



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:33 PM GMT

PDB ID : 1G21
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 3.00 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

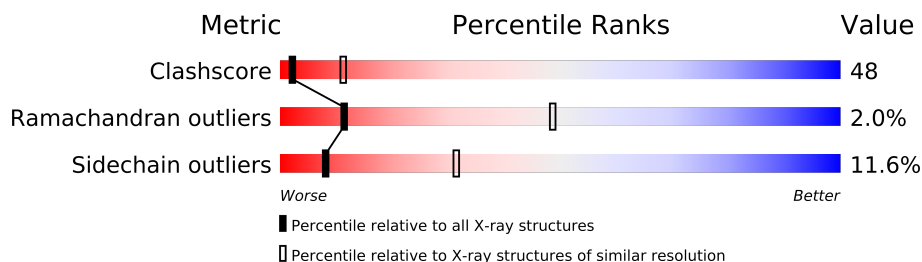
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24237 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

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

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

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

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

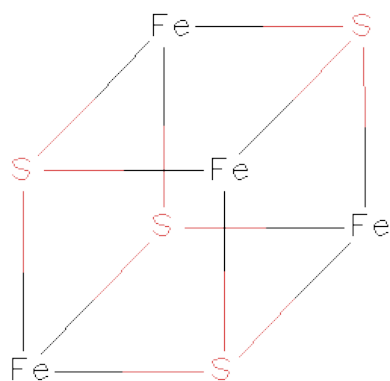
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

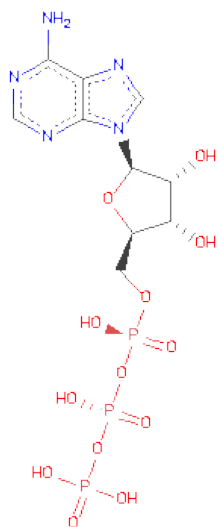
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



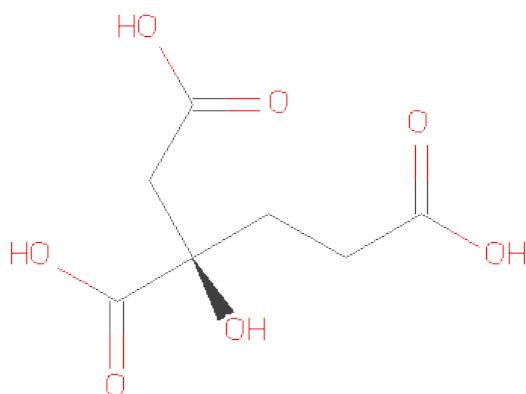
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	Fe	S	0	0
			8	4	4		
6	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



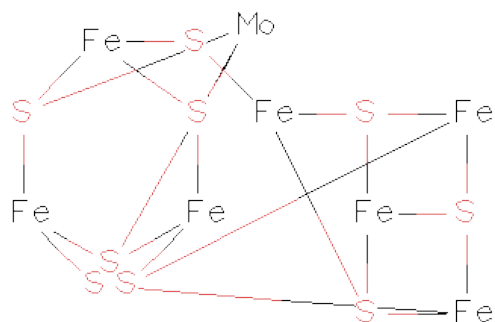
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is 3-HYDROXY-3-CARBOXY-ADIPIACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



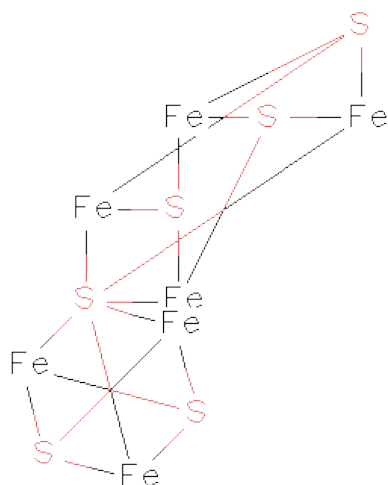
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			14	7	7		
8	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 9 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



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

- Molecule 10 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



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

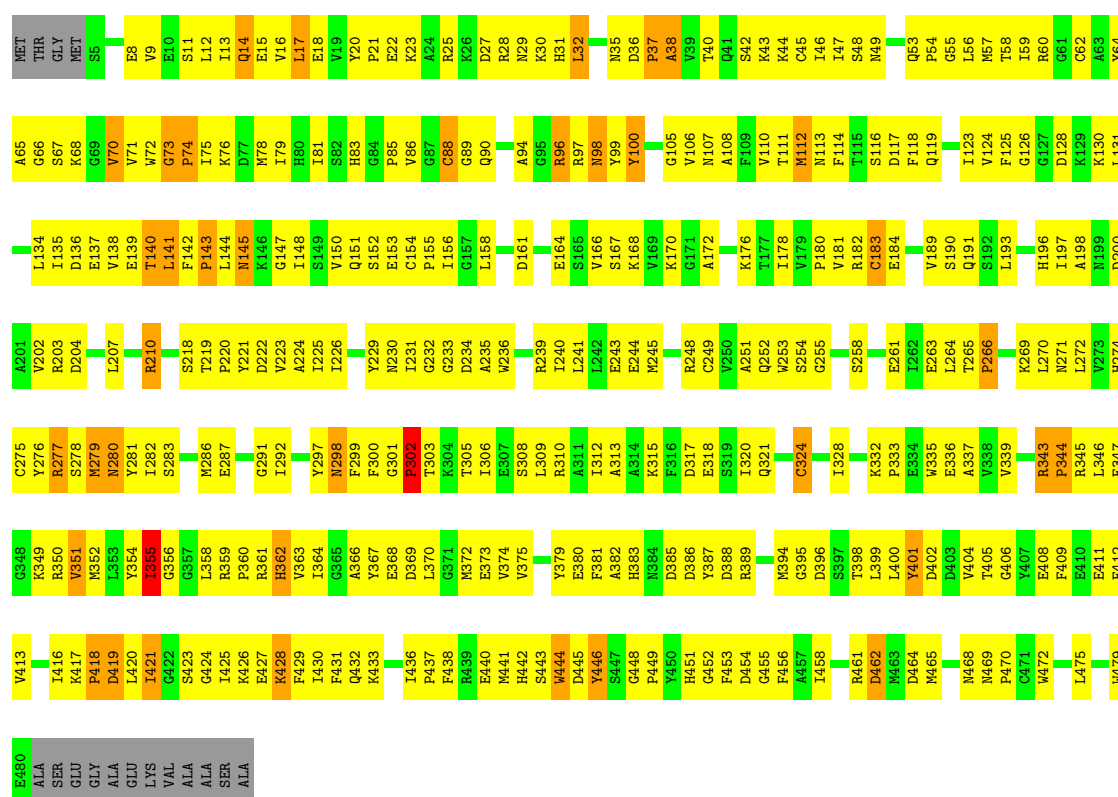
3 Residue-property plots

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.

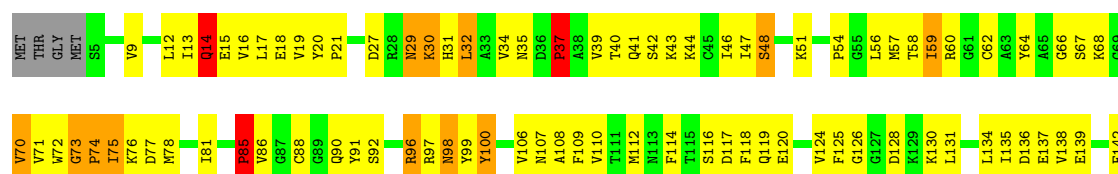
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain A:



• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain C:



P143	T219	S283	Y354	G422	LYS
L144	P220	R284	I355	S423	VAL
M145	Y221	H285	G356	G424	ALA
	D222	M286	G357	T425	ALA
	V223	E287	L358	K426	SER
I148	A224	E288	R359	E427	ALA
V150	I225		P360	K428	
Q151	I226		R361	F429	
S152		G291	R362	F430	
E153	Y229	I292	V363	F431	
C154	N230	Y297	I364	Q432	
P155	I231	L298	G365	K433	
I156	G232	N299	G366	T436	
	G233	F293	Y367	F437	
	D234	F300	E368	F438	
	A235	P302	D369	E439	
	W236	T303	L370	R439	
E164		K304	G371	E440	
S165	R239	T305	M372	M441	
V166	L240	I306	E373	H442	
S167	L241	E307	V374	S443	
P168		S308	V375	D444	
V169	E244	L309		Y446	
K170	M245	R310	Y379	S447	
G171		A311	F381	G448	
A172		T312	A382	F449	
	R248	A313	H383	Y450	
I178	C249	K314	R384	H451	
V179	V250	K315	D385	G452	
P180	A251	F316	K386	F453	
V181	Q252	D317	Y387	T454	
R182	W253	E318	D388	G456	
C183	S254	S319	R389	A457	
E184	D256	T320	M394	T458	
G185	G257	Q321	G395	R461	
F186	F258		D396	D462	
R187	S259	C324	S397	M463	
	S260		T398	K464	
S190	E261		L399	M465	
Q191	L262		K400	T466	
L193	L263		Y401	L467	
	L264		D402	M468	
H196	T265		D403	M469	
I197	P266		V404	P470	
A198	K267		T405	C471	
H199	V268		E408	V472	
D200	K269		F409	L475	
	L270		F412		
R203	N271		V413		
D204	L272		F416	ALA	
W205	W273		V417	SER	
V206	H274		I418	GLU	
L207	C275		P418	GLY	
G208	Y276		D419	ALA	
G209	R277		L420		
R210	S278		I421		
	W279				
F216	N280				
A217	Y281				
S218	I282				

• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

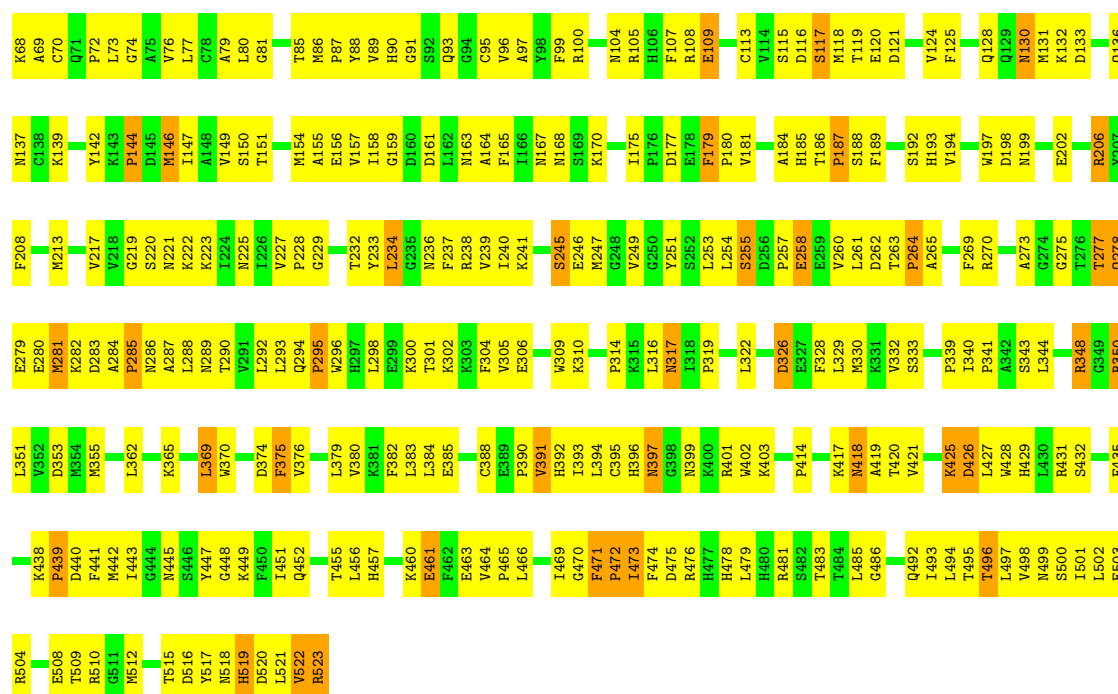
Chain B:

MET	A69	G134	N199	F269	P339	S413	D475
S2	C70	L135	E202	F269	P340	P414	R476
Q3	Q71	N136	G203	A273	I340	P415	R477
V5	P72	N137	I204	G274	A342	Y415	L479
I8	G74	K139	A205	G275	S343	N418	T483
	A75	Y142	R206	T276	L344	A419	L484
Y12	V76	K143	Y207	T277	T345	T420	T485
P13	L77	P144	F208	Q278	K346	V421	L486
L14	L80	D145	T209	E279	E347	Y422	M491
F15	G81	M146	K211	M281	R348	I423	Q492
	F82	I147	S212	D282	G349	K424	I493
D19	E83	A148	M213	D283	R350	K425	I494
Y20	K84	V149	K216	A284	L351	D426	T495
M23	K85	S150	V217	P285	V352	L427	T496
L24	M86	T151	G219	N286	K354	W428	L497
K27	Y88	C153	G218	L288	M355	H429	V498
R28	H90	M154	S220	N289	T356	R431	M499
F31	G94	A155	N221	T290	D357	S432	S500
E32	C95	V157	K223	L292	S358	L433	I501
E33	G96	I158	E225	Q294	H359	V434	E503
K34	Y97	D160	T226	P295	L362	T436	R504
P36	A98	E161	V227	W296	R366	D437	D506
Q37	F99	L162	G229	H297	F367	K438	E507
D38	R100	M163		L298	P439	P439	E508
K39	M104	F165	T232	T301	M442	M442	T509
T40	R105	I166	Y233	K302	L443	L443	R510
D41	H106	N167	L234	A303	G444	G444	G511
E42	F107	S168	G235	F304	S445	S445	M512
V43	R108	K170	N236	V305	Y447	Y447	T515
F44	F44	K171	F237	E306	G448	G448	D516
Q45	E109	E172	R238	K309	K449	K449	Y517
V46	P110		V239	K310	F450	F450	N518
T47	C113	I175	K241	P314	T451	T451	R519
T48	V114	D177	S245	R315	L455	L455	D520
T49	S115	E178	E246	L316	W457	W457	V522
Y51	D116	F179	M247	R317	G458	G458	R523
Y52	Q53	P180	G248	I318	G459	G459	
E54	L55	V181	V249	P319	K460	K460	
		P182		L322	E461	E461	
		H185	L253		F462	F462	
		T186	L254		E463	E463	
		S188	S255		V464	V464	
			D266		P465	P465	
			P257		L466	L466	
			E258		I467	I467	
			E259		R468	R468	
			V260		L469	L469	
			L261		W402	W402	
			D262		F471	F471	
			T263		P472	P472	
			N130		I473	I473	
			T194		F474	F474	
			T195				
			G196				
			W197				
			D198				

• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

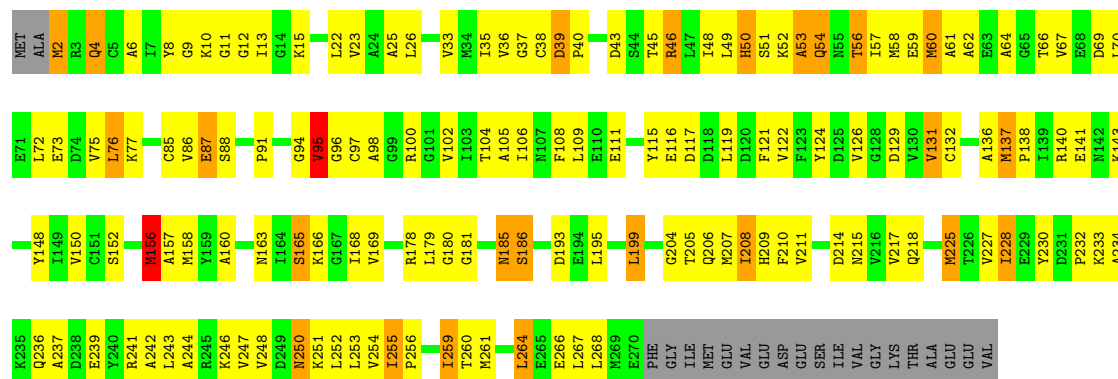
Chain D:

MET	Y52
S2	Q53
Q3	E54
Q4	L55
V5	F57
	Q58
I8	R59
K9	A61
A10	L62
S11	T63
Y12	V64
P13	M65
L14	P66
F15	A67
D19	
Y20	
M23	
L24	
K27	
R28	
F31	
E32	
E33	
K34	
Y35	
P36	
Q37	
D38	
K39	
T40	
D41	
Y42	
V43	
F44	
Q45	
W46	
T47	
T48	
T49	



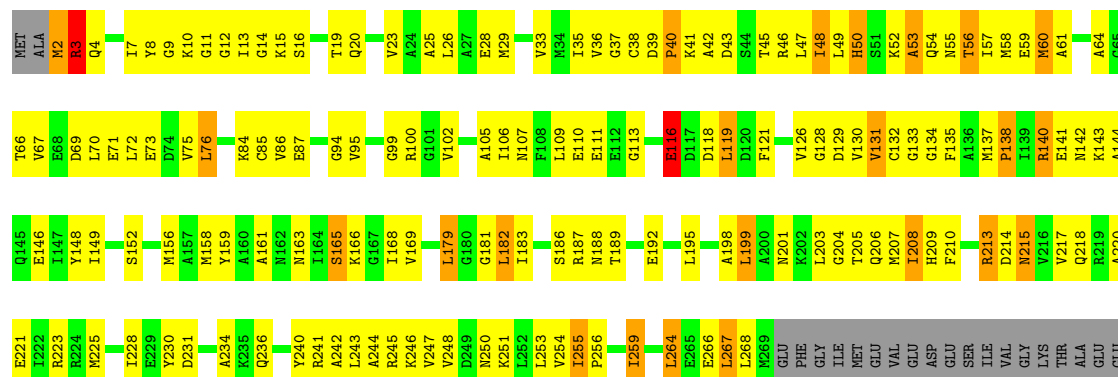
• Molecule 3: NITROGENASE IRON PROTEIN

Chain E:



• Molecule 3: NITROGENASE IRON PROTEIN

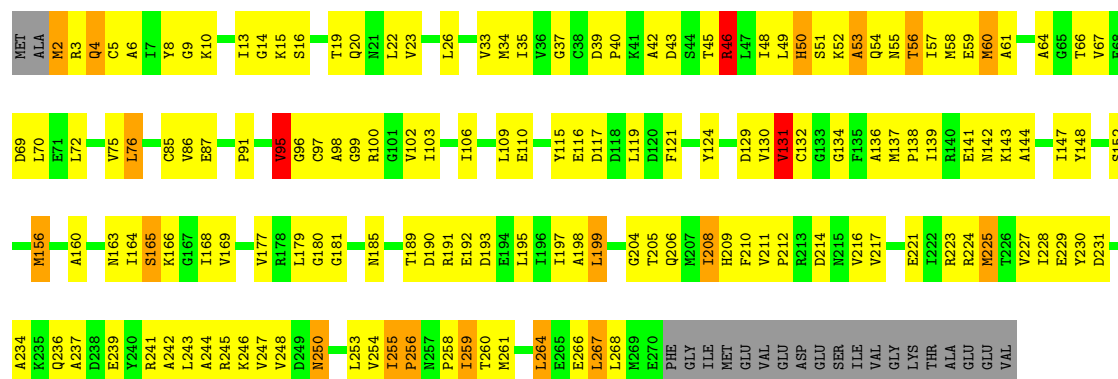
Chain F:



VAL

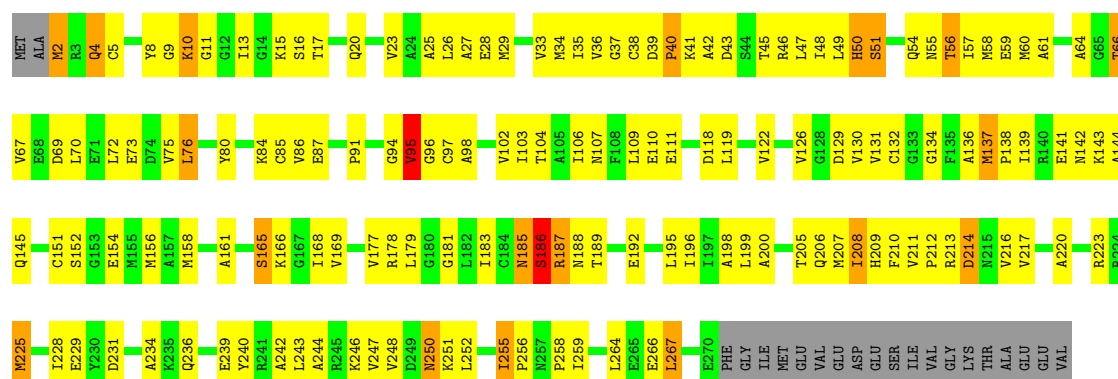
- Molecule 3: NITROGENASE IRON PROTEIN

Chain G:



- Molecule 3: NITROGENASE IRON PROTEIN

Chain H:



4 Data and refinement statistics

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	110.50Å 121.50Å 264.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	71.6 (20.00-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24237	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.50	0/3864	0.73	2/5212 (0.0%)
1	C	0.48	0/3864	0.73	2/5212 (0.0%)
2	B	0.54	0/4276	0.82	7/5782 (0.1%)
2	D	0.50	1/4276 (0.0%)	0.88	15/5782 (0.3%)
3	E	0.51	0/2052	0.80	2/2764 (0.1%)
3	F	0.55	1/2043 (0.0%)	0.84	4/2752 (0.1%)
3	G	0.47	0/2052	0.75	0/2764
3	H	0.54	1/2052 (0.0%)	0.81	1/2764 (0.0%)
All	All	0.51	3/24479 (0.0%)	0.80	33/33032 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	40	PRO	N-CD	5.37	1.55	1.47
3	F	40	PRO	N-CD	5.31	1.55	1.47
2	D	109	GLU	C-N	-5.08	1.24	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	TYR	C-N-CD	-21.77	72.71	120.60
2	B	12	TYR	C-N-CD	-20.40	75.71	120.60
2	B	12	TYR	C-N-CA	13.32	177.95	122.00
2	D	12	TYR	C-N-CA	12.49	174.45	122.00
1	A	88	CYS	CA-CB-SG	-10.83	94.51	114.00
2	D	95	CYS	CA-CB-SG	-10.59	94.93	114.00
2	D	350	ARG	NE-CZ-NH2	9.26	124.93	120.30
2	D	348	ARG	NE-CZ-NH1	-7.22	116.69	120.30
3	F	116	GLU	N-CA-C	7.09	130.14	111.00
2	D	350	ARG	NE-CZ-NH1	-7.08	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	206	ARG	NE-CZ-NH1	-7.06	116.77	120.30
2	D	348	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	D	13	PRO	CA-N-CD	-6.80	101.98	111.50
2	D	471	PHE	C-N-CD	-6.77	105.71	120.60
2	D	59	ARG	NE-CZ-NH1	-6.75	116.92	120.30
3	F	3	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	D	431	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	E	156	MET	CG-SD-CE	-6.67	89.53	100.20
2	B	471	PHE	C-N-CD	-6.61	106.06	120.60
3	E	39	ASP	CB-CG-OD2	6.53	124.18	118.30
2	B	13	PRO	CA-N-CD	-6.35	102.61	111.50
3	H	186	SER	N-CA-C	6.29	127.99	111.00
2	B	439	PRO	CA-N-CD	-6.26	102.73	111.50
3	F	3	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	F	119	LEU	N-CA-C	5.99	127.16	111.00
2	D	206	ARG	NE-CZ-NH2	5.84	123.22	120.30
2	D	59	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	38	ALA	N-CA-C	5.78	126.61	111.00
2	B	116	ASP	N-CA-C	-5.64	95.78	111.00
1	C	14	GLN	CB-CA-C	5.62	121.64	110.40
2	B	257	PRO	CA-N-CD	-5.61	103.65	111.50
2	D	431	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	143	PRO	CA-N-CD	-5.01	104.48	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3776	0	3709	452	0
1	C	3776	0	3709	490	0
2	B	4170	0	4076	441	0
2	D	4170	0	4076	461	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2029	0	2040	150	0
3	F	2020	0	2034	166	0
3	G	2029	0	2041	158	0
3	H	2029	0	2041	153	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	F	8	0	0	0	0
6	G	8	0	0	0	0
7	E	31	0	12	4	0
7	F	31	0	12	6	0
7	G	31	0	12	11	0
7	H	31	0	12	6	0
8	A	14	0	6	1	0
8	C	14	0	6	2	0
9	A	17	0	0	4	0
9	C	17	0	0	7	0
10	A	15	0	0	1	0
10	D	15	0	0	3	0
All	All	24237	0	23786	2236	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

All (2236) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:39:ASP:OD1	3:F:40:PRO:HD2	1.28	1.29
2:D:91:GLY:HA2	2:D:118:MET:CE	1.62	1.28
1:C:124:VAL:HG21	3:H:58:MET:CE	1.70	1.21
1:A:355:ILE:HG23	1:A:356:GLY:H	0.99	1.15
3:F:39:ASP:OD1	3:F:40:PRO:CD	1.95	1.13
2:B:471:PHE:CD2	2:B:472:PRO:HD3	1.83	1.12
1:C:433:LYS:NZ	2:D:263:THR:HG23	1.66	1.10
3:F:106:ILE:CD1	3:F:138:PRO:HD3	1.82	1.09
1:C:355:ILE:CG2	1:C:356:GLY:H	1.63	1.08
2:B:128:GLN:HG3	2:B:132:LYS:HE3	1.09	1.06
1:A:355:ILE:CG2	1:A:360:PRO:CD	2.33	1.06
1:C:124:VAL:HG21	3:H:58:MET:HE2	1.13	1.06
1:A:86:VAL:HG11	2:B:68:LYS:HE3	1.36	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:355:ILE:HG22	1:C:356:GLY:N	1.62	1.04
2:D:86:MET:HE2	2:D:87:PRO:HD2	1.37	1.04
1:C:167:SER:CB	1:C:180:PRO:HG3	1.86	1.04
1:C:167:SER:HB2	1:C:180:PRO:HG3	1.40	1.04
3:G:56:THR:HG23	3:G:59:GLU:HB2	1.40	1.03
2:B:128:GLN:CG	2:B:132:LYS:HE3	1.88	1.03
3:E:156:MET:SD	7:F:6292:ATP:H4'	1.99	1.02
1:A:355:ILE:HG22	1:A:360:PRO:CD	1.89	1.01
1:C:58:THR:HG22	1:C:60:ARG:H	1.25	1.01
2:D:91:GLY:HA2	2:D:118:MET:HE3	1.02	1.01
3:H:56:THR:HG23	3:H:59:GLU:HB2	1.41	1.01
1:C:346:LEU:HD12	1:C:372:MET:SD	2.00	1.01
2:B:212:SER:O	2:B:216:LYS:HE3	1.61	1.00
3:H:23:VAL:HG21	3:H:35:ILE:HD11	1.43	1.00
2:D:86:MET:CE	2:D:87:PRO:HD2	1.92	1.00
2:B:289:ASN:HD21	2:B:314:PRO:HD3	1.27	0.99
3:H:225:MET:HE3	3:H:229:GLU:OE2	1.63	0.99
3:F:242:ALA:O	3:F:246:LYS:HG2	1.62	0.98
1:A:355:ILE:HG23	1:A:356:GLY:N	1.74	0.98
1:A:97:ARG:NH2	1:A:99:TYR:OH	1.95	0.98
7:G:7292:ATP:H5'2	3:H:156:MET:SD	2.02	0.98
1:C:253:TRP:CZ3	1:C:282:ILE:HD13	1.99	0.97
1:C:253:TRP:HZ3	1:C:282:ILE:HD13	1.25	0.97
1:A:355:ILE:CG2	1:A:360:PRO:HD3	1.93	0.97
2:B:220:SER:HB2	2:B:286:ASN:HB3	1.41	0.97
3:E:4:GLN:NE2	3:E:143:LYS:O	1.98	0.97
2:B:260:VAL:HG22	2:B:273:ALA:O	1.64	0.96
1:C:426:LYS:HZ1	2:D:97:ALA:HB1	1.26	0.96
1:A:167:SER:HB2	1:A:180:PRO:HG3	1.46	0.96
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.48	0.96
3:E:56:THR:HG23	3:E:59:GLU:HB3	1.46	0.96
1:C:389:ARG:HG3	1:C:389:ARG:HH11	1.30	0.95
1:A:229:TYR:HA	1:A:254:SER:O	1.68	0.94
1:C:355:ILE:HG22	1:C:356:GLY:H	0.79	0.94
1:C:59:ILE:HG23	1:C:426:LYS:HD2	1.48	0.94
3:G:217:VAL:HG21	7:G:7292:ATP:H2	1.32	0.94
1:A:27:ASP:O	1:A:30:LYS:HG2	1.67	0.94
1:A:346:LEU:HD12	1:A:370:LEU:HD12	1.47	0.94
3:F:56:THR:O	3:F:60:MET:HB2	1.67	0.93
2:B:206:ARG:HG3	2:B:304:PHE:CZ	2.02	0.93
1:C:433:LYS:NZ	2:D:263:THR:CG2	2.31	0.93
1:A:355:ILE:CG2	1:A:356:GLY:N	2.31	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:35:ILE:CD1	3:E:48:ILE:HD12	1.98	0.93
1:C:209:LYS:HE2	1:C:263:GLU:OE1	1.69	0.93
3:G:189:THR:HG22	3:G:190:ASP:H	1.33	0.92
1:A:355:ILE:CG2	1:A:356:GLY:H	1.78	0.92
3:F:13:ILE:O	3:F:187:ARG:NH2	2.03	0.92
3:F:186:SER:HB3	3:F:210:PHE:CZ	2.04	0.91
1:C:426:LYS:NZ	2:D:97:ALA:HB1	1.84	0.91
1:C:342:TYR:O	1:C:345:ARG:HG3	1.70	0.91
2:D:220:SER:HB2	2:D:286:ASN:HB3	1.49	0.91
2:B:85:THR:HG22	2:B:146:MET:HB3	1.53	0.91
1:A:218:SER:OG	1:A:269:LYS:HE2	1.72	0.90
2:B:238:ARG:HE	2:B:258:GLU:CG	1.85	0.90
2:B:142:TYR:O	2:B:144:PRO:HD3	1.70	0.90
3:F:42:ALA:HA	3:F:87:GLU:OE1	1.72	0.90
2:D:471:PHE:CD2	2:D:472:PRO:HD3	2.07	0.89
1:C:355:ILE:HD12	1:C:359:ARG:HB2	1.52	0.89
2:D:3:GLN:HA	2:D:3:GLN:HE21	1.38	0.89
1:C:20:TYR:OH	1:C:408:GLU:HG2	1.72	0.88
2:B:3:GLN:HE21	2:B:3:GLN:HA	1.39	0.88
1:C:433:LYS:HZ1	2:D:263:THR:HG23	1.37	0.88
1:A:405:THR:OG1	1:A:408:GLU:HG3	1.74	0.88
1:C:138:VAL:HG13	2:D:62:LEU:HD13	1.53	0.88
2:B:457:HIS:HD2	2:D:512:MET:HB3	1.39	0.87
2:B:77:LEU:HA	2:B:80:LEU:HD12	1.56	0.87
1:A:182:ARG:O	1:A:197:ILE:HG21	1.74	0.87
2:D:91:GLY:CA	2:D:118:MET:HE3	1.98	0.87
1:A:167:SER:CB	1:A:180:PRO:HG3	2.04	0.87
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.56	0.87
1:A:355:ILE:HG21	1:A:360:PRO:HD3	1.55	0.87
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.57	0.87
2:D:91:GLY:CA	2:D:118:MET:CE	2.52	0.87
2:B:512:MET:HB3	2:D:457:HIS:HD2	1.38	0.86
1:A:20:TYR:OH	1:A:408:GLU:HG2	1.74	0.86
2:B:517:TYR:O	1:C:99:TYR:CE1	2.28	0.86
2:B:90:HIS:N	2:B:150:SER:O	2.07	0.86
2:B:90:HIS:HA	2:B:116:ASP:OD1	1.74	0.86
2:D:64:VAL:O	2:D:426:ASP:OD1	1.94	0.86
2:D:85:THR:HG22	2:D:146:MET:HB3	1.55	0.86
3:F:241:ARG:O	3:F:245:ARG:HG3	1.76	0.86
2:B:130:ASN:ND2	2:B:130:ASN:H	1.70	0.85
1:C:71:VAL:HG11	1:C:198:ALA:HB1	1.58	0.85
3:G:243:LEU:O	3:G:247:VAL:HG23	1.77	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:350:ARG:HG2	2:D:264:PRO:HG3	1.59	0.85
3:F:13:ILE:HA	3:F:187:ARG:HH21	1.42	0.85
2:D:496:THR:O	2:D:500:SER:OG	1.95	0.84
1:A:277:ARG:CZ	1:A:383:HIS:CD2	2.60	0.84
2:D:260:VAL:HG23	2:D:273:ALA:O	1.77	0.84
1:A:58:THR:HG22	1:A:60:ARG:H	1.42	0.84
2:B:206:ARG:HG3	2:B:304:PHE:CE1	2.13	0.84
1:A:388:ASP:OD1	1:A:389:ARG:HG3	1.78	0.84
2:B:161:ASP:O	2:B:165:PHE:CD1	2.31	0.84
2:B:397:ASN:H	2:B:397:ASN:HD22	1.24	0.84
2:D:238:ARG:HE	2:D:258:GLU:CG	1.90	0.84
2:D:362:LEU:HD11	2:D:498:VAL:HG22	1.59	0.84
1:C:27:ASP:O	1:C:30:LYS:HG3	1.77	0.84
1:A:219:THR:HG22	1:A:221:TYR:H	1.42	0.84
3:H:54:GLN:HG3	3:H:55:ASN:H	1.43	0.83
3:G:217:VAL:HG22	3:G:227:VAL:HG21	1.61	0.83
2:D:397:ASN:H	2:D:397:ASN:HD22	1.26	0.83
3:G:42:ALA:HA	3:G:87:GLU:OE1	1.78	0.83
3:E:37:GLY:HA3	3:E:87:GLU:OE2	1.78	0.83
2:B:289:ASN:ND2	2:B:314:PRO:HD3	1.93	0.83
1:C:449:PRO:HG2	2:D:15:PHE:HZ	1.43	0.83
1:C:182:ARG:O	1:C:197:ILE:HG21	1.78	0.83
2:B:331:LYS:O	2:B:335:ILE:HG12	1.79	0.83
2:B:220:SER:N	2:B:286:ASN:O	2.11	0.83
1:C:234:ASP:HB3	1:C:451:HIS:CG	2.14	0.83
3:G:241:ARG:O	3:G:245:ARG:HG3	1.79	0.83
1:A:385:ASP:O	1:A:388:ASP:OD1	1.96	0.82
2:D:452:GLN:NE2	2:D:465:PRO:HA	1.94	0.82
1:A:343:ARG:O	1:A:347:GLU:HG3	1.80	0.82
3:F:106:ILE:HD11	3:F:138:PRO:HD3	1.61	0.82
1:C:219:THR:HG22	1:C:221:TYR:H	1.42	0.82
1:C:167:SER:HB2	1:C:180:PRO:CG	2.08	0.82
3:E:12:GLY:HA2	3:F:156:MET:CE	2.09	0.82
1:C:405:THR:OG1	1:C:408:GLU:HG3	1.79	0.82
1:C:298:ASN:HB2	1:C:362:HIS:HE2	1.43	0.82
2:B:452:GLN:NE2	2:B:465:PRO:HA	1.95	0.82
1:C:124:VAL:CG2	3:H:58:MET:HE2	2.06	0.81
2:B:397:ASN:H	2:B:397:ASN:ND2	1.79	0.81
1:C:57:MET:HE1	2:D:100:ARG:CZ	2.10	0.81
1:C:57:MET:CE	2:D:100:ARG:NH2	2.44	0.81
2:D:397:ASN:H	2:D:397:ASN:ND2	1.79	0.81
3:G:37:GLY:HA3	3:G:87:GLU:OE2	1.80	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:326:ASP:OD2	2:D:348:ARG:HD2	1.81	0.81
2:D:161:ASP:O	2:D:165:PHE:CD1	2.34	0.81
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.43	0.81
2:D:130:ASN:H	2:D:130:ASN:ND2	1.79	0.81
2:B:197:TRP:CE3	2:B:229:GLY:HA2	2.15	0.80
3:H:56:THR:O	3:H:60:MET:HB2	1.81	0.80
1:C:210:ARG:HH11	1:C:264:LEU:HD21	1.46	0.80
2:B:59:ARG:NH2	2:B:429:HIS:CE1	2.50	0.80
1:A:355:ILE:HG22	1:A:360:PRO:CG	2.11	0.80
2:B:59:ARG:HH22	2:B:429:HIS:CE1	2.00	0.80
3:H:137:MET:HB3	3:H:138:PRO:HD3	1.63	0.80
2:D:238:ARG:HD3	2:D:258:GLU:HG3	1.64	0.80
1:A:234:ASP:HB3	1:A:451:HIS:CG	2.17	0.80
1:C:186:PHE:HE1	3:G:100:ARG:HH21	1.29	0.80
2:D:151:THR:CG2	2:D:186:THR:H	1.94	0.80
3:H:231:ASP:OD2	3:H:234:ALA:HB2	1.81	0.80
3:H:244:ALA:O	3:H:248:VAL:HG23	1.82	0.80
1:A:355:ILE:HG21	1:A:360:PRO:CD	2.09	0.79
3:H:106:ILE:CD1	3:H:138:PRO:HD3	2.12	0.79
2:B:158:ILE:O	3:F:133:GLY:HA3	1.81	0.79
1:C:97:ARG:NH1	1:C:446:TYR:HA	1.96	0.79
3:G:49:LEU:O	3:G:50:HIS:HB2	1.80	0.79
1:C:59:ILE:HD13	1:C:427:GLU:OE2	1.82	0.79
1:C:170:LYS:O	1:C:178:ILE:HD12	1.82	0.79
1:A:31:HIS:O	1:A:46:ILE:HD11	1.83	0.79
3:F:43:ASP:HB2	3:F:46:ARG:HD3	1.62	0.79
2:D:305:VAL:HG13	2:D:309:TRP:CE3	2.17	0.79
3:F:204:GLY:O	3:F:254:VAL:HG21	1.83	0.79
1:A:97:ARG:HH21	2:D:520:ASP:CG	1.86	0.78
2:B:151:THR:OG1	2:B:155:ALA:HB3	1.82	0.78
2:D:369:LEU:HD21	2:D:393:ILE:HG12	1.65	0.78
2:D:238:ARG:CD	2:D:258:GLU:HG3	2.13	0.78
3:E:35:ILE:HD11	3:E:48:ILE:HD12	1.65	0.78
2:D:238:ARG:NE	2:D:258:GLU:HG3	1.98	0.78
3:E:61:ALA:HB2	3:E:70:LEU:HD12	1.64	0.78
2:B:85:THR:HG21	2:B:146:MET:HE1	1.66	0.78
2:B:65:ASN:O	2:B:427:LEU:HB2	1.82	0.78
2:D:77:LEU:HA	2:D:80:LEU:HD12	1.66	0.78
2:B:496:THR:O	2:B:500:SER:OG	2.00	0.78
1:A:75:ILE:HG21	1:A:78:MET:CE	2.14	0.78
1:C:167:SER:CB	1:C:180:PRO:CG	2.61	0.78
1:C:389:ARG:CG	1:C:389:ARG:HH11	1.97	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:298:ASN:HD22	1:C:299:PHE:N	1.81	0.78
1:C:58:THR:HG22	1:C:60:ARG:N	1.97	0.78
1:C:433:LYS:HZ3	2:D:263:THR:CG2	1.95	0.78
3:H:49:LEU:O	3:H:50:HIS:HB2	1.84	0.78
2:D:128:GLN:HE22	2:D:168:ASN:HD22	1.31	0.78
2:B:279:GLU:OE1	2:B:282:LYS:HD2	1.83	0.78
2:D:233:TYR:HB2	2:D:236:ASN:HD22	1.50	0.77
2:D:91:GLY:HA2	2:D:118:MET:HE2	1.63	0.77
1:C:253:TRP:HE1	1:C:265:THR:HG1	1.31	0.77
2:B:142:TYR:C	2:B:144:PRO:HD3	2.05	0.77
1:C:57:MET:HE1	2:D:100:ARG:NH2	2.00	0.77
1:A:433:LYS:NZ	2:B:263:THR:O	2.17	0.77
1:A:59:ILE:HG23	1:A:426:LYS:HD2	1.65	0.77
1:A:355:ILE:CG2	1:A:360:PRO:HD2	2.14	0.77
1:C:355:ILE:HD11	1:C:441:MET:HB3	1.67	0.77
3:E:94:GLY:O	3:E:95:VAL:HG23	1.85	0.77
1:C:355:ILE:HB	1:C:360:PRO:CD	2.14	0.77
1:C:355:ILE:HB	1:C:360:PRO:HG3	1.65	0.77
1:C:75:ILE:HG21	1:C:78:MET:CE	2.15	0.77
1:A:465:MET:O	1:A:469:ASN:HB2	1.85	0.77
1:A:429:PHE:CB	2:B:110:PRO:HD3	2.15	0.77
2:B:329:LEU:HD13	2:B:344:LEU:HD13	1.65	0.76
2:D:217:VAL:HB	2:D:220:SER:OG	1.84	0.76
1:C:40:THR:O	1:C:40:THR:HG22	1.86	0.76
1:C:193:LEU:O	1:C:197:ILE:HG13	1.84	0.76
1:C:385:ASP:HA	1:C:388:ASP:OD2	1.85	0.76
1:A:251:ALA:HA	1:A:261:GLU:HG2	1.65	0.76
1:C:131:LEU:O	1:C:135:ILE:HG13	1.86	0.76
1:C:433:LYS:HZ1	2:D:263:THR:CG2	1.95	0.76
1:A:71:VAL:HG11	1:A:198:ALA:HB1	1.68	0.76
2:D:262:ASP:O	2:D:264:PRO:HD3	1.85	0.76
2:D:86:MET:HE2	2:D:87:PRO:CD	2.14	0.76
2:B:369:LEU:HD12	2:B:379:LEU:HD23	1.67	0.76
2:D:116:ASP:HB2	2:D:130:ASN:HB2	1.68	0.75
2:D:329:LEU:HD13	2:D:344:LEU:HD13	1.68	0.75
1:A:355:ILE:HG22	1:A:360:PRO:HD2	1.67	0.75
3:H:186:SER:HB3	3:H:210:PHE:CZ	2.22	0.75
1:C:30:LYS:NZ	1:C:47:ILE:HD13	2.02	0.75
3:H:166:LYS:O	3:H:169:VAL:HG12	1.86	0.75
2:D:46:TRP:O	2:D:49:THR:HG22	1.86	0.75
2:B:197:TRP:CZ3	2:B:229:GLY:HA2	2.22	0.75
3:G:56:THR:O	3:G:60:MET:HB2	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:49:THR:HG23	2:D:52:TYR:H	1.52	0.75
2:B:170:LYS:HD2	2:B:177:ASP:HA	1.69	0.75
1:A:429:PHE:HB3	2:B:110:PRO:HD3	1.69	0.74
1:C:355:ILE:HB	1:C:360:PRO:CG	2.17	0.74
1:A:388:ASP:OD1	1:A:389:ARG:N	2.20	0.74
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.50	0.74
3:H:141:GLU:O	3:H:142:ASN:HB2	1.86	0.74
3:G:56:THR:HG23	3:G:59:GLU:CB	2.17	0.74
3:G:181:GLY:HA2	3:G:205:THR:OG1	1.88	0.74
2:B:129:GLN:NE2	2:B:132:LYS:HD2	2.03	0.74
1:C:57:MET:CE	2:D:100:ARG:CZ	2.65	0.74
2:D:68:LYS:HG2	2:D:396:HIS:HD2	1.52	0.74
3:H:55:ASN:HB3	3:H:60:MET:SD	2.27	0.74
2:B:217:VAL:HB	2:B:220:SER:OG	1.87	0.74
1:C:251:ALA:HA	1:C:261:GLU:HG2	1.70	0.74
3:F:206:GLN:NE2	3:F:250:ASN:OD1	2.21	0.74
3:F:56:THR:HG23	3:F:59:GLU:HB2	1.70	0.74
2:D:170:LYS:HD2	2:D:177:ASP:HA	1.70	0.74
2:B:233:TYR:HB2	2:B:236:ASN:HD22	1.52	0.74
1:C:31:HIS:O	1:C:46:ILE:HD11	1.88	0.73
1:A:276:TYR:HB3	1:A:361:ARG:HH22	1.53	0.73
2:B:128:GLN:O	2:B:132:LYS:HG3	1.88	0.73
3:H:106:ILE:HD13	3:H:138:PRO:HD3	1.71	0.73
2:D:28:ARG:HA	2:D:32:GLU:HG3	1.69	0.73
2:D:65:ASN:O	2:D:427:LEU:HB2	1.89	0.73
3:H:60:MET:HB3	3:H:70:LEU:HD11	1.69	0.73
1:A:131:LEU:O	1:A:135:ILE:HG13	1.88	0.73
1:A:360:PRO:HB2	1:A:379:TYR:CE2	2.24	0.73
2:B:151:THR:CG2	2:B:186:THR:H	2.01	0.73
1:C:56:LEU:O	1:C:57:MET:HB2	1.87	0.73
1:A:280:ASN:N	1:A:280:ASN:HD22	1.86	0.73
3:F:183:ILE:HD13	3:F:243:LEU:HD11	1.70	0.73
1:A:210:ARG:HH11	1:A:264:LEU:HD21	1.52	0.73
1:C:355:ILE:HD12	1:C:359:ARG:CB	2.18	0.73
1:C:116:SER:O	1:C:130:LYS:HE2	1.86	0.73
2:B:178:GLU:O	2:B:180:PRO:HD3	1.89	0.73
2:B:238:ARG:HE	2:B:258:GLU:HG2	1.53	0.73
3:F:110:GLU:OE2	3:F:143:LYS:NZ	2.22	0.73
3:G:23:VAL:HG21	3:G:35:ILE:HD11	1.70	0.73
1:C:124:VAL:HG21	3:H:58:MET:HE3	1.71	0.73
1:C:86:VAL:HG21	2:D:68:LYS:HE3	1.71	0.73
3:E:57:ILE:HG12	3:E:75:VAL:HG21	1.71	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:207:MET:CE	3:F:210:PHE:HB2	2.20	0.72
3:G:106:ILE:HD12	3:G:137:MET:HB3	1.71	0.72
1:C:98:ASN:H	1:C:98:ASN:ND2	1.87	0.72
3:F:49:LEU:O	3:F:50:HIS:HB2	1.89	0.72
2:D:238:ARG:HE	2:D:258:GLU:HG3	1.50	0.72
3:F:23:VAL:HG21	3:F:35:ILE:HD11	1.71	0.72
2:B:305:VAL:HG13	2:B:309:TRP:CE3	2.23	0.72
1:A:298:ASN:HB2	1:A:362:HIS:HE2	1.54	0.72
3:F:54:GLN:HG3	3:F:55:ASN:H	1.54	0.72
3:H:39:ASP:OD1	3:H:40:PRO:HD2	1.88	0.72
3:G:22:LEU:HD11	3:G:247:VAL:HG21	1.72	0.72
3:E:57:ILE:HG13	3:E:75:VAL:HG11	1.71	0.72
1:C:433:LYS:HZ3	2:D:263:THR:HG23	1.53	0.72
2:B:512:MET:CB	2:D:457:HIS:HD2	2.02	0.72
2:D:260:VAL:CG2	2:D:273:ALA:O	2.36	0.72
2:B:422:TYR:HD2	2:B:425:LYS:HZ2	1.36	0.72
1:C:280:ASN:HD22	1:C:280:ASN:N	1.87	0.72
2:D:146:MET:CG	2:D:180:PRO:HB2	2.19	0.72
2:D:124:VAL:HG11	3:G:58:MET:HG3	1.71	0.72
2:B:362:LEU:HD11	2:B:498:VAL:HG22	1.72	0.72
2:B:139:LYS:HG3	2:B:179:PHE:CE1	2.25	0.72
2:B:14:LEU:HD12	2:B:14:LEU:O	1.90	0.72
3:F:13:ILE:CA	3:F:187:ARG:HH21	2.03	0.72
1:A:193:LEU:O	1:A:197:ILE:HG13	1.89	0.72
2:D:12:TYR:CD2	2:D:13:PRO:HD3	2.25	0.72
2:B:238:ARG:NE	2:B:258:GLU:HG3	2.05	0.71
2:B:49:THR:HG23	2:B:52:TYR:H	1.53	0.71
2:D:301:THR:O	2:D:305:VAL:HG23	1.89	0.71
1:A:151:GLN:NE2	1:A:181:VAL:HG11	2.04	0.71
1:C:15:GLU:O	1:C:18:GLU:HB2	1.90	0.71
2:B:85:THR:HG21	2:B:146:MET:CE	2.20	0.71
1:C:280:ASN:ND2	1:C:281:TYR:H	1.88	0.71
1:A:277:ARG:NE	1:A:383:HIS:CD2	2.58	0.71
2:B:301:THR:O	2:B:305:VAL:HG23	1.89	0.71
2:D:283:ASP:O	2:D:283:ASP:OD1	2.08	0.71
3:E:56:THR:O	3:E:60:MET:HB2	1.91	0.71
1:A:138:VAL:HG21	1:A:148:ILE:CD1	2.20	0.71
1:A:479:TRP:HZ3	2:D:326:ASP:HB3	1.53	0.71
1:A:258:SER:HB2	1:A:261:GLU:HB2	1.72	0.71
1:A:128:ASP:HB3	1:A:166:VAL:HG21	1.70	0.71
3:E:204:GLY:O	3:E:254:VAL:HG21	1.89	0.71
2:B:302:LYS:HE2	2:B:306:GLU:OE2	1.91	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:THR:HG22	1:A:60:ARG:N	2.03	0.71
1:A:98:ASN:H	1:A:98:ASN:ND2	1.89	0.71
3:G:141:GLU:O	3:G:142:ASN:HB2	1.90	0.71
3:G:217:VAL:CG2	7:G:7292:ATP:H2	2.03	0.71
2:B:346:LYS:HG3	2:D:264:PRO:HG2	1.73	0.71
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.72	0.71
3:G:56:THR:CG2	3:G:59:GLU:HB2	2.19	0.71
3:F:60:MET:HB3	3:F:70:LEU:HD11	1.72	0.71
2:B:262:ASP:OD2	2:D:350:ARG:NE	2.24	0.71
2:D:130:ASN:ND2	2:D:130:ASN:N	2.39	0.70
3:F:55:ASN:HB3	3:F:60:MET:SD	2.31	0.70
2:B:512:MET:HE2	2:D:457:HIS:CB	2.21	0.70
1:A:75:ILE:HG21	1:A:78:MET:HE3	1.73	0.70
1:C:360:PRO:HB2	1:C:379:TYR:CE2	2.26	0.70
2:D:146:MET:CE	2:D:208:PHE:CZ	2.73	0.70
3:F:195:LEU:HD21	3:F:268:LEU:HD23	1.73	0.70
1:C:430:ILE:HG12	2:D:269:PHE:CE1	2.26	0.70
1:C:138:VAL:HG21	1:C:148:ILE:CD1	2.21	0.70
1:A:105:GLY:HA2	1:A:112:MET:HE1	1.71	0.70
2:B:45:GLN:O	2:B:48:THR:HG22	1.91	0.70
1:C:159:ILE:HD12	3:H:97:CYS:HB2	1.72	0.70
3:G:259:ILE:HD12	3:G:264:LEU:HD23	1.72	0.70
2:D:292:LEU:O	2:D:295:PRO:HD3	1.90	0.70
1:A:298:ASN:HB2	1:A:362:HIS:NE2	2.07	0.70
1:A:352:MET:HB3	1:A:421:ILE:HG23	1.74	0.70
1:C:346:LEU:CD1	1:C:372:MET:SD	2.79	0.70
3:F:244:ALA:O	3:F:248:VAL:HG23	1.92	0.70
1:C:355:ILE:CG2	9:C:3496:CFM:S3A	2.80	0.70
2:B:46:TRP:O	2:B:49:THR:HG22	1.92	0.70
1:C:465:MET:O	1:C:469:ASN:HB2	1.92	0.70
1:C:425:ILE:HG22	8:C:3494:HCA:C6	2.21	0.70
3:E:23:VAL:HG12	3:E:33:VAL:HG11	1.73	0.70
2:B:238:ARG:CD	2:B:258:GLU:HG3	2.22	0.70
2:D:96:VAL:HG13	2:D:113:CYS:SG	2.32	0.70
3:E:35:ILE:HD12	3:E:48:ILE:HD12	1.73	0.70
2:D:142:TYR:O	2:D:144:PRO:HD3	1.90	0.70
3:G:224:ARG:O	3:G:225:MET:HG2	1.92	0.70
3:E:12:GLY:HA2	3:F:156:MET:HE3	1.73	0.69
1:A:35:ASN:HB2	1:A:400:LEU:HD11	1.74	0.69
1:C:30:LYS:HZ2	1:C:47:ILE:HD13	1.55	0.69
1:A:350:ARG:HH11	1:A:375:VAL:HG11	1.56	0.69
3:H:223:ARG:HG2	3:H:223:ARG:O	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:355:ILE:HG22	9:C:3496:CFM:S3A	2.31	0.69
2:B:238:ARG:NE	2:B:258:GLU:CG	2.55	0.69
2:D:128:GLN:HE22	2:D:168:ASN:ND2	1.89	0.69
1:C:298:ASN:HB2	1:C:362:HIS:NE2	2.06	0.69
2:D:403:LYS:NZ	2:D:421:VAL:HB	2.07	0.69
2:D:45:GLN:O	2:D:48:THR:HG22	1.92	0.69
3:E:11:GLY:HA2	7:E:5292:ATP:O1G	1.93	0.69
1:A:86:VAL:CG1	2:B:68:LYS:HE3	2.19	0.69
1:C:134:LEU:HD12	2:D:61:ALA:O	1.92	0.69
3:G:156:MET:SD	7:H:8292:ATP:H4'	2.32	0.69
2:D:394:LEU:HD23	2:D:395:CYS:N	2.07	0.69
3:H:56:THR:HG23	3:H:59:GLU:CB	2.22	0.69
1:A:116:SER:O	1:A:130:LYS:HE2	1.93	0.69
2:B:124:VAL:HG11	3:E:58:MET:HG3	1.74	0.69
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.27	0.69
2:D:146:MET:HG3	2:D:180:PRO:CB	2.21	0.69
1:A:421:ILE:HD11	1:A:436:ILE:HG21	1.75	0.69
2:D:213:MET:HE1	2:D:309:TRP:HA	1.74	0.69
1:A:64:TYR:CE2	1:A:88:CYS:HB3	2.28	0.69
1:A:446:TYR:CE2	2:D:522:VAL:HG23	2.28	0.68
2:B:59:ARG:NH2	2:B:426:ASP:OD2	2.26	0.68
1:A:99:TYR:CE1	2:D:517:TYR:O	2.47	0.68
1:C:274:HIS:O	1:C:358:LEU:HD11	1.93	0.68
3:H:50:HIS:O	3:H:51:SER:HB3	1.94	0.68
2:B:130:ASN:HD22	2:B:130:ASN:H	1.41	0.68
1:C:449:PRO:HG2	2:D:15:PHE:CZ	2.28	0.68
1:C:154:CYS:HB2	1:C:155:PRO:CD	2.23	0.68
1:C:62:CYS:O	1:C:191:GLN:HA	1.94	0.68
3:G:192:GLU:HB3	3:G:210:PHE:HE2	1.58	0.68
2:D:322:LEU:O	2:D:326:ASP:OD1	2.12	0.68
3:E:181:GLY:HA2	3:E:205:THR:OG1	1.93	0.68
3:F:26:LEU:HD12	3:F:29:MET:CE	2.23	0.68
3:H:57:ILE:HG12	3:H:75:VAL:HG21	1.75	0.68
1:A:189:VAL:HG23	1:A:190:SER:N	2.08	0.68
1:C:48:SER:HB3	1:C:402:ASP:OD2	1.94	0.68
1:C:287:GLU:O	1:C:291:GLY:HA2	1.93	0.68
3:E:23:VAL:HG21	3:E:35:ILE:HD11	1.76	0.68
2:B:238:ARG:HE	2:B:258:GLU:HG3	1.59	0.68
1:C:359:ARG:HH11	1:C:359:ARG:HG3	1.58	0.68
1:C:343:ARG:O	1:C:347:GLU:HG3	1.94	0.68
1:C:209:LYS:HE2	1:C:263:GLU:CD	2.12	0.68
2:B:517:TYR:O	1:C:99:TYR:CD1	2.47	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:74:PRO:HG3	1:C:98:ASN:OD1	1.94	0.68
1:A:105:GLY:HA2	1:A:112:MET:CE	2.23	0.68
1:C:68:LYS:O	1:C:68:LYS:HD3	1.94	0.68
1:A:280:ASN:ND2	1:A:281:TYR:H	1.92	0.67
1:C:355:ILE:CB	1:C:360:PRO:HD3	2.24	0.67
1:A:74:PRO:HG3	1:A:98:ASN:OD1	1.94	0.67
1:A:449:PRO:HG2	2:B:15:PHE:HZ	1.58	0.67
2:D:222:LYS:HA	2:D:288:LEU:HD21	1.77	0.67
1:C:137:GLU:OE1	2:D:59:ARG:HG3	1.94	0.67
1:C:404:VAL:HG23	1:C:408:GLU:HB2	1.77	0.67
1:C:253:TRP:CZ3	1:C:282:ILE:CD1	2.76	0.67
1:A:346:LEU:HD12	1:A:370:LEU:CD1	2.21	0.67
2:B:91:GLY:HA2	2:B:118:MET:SD	2.34	0.67
2:B:326:ASP:HB3	1:C:479:TRP:HZ3	1.58	0.67
1:A:441:MET:SD	1:A:444:TRP:HZ3	2.17	0.67
2:B:254:LEU:HB3	2:B:281:MET:HE2	1.77	0.67
2:D:375:PHE:HE2	2:D:470:GLY:HA2	1.59	0.67
3:E:10:LYS:H	3:E:13:ILE:CD1	2.08	0.67
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.29	0.67
3:E:195:LEU:HD21	3:E:268:LEU:HD23	1.77	0.67
2:B:314:PRO:HB3	2:B:316:LEU:HD13	1.75	0.67
1:C:352:MET:HB3	1:C:421:ILE:HG23	1.77	0.67
1:C:275:CYS:HA	1:C:358:LEU:HD13	1.75	0.67
3:E:185:ASN:HA	3:E:211:VAL:HB	1.76	0.67
2:D:225:ASN:HB2	2:D:290:THR:HA	1.77	0.67
1:C:332:LYS:O	1:C:336:GLU:HG3	1.94	0.67
2:B:130:ASN:ND2	2:B:130:ASN:N	2.40	0.67
1:C:229:TYR:HA	1:C:254:SER:O	1.93	0.67
1:A:168:LYS:O	1:A:172:ALA:HB2	1.94	0.67
3:E:13:ILE:O	3:E:185:ASN:ND2	2.28	0.67
1:A:178:ILE:O	1:A:180:PRO:HD3	1.95	0.67
3:F:37:GLY:HA3	3:F:87:GLU:OE2	1.95	0.66
2:D:294:GLN:HB3	2:D:374:ASP:OD2	1.94	0.66
1:A:97:ARG:NH2	2:D:520:ASP:OD2	2.28	0.66
1:C:265:THR:HB	1:C:266:PRO:HD3	1.78	0.66
3:E:35:ILE:HD11	3:E:48:ILE:CD1	2.24	0.66
1:C:144:LEU:CG	2:D:43:VAL:HG21	2.25	0.66
1:A:359:ARG:NH1	1:A:359:ARG:HG3	2.08	0.66
1:A:444:TRP:CE3	1:A:444:TRP:HA	2.28	0.66
1:A:14:GLN:O	1:A:18:GLU:HG3	1.95	0.66
2:D:88:TYR:HB2	2:D:147:ILE:HG22	1.77	0.66
3:G:115:TYR:C	3:G:117:ASP:H	1.97	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:ARG:NH1	1:A:446:TYR:HA	2.10	0.66
1:C:75:ILE:HG21	1:C:78:MET:HE3	1.77	0.66
1:A:239:ARG:HG3	1:A:249:CYS:SG	2.36	0.66
2:D:81:GLY:HA2	2:D:257:PRO:HD3	1.78	0.66
1:C:433:LYS:NZ	2:D:263:THR:O	2.28	0.66
2:D:220:SER:N	2:D:286:ASN:O	2.28	0.66
2:B:37:GLN:HG3	2:B:41:ASP:OD1	1.95	0.66
2:D:37:GLN:HG3	2:D:41:ASP:OD1	1.95	0.66
2:D:107:PHE:CE2	2:D:261:LEU:HD23	2.31	0.66
3:H:45:THR:HG21	3:H:85:CYS:HB3	1.77	0.66
2:D:146:MET:CE	2:D:208:PHE:CE1	2.79	0.66
1:C:230:ASN:HB2	1:C:235:ALA:CB	2.25	0.66
1:C:235:ALA:HB1	1:C:252:GLN:HE21	1.61	0.66
1:C:210:ARG:NH1	1:C:264:LEU:HD21	2.10	0.66
1:C:99:TYR:CE2	1:C:232:GLY:HA2	2.31	0.66
1:C:302:PRO:HD3	1:C:456:PHE:CG	2.30	0.66
1:C:303:THR:HG22	1:C:369:ASP:OD1	1.95	0.66
3:G:179:LEU:HD12	3:G:256:PRO:HG3	1.78	0.66
1:A:303:THR:HG22	1:A:369:ASP:OD1	1.95	0.66
1:A:425:ILE:HD11	2:B:105:ARG:HG2	1.78	0.66
3:H:86:VAL:HG21	3:H:109:LEU:HD11	1.78	0.66
2:B:107:PHE:CE2	2:B:261:LEU:HD23	2.31	0.66
1:C:85:PRO:HG3	2:D:189:PHE:HB3	1.77	0.66
3:G:231:ASP:OD2	3:G:234:ALA:HB2	1.95	0.66
1:C:138:VAL:HG21	1:C:148:ILE:HD11	1.78	0.65
2:D:146:MET:HE2	2:D:208:PHE:CZ	2.31	0.65
3:G:224:ARG:C	3:G:225:MET:HG2	2.16	0.65
3:E:2:MET:HB2	3:E:119:LEU:O	1.95	0.65
3:G:57:ILE:CG1	3:G:75:VAL:HG11	2.26	0.65
1:A:138:VAL:HG21	1:A:148:ILE:HD11	1.78	0.65
1:A:401:TYR:HB2	1:A:404:VAL:HB	1.77	0.65
3:F:106:ILE:HD12	3:F:138:PRO:HD3	1.78	0.65
3:H:137:MET:HB3	3:H:138:PRO:CD	2.25	0.65
2:B:89:VAL:HG22	2:B:150:SER:HB2	1.77	0.65
2:B:164:ALA:O	2:B:168:ASN:ND2	2.28	0.65
1:C:68:LYS:HD3	1:C:68:LYS:C	2.17	0.65
3:G:61:ALA:HB2	3:G:70:LEU:HD12	1.78	0.65
3:F:189:THR:OG1	3:F:192:GLU:HB2	1.95	0.65
2:D:302:LYS:HE2	2:D:306:GLU:OE2	1.97	0.65
1:A:417:LYS:N	1:A:418:PRO:HD3	2.12	0.65
2:B:47:THR:HA	2:B:52:TYR:CG	2.32	0.65
1:A:76:LYS:O	1:A:108:ALA:HA	1.95	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:THR:HG21	1:A:60:ARG:HB2	1.77	0.65
3:F:57:ILE:HG12	3:F:75:VAL:HG21	1.78	0.65
3:G:87:GLU:OE2	3:G:87:GLU:HA	1.97	0.65
2:D:146:MET:HA	2:D:179:PHE:HE2	1.61	0.65
2:D:260:VAL:HG22	2:D:273:ALA:H	1.60	0.65
2:D:284:ALA:HB3	2:D:285:PRO:HD3	1.79	0.65
1:C:35:ASN:HB2	1:C:400:LEU:HD11	1.79	0.65
2:D:56:ASN:O	2:D:59:ARG:HB2	1.97	0.65
2:B:130:ASN:HD22	2:B:130:ASN:N	1.94	0.65
1:C:350:ARG:HH11	1:C:375:VAL:HG11	1.61	0.65
3:F:2:MET:HB2	3:F:119:LEU:O	1.97	0.65
3:G:189:THR:HG22	3:G:190:ASP:N	2.10	0.64
1:C:404:VAL:CG2	1:C:408:GLU:HB2	2.27	0.64
3:E:54:GLN:HG2	3:E:77:LYS:HZ2	1.62	0.64
3:E:207:MET:CE	3:E:210:PHE:HB2	2.25	0.64
3:H:15:LYS:N	7:H:8292:ATP:O1B	2.29	0.64
2:D:81:GLY:CA	2:D:257:PRO:HD3	2.28	0.64
3:E:54:GLN:HG2	3:E:77:LYS:NZ	2.13	0.64
2:D:142:TYR:C	2:D:144:PRO:HD3	2.18	0.64
1:C:332:LYS:HG2	1:C:336:GLU:OE2	1.98	0.64
1:C:355:ILE:O	1:C:380:GLU:HG2	1.97	0.64
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.30	0.64
1:C:17:LEU:HD11	1:C:29:ASN:HA	1.78	0.64
1:C:37:PRO:HD3	1:C:396:ASP:HA	1.79	0.64
2:D:57:PHE:CD2	2:D:425:LYS:NZ	2.66	0.64
2:B:397:ASN:ND2	2:B:397:ASN:N	2.45	0.64
2:D:239:VAL:HG11	2:D:483:THR:HG21	1.79	0.64
1:A:444:TRP:HA	1:A:444:TRP:HE3	1.61	0.64
2:D:362:LEU:HD11	2:D:498:VAL:CG2	2.26	0.64
3:E:52:LYS:O	3:E:53:ALA:HB2	1.98	0.64
1:A:275:CYS:SG	1:A:278:SER:HB2	2.38	0.64
2:D:124:VAL:HG21	3:G:58:MET:HE1	1.80	0.64
3:H:187:ARG:NH2	3:H:195:LEU:CD2	2.61	0.64
3:G:206:GLN:NE2	3:G:250:ASN:OD1	2.30	0.64
1:A:99:TYR:CE2	1:A:232:GLY:HA2	2.33	0.64
2:D:86:MET:CE	2:D:87:PRO:CD	2.71	0.64
2:B:146:MET:HA	2:B:179:PHE:HE2	1.61	0.64
2:D:206:ARG:HG2	2:D:304:PHE:CE1	2.33	0.64
3:H:250:ASN:HD22	3:H:250:ASN:C	2.00	0.64
3:F:220:ALA:HB1	3:F:225:MET:O	1.97	0.64
1:A:405:THR:OG1	1:A:408:GLU:CG	2.46	0.64
3:G:34:MET:HB2	3:G:119:LEU:CD1	2.27	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:37:GLY:HA3	3:H:87:GLU:OE2	1.97	0.64
1:A:332:LYS:O	1:A:336:GLU:HG3	1.98	0.64
1:C:76:LYS:O	1:C:108:ALA:HA	1.98	0.64
2:B:119:THR:HG22	2:B:120:GLU:H	1.63	0.64
1:A:35:ASN:CB	1:A:400:LEU:HD11	2.28	0.64
1:C:138:VAL:HG13	2:D:62:LEU:CD1	2.28	0.63
1:C:209:LYS:CE	1:C:263:GLU:OE1	2.45	0.63
2:D:47:THR:HA	2:D:52:TYR:CG	2.32	0.63
1:C:458:ILE:HG23	1:C:461:ARG:NH2	2.14	0.63
1:C:144:LEU:HD11	2:D:43:VAL:HG21	1.80	0.63
1:A:207:LEU:HD11	1:A:266:PRO:CG	2.28	0.63
1:C:359:ARG:NH1	1:C:359:ARG:HG3	2.12	0.63
1:C:423:SER:HB3	1:C:427:GLU:HG3	1.80	0.63
2:B:64:VAL:O	2:B:426:ASP:OD1	2.16	0.63
1:C:276:TYR:O	1:C:280:ASN:HB3	1.99	0.63
1:A:302:PRO:HD3	1:A:456:PHE:CG	2.34	0.63
1:C:58:THR:CG2	1:C:60:ARG:H	2.08	0.63
1:A:230:ASN:HB2	1:A:235:ALA:CB	2.28	0.63
2:D:128:GLN:NE2	2:D:168:ASN:ND2	2.46	0.63
1:C:9:VAL:O	1:C:13:ILE:HG13	1.98	0.63
1:A:276:TYR:O	1:A:280:ASN:HB3	1.99	0.63
1:A:35:ASN:HB2	1:A:400:LEU:CD1	2.29	0.63
1:C:433:LYS:CE	2:D:263:THR:HG23	2.28	0.63
1:C:178:ILE:O	1:C:180:PRO:HD2	1.99	0.63
2:B:3:GLN:HE21	2:B:3:GLN:CA	2.09	0.63
1:C:12:LEU:O	1:C:16:VAL:HG23	1.98	0.63
2:B:238:ARG:HD3	2:B:258:GLU:HG3	1.79	0.63
2:D:3:GLN:HE21	2:D:3:GLN:CA	2.09	0.63
3:E:98:ALA:O	3:E:102:VAL:HG23	1.98	0.63
2:D:502:LEU:HD22	2:D:523:ARG:HD3	1.80	0.63
3:G:45:THR:HG21	3:G:85:CYS:HB3	1.81	0.63
3:E:129:ASP:HB3	3:E:131:VAL:HG12	1.80	0.63
2:B:460:LYS:HE3	2:B:507:GLU:OE2	1.99	0.63
3:G:13:ILE:O	3:G:185:ASN:ND2	2.32	0.63
1:A:23:LYS:NZ	2:B:133:ASP:OD2	2.15	0.63
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.81	0.63
1:C:423:SER:CB	1:C:427:GLU:HG3	2.29	0.63
1:C:167:SER:OG	1:C:180:PRO:HG3	1.98	0.63
2:B:47:THR:OG1	2:B:431:ARG:NH1	2.31	0.63
1:A:419:ASP:O	1:A:437:PRO:HD2	1.99	0.62
2:B:225:ASN:HB2	2:B:290:THR:HA	1.81	0.62
1:C:253:TRP:HZ3	1:C:282:ILE:CD1	2.06	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:400:LEU:HD12	1:C:400:LEU:N	2.13	0.62
2:D:90:HIS:ND1	2:D:116:ASP:OD2	2.32	0.62
1:C:309:LEU:HD11	1:C:453:PHE:HE1	1.64	0.62
1:A:58:THR:CG2	1:A:60:ARG:HB2	2.28	0.62
3:H:134:GLY:O	3:H:137:MET:HB2	1.99	0.62
2:B:239:VAL:HG11	2:B:483:THR:HG21	1.80	0.62
3:G:23:VAL:HA	3:G:26:LEU:HB2	1.81	0.62
3:F:13:ILE:HA	3:F:187:ARG:NH2	2.12	0.62
3:F:7:ILE:HD12	3:F:19:THR:OG1	2.00	0.62
2:D:222:LYS:HG2	2:D:222:LYS:O	1.97	0.62
1:A:302:PRO:HD3	1:A:456:PHE:CD1	2.34	0.62
2:D:279:GLU:OE2	2:D:282:LYS:HD2	1.99	0.62
1:C:144:LEU:HD11	2:D:43:VAL:CG2	2.29	0.62
3:E:91:PRO:HD2	3:E:98:ALA:HB2	1.81	0.62
3:H:42:ALA:HA	3:H:87:GLU:OE1	1.99	0.62
3:G:57:ILE:HG12	3:G:75:VAL:HG21	1.82	0.62
3:E:166:LYS:O	3:E:169:VAL:HG12	2.00	0.62
1:A:170:LYS:O	1:A:178:ILE:HD12	1.99	0.62
3:E:87:GLU:OE2	3:E:87:GLU:HA	1.99	0.62
2:D:284:ALA:HB3	2:D:285:PRO:CD	2.30	0.62
2:B:499:ASN:O	2:B:503:GLU:HG3	2.00	0.62
3:H:16:SER:O	3:H:20:GLN:HG3	2.00	0.62
1:A:189:VAL:HG23	1:A:190:SER:H	1.65	0.62
1:A:280:ASN:H	1:A:280:ASN:HD22	1.45	0.62
1:C:298:ASN:CG	1:C:362:HIS:CD2	2.74	0.62
3:G:212:PRO:HB2	3:G:236:GLN:HE21	1.65	0.62
2:B:392:HIS:ND1	2:B:433:LEU:HD12	2.15	0.62
2:B:509:THR:HA	2:B:515:THR:HB	1.82	0.62
3:E:215:ASN:HA	3:E:218:GLN:OE1	2.00	0.62
2:B:520:ASP:O	2:D:449:LYS:NZ	2.33	0.62
3:F:57:ILE:HD12	3:F:105:ALA:HB1	1.81	0.61
1:A:75:ILE:HG21	1:A:78:MET:HE2	1.80	0.61
2:B:322:LEU:O	2:B:326:ASP:OD1	2.18	0.61
2:D:369:LEU:HD23	2:D:393:ILE:HA	1.82	0.61
3:F:195:LEU:O	3:F:198:ALA:HB3	2.00	0.61
3:F:86:VAL:HG21	3:F:109:LEU:HD11	1.82	0.61
3:G:129:ASP:HB3	3:G:131:VAL:HG12	1.82	0.61
2:B:471:PHE:CD2	2:B:472:PRO:CD	2.74	0.61
2:D:238:ARG:HE	2:D:258:GLU:HG2	1.63	0.61
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.31	0.61
1:C:218:SER:OG	1:C:269:LYS:HE2	2.00	0.61
2:B:375:PHE:HE2	2:B:470:GLY:HA2	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:300:PHE:HB3	1:C:366:ALA:HB2	1.82	0.61
1:C:444:TRP:CE3	1:C:444:TRP:HA	2.36	0.61
3:H:87:GLU:OE2	3:H:87:GLU:HA	2.01	0.61
3:G:204:GLY:O	3:G:254:VAL:HG21	2.00	0.61
3:E:131:VAL:HG22	3:E:132:CYS:N	2.15	0.61
1:C:274:HIS:O	1:C:358:LEU:CD1	2.48	0.61
3:E:217:VAL:HB	7:E:5292:ATP:C2	2.36	0.61
3:G:9:GLY:O	3:G:15:LYS:HE2	2.00	0.61
2:B:124:VAL:HG21	3:E:58:MET:HE1	1.82	0.61
3:E:23:VAL:CG1	3:E:33:VAL:HG11	2.31	0.61
1:A:219:THR:HG23	1:A:220:PRO:HD2	1.83	0.61
1:A:225:ILE:HD11	1:A:249:CYS:SG	2.39	0.61
2:D:70:CYS:O	2:D:193:HIS:HA	2.01	0.61
2:D:146:MET:CE	2:D:208:PHE:HZ	2.13	0.61
1:A:141:LEU:HD23	2:B:59:ARG:HD2	1.81	0.61
2:B:56:ASN:O	2:B:59:ARG:HB2	2.01	0.61
2:D:222:LYS:HA	2:D:288:LEU:CD2	2.31	0.61
1:A:332:LYS:HG2	1:A:336:GLU:OE2	2.00	0.61
2:B:328:PHE:O	2:B:332:VAL:HG23	2.01	0.61
1:C:96:ARG:HH11	1:C:96:ARG:HG2	1.66	0.61
2:B:302:LYS:O	2:B:306:GLU:HG3	2.01	0.61
3:G:223:ARG:O	3:G:224:ARG:HB2	2.01	0.61
2:D:317:ASN:ND2	2:D:317:ASN:H	1.98	0.61
3:G:106:ILE:CD1	3:G:137:MET:HB3	2.31	0.61
3:H:64:ALA:HB1	3:H:69:ASP:HB3	1.82	0.61
3:F:242:ALA:O	3:F:246:LYS:CG	2.43	0.60
1:C:57:MET:HE3	2:D:100:ARG:NH1	2.15	0.60
3:H:38:CYS:HB3	3:H:102:VAL:HG13	1.83	0.60
2:B:105:ARG:HB2	2:B:474:PHE:CE2	2.36	0.60
1:A:277:ARG:CZ	1:A:383:HIS:HD2	2.12	0.60
2:D:72:PRO:HB2	2:D:99:PHE:CZ	2.35	0.60
1:C:389:ARG:CG	1:C:389:ARG:NH1	2.61	0.60
3:E:237:ALA:O	3:E:241:ARG:HG3	2.01	0.60
2:D:370:TRP:HH2	2:D:448:GLY:HA3	1.66	0.60
1:A:309:LEU:HD11	1:A:453:PHE:HE1	1.66	0.60
1:A:355:ILE:O	1:A:380:GLU:HG2	2.01	0.60
1:C:178:ILE:HG22	1:C:180:PRO:HD3	1.83	0.60
2:B:422:TYR:HD2	2:B:425:LYS:HD2	1.64	0.60
1:C:222:ASP:OD1	1:C:248:ARG:NH1	2.34	0.60
2:B:131:MET:HG2	2:B:165:PHE:HB3	1.83	0.60
1:A:404:VAL:HG23	1:A:408:GLU:HB2	1.83	0.60
3:G:212:PRO:HB2	3:G:236:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:341:LYS:HD2	2:D:5:VAL:CG1	2.31	0.60
1:A:222:ASP:OD1	1:A:248:ARG:NH1	2.35	0.60
1:C:421:ILE:HD11	1:C:436:ILE:HG21	1.83	0.60
3:G:22:LEU:HD23	3:G:22:LEU:O	2.02	0.60
2:B:247:MET:HE3	2:B:340:ILE:HA	1.84	0.60
2:D:499:ASN:O	2:D:503:GLU:HG3	2.01	0.60
3:E:179:LEU:HD12	3:E:256:PRO:HG3	1.82	0.60
2:B:129:GLN:NE2	2:B:129:GLN:HA	2.17	0.60
2:B:236:ASN:HA	2:B:239:VAL:HG12	1.84	0.60
1:C:35:ASN:CB	1:C:400:LEU:HD11	2.32	0.60
2:D:328:PHE:O	2:D:332:VAL:HG23	2.02	0.60
3:E:243:LEU:O	3:E:247:VAL:HG23	2.02	0.60
1:C:433:LYS:HE3	2:D:263:THR:O	2.01	0.60
3:H:26:LEU:HD12	3:H:29:MET:CE	2.32	0.60
2:B:142:TYR:C	2:B:144:PRO:CD	2.69	0.60
1:C:186:PHE:HB3	2:D:154:MET:CE	2.31	0.60
1:A:9:VAL:O	1:A:13:ILE:HG13	2.01	0.59
2:B:503:GLU:HG2	2:D:476:ARG:HH11	1.66	0.59
2:D:119:THR:HG22	2:D:120:GLU:H	1.67	0.59
1:C:417:LYS:N	1:C:418:PRO:HD3	2.17	0.59
3:H:243:LEU:O	3:H:247:VAL:HG23	2.01	0.59
1:C:32:LEU:N	1:C:32:LEU:HD23	2.18	0.59
3:G:40:PRO:HG3	3:G:98:ALA:HB1	1.84	0.59
3:F:146:GLU:HG2	3:F:253:LEU:HD22	1.83	0.59
3:E:10:LYS:O	3:E:13:ILE:HG12	2.02	0.59
2:D:131:MET:HG2	2:D:165:PHE:HB3	1.83	0.59
1:A:355:ILE:HG21	1:A:359:ARG:HB2	1.83	0.59
2:D:59:ARG:NH1	2:D:429:HIS:CE1	2.71	0.59
3:F:20:GLN:NE2	3:F:47:LEU:HD12	2.18	0.59
3:G:217:VAL:HG22	3:G:227:VAL:CG2	2.31	0.59
2:D:394:LEU:HD23	2:D:394:LEU:C	2.23	0.59
1:C:230:ASN:HB2	1:C:235:ALA:HB3	1.82	0.59
2:B:81:GLY:CA	2:B:257:PRO:HD3	2.32	0.59
1:A:207:LEU:HD11	1:A:266:PRO:HG3	1.84	0.59
1:C:42:SER:HB3	1:C:46:ILE:HG22	1.83	0.59
1:C:280:ASN:H	1:C:280:ASN:HD22	1.49	0.59
2:B:212:SER:O	2:B:216:LYS:CE	2.45	0.59
2:D:236:ASN:HA	2:D:239:VAL:HG12	1.85	0.59
1:A:128:ASP:OD1	1:A:161:ASP:HB3	2.02	0.59
2:D:448:GLY:C	2:D:466:LEU:HD22	2.22	0.59
1:A:287:GLU:O	1:A:291:GLY:HA2	2.01	0.59
1:A:423:SER:OG	1:A:427:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:479:TRP:CZ3	2:D:326:ASP:HB3	2.36	0.59
1:C:96:ARG:NH1	1:C:96:ARG:HG2	2.18	0.59
3:F:45:THR:HG21	3:F:85:CYS:HB3	1.84	0.59
2:D:118:MET:HE1	2:D:155:ALA:HB2	1.85	0.59
3:F:106:ILE:HD12	3:F:137:MET:CG	2.32	0.59
1:C:424:GLY:CA	1:C:442:HIS:HD2	2.16	0.59
1:C:405:THR:OG1	1:C:408:GLU:CG	2.50	0.59
2:D:494:LEU:O	2:D:498:VAL:HG23	2.02	0.59
2:D:362:LEU:CD1	2:D:498:VAL:HG22	2.30	0.59
1:A:425:ILE:CD1	2:B:105:ARG:HG2	2.33	0.59
1:C:355:ILE:CG2	1:C:356:GLY:N	2.36	0.59
3:E:88:SER:HA	3:E:105:ALA:CB	2.33	0.59
3:F:198:ALA:HB1	3:F:267:LEU:HD21	1.84	0.59
1:C:433:LYS:CE	2:D:263:THR:O	2.50	0.59
2:B:213:MET:HE1	2:B:309:TRP:HA	1.84	0.59
2:B:494:LEU:O	2:B:498:VAL:HG23	2.03	0.59
1:C:230:ASN:OD1	1:C:233:GLY:CA	2.51	0.59
3:G:191:ARG:O	3:G:195:LEU:HB2	2.03	0.59
3:H:55:ASN:HD22	3:H:55:ASN:N	1.99	0.58
3:H:55:ASN:ND2	3:H:55:ASN:N	2.50	0.58
2:B:397:ASN:N	2:B:397:ASN:HD22	1.88	0.58
1:A:350:ARG:HD2	1:A:375:VAL:HG11	1.85	0.58
1:C:230:ASN:OD1	1:C:233:GLY:HA2	2.03	0.58
1:C:128:ASP:HB3	1:C:166:VAL:HG21	1.85	0.58
3:E:255:ILE:HG22	3:E:255:ILE:O	2.02	0.58
1:C:298:ASN:ND2	1:C:298:ASN:C	2.57	0.58
1:A:280:ASN:HD22	1:A:281:TYR:H	1.50	0.58
2:B:91:GLY:O	2:B:116:ASP:O	2.20	0.58
1:A:479:TRP:CD2	2:D:340:ILE:HD12	2.38	0.58
2:B:375:PHE:C	2:B:375:PHE:HD1	2.06	0.58
2:B:394:LEU:HD23	2:B:395:CYS:N	2.18	0.58
2:B:162:LEU:HD12	2:B:185:HIS:HD2	1.68	0.58
1:A:32:LEU:HD23	1:A:32:LEU:N	2.18	0.58
2:B:72:PRO:HB2	2:B:99:PHE:CZ	2.38	0.58
1:A:404:VAL:CG2	1:A:408:GLU:HB2	2.33	0.58
3:F:207:MET:HE3	3:F:210:PHE:HB2	1.86	0.58
2:D:124:VAL:HG21	3:G:58:MET:CE	2.33	0.58
1:C:75:ILE:HG21	1:C:78:MET:HE2	1.86	0.58
3:F:72:LEU:HD11	3:F:76:LEU:HD12	1.86	0.58
2:B:449:LYS:NZ	2:D:520:ASP:O	2.35	0.58
3:H:49:LEU:HD11	3:H:85:CYS:HB2	1.85	0.58
2:B:56:ASN:OD1	2:B:59:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:MET:HE1	1:A:309:LEU:HD22	1.84	0.58
1:C:299:PHE:HB3	1:C:452:GLY:H	1.69	0.58
3:E:91:PRO:HB2	3:E:95:VAL:O	2.03	0.58
3:F:148:TYR:CE2	3:F:208:ILE:HD12	2.39	0.58
2:D:130:ASN:N	2:D:130:ASN:HD22	2.00	0.58
3:F:57:ILE:HG13	3:F:75:VAL:HG11	1.86	0.58
2:D:128:GLN:O	2:D:132:LYS:HG3	2.03	0.58
2:B:246:GLU:OE2	2:B:343:SER:HB2	2.03	0.58
3:F:215:ASN:HA	3:F:218:GLN:OE1	2.04	0.58
2:B:283:ASP:O	2:B:283:ASP:OD1	2.22	0.58
2:D:151:THR:OG1	2:D:155:ALA:HB3	2.03	0.58
1:A:426:LYS:HE3	2:B:97:ALA:O	2.04	0.58
1:C:277:ARG:NH2	1:C:280:ASN:OD1	2.35	0.58
1:A:300:PHE:HB3	1:A:366:ALA:HB2	1.85	0.58
1:C:298:ASN:C	1:C:298:ASN:HD22	2.03	0.58
2:B:129:GLN:HE21	2:B:129:GLN:HA	1.69	0.58
1:C:419:ASP:O	1:C:437:PRO:HD2	2.04	0.58
2:B:124:VAL:HG21	3:E:58:MET:CE	2.34	0.58
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.84	0.58
2:B:523:ARG:HG3	2:D:475:ASP:HA	1.85	0.58
1:C:440:GLU:HB2	1:C:445:ASP:HB2	1.85	0.58
3:E:136:ALA:HB2	3:F:94:GLY:CA	2.34	0.58
2:B:314:PRO:CB	2:B:316:LEU:HD13	2.34	0.58
3:F:13:ILE:C	3:F:187:ARG:NH2	2.57	0.58
2:B:3:GLN:NE2	2:B:3:GLN:HA	2.17	0.58
2:B:457:HIS:HD2	2:D:512:MET:CB	2.15	0.58
1:A:224:ALA:CB	1:A:251:ALA:HB3	2.34	0.58
1:A:150:VAL:O	1:A:181:VAL:HG12	2.04	0.58
2:B:70:CYS:HB2	2:B:188:SER:HB3	1.85	0.58
3:E:115:TYR:O	3:E:117:ASP:N	2.30	0.58
1:C:444:TRP:HE3	1:C:444:TRP:HA	1.68	0.57
1:A:116:SER:O	1:A:130:LYS:CE	2.52	0.57
2:D:158:ILE:HG22	3:G:97:CYS:HB2	1.85	0.57
3:F:8:TYR:CE1	3:F:126:VAL:HG21	2.38	0.57
2:B:370:TRP:HH2	2:B:448:GLY:HA3	1.68	0.57
1:C:124:VAL:CG2	3:H:58:MET:CE	2.64	0.57
1:C:360:PRO:HB2	1:C:379:TYR:CZ	2.39	0.57
1:C:401:TYR:HB2	1:C:404:VAL:HB	1.85	0.57
1:C:66:GLY:O	1:C:70:VAL:HG22	2.04	0.57
2:B:57:PHE:HE2	2:B:425:LYS:NZ	2.01	0.57
1:A:210:ARG:NH1	1:A:264:LEU:HD21	2.19	0.57
2:D:375:PHE:C	2:D:375:PHE:HD1	2.06	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:35:ASN:HB2	1:C:400:LEU:CD1	2.34	0.57
3:G:131:VAL:HG22	3:G:132:CYS:N	2.19	0.57
1:A:400:LEU:N	1:A:400:LEU:HD12	2.19	0.57
1:A:231:ILE:O	1:A:234:ASP:OD2	2.23	0.57
2:B:467:ILE:HD13	2:B:497:LEU:HD23	1.87	0.57
3:F:49:LEU:O	3:F:50:HIS:CB	2.52	0.57
2:D:317:ASN:HD22	2:D:317:ASN:H	1.51	0.57
3:G:166:LYS:O	3:G:169:VAL:HG12	2.04	0.57
1:C:151:GLN:NE2	1:C:181:VAL:HG11	2.19	0.57
2:D:197:TRP:CE3	2:D:229:GLY:HA2	2.39	0.57
2:B:471:PHE:HD2	2:B:472:PRO:HD3	1.62	0.57
2:D:375:PHE:C	2:D:375:PHE:CD1	2.77	0.57
2:D:390:PRO:O	2:D:419:ALA:HB1	2.04	0.57
3:F:141:GLU:O	3:F:142:ASN:HB2	2.02	0.57
2:D:91:GLY:CA	2:D:118:MET:HE2	2.28	0.57
1:C:58:THR:HG22	1:C:59:ILE:N	2.19	0.57
3:H:45:THR:OG1	3:H:49:LEU:HD12	2.04	0.57
1:A:167:SER:HB2	1:A:180:PRO:CG	2.28	0.57
3:G:91:PRO:HB2	3:G:95:VAL:O	2.03	0.57
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.86	0.57
3:F:199:LEU:O	3:F:203:LEU:HB2	2.04	0.57
1:A:36:ASP:OD1	1:A:38:ALA:HB3	2.04	0.57
3:H:4:GLN:HB3	3:H:122:VAL:HB	1.87	0.57
1:C:299:PHE:CD2	1:C:305:THR:HG23	2.40	0.57
1:C:355:ILE:HD11	1:C:441:MET:CB	2.33	0.57
2:D:397:ASN:N	2:D:397:ASN:HD22	1.89	0.57
2:B:502:LEU:HD22	2:B:523:ARG:HD3	1.84	0.57
1:C:17:LEU:CD1	1:C:29:ASN:HA	2.35	0.57
2:B:375:PHE:C	2:B:375:PHE:CD1	2.77	0.57
2:B:375:PHE:CZ	2:B:469:ILE:HG22	2.39	0.57
1:A:124:VAL:HG21	3:F:58:MET:CE	2.35	0.57
1:C:352:MET:HE1	1:C:413:VAL:HA	1.86	0.57
2:D:128:GLN:NE2	2:D:165:PHE:HA	2.15	0.57
2:D:154:MET:O	2:D:158:ILE:HG12	2.04	0.57
3:F:23:VAL:HA	3:F:26:LEU:HB2	1.86	0.57
3:H:250:ASN:ND2	3:H:250:ASN:C	2.58	0.57
2:B:473:ILE:HG21	2:B:479:LEU:HD22	1.87	0.57
1:C:429:PHE:O	1:C:433:LYS:HG2	2.05	0.57
1:C:298:ASN:ND2	1:C:299:PHE:N	2.53	0.57
3:H:35:ILE:CD1	3:H:48:ILE:HD12	2.35	0.57
2:D:3:GLN:HA	2:D:3:GLN:NE2	2.17	0.57
2:D:238:ARG:NE	2:D:258:GLU:CG	2.60	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:280:ASN:HD22	1:C:281:TYR:H	1.53	0.57
1:C:34:VAL:CG1	1:C:397:SER:HA	2.35	0.57
1:A:446:TYR:CE2	2:D:522:VAL:CG2	2.87	0.57
1:A:446:TYR:HE2	2:D:522:VAL:CG2	2.18	0.57
3:H:26:LEU:HD12	3:H:29:MET:HE3	1.86	0.57
3:E:56:THR:HG23	3:E:59:GLU:CB	2.30	0.57
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.19	0.57
1:C:280:ASN:ND2	1:C:281:TYR:N	2.52	0.57
3:G:57:ILE:HG13	3:G:75:VAL:HG11	1.87	0.57
1:A:287:GLU:HA	1:A:292:ILE:H	1.69	0.57
3:H:94:GLY:O	3:H:95:VAL:HG23	2.04	0.57
3:E:208:ILE:O	3:E:246:LYS:HE3	2.05	0.57
3:F:106:ILE:HD11	3:F:138:PRO:CD	2.35	0.57
2:D:62:LEU:HD21	2:D:64:VAL:CG2	2.34	0.57
1:C:207:LEU:HD11	1:C:266:PRO:HD3	1.86	0.57
1:A:230:ASN:OD1	1:A:233:GLY:HA2	2.04	0.57
2:B:206:ARG:CG	2:B:304:PHE:CE1	2.88	0.57
1:A:251:ALA:HA	1:A:261:GLU:CG	2.34	0.57
1:C:425:ILE:HG22	8:C:3494:HCA:O3	2.05	0.57
3:G:16:SER:O	3:G:20:GLN:HG3	2.05	0.57
2:B:459:GLY:HA3	2:B:461:GLU:OE1	2.04	0.57
3:E:100:ARG:O	3:E:100:ARG:HD2	2.04	0.57
1:A:421:ILE:HD11	1:A:436:ILE:CG2	2.34	0.56
1:C:423:SER:OG	1:C:427:GLU:HG3	2.05	0.56
1:C:396:ASP:O	1:C:397:SER:HB2	2.05	0.56
3:F:107:ASN:O	3:F:111:GLU:HB2	2.05	0.56
2:D:456:LEU:HD13	2:D:463:GLU:OE2	2.05	0.56
3:F:56:THR:HG23	3:F:59:GLU:CB	2.35	0.56
1:A:68:LYS:HD3	1:A:68:LYS:O	2.06	0.56
1:A:380:GLU:HG3	1:A:381:PHE:CD2	2.41	0.56
1:C:351:VAL:HG11	1:C:367:TYR:CE2	2.40	0.56
3:H:45:THR:CG2	3:H:85:CYS:HB3	2.34	0.56
2:B:238:ARG:HD3	2:B:258:GLU:CD	2.26	0.56
1:C:144:LEU:CD1	2:D:43:VAL:HG21	2.35	0.56
1:A:429:PHE:HB2	2:B:110:PRO:HD3	1.86	0.56
3:H:141:GLU:O	3:H:142:ASN:CB	2.51	0.56
2:D:67:ALA:HB3	2:D:396:HIS:HB2	1.87	0.56
3:G:141:GLU:O	3:G:142:ASN:CB	2.52	0.56
2:D:403:LYS:HZ1	2:D:421:VAL:HB	1.68	0.56
3:G:57:ILE:HG12	3:G:75:VAL:HG11	1.88	0.56
3:F:45:THR:CG2	3:F:85:CYS:HB3	2.35	0.56
3:E:115:TYR:C	3:E:117:ASP:H	2.08	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:GLN:NE2	2:B:447:TYR:CZ	2.73	0.56
3:G:86:VAL:HG21	3:G:109:LEU:HD11	1.87	0.56
2:D:246:GLU:OE2	2:D:343:SER:HB2	2.05	0.56
3:G:72:LEU:HD11	3:G:76:LEU:HD12	1.87	0.56
2:D:442:MET:HG3	2:D:464:VAL:HG12	1.86	0.56
1:A:97:ARG:NH2	2:D:520:ASP:CG	2.58	0.56
1:C:97:ARG:CZ	1:C:446:TYR:HA	2.34	0.56
1:A:277:ARG:HE	1:A:383:HIS:HE2	1.52	0.56
2:B:309:TRP:O	2:B:310:LYS:HB2	2.04	0.56
2:B:503:GLU:HG2	2:D:476:ARG:NH1	2.21	0.56
2:B:375:PHE:HZ	2:B:469:ILE:HG22	1.69	0.56
2:D:314:PRO:CB	2:D:316:LEU:HD13	2.35	0.56
1:A:97:ARG:NH2	2:D:520:ASP:OD1	2.36	0.56
3:G:217:VAL:HG21	7:G:7292:ATP:C2	2.28	0.56
2:B:456:LEU:HD13	2:B:463:GLU:OE2	2.05	0.56
1:C:351:VAL:HG23	1:C:420:LEU:HB3	1.88	0.56
2:B:118:MET:HB3	2:B:154:MET:HE1	1.88	0.56
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.21	0.56
1:A:449:PRO:HG2	2:B:15:PHE:CZ	2.40	0.56
1:C:239:ARG:NH1	1:C:252:GLN:OE1	2.38	0.56
2:D:390:PRO:O	2:D:419:ALA:CB	2.54	0.56
1:A:458:ILE:HG23	1:A:461:ARG:NH2	2.20	0.56
3:H:57:ILE:HG13	3:H:75:VAL:HG11	1.88	0.56
2:D:442:MET:HG3	2:D:464:VAL:CG1	2.35	0.56
1:A:265:THR:HG22	1:A:286:MET:HE2	1.87	0.56
1:C:118:PHE:CZ	1:C:156:ILE:HD11	2.41	0.56
1:A:423:SER:CB	1:A:427:GLU:HG3	2.36	0.56
1:C:287:GLU:HA	1:C:292:ILE:H	1.69	0.56
2:B:239:VAL:HG11	2:B:483:THR:CG2	2.36	0.56
1:C:245:MET:HE1	1:C:309:LEU:HD22	1.88	0.56
1:C:426:LYS:NZ	2:D:97:ALA:CB	2.66	0.55
2:D:239:VAL:HG11	2:D:483:THR:CG2	2.36	0.55
2:D:289:ASN:ND2	2:D:314:PRO:HD3	2.21	0.55
3:F:137:MET:HB3	3:F:138:PRO:CD	2.36	0.55
2:D:67:ALA:HB3	2:D:396:HIS:CB	2.37	0.55
3:F:243:LEU:O	3:F:247:VAL:HG23	2.06	0.55
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.70	0.55
2:B:50:LYS:HG3	2:B:436:THR:HG22	1.87	0.55
1:A:280:ASN:ND2	1:A:281:TYR:N	2.54	0.55
2:D:59:ARG:HH12	2:D:429:HIS:CE1	2.25	0.55
1:C:265:THR:HG22	1:C:286:MET:HE2	1.88	0.55
1:C:210:ARG:HH11	1:C:264:LEU:CD2	2.17	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:517:TYR:O	1:C:99:TYR:HE1	1.85	0.55
1:C:358:LEU:O	1:C:362:HIS:HB2	2.06	0.55
2:B:125:PHE:CZ	3:E:58:MET:O	2.58	0.55
3:F:43:ASP:CB	3:F:46:ARG:HD3	2.34	0.55
1:A:70:VAL:CG2	1:A:71:VAL:N	2.69	0.55
2:D:88:TYR:HB2	2:D:147:ILE:CG2	2.37	0.55
1:C:235:ALA:HB1	1:C:252:GLN:NE2	2.20	0.55
1:A:17:LEU:HD21	1:A:28:ARG:HB2	1.88	0.55
1:C:358:LEU:HD22	9:C:3496:CFM:S4A	2.47	0.55
3:E:15:LYS:N	7:E:5292:ATP:O1B	2.40	0.55
1:A:37:PRO:HD3	1:A:396:ASP:HA	1.87	0.55
3:E:8:TYR:CE1	3:E:126:VAL:HG21	2.42	0.55
1:C:119:GLN:HA	1:C:119:GLN:OE1	2.05	0.55
1:A:351:VAL:HG11	1:A:367:TYR:CE2	2.41	0.55
1:C:351:VAL:CG1	1:C:374:VAL:HG22	2.36	0.55
1:C:346:LEU:HG	1:C:370:LEU:HD12	1.89	0.55
1:A:136:ASP:O	1:A:140:THR:HG22	2.07	0.55
2:B:238:ARG:HD3	2:B:258:GLU:CG	2.36	0.55
2:D:260:VAL:HG22	2:D:273:ALA:N	2.21	0.55
2:B:228:PRO:O	2:B:294:GLN:HG3	2.07	0.55
1:A:144:LEU:CG	2:B:43:VAL:HG21	2.37	0.55
2:B:422:TYR:CD2	2:B:425:LYS:HD2	2.42	0.55
3:G:61:ALA:HB2	3:G:70:LEU:CD1	2.36	0.55
2:D:90:HIS:O	2:D:151:THR:HA	2.05	0.55
1:A:355:ILE:CB	1:A:360:PRO:HD3	2.37	0.55
1:C:433:LYS:NZ	2:D:263:THR:HG22	2.22	0.55
3:G:14:GLY:HA3	3:G:185:ASN:HD22	1.70	0.55
3:F:13:ILE:C	3:F:187:ARG:HH21	2.09	0.55
1:A:277:ARG:NE	1:A:383:HIS:NE2	2.53	0.55
3:H:20:GLN:OE1	3:H:47:LEU:HB2	2.06	0.55
1:C:98:ASN:N	1:C:98:ASN:ND2	2.52	0.55
3:F:26:LEU:HD12	3:F:29:MET:HE3	1.87	0.55
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.89	0.55
1:A:138:VAL:HG23	1:A:139:GLU:H	1.72	0.55
1:A:151:GLN:HA	1:A:181:VAL:HG13	1.89	0.55
1:A:332:LYS:N	1:A:333:PRO:HD2	2.21	0.55
3:E:208:ILE:HG22	3:E:209:HIS:N	2.22	0.55
1:A:138:VAL:HG13	2:B:62:LEU:HD22	1.88	0.55
3:E:23:VAL:HA	3:E:26:LEU:HB2	1.88	0.55
2:D:128:GLN:NE2	2:D:168:ASN:HD22	2.01	0.55
3:H:138:PRO:O	3:H:143:LYS:CB	2.55	0.55
3:G:239:GLU:O	3:G:242:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:CYS:HA	1:A:358:LEU:HD13	1.87	0.54
1:C:380:GLU:HG3	1:C:381:PHE:CD2	2.42	0.54
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.07	0.54
1:A:99:TYR:CD1	2:D:517:TYR:O	2.61	0.54
1:C:346:LEU:HD11	1:C:463:MET:HB2	1.88	0.54
2:B:512:MET:HB3	2:D:457:HIS:CD2	2.30	0.54
1:C:224:ALA:CB	1:C:251:ALA:HB3	2.38	0.54
2:B:70:CYS:O	2:B:193:HIS:HA	2.06	0.54
2:B:434:VAL:HG12	2:B:439:PRO:HG2	1.88	0.54
2:D:219:GLY:N	2:D:287:ALA:O	2.40	0.54
1:C:355:ILE:CG2	1:C:360:PRO:HD3	2.37	0.54
3:E:61:ALA:HB1	3:E:67:VAL:HA	1.89	0.54
3:H:39:ASP:OD1	3:H:40:PRO:CD	2.56	0.54
1:C:332:LYS:N	1:C:333:PRO:HD2	2.22	0.54
1:A:225:ILE:CD1	1:A:249:CYS:SG	2.95	0.54
1:A:239:ARG:NH1	1:A:252:GLN:OE1	2.40	0.54
3:H:144:ALA:O	3:H:177:VAL:HG23	2.08	0.54
3:H:2:MET:HB2	3:H:119:LEU:O	2.07	0.54
3:F:213:ARG:HG2	7:F:6292:ATP:H2	1.72	0.54
1:A:134:LEU:HD12	2:B:61:ALA:O	2.08	0.54
2:B:457:HIS:CD2	2:D:512:MET:HB3	2.31	0.54
1:C:324:CYS:SG	1:C:328:ILE:HD11	2.48	0.54
1:C:41:GLN:HE21	1:C:43:LYS:HG3	1.73	0.54
3:E:12:GLY:HA2	3:F:156:MET:HE1	1.86	0.54
2:B:227:VAL:HG12	2:B:298:LEU:HD13	1.90	0.54
1:A:131:LEU:HD12	1:A:166:VAL:HG11	1.89	0.54
1:C:358:LEU:CD2	9:C:3496:CFM:S4A	2.96	0.54
2:B:217:VAL:O	2:B:286:ASN:HA	2.07	0.54
3:G:244:ALA:O	3:G:248:VAL:HG23	2.07	0.54
3:H:198:ALA:HB1	3:H:267:LEU:HD21	1.89	0.54
2:B:413:SER:OG	2:B:415:TYR:HD1	1.90	0.54
2:D:401:ARG:HB2	2:D:401:ARG:HH11	1.73	0.54
1:A:298:ASN:ND2	1:A:300:PHE:H	2.06	0.54
1:A:35:ASN:HD21	1:A:394:MET:HB2	1.73	0.54
1:A:81:ILE:HD13	1:A:134:LEU:CD2	2.37	0.54
2:B:146:MET:HA	2:B:179:PHE:CE2	2.41	0.54
2:B:118:MET:CE	2:B:127:GLY:HA3	2.37	0.54
2:D:375:PHE:HZ	2:D:469:ILE:HG22	1.72	0.54
3:E:195:LEU:HD21	3:E:268:LEU:CD2	2.38	0.54
3:E:165:SER:HB2	3:E:256:PRO:HB3	1.89	0.54
3:F:25:ALA:HB2	3:F:228:ILE:CD1	2.38	0.54
3:E:43:ASP:HB2	3:E:46:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:91:GLY:N	2:D:116:ASP:OD1	2.34	0.54
1:A:356:GLY:O	1:A:379:TYR:HD2	1.91	0.54
1:C:81:ILE:HD13	1:C:134:LEU:CD2	2.37	0.54
2:B:356:THR:HG22	1:C:471:CYS:SG	2.48	0.54
2:D:188:SER:HB3	10:D:3498:CLF:S3B	2.48	0.54
1:C:239:ARG:HG3	1:C:249:CYS:SG	2.48	0.54
2:B:81:GLY:O	2:B:275:GLY:HA2	2.07	0.54
3:H:187:ARG:NH2	3:H:195:LEU:HD22	2.23	0.54
1:A:265:THR:HB	1:A:266:PRO:HD3	1.88	0.54
2:D:314:PRO:HB2	2:D:316:LEU:HD13	1.88	0.54
2:D:473:ILE:HG21	2:D:479:LEU:HD22	1.90	0.54
1:A:230:ASN:HB2	1:A:235:ALA:HB3	1.87	0.54
2:D:124:VAL:HG11	3:G:58:MET:HE2	1.88	0.54
1:C:430:ILE:HG23	2:D:269:PHE:CD1	2.43	0.54
2:B:81:GLY:HA2	2:B:257:PRO:HD3	1.90	0.54
3:F:179:LEU:HB2	3:F:256:PRO:HG3	1.90	0.54
3:H:242:ALA:O	3:H:246:LYS:HG2	2.08	0.54
3:G:193:ASP:O	3:G:197:ILE:HG13	2.07	0.54
1:A:423:SER:HB3	1:A:427:GLU:HG3	1.90	0.54
3:H:23:VAL:HA	3:H:26:LEU:HB2	1.88	0.54
2:D:161:ASP:O	2:D:165:PHE:HD1	1.86	0.54
1:A:106:VAL:HG21	2:B:44:PHE:HB2	1.90	0.54
2:B:39:LYS:O	2:B:43:VAL:HG23	2.08	0.54
2:D:236:ASN:HB3	2:D:485:LEU:HD22	1.89	0.54
1:C:240:ILE:HG23	1:C:241:LEU:N	2.23	0.54
3:F:166:LYS:O	3:F:169:VAL:HG12	2.07	0.54
2:B:442:MET:HG3	2:B:464:VAL:HG12	1.90	0.54
3:E:186:SER:N	3:E:211:VAL:O	2.26	0.53
3:F:15:LYS:N	7:F:6292:ATP:O1B	2.41	0.53
7:G:7292:ATP:C5'	3:H:156:MET:SD	2.89	0.53
3:G:189:THR:HB	3:G:192:GLU:HG2	1.90	0.53
2:D:39:LYS:HA	2:D:42:GLU:HB2	1.90	0.53
2:D:238:ARG:HD3	2:D:258:GLU:CG	2.36	0.53
3:F:25:ALA:O	3:F:28:GLU:HB3	2.08	0.53
1:A:298:ASN:C	1:A:298:ASN:HD22	2.11	0.53
3:F:207:MET:HE1	3:F:210:PHE:HB2	1.91	0.53
1:C:70:VAL:CG2	1:C:71:VAL:N	2.71	0.53
3:E:57:ILE:CG1	3:E:75:VAL:HG11	2.38	0.53
1:C:458:ILE:HG22	1:C:462:ASP:OD2	2.08	0.53
3:F:3:ARG:HG3	3:F:3:ARG:HH11	1.73	0.53
2:B:418:ASN:ND2	2:B:418:ASN:O	2.41	0.53
1:A:99:TYR:HE2	1:A:232:GLY:HA2	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:186:SER:HB2	3:F:192:GLU:OE1	2.07	0.53
1:C:57:MET:HB2	2:D:142:TYR:OH	2.09	0.53
1:C:230:ASN:O	1:C:230:ASN:OD1	2.26	0.53
1:C:350:ARG:HD2	1:C:375:VAL:HG11	1.91	0.53
1:C:37:PRO:HD2	1:C:396:ASP:CG	2.29	0.53
2:D:91:GLY:O	2:D:116:ASP:O	2.27	0.53
1:C:60:ARG:HD3	1:C:190:SER:HB3	1.89	0.53
3:G:95:VAL:HG12	3:G:95:VAL:O	2.09	0.53
1:A:224:ALA:HB1	1:A:251:ALA:HB3	1.90	0.53
1:C:417:LYS:N	1:C:418:PRO:CD	2.72	0.53
1:A:299:PHE:CD2	1:A:305:THR:HG23	2.43	0.53
1:A:35:ASN:ND2	1:A:394:MET:HB2	2.23	0.53
1:C:30:LYS:NZ	1:C:47:ILE:CD1	2.71	0.53
1:C:186:PHE:HE1	3:G:100:ARG:NH2	2.02	0.53
2:D:369:LEU:CD2	2:D:393:ILE:HA	2.38	0.53
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.49	0.53
3:G:131:VAL:CG2	3:G:132:CYS:N	2.71	0.53
2:B:394:LEU:HD23	2:B:394:LEU:C	2.28	0.53
2:D:156:GLU:HG3	2:D:187:PRO:HA	1.91	0.53
1:A:59:ILE:HD13	1:A:427:GLU:OE2	2.09	0.53
3:H:138:PRO:O	3:H:143:LYS:HB2	2.08	0.53
1:C:14:GLN:O	1:C:18:GLU:HG3	2.08	0.53
2:D:375:PHE:CZ	2:D:469:ILE:HG22	2.42	0.53
1:C:306:ILE:HD11	1:C:335:TRP:NE1	2.23	0.53
1:A:15:GLU:O	1:A:18:GLU:HB2	2.09	0.53
2:B:241:LYS:O	2:B:245:SER:HB2	2.08	0.53
3:G:255:ILE:HG22	3:G:255:ILE:O	2.07	0.53
3:F:39:ASP:OD1	3:F:40:PRO:N	2.42	0.53
1:C:271:ASN:OD1	1:C:286:MET:HE2	2.09	0.53
3:E:35:ILE:CD1	3:E:48:ILE:CD1	2.79	0.53
1:A:124:VAL:HG21	3:F:58:MET:HE1	1.91	0.53
3:F:259:ILE:HD12	3:F:264:LEU:HD23	1.89	0.53
1:C:90:GLN:O	1:C:90:GLN:HG3	2.09	0.53
2:B:129:GLN:CA	2:B:129:GLN:HE21	2.22	0.53
2:D:139:LYS:HG3	2:D:179:PHE:CE1	2.43	0.53
1:C:99:TYR:HE2	1:C:232:GLY:HA2	1.74	0.53
2:D:322:LEU:HD11	2:D:348:ARG:HH21	1.73	0.53
3:E:61:ALA:N	3:E:70:LEU:HD11	2.24	0.53
1:C:277:ARG:NE	1:C:277:ARG:HA	2.23	0.53
1:C:302:PRO:HD3	1:C:456:PHE:CD1	2.44	0.53
2:D:76:VAL:HG13	2:D:87:PRO:HB3	1.90	0.53
3:H:61:ALA:HB1	3:H:67:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:237:ALA:O	3:G:241:ARG:HG3	2.09	0.53
1:C:57:MET:HE3	2:D:100:ARG:CZ	2.38	0.53
2:D:451:ILE:O	2:D:455:THR:HG23	2.09	0.53
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.44	0.53
1:C:298:ASN:ND2	1:C:300:PHE:H	2.07	0.53
2:B:38:ASP:O	2:B:42:GLU:HG3	2.08	0.53
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.90	0.53
3:H:217:VAL:HG11	7:H:8292:ATP:C8	2.44	0.53
1:C:428:LYS:HD2	1:C:440:GLU:HG3	1.91	0.53
2:D:289:ASN:HD21	2:D:314:PRO:HD3	1.74	0.53
1:C:200:ASP:O	1:C:203:ARG:HG3	2.09	0.53
2:B:351:LEU:O	2:B:355:MET:HG3	2.09	0.53
1:A:355:ILE:HD13	1:A:359:ARG:HB2	1.91	0.52
3:H:137:MET:CB	3:H:138:PRO:CD	2.87	0.52
3:G:33:VAL:HG22	3:G:121:PHE:HB2	1.91	0.52
1:A:424:GLY:HA2	1:A:442:HIS:HD2	1.73	0.52
3:E:4:GLN:CD	3:E:143:LYS:O	2.48	0.52
2:D:43:VAL:O	2:D:47:THR:HG23	2.10	0.52
2:D:516:ASP:O	2:D:519:HIS:HB2	2.09	0.52
3:H:217:VAL:HG11	7:H:8292:ATP:N7	2.24	0.52
2:D:81:GLY:O	2:D:275:GLY:HA2	2.08	0.52
1:C:428:LYS:HD2	1:C:440:GLU:CG	2.39	0.52
3:G:4:GLN:NE2	3:G:124:TYR:OH	2.41	0.52
2:D:184:ALA:O	2:D:186:THR:HG23	2.10	0.52
1:A:413:VAL:HG21	1:A:431:PHE:CE2	2.44	0.52
1:C:138:VAL:CG1	2:D:62:LEU:HD13	2.34	0.52
1:C:144:LEU:HG	2:D:43:VAL:HG21	1.90	0.52
1:C:224:ALA:HB1	1:C:251:ALA:HB3	1.91	0.52
1:C:13:ILE:O	1:C:17:LEU:HG	2.08	0.52
2:B:219:GLY:N	2:B:287:ALA:O	2.42	0.52
3:F:64:ALA:HB1	3:F:69:ASP:HB3	1.90	0.52
3:G:64:ALA:HB1	3:G:69:ASP:HB3	1.90	0.52
1:C:207:LEU:HD11	1:C:266:PRO:CD	2.40	0.52
1:A:67:SER:OG	1:A:183:CYS:HB3	2.10	0.52
1:C:440:GLU:HB2	1:C:445:ASP:CB	2.39	0.52
2:B:510:ARG:HG2	2:B:510:ARG:O	2.08	0.52
1:A:387:TYR:OH	1:A:402:ASP:HB2	2.10	0.52
1:C:58:THR:HG21	1:C:60:ARG:HB2	1.90	0.52
3:E:10:LYS:HZ3	3:E:156:MET:HG3	1.75	0.52
1:C:216:PHE:CE1	1:C:264:LEU:HD13	2.45	0.52
3:F:87:GLU:HA	3:F:87:GLU:OE2	2.10	0.52
2:B:116:ASP:OD1	2:B:116:ASP:N	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:57:PHE:CE2	2:B:425:LYS:NZ	2.77	0.52
2:D:68:LYS:HG2	2:D:396:HIS:CD2	2.39	0.52
3:H:154:GLU:O	3:H:158:MET:HG3	2.10	0.52
1:A:355:ILE:HG21	1:A:360:PRO:HD2	1.87	0.52
3:E:10:LYS:H	3:E:13:ILE:HD11	1.74	0.52
3:E:33:VAL:HG22	3:E:121:PHE:HB2	1.91	0.52
2:D:510:ARG:HB2	2:D:519:HIS:NE2	2.24	0.52
3:F:195:LEU:HD12	3:F:267:LEU:HD22	1.91	0.52
2:B:340:ILE:HD12	1:C:479:TRP:CD2	2.44	0.52
2:B:448:GLY:C	2:B:466:LEU:HD22	2.30	0.52
3:F:106:ILE:HD13	3:F:138:PRO:HD3	1.86	0.52
3:F:186:SER:HA	3:F:192:GLU:CD	2.30	0.52
1:A:382:ALA:HB1	1:A:386:ASP:CB	2.40	0.52
2:B:59:ARG:NH2	2:B:429:HIS:HE1	2.07	0.52
3:E:131:VAL:CG2	3:E:132:CYS:N	2.71	0.52
2:B:151:THR:HG23	2:B:186:THR:H	1.74	0.52
2:B:452:GLN:CD	2:D:510:ARG:NH1	2.63	0.52
3:E:61:ALA:HB2	3:E:70:LEU:CD1	2.35	0.52
3:H:212:PRO:HG2	3:H:239:GLU:OE2	2.09	0.52
2:B:451:ILE:O	2:B:455:THR:HG23	2.09	0.52
2:D:397:ASN:N	2:D:397:ASN:ND2	2.45	0.52
2:D:88:TYR:CB	2:D:147:ILE:HG22	2.40	0.52
2:B:442:MET:HG3	2:B:464:VAL:CG1	2.39	0.52
2:D:391:VAL:HG12	2:D:392:HIS:CE1	2.45	0.52
1:C:159:ILE:CD1	3:H:97:CYS:HB2	2.39	0.52
1:C:424:GLY:HA2	1:C:442:HIS:HD2	1.75	0.52
2:D:302:LYS:O	2:D:306:GLU:HG3	2.10	0.52
2:D:241:LYS:O	2:D:245:SER:HB2	2.10	0.52
1:A:72:TRP:CZ2	1:A:202:VAL:HG22	2.45	0.52
3:F:106:ILE:HD12	3:F:137:MET:HG2	1.93	0.51
1:C:421:ILE:HD11	1:C:436:ILE:CG2	2.38	0.51
3:G:185:ASN:HA	3:G:211:VAL:HB	1.92	0.51
1:A:136:ASP:OD1	1:A:170:LYS:NZ	2.28	0.51
3:F:57:ILE:CG1	3:F:75:VAL:HG11	2.40	0.51
1:A:355:ILE:CD1	1:A:359:ARG:HB2	2.40	0.51
2:B:391:VAL:HG12	2:B:392:HIS:CE1	2.45	0.51
1:C:40:THR:O	1:C:40:THR:CG2	2.57	0.51
1:A:131:LEU:HD11	1:A:135:ILE:HD11	1.93	0.51
3:G:223:ARG:HG2	3:G:223:ARG:O	2.11	0.51
2:D:197:TRP:HZ2	2:D:255:SER:HG	1.55	0.51
1:A:299:PHE:HB3	1:A:452:GLY:H	1.75	0.51
1:A:55:GLY:HA2	2:B:114:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:247:MET:HE3	2:D:340:ILE:HA	1.91	0.51
1:C:385:ASP:OD2	1:C:385:ASP:C	2.48	0.51
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.40	0.51
2:D:317:ASN:N	2:D:317:ASN:ND2	2.57	0.51
2:D:456:LEU:HD11	2:D:460:LYS:HD2	1.92	0.51
1:C:250:VAL:HG13	2:D:31:PHE:CD2	2.45	0.51
1:A:116:SER:HA	1:A:134:LEU:CD1	2.40	0.51
2:B:512:MET:HE1	2:D:44:PHE:HE1	1.76	0.51
2:B:512:MET:HE2	2:D:457:HIS:CG	2.45	0.51
2:B:156:GLU:HG3	2:B:187:PRO:HA	1.93	0.51
2:D:309:TRP:O	2:D:310:LYS:HB2	2.10	0.51
1:C:385:ASP:OD2	1:C:386:ASP:OD1	2.29	0.51
2:B:82:PHE:CZ	2:B:255:SER:HB2	2.46	0.51
3:G:148:TYR:CE2	3:G:208:ILE:HD12	2.45	0.51
2:D:293:LEU:HD22	2:D:319:PRO:HG2	1.91	0.51
2:B:289:ASN:ND2	2:B:314:PRO:CD	2.71	0.51
2:B:118:MET:HE3	2:B:160:ASP:OD2	2.11	0.51
1:C:35:ASN:ND2	1:C:395:GLY:O	2.44	0.51
2:B:434:VAL:HA	2:B:439:PRO:HD2	1.92	0.51
1:C:72:TRP:O	1:C:73:GLY:C	2.49	0.51
2:D:351:LEU:O	2:D:355:MET:HG3	2.09	0.51
1:C:116:SER:HA	1:C:134:LEU:CD1	2.41	0.51
1:C:449:PRO:CG	2:D:15:PHE:HZ	2.18	0.51
2:B:76:VAL:HG13	2:B:87:PRO:HB3	1.92	0.51
1:C:42:SER:O	1:C:46:ILE:O	2.28	0.51
1:C:221:TYR:O	1:C:223:VAL:HG13	2.10	0.51
2:D:509:THR:HG21	2:D:518:ASN:HD22	1.76	0.51
3:G:160:ALA:HA	3:G:163:ASN:HB3	1.93	0.51
2:D:263:THR:OG1	2:D:270:ARG:HD2	2.11	0.51
1:C:275:CYS:SG	1:C:278:SER:HB2	2.51	0.51
1:C:364:ILE:O	1:C:367:TYR:HB2	2.11	0.51
3:F:186:SER:HB3	3:F:210:PHE:HZ	1.65	0.51
2:D:206:ARG:HG2	2:D:304:PHE:CZ	2.45	0.51
3:G:208:ILE:O	3:G:246:LYS:HD3	2.11	0.51
1:A:337:ALA:HB1	2:B:5:VAL:HG21	1.93	0.51
3:E:217:VAL:HG22	3:E:227:VAL:HG21	1.93	0.51
3:H:40:PRO:HG3	3:H:98:ALA:HB1	1.93	0.51
2:B:445:ASN:OD1	2:B:447:TYR:HB2	2.11	0.51
3:E:206:GLN:NE2	3:E:250:ASN:OD1	2.44	0.51
3:E:73:GLU:OE1	3:E:73:GLU:N	2.44	0.51
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.91	0.51
3:F:10:LYS:O	3:F:13:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:181:VAL:N	2:B:182:PRO:HD3	2.26	0.51
2:B:422:TYR:HB3	2:B:425:LYS:HD2	1.91	0.51
3:G:98:ALA:O	3:G:102:VAL:HG23	2.10	0.51
1:C:277:ARG:HE	1:C:277:ARG:HA	1.76	0.51
1:A:280:ASN:N	1:A:280:ASN:ND2	2.58	0.51
1:A:355:ILE:HG22	1:A:360:PRO:HG2	1.92	0.51
1:A:16:VAL:HG11	1:A:408:GLU:HA	1.92	0.51
1:C:134:LEU:HG	2:D:62:LEU:HB2	1.92	0.51
3:E:10:LYS:H	3:E:13:ILE:HD13	1.75	0.51
3:F:16:SER:OG	7:F:6292:ATP:O2A	2.29	0.51
1:A:277:ARG:NE	1:A:383:HIS:HE2	2.08	0.51
2:D:125:PHE:HA	3:G:91:PRO:HB3	1.93	0.51
1:C:258:SER:HB2	1:C:261:GLU:HB2	1.93	0.51
2:B:523:ARG:CG	2:D:475:ASP:HA	2.40	0.51
1:C:200:ASP:HA	1:C:203:ARG:HG2	1.92	0.51
3:F:236:GLN:HG2	3:F:240:TYR:CE2	2.45	0.51
3:H:72:LEU:HD11	3:H:76:LEU:CD1	2.41	0.51
1:A:355:ILE:HG23	9:A:1496:CFM:S3A	2.51	0.50
1:C:351:VAL:HG12	1:C:374:VAL:HG22	1.94	0.50
3:H:49:LEU:O	3:H:50:HIS:CB	2.57	0.50
2:B:118:MET:HE2	2:B:127:GLY:HA3	1.93	0.50
2:B:88:TYR:HB2	2:B:147:ILE:HG23	1.92	0.50
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.26	0.50
3:E:52:LYS:O	3:E:53:ALA:CB	2.60	0.50
3:H:131:VAL:HG22	3:H:132:CYS:SG	2.51	0.50
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.12	0.50
1:C:471:CYS:SG	1:C:472:TRP:N	2.83	0.50
1:C:266:PRO:O	1:C:292:ILE:HD11	2.11	0.50
1:A:141:LEU:CD2	2:B:59:ARG:HD2	2.41	0.50
3:H:207:MET:CE	3:H:210:PHE:HB2	2.41	0.50
1:C:230:ASN:HB2	1:C:235:ALA:HB2	1.92	0.50
1:C:239:ARG:HB3	2:D:23:MET:HE1	1.94	0.50
1:C:34:VAL:HG13	1:C:397:SER:HA	1.94	0.50
1:C:241:LEU:HD21	1:C:453:PHE:HD1	1.75	0.50
2:B:222:LYS:HD3	2:B:288:LEU:HD21	1.93	0.50
2:B:390:PRO:O	2:B:419:ALA:HB1	2.11	0.50
3:H:107:ASN:O	3:H:111:GLU:HB2	2.10	0.50
3:F:52:LYS:O	3:F:53:ALA:HB2	2.11	0.50
2:D:146:MET:HA	2:D:179:PHE:CE2	2.45	0.50
2:D:146:MET:HE3	2:D:208:PHE:CZ	2.46	0.50
1:C:405:THR:H	1:C:408:GLU:HG3	1.76	0.50
2:B:118:MET:HB3	2:B:154:MET:CE	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:369:LEU:HD21	2:B:393:ILE:HG12	1.93	0.50
1:A:151:GLN:CD	1:A:181:VAL:HG11	2.32	0.50
3:G:115:TYR:C	3:G:117:ASP:N	2.64	0.50
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.26	0.50
2:B:70:CYS:CB	2:B:188:SER:HB3	2.41	0.50
3:G:96:GLY:O	3:H:132:CYS:HB2	2.12	0.50
3:H:179:LEU:HB2	3:H:256:PRO:HG3	1.94	0.50
1:C:429:PHE:CZ	2:D:108:ARG:HA	2.46	0.50
1:C:343:ARG:HG3	1:C:370:LEU:O	2.11	0.50
2:D:146:MET:HE3	2:D:208:PHE:HZ	1.76	0.50
2:B:206:ARG:CG	2:B:304:PHE:CZ	2.88	0.50
1:A:144:LEU:HD22	2:B:35:TYR:CD1	2.46	0.50
1:C:186:PHE:HB3	2:D:154:MET:HE2	1.93	0.50
1:A:46:ILE:HG12	1:A:47:ILE:N	2.25	0.50
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.46	0.50
2:B:284:ALA:HB3	2:B:285:PRO:CD	2.41	0.50
1:C:226:ILE:HG23	1:C:279:MET:HG2	1.93	0.50
3:H:73:GLU:N	3:H:73:GLU:OE1	2.44	0.50
2:D:91:GLY:N	2:D:118:MET:HE2	2.25	0.50
1:C:106:VAL:HG21	2:D:44:PHE:HB2	1.93	0.50
2:D:234:LEU:O	2:D:238:ARG:HG2	2.12	0.50
2:B:422:TYR:HD2	2:B:425:LYS:CD	2.23	0.50
1:C:277:ARG:NH1	1:C:383:HIS:CG	2.79	0.50
3:G:264:LEU:O	3:G:267:LEU:HB2	2.11	0.50
2:D:254:LEU:HB3	2:D:281:MET:HE2	1.94	0.50
2:D:254:LEU:HD13	2:D:281:MET:HE1	1.93	0.50
3:F:165:SER:HA	3:F:168:ILE:HD12	1.91	0.50
3:G:52:LYS:O	3:G:53:ALA:HB2	2.12	0.50
1:C:164:GLU:HA	1:C:180:PRO:HB3	1.93	0.50
3:H:54:GLN:HG3	3:H:55:ASN:N	2.21	0.50
2:B:522:VAL:HG23	1:C:446:TYR:CE2	2.46	0.50
2:D:39:LYS:O	2:D:43:VAL:HG23	2.12	0.50
3:G:225:MET:CE	3:G:230:TYR:HA	2.41	0.50
3:E:148:TYR:CD2	3:E:208:ILE:HD12	2.46	0.50
3:E:4:GLN:HB3	3:E:122:VAL:HB	1.94	0.50
1:A:57:MET:HE3	2:B:100:ARG:CZ	2.42	0.50
1:A:57:MET:CG	2:B:142:TYR:CZ	2.94	0.50
3:G:100:ARG:HD2	3:G:100:ARG:O	2.10	0.50
3:G:137:MET:CB	3:G:138:PRO:HD3	2.42	0.50
1:C:151:GLN:HA	1:C:181:VAL:HG13	1.93	0.50
1:A:430:ILE:HG12	2:B:269:PHE:CE1	2.47	0.50
1:A:359:ARG:HB2	1:A:360:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:342:TYR:O	1:C:343:ARG:C	2.50	0.50
1:A:230:ASN:HB2	1:A:235:ALA:HB2	1.92	0.50
3:F:201:ASN:C	3:F:203:LEU:H	2.15	0.50
1:A:354:TYR:CE1	1:A:404:VAL:HG12	2.46	0.50
2:D:180:PRO:HG2	2:D:278:GLN:OE1	2.12	0.50
2:D:445:ASN:OD1	2:D:447:TYR:HB2	2.12	0.50
1:C:231:ILE:O	1:C:234:ASP:OD2	2.30	0.50
3:H:103:ILE:HG12	3:H:137:MET:HG2	1.93	0.50
3:H:141:GLU:HA	3:H:141:GLU:OE1	2.12	0.50
2:D:382:PHE:HD1	2:D:385:GLU:OE2	1.95	0.50
3:F:231:ASP:OD2	3:F:234:ALA:HB2	2.11	0.50
3:F:131:VAL:HG22	3:F:132:CYS:SG	2.51	0.50
1:C:349:LYS:O	1:C:372:MET:HA	2.12	0.49
1:A:385:ASP:O	1:A:388:ASP:CG	2.51	0.49
2:D:510:ARG:O	2:D:510:ARG:CG	2.60	0.49
2:B:326:ASP:HB3	1:C:479:TRP:CZ3	2.43	0.49
2:B:326:ASP:OD2	2:B:348:ARG:NE	2.43	0.49
1:A:351:VAL:CG1	1:A:374:VAL:HG22	2.42	0.49
1:C:138:VAL:HG23	1:C:139:GLU:H	1.77	0.49
3:G:55:ASN:HB3	3:G:60:MET:SD	2.52	0.49
1:A:151:GLN:HA	1:A:181:VAL:CG1	2.42	0.49
1:A:62:CYS:O	1:A:191:GLN:HA	2.12	0.49
3:H:161:ALA:O	3:H:165:SER:OG	2.30	0.49
1:C:107:ASN:O	1:C:107:ASN:ND2	2.45	0.49
1:A:40:THR:O	1:A:40:THR:HG22	2.13	0.49
1:A:221:TYR:CE2	1:A:320:ILE:HD11	2.47	0.49
1:A:106:VAL:HG12	1:A:144:LEU:HD12	1.94	0.49
2:B:236:ASN:HB3	2:B:485:LEU:HD22	1.93	0.49
1:C:37:PRO:HG2	1:C:396:ASP:HB2	1.93	0.49
3:G:43:ASP:HB2	3:G:46:ARG:HD3	1.93	0.49
2:B:53:GLN:OE1	2:B:432:SER:HB3	2.12	0.49
1:A:298:ASN:ND2	1:A:298:ASN:C	2.65	0.49
2:B:156:GLU:CD	2:B:187:PRO:HG3	2.33	0.49
3:G:34:MET:HB2	3:G:119:LEU:HD11	1.92	0.49
2:B:247:MET:HB3	2:B:249:VAL:HG23	1.93	0.49
2:B:224:ILE:HD12	2:B:249:VAL:CG1	2.42	0.49
2:D:495:THR:HG22	2:D:499:ASN:ND2	2.27	0.49
3:E:141:GLU:HA	3:E:141:GLU:OE1	2.13	0.49
2:D:251:TYR:CD1	2:D:251:TYR:C	2.85	0.49
1:A:35:ASN:ND2	1:A:395:GLY:O	2.46	0.49
2:B:59:ARG:CZ	2:B:429:HIS:CE1	2.96	0.49
2:B:43:VAL:O	2:B:47:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:102:VAL:O	3:G:106:ILE:HG13	2.13	0.49
2:D:403:LYS:HZ2	2:D:421:VAL:HB	1.77	0.49
1:C:236:TRP:HA	2:D:23:MET:HE1	1.95	0.49
3:F:72:LEU:HD11	3:F:76:LEU:CD1	2.42	0.49
1:C:125:PHE:O	1:C:126:GLY:O	2.30	0.49
2:D:93:GLN:HB3	2:D:117:SER:OG	2.13	0.49
1:A:359:ARG:HG2	9:A:1496:CFM:S3A	2.52	0.49
1:A:196:HIS:HA	1:A:281:TYR:CD1	2.47	0.49
1:A:405:THR:H	1:A:408:GLU:HG3	1.77	0.49
3:G:192:GLU:HB3	3:G:210:PHE:CE2	2.44	0.49
1:C:280:ASN:N	1:C:280:ASN:ND2	2.59	0.49
3:F:195:LEU:HD21	3:F:268:LEU:CD2	2.40	0.49
1:A:203:ARG:HA	1:A:207:LEU:HB3	1.93	0.49
2:B:222:LYS:HA	2:B:288:LEU:HD21	1.95	0.49
1:A:83:HIS:O	1:A:153:GLU:HG3	2.12	0.49
3:E:10:LYS:O	3:E:11:GLY:C	2.49	0.49
3:G:110:GLU:OE2	3:G:143:LYS:NZ	2.45	0.49
3:E:180:GLY:HA2	3:E:253:LEU:HD23	1.93	0.49
2:D:19:ASP:OD2	2:D:20:TYR:N	2.45	0.49
1:C:272:LEU:HD13	1:C:312:ILE:HD13	1.93	0.49
3:G:50:HIS:NE2	3:G:229:GLU:OE2	2.40	0.49
2:B:249:VAL:HG13	2:B:336:SER:HB2	1.94	0.49
1:C:399:LEU:HD21	1:C:412:PHE:CD2	2.47	0.49
2:B:125:PHE:HE2	3:E:62:ALA:HB2	1.78	0.49
2:B:206:ARG:HH11	2:B:210:LEU:HD22	1.78	0.49
1:C:144:LEU:HD21	2:D:43:VAL:HG21	1.94	0.49
1:C:196:HIS:HA	1:C:281:TYR:CD1	2.47	0.49
1:C:280:ASN:O	1:C:284:ARG:HG3	2.13	0.49
1:A:210:ARG:HG3	1:A:263:GLU:HB3	1.95	0.49
1:A:203:ARG:HG3	1:A:204:ASP:OD2	2.12	0.49
2:B:296:TRP:CZ3	2:B:402:TRP:HA	2.47	0.49
1:A:399:LEU:HD21	1:A:412:PHE:CD2	2.47	0.49
2:D:64:VAL:HB	2:D:428:TRP:CB	2.43	0.49
1:C:342:TYR:OH	2:D:8:ILE:HD11	2.12	0.49
2:D:44:PHE:CD2	2:D:44:PHE:C	2.86	0.49
2:B:39:LYS:HA	2:B:42:GLU:HB2	1.95	0.49
1:C:76:LYS:HD3	1:C:256:ASP:OD2	2.13	0.49
2:D:197:TRP:CZ3	2:D:229:GLY:HA2	2.48	0.49
1:C:41:GLN:HG3	1:C:43:LYS:H	1.76	0.49
1:C:342:TYR:HA	1:C:345:ARG:HD2	1.94	0.48
1:A:138:VAL:HG23	1:A:139:GLU:N	2.27	0.48
3:F:61:ALA:HB1	3:F:67:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:186:SER:C	3:F:188:ASN:H	2.17	0.48
2:B:227:VAL:CG1	2:B:298:LEU:HD13	2.43	0.48
3:G:39:ASP:OD1	3:G:40:PRO:HD2	2.13	0.48
3:H:231:ASP:OD2	3:H:234:ALA:CB	2.56	0.48
2:B:107:PHE:CZ	2:B:232:THR:HB	2.48	0.48
2:B:133:ASP:O	2:B:136:GLN:N	2.46	0.48
2:D:254:LEU:O	2:D:255:SER:CB	2.61	0.48
3:E:43:ASP:HB2	3:E:46:ARG:HD3	1.93	0.48
3:E:264:LEU:O	3:E:267:LEU:HB2	2.13	0.48
1:A:298:ASN:HD22	1:A:299:PHE:N	2.10	0.48
1:C:167:SER:HB3	1:C:180:PRO:HD3	1.95	0.48
2:D:146:MET:CE	2:D:208:PHE:HE1	2.26	0.48
2:B:161:ASP:O	2:B:165:PHE:HD1	1.89	0.48
3:E:38:CYS:HB3	3:E:102:VAL:HG13	1.95	0.48
3:G:2:MET:HB2	3:G:119:LEU:O	2.13	0.48
1:C:98:ASN:HD22	1:C:98:ASN:N	2.09	0.48
1:A:349:LYS:O	1:A:372:MET:HA	2.13	0.48
1:A:449:PRO:CG	2:B:15:PHE:HZ	2.25	0.48
2:D:495:THR:HG22	2:D:499:ASN:HD22	1.78	0.48
2:B:241:LYS:NZ	2:B:256:ASP:OD2	2.45	0.48
3:F:255:ILE:HG22	3:F:255:ILE:O	2.12	0.48
2:B:422:TYR:OH	2:B:433:LEU:HD11	2.13	0.48
2:D:12:TYR:O	2:D:12:TYR:CD2	2.66	0.48
1:A:110:VAL:C	1:A:112:MET:H	2.15	0.48
2:D:199:ASN:HD22	2:D:199:ASN:N	2.10	0.48
1:A:58:THR:HG22	1:A:59:ILE:N	2.28	0.48
3:H:23:VAL:HG21	3:H:35:ILE:CD1	2.28	0.48
1:C:66:GLY:HA2	1:C:70:VAL:HG13	1.95	0.48
2:B:278:GLN:HG2	2:B:278:GLN:H	1.50	0.48
3:G:115:TYR:O	3:G:117:ASP:N	2.38	0.48
1:A:416:ILE:C	1:A:418:PRO:HD3	2.34	0.48
1:A:167:SER:HB3	1:A:178:ILE:HG22	1.94	0.48
2:B:186:THR:N	2:B:187:PRO:HD3	2.29	0.48
1:C:251:ALA:HA	1:C:261:GLU:CG	2.41	0.48
1:C:430:ILE:HG12	2:D:269:PHE:HE1	1.75	0.48
3:H:165:SER:HA	3:H:168:ILE:HD12	1.96	0.48
3:G:224:ARG:C	3:G:225:MET:CG	2.82	0.48
1:C:245:MET:CE	1:C:309:LEU:HD22	2.43	0.48
2:B:471:PHE:CE2	2:B:472:PRO:HD3	2.41	0.48
3:E:156:MET:HG2	3:E:157:ALA:N	2.29	0.48
2:D:238:ARG:NH1	2:D:262:ASP:OD2	2.46	0.48
1:A:68:LYS:C	1:A:68:LYS:HD3	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:TRP:O	1:A:73:GLY:C	2.51	0.48
3:G:14:GLY:HA3	3:G:185:ASN:ND2	2.29	0.48
1:C:389:ARG:HG3	1:C:389:ARG:NH1	2.11	0.48
2:B:44:PHE:CD2	2:B:44:PHE:C	2.86	0.48
2:D:479:LEU:HD12	2:D:479:LEU:N	2.28	0.48
2:B:388:CYS:O	2:B:390:PRO:HD3	2.14	0.48
1:A:324:CYS:SG	1:A:328:ILE:HD11	2.53	0.48
1:A:351:VAL:HG23	1:A:420:LEU:HB3	1.95	0.48
1:A:81:ILE:HD12	1:A:148:ILE:HG21	1.95	0.48
1:A:219:THR:C	1:A:221:TYR:H	2.17	0.48
2:B:362:LEU:HD11	2:B:498:VAL:CG2	2.42	0.48
2:B:247:MET:HA	2:B:341:PRO:HG3	1.96	0.48
2:B:81:GLY:HA3	2:B:257:PRO:HD3	1.96	0.48
2:B:192:SER:OG	2:B:194:VAL:HG22	2.14	0.48
1:C:125:PHE:C	1:C:126:GLY:O	2.49	0.48
2:D:20:TYR:O	2:D:24:LEU:HG	2.13	0.48
3:E:72:LEU:HD11	3:E:76:LEU:CD1	2.44	0.48
3:E:160:ALA:HA	3:E:163:ASN:HB3	1.96	0.48
1:A:373:GLU:HG3	1:A:373:GLU:O	2.12	0.48
1:C:355:ILE:HG21	1:C:359:ARG:HB2	1.96	0.48
2:D:146:MET:HG2	2:D:180:PRO:O	2.13	0.48
2:B:475:ASP:HA	2:D:523:ARG:HG3	1.95	0.48
2:B:247:MET:CE	2:B:340:ILE:HA	2.44	0.48
3:G:72:LEU:HD11	3:G:76:LEU:CD1	2.43	0.48
3:H:151:CYS:SG	3:H:196:ILE:HD12	2.54	0.48
1:A:119:GLN:HA	1:A:119:GLN:OE1	2.12	0.48
3:F:16:SER:O	3:F:20:GLN:HG3	2.13	0.47
1:C:457:ALA:CB	2:D:3:GLN:HG2	2.44	0.47
2:B:181:VAL:O	2:B:181:VAL:HG12	2.12	0.47
3:G:132:CYS:HB2	3:H:96:GLY:O	2.14	0.47
1:C:428:LYS:O	1:C:432:GLN:HG3	2.14	0.47
2:B:108:ARG:NH2	2:B:477:HIS:CD2	2.82	0.47
2:D:89:VAL:HG22	2:D:150:SER:HB2	1.96	0.47
1:A:240:ILE:HG23	1:A:241:LEU:N	2.29	0.47
1:A:280:ASN:H	1:A:280:ASN:ND2	2.10	0.47
1:C:138:VAL:O	1:C:142:PHE:N	2.42	0.47
3:F:213:ARG:HG2	7:F:6292:ATP:C2	2.49	0.47
3:H:56:THR:CG2	3:H:59:GLU:HB2	2.28	0.47
2:D:238:ARG:HG3	2:D:238:ARG:HH21	1.78	0.47
1:C:337:ALA:HB1	2:D:5:VAL:HG21	1.96	0.47
3:F:201:ASN:C	3:F:203:LEU:N	2.66	0.47
2:B:86:MET:HG2	2:B:138:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:22:LEU:O	3:E:22:LEU:HD23	2.14	0.47
1:C:142:PHE:O	1:C:145:ASN:ND2	2.47	0.47
2:B:475:ASP:HA	2:D:523:ARG:CG	2.44	0.47
2:D:379:LEU:HD21	2:D:443:ILE:HG21	1.95	0.47
1:C:277:ARG:HD2	1:C:386:ASP:OD2	2.14	0.47
2:B:180:PRO:HG2	2:B:278:GLN:OE1	2.14	0.47
2:B:254:LEU:O	2:B:255:SER:HB3	2.14	0.47
3:E:207:MET:HE3	3:E:210:PHE:HB2	1.94	0.47
1:A:301:GLY:HA2	1:A:456:PHE:CD1	2.48	0.47
3:H:179:LEU:HD23	3:H:181:GLY:H	1.79	0.47
3:E:106:ILE:HD12	3:E:137:MET:HB3	1.95	0.47
2:D:192:SER:OG	2:D:194:VAL:HG22	2.14	0.47
1:A:355:ILE:CG2	9:A:1496:CFM:S3A	3.02	0.47
1:A:16:VAL:HG21	1:A:412:PHE:CE1	2.48	0.47
2:D:217:VAL:O	2:D:286:ASN:HA	2.14	0.47
2:B:139:LYS:CG	2:B:179:PHE:CE1	2.97	0.47
2:B:85:THR:CG2	2:B:146:MET:CE	2.91	0.47
1:C:219:THR:HG23	1:C:220:PRO:HD2	1.96	0.47
2:D:509:THR:HA	2:D:515:THR:HB	1.96	0.47
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.95	0.47
1:A:449:PRO:O	1:A:455:GLY:HA2	2.13	0.47
1:C:302:PRO:O	1:C:306:ILE:HG13	2.15	0.47
2:B:71:GLN:HG2	2:B:192:SER:O	2.15	0.47
2:B:318:ILE:O	2:B:318:ILE:HG23	2.15	0.47
3:G:216:VAL:O	3:G:216:VAL:HG12	2.15	0.47
3:H:208:ILE:HG22	3:H:209:HIS:N	2.30	0.47
1:C:361:ARG:HB3	1:C:379:TYR:OH	2.13	0.47
3:E:10:LYS:NZ	3:E:156:MET:HG3	2.29	0.47
1:C:20:TYR:HH	1:C:408:GLU:HG2	1.73	0.47
2:B:247:MET:HE2	2:B:339:PRO:O	2.13	0.47
3:H:179:LEU:HD12	3:H:256:PRO:HG3	1.96	0.47
3:E:236:GLN:O	3:E:236:GLN:CG	2.62	0.47
1:A:298:ASN:CG	1:A:362:HIS:CD2	2.88	0.47
1:A:399:LEU:HD23	1:A:416:ILE:HD11	1.97	0.47
1:A:427:GLU:HB2	1:A:431:PHE:HE1	1.78	0.47
2:B:522:VAL:HB	2:D:474:PHE:HB3	1.96	0.47
2:D:494:LEU:HD23	2:D:494:LEU:C	2.35	0.47
2:D:509:THR:O	2:D:516:ASP:HA	2.15	0.47
2:B:392:HIS:CG	2:B:433:LEU:HD12	2.49	0.47
2:D:369:LEU:HD23	2:D:369:LEU:O	2.14	0.47
3:G:34:MET:HB2	3:G:119:LEU:HD13	1.96	0.47
3:F:3:ARG:NH2	3:F:146:GLU:OE1	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:203:ARG:HG3	1:C:204:ASP:OD2	2.15	0.47
1:A:424:GLY:CA	1:A:442:HIS:HD2	2.27	0.47
2:B:382:PHE:HD1	2:B:385:GLU:OE2	1.98	0.47
1:A:118:PHE:CZ	1:A:156:ILE:HD11	2.49	0.47
1:A:352:MET:CE	1:A:418:PRO:HG2	2.45	0.47
1:A:58:THR:CG2	1:A:60:ARG:H	2.20	0.47
1:C:60:ARG:HG2	1:C:380:GLU:O	2.14	0.47
1:C:138:VAL:HG23	1:C:139:GLU:N	2.30	0.47
1:C:346:LEU:HB3	1:C:372:MET:CG	2.45	0.47
1:A:57:MET:SD	2:B:113:CYS:O	2.73	0.47
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.50	0.47
2:B:512:MET:CB	2:D:457:HIS:CD2	2.92	0.47
2:B:512:MET:HE2	2:D:457:HIS:HB2	1.94	0.47
1:A:144:LEU:HG	2:B:43:VAL:HG21	1.96	0.47
3:G:137:MET:O	3:G:143:LYS:HG3	2.15	0.47
3:G:50:HIS:O	3:G:51:SER:HB3	2.14	0.47
2:B:367:PHE:CD2	2:B:443:ILE:HD11	2.49	0.47
1:A:210:ARG:HH11	1:A:264:LEU:CD2	2.26	0.47
3:E:57:ILE:HD12	3:E:105:ALA:HB1	1.96	0.47
3:F:26:LEU:CD1	3:F:244:ALA:HB1	2.43	0.47
1:A:168:LYS:O	1:A:172:ALA:CB	2.61	0.47
2:B:71:GLN:O	2:B:196:GLY:HA3	2.15	0.47
2:D:254:LEU:O	2:D:255:SER:HB3	2.14	0.47
1:C:168:LYS:O	1:C:172:ALA:HB2	2.15	0.47
3:G:147:ILE:HD11	3:G:177:VAL:HG21	1.97	0.47
1:A:42:SER:C	1:A:44:LYS:N	2.65	0.47
3:G:180:GLY:HA2	3:G:253:LEU:HD23	1.96	0.47
1:A:100:TYR:N	1:A:100:TYR:CD2	2.83	0.47
3:F:223:ARG:O	3:F:223:ARG:HG2	2.14	0.47
1:A:359:ARG:O	1:A:363:VAL:HG13	2.15	0.47
1:C:442:HIS:HA	9:C:3496:CFM:S4B	2.55	0.47
3:F:13:ILE:CA	3:F:187:ARG:NH2	2.73	0.47
3:E:39:ASP:OD1	3:E:40:PRO:N	2.47	0.47
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.96	0.47
3:G:199:LEU:CD1	3:G:259:ILE:HD11	2.45	0.47
2:D:96:VAL:CG1	2:D:113:CYS:SG	3.03	0.47
2:B:495:THR:HG22	2:B:499:ASN:ND2	2.30	0.47
3:F:146:GLU:HG2	3:F:253:LEU:CD2	2.45	0.47
1:C:373:GLU:HG3	1:C:373:GLU:O	2.15	0.47
2:D:90:HIS:HA	2:D:116:ASP:OD1	2.15	0.47
1:A:426:LYS:HA	2:B:104:ASN:HD21	1.79	0.47
1:C:413:VAL:HG21	1:C:431:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:156:MET:HE3	3:F:12:GLY:HA2	1.97	0.47
1:C:97:ARG:NH1	1:C:446:TYR:CA	2.74	0.47
1:C:20:TYR:OH	1:C:408:GLU:CG	2.56	0.47
3:F:43:ASP:N	3:F:43:ASP:OD1	2.47	0.47
2:D:284:ALA:CB	2:D:285:PRO:CD	2.92	0.47
3:G:223:ARG:HD2	3:G:230:TYR:CE1	2.50	0.47
3:G:195:LEU:HD21	3:G:268:LEU:CD2	2.45	0.47
1:A:145:ASN:ND2	1:A:147:GLY:H	2.13	0.47
1:C:464:ASP:OD1	1:C:468:ASN:ND2	2.48	0.47
1:A:158:LEU:HD21	2:B:123:ALA:HB1	1.96	0.47
1:A:253:TRP:CZ3	1:A:282:ILE:HG12	2.49	0.47
2:B:106:HIS:CE1	2:B:471:PHE:HD1	2.32	0.47
1:C:207:LEU:HD11	1:C:266:PRO:CG	2.45	0.47
3:H:57:ILE:CG1	3:H:75:VAL:HG11	2.45	0.47
1:C:399:LEU:C	1:C:400:LEU:HD12	2.35	0.47
2:D:456:LEU:CD1	2:D:460:LYS:HD2	2.44	0.47
1:A:428:LYS:HG2	1:A:438:PHE:CD2	2.50	0.47
2:B:163:ASN:OD1	2:B:167:ASN:ND2	2.48	0.47
3:F:46:ARG:NH2	3:F:221:GLU:HG3	2.30	0.46
2:D:105:ARG:HB2	2:D:474:PHE:CE2	2.50	0.46
3:G:22:LEU:HD23	3:G:22:LEU:C	2.34	0.46
2:D:370:TRP:HA	2:D:394:LEU:O	2.15	0.46
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.55	0.46
2:B:506:ASP:O	2:B:510:ARG:HB2	2.15	0.46
3:G:148:TYR:CE2	3:G:208:ILE:CD1	2.99	0.46
3:E:250:ASN:ND2	3:E:252:LEU:H	2.14	0.46
2:B:380:VAL:O	2:B:383:LEU:HB2	2.15	0.46
1:A:245:MET:HG3	1:A:324:CYS:HA	1.97	0.46
1:A:86:VAL:HG21	2:B:68:LYS:HE2	1.97	0.46
2:B:238:ARG:CD	2:B:258:GLU:CG	2.90	0.46
2:D:493:ILE:O	2:D:497:LEU:HG	2.14	0.46
3:G:19:THR:O	3:G:23:VAL:HG22	2.16	0.46
1:C:428:LYS:HG3	1:C:438:PHE:CD2	2.51	0.46
2:B:376:VAL:O	2:B:380:VAL:HG23	2.14	0.46
1:C:91:TYR:OH	2:D:73:LEU:HB2	2.15	0.46
2:D:163:ASN:OD1	2:D:167:ASN:ND2	2.49	0.46
2:D:62:LEU:CD2	2:D:64:VAL:HG23	2.46	0.46
1:C:64:TYR:HB2	10:D:3498:CLF:S3A	2.56	0.46
1:C:150:VAL:O	1:C:181:VAL:HG12	2.15	0.46
1:C:203:ARG:NE	1:C:204:ASP:OD2	2.48	0.46
3:E:22:LEU:C	3:E:22:LEU:HD23	2.36	0.46
2:B:226:ILE:O	2:B:228:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:41:LYS:O	3:H:42:ALA:HB3	2.15	0.46
3:H:187:ARG:O	3:H:188:ASN:HB3	2.16	0.46
1:A:48:SER:HB3	1:A:387:TYR:CE1	2.51	0.46
2:B:401:ARG:HH11	2:B:401:ARG:HB2	1.81	0.46
1:A:358:LEU:HD12	1:A:361:ARG:HH21	1.80	0.46
3:H:61:ALA:HB2	3:H:70:LEU:HD12	1.96	0.46
1:A:385:ASP:OD1	1:A:386:ASP:OD1	2.33	0.46
2:D:369:LEU:HD12	2:D:379:LEU:HD23	1.97	0.46
1:C:276:TYR:O	1:C:276:TYR:CG	2.68	0.46
1:C:229:TYR:N	1:C:229:TYR:CD1	2.83	0.46
2:B:326:ASP:O	2:B:330:MET:HG3	2.15	0.46
3:H:66:THR:O	3:H:69:ASP:HB2	2.15	0.46
3:E:148:TYR:CE2	3:E:208:ILE:CD1	2.99	0.46
1:A:89:GLY:C	1:A:113:ASN:ND2	2.69	0.46
1:A:142:PHE:N	1:A:143:PRO:HD3	2.31	0.46
3:F:73:GLU:N	3:F:73:GLU:OE1	2.45	0.46
2:B:474:PHE:HB3	2:D:522:VAL:HB	1.96	0.46
3:G:39:ASP:OD1	3:G:40:PRO:N	2.49	0.46
3:H:39:ASP:OD2	3:H:41:LYS:HB2	2.16	0.46
1:A:98:ASN:H	1:A:98:ASN:HD22	1.61	0.46
3:H:187:ARG:HH21	3:H:195:LEU:HD22	1.80	0.46
3:H:76:LEU:HD21	3:H:84:LYS:HD3	1.97	0.46
2:D:90:HIS:HB3	2:D:150:SER:O	2.15	0.46
1:A:425:ILE:HG22	8:A:1494:HCA:C6	2.46	0.46
3:G:212:PRO:O	7:G:7292:ATP:N6	2.44	0.46
3:F:57:ILE:HG13	3:F:87:GLU:O	2.16	0.46
1:A:128:ASP:HB3	1:A:166:VAL:CG2	2.41	0.46
1:A:131:LEU:CD1	1:A:166:VAL:HG11	2.45	0.46
2:D:448:GLY:O	2:D:466:LEU:HD22	2.15	0.46
1:C:51:LYS:HE3	2:D:119:THR:OG1	2.15	0.46
3:H:183:ILE:HD13	3:H:243:LEU:HD11	1.98	0.46
1:A:90:GLN:NE2	2:B:447:TYR:CE1	2.84	0.46
1:C:58:THR:CG2	1:C:60:ARG:HB2	2.45	0.46
2:B:227:VAL:HG12	2:B:298:LEU:CD1	2.45	0.46
3:G:179:LEU:CD1	3:G:256:PRO:HG3	2.46	0.46
2:B:257:PRO:HB3	2:B:261:LEU:HD22	1.98	0.46
1:A:458:ILE:HG22	1:A:462:ASP:OD2	2.16	0.46
3:H:129:ASP:HB3	3:H:131:VAL:HG12	1.98	0.46
2:B:222:LYS:HA	2:B:288:LEU:CD2	2.46	0.46
3:H:181:GLY:HA2	3:H:205:THR:OG1	2.16	0.46
3:E:58:MET:SD	3:E:104:THR:HG21	2.56	0.46
1:C:449:PRO:O	1:C:455:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:144:LEU:CD2	2:D:43:VAL:HG21	2.46	0.46
1:C:186:PHE:CE1	3:G:100:ARG:NH2	2.81	0.46
1:C:302:PRO:HG3	1:C:335:TRP:HB2	1.98	0.46
1:C:168:LYS:O	1:C:172:ALA:CB	2.64	0.46
2:B:318:ILE:HD12	2:B:374:ASP:HB3	1.98	0.46
1:A:22:GLU:HA	1:A:25:ARG:HB3	1.98	0.46
2:D:157:VAL:C	2:D:159:GLY:H	2.19	0.46
2:D:418:ASN:ND2	2:D:418:ASN:O	2.49	0.46
2:D:38:ASP:O	2:D:42:GLU:HG3	2.16	0.45
2:B:147:ILE:O	2:B:181:VAL:HA	2.15	0.45
3:E:50:HIS:O	3:E:51:SER:HB3	2.15	0.45
1:C:416:ILE:C	1:C:418:PRO:HD3	2.37	0.45
3:H:72:LEU:HD11	3:H:76:LEU:HD12	1.98	0.45
2:B:390:PRO:O	2:B:419:ALA:CB	2.64	0.45
3:E:72:LEU:HD11	3:E:76:LEU:HD12	1.98	0.45
1:A:297:TYR:HB2	1:A:308:SER:OG	2.16	0.45
1:C:380:GLU:HG3	1:C:381:PHE:HD2	1.81	0.45
2:B:227:VAL:HB	2:B:292:LEU:HD23	1.97	0.45
2:D:380:VAL:O	2:D:383:LEU:HB2	2.17	0.45
1:C:165:SER:O	1:C:168:LYS:HB2	2.16	0.45
1:C:110:VAL:C	1:C:112:MET:H	2.20	0.45
1:C:144:LEU:HD22	2:D:35:TYR:CD1	2.51	0.45
2:B:329:LEU:CD1	2:B:344:LEU:HD13	2.41	0.45
2:D:257:PRO:HB3	2:D:261:LEU:HD22	1.98	0.45
1:C:239:ARG:HD3	2:D:23:MET:SD	2.55	0.45
3:H:192:GLU:HA	3:H:195:LEU:HB3	1.98	0.45
1:C:107:ASN:ND2	1:C:107:ASN:C	2.67	0.45
1:A:272:LEU:HD13	1:A:312:ILE:HD13	1.98	0.45
2:D:185:HIS:C	2:D:187:PRO:HD3	2.36	0.45
1:A:245:MET:CE	1:A:309:LEU:HD22	2.47	0.45
1:A:56:LEU:O	1:A:405:THR:HB	2.16	0.45
1:C:359:ARG:O	1:C:363:VAL:HG13	2.16	0.45
1:C:46:ILE:HG12	1:C:47:ILE:N	2.31	0.45
1:A:219:THR:HG22	1:A:221:TYR:N	2.21	0.45
1:C:230:ASN:O	1:C:230:ASN:CG	2.54	0.45
2:B:67:ALA:HB3	2:B:396:HIS:HB2	1.98	0.45
3:G:8:TYR:HD2	3:G:130:VAL:HG22	1.82	0.45
3:H:43:ASP:OD1	3:H:43:ASP:N	2.49	0.45
1:C:298:ASN:CB	1:C:362:HIS:NE2	2.79	0.45
2:D:56:ASN:O	2:D:59:ARG:CB	2.64	0.45
3:F:23:VAL:HG12	3:F:33:VAL:HG11	1.99	0.45
3:E:158:MET:HE1	3:E:195:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:ARG:HD3	2:B:23:MET:SD	2.57	0.45
3:E:136:ALA:HB2	3:F:94:GLY:HA2	1.98	0.45
1:A:125:PHE:C	1:A:126:GLY:O	2.54	0.45
3:H:8:TYR:CE1	3:H:126:VAL:HG21	2.52	0.45
1:A:189:VAL:CG2	1:A:190:SER:N	2.76	0.45
2:B:472:PRO:HB3	2:B:474:PHE:CE2	2.51	0.45
1:C:58:THR:CG2	1:C:59:ILE:N	2.79	0.45
1:C:253:TRP:NE1	1:C:265:THR:OG1	2.34	0.45
1:A:57:MET:HE3	2:B:100:ARG:NH1	2.32	0.45
2:B:90:HIS:O	2:B:151:THR:HA	2.16	0.45
2:B:122:ALA:HB3	2:B:154:MET:HE1	1.99	0.45
1:A:141:LEU:HA	1:A:141:LEU:HD12	1.84	0.45
3:H:103:ILE:HA	3:H:137:MET:HG3	1.99	0.45
1:C:239:ARG:HD3	2:D:23:MET:CG	2.47	0.45
3:E:207:MET:HE1	3:E:210:PHE:HB2	1.96	0.45
2:B:119:THR:HG22	2:B:120:GLU:N	2.31	0.45
3:G:4:GLN:HE21	3:G:124:TYR:HE2	1.65	0.45
3:F:38:CYS:HB3	3:F:102:VAL:HG13	1.98	0.45
3:F:113:GLY:HA2	3:F:116:GLU:OE1	2.17	0.45
2:D:330:MET:O	2:D:333:SER:HB3	2.16	0.45
1:A:276:TYR:O	1:A:280:ASN:CB	2.64	0.45
1:A:360:PRO:HB2	1:A:379:TYR:CZ	2.52	0.45
1:C:81:ILE:HD12	1:C:148:ILE:HG21	1.98	0.45
1:C:210:ARG:HH22	2:D:33:GLU:CD	2.20	0.45
2:B:85:THR:HA	2:B:146:MET:O	2.17	0.45
2:B:234:LEU:O	2:B:238:ARG:HG2	2.17	0.45
2:B:56:ASN:O	2:B:59:ARG:HD3	2.17	0.45
2:D:233:TYR:CB	2:D:236:ASN:HD22	2.25	0.45
3:F:3:ARG:NH1	3:F:3:ARG:HG3	2.31	0.45
3:E:255:ILE:O	3:E:255:ILE:CG2	2.63	0.45
1:A:448:GLY:HA3	1:A:458:ILE:HD13	1.98	0.45
3:E:25:ALA:HB2	3:E:228:ILE:CD1	2.47	0.45
1:A:381:PHE:CZ	9:A:1496:CFM:S2B	3.10	0.45
1:A:35:ASN:ND2	1:A:394:MET:CB	2.80	0.45
3:F:217:VAL:HG11	7:F:6292:ATP:N7	2.32	0.45
1:C:457:ALA:HB3	2:D:3:GLN:HG2	1.99	0.45
2:B:122:ALA:O	2:B:126:GLY:N	2.48	0.45
1:A:343:ARG:N	1:A:344:PRO:CD	2.80	0.45
2:B:494:LEU:HD23	2:B:494:LEU:C	2.37	0.45
1:A:98:ASN:ND2	1:A:98:ASN:N	2.57	0.45
1:A:350:ARG:O	1:A:419:ASP:OD1	2.35	0.45
3:E:49:LEU:O	3:E:50:HIS:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:3:ARG:NH1	3:F:121:PHE:CZ	2.84	0.45
1:A:36:ASP:O	1:A:38:ALA:N	2.50	0.45
1:A:190:SER:HB2	1:A:381:PHE:HB3	1.99	0.45
1:C:167:SER:HB3	1:C:178:ILE:HG22	1.98	0.45
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.50	0.45
2:D:284:ALA:CB	2:D:285:PRO:HD3	2.45	0.45
1:C:448:GLY:HA3	1:C:458:ILE:HD13	1.99	0.45
1:C:337:ALA:CB	2:D:5:VAL:HG21	2.46	0.45
1:A:90:GLN:N	1:A:113:ASN:HD21	2.15	0.45
3:E:244:ALA:O	3:E:248:VAL:HG23	2.17	0.45
2:D:137:ASN:HD22	2:D:137:ASN:N	2.14	0.45
2:D:90:HIS:CE1	2:D:116:ASP:OD2	2.70	0.45
2:B:212:SER:C	2:B:216:LYS:HE3	2.36	0.45
2:D:497:LEU:O	2:D:500:SER:N	2.50	0.45
1:C:221:TYR:CE2	1:C:320:ILE:HD11	2.52	0.45
3:H:231:ASP:OD2	3:H:234:ALA:N	2.50	0.45
1:C:37:PRO:HD2	1:C:396:ASP:OD1	2.17	0.45
2:B:70:CYS:HB2	2:B:72:PRO:HD2	1.99	0.45
1:C:297:TYR:HB2	1:C:308:SER:OG	2.17	0.45
2:D:277:THR:O	2:D:280:GLU:HB3	2.16	0.45
1:C:260:SER:HB2	2:D:33:GLU:OE1	2.17	0.44
3:E:158:MET:CE	3:E:195:LEU:HG	2.47	0.44
2:D:147:ILE:O	2:D:181:VAL:HA	2.16	0.44
3:G:160:ALA:O	3:G:164:ILE:HG13	2.17	0.44
3:F:149:ILE:O	3:F:182:LEU:HA	2.16	0.44
1:C:124:VAL:O	3:H:97:CYS:N	2.42	0.44
1:A:9:VAL:O	1:A:12:LEU:HB3	2.16	0.44
1:A:35:ASN:HB3	1:A:398:THR:OG1	2.16	0.44
2:D:426:ASP:OD1	2:D:428:TRP:N	2.49	0.44
3:H:220:ALA:HB1	3:H:225:MET:O	2.17	0.44
1:C:232:GLY:O	1:C:449:PRO:HG3	2.17	0.44
2:B:512:MET:HG2	2:D:457:HIS:CD2	2.52	0.44
1:A:271:ASN:OD1	1:A:286:MET:HE2	2.17	0.44
3:E:136:ALA:HB2	3:F:94:GLY:HA3	1.99	0.44
1:A:253:TRP:CH2	1:A:282:ILE:HG12	2.52	0.44
3:E:225:MET:CE	3:E:230:TYR:HA	2.47	0.44
1:A:310:ARG:O	1:A:313:ALA:HB3	2.17	0.44
7:G:7292:ATP:H4'	3:H:156:MET:SD	2.57	0.44
1:C:186:PHE:CB	2:D:154:MET:CE	2.95	0.44
3:H:236:GLN:HE22	7:H:8292:ATP:N6	2.15	0.44
2:D:81:GLY:HA3	2:D:257:PRO:HD3	2.00	0.44
1:A:306:ILE:HD11	1:A:335:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:129:ASP:CB	3:E:131:VAL:HG12	2.47	0.44
2:B:284:ALA:HB3	2:B:285:PRO:HD3	2.00	0.44
3:G:43:ASP:N	3:G:43:ASP:OD1	2.50	0.44
2:D:426:ASP:H	2:D:429:HIS:CE1	2.36	0.44
1:C:219:THR:C	1:C:221:TYR:H	2.19	0.44
1:A:144:LEU:HD21	2:B:43:VAL:HG21	1.99	0.44
2:D:369:LEU:CD2	2:D:369:LEU:N	2.80	0.44
3:E:148:TYR:CE2	3:E:208:ILE:HD12	2.52	0.44
2:B:67:ALA:HB3	2:B:396:HIS:CB	2.46	0.44
2:D:133:ASP:O	2:D:136:GLN:N	2.50	0.44
2:B:353:ASP:OD2	2:D:109:GLU:OE2	2.35	0.44
2:D:14:LEU:HD12	2:D:14:LEU:O	2.17	0.44
1:A:417:LYS:N	1:A:418:PRO:CD	2.78	0.44
2:B:314:PRO:HB3	2:B:316:LEU:CD1	2.46	0.44
1:A:277:ARG:NH2	1:A:383:HIS:CD2	2.84	0.44
2:B:168:ASN:O	2:B:172:GLU:HB2	2.17	0.44
3:H:138:PRO:O	3:H:143:LYS:HB3	2.17	0.44
2:D:285:PRO:HG3	2:D:309:TRP:CD1	2.53	0.44
1:C:280:ASN:H	1:C:280:ASN:ND2	2.14	0.44
3:H:213:ARG:HG3	7:H:8292:ATP:H2	1.83	0.44
2:B:12:TYR:OH	2:D:508:GLU:HB3	2.17	0.44
3:H:255:ILE:HG22	3:H:255:ILE:O	2.16	0.44
1:C:59:ILE:CD1	1:C:427:GLU:OE2	2.58	0.44
1:A:57:MET:HG2	2:B:142:TYR:CE1	2.53	0.44
2:B:88:TYR:O	2:B:150:SER:N	2.50	0.44
3:H:110:GLU:OE2	3:H:143:LYS:NZ	2.51	0.44
1:C:35:ASN:HD21	1:C:394:MET:HB2	1.83	0.44
3:E:165:SER:HA	3:E:168:ILE:HD12	2.00	0.44
1:A:100:TYR:OH	1:A:111:THR:HG23	2.16	0.44
3:F:102:VAL:HG21	3:F:135:PHE:CE1	2.53	0.44
3:E:64:ALA:HB1	3:E:69:ASP:HB3	1.99	0.44
1:C:265:THR:HG22	1:C:286:MET:CE	2.48	0.44
3:E:6:ALA:HA	3:E:124:TYR:HB2	1.99	0.44
2:D:146:MET:HE1	2:D:208:PHE:HE1	1.83	0.44
3:G:189:THR:CG2	3:G:190:ASP:H	2.15	0.44
2:B:143:LYS:N	2:B:144:PRO:CD	2.80	0.44
1:C:193:LEU:HG	1:C:197:ILE:HD11	1.98	0.44
3:F:195:LEU:CD1	3:F:267:LEU:HD22	2.48	0.44
2:D:365:LYS:HG3	2:D:501:ILE:CD1	2.47	0.44
1:A:475:LEU:HD13	2:B:265:ALA:O	2.17	0.44
1:A:274:HIS:HB2	1:A:297:TYR:CE2	2.52	0.44
3:H:50:HIS:HE1	3:H:225:MET:HB3	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:MET:HG3	2:B:142:TYR:CZ	2.53	0.44
1:C:70:VAL:CG2	1:C:71:VAL:HG23	2.47	0.44
2:D:124:VAL:HG22	3:G:100:ARG:HG3	2.00	0.44
2:B:158:ILE:HG22	3:E:97:CYS:HB2	2.00	0.44
1:A:469:ASN:CG	1:A:470:PRO:HD2	2.37	0.44
3:F:4:GLN:HB2	3:F:144:ALA:HA	2.00	0.44
3:G:33:VAL:HG12	3:G:34:MET:N	2.33	0.44
3:G:198:ALA:HB1	3:G:267:LEU:HD21	2.00	0.44
3:F:159:TYR:HA	3:F:264:LEU:HD11	2.00	0.44
3:H:25:ALA:O	3:H:28:GLU:HB3	2.17	0.44
3:E:86:VAL:HG21	3:E:109:LEU:HD11	2.00	0.44
3:E:9:GLY:C	3:E:15:LYS:HE3	2.39	0.44
3:H:23:VAL:O	3:H:27:ALA:N	2.47	0.44
2:D:278:GLN:HG2	2:D:278:GLN:H	1.51	0.44
3:G:39:ASP:OD1	3:G:40:PRO:CD	2.66	0.44
2:B:41:ASP:O	2:B:45:GLN:HG2	2.18	0.44
3:F:76:LEU:HD21	3:F:84:LYS:HB3	1.99	0.44
2:D:479:LEU:N	2:D:479:LEU:CD1	2.81	0.44
1:A:229:TYR:CD1	1:A:229:TYR:N	2.86	0.43
3:G:91:PRO:HD2	3:G:98:ALA:HB2	1.99	0.43
3:F:46:ARG:HH21	3:F:221:GLU:HG3	1.83	0.43
1:A:181:VAL:HG13	1:A:181:VAL:O	2.18	0.43
1:C:469:ASN:CG	1:C:470:PRO:HD2	2.38	0.43
1:A:64:TYR:C	1:A:66:GLY:N	2.71	0.43
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.32	0.43
1:A:283:SER:HA	1:A:286:MET:HB2	2.00	0.43
3:G:86:VAL:HG21	3:G:109:LEU:CD1	2.49	0.43
1:C:168:LYS:HE3	1:C:205:TRP:HH2	1.82	0.43
3:G:165:SER:HA	3:G:168:ILE:HD12	2.00	0.43
1:A:364:ILE:O	1:A:367:TYR:HB2	2.18	0.43
1:C:359:ARG:CZ	1:C:444:TRP:CZ2	3.01	0.43
1:C:427:GLU:HB2	1:C:431:PHE:HE1	1.83	0.43
3:G:15:LYS:N	7:G:7292:ATP:O1B	2.51	0.43
3:F:61:ALA:HB2	3:F:70:LEU:HD12	2.00	0.43
3:F:152:SER:HB2	3:F:187:ARG:HG2	2.00	0.43
2:B:198:ASP:CG	2:B:298:LEU:HA	2.38	0.43
2:B:426:ASP:OD1	2:B:428:TRP:N	2.50	0.43
2:B:208:PHE:HB3	2:B:282:LYS:HA	1.98	0.43
2:D:375:PHE:CE2	2:D:470:GLY:HA2	2.46	0.43
3:G:61:ALA:HB1	3:G:67:VAL:HA	2.00	0.43
2:B:437:ASP:O	2:B:439:PRO:HD3	2.18	0.43
1:A:305:THR:O	1:A:309:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:E:5292:ATP:H4'	3:F:156:MET:SD	2.58	0.43
1:C:283:SER:HA	1:C:286:MET:HB2	2.01	0.43
2:B:512:MET:CE	2:D:457:HIS:CG	3.01	0.43
2:B:512:MET:HE3	2:D:457:HIS:CD2	2.53	0.43
2:D:49:THR:CG2	2:D:52:TYR:H	2.28	0.43
3:H:206:GLN:NE2	3:H:250:ASN:OD1	2.50	0.43
1:C:179:VAL:O	1:C:181:VAL:N	2.49	0.43
2:B:293:LEU:HD22	2:B:319:PRO:HG2	2.00	0.43
2:D:104:ASN:O	2:D:108:ARG:N	2.44	0.43
1:C:138:VAL:CG1	2:D:62:LEU:CD1	2.94	0.43
3:H:48:ILE:HG23	3:H:80:TYR:HB3	2.00	0.43
3:F:42:ALA:CA	3:F:87:GLU:OE1	2.55	0.43
2:D:472:PRO:HB3	2:D:474:PHE:CE2	2.54	0.43
2:B:228:PRO:HG3	2:B:253:LEU:HD11	2.00	0.43
1:A:433:LYS:HE2	2:D:353:ASP:OD2	2.19	0.43
2:B:175:ILE:HG13	2:B:175:ILE:O	2.18	0.43
1:C:35:ASN:ND2	1:C:394:MET:HB2	2.33	0.43
1:A:125:PHE:O	1:A:126:GLY:O	2.35	0.43
2:D:53:GLN:OE1	2:D:432:SER:HB3	2.18	0.43
2:B:352:VAL:HG11	1:C:475:LEU:HD22	2.01	0.43
1:A:431:PHE:N	1:A:431:PHE:CD1	2.87	0.43
1:A:57:MET:HG2	2:B:142:TYR:CZ	2.53	0.43
1:C:97:ARG:NH2	1:C:99:TYR:OH	2.44	0.43
1:C:219:THR:HG22	1:C:221:TYR:N	2.22	0.43
1:A:70:VAL:CG2	1:A:71:VAL:HG23	2.48	0.43
2:D:41:ASP:O	2:D:45:GLN:HG2	2.19	0.43
2:D:69:ALA:HB3	2:D:193:HIS:HB3	2.00	0.43
2:B:71:GLN:OE1	2:B:195:THR:HG22	2.19	0.43
1:C:312:ILE:O	1:C:316:PHE:CD1	2.71	0.43
3:G:260:THR:O	3:G:261:MET:C	2.56	0.43
1:C:100:TYR:N	1:C:100:TYR:CD2	2.87	0.43
1:A:240:ILE:O	1:A:244:GLU:HG3	2.18	0.43
1:A:361:ARG:HG2	1:A:362:HIS:N	2.34	0.43
1:A:20:TYR:OH	1:A:408:GLU:CG	2.58	0.43
1:C:136:ASP:CG	1:C:170:LYS:HZ1	2.22	0.43
2:D:208:PHE:HB3	2:D:282:LYS:HA	2.01	0.43
2:B:475:ASP:O	2:D:502:LEU:HD13	2.18	0.43
2:D:227:VAL:HG12	2:D:298:LEU:HD13	2.00	0.43
3:G:208:ILE:HG22	3:G:209:HIS:N	2.33	0.43
1:A:276:TYR:CD1	1:A:280:ASN:HB3	2.53	0.43
1:A:8:GLU:O	1:A:12:LEU:N	2.49	0.43
1:C:298:ASN:HD21	1:C:300:PHE:HD1	1.64	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:413:VAL:HG11	1:C:431:PHE:HD2	1.84	0.43
1:C:142:PHE:N	1:C:143:PRO:CD	2.81	0.43
1:A:148:ILE:O	1:A:178:ILE:HA	2.18	0.43
2:B:346:LYS:HG3	2:D:264:PRO:CG	2.47	0.43
2:B:369:LEU:N	2:B:369:LEU:HD23	2.33	0.43
1:A:76:LYS:HA	1:A:110:VAL:HG23	2.01	0.43
3:H:236:GLN:HG2	3:H:240:TYR:CE2	2.53	0.43
3:G:195:LEU:HD11	3:G:268:LEU:HD23	2.01	0.43
1:A:337:ALA:CB	2:B:5:VAL:HG21	2.49	0.43
2:D:14:LEU:C	2:D:14:LEU:HD12	2.38	0.43
1:C:315:LYS:HA	1:C:315:LYS:HD3	1.72	0.43
1:C:57:MET:CG	2:D:142:TYR:CZ	3.01	0.43
1:A:65:ALA:O	1:A:70:VAL:HG13	2.19	0.43
2:D:329:LEU:CD1	2:D:344:LEU:HD13	2.44	0.43
1:C:98:ASN:HB3	1:C:229:TYR:O	2.19	0.43
3:F:225:MET:HE2	3:F:230:TYR:HA	2.01	0.43
3:F:141:GLU:O	3:F:142:ASN:CB	2.67	0.43
1:A:158:LEU:CD2	2:B:123:ALA:HB1	2.48	0.43
3:E:199:LEU:CD1	3:E:259:ILE:HD11	2.47	0.43
1:A:54:PRO:HB2	2:B:134:GLY:CA	2.48	0.43
2:D:238:ARG:HG3	2:D:238:ARG:NH2	2.34	0.43
3:F:19:THR:O	3:F:23:VAL:HG22	2.17	0.43
3:G:6:ALA:HA	3:G:124:TYR:HB2	2.01	0.43
2:B:137:ASN:HD22	2:B:137:ASN:N	2.17	0.43
2:B:199:ASN:N	2:B:199:ASN:HD22	2.16	0.43
1:A:399:LEU:C	1:A:400:LEU:HD12	2.40	0.43
3:F:11:GLY:HA2	3:F:15:LYS:HE3	2.01	0.43
3:G:217:VAL:CG2	7:G:7292:ATP:C2	2.96	0.43
1:A:134:LEU:HG	2:B:62:LEU:HD13	2.00	0.43
2:B:179:PHE:C	2:B:179:PHE:CD2	2.93	0.43
2:D:498:VAL:O	2:D:502:LEU:HG	2.19	0.43
2:D:124:VAL:HG11	3:G:58:MET:CG	2.46	0.43
2:D:228:PRO:HD2	2:D:254:LEU:O	2.18	0.43
1:C:88:CYS:HB2	1:C:153:GLU:OE1	2.19	0.43
2:B:94:GLY:O	2:B:97:ALA:HB3	2.19	0.42
1:C:359:ARG:HH11	1:C:359:ARG:CG	2.27	0.42
1:C:431:PHE:N	1:C:431:PHE:CD1	2.86	0.42
2:D:86:MET:HE3	2:D:87:PRO:CD	2.48	0.42
3:H:67:VAL:HG21	3:H:104:THR:HG21	2.00	0.42
2:D:8:ILE:H	2:D:8:ILE:HG13	1.66	0.42
3:H:33:VAL:HG12	3:H:34:MET:N	2.34	0.42
3:G:217:VAL:O	3:G:221:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:212:PRO:C	3:G:236:GLN:HE22	2.22	0.42
1:C:71:VAL:CG1	1:C:198:ALA:HB1	2.40	0.42
1:A:223:VAL:HG12	1:A:270:LEU:HB3	2.00	0.42
2:B:362:LEU:CD1	2:B:498:VAL:HG22	2.47	0.42
2:D:198:ASP:CG	2:D:298:LEU:HA	2.40	0.42
2:B:322:LEU:HD11	2:B:348:ARG:NE	2.34	0.42
2:B:71:GLN:N	2:B:72:PRO:CD	2.81	0.42
3:E:115:TYR:C	3:E:117:ASP:N	2.72	0.42
1:A:89:GLY:C	1:A:113:ASN:HD21	2.22	0.42
2:B:256:ASP:C	2:B:256:ASP:OD1	2.57	0.42
3:G:139:ILE:HG21	3:G:147:ILE:HD11	2.02	0.42
1:C:310:ARG:O	1:C:313:ALA:HB3	2.19	0.42
1:A:440:GLU:HB2	1:A:445:ASP:HB2	2.00	0.42
1:A:363:VAL:O	1:A:367:TYR:HD1	2.02	0.42
1:C:356:GLY:CA	1:C:381:PHE:CE2	3.02	0.42
2:D:64:VAL:HG12	2:D:428:TRP:HB2	2.01	0.42
1:C:210:ARG:NH2	2:D:33:GLU:OE1	2.47	0.42
2:B:197:TRP:CE3	2:B:298:LEU:HD21	2.53	0.42
1:C:383:HIS:N	1:C:383:HIS:ND1	2.67	0.42
2:B:498:VAL:O	2:B:502:LEU:HG	2.19	0.42
2:B:502:LEU:HD13	2:D:475:ASP:O	2.18	0.42
1:C:90:GLN:HE22	2:D:66:PRO:C	2.21	0.42
1:A:282:ILE:O	1:A:282:ILE:HD12	2.19	0.42
1:A:49:ASN:ND2	1:A:189:VAL:HG21	2.34	0.42
2:B:443:ILE:HA	2:B:467:ILE:O	2.19	0.42
2:B:233:TYR:CB	2:B:236:ASN:HD22	2.28	0.42
1:A:226:ILE:HG23	1:A:279:MET:HG2	2.01	0.42
1:A:464:ASP:OD1	1:A:468:ASN:ND2	2.51	0.42
1:A:176:LYS:HB2	1:A:176:LYS:HE3	1.84	0.42
3:F:9:GLY:O	3:F:15:LYS:HE2	2.20	0.42
2:B:181:VAL:N	2:B:182:PRO:CD	2.83	0.42
3:G:138:PRO:O	3:G:144:ALA:HB3	2.18	0.42
3:H:217:VAL:CG2	3:H:236:GLN:HE21	2.32	0.42
1:A:303:THR:HG22	1:A:369:ASP:CG	2.39	0.42
1:A:302:PRO:HG3	1:A:335:TRP:HB2	2.01	0.42
2:B:492:GLN:O	2:B:493:ILE:C	2.58	0.42
3:H:145:GLN:HA	3:H:177:VAL:HA	2.01	0.42
3:H:10:LYS:H	3:H:13:ILE:HD13	1.84	0.42
3:E:108:PHE:O	3:E:111:GLU:N	2.52	0.42
2:B:19:ASP:OD2	2:B:20:TYR:N	2.51	0.42
1:C:77:ASP:N	1:C:77:ASP:OD2	2.52	0.42
3:F:137:MET:HB3	3:F:138:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:274:HIS:HE2	1:C:300:PHE:HE1	1.65	0.42
1:C:442:HIS:CE1	9:C:3496:CFM:S1B	3.12	0.42
1:C:363:VAL:O	1:C:367:TYR:HD1	2.01	0.42
2:D:3:GLN:OE1	2:D:9:LYS:O	2.37	0.42
1:A:193:LEU:HG	1:A:197:ILE:HD11	2.01	0.42
1:A:54:PRO:HB3	2:B:116:ASP:HA	2.01	0.42
2:B:407:ASP:O	2:B:410:LEU:HB2	2.19	0.42
1:A:222:ASP:OD1	1:A:248:ARG:HG2	2.20	0.42
2:D:199:ASN:ND2	2:D:199:ASN:N	2.67	0.42
1:A:114:PHE:HE2	1:A:142:PHE:CE1	2.37	0.42
2:B:149:VAL:HG21	2:B:166:ILE:HD11	2.01	0.42
3:G:99:GLY:O	3:G:134:GLY:HA3	2.19	0.42
1:A:86:VAL:HG21	2:B:68:LYS:CE	2.49	0.42
1:C:167:SER:HB3	1:C:180:PRO:CD	2.50	0.42
1:A:57:MET:SD	2:B:114:VAL:HG12	2.59	0.42
1:C:382:ALA:HB1	1:C:386:ASP:CB	2.49	0.42
2:B:339:PRO:O	2:B:341:PRO:HD3	2.19	0.42
3:F:179:LEU:CB	3:F:256:PRO:HG3	2.49	0.42
1:A:440:GLU:HB2	1:A:445:ASP:CB	2.49	0.42
1:C:109:PHE:N	1:C:109:PHE:CD1	2.87	0.42
1:A:274:HIS:HE1	1:A:299:PHE:H	1.68	0.42
1:C:356:GLY:HA2	1:C:381:PHE:CE2	2.55	0.42
2:D:426:ASP:OD1	2:D:426:ASP:C	2.57	0.42
3:F:20:GLN:O	3:F:48:ILE:HD11	2.18	0.42
3:G:14:GLY:CA	7:G:7292:ATP:O1B	2.68	0.42
2:B:522:VAL:CG2	1:C:446:TYR:CE2	3.03	0.42
1:C:405:THR:CB	1:C:408:GLU:HG3	2.49	0.42
1:A:389:ARG:HG3	1:A:389:ARG:HH11	1.84	0.42
1:A:219:THR:HG23	1:A:220:PRO:CD	2.49	0.42
3:E:40:PRO:HG3	3:E:98:ALA:HB1	2.02	0.42
1:A:239:ARG:NH2	2:B:27:LYS:HG3	2.35	0.42
3:H:250:ASN:ND2	3:H:251:LYS:N	2.67	0.42
3:E:45:THR:OG1	3:E:49:LEU:HD12	2.18	0.42
3:F:179:LEU:HB2	3:F:256:PRO:CG	2.50	0.42
3:E:137:MET:CB	3:E:138:PRO:HD3	2.49	0.42
3:E:36:VAL:HA	3:E:86:VAL:HG23	2.01	0.42
2:D:240:ILE:HA	2:D:240:ILE:HD13	1.94	0.42
1:A:189:VAL:CG2	1:A:190:SER:H	2.30	0.42
1:A:12:LEU:O	1:A:16:VAL:HG23	2.19	0.42
1:A:138:VAL:CG1	2:B:62:LEU:HD22	2.48	0.42
1:A:193:LEU:HA	1:A:193:LEU:HD12	1.85	0.42
2:D:74:GLY:HA3	2:D:193:HIS:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:28:ARG:HA	2:B:32:GLU:HG3	2.02	0.42
3:H:185:ASN:HD21	3:H:211:VAL:CG1	2.33	0.42
1:A:298:ASN:HD21	1:A:300:PHE:HB2	1.85	0.42
1:C:57:MET:CE	2:D:100:ARG:NH1	2.82	0.42
2:D:322:LEU:HD11	2:D:348:ARG:NH2	2.34	0.42
2:D:165:PHE:H	2:D:165:PHE:HD1	1.67	0.42
1:A:144:LEU:HD11	2:B:43:VAL:HG21	2.02	0.42
1:C:86:VAL:CG2	2:D:68:LYS:HE3	2.47	0.42
2:B:236:ASN:OD1	2:B:485:LEU:N	2.53	0.42
3:G:23:VAL:HG12	3:G:33:VAL:HG11	2.02	0.42
3:F:158:MET:HE1	3:F:195:LEU:HG	2.01	0.42
1:A:239:ARG:NH1	2:B:27:LYS:HD2	2.35	0.42
2:B:469:ILE:HD13	2:B:493:ILE:CD1	2.50	0.42
1:A:48:SER:CB	1:A:402:ASP:OD2	2.68	0.42
2:D:339:PRO:O	2:D:341:PRO:HD3	2.19	0.42
2:D:438:LYS:HA	2:D:439:PRO:HD2	1.95	0.42
1:C:114:PHE:N	1:C:114:PHE:CD1	2.88	0.42
1:C:355:ILE:HG21	9:C:3496:CFM:S3A	2.59	0.42
2:B:57:PHE:C	2:B:59:ARG:H	2.22	0.42
1:C:128:ASP:HB3	1:C:166:VAL:CG2	2.49	0.42
3:G:136:ALA:HB2	3:H:94:GLY:HA2	2.01	0.42
1:A:352:MET:HE1	1:A:418:PRO:HG2	2.00	0.41
1:A:425:ILE:HG23	1:A:426:LYS:N	2.35	0.41
1:C:112:MET:HE1	2:D:428:TRP:CZ3	2.54	0.41
2:D:146:MET:HE2	2:D:208:PHE:CE1	2.49	0.41
3:F:186:SER:HA	3:F:192:GLU:OE2	2.20	0.41
1:A:141:LEU:HD21	2:B:56:ASN:HA	2.02	0.41
2:B:204:ILE:HG23	2:B:208:PHE:HE1	1.85	0.41
3:F:4:GLN:HB2	3:F:143:LYS:O	2.20	0.41
1:A:98:ASN:HD22	1:A:98:ASN:N	2.16	0.41
2:D:375:PHE:HE2	2:D:470:GLY:CA	2.31	0.41
1:C:302:PRO:CD	1:C:456:PHE:CD1	3.03	0.41
1:C:239:ARG:NH1	2:D:27:LYS:HD2	2.35	0.41
2:D:206:ARG:CG	2:D:304:PHE:CZ	3.03	0.41
2:D:365:LYS:O	2:D:388:CYS:HB3	2.19	0.41
3:H:185:ASN:HD21	3:H:211:VAL:HG12	1.85	0.41
3:H:136:ALA:O	3:H:139:ILE:HG12	2.20	0.41
1:C:318:GLU:HA	1:C:321:GLN:OE1	2.20	0.41
1:C:39:VAL:HG23	1:C:39:VAL:O	2.19	0.41
1:A:318:GLU:HA	1:A:321:GLN:OE1	2.20	0.41
3:E:260:THR:O	3:E:261:MET:C	2.58	0.41
1:A:355:ILE:HB	1:A:360:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:427:GLU:O	1:C:431:PHE:CD1	2.73	0.41
1:A:134:LEU:HG	2:B:62:LEU:CD1	2.50	0.41
2:B:118:MET:HE3	2:B:127:GLY:HA3	2.02	0.41
1:A:277:ARG:HD3	1:A:386:ASP:OD2	2.21	0.41
3:G:103:ILE:HG12	3:G:137:MET:HG2	2.02	0.41
3:H:166:LYS:HA	3:H:258:PRO:HG3	2.02	0.41
3:H:98:ALA:O	3:H:102:VAL:HG23	2.20	0.41
1:A:96:ARG:NH1	1:A:98:ASN:OD1	2.53	0.41
2:B:330:MET:O	2:B:333:SER:HB3	2.19	0.41
1:C:76:LYS:HG2	1:C:257:GLY:O	2.20	0.41
3:E:96:GLY:O	3:F:132:CYS:HB2	2.19	0.41
3:H:185:ASN:HD22	3:H:185:ASN:HA	1.40	0.41
2:D:221:ASN:O	2:D:223:LYS:HG3	2.20	0.41
1:C:210:ARG:HG3	1:C:263:GLU:HB3	2.01	0.41
1:A:70:VAL:HG23	1:A:71:VAL:N	2.35	0.41
2:B:393:ILE:HD12	2:B:410:LEU:HD11	2.03	0.41
1:A:239:ARG:O	1:A:243:GLU:HG3	2.20	0.41
3:F:36:VAL:HA	3:F:86:VAL:HG23	2.02	0.41
2:B:395:CYS:O	2:B:423:ILE:HA	2.21	0.41
2:D:388:CYS:O	2:D:390:PRO:HD3	2.21	0.41
3:E:100:ARG:C	3:E:100:ARG:HD2	2.40	0.41
3:H:165:SER:HB3	3:H:179:LEU:HD12	2.02	0.41
1:C:226:ILE:O	1:C:226:ILE:HG22	2.20	0.41
1:C:358:LEU:HD11	1:C:362:HIS:ND1	2.36	0.41
1:C:364:ILE:O	1:C:368:GLU:HG2	2.21	0.41
3:G:185:ASN:OD1	7:G:7292:ATP:N6	2.54	0.41
2:D:492:GLN:O	2:D:493:ILE:C	2.56	0.41
1:A:221:TYR:O	1:A:223:VAL:HG13	2.20	0.41
2:B:294:GLN:HB2	2:B:297:HIS:CE1	2.55	0.41
2:D:369:LEU:HD11	2:D:380:VAL:CG2	2.50	0.41
1:A:454:ASP:HB3	2:B:14:LEU:HD21	2.01	0.41
3:F:198:ALA:CB	3:F:267:LEU:HD21	2.50	0.41
3:H:214:ASP:OD2	3:H:216:VAL:HG23	2.20	0.41
2:D:375:PHE:O	2:D:375:PHE:HD1	2.03	0.41
10:A:1498:CLF:S3B	2:B:72:PRO:HG2	2.60	0.41
3:F:163:ASN:O	3:F:166:LYS:HB3	2.21	0.41
2:D:237:PHE:O	2:D:241:LYS:HG3	2.21	0.41
2:D:414:PRO:HA	2:D:417:LYS:HG3	2.02	0.41
2:B:277:THR:O	2:B:280:GLU:HB3	2.20	0.41
1:A:352:MET:HE1	1:A:413:VAL:HA	2.02	0.41
1:C:346:LEU:HB3	1:C:372:MET:HG3	2.02	0.41
1:C:349:LYS:HD3	1:C:419:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:146:MET:HE2	2:D:208:PHE:HZ	1.79	0.41
1:A:230:ASN:OD1	1:A:233:GLY:CA	2.68	0.41
1:A:339:VAL:HG13	1:A:343:ARG:HB2	2.01	0.41
1:A:144:LEU:HD22	2:B:35:TYR:CE1	2.56	0.41
2:B:366:ARG:HB3	2:B:391:VAL:HG21	2.01	0.41
2:B:39:LYS:HD2	2:B:42:GLU:OE1	2.21	0.41
2:D:170:LYS:HD3	2:D:175:ILE:HG13	2.02	0.41
2:D:427:LEU:HA	2:D:427:LEU:HD23	1.91	0.41
1:A:131:LEU:HD13	1:A:131:LEU:C	2.40	0.41
1:A:349:LYS:HD3	1:A:419:ASP:OD2	2.20	0.41
1:A:236:TRP:HA	2:B:23:MET:HE1	2.02	0.41
3:H:36:VAL:HA	3:H:86:VAL:HG23	2.02	0.41
1:C:37:PRO:HD2	1:C:396:ASP:CB	2.51	0.41
3:H:200:ALA:O	3:H:205:THR:O	2.39	0.41
1:A:411:GLU:HA	1:A:411:GLU:OE1	2.19	0.41
1:A:405:THR:O	1:A:406:GLY:C	2.57	0.41
2:B:125:PHE:CE2	3:E:62:ALA:HB2	2.55	0.41
1:C:404:VAL:HG22	1:C:408:GLU:HB2	2.02	0.41
1:C:30:LYS:HZ1	1:C:47:ILE:CD1	2.33	0.41
1:A:141:LEU:HD12	2:B:52:TYR:CE1	2.56	0.41
1:A:67:SER:HB3	1:A:151:GLN:NE2	2.35	0.41
2:B:262:ASP:O	2:B:264:PRO:HD3	2.21	0.41
1:C:16:VAL:HG21	1:C:412:PHE:CE1	2.55	0.41
2:B:74:GLY:HA3	2:B:193:HIS:O	2.19	0.41
3:E:106:ILE:CD1	3:E:137:MET:HB3	2.50	0.41
3:F:100:ARG:O	3:F:100:ARG:HD2	2.20	0.41
1:A:364:ILE:O	1:A:368:GLU:HG2	2.20	0.41
1:A:164:GLU:HA	1:A:180:PRO:HB3	2.03	0.41
2:D:362:LEU:HD21	2:D:497:LEU:HB2	2.03	0.41
3:F:23:VAL:CG1	3:F:33:VAL:HG11	2.51	0.41
2:D:227:VAL:HB	2:D:292:LEU:HD23	2.02	0.41
3:H:195:LEU:O	3:H:198:ALA:HB3	2.21	0.41
3:H:91:PRO:HB2	3:H:95:VAL:O	2.20	0.41
3:E:242:ALA:O	3:E:246:LYS:HG2	2.21	0.41
3:F:102:VAL:HG21	3:F:135:PHE:CD1	2.56	0.41
2:B:84:LYS:HD3	2:B:145:ASP:CG	2.41	0.41
2:D:440:ASP:HB3	2:D:441:PHE:CE1	2.56	0.41
2:D:481:ARG:HB3	2:D:481:ARG:CZ	2.50	0.41
2:D:186:THR:N	2:D:187:PRO:HD3	2.36	0.41
1:C:359:ARG:N	1:C:360:PRO:CD	2.83	0.41
2:D:179:PHE:C	2:D:179:PHE:CD2	2.94	0.41
2:B:125:PHE:HZ	3:E:58:MET:O	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:445:ASN:HB2	2:D:472:PRO:O	2.20	0.41
2:B:76:VAL:O	2:B:80:LEU:HG	2.20	0.41
1:C:106:VAL:HG12	1:C:144:LEU:HD12	2.02	0.41
2:D:510:ARG:O	2:D:510:ARG:HG2	2.21	0.41
2:D:142:TYR:C	2:D:144:PRO:CD	2.88	0.41
1:C:277:ARG:CA	1:C:277:ARG:HE	2.33	0.41
3:G:26:LEU:CD1	3:G:244:ALA:HB1	2.51	0.41
2:B:309:TRP:CD1	2:B:309:TRP:N	2.85	0.41
1:C:402:ASP:O	1:C:403:ASP:HB3	2.21	0.41
3:F:208:ILE:HG22	3:F:209:HIS:N	2.35	0.41
1:C:475:LEU:HD13	2:D:265:ALA:O	2.21	0.41
1:C:67:SER:HB3	1:C:183:CYS:HB3	2.02	0.41
2:B:358:SER:OG	2:D:478:HIS:NE2	2.53	0.41
3:F:99:GLY:O	3:F:134:GLY:HA3	2.20	0.41
2:B:31:PHE:CD1	2:B:31:PHE:N	2.89	0.41
3:H:70:LEU:HD23	3:H:70:LEU:HA	1.76	0.41
1:C:346:LEU:HB3	1:C:372:MET:SD	2.61	0.41
3:H:23:VAL:HG12	3:H:33:VAL:HG11	2.03	0.41
3:E:4:GLN:NE2	3:E:124:TYR:OH	2.54	0.41
2:B:512:MET:CE	2:D:457:HIS:CD2	3.04	0.41
2:B:421:VAL:HG12	2:B:422:TYR:N	2.35	0.41
3:G:95:VAL:CG1	3:G:95:VAL:O	2.62	0.41
1:A:224:ALA:HB2	1:A:251:ALA:HB3	2.01	0.41
2:B:170:LYS:HD3	2:B:175:ILE:HG13	2.03	0.41
1:C:86:VAL:HB	1:C:117:ASP:OD2	2.19	0.41
3:H:9:GLY:C	3:H:15:LYS:HE3	2.41	0.41
3:H:214:ASP:O	3:H:217:VAL:HG23	2.21	0.41
2:D:188:SER:HB2	10:D:3498:CLF:S2B	2.61	0.41
1:A:207:LEU:HD11	1:A:266:PRO:HD3	2.03	0.41
2:B:495:THR:HG22	2:B:499:ASN:HD22	1.86	0.41
2:D:70:CYS:O	2:D:193:HIS:CA	2.69	0.41
2:D:365:LYS:HG3	2:D:501:ILE:HD11	2.02	0.41
1:A:461:ARG:HG3	2:B:8:ILE:HD12	2.03	0.41
3:F:161:ALA:O	3:F:165:SER:OG	2.39	0.41
1:A:428:LYS:O	1:A:432:GLN:HG3	2.20	0.41
1:A:443:SER:C	1:A:445:ASP:N	2.74	0.41
2:B:20:TYR:O	2:B:24:LEU:HG	2.21	0.41
2:D:296:TRP:CZ3	2:D:402:TRP:HA	2.55	0.41
2:D:461:GLU:HG3	2:D:461:GLU:O	2.21	0.41
2:D:399:ASN:C	2:D:399:ASN:OD1	2.60	0.41
1:A:241:LEU:HD11	1:A:453:PHE:CD1	2.56	0.41
2:B:125:PHE:HZ	3:E:59:GLU:HA	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:MET:CE	2:B:100:ARG:CZ	2.99	0.41
3:G:100:ARG:NH1	3:G:103:ILE:CG2	2.84	0.41
3:F:41:LYS:HB3	3:F:43:ASP:OD1	2.21	0.41
3:G:199:LEU:HD11	3:G:259:ILE:HD11	2.03	0.41
1:C:301:GLY:HA2	1:C:456:PHE:CD1	2.56	0.41
1:C:222:ASP:OD1	1:C:248:ARG:HG2	2.20	0.41
2:D:456:LEU:HD11	2:D:460:LYS:CD	2.51	0.41
3:F:179:LEU:HD12	3:F:256:PRO:HG3	2.02	0.41
3:F:129:ASP:HB3	3:F:131:VAL:HG12	2.03	0.41
1:A:79:ILE:HG13	1:A:145:ASN:HB2	2.02	0.41
2:D:221:ASN:CG	2:D:223:LYS:HD3	2.41	0.41
1:A:413:VAL:HG11	1:A:431:PHE:HD2	1.85	0.40
1:C:148:ILE:O	1:C:178:ILE:HA	2.21	0.40
3:E:61:ALA:HA	3:E:70:LEU:HG	2.03	0.40
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.27	0.40
1:C:240:ILE:O	1:C:244:GLU:HG3	2.21	0.40
1:C:96:ARG:HH11	1:C:96:ARG:CG	2.33	0.40
2:B:69:ALA:HB3	2:B:193:HIS:HB3	2.03	0.40
1:A:90:GLN:N	1:A:113:ASN:ND2	2.68	0.40
2:B:510:ARG:CG	2:B:510:ARG:O	2.70	0.40
1:A:48:SER:HB2	1:A:402:ASP:OD2	2.21	0.40
3:E:225:MET:HE2	3:E:230:TYR:HB2	2.03	0.40
2:B:54:GLU:O	2:B:58:GLN:HG3	2.22	0.40
1:A:107:ASN:O	1:A:107:ASN:ND2	2.53	0.40
2:D:62:LEU:HD23	2:D:64:VAL:HG23	2.02	0.40
3:E:13:ILE:HD12	3:E:150:VAL:O	2.20	0.40
3:H:50:HIS:O	3:H:51:SER:CB	2.61	0.40
1:A:218:SER:OG	1:A:269:LYS:CE	2.57	0.40
2:D:247:MET:CE	2:D:340:ILE:HA	2.51	0.40
1:A:258:SER:HB2	1:A:261:GLU:H	1.86	0.40
3:H:186:SER:CB	3:H:210:PHE:CZ	3.00	0.40
3:F:158:MET:CE	3:F:195:LEU:HG	2.51	0.40
3:G:223:ARG:O	3:G:224:ARG:CB	2.63	0.40
1:A:207:LEU:HD11	1:A:266:PRO:CD	2.52	0.40
2:B:185:HIS:CE1	3:F:140:ARG:HH12	2.39	0.40
1:C:204:ASP:HB2	1:C:205:TRP:CD1	2.57	0.40
1:A:42:SER:O	1:A:43:LYS:C	2.60	0.40
1:A:94:ALA:HB3	2:D:521:LEU:HD22	2.03	0.40
1:A:367:TYR:O	1:A:368:GLU:C	2.59	0.40
1:A:427:GLU:HB2	1:A:431:PHE:CE1	2.56	0.40
2:D:79:ALA:O	2:D:80:LEU:C	2.58	0.40
2:B:224:ILE:HD12	2:B:249:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:16:VAL:O	1:C:19:VAL:HG22	2.21	0.40
1:A:200:ASP:HA	1:A:203:ARG:HG2	2.03	0.40
3:E:131:VAL:HG22	3:E:132:CYS:SG	2.61	0.40
3:E:179:LEU:HB2	3:E:256:PRO:HG3	2.02	0.40
1:C:43:LYS:HE2	1:C:384:ASN:ND2	2.36	0.40
2:B:32:GLU:O	2:B:33:GLU:C	2.59	0.40
1:A:8:GLU:O	1:A:11:SER:N	2.55	0.40
2:D:247:MET:CB	2:D:249:VAL:HG23	2.50	0.40
3:G:106:ILE:HD12	3:G:137:MET:CB	2.46	0.40
3:E:94:GLY:O	3:E:95:VAL:CG2	2.64	0.40
1:A:67:SER:HB2	1:A:183:CYS:CB	2.52	0.40
1:C:9:VAL:HB	1:C:34:VAL:HG22	2.04	0.40
1:A:265:THR:HG22	1:A:286:MET:CE	2.49	0.40
1:C:245:MET:HG3	1:C:324:CYS:HA	2.04	0.40
2:B:415:TYR:CD1	2:B:415:TYR:N	2.90	0.40
1:C:250:VAL:HA	2:D:31:PHE:CE2	2.55	0.40
2:B:293:LEU:O	2:B:318:ILE:HA	2.20	0.40
1:A:118:PHE:HD1	1:A:123:ILE:HD13	1.86	0.40
3:H:185:ASN:ND2	3:H:211:VAL:CG1	2.84	0.40
3:E:233:LYS:O	3:E:234:ALA:C	2.59	0.40
1:A:315:LYS:HD3	1:A:315:LYS:HA	1.79	0.40
3:E:239:GLU:OE1	3:E:239:GLU:HA	2.22	0.40
1:C:437:PRO:HA	1:C:472:TRP:CH2	2.55	0.40
1:A:229:TYR:O	1:A:230:ASN:HB3	2.21	0.40
3:F:187:ARG:HD3	3:F:187:ARG:HA	1.90	0.40
1:C:106:VAL:HG21	2:D:44:PHE:HD1	1.87	0.40
2:B:161:ASP:OD2	2:B:164:ALA:HB2	2.21	0.40
2:D:131:MET:CE	2:D:149:VAL:HG11	2.51	0.40
2:D:161:ASP:OD2	2:D:164:ALA:HB2	2.21	0.40
2:B:227:VAL:HA	2:B:228:PRO:HD2	1.95	0.40
1:A:137:GLU:O	1:A:141:LEU:HB2	2.21	0.40
2:B:43:VAL:O	2:B:46:TRP:HB3	2.21	0.40
2:D:376:VAL:O	2:D:380:VAL:HG23	2.21	0.40
3:F:26:LEU:HD12	3:F:244:ALA:HB1	2.03	0.40
3:F:26:LEU:HD12	3:F:29:MET:HE2	2.02	0.40
3:H:250:ASN:ND2	3:H:252:LEU:N	2.70	0.40
2:B:516:ASP:O	2:B:519:HIS:HB2	2.21	0.40
2:B:359:HIS:NE2	1:C:466:THR:HG23	2.36	0.40
2:B:240:ILE:HA	2:B:240:ILE:HD13	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	474/492 (96%)	420 (89%)	47 (10%)	7 (2%)	15	58
1	C	474/492 (96%)	415 (88%)	52 (11%)	7 (2%)	15	58
2	B	520/523 (99%)	470 (90%)	43 (8%)	7 (1%)	18	62
2	D	520/523 (99%)	450 (86%)	60 (12%)	10 (2%)	12	51
3	E	266/289 (92%)	232 (87%)	29 (11%)	5 (2%)	12	51
3	F	265/289 (92%)	232 (88%)	25 (9%)	8 (3%)	7	34
3	G	266/289 (92%)	225 (85%)	33 (12%)	8 (3%)	7	34
3	H	266/289 (92%)	234 (88%)	24 (9%)	8 (3%)	7	34
All	All	3051/3186 (96%)	2678 (88%)	313 (10%)	60 (2%)	11	48

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	PRO
2	B	391	VAL
2	D	13	PRO
2	D	439	PRO
3	E	53	ALA
3	F	50	HIS
3	G	95	VAL
3	H	50	HIS
3	H	186	SER
2	D	391	VAL
3	E	95	VAL
3	E	116	GLU
3	F	53	ALA
3	F	116	GLU
3	G	50	HIS
3	G	53	ALA
3	H	118	ASP
1	C	37	PRO
2	D	117	SER

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Mol	Chain	Res	Type
2	D	255	SER
3	F	128	GLY
3	G	258	PRO
1	A	302	PRO
1	C	85	PRO
3	F	215	ASN
3	G	116	GLU
3	G	131	VAL
3	H	51	SER
1	A	355	ILE
2	B	255	SER
2	D	187	PRO
3	E	140	ARG
3	H	189	THR
1	A	73	GLY
1	A	117	ASP
1	A	255	GLY
2	B	187	PRO
2	B	473	ILE
1	C	73	GLY
1	C	254	SER
2	D	258	GLU
3	E	50	HIS
3	G	46	ARG
1	C	255	GLY
3	F	14	GLY
3	F	130	VAL
1	A	37	PRO
1	C	180	PRO
2	D	473	ILE
3	H	130	VAL
2	B	228	PRO
1	C	355	ILE
2	D	66	PRO
2	D	486	GLY
3	H	11	GLY
3	H	95	VAL
1	A	85	PRO
2	B	319	PRO
3	F	138	PRO
3	G	256	PRO

5.3.2 Protein sidechains ⓘ

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	405/415 (98%)	362 (89%)	43 (11%)	10	36
1	C	405/415 (98%)	357 (88%)	48 (12%)	8	30
2	B	453/455 (100%)	398 (88%)	55 (12%)	7	29
2	D	453/455 (100%)	411 (91%)	42 (9%)	13	45
3	E	216/233 (93%)	186 (86%)	30 (14%)	5	23
3	F	215/233 (92%)	190 (88%)	25 (12%)	8	31
3	G	216/233 (93%)	188 (87%)	28 (13%)	6	26
3	H	216/233 (93%)	189 (88%)	27 (12%)	7	28
All	All	2579/2672 (96%)	2281 (88%)	298 (12%)	8	31

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	17	LEU
1	A	21	PRO
1	A	29	ASN
1	A	32	LEU
1	A	45	CYS
1	A	70	VAL
1	A	74	PRO
1	A	96	ARG
1	A	98	ASN
1	A	100	TYR
1	A	112	MET
1	A	140	THR
1	A	141	LEU
1	A	143	PRO
1	A	145	ASN
1	A	152	SER
1	A	183	CYS
1	A	184	GLU
1	A	210	ARG
1	A	266	PRO

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	279	MET
1	A	280	ASN
1	A	298	ASN
1	A	302	PRO
1	A	317	ASP
1	A	324	CYS
1	A	343	ARG
1	A	344	PRO
1	A	345	ARG
1	A	351	VAL
1	A	355	ILE
1	A	362	HIS
1	A	401	TYR
1	A	409	PHE
1	A	418	PRO
1	A	419	ASP
1	A	421	ILE
1	A	428	LYS
1	A	444	TRP
1	A	446	TYR
1	A	462	ASP
2	B	3	GLN
2	B	13	PRO
2	B	14	LEU
2	B	31	PHE
2	B	41	ASP
2	B	54	GLU
2	B	66	PRO
2	B	83	GLU
2	B	115	SER
2	B	116	ASP
2	B	121	ASP
2	B	130	ASN
2	B	144	PRO
2	B	153	CYS
2	B	154	MET
2	B	172	GLU
2	B	179	PHE
2	B	180	PRO
2	B	182	PRO
2	B	187	PRO

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Mol	Chain	Res	Type
2	B	188	SER
2	B	197	TRP
2	B	202	GLU
2	B	206	ARG
2	B	234	LEU
2	B	238	ARG
2	B	245	SER
2	B	260	VAL
2	B	263	THR
2	B	264	PRO
2	B	277	THR
2	B	278	GLN
2	B	279	GLU
2	B	281	MET
2	B	314	PRO
2	B	326	ASP
2	B	339	PRO
2	B	341	PRO
2	B	350	ARG
2	B	375	PHE
2	B	384	LEU
2	B	397	ASN
2	B	414	PRO
2	B	418	ASN
2	B	420	THR
2	B	426	ASP
2	B	435	PHE
2	B	461	GLU
2	B	472	PRO
2	B	491	MET
2	B	496	THR
2	B	504	ARG
2	B	519	HIS
2	B	522	VAL
2	B	523	ARG
1	C	14	GLN
1	C	21	PRO
1	C	29	ASN
1	C	30	LYS
1	C	32	LEU
1	C	37	PRO
1	C	44	LYS

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Mol	Chain	Res	Type
1	C	48	SER
1	C	54	PRO
1	C	59	ILE
1	C	70	VAL
1	C	74	PRO
1	C	75	ILE
1	C	85	PRO
1	C	92	SER
1	C	96	ARG
1	C	98	ASN
1	C	100	TYR
1	C	120	GLU
1	C	155	PRO
1	C	184	GLU
1	C	187	ARG
1	C	203	ARG
1	C	240	ILE
1	C	252	GLN
1	C	258	SER
1	C	266	PRO
1	C	267	LYS
1	C	279	MET
1	C	280	ASN
1	C	288	GLU
1	C	298	ASN
1	C	302	PRO
1	C	317	ASP
1	C	324	CYS
1	C	345	ARG
1	C	346	LEU
1	C	360	PRO
1	C	362	HIS
1	C	383	HIS
1	C	398	THR
1	C	401	TYR
1	C	409	PHE
1	C	419	ASP
1	C	421	ILE
1	C	444	TRP
1	C	446	TYR
1	C	462	ASP
2	D	3	GLN

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Mol	Chain	Res	Type
2	D	11	SER
2	D	13	PRO
2	D	14	LEU
2	D	31	PHE
2	D	41	ASP
2	D	54	GLU
2	D	62	LEU
2	D	121	ASP
2	D	130	ASN
2	D	144	PRO
2	D	146	MET
2	D	179	PHE
2	D	202	GLU
2	D	234	LEU
2	D	245	SER
2	D	253	LEU
2	D	264	PRO
2	D	277	THR
2	D	278	GLN
2	D	281	MET
2	D	285	PRO
2	D	295	PRO
2	D	300	LYS
2	D	317	ASN
2	D	326	ASP
2	D	369	LEU
2	D	375	PHE
2	D	384	LEU
2	D	397	ASN
2	D	418	ASN
2	D	420	THR
2	D	425	LYS
2	D	426	ASP
2	D	435	PHE
2	D	461	GLU
2	D	472	PRO
2	D	496	THR
2	D	504	ARG
2	D	519	HIS
2	D	522	VAL
2	D	523	ARG
3	E	2	MET

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Mol	Chain	Res	Type
3	E	4	GLN
3	E	46	ARG
3	E	54	GLN
3	E	56	THR
3	E	60	MET
3	E	66	THR
3	E	76	LEU
3	E	87	GLU
3	E	95	VAL
3	E	131	VAL
3	E	137	MET
3	E	152	SER
3	E	156	MET
3	E	165	SER
3	E	185	ASN
3	E	186	SER
3	E	193	ASP
3	E	199	LEU
3	E	208	ILE
3	E	214	ASP
3	E	225	MET
3	E	228	ILE
3	E	232	PRO
3	E	250	ASN
3	E	251	LYS
3	E	255	ILE
3	E	259	ILE
3	E	264	LEU
3	E	266	GLU
3	F	2	MET
3	F	3	ARG
3	F	48	ILE
3	F	56	THR
3	F	60	MET
3	F	66	THR
3	F	71	GLU
3	F	76	LEU
3	F	95	VAL
3	F	118	ASP
3	F	131	VAL
3	F	140	ARG
3	F	165	SER

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Mol	Chain	Res	Type
3	F	179	LEU
3	F	182	LEU
3	F	199	LEU
3	F	208	ILE
3	F	213	ARG
3	F	214	ASP
3	F	251	LYS
3	F	255	ILE
3	F	259	ILE
3	F	264	LEU
3	F	266	GLU
3	F	267	LEU
3	G	2	MET
3	G	3	ARG
3	G	4	GLN
3	G	5	CYS
3	G	10	LYS
3	G	46	ARG
3	G	48	ILE
3	G	54	GLN
3	G	56	THR
3	G	60	MET
3	G	66	THR
3	G	76	LEU
3	G	95	VAL
3	G	131	VAL
3	G	152	SER
3	G	156	MET
3	G	165	SER
3	G	199	LEU
3	G	208	ILE
3	G	214	ASP
3	G	225	MET
3	G	228	ILE
3	G	250	ASN
3	G	255	ILE
3	G	259	ILE
3	G	264	LEU
3	G	266	GLU
3	G	267	LEU
3	H	2	MET
3	H	4	GLN

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Mol	Chain	Res	Type
3	H	5	CYS
3	H	10	LYS
3	H	17	THR
3	H	46	ARG
3	H	56	THR
3	H	66	THR
3	H	76	LEU
3	H	95	VAL
3	H	137	MET
3	H	152	SER
3	H	165	SER
3	H	178	ARG
3	H	185	ASN
3	H	187	ARG
3	H	199	LEU
3	H	208	ILE
3	H	214	ASP
3	H	225	MET
3	H	228	ILE
3	H	250	ASN
3	H	255	ILE
3	H	259	ILE
3	H	264	LEU
3	H	266	GLU
3	H	267	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	53	GLN
1	A	113	ASN
1	A	145	ASN
1	A	191	GLN
1	A	199	ASN
1	A	274	HIS
1	A	280	ASN
1	A	298	ASN
1	A	362	HIS
1	A	432	GLN
1	A	442	HIS

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Mol	Chain	Res	Type
2	B	3	GLN
2	B	18	GLN
2	B	71	GLN
2	B	128	GLN
2	B	129	GLN
2	B	130	ASN
2	B	137	ASN
2	B	167	ASN
2	B	168	ASN
2	B	185	HIS
2	B	225	ASN
2	B	289	ASN
2	B	397	ASN
2	B	418	ASN
2	B	429	HIS
2	B	452	GLN
2	B	457	HIS
2	B	480	HIS
2	B	518	ASN
1	C	35	ASN
1	C	151	GLN
1	C	280	ASN
1	C	298	ASN
1	C	362	HIS
1	C	384	ASN
1	C	432	GLN
1	C	476	GLN
2	D	3	GLN
2	D	18	GLN
2	D	58	GLN
2	D	104	ASN
2	D	129	GLN
2	D	130	ASN
2	D	137	ASN
2	D	167	ASN
2	D	168	ASN
2	D	199	ASN
2	D	225	ASN
2	D	268	GLN
2	D	294	GLN
2	D	317	ASN
2	D	396	HIS

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Mol	Chain	Res	Type
2	D	397	ASN
2	D	452	GLN
2	D	457	HIS
2	D	518	ASN
3	E	4	GLN
3	E	107	ASN
3	E	206	GLN
3	E	236	GLN
3	E	250	ASN
3	F	4	GLN
3	F	107	ASN
3	F	206	GLN
3	F	250	ASN
3	G	4	GLN
3	G	54	GLN
3	G	206	GLN
3	G	236	GLN
3	G	250	ASN
3	H	4	GLN
3	H	54	GLN
3	H	55	ASN
3	H	107	ASN
3	H	185	ASN
3	H	206	GLN
3	H	236	GLN
3	H	250	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	HCA	A	1494	9	13,13,13	2.30	4 (30%)	18,18,18	2.45	7 (38%)
9	CFM	A	1496	1,8	18,24,24	8.09	15 (83%)	0,45,45	0.00	-
10	CLF	A	1498	1,2	18,24,24	73.78	17 (94%)	0,57,57	0.00	-
8	HCA	C	3494	9	13,13,13	2.16	3 (23%)	18,18,18	2.55	6 (33%)
9	CFM	C	3496	1,8	18,24,24	4.48	10 (55%)	0,45,45	0.00	-
10	CLF	D	3498	1,2	18,24,24	74.02	16 (88%)	0,57,57	0.00	-
7	ATP	E	5292	4	33,33,33	1.28	3 (9%)	52,52,52	1.28	6 (11%)
6	SF4	F	5290	3	12,12,12	6.54	8 (66%)	0,24,24	0.00	-
7	ATP	F	6292	4	33,33,33	1.37	4 (12%)	52,52,52	1.37	6 (11%)
6	SF4	G	7290	3	12,12,12	3.05	8 (66%)	0,24,24	0.00	-
7	ATP	G	7292	4	33,33,33	1.69	7 (21%)	52,52,52	1.38	5 (9%)
7	ATP	H	8292	4	33,33,33	1.32	4 (12%)	52,52,52	1.33	7 (13%)

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
8	HCA	A	1494	9	-	0/17/17/17	0/0/0/0
9	CFM	A	1496	1,8	-	0/0/84/84	0/0/8/8
10	CLF	A	1498	1,2	-	0/0/132/132	0/0/10/10
8	HCA	C	3494	9	-	0/17/17/17	0/0/0/0
9	CFM	C	3496	1,8	-	0/0/84/84	0/0/8/8
10	CLF	D	3498	1,2	-	0/0/132/132	0/0/10/10
7	ATP	E	5292	4	-	0/22/38/38	0/1/3/3
6	SF4	F	5290	3	-	0/0/48/48	0/0/5/5
7	ATP	F	6292	4	-	0/22/38/38	0/1/3/3
6	SF4	G	7290	3	-	0/0/48/48	0/0/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	G	7292	4	-	0/22/38/38	0/1/3/3
7	ATP	H	8292	4	-	0/22/38/38	0/1/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1498	CLF	S4A-FE2	235.04	3.91	2.33
10	D	3498	CLF	S4A-FE2	231.19	3.88	2.33
10	D	3498	CLF	S3A-FE1	210.23	3.74	2.33
10	A	1498	CLF	S3A-FE1	202.59	3.69	2.33
9	A	1496	CFM	S1B-FE5	-22.57	2.18	2.33
10	A	1498	CLF	S2A-FE3	-17.38	2.21	2.33
10	A	1498	CLF	S2A-FE2	-16.85	2.21	2.33
10	D	3498	CLF	S2B-FE7	-15.41	2.22	2.33
10	A	1498	CLF	S2A-FE1	-12.91	2.24	2.33
9	A	1496	CFM	S4A-FE4	-12.62	2.24	2.33
10	D	3498	CLF	S2A-FE3	-12.55	2.24	2.33
10	A	1498	CLF	S3B-FE7	-12.11	2.25	2.33
10	A	1498	CLF	S2B-FE7	-11.93	2.25	2.33
10	A	1498	CLF	S3B-FE8	-10.89	2.25	2.33
10	A	1498	CLF	S4A-FE4	-10.61	2.26	2.33
9	A	1496	CFM	S2A-FE2	-10.40	2.26	2.33
10	A	1498	CLF	S4B-FE5	-10.31	2.26	2.33
9	C	3496	CFM	S1B-FE6	-10.07	2.26	2.33
10	D	3498	CLF	S4B-FE5	-9.92	2.26	2.33
6	F	5290	SF4	S2-FE1	-9.61	2.26	2.33
9	A	1496	CFM	S3B-FE7	-9.48	2.26	2.33
9	C	3496	CFM	S4A-FE4	-9.18	2.27	2.33
6	F	5290	SF4	S3-FE2	9.12	2.39	2.33
10	D	3498	CLF	S3B-FE6	-9.02	2.27	2.33
6	F	5290	SF4	S2-FE3	8.74	2.39	2.33
10	D	3498	CLF	S2B-FE5	-8.64	2.27	2.33
10	A	1498	CLF	S3A-FE4	-8.53	2.27	2.33
10	D	3498	CLF	S2A-FE1	-8.34	2.27	2.33
6	F	5290	SF4	S4-FE1	8.13	2.38	2.33
10	A	1498	CLF	S4B-FE8	-8.01	2.27	2.33
10	D	3498	CLF	S4A-FE3	-8.00	2.27	2.33
6	F	5290	SF4	S3-FE4	-7.87	2.28	2.33
10	D	3498	CLF	S3A-FE4	-7.68	2.28	2.33
9	A	1496	CFM	MO1-S3B	7.53	2.39	2.31
9	C	3496	CFM	S1B-FE5	-7.24	2.28	2.33
9	A	1496	CFM	S1B-FE6	-7.14	2.28	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	5290	SF4	S1-FE2	-7.05	2.28	2.33
10	A	1498	CLF	S2B-FE6	-6.97	2.28	2.33
9	A	1496	CFM	MO1-S1B	-6.93	2.24	2.31
9	A	1496	CFM	S4A-FE1	-6.89	2.28	2.33
6	F	5290	SF4	S1-FE4	6.69	2.37	2.33
10	D	3498	CLF	S2A-FE2	-6.38	2.29	2.33
10	A	1498	CLF	S2B-FE5	-6.36	2.29	2.33
8	A	1494	HCA	O5-C7	6.34	1.44	1.22
8	C	3494	HCA	O5-C7	6.10	1.43	1.22
10	D	3498	CLF	S2B-FE6	-5.79	2.29	2.33
6	F	5290	SF4	S4-FE3	-5.76	2.29	2.33
6	G	7290	SF4	S3-FE4	-5.73	2.29	2.33
10	A	1498	CLF	S3A-FE3	-5.68	2.29	2.33
10	A	1498	CLF	S4A-FE3	-5.49	2.29	2.33
10	D	3498	CLF	S3B-FE8	-5.20	2.29	2.33
9	C	3496	CFM	S4B-FE7	-4.89	2.30	2.33
9	C	3496	CFM	S4A-FE3	-4.86	2.30	2.33
7	G	7292	ATP	C4-N3	4.83	1.43	1.35
9	A	1496	CFM	S2A-FE3	-4.75	2.30	2.33
9	C	3496	CFM	S1A-FE4	4.71	2.36	2.33
10	D	3498	CLF	S3B-FE7	-4.37	2.30	2.33
10	A	1498	CLF	S3B-FE6	-4.23	2.30	2.33
9	C	3496	CFM	MO1-S4B	4.09	2.36	2.31
6	G	7290	SF4	S3-FE2	-4.08	2.30	2.33
9	A	1496	CFM	S1A-FE2	4.07	2.36	2.33
6	G	7290	SF4	S4-FE2	-4.02	2.30	2.33
6	G	7290	SF4	S1-FE2	-3.98	2.30	2.33
7	E	5292	ATP	PB-O3A	-3.91	1.52	1.59
9	A	1496	CFM	S4B-FE5	3.89	2.35	2.33
9	C	3496	CFM	S4A-FE1	-3.69	2.30	2.33
7	G	7292	ATP	O4'-C1'	3.65	1.47	1.41
9	A	1496	CFM	S4A-FE3	3.57	2.35	2.33
9	A	1496	CFM	S1A-FE1	-3.48	2.30	2.33
7	H	8292	ATP	PB-O3A	-3.46	1.53	1.59
7	G	7292	ATP	PB-O3A	-3.38	1.53	1.59
7	F	6292	ATP	PB-O3A	-3.37	1.53	1.59
9	A	1496	CFM	S1A-FE4	-3.32	2.31	2.33
9	C	3496	CFM	S2A-FE3	3.29	2.35	2.33
9	A	1496	CFM	S4B-FE7	-3.16	2.31	2.33
10	D	3498	CLF	S4B-FE8	-2.89	2.31	2.33
10	D	3498	CLF	S4B-FE7	-2.84	2.31	2.33
6	G	7290	SF4	S3-FE1	2.81	2.35	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	7292	ATP	C2'-C1'	2.81	1.57	1.53
7	F	6292	ATP	C4-N9	-2.79	1.33	1.37
7	E	5292	ATP	C4-N3	2.74	1.39	1.35
8	C	3494	HCA	O3-C6	2.68	1.31	1.22
8	A	1494	HCA	O3-C6	2.63	1.31	1.22
6	G	7290	SF4	S1-FE3	-2.62	2.31	2.33
6	G	7290	SF4	S2-FE4	-2.54	2.31	2.33
8	A	1494	HCA	O6-C7	-2.53	1.20	1.30
7	F	6292	ATP	PB-O3B	2.51	1.64	1.59
8	A	1494	HCA	O1-C1	2.48	1.31	1.22
7	G	7292	ATP	C2-N3	2.47	1.37	1.32
6	G	7290	SF4	S2-FE3	-2.45	2.31	2.33
7	H	8292	ATP	C8-N7	-2.34	1.30	1.34
7	F	6292	ATP	PG-O3B	2.27	1.64	1.60
7	H	8292	ATP	PB-O2B	-2.20	1.45	1.55
7	G	7292	ATP	PG-O2G	-2.13	1.46	1.54
8	C	3494	HCA	O6-C7	-2.13	1.22	1.30
7	H	8292	ATP	C4-N9	-2.07	1.34	1.37
7	G	7292	ATP	PB-O2B	-2.05	1.45	1.55
9	C	3496	CFM	MO1-S3B	-2.05	2.29	2.31
7	E	5292	ATP	PG-O2G	-2.04	1.47	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3494	HCA	O6-C7-C3	7.38	123.62	112.89
8	A	1494	HCA	O6-C7-C3	6.17	121.86	112.89
8	A	1494	HCA	O5-C7-C3	-4.90	115.44	122.20
7	E	5292	ATP	O4'-C1'-C2'	-4.42	99.99	106.77
7	G	7292	ATP	C8-N9-C4	-4.37	103.56	106.90
7	H	8292	ATP	O4'-C1'-C2'	-4.24	100.27	106.77
7	G	7292	ATP	O4'-C1'-C2'	-4.11	100.47	106.77
7	F	6292	ATP	O4'-C1'-C2'	-4.02	100.62	106.77
8	C	3494	HCA	O5-C7-C3	-3.87	116.87	122.20
7	F	6292	ATP	C3'-C2'-C1'	3.85	106.93	100.91
7	F	6292	ATP	C4-C5-N7	3.83	112.80	109.52
7	H	8292	ATP	C4-C5-N7	3.72	112.71	109.52
8	C	3494	HCA	O2-C1-O1	-3.45	114.52	123.30
7	G	7292	ATP	O3'-C3'-C4'	-3.27	101.46	111.08
8	A	1494	HCA	C4-C3-C7	-3.11	103.03	110.31
7	H	8292	ATP	C3'-C2'-C1'	3.08	105.73	100.91
8	C	3494	HCA	O2-C1-C2	3.07	125.44	114.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	7292	ATP	C4'-O4'-C1'	2.90	112.89	109.75
7	E	5292	ATP	C4-C5-N7	2.86	111.97	109.52
7	F	6292	ATP	O3'-C3'-C4'	-2.71	103.11	111.08
8	A	1494	HCA	C5-C4-C3	2.65	123.60	115.10
7	E	5292	ATP	O3G-PG-O2G	2.59	117.68	107.61
7	H	8292	ATP	PA-O3A-PB	2.57	139.23	131.68
7	E	5292	ATP	C8-N9-C4	-2.56	104.94	106.90
8	C	3494	HCA	O4-C6-O3	-2.56	116.79	123.30
8	A	1494	HCA	O2-C1-O1	-2.55	116.81	123.30
7	H	8292	ATP	O3G-PG-O2G	2.52	117.41	107.61
7	G	7292	ATP	C3'-C2'-C1'	2.46	104.75	100.91
8	C	3494	HCA	O4-C6-C5	2.38	122.62	114.22
7	F	6292	ATP	C8-N9-C4	-2.36	105.10	106.90
7	H	8292	ATP	C8-N9-C4	-2.22	105.20	106.90
7	H	8292	ATP	O3'-C3'-C4'	-2.20	104.60	111.08
7	E	5292	ATP	C3'-C2'-C1'	2.16	104.28	100.91
7	E	5292	ATP	O4'-C1'-N9	2.11	110.40	108.44
7	F	6292	ATP	O3G-PG-O2G	2.07	115.68	107.61
8	A	1494	HCA	O2-C1-C2	2.07	121.91	114.63
8	A	1494	HCA	O4-C6-O3	-2.00	118.20	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.