1	I	14	GLN
1	I	35	ASN
1	I	49	ASN
1	I	83	HIS
1	I	107	ASN
1	I	113	ASN
1	I	271	ASN
1	I	432	GLN
2	J	37	GLN
2	J	45	GLN
2	J	104	ASN
2	J	128	GLN
2	J	137	ASN
2	J	268	GLN
2	J	278	GLN
2	J	286	ASN

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Mol	Chain	Res	Type
2	J	294	GLN
2	J	478	HIS
2	J	499	ASN
2	J	513	GLN
2	J	518	ASN
2	J	519	HIS
1	K	14	GLN
1	K	35	ASN
1	K	49	ASN
1	K	107	ASN
1	K	113	ASN
1	K	432	GLN
2	L	37	GLN
2	L	45	GLN
2	L	104	ASN
2	L	128	GLN
2	L	137	ASN
2	L	268	GLN
2	L	278	GLN
2	L	286	ASN
2	L	499	ASN
2	L	513	GLN
2	L	519	HIS
3	M	50	HIS
3	M	107	ASN
3	M	162	ASN
3	M	173	ASN
3	M	185	ASN
3	M	188	ASN
3	M	236	GLN
3	N	20	GLN
3	N	50	HIS
3	N	54	GLN
3	N	55	ASN
3	N	142	ASN
3	N	145	GLN
3	N	162	ASN
3	N	185	ASN
3	N	201	ASN
3	O	50	HIS
3	O	107	ASN
3	O	162	ASN

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Mol	Chain	Res	Type
3	O	173	ASN
3	O	185	ASN
3	O	188	ASN
3	O	236	GLN
3	P	20	GLN
3	P	50	HIS
3	P	54	GLN
3	P	55	ASN
3	P	142	ASN
3	P	145	GLN
3	P	162	ASN
3	P	185	ASN
3	P	201	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
5	HCA	A	6494	6	4,13,13	2.98	2 (50%)	3,18,18	1.71	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CFM	A	6496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	A	6498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
5	HCA	C	7494	6	4,13,13	3.22	1 (25%)	3,18,18	2.05	1 (33%)
6	CFM	C	7496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	D	7498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	SF4	E	290	3	0,12,12	0.00	-	0,24,24	0.00	-
8	SF4	G	1290	3	0,12,12	0.00	-	0,24,24	0.00	-
5	HCA	I	8494	6	4,13,13	2.43	2 (50%)	3,18,18	1.67	1 (33%)
6	CFM	I	8496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	J	8498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
5	HCA	K	9494	6	4,13,13	3.14	2 (50%)	3,18,18	2.23	1 (33%)
6	CFM	K	9496	1,5	0,24,24	0.00	-	0,45,45	0.00	-
7	CLF	K	9498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
8	SF4	N	2290	3	0,12,12	0.00	-	0,24,24	0.00	-
8	SF4	P	3290	3	0,12,12	0.00	-	0,24,24	0.00	-

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
5	HCA	A	6494	6	-	0/7/17/17	0/0/0/0
6	CFM	A	6496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	A	6498	1,2	-	0/0/132/132	0/12/10/10
5	HCA	C	7494	6	-	0/7/17/17	0/0/0/0
6	CFM	C	7496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	D	7498	1,2	-	0/0/132/132	0/12/10/10
8	SF4	E	290	3	-	0/0/48/48	0/6/5/5
8	SF4	G	1290	3	-	0/0/48/48	0/6/5/5
5	HCA	I	8494	6	-	0/7/17/17	0/0/0/0
6	CFM	I	8496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	J	8498	1,2	-	0/0/132/132	0/12/10/10
5	HCA	K	9494	6	-	0/7/17/17	0/0/0/0
6	CFM	K	9496	1,5	-	0/0/84/84	0/0/8/8
7	CLF	K	9498	1,2	-	0/0/132/132	0/12/10/10
8	SF4	N	2290	3	-	0/0/48/48	0/6/5/5
8	SF4	P	3290	3	-	0/0/48/48	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6494	HCA	C2-C3	-3.84	1.48	1.54
5	K	9494	HCA	C2-C3	-2.85	1.50	1.54
5	I	8494	HCA	C2-C3	-2.14	1.51	1.54
5	I	8494	HCA	O7-C3	4.33	1.50	1.43
5	A	6494	HCA	O7-C3	4.36	1.50	1.43
5	K	9494	HCA	O7-C3	5.53	1.52	1.43
5	C	7494	HCA	O7-C3	6.08	1.53	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	9494	HCA	C3-C2-C1	-3.75	108.96	114.96
5	C	7494	HCA	C3-C2-C1	-3.53	109.32	114.96
5	I	8494	HCA	C3-C2-C1	-2.87	110.38	114.96
5	A	6494	HCA	C3-C2-C1	-2.84	110.41	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	6494	HCA	1	0
6	A	6496	CFM	7	0
7	A	6498	CLF	4	0
5	C	7494	HCA	1	0
6	C	7496	CFM	5	0
7	D	7498	CLF	3	0
8	E	290	SF4	2	0
8	G	1290	SF4	2	0
5	I	8494	HCA	1	0
6	I	8496	CFM	3	0
7	J	8498	CLF	3	0
5	K	9494	HCA	1	0
6	K	9496	CFM	3	0
7	K	9498	CLF	3	0
8	N	2290	SF4	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.