



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:30 am BST

PDB ID : 4HNU
Title : crystal structure of K442E mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

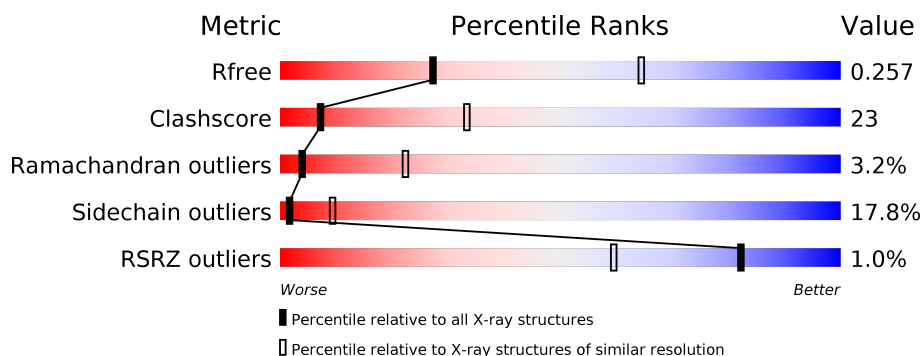
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1173	<div> <div>2%</div> <div> <div>49%</div> <div>31%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	1173	<div> <div>47%</div> <div>31%</div> <div>6%</div> <div>16%</div> </div>
1	C	1173	<div> <div>%</div> <div> <div>47%</div> <div>32%</div> <div>10%</div> <div>10%</div> </div> </div>
1	D	1173	<div> <div>%</div> <div> <div>46%</div> <div>30%</div> <div>7%</div> <div>16%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8342	5291	1403	1621	27			
1	B	989	Total	C	N	O	S	0	0	0
			7838	4974	1320	1518	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8379	5312	1411	1628	28			
1	D	989	Total	C	N	O	S	0	0	0
			7838	4974	1320	1518	26			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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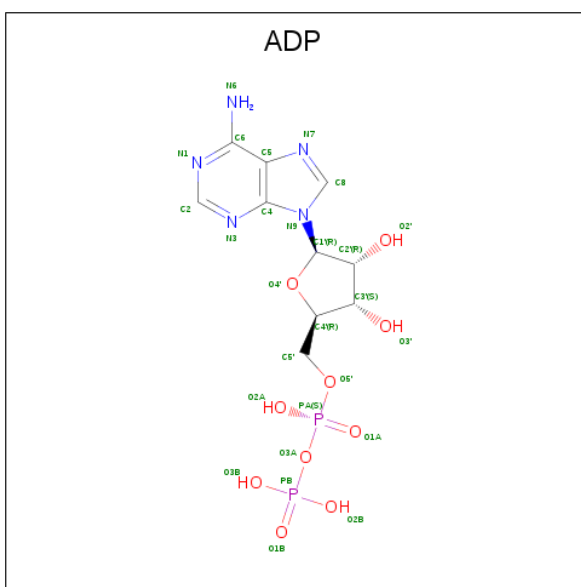
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
A	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

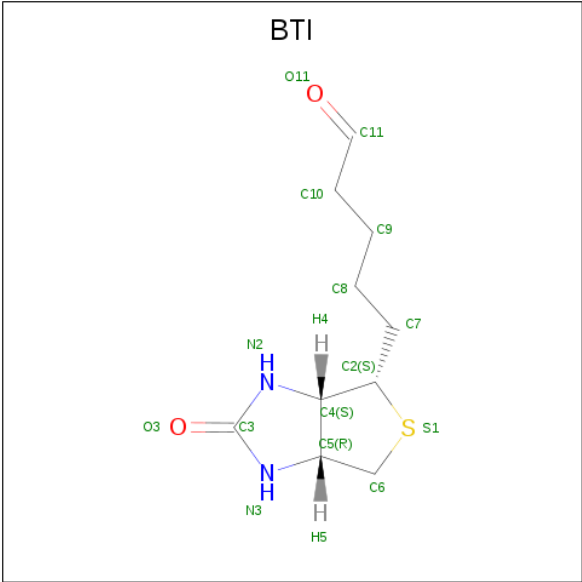


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn		
			1	1	0	0
3	A	1	Total	Mn		
			1	1	0	0
3	D	1	Total	Mn		
			1	1	0	0
3	C	1	Total	Mn		
			1	1	0	0

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).

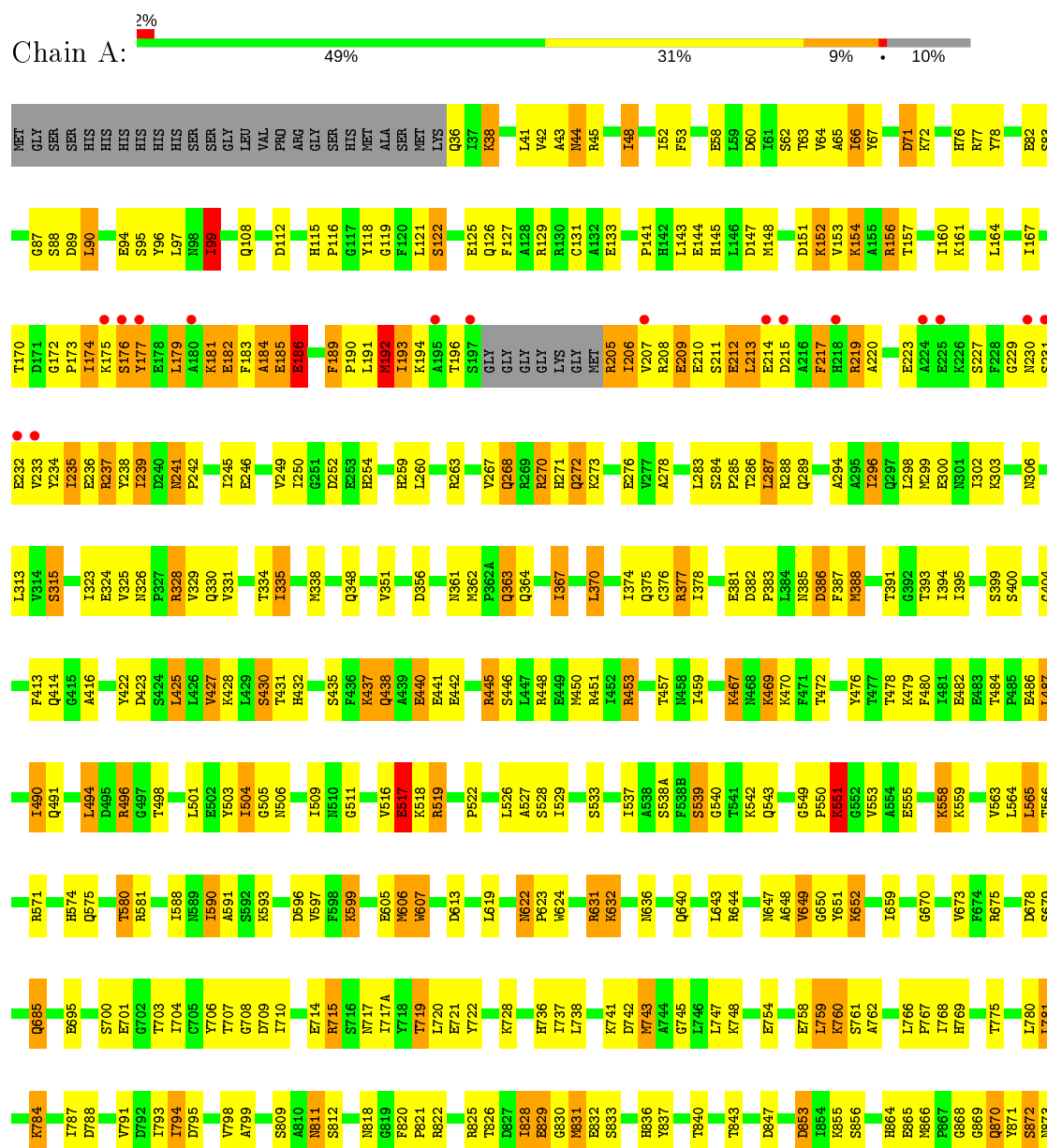


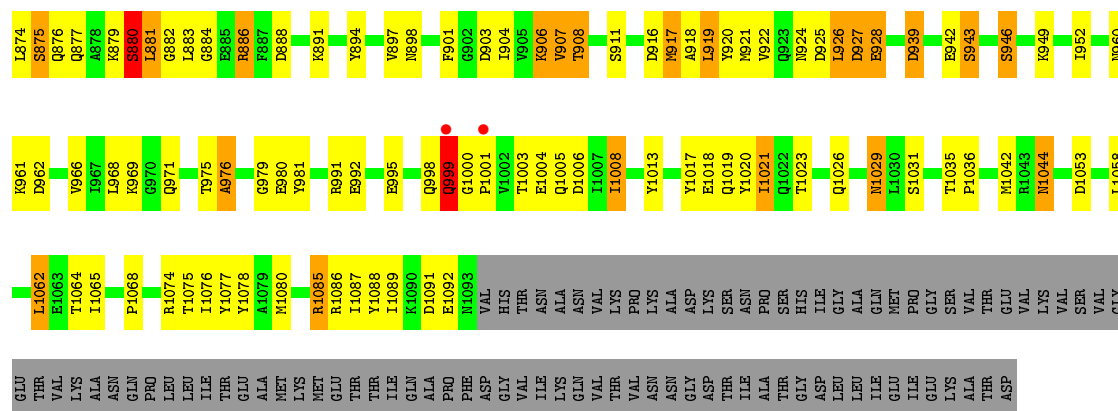
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	15	10	2	2	1	0	0

3 Residue-property plots

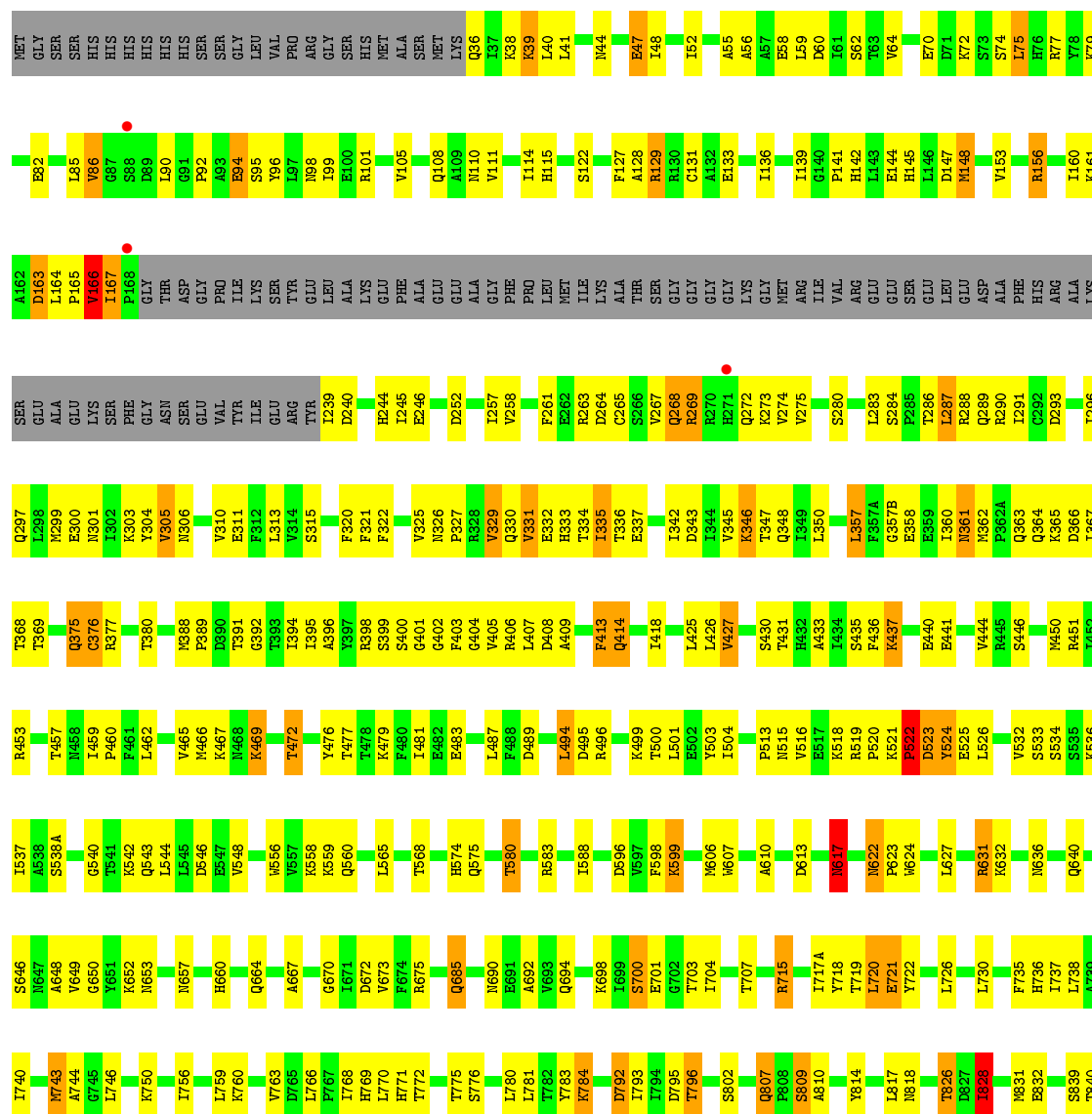
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase

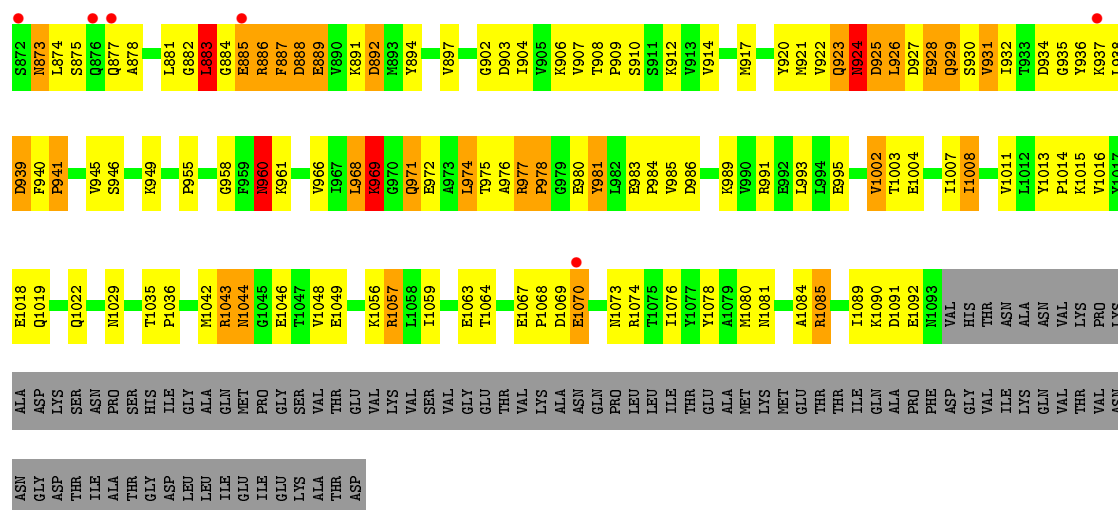


V841	V821	V1016	LYS
Y844	Y922	Y1017	ALA
Y845	Y923	Q1018	ASP
S846	Y924	Q1019	GLY
E849	D925	T1023	THR
S852	D926	R1024	ASN
D853	D927	R1024	PRO
I854	E928	Y1027	ALA
S855	Q929	Y1027	THR
S856	S930	L1030	GLY
P857	S931	S1031	ASP
	I932	L1032	LEU
	Y933	L1032	ALA
I861	D934	M1042	ILE
H864	G935	R1043	GLU
H865	L938	N1044	GLY
H866	S943	E1049	LYS
P867	Y944	I1050	VAL
G868	F948	E1051	THR
G869	K949	I1052	GLU
Q870	G950	D1053	VAL
Y871	E951	K1056	VAL
		R1057	GLY
S875	F959	L1062	GLU
Q876	N960	L1062	THR
K879	L963	I1065	VAL
S880	L963	I1065	LYS
L881	Q964	D1069	ALA
G884	K969	E1070	ASN
	L982	N1071	GLN
		R1074	PRO
K891	V985	T1075	LEU
D892	D986	M1080	ILE
M893	K989	Q1083	THR
R896	V990	A1084	GLU
V897	R991	R1085	ALA
N898	L994	R1086	MET
F901	F997	I1087	THR
K906	Q998	Y1088	THR
V907	Q999	I1089	THR
T908	G1000	K1090	ILE
P909	P1001	D1091	GLN
S910	V1002	E1092	ALA
S911	T1003	N1093	PRO
K912	D1006	VAL	PHE
V913	I1007	HIS	ASP
D916	I1008	THR	GLY
M917	Y1013	ASN	VAL
A918	P1014	LYS	THR
L919	K1015	VAL	VAL
Y920		PRO	

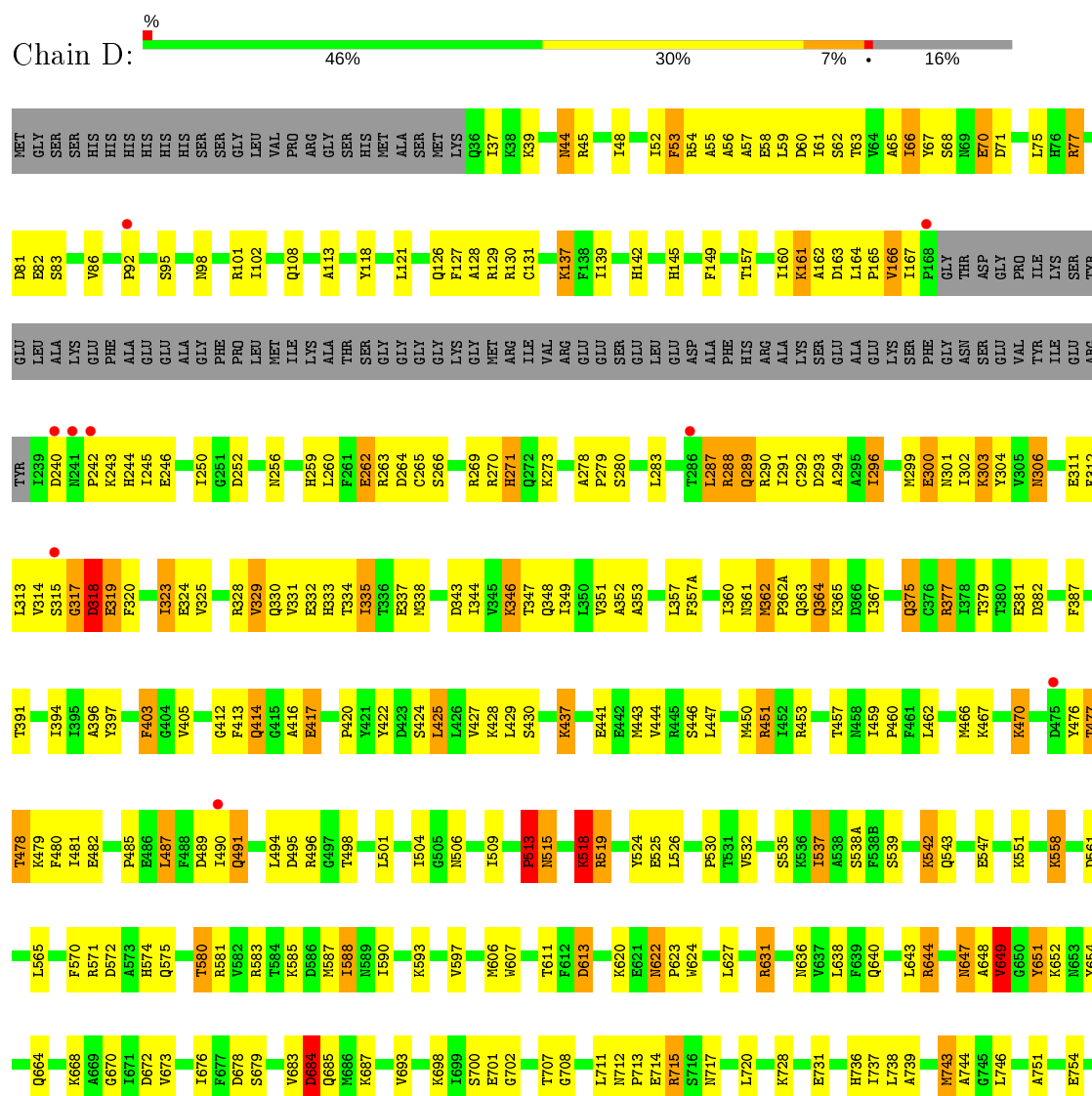
• Molecule 1: Pyruvate carboxylase



Y93	P165	K346	H432	V510	L578	S679	I793
E94	V166	T347	A433	Q511	A979	D684	I794
L97	P167	Q348	S434	P512	T580	Q685	D795
N98	P168	G354	S435	P513	S581	Q686	T796
I99	G169	G354	K436	N515	V582	V687	A797
E100	T170	E358	Q437	V516	T583	V688	A799
R101	D171	E359	Q438	E517	N589	A689	G803
I102	G172	E360	A439	R519	R589	N690	L804
T103	I174	I360	E440	R519	I590	N690	L804
D104	E185	M362	E441	P520	E441	Q694	T805
K107	A180	K365	M443	K521	M443	F698	S806
Q108	E182	D366	V444	Y524	V698	K698	O807
M109	F183	D366	M450	E525	E605	T699	P808
N110	A184	T369	R451	L526	M606	S700	S809
A113	E185	L370	R452	A527	M607	E701	A810
I114	F189	G371	R453	S528	L614	N712	N811
H115	P190	Y372	K456	P530	V614	N712	S812
P116	P190	A373	K456	T531	A615	E713	L813
G117	M192	Q375	I459	S534	F618	T719	Y814
Y118	M193	C376	P460	S535	L619	T719	N818
F119	K194	R377	R459	K536	N622	E721	P821
G120	A195	I378	M466	S538A	P623	E731	R822
L121	T196	T379	K467	F539B	W624	H736	H823
S122	S197	T380	M468	S539	R629	I737	I828
E123	G198	E381	K469	G540	R629	I737	E932
N124	G199	I296	T472	T541	R631	L738	S833
E125	G199	D382	T473	K542	K632	A739	L834
V42	Q126	P383	G474	Q543	L643	M743	Y837
A43	I206	L384	S473	L544	A645	I756	N838
M44	D207	N301	G474	V548	S645	G757	S839
R45	E208	N302	T477	G549	P646	E758	T840
R130	E209	I302	T477	P550	N647	L759	V841
R54	E210	V303	T477	G552	A648	K760	R842
E133	S211	N306	A396	V553	V649	S761	Y844
E134	E212	I306	Y397	K558	D489	A762	S845
G135	E213	T309	R398	K559	I490	V763	S846
I136	E214	E311	S399	D560	Q491	D765	D847
L139	D215	F320	F403	D561	F492	I768	F848
H142	F217	I323	G404	T568	S493		F849
L143	R219	E324	L407	T569	L494		P855
E144	A220	P327	F413	T569	D562		D856
H145	E223	R328	Q414	L564	V663		N657
D147	S74	V329	I418	L565	L564		D773
M148	L75	Q330	I418	T566	D496		D774
F149	H76	V331	D423	D567	G497		T775
G150	L85	F228	S424	T568	H660		N778
D151	S231	F228	L425	T569	H661		I778
K152	G87	S231	E502	P570	I671		L781
V153	E232	I335	Y503	H571	D672		K784
K154	V233	N338	V427	D572	R675		I787
A155	Y234	T342	K428	L573	L676		Y871
R156	I235	D343	L429	H574	F677		Q870
L164	E236	T431	S430	T508			Y871
	R237			I509			



• Molecule 1: Pyruvate carboxylase



GLY	HIS	E1051	I926	F848	E758
ASP	ILE	I1052	D927	E849	L759
LEU	GLY	D1053	Q928		K760
ILE	ALA	I1054	Q929	I854	S761
ILE	GLN	K1055	S930	K855	A762
PRO	MET	K1056		S856	V763
GLY	PRO	K1057	Q935	P857	D765
LYS	GLY	L1058		M858	L766
ALA	SER	L1059	I938	T859	P767
THR	VAL	I1060	D939	E860	I768
ASP	THR	I1061	F940	I861	H769
	GLU	L1062		Y862	
	VAL	E1063	V944	Q863	T772
	LYS	T1064	V945	H864	H773
	VAL	I1065	S946	E865	D774
	SER	S1066	F947	M866	T775
	VAL	E1067	F948	P867	S776
	GLY	P1068	K949	G868	G777
	GLU	D1069	Q950	G869	N778
	THR	E1070	E951	Q870	
	VAL	N1071	I952	Y871	L781
	LYS	G1072		S872	
	ALA	N1073	N960	N873	K784
	ASN	R1074	K961	L874	
	GLN	T1075	D962	S875	V791
	PRO	I1076	I963	Q876	
	LEU	I1077		Q877	
	ILE	Y1078	V966	A878	A799
	THR	A1079	I967	K879	S800
	GLU	M1080	T975	S880	M801
	ALA	N1081	A976	L881	S802
	MET	G1082	R977	G882	Q807
	LYS	Q1083		L883	P808
	MET	A1084	E983	G884	S809
	GLU	R1085		E885	A310
	THR	R1086		R886	N811
	THR	I1087	D986	F887	
	ILE	Y1088			Y814
	GLN	K1089	R991	K891	
	ALA	K1090	L994	R896	N818
	PHE		E995	V897	G819
	ASP	N1093	E996		F820
	GLY	VAL	Q997	F901	P821
	VAL	HIS	Q998		R822
	ILE	THR	Q999	V905	B823
	LYS	ASN	G1000	K906	L824
	LYS	ALA	P1001	V907	
	GLN	ASN		T908	I828
	VAL	VAL	Q1005	P909	E829
	THR	LYS			E832
	VAL	PRO	I1008	V914	
	ASN	LYS	Y1013	M917	Y837
	GLY	ALA		A918	T840
	ASP	LYS	E1018	I919	V841
	THR	SER		Y920	B842
	ILE	ASN	T1035		T843
	ALA	PRO		N924	
	THR	SER	M1042	D925	D847

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.57Å 258.52Å 126.90Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.00) 98.4 (29.72-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.257	Depositor DCC
R_{free} test set	5765 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32443	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.60	0/8504	0.69	3/11500 (0.0%)
1	B	0.46	2/7990 (0.0%)	0.57	0/10811
1	C	0.53	5/8542 (0.1%)	0.61	3/11549 (0.0%)
1	D	0.59	2/7990 (0.0%)	0.68	4/10811 (0.0%)
All	All	0.55	9/33026 (0.0%)	0.64	10/44671 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	3
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	515	ASN	N-CA	6.54	1.59	1.46
1	B	513	PRO	CA-C	6.53	1.66	1.52
1	C	513	PRO	CA-C	6.13	1.65	1.52
1	C	441	GLU	CG-CD	5.96	1.60	1.51
1	B	515	ASN	N-CA	5.89	1.58	1.46
1	C	849	GLU	N-CA	5.67	1.57	1.46
1	D	513	PRO	CA-C	5.55	1.64	1.52
1	C	376	CYS	CB-SG	-5.34	1.73	1.81
1	D	315	SER	CA-C	5.16	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLU	CA-C-N	-7.39	100.94	117.20
1	C	513	PRO	CA-N-CD	7.06	121.59	111.70
1	C	513	PRO	N-CA-CB	-5.95	96.05	102.60
1	D	315	SER	N-CA-CB	-5.93	101.61	110.50
1	D	849	GLU	CA-C-N	5.54	129.38	117.20
1	C	427	VAL	CB-CA-C	-5.44	101.06	111.40
1	D	513	PRO	N-CA-C	5.29	125.85	112.10
1	A	441	GLU	O-C-N	5.28	131.15	122.70
1	D	849	GLU	C-N-CA	-5.16	108.81	121.70
1	A	788	ASP	CB-CG-OD2	5.13	122.91	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	GLU	Peptide
1	A	174	ILE	Peptide
1	A	215	ASP	Peptide
1	B	357(B)	GLY	Peptide
1	B	522	PRO	Peptide
1	C	193	ILE	Peptide
1	D	167	ILE	Peptide
1	D	651	TYR	Peptide
1	D	999	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8342	0	8246	393	0
1	B	7838	0	7764	331	0
1	C	8379	0	8284	385	0
1	D	7838	0	7764	365	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	15	0	16	4	0
All	All	32443	0	32086	1456	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:LYS:HD2	1:D:961:LYS:N	1.59	1.14
1:C:437:LYS:HD3	1:C:437:LYS:H	0.98	1.13
1:D:961:LYS:H	1:D:961:LYS:CD	1.59	1.12
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.84	1.11
1:A:866:MET:HE3	1:A:870:GLN:HG2	1.26	1.11
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.03	1.11
1:A:338:MET:HE1	1:A:430:SER:CB	1.82	1.09
1:D:999:GLN:HG2	1:D:1000:GLY:N	1.58	1.09
1:C:156:ARG:NH2	1:C:170:THR:O	1.85	1.08
1:C:338:MET:CE	1:C:430:SER:HB3	1.85	1.06
1:C:870:GLN:HG3	1:C:870:GLN:O	1.50	1.05
1:A:338:MET:HE1	1:A:430:SER:HB2	1.06	1.05
1:D:513:PRO:HD3	4:D:1201:BTI:H11	1.39	1.05
1:C:874:LEU:HD23	1:C:874:LEU:O	1.57	1.04
1:D:413:PHE:CE2	1:D:416:ALA:HB2	1.93	1.03
1:C:437:LYS:HD3	1:C:437:LYS:N	1.61	1.03
1:C:438:GLN:HG2	1:C:441:GLU:OE1	1.58	1.03
1:B:907:VAL:O	1:B:911:SER:HB3	1.58	1.02
1:A:883:LEU:HD22	1:A:886:ARG:NH1	1.75	1.02
1:C:828:ILE:HD12	1:C:828:ILE:H	1.21	1.02
1:D:917:MET:HG2	1:D:944:VAL:HG21	1.40	1.02
1:A:883:LEU:HD22	1:A:886:ARG:HH12	1.26	1.01
1:D:999:GLN:CG	1:D:1000:GLY:H	1.75	0.99
1:A:338:MET:CE	1:A:430:SER:HB2	1.93	0.98
1:D:999:GLN:HG2	1:D:1000:GLY:H	0.82	0.97
1:D:873:ASN:HD22	1:D:873:ASN:N	1.58	0.97
1:D:256:ASN:O	1:D:357:LEU:HD21	1.64	0.97
1:C:451:ARG:NH1	1:C:451:ARG:HG2	1.77	0.96
1:A:44:ASN:HD22	1:A:45:ARG:H	1.05	0.96
1:D:811:ASN:H	1:D:811:ASN:HD22	0.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASN:HD22	1:D:45:ARG:H	1.09	0.96
1:A:245:ILE:HD13	1:A:283:LEU:HD11	1.48	0.95
1:C:494:LEU:HB2	1:C:496:ARG:NH2	1.81	0.95
1:A:237:ARG:HH11	1:A:237:ARG:HG2	1.29	0.95
1:C:437:LYS:CD	1:C:437:LYS:H	1.77	0.95
1:A:209:GLU:HA	1:A:213:LEU:HD21	1.49	0.94
1:C:1076:ILE:HD12	1:C:1089:ILE:CD1	1.98	0.94
1:C:995:GLU:HG3	1:C:1002:VAL:HG21	1.47	0.93
1:D:811:ASN:N	1:D:811:ASN:HD22	1.67	0.92
1:B:275:VAL:HG21	1:B:466:MET:CE	1.99	0.92
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.08	0.92
1:A:864:HIS:HD2	1:A:866:MET:H	1.17	0.91
1:C:196:THR:O	1:C:197:SER:HB2	1.71	0.90
1:D:961:LYS:HD2	1:D:961:LYS:H	0.74	0.90
1:B:704:ILE:HD11	1:B:730:LEU:HD12	1.52	0.90
1:B:275:VAL:HG21	1:B:466:MET:HE3	1.54	0.89
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.07	0.89
1:B:47:GLU:HG3	1:B:48:ILE:N	1.84	0.89
1:A:338:MET:CE	1:A:430:SER:CB	2.51	0.89
1:D:513:PRO:O	1:D:515:ASN:HB2	1.71	0.89
1:B:1008:ILE:HD13	1:B:1008:ILE:H	1.34	0.88
1:C:995:GLU:CG	1:C:1002:VAL:HG21	2.03	0.87
1:C:44:ASN:ND2	1:C:45:ARG:H	1.73	0.87
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.56	0.87
1:C:44:ASN:HD22	1:C:45:ARG:N	1.73	0.87
1:C:878:ALA:HA	1:C:883:LEU:HD12	1.56	0.87
1:A:700:SER:H	1:A:736:HIS:HD2	1.13	0.87
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.54	0.87
1:B:999:GLN:HE21	1:B:1001:PRO:HG3	1.40	0.86
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.06	0.86
1:A:1042:MET:HE3	1:A:1062:LEU:HB2	1.58	0.86
1:C:44:ASN:HD22	1:C:45:ARG:H	0.88	0.86
1:C:306:ASN:OD1	1:C:348:GLN:HG2	1.75	0.85
1:C:338:MET:HE1	1:C:430:SER:HB3	1.57	0.85
1:A:622:ASN:ND2	1:A:624:TRP:H	1.74	0.85
1:A:998:GLN:HB3	1:A:999:GLN:HE21	1.39	0.85
1:C:849:GLU:O	1:C:852:SER:O	1.93	0.85
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.59	0.84
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.59	0.84
1:C:1076:ILE:HD12	1:C:1089:ILE:HD13	1.59	0.84
1:D:44:ASN:HD22	1:D:45:ARG:N	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:HIS:CD2	1:D:337:GLU:OE2	2.30	0.84
1:A:313:LEU:HD22	1:A:323:ILE:HD11	1.60	0.84
1:A:1018:GLU:OE1	1:A:1018:GLU:HA	1.76	0.84
1:B:853:ASP:O	1:B:855:LYS:HD3	1.78	0.83
1:D:873:ASN:ND2	1:D:873:ASN:N	2.25	0.83
1:C:69:ASN:O	1:C:72:LYS:HG3	1.79	0.83
1:A:484:THR:HB	1:A:487:LEU:HD22	1.60	0.83
1:B:329:VAL:HG22	1:B:348:GLN:HE22	1.42	0.83
1:C:191:LEU:HD13	1:C:235:ILE:HD11	1.60	0.83
1:B:700:SER:H	1:B:736:HIS:HD2	1.23	0.83
1:A:811:ASN:H	1:A:811:ASN:HD22	1.22	0.83
1:A:219:ARG:HE	1:A:219:ARG:HA	1.44	0.83
1:B:897:VAL:HG22	1:B:921:MET:HE1	1.60	0.82
1:C:451:ARG:HH11	1:C:451:ARG:CG	1.90	0.82
1:D:263:ARG:NH2	1:D:330:GLN:HE21	1.77	0.82
1:A:118:TYR:HB2	1:A:328:ARG:HH11	1.42	0.82
1:A:883:LEU:CD2	1:A:886:ARG:HH12	1.91	0.82
1:C:142:HIS:H	1:C:145:HIS:HD2	1.28	0.82
1:A:381:GLU:O	1:A:383:PRO:HD3	1.79	0.82
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.78	0.81
1:C:269:ARG:HG3	1:C:270:ARG:H	1.45	0.81
1:D:44:ASN:ND2	1:D:45:ARG:H	1.77	0.81
1:B:47:GLU:HG3	1:B:48:ILE:H	1.43	0.81
1:D:864:HIS:HD2	1:D:866:MET:H	1.29	0.81
1:A:632:LYS:CB	1:A:632:LYS:NZ	2.44	0.81
1:A:382:ASP:OD2	1:A:385:ASN:HB3	1.81	0.81
1:C:278:ALA:HB3	1:C:335:ILE:HG23	1.62	0.81
1:A:184:ALA:HB1	1:A:185:GLU:OE2	1.81	0.80
1:B:239:ILE:O	1:B:239:ILE:HG22	1.82	0.80
1:A:118:TYR:HB2	1:A:328:ARG:NH1	1.96	0.80
1:C:650:GLY:HA2	1:C:1013:TYR:CE1	2.17	0.80
1:C:438:GLN:HA	1:C:441:GLU:OE1	1.81	0.80
1:C:571:ARG:NH1	1:C:575:GLN:OE1	2.15	0.80
1:A:335:ILE:HD11	1:A:374:ILE:C	2.01	0.79
1:B:395:ILE:HD12	1:B:1086:ARG:O	1.83	0.79
1:C:502:GLU:OE1	1:C:502:GLU:HA	1.82	0.79
1:C:1056:LYS:O	1:C:1057:ARG:HB3	1.82	0.79
1:D:811:ASN:H	1:D:811:ASN:ND2	1.79	0.79
1:A:1044:ASN:N	1:A:1044:ASN:HD22	1.78	0.79
1:C:922:VAL:C	1:C:924:ASN:H	1.85	0.79
1:A:811:ASN:H	1:A:811:ASN:ND2	1.78	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.65	0.79
1:A:883:LEU:CD2	1:A:886:ARG:NH1	2.45	0.79
1:C:235:ILE:O	1:C:235:ILE:HG12	1.82	0.79
1:C:920:TYR:O	1:C:924:ASN:HB2	1.82	0.79
1:D:296:ILE:O	1:D:300:GLU:HB2	1.82	0.79
1:C:444:VAL:HG23	1:C:466:MET:HB3	1.64	0.79
1:B:784:LYS:HG3	1:C:781:LEU:HD21	1.65	0.79
1:B:646:SER:HB3	1:B:685:GLN:HE22	1.48	0.78
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.62	0.78
1:B:525:GLU:HB3	1:B:840:THR:HG23	1.64	0.78
1:D:289:GLN:NE2	1:D:289:GLN:HA	1.98	0.78
1:A:268:GLN:HB2	1:A:272:GLN:O	1.83	0.78
1:B:540:GLY:H	1:B:543:GLN:HE21	1.29	0.78
1:B:897:VAL:HG22	1:B:921:MET:CE	2.13	0.78
1:C:136:ILE:N	1:C:136:ILE:HD13	1.97	0.78
1:C:216:ALA:O	1:C:220:ALA:HB3	1.84	0.78
1:C:622:ASN:ND2	1:C:624:TRP:H	1.81	0.78
1:A:640:GLN:HG3	1:A:673:VAL:HB	1.64	0.78
1:A:1044:ASN:HD22	1:A:1044:ASN:H	1.31	0.77
1:D:349:ILE:O	1:D:349:ILE:HG22	1.83	0.77
1:A:48:ILE:O	1:A:52:ILE:HG12	1.85	0.77
1:C:191:LEU:HD23	1:C:237:ARG:HA	1.65	0.77
1:D:1052:ILE:HG22	1:D:1053:ASP:H	1.50	0.77
1:D:622:ASN:HD22	1:D:623:PRO:N	1.83	0.77
1:C:921:MET:HA	1:C:926:LEU:HD12	1.65	0.77
1:C:437:LYS:N	1:C:437:LYS:CD	2.39	0.76
1:A:1003:THR:HG23	1:A:1006:ASP:H	1.50	0.76
1:C:828:ILE:CD1	1:C:828:ILE:H	1.92	0.76
1:C:153:VAL:HG21	1:C:173:PRO:HD3	1.66	0.76
1:D:447:LEU:HD11	1:D:462:LEU:HB3	1.66	0.76
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.68	0.75
1:C:396:ALA:HA	1:C:414:GLN:OE1	1.86	0.75
1:C:738:LEU:HD23	1:C:768:ILE:HG12	1.68	0.75
1:A:866:MET:CE	1:A:871:TYR:HA	2.17	0.75
1:C:125:GLU:OE2	1:C:147:ASP:HB2	1.85	0.75
1:C:168:PRO:HG2	1:C:237:ARG:HD3	1.68	0.75
1:B:704:ILE:HD11	1:B:730:LEU:CD1	2.17	0.75
1:D:142:HIS:HB2	1:D:145:HIS:CD2	2.21	0.75
1:A:145:HIS:HE1	1:A:302:ILE:O	1.69	0.75
1:C:213:LEU:O	1:C:215:ASP:N	2.20	0.75
1:C:338:MET:HE2	1:C:430:SER:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:ND2	1:B:48:ILE:HG21	2.02	0.75
1:C:712:ASN:OD1	1:C:714:GLU:HG3	1.86	0.75
1:A:259:HIS:HB3	1:A:296:ILE:CD1	2.17	0.74
1:A:866:MET:HE2	1:A:871:TYR:HA	1.68	0.74
1:C:338:MET:HE1	1:C:430:SER:CB	2.16	0.74
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.52	0.74
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.20	0.74
1:A:700:SER:H	1:A:736:HIS:CD2	2.03	0.74
1:C:189:PHE:HB3	1:C:209:GLU:HA	1.69	0.74
1:D:746:LEU:HD11	1:D:865:GLU:HG2	1.70	0.74
1:D:917:MET:CG	1:D:944:VAL:HG21	2.17	0.74
1:B:1008:ILE:N	1:B:1008:ILE:HD13	2.02	0.73
1:C:129:ARG:HB2	1:C:143:LEU:HD11	1.70	0.73
1:A:235:ILE:HG13	1:A:236:GLU:N	2.01	0.73
1:A:866:MET:HE3	1:A:870:GLN:CG	2.13	0.73
1:A:170:THR:HG22	1:A:172:GLY:O	1.88	0.73
1:A:828:ILE:HD12	1:A:829:GLU:H	1.52	0.73
1:B:719:THR:H	1:B:722:TYR:HB3	1.53	0.73
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.53	0.73
1:C:622:ASN:HD22	1:C:624:TRP:H	1.36	0.73
1:C:922:VAL:O	1:C:924:ASN:N	2.22	0.73
1:B:959:PHE:CD1	1:B:964:GLN:NE2	2.57	0.73
1:C:1067:GLU:HA	1:C:1074:ARG:HH21	1.52	0.73
1:D:513:PRO:O	1:D:515:ASN:CB	2.36	0.73
1:D:501:LEU:HD13	1:D:1078:TYR:CD1	2.24	0.73
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.71	0.73
1:A:94:GLU:HG3	1:A:94:GLU:O	1.87	0.73
1:C:103:ILE:O	1:C:107:LYS:HG3	1.89	0.72
1:D:622:ASN:ND2	1:D:624:TRP:H	1.87	0.72
1:C:1067:GLU:OE1	1:C:1074:ARG:NH2	2.21	0.72
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.19	0.72
1:B:898:ASN:ND2	1:B:906:LYS:HE3	2.04	0.72
1:B:927:ASP:HB2	1:B:930:SER:OG	1.90	0.72
1:C:828:ILE:HD12	1:C:828:ILE:N	2.03	0.72
1:A:239:ILE:HD11	1:A:315:SER:CB	2.19	0.72
1:A:565:LEU:O	1:A:565:LEU:HD23	1.90	0.72
1:A:237:ARG:NH1	1:A:237:ARG:HG2	2.03	0.72
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.25	0.72
1:A:404:GLY:HA3	1:A:442:GLU:OE1	1.90	0.72
1:B:700:SER:H	1:B:736:HIS:CD2	2.07	0.72
1:A:153:VAL:HG21	1:A:173:PRO:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:GLY:H	1:B:543:GLN:NE2	1.88	0.71
1:D:53:PHE:HA	1:D:63:THR:HG21	1.72	0.71
1:B:640:GLN:HG3	1:B:673:VAL:HB	1.70	0.71
1:D:960:ASN:HB3	1:D:963:LEU:HB3	1.71	0.71
1:B:343:ASP:CG	1:B:346:LYS:HB2	2.11	0.71
1:B:1008:ILE:CD1	1:B:1008:ILE:H	2.04	0.71
1:D:518:LYS:HD2	1:D:518:LYS:C	2.11	0.71
1:B:306:ASN:OD1	1:B:348:GLN:HG3	1.91	0.71
1:D:453:ARG:HH12	1:D:495:ASP:HB3	1.55	0.71
1:B:477:THR:OG1	1:B:479:LYS:HB2	1.91	0.71
1:D:164:LEU:HD13	1:D:294:ALA:HB1	1.73	0.71
1:D:840:THR:O	1:D:843:THR:HB	1.90	0.71
1:B:144:GLU:O	1:B:148:MET:HB2	1.91	0.71
1:A:382:ASP:O	1:A:387:PHE:HA	1.90	0.71
1:B:898:ASN:HD22	1:B:906:LYS:HE3	1.56	0.71
1:A:164:LEU:HD22	1:A:294:ALA:HB1	1.72	0.71
1:D:391:THR:HG21	1:D:420:PRO:HB3	1.73	0.71
1:A:179:LEU:HG	1:A:217:PHE:HE2	1.56	0.70
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.24	0.70
1:A:632:LYS:HB2	1:A:632:LYS:NZ	2.06	0.70
1:C:259:HIS:O	1:C:260:LEU:HD23	1.91	0.70
1:A:622:ASN:HD22	1:A:624:TRP:H	1.38	0.70
1:C:525:GLU:OE2	1:C:525:GLU:HA	1.91	0.70
1:C:968:LEU:O	1:C:969:LYS:C	2.30	0.70
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.73	0.70
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.26	0.70
1:D:622:ASN:C	1:D:622:ASN:HD22	1.94	0.70
1:A:1000:GLY:H	1:A:1001:PRO:HD2	1.56	0.70
1:B:893:MET:O	1:B:897:VAL:HG23	1.92	0.70
1:C:166:VAL:HG12	1:C:167:ILE:H	1.55	0.70
1:A:173:PRO:HA	1:A:234:TYR:HB3	1.73	0.69
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.28	0.69
1:C:130:ARG:O	1:C:134:GLU:HG2	1.92	0.69
1:D:513:PRO:CD	4:D:1201:BTI:H11	2.20	0.69
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.75	0.69
1:B:363:GLN:OE1	1:B:363:GLN:HA	1.92	0.69
1:A:644:ARG:NH2	1:A:908:THR:CG2	2.56	0.69
1:D:142:HIS:HB2	1:D:145:HIS:HD2	1.56	0.69
1:A:191:LEU:O	1:A:238:TYR:HB2	1.92	0.69
1:B:395:ILE:HB	1:B:1086:ARG:HB2	1.74	0.69
1:C:544:LEU:HD23	1:C:553:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HG	1:B:499:LYS:HE2	1.73	0.69
1:C:494:LEU:HB2	1:C:496:ARG:HH22	1.58	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.28	0.69
1:D:700:SER:H	1:D:736:HIS:HD2	1.39	0.69
1:A:254:HIS:CD2	1:A:356:ASP:HB2	2.27	0.68
1:B:275:VAL:HG21	1:B:466:MET:HE1	1.74	0.68
1:A:193:ILE:O	1:A:193:ILE:HG23	1.94	0.68
1:B:457:THR:OG1	1:B:459:ILE:HG12	1.93	0.68
1:D:334:THR:HA	1:D:337:GLU:HG3	1.74	0.68
1:B:704:ILE:N	1:B:704:ILE:HD13	2.06	0.68
1:D:580:THR:CG2	1:D:611:THR:HG22	2.23	0.68
1:B:770:LEU:HD12	1:B:771:HIS:N	2.08	0.68
1:D:542:LYS:HE2	1:D:631:ARG:NH2	2.09	0.68
1:C:864:HIS:CD2	1:C:866:MET:HG3	2.28	0.68
1:C:92:PRO:HD2	1:C:94:GLU:OE2	1.94	0.68
1:D:1071:ASN:HB3	1:D:1073:ASN:ND2	2.07	0.68
1:D:960:ASN:HD22	1:D:963:LEU:H	1.42	0.68
1:D:1076:ILE:CD1	1:D:1089:ILE:HD13	2.23	0.68
1:D:684:ASP:HA	1:D:687:LYS:HE2	1.75	0.68
1:A:254:HIS:HD2	1:A:356:ASP:HB2	1.58	0.67
1:A:144:GLU:O	1:A:148:MET:HB2	1.94	0.67
1:A:820:PHE:HB3	1:A:821:PRO:CD	2.24	0.67
1:C:144:GLU:O	1:C:148:MET:HB2	1.93	0.67
1:D:453:ARG:HH22	1:D:495:ASP:HB2	1.59	0.67
1:A:540:GLY:H	1:A:543:GLN:HE21	1.43	0.67
1:B:1085:ARG:HG3	1:B:1086:ARG:H	1.59	0.67
1:B:156:ARG:NH2	1:B:167:ILE:HG12	2.09	0.67
1:C:574:HIS:CD2	1:C:582:VAL:HB	2.30	0.67
1:A:709:ASP:OD1	1:A:748:LYS:NZ	2.26	0.67
1:A:90:LEU:HD22	1:A:95:SER:HA	1.76	0.67
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.24	0.67
1:A:949:LYS:HE3	1:A:971:GLN:OE1	1.95	0.67
1:D:252:ASP:HA	1:D:351:VAL:HG13	1.77	0.67
1:B:142:HIS:H	1:B:145:HIS:HD2	1.43	0.67
1:B:413:PHE:O	1:B:414:GLN:HB2	1.93	0.67
1:B:700:SER:N	1:B:736:HIS:HD2	1.93	0.67
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.42	0.67
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.76	0.67
1:B:41:LEU:HB2	1:B:111:VAL:HG21	1.76	0.67
1:C:269:ARG:HH11	1:C:269:ARG:HB2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:SER:HA	1:C:543:GLN:HG3	1.77	0.67
1:D:999:GLN:CG	1:D:1000:GLY:N	2.43	0.66
1:C:104:ASP:O	1:C:108:GLN:NE2	2.28	0.66
1:A:44:ASN:HD22	1:A:45:ARG:N	1.88	0.66
1:A:1029:ASN:HD22	1:A:1029:ASN:C	1.99	0.66
1:C:494:LEU:HB2	1:C:496:ARG:HH21	1.56	0.66
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.10	0.66
1:C:116:PRO:HB2	1:C:122:SER:HA	1.78	0.66
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.94	0.66
1:D:864:HIS:CD2	1:D:866:MET:H	2.14	0.66
1:A:338:MET:CE	1:A:430:SER:HB3	2.25	0.66
1:A:644:ARG:NH2	1:A:908:THR:HG21	2.11	0.66
1:B:64:VAL:HG22	1:B:82:GLU:HG3	1.77	0.66
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.78	0.66
1:A:205:ARG:N	1:A:205:ARG:HE	1.94	0.65
1:B:1085:ARG:HG3	1:B:1086:ARG:N	2.10	0.65
1:B:334:THR:HG22	1:B:406:ARG:NH2	2.11	0.65
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.60	0.65
1:C:1043:ARG:HB3	1:C:1043:ARG:HH11	1.62	0.65
1:C:811:ASN:H	1:C:811:ASN:HD22	1.43	0.65
1:D:332:GLU:HA	1:D:375:GLN:HE21	1.62	0.65
1:D:881:LEU:N	1:D:881:LEU:HD23	2.11	0.65
1:B:459:ILE:HB	1:B:460:PRO:CD	2.27	0.65
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.26	0.65
1:C:329:VAL:HG22	1:C:348:GLN:HE22	1.61	0.65
1:A:632:LYS:HB3	1:A:632:LYS:HZ3	1.61	0.65
1:B:503:TYR:HB2	1:B:1027:TYR:CD2	2.31	0.65
1:A:363:GLN:HA	1:A:363:GLN:NE2	2.11	0.65
1:C:438:GLN:O	1:C:441:GLU:HG2	1.96	0.65
1:C:991:ARG:NH1	1:C:1002:VAL:O	2.30	0.65
1:C:882:GLY:C	1:C:884:GLY:H	2.00	0.65
1:C:910:SER:O	1:C:914:VAL:HG23	1.97	0.65
1:A:99:ILE:HD13	1:A:127:PHE:HB2	1.78	0.64
1:B:771:HIS:HB2	1:B:795:ASP:OD2	1.98	0.64
1:D:870:GLN:O	1:D:873:ASN:N	2.30	0.64
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.78	0.64
1:A:632:LYS:HZ2	1:A:632:LYS:HB2	1.61	0.64
1:D:920:TYR:OH	1:D:938:LEU:O	2.16	0.64
1:C:700:SER:H	1:C:736:HIS:HD2	1.45	0.64
1:B:479:LYS:O	1:B:483:GLU:HG2	1.98	0.64
1:A:679:SER:HB2	1:A:908:THR:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:ASN:ND2	1:B:624:TRP:H	1.95	0.64
1:A:145:HIS:CE1	1:A:302:ILE:O	2.50	0.64
1:B:701:GLU:OE2	1:B:737:ILE:HG21	1.97	0.64
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.80	0.64
1:D:262:GLU:OE2	1:D:279:PRO:HB3	1.98	0.64
1:D:811:ASN:N	1:D:811:ASN:ND2	2.36	0.64
1:A:241:ASN:N	1:A:242:PRO:HD3	2.12	0.64
1:A:377:ARG:HG2	1:A:425:LEU:HD22	1.79	0.64
1:A:1087:ILE:HG22	1:A:1089:ILE:HD11	1.79	0.64
1:A:918:ALA:O	1:A:922:VAL:HG23	1.98	0.63
1:C:622:ASN:HD22	1:C:622:ASN:C	2.02	0.63
1:C:114:ILE:HG13	1:C:136:ILE:HG21	1.80	0.63
1:C:241:ASN:N	1:C:242:PRO:HD3	2.11	0.63
1:D:394:ILE:HG22	1:D:394:ILE:O	1.97	0.63
1:D:870:GLN:O	1:D:871:TYR:C	2.36	0.63
1:C:849:GLU:C	1:C:852:SER:O	2.36	0.63
1:C:1076:ILE:CD1	1:C:1089:ILE:HD13	2.29	0.63
1:C:495:ASP:HB3	1:C:498:THR:HB	1.79	0.63
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.78	0.63
1:D:98:ASN:O	1:D:102:ILE:HD12	1.98	0.63
1:B:311:GLU:OE1	1:B:326:ASN:ND2	2.32	0.63
1:D:453:ARG:HH22	1:D:495:ASP:CB	2.11	0.63
1:C:884:GLY:O	1:C:885:GLU:HB2	1.99	0.62
1:A:213:LEU:HD23	1:A:213:LEU:N	2.13	0.62
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.81	0.62
1:A:329:VAL:HG21	1:A:348:GLN:OE1	1.99	0.62
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.63	0.62
1:C:189:PHE:H	1:C:190:PRO:HD3	1.65	0.62
1:D:382:ASP:O	1:D:387:PHE:HA	1.99	0.62
1:B:792:ASP:N	1:B:792:ASP:OD2	2.31	0.62
1:C:606:MET:HE1	1:C:607:TRP:HB2	1.82	0.62
1:D:287:LEU:HD22	1:D:291:ILE:HD11	1.80	0.62
1:A:245:ILE:HD13	1:A:283:LEU:CD1	2.27	0.62
1:A:632:LYS:HB3	1:A:632:LYS:NZ	2.14	0.62
1:B:864:HIS:CD2	1:B:866:MET:HG3	2.35	0.62
1:C:142:HIS:N	1:C:145:HIS:HD2	1.98	0.62
1:C:278:ALA:CB	1:C:335:ILE:HG23	2.28	0.62
1:D:1069:ASP:O	1:D:1072:GLY:N	2.32	0.62
1:A:239:ILE:HD11	1:A:315:SER:HB2	1.81	0.62
1:A:540:GLY:N	1:A:543:GLN:HE21	1.97	0.62
1:A:927:ASP:OD2	1:A:928:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASN:OD1	1:B:348:GLN:CG	2.48	0.62
1:B:459:ILE:HB	1:B:460:PRO:HD3	1.80	0.62
1:C:494:LEU:CD2	1:C:496:ARG:HH21	2.13	0.62
1:A:239:ILE:HD11	1:A:315:SER:HB3	1.81	0.62
1:B:409:ALA:HA	1:B:427:VAL:HG12	1.80	0.62
1:D:1042:MET:CE	1:D:1062:LEU:HB2	2.30	0.62
1:D:570:PHE:O	1:D:574:HIS:HE1	1.82	0.62
1:A:394:ILE:O	1:A:414:GLN:O	2.18	0.61
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.82	0.61
1:A:728:LYS:HE2	1:A:762:ALA:HB1	1.82	0.61
1:D:289:GLN:HA	1:D:289:GLN:HE21	1.64	0.61
1:D:587:MET:O	1:D:590:ILE:HD12	2.00	0.61
1:B:263:ARG:HH21	1:B:330:GLN:NE2	1.97	0.61
1:C:849:GLU:O	1:C:852:SER:C	2.38	0.61
1:C:296:ILE:O	1:C:300:GLU:HB2	1.99	0.61
1:B:437:LYS:O	1:B:441:GLU:HG2	1.99	0.61
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.30	0.61
1:C:87:GLY:O	1:C:90:LEU:N	2.28	0.61
1:B:52:ILE:HD13	1:B:345:VAL:HG11	1.82	0.61
1:D:1076:ILE:CD1	1:D:1089:ILE:CD1	2.79	0.61
1:A:571:ARG:HH11	1:A:575:GLN:NE2	1.98	0.61
1:B:264:ASP:HB2	1:B:280:SER:HB2	1.82	0.61
1:B:286:THR:O	1:B:290:ARG:HG3	2.01	0.61
1:C:499:LYS:O	1:C:502:GLU:HB2	2.00	0.61
1:A:67:TYR:HA	1:A:96:TYR:OH	2.01	0.61
1:B:465:VAL:HG22	1:B:487:LEU:HD23	1.82	0.61
1:C:1078:TYR:HB2	1:C:1085:ARG:O	2.00	0.61
1:C:269:ARG:NH1	1:C:269:ARG:HB2	2.15	0.61
1:C:874:LEU:O	1:C:874:LEU:CD2	2.41	0.61
1:A:87:GLY:C	1:A:89:ASP:H	2.04	0.61
1:B:738:LEU:HD23	1:B:768:ILE:HD13	1.82	0.61
1:D:357(A):PHE:HE2	1:D:363:GLN:HA	1.65	0.61
1:A:192:MET:CE	1:A:238:TYR:HD1	2.14	0.61
1:A:1044:ASN:ND2	1:A:1044:ASN:H	1.98	0.60
1:A:906:LYS:HZ3	1:A:906:LYS:HB2	1.66	0.60
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.31	0.60
1:B:86:VAL:HG12	1:B:86:VAL:O	2.01	0.60
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.65	0.60
1:C:375:GLN:HG3	1:C:376:CYS:N	2.16	0.60
1:C:922:VAL:C	1:C:924:ASN:N	2.55	0.60
1:B:156:ARG:HH21	1:B:167:ILE:HG12	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:HD12	1:C:86:VAL:HG21	1.83	0.60
1:A:425:LEU:HD12	1:A:425:LEU:C	2.22	0.60
1:D:39:LYS:HG3	1:D:62:SER:HB3	1.83	0.60
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.82	0.60
1:C:864:HIS:HD2	1:C:866:MET:H	1.48	0.60
1:B:263:ARG:HH21	1:B:330:GLN:HE21	1.49	0.60
1:B:744:ALA:HB3	1:B:746:LEU:HG	1.83	0.60
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.67	0.60
1:C:210:GLU:O	1:C:212:GLU:N	2.35	0.60
1:A:856:SER:OG	1:D:800:SER:HA	2.01	0.60
1:A:866:MET:HG2	1:A:894:TYR:CE2	2.36	0.60
1:C:118:TYR:CZ	1:C:331:VAL:HG22	2.36	0.60
1:C:926:LEU:HB3	1:C:930:SER:HB3	1.84	0.60
1:D:613:ASP:HB2	1:D:1013:TYR:CZ	2.37	0.60
1:A:383:PRO:HA	1:A:387:PHE:CE2	2.36	0.60
1:C:927:ASP:OD1	1:C:929:GLN:HG2	2.02	0.59
1:D:1076:ILE:HD11	1:D:1089:ILE:HD13	1.83	0.59
1:A:719:THR:O	1:A:722:TYR:N	2.34	0.59
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.60	0.59
1:C:261:PHE:CD1	1:C:369:THR:CG2	2.84	0.59
1:C:386:ASP:O	1:C:387:PHE:HB2	2.01	0.59
1:D:269:ARG:HG3	1:D:270:ARG:H	1.66	0.59
1:D:343:ASP:CG	1:D:346:LYS:HB2	2.21	0.59
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.83	0.59
1:A:1044:ASN:N	1:A:1044:ASN:ND2	2.50	0.59
1:B:469:LYS:H	1:B:469:LYS:HD3	1.67	0.59
1:C:269:ARG:HH11	1:C:269:ARG:CB	2.15	0.59
1:C:882:GLY:O	1:C:884:GLY:N	2.34	0.59
1:D:1076:ILE:HD13	1:D:1089:ILE:CD1	2.32	0.59
1:B:245:ILE:HG12	1:B:283:LEU:HD11	1.84	0.59
1:C:335:ILE:HD11	1:C:374:ILE:C	2.23	0.59
1:D:290:ARG:HE	1:D:320:PHE:HE1	1.50	0.59
1:D:349:ILE:CG2	1:D:349:ILE:O	2.50	0.59
1:D:558:LYS:HD2	1:D:765:ASP:O	2.02	0.59
1:A:52:ILE:HD12	1:A:115:HIS:CD2	2.37	0.59
1:C:494:LEU:HD23	1:C:496:ARG:HH21	1.67	0.59
1:C:870:GLN:CG	1:C:870:GLN:O	2.37	0.59
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.38	0.59
1:A:738:LEU:HD21	1:A:759:LEU:CD1	2.33	0.59
1:C:871:TYR:O	1:C:875:SER:HB2	2.03	0.59
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ALA:HB2	1:D:335:ILE:HG23	1.85	0.59
1:A:254:HIS:HD2	1:A:356:ASP:CB	2.15	0.59
1:C:1043:ARG:HD3	1:C:1046:GLU:HB2	1.85	0.59
1:C:189:PHE:H	1:C:190:PRO:CD	2.16	0.59
1:A:413:PHE:CE2	1:A:416:ALA:HB2	2.38	0.58
1:B:763:VAL:C	1:B:766:LEU:H	2.06	0.58
1:C:41:LEU:HD23	1:C:41:LEU:C	2.23	0.58
1:A:209:GLU:HA	1:A:213:LEU:CD2	2.28	0.58
1:A:866:MET:CE	1:A:870:GLN:HG2	2.16	0.58
1:B:322:PHE:HE2	1:B:325:VAL:HG23	1.68	0.58
1:C:438:GLN:HA	1:C:441:GLU:CD	2.24	0.58
1:D:530:PRO:HB2	1:D:593:LYS:HD3	1.85	0.58
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.36	0.58
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.18	0.58
1:D:331:VAL:HG11	1:D:377:ARG:HD3	1.84	0.58
1:D:917:MET:HG2	1:D:944:VAL:CG2	2.27	0.58
1:A:313:LEU:HD22	1:A:323:ILE:CD1	2.33	0.58
1:A:921:MET:HG2	1:A:926:LEU:HB3	1.85	0.58
1:C:269:ARG:CG	1:C:270:ARG:H	2.17	0.58
1:B:413:PHE:O	1:B:414:GLN:CB	2.48	0.58
1:D:477:THR:C	1:D:479:LYS:H	2.05	0.58
1:D:53:PHE:CZ	1:D:65:ALA:HB2	2.38	0.58
1:D:644:ARG:NH1	1:D:908:THR:HG22	2.19	0.58
1:A:864:HIS:CD2	1:A:866:MET:CG	2.76	0.58
1:B:39:LYS:HG3	1:B:111:VAL:HA	1.84	0.58
1:B:437:LYS:HE3	1:B:437:LYS:CA	2.34	0.58
1:C:650:GLY:HA2	1:C:1013:TYR:HE1	1.65	0.58
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.85	0.58
1:D:828:ILE:O	1:D:832:GLU:HG2	2.02	0.58
1:A:273:LYS:HB3	1:A:276:GLU:OE2	2.04	0.58
1:B:332:GLU:HA	1:B:375:GLN:NE2	2.19	0.58
1:B:376:CYS:SG	1:B:462:LEU:HD13	2.43	0.58
1:C:572:ASP:HB3	1:C:807:GLN:NE2	2.19	0.58
1:B:406:ARG:NH1	1:D:403:PHE:HB2	2.19	0.58
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.68	0.58
1:A:644:ARG:HG2	1:A:647:ASN:OD1	2.02	0.58
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.58
1:C:205:ARG:NH1	1:C:223:GLU:OE1	2.36	0.58
1:C:940:PHE:HB3	1:C:941:PRO:HD2	1.86	0.58
1:A:296:ILE:O	1:A:300:GLU:HB2	2.04	0.58
1:B:999:GLN:HG2	1:B:1000:GLY:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LYS:O	1:D:245:ILE:HG12	2.03	0.58
1:D:580:THR:HG22	1:D:611:THR:HG22	1.86	0.58
1:A:799:ALA:H	1:A:811:ASN:ND2	2.02	0.57
1:C:794:ILE:HD12	1:C:796:THR:HG23	1.86	0.57
1:D:622:ASN:ND2	1:D:624:TRP:N	2.52	0.57
1:A:590:ILE:HG12	1:A:837:TYR:CD2	2.39	0.57
1:A:871:TYR:HE1	1:A:891:LYS:HD2	1.68	0.57
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.85	0.57
1:D:791:VAL:O	1:D:822:ARG:NH2	2.36	0.57
1:A:400:SER:CB	1:A:446:SER:HB2	2.35	0.57
1:A:622:ASN:C	1:A:622:ASN:HD22	2.06	0.57
1:C:494:LEU:HD23	1:C:496:ARG:NH2	2.20	0.57
1:D:413:PHE:CD2	1:D:416:ALA:HB2	2.39	0.57
1:D:861:ILE:HG13	1:D:862:TYR:N	2.18	0.57
1:B:949:LYS:O	1:B:951:GLU:N	2.37	0.57
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.36	0.57
1:A:503:TYR:O	1:A:504:ILE:C	2.42	0.57
1:B:544:LEU:O	1:B:548:VAL:HG22	2.05	0.57
1:B:770:LEU:HD12	1:B:771:HIS:H	1.68	0.57
1:C:121:LEU:HB3	1:C:127:PHE:CD2	2.39	0.57
1:C:989:LYS:O	1:C:993:LEU:HB2	2.04	0.57
1:D:1052:ILE:O	1:D:1053:ASP:C	2.40	0.57
1:D:640:GLN:HG3	1:D:673:VAL:CG1	2.34	0.57
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.85	0.57
1:C:549:GLY:O	1:C:553:VAL:HG23	2.03	0.57
1:C:960:ASN:N	1:C:960:ASN:OD1	2.37	0.57
1:A:239:ILE:O	1:A:239:ILE:HG13	2.03	0.57
1:B:335:ILE:HG22	1:B:336:THR:N	2.20	0.57
1:B:740:ILE:HD11	1:B:759:LEU:HD12	1.87	0.57
1:B:986:ASP:OD1	1:B:989:LYS:HG3	2.04	0.57
1:C:1019:GLN:HA	1:C:1022:GLN:HE21	1.70	0.57
1:C:113:ALA:HB1	1:C:139:ILE:HD11	1.86	0.57
1:C:378:ILE:N	1:C:378:ILE:CD1	2.68	0.57
1:D:128:ALA:O	1:D:131:CYS:HB2	2.05	0.57
1:A:509:ILE:CD1	1:A:1065:ILE:HG21	2.35	0.57
1:C:517:GLU:O	1:C:519:ARG:N	2.37	0.57
1:C:75:LEU:HG	1:C:413:PHE:CD2	2.40	0.57
1:A:267:VAL:HG23	1:A:476:TYR:CE2	2.40	0.56
1:B:329:VAL:HG22	1:B:348:GLN:NE2	2.14	0.56
1:C:701:GLU:HG2	1:C:739:ALA:HB2	1.87	0.56
1:C:917:MET:O	1:C:921:MET:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:997:GLU:OE2	1:D:1018:GLU:OE1	2.23	0.56
1:B:406:ARG:CZ	1:D:403:PHE:HB2	2.36	0.56
1:C:955:PRO:HG2	1:C:958:GLY:HA2	1.86	0.56
1:D:362(A):PRO:HB2	1:D:367:ILE:HG13	1.87	0.56
1:A:362:MET:CE	1:A:367:ILE:HD11	2.35	0.56
1:C:399:SER:HA	1:C:450:MET:HE2	1.87	0.56
1:A:119:GLY:N	1:A:122:SER:OG	2.38	0.56
1:A:129:ARG:O	1:A:133:GLU:HG3	2.06	0.56
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.39	0.56
1:C:98:ASN:O	1:C:102:ILE:HD12	2.05	0.56
1:D:317:GLY:O	1:D:318:ASP:C	2.44	0.56
1:D:363:GLN:HG3	1:D:365:LYS:HG3	1.87	0.56
1:D:446:SER:O	1:D:450:MET:HG2	2.05	0.56
1:A:118:TYR:CB	1:A:328:ARG:HH11	2.14	0.56
1:C:270:ARG:HH11	1:C:271:HIS:CD2	2.24	0.56
1:C:37:ILE:CD1	1:C:113:ALA:HB2	2.35	0.56
1:D:1077:TYR:HD1	1:D:1077:TYR:N	2.04	0.56
1:B:77:ARG:HH12	1:D:1059:ILE:CD1	2.18	0.56
1:C:544:LEU:O	1:C:548:VAL:HG22	2.05	0.56
1:D:379:THR:OG1	1:D:381:GLU:HB2	2.05	0.56
1:D:581:ARG:HD2	1:D:848:PHE:CE2	2.40	0.56
1:A:446:SER:O	1:A:450:MET:HG3	2.05	0.56
1:A:44:ASN:ND2	1:A:45:ARG:H	1.88	0.56
1:B:999:GLN:HG2	1:B:1000:GLY:N	2.21	0.56
1:C:343:ASP:OD2	1:C:346:LYS:HB2	2.06	0.56
1:C:878:ALA:HA	1:C:883:LEU:CD1	2.31	0.56
1:B:322:PHE:CE2	1:B:325:VAL:HG23	2.40	0.56
1:C:1068:PRO:HD3	1:C:1074:ARG:NE	2.21	0.56
1:C:215:ASP:HB3	1:C:219:ARG:HH22	1.71	0.56
1:D:62:SER:HA	1:D:81:ASP:OD1	2.05	0.56
1:D:760:LYS:HD3	1:D:768:ILE:HD12	1.88	0.56
1:A:437:LYS:H	1:A:437:LYS:CD	2.18	0.56
1:A:866:MET:HE2	1:A:871:TYR:CA	2.35	0.56
1:C:207:VAL:O	1:C:207:VAL:HG12	2.04	0.56
1:C:657:ASN:OD1	1:C:984:PRO:HA	2.06	0.56
1:D:746:LEU:CD1	1:D:865:GLU:HG2	2.36	0.56
1:A:121:LEU:HB3	1:A:127:PHE:CD2	2.41	0.55
1:A:875:SER:C	1:A:877:GLN:H	2.08	0.55
1:C:166:VAL:HG12	1:C:167:ILE:N	2.21	0.55
1:C:347:THR:HG23	1:C:360:ILE:HD13	1.88	0.55
1:C:920:TYR:OH	1:C:938:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:ILE:CG1	1:D:837:TYR:CE2	2.90	0.55
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.29	0.55
1:C:210:GLU:C	1:C:212:GLU:H	2.10	0.55
1:D:1077:TYR:CD1	1:D:1077:TYR:N	2.74	0.55
1:A:596:ASP:O	1:A:599:LYS:HG2	2.06	0.55
1:C:1043:ARG:HH11	1:C:1043:ARG:CB	2.19	0.55
1:C:194:LYS:HD3	1:C:236:GLU:OE2	2.06	0.55
1:A:1088:TYR:C	1:A:1089:ILE:HD12	2.27	0.55
1:B:269:ARG:O	1:B:272:GLN:HB2	2.06	0.55
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.53	0.55
1:B:289:GLN:O	1:B:293:ASP:HB2	2.07	0.55
1:B:871:TYR:CD1	1:B:871:TYR:O	2.60	0.55
1:C:213:LEU:C	1:C:215:ASP:H	2.09	0.55
1:C:378:ILE:N	1:C:378:ILE:HD12	2.22	0.55
1:C:513:PRO:O	1:C:515:ASN:HB2	2.07	0.55
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.72	0.55
1:A:897:VAL:HG21	1:A:917:MET:HB3	1.89	0.55
1:B:142:HIS:H	1:B:145:HIS:CD2	2.25	0.55
1:D:381:GLU:HG2	1:D:387:PHE:O	2.07	0.55
1:D:1042:MET:HE1	1:D:1062:LEU:HB2	1.88	0.55
1:A:334:THR:HG21	1:A:430:SER:OG	2.06	0.55
1:B:622:ASN:HD22	1:B:623:PRO:N	2.04	0.55
1:D:701:GLU:OE2	1:D:769:HIS:ND1	2.36	0.55
1:B:55:ALA:HA	1:B:58:GLU:OE1	2.07	0.55
1:B:622:ASN:HD22	1:B:622:ASN:C	2.09	0.55
1:C:135:GLY:C	1:C:136:ILE:HD13	2.27	0.55
1:C:811:ASN:H	1:C:811:ASN:ND2	2.04	0.55
1:D:142:HIS:H	1:D:145:HIS:HD2	1.53	0.55
1:A:335:ILE:HD13	1:A:375:GLN:HB2	1.87	0.54
1:B:329:VAL:CG2	1:B:348:GLN:HE22	2.18	0.54
1:C:425:LEU:HD12	1:C:425:LEU:C	2.28	0.54
1:D:113:ALA:HB1	1:D:139:ILE:HD11	1.88	0.54
1:B:48:ILE:O	1:B:52:ILE:HG12	2.08	0.54
1:B:864:HIS:HD2	1:B:866:MET:HG3	1.72	0.54
1:D:717:ASN:H	1:D:717:ASN:HD22	1.55	0.54
1:A:504:ILE:CG2	1:A:1042:MET:HG3	2.37	0.54
1:B:719:THR:HG22	1:B:720:LEU:N	2.21	0.54
1:B:934:ASP:O	1:B:938:LEU:HG	2.07	0.54
1:D:244:HIS:HD2	1:D:265:CYS:HB2	1.72	0.54
1:A:828:ILE:HD12	1:A:829:GLU:N	2.21	0.54
1:A:864:HIS:CG	1:A:866:MET:HG3	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:ASN:ND2	1:B:1093:ASN:O	2.41	0.54
1:D:86:VAL:HG11	1:D:95:SER:O	2.08	0.54
1:B:47:GLU:CG	1:B:48:ILE:N	2.63	0.54
1:D:283:LEU:HD22	1:D:287:LEU:HD13	1.88	0.54
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.70	0.54
1:D:927:ASP:HB3	1:D:930:SER:OG	2.08	0.54
1:B:690:ASN:O	1:B:694:GLN:HG2	2.08	0.54
1:C:886:ARG:O	1:C:888:ASP:N	2.41	0.54
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.43	0.54
1:A:1029:ASN:C	1:A:1029:ASN:ND2	2.58	0.54
1:A:43:ALA:HA	1:A:66:ILE:CD1	2.38	0.54
1:B:357:LEU:O	1:B:362:MET:HB3	2.08	0.54
1:B:780:LEU:HD13	1:C:778:ASN:ND2	2.23	0.54
1:C:45:ARG:HA	1:C:76:HIS:CD2	2.43	0.54
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.88	0.54
1:B:114:ILE:HG13	1:B:136:ILE:HG21	1.90	0.54
1:C:329:VAL:HG22	1:C:348:GLN:NE2	2.23	0.54
1:C:507:VAL:HA	1:C:511:GLY:O	2.07	0.54
1:C:796:THR:HB	1:C:810:ALA:HB2	1.89	0.54
1:A:555:GLU:O	1:A:558:LYS:HG3	2.06	0.54
1:B:252:ASP:HB3	1:B:357:LEU:HD23	1.90	0.54
1:B:394:ILE:HG13	1:B:418:ILE:HD13	1.90	0.54
1:B:927:ASP:H	1:B:930:SER:HB2	1.73	0.54
1:B:959:PHE:HD1	1:B:964:GLN:NE2	2.05	0.54
1:C:270:ARG:HH11	1:C:271:HIS:HD2	1.55	0.53
1:D:1075:THR:CG2	1:D:1077:TYR:HE1	2.21	0.53
1:A:263:ARG:HG2	1:A:278:ALA:HB2	1.90	0.53
1:B:999:GLN:NE2	1:B:1001:PRO:HG3	2.19	0.53
1:B:337:GLU:HG2	1:B:342:ILE:O	2.08	0.53
1:A:58:GLU:HB3	1:C:441:GLU:HG3	1.91	0.53
1:C:864:HIS:HD2	1:C:866:MET:HG3	1.72	0.53
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.38	0.53
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.41	0.53
1:A:498:THR:HG23	1:A:1085:ARG:HH12	1.74	0.53
1:B:1091:ASP:C	1:B:1093:ASN:H	2.11	0.53
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.90	0.53
1:C:438:GLN:CG	1:C:441:GLU:OE1	2.43	0.53
1:C:645:ALA:N	1:C:677:PHE:O	2.39	0.53
1:D:1065:ILE:HG22	1:D:1066:SER:H	1.72	0.53
1:B:398:ARG:HH22	1:B:1085:ARG:HH21	1.54	0.53
1:D:506:ASN:ND2	4:D:1201:BTI:H92	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:GLN:O	1:D:879:LYS:N	2.33	0.53
1:C:1076:ILE:HD12	1:C:1089:ILE:HD11	1.88	0.53
1:C:840:THR:O	1:C:843:THR:HB	2.09	0.53
1:D:318:ASP:O	1:D:319:GLU:HB2	2.08	0.53
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.90	0.53
1:A:811:ASN:N	1:A:811:ASN:HD22	2.01	0.53
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.91	0.53
1:B:866:MET:HB3	1:B:870:GLN:HB3	1.91	0.53
1:C:1044:ASN:N	1:C:1044:ASN:HD22	2.07	0.53
1:C:170:THR:HB	1:C:172:GLY:O	2.07	0.53
1:C:647:ASN:ND2	1:C:652:LYS:O	2.40	0.53
1:A:644:ARG:NH2	1:A:908:THR:HG22	2.24	0.53
1:B:94:GLU:O	1:B:96:TYR:N	2.41	0.53
1:C:215:ASP:HB3	1:C:219:ARG:NH2	2.23	0.53
1:D:640:GLN:HG3	1:D:673:VAL:HB	1.89	0.53
1:A:284:SER:OG	1:A:287:LEU:HB2	2.09	0.53
1:B:398:ARG:NH2	1:B:1085:ARG:HE	2.07	0.53
1:B:141:PRO:HA	1:B:305:VAL:HG12	1.91	0.53
1:B:704:ILE:CD1	1:B:730:LEU:CD1	2.85	0.53
1:C:266:SER:O	1:C:478:THR:HA	2.09	0.53
1:B:504:ILE:HG21	1:B:1042:MET:HG3	1.91	0.53
1:B:949:LYS:O	1:B:950:GLY:C	2.47	0.53
1:D:622:ASN:HD21	1:D:624:TRP:H	1.56	0.53
1:A:719:THR:O	1:A:721:GLU:N	2.43	0.53
1:D:413:PHE:CZ	1:D:416:ALA:HB2	2.44	0.53
1:B:267:VAL:HG22	1:B:476:TYR:CE2	2.44	0.52
1:C:928:GLU:O	1:C:931:VAL:HG12	2.09	0.52
1:D:539:SER:HA	1:D:543:GLN:HG3	1.91	0.52
1:A:1089:ILE:HD12	1:A:1089:ILE:N	2.24	0.52
1:A:174:ILE:HD12	1:A:179:LEU:HD12	1.90	0.52
1:A:189:PHE:CD2	1:A:208:ARG:HD2	2.44	0.52
1:B:1042:MET:HE3	1:B:1062:LEU:HD12	1.91	0.52
1:B:436:PHE:HE2	1:B:472:THR:HA	1.74	0.52
1:B:532:VAL:HB	1:B:537:ILE:HD11	1.89	0.52
1:B:730:LEU:HD22	1:B:735:PHE:CE1	2.44	0.52
1:A:703:THR:HG21	1:A:741:LYS:HB2	1.90	0.52
1:C:342:ILE:HG13	1:C:362:MET:HE1	1.90	0.52
1:A:631:ARG:HG2	1:A:670:GLY:HA3	1.92	0.52
1:A:799:ALA:H	1:A:811:ASN:HD21	1.56	0.52
1:B:660:HIS:CD2	1:B:692:ALA:HB2	2.45	0.52
1:C:648:ALA:HB2	1:C:659:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:ALA:H	1:C:811:ASN:ND2	2.07	0.52
1:D:323:ILE:HG22	1:D:324:GLU:HG2	1.91	0.52
1:D:897:VAL:HG12	1:D:914:VAL:HG13	1.92	0.52
1:A:283:LEU:CD2	1:A:287:LEU:HD13	2.38	0.52
1:A:152:LYS:CE	1:A:324:GLU:HB3	2.40	0.52
1:B:841:VAL:O	1:B:844:TYR:HB2	2.09	0.52
1:C:866:MET:HG2	1:C:894:TYR:CZ	2.44	0.52
1:D:447:LEU:CD1	1:D:462:LEU:HB3	2.39	0.52
1:A:404:GLY:O	1:A:431:THR:HA	2.09	0.52
1:A:622:ASN:HD22	1:A:623:PRO:N	2.08	0.52
1:D:357:LEU:HA	1:D:360:ILE:HD12	1.91	0.52
1:A:539:SER:HB2	1:A:543:GLN:HG2	1.90	0.52
1:A:742:ASP:OD2	1:A:745:GLY:HA2	2.10	0.52
1:C:938:LEU:O	1:C:939:ASP:C	2.48	0.52
1:D:48:ILE:O	1:D:52:ILE:HD12	2.09	0.52
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.92	0.52
1:A:241:ASN:N	1:A:242:PRO:CD	2.72	0.52
1:A:437:LYS:H	1:A:437:LYS:HD2	1.75	0.52
1:B:743:MET:SD	1:B:743:MET:N	2.75	0.52
1:C:289:GLN:OE1	1:C:289:GLN:HA	2.09	0.52
1:C:571:ARG:HH21	1:C:605:GLU:CD	2.13	0.52
1:A:448:ARG:HH22	1:A:467:LYS:HE2	1.74	0.52
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.25	0.52
1:D:711:LEU:HG	1:D:751:ALA:HB2	1.90	0.52
1:B:320:PHE:C	1:B:321:PHE:CD1	2.84	0.52
1:C:814:TYR:CZ	1:C:828:ILE:CG1	2.93	0.52
1:D:717:ASN:N	1:D:717:ASN:HD22	2.08	0.52
1:D:799:ALA:O	1:D:802:SER:OG	2.19	0.52
1:D:252:ASP:OD2	1:D:256:ASN:N	2.42	0.51
1:D:878:ALA:O	1:D:883:LEU:HB2	2.09	0.51
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.92	0.51
1:A:494:LEU:HD22	1:A:496:ARG:HH22	1.74	0.51
1:D:137:LYS:HD2	1:D:352:ALA:HB1	1.92	0.51
1:D:524:TYR:HD2	1:D:843:THR:HG22	1.76	0.51
1:D:866:MET:HE2	1:D:874:LEU:HD22	1.91	0.51
1:B:401:GLY:O	1:D:54:ARG:NH1	2.43	0.51
1:C:169:GLY:CA	1:C:236:GLU:HA	2.40	0.51
1:C:563:VAL:HG11	1:C:787:ILE:HG12	1.93	0.51
1:D:357(A):PHE:CE2	1:D:363:GLN:HA	2.44	0.51
1:C:874:LEU:O	1:C:878:ALA:HB2	2.10	0.51
1:D:290:ARG:HH11	1:D:290:ARG:HG3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:HB2	1:A:122:SER:HA	1.92	0.51
1:D:581:ARG:HG3	1:D:848:PHE:CD2	2.46	0.51
1:A:183:PHE:O	1:A:186:GLU:CG	2.58	0.51
1:A:549:GLY:O	1:A:553:VAL:HG23	2.11	0.51
1:A:64:VAL:HG22	1:A:82:GLU:HB2	1.91	0.51
1:B:398:ARG:HH22	1:B:1085:ARG:NH2	2.09	0.51
1:B:446:SER:O	1:B:450:MET:HG3	2.10	0.51
1:B:881:LEU:CD2	1:B:923:GLN:OE1	2.59	0.51
1:C:211:SER:O	1:C:214:GLU:HB2	2.11	0.51
1:C:495:ASP:CB	1:C:498:THR:HB	2.40	0.51
1:C:41:LEU:HD23	1:C:42:VAL:N	2.26	0.51
1:D:1051:GLU:OE2	1:D:1057:ARG:NH1	2.44	0.51
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.93	0.51
1:B:377:ARG:HG2	1:B:425:LEU:CD1	2.40	0.51
1:B:986:ASP:O	1:B:990:VAL:HG23	2.11	0.51
1:D:574:HIS:CD2	1:D:580:THR:HA	2.46	0.51
1:D:651:TYR:CZ	1:D:652:LYS:HD3	2.46	0.51
1:A:1076:ILE:HG13	1:A:1089:ILE:HD13	1.93	0.51
1:B:115:HIS:HB2	1:B:139:ILE:HD12	1.93	0.51
1:B:85:LEU:HD12	1:B:86:VAL:H	1.74	0.51
1:C:170:THR:HB	1:C:172:GLY:H	1.76	0.51
1:C:652:LYS:HG3	1:C:653:ASN:H	1.76	0.51
1:A:877:GLN:NE2	1:A:919:LEU:CD2	2.74	0.51
1:A:540:GLY:H	1:A:543:GLN:NE2	2.06	0.50
1:B:304:TYR:OH	1:B:327:PRO:HA	2.10	0.50
1:B:440:GLU:O	1:B:444:VAL:HG23	2.10	0.50
1:B:85:LEU:HD12	1:B:86:VAL:N	2.26	0.50
1:A:866:MET:HE1	1:A:871:TYR:HA	1.94	0.50
1:B:75:LEU:HG	1:B:413:PHE:CD2	2.47	0.50
1:C:189:PHE:N	1:C:190:PRO:CD	2.74	0.50
1:D:259:HIS:C	1:D:260:LEU:HD23	2.31	0.50
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.46	0.50
1:D:874:LEU:O	1:D:887:PHE:CE1	2.64	0.50
1:C:1004:GLU:HA	1:C:1007:ILE:HG13	1.93	0.50
1:C:267:VAL:HG23	1:C:476:TYR:CE2	2.47	0.50
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.47	0.50
1:B:1006:ASP:HB3	1:B:1017:TYR:OH	2.11	0.50
1:B:1086:ARG:NH2	1:D:1063:GLU:OE1	2.44	0.50
1:A:539:SER:CB	1:A:543:GLN:HG2	2.42	0.50
1:C:375:GLN:HE22	1:C:428:LYS:HD3	1.77	0.50
1:C:775:THR:HG21	1:C:861:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:O	1:D:53:PHE:C	2.50	0.50
1:D:738:LEU:HD12	1:D:739:ALA:H	1.77	0.50
1:B:404:GLY:O	1:B:431:THR:HA	2.11	0.50
1:B:856:SER:CB	1:B:857:PRO:HD2	2.41	0.50
1:C:924:ASN:O	1:C:925:ASP:HB2	2.11	0.50
1:D:678:ASP:OD2	1:D:685:GLN:NE2	2.44	0.50
1:B:652:LYS:CG	1:B:653:ASN:N	2.75	0.50
1:C:234:TYR:CE1	1:C:236:GLU:HG3	2.47	0.50
1:C:40:LEU:HD12	1:C:113:ALA:HB3	1.94	0.50
1:D:477:THR:O	1:D:479:LYS:N	2.45	0.50
1:D:856:SER:HB2	1:D:857:PRO:HD2	1.94	0.50
1:A:170:THR:OG1	1:A:235:ILE:HG23	2.11	0.50
1:A:259:HIS:HB3	1:A:296:ILE:HD12	1.94	0.50
1:B:297:GLN:O	1:B:301:ASN:HB2	2.12	0.50
1:B:377:ARG:HG2	1:B:425:LEU:HD11	1.94	0.50
1:D:56:ALA:O	1:D:57:ALA:C	2.49	0.50
1:A:1087:ILE:HG22	1:A:1089:ILE:CD1	2.42	0.50
1:A:504:ILE:HG21	1:A:1042:MET:HG3	1.93	0.50
1:A:784:LYS:C	1:A:784:LYS:HD3	2.32	0.50
1:B:583:ARG:NH2	1:B:1030:LEU:O	2.44	0.50
1:B:596:ASP:O	1:B:599:LYS:HG2	2.12	0.50
1:B:398:ARG:NE	1:B:1083:GLN:HB3	2.25	0.49
1:B:333:HIS:O	1:B:334:THR:C	2.51	0.49
1:B:575:GLN:NE2	1:B:610:ALA:H	2.10	0.49
1:C:889:GLU:HA	1:C:892:ASP:OD1	2.11	0.49
1:A:991:ARG:NH1	1:A:1004:GLU:OE1	2.39	0.49
1:A:529:ILE:HD12	1:A:837:TYR:HE1	1.77	0.49
1:B:1092:GLU:O	1:B:1093:ASN:HB3	2.12	0.49
1:B:287:LEU:HD22	1:B:291:ILE:HD11	1.94	0.49
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.94	0.49
1:D:164:LEU:HD13	1:D:294:ALA:CB	2.40	0.49
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.27	0.49
1:D:561:ASP:O	1:D:822:ARG:HD2	2.12	0.49
1:D:986:ASP:OD2	1:D:986:ASP:C	2.48	0.49
1:A:877:GLN:NE2	1:A:919:LEU:HD23	2.25	0.49
1:B:141:PRO:HB2	1:B:145:HIS:CD2	2.46	0.49
1:B:44:ASN:ND2	1:B:48:ILE:CG2	2.74	0.49
1:B:565:LEU:HD21	1:B:826:THR:HG21	1.95	0.49
1:C:130:ARG:HB3	1:C:130:ARG:CZ	2.41	0.49
1:C:846:SER:HA	1:C:849:GLU:HG2	1.95	0.49
1:C:976:ALA:HB3	1:C:981:TYR:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:TYR:CD2	1:A:1021:ILE:HD12	2.47	0.49
1:A:1087:ILE:CG2	1:A:1089:ILE:HD11	2.42	0.49
1:A:869:GLY:O	1:A:870:GLN:C	2.50	0.49
1:B:652:LYS:HG3	1:B:653:ASN:H	1.77	0.49
1:B:631:ARG:HG2	1:B:670:GLY:HA3	1.94	0.49
1:C:873:ASN:O	1:C:877:GLN:HG2	2.12	0.49
1:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.94	0.49
1:A:87:GLY:C	1:A:89:ASP:N	2.66	0.49
1:B:165:PRO:O	1:B:166:VAL:HG13	2.12	0.49
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.47	0.49
1:C:529:ILE:HG21	1:C:589:ASN:HB3	1.95	0.49
1:A:208:ARG:HH11	1:A:208:ARG:HG2	1.76	0.49
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.93	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:A:242:PRO:O	1:A:478:THR:HG23	2.13	0.49
1:B:704:ILE:HG12	1:B:738:LEU:HD11	1.94	0.49
1:B:879:LYS:HG3	1:B:884:GLY:HA3	1.95	0.49
1:B:574:HIS:CD2	1:B:580:THR:HA	2.48	0.49
1:B:701:GLU:OE2	1:B:737:ILE:CG2	2.59	0.49
1:C:114:ILE:HG13	1:C:136:ILE:CG2	2.43	0.49
1:C:136:ILE:N	1:C:136:ILE:CD1	2.69	0.49
1:C:597:VAL:HG11	1:C:834:LEU:HD12	1.95	0.49
1:D:873:ASN:ND2	1:D:873:ASN:H	2.07	0.49
1:A:820:PHE:HB3	1:A:821:PRO:HD2	1.94	0.49
1:B:763:VAL:HB	1:B:766:LEU:HB2	1.95	0.49
1:C:622:ASN:HD22	1:C:623:PRO:N	2.11	0.49
1:A:715:ARG:NH1	1:A:865:GLU:OE2	2.46	0.49
1:B:395:ILE:HG12	1:B:453:ARG:O	2.13	0.49
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.28	0.49
1:D:252:ASP:HA	1:D:351:VAL:CG1	2.43	0.49
1:D:728:LYS:HE2	1:D:762:ALA:HB1	1.95	0.49
1:D:917:MET:CG	1:D:944:VAL:CG2	2.89	0.49
1:A:71:ASP:OD2	1:A:422:TYR:CE1	2.65	0.48
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.59	0.48
1:B:99:ILE:HG23	1:B:127:PHE:HA	1.95	0.48
1:C:59:LEU:O	1:C:60:ASP:HB3	2.13	0.48
1:A:208:ARG:NH1	1:A:208:ARG:HG2	2.28	0.48
1:A:385:ASN:O	1:A:387:PHE:N	2.46	0.48
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.95	0.48
1:D:1053:ASP:O	1:D:1054:LYS:C	2.51	0.48
1:D:506:ASN:HD22	4:D:1201:BTI:H92	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:ILE:HD13	1:D:1074:ARG:HD3	1.96	0.48
1:A:177:TYR:C	1:A:179:LEU:N	2.67	0.48
1:A:329:VAL:CG2	1:A:348:GLN:OE1	2.61	0.48
1:B:772:THR:HG22	1:B:783:TYR:CZ	2.48	0.48
1:C:191:LEU:HA	1:C:237:ARG:HA	1.95	0.48
1:C:615:ALA:HA	1:C:619:LEU:HB2	1.95	0.48
1:D:412:GLY:O	1:D:413:PHE:HB3	2.14	0.48
1:D:587:MET:HA	1:D:590:ILE:HD11	1.95	0.48
1:A:435:SER:OG	1:A:438:GLN:HB2	2.14	0.48
1:A:469:LYS:HD2	1:A:469:LYS:HA	1.58	0.48
1:A:784:LYS:HD3	1:A:784:LYS:O	2.12	0.48
1:B:258:VAL:HB	1:B:364:GLN:OE1	2.13	0.48
1:C:924:ASN:O	1:C:925:ASP:CB	2.60	0.48
1:D:504:ILE:CG2	1:D:1042:MET:HG3	2.44	0.48
1:D:1071:ASN:HB3	1:D:1073:ASN:HD22	1.79	0.48
1:D:1089:ILE:CG2	1:D:1090:LYS:N	2.76	0.48
1:D:397:TYR:HA	1:D:451:ARG:O	2.13	0.48
1:A:364:GLN:HA	1:A:367:ILE:HG13	1.94	0.48
1:A:38:LYS:HE2	1:A:38:LYS:HB3	1.61	0.48
1:B:565:LEU:HD11	1:B:598:PHE:HE2	1.79	0.48
1:B:802:SER:OG	1:B:809:SER:HB2	2.14	0.48
1:C:1019:GLN:HA	1:C:1022:GLN:NE2	2.28	0.48
1:C:580:THR:HB	1:C:614:VAL:HG21	1.94	0.48
1:C:938:LEU:O	1:C:939:ASP:O	2.32	0.48
1:D:590:ILE:HG13	1:D:837:TYR:CE2	2.48	0.48
1:A:78:TYR:CE2	1:C:1081:ASN:HA	2.49	0.48
1:B:287:LEU:O	1:B:291:ILE:HG13	2.14	0.48
1:C:152:LYS:HE2	1:C:324:GLU:OE2	2.13	0.48
1:C:278:ALA:CB	1:C:335:ILE:CG2	2.91	0.48
1:C:756:ILE:O	1:C:760:LYS:HB2	2.14	0.48
1:D:429:LEU:HD23	1:D:443:MET:SD	2.53	0.48
1:A:871:TYR:HE1	1:A:891:LYS:CD	2.25	0.48
1:A:94:GLU:O	1:A:94:GLU:CG	2.58	0.48
1:B:580:THR:HG21	1:B:610:ALA:HB3	1.96	0.48
1:C:360:ILE:O	1:C:362:MET:N	2.46	0.48
1:D:1065:ILE:HG23	1:D:1076:ILE:HG13	1.95	0.48
1:D:983:GLU:OE2	1:D:983:GLU:HA	2.13	0.48
1:A:1003:THR:HG22	1:A:1006:ASP:OD2	2.14	0.48
1:A:791:VAL:O	1:A:822:ARG:NH2	2.37	0.48
1:C:570:PHE:O	1:C:574:HIS:HE1	1.96	0.48
1:D:664:GLN:O	1:D:668:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LEU:HD12	1:D:165:PRO:HD2	1.96	0.48
1:B:284:SER:OG	1:B:287:LEU:HB2	2.14	0.48
1:C:213:LEU:C	1:C:215:ASP:N	2.67	0.48
1:D:118:TYR:CZ	1:D:331:VAL:HG22	2.49	0.48
1:A:156:ARG:NH1	1:A:167:ILE:O	2.47	0.47
1:A:313:LEU:CD2	1:A:323:ILE:HD11	2.39	0.47
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.96	0.47
1:C:438:GLN:HA	1:C:441:GLU:HG2	1.97	0.47
1:C:882:GLY:C	1:C:884:GLY:N	2.67	0.47
1:D:66:ILE:HB	1:D:86:VAL:HG23	1.96	0.47
1:D:896:ARG:HD2	1:D:928:GLU:OE2	2.13	0.47
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.95	0.47
1:D:1075:THR:HG22	1:D:1077:TYR:CE1	2.49	0.47
1:A:1003:THR:CG2	1:A:1006:ASP:H	2.24	0.47
1:B:1042:MET:HE1	1:B:1062:LEU:HB2	1.95	0.47
1:C:738:LEU:HD21	1:C:759:LEU:HD13	1.97	0.47
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.79	0.47
1:B:286:THR:O	1:B:290:ARG:CG	2.62	0.47
1:B:396:ALA:HB3	1:B:453:ARG:HB2	1.96	0.47
1:B:652:LYS:HG3	1:B:653:ASN:N	2.29	0.47
1:D:593:LYS:O	1:D:597:VAL:HG23	2.15	0.47
1:D:883:LEU:O	1:D:886:ARG:HG2	2.15	0.47
1:A:189:PHE:CE2	1:A:208:ARG:HD2	2.50	0.47
1:A:879:LYS:C	1:A:881:LEU:H	2.18	0.47
1:B:565:LEU:HD21	1:B:826:THR:CG2	2.44	0.47
1:C:381:GLU:O	1:C:383:PRO:HD3	2.15	0.47
1:C:644:ARG:HA	1:C:677:PHE:CE1	2.49	0.47
1:C:686:MET:O	1:C:687:LYS:C	2.53	0.47
1:D:720:LEU:HD21	1:D:758:GLU:CG	2.37	0.47
1:A:263:ARG:HH21	1:A:330:GLN:HE21	1.63	0.47
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.80	0.47
1:B:36:GLN:O	1:B:36:GLN:HG2	2.15	0.47
1:B:519:ARG:CB	1:B:520:PRO:CD	2.90	0.47
1:B:740:ILE:HD11	1:B:759:LEU:CD1	2.44	0.47
1:C:902:GLY:O	1:C:903:ASP:HB3	2.15	0.47
1:B:414:GLN:OE1	1:D:1082:GLY:O	2.32	0.47
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.95	0.47
1:A:193:ILE:O	1:A:193:ILE:CG2	2.60	0.47
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.44	0.47
1:A:979:GLY:O	1:A:981:TYR:N	2.47	0.47
1:B:556:TRP:O	1:B:560:GLN:NE2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:HIS:HD2	1:B:866:MET:H	1.63	0.47
1:A:239:ILE:CD1	1:A:315:SER:HB3	2.44	0.47
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.97	0.47
1:B:394:ILE:O	1:B:414:GLN:O	2.33	0.47
1:B:59:LEU:HD22	1:B:350:LEU:HD21	1.97	0.47
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.47
1:C:130:ARG:NH1	1:C:133:GLU:OE1	2.47	0.47
1:C:814:TYR:CZ	1:C:828:ILE:HG13	2.49	0.47
1:D:760:LYS:CD	1:D:768:ILE:HD12	2.44	0.47
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.65	0.47
1:B:867:PRO:O	1:B:870:GLN:HB2	2.14	0.47
1:D:712:ASN:OD1	1:D:714:GLU:HG2	2.15	0.47
1:A:325:VAL:CG1	1:A:326:ASN:N	2.77	0.47
1:A:853:ASP:OD2	1:A:853:ASP:N	2.41	0.47
1:A:875:SER:C	1:A:877:GLN:N	2.68	0.47
1:A:879:LYS:O	1:A:881:LEU:N	2.48	0.47
1:A:979:GLY:C	1:A:981:TYR:H	2.18	0.47
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.70	0.47
1:C:606:MET:HE1	1:C:671:ILE:HD11	1.95	0.47
1:C:760:LYS:NZ	1:C:792:ASP:OD2	2.46	0.47
1:D:54:ARG:O	1:D:58:GLU:HG3	2.15	0.47
1:D:938:LEU:O	1:D:939:ASP:HB3	2.14	0.47
1:A:440:GLU:HG2	1:A:440:GLU:O	2.15	0.46
1:B:129:ARG:O	1:B:133:GLU:HG3	2.15	0.46
1:B:501:LEU:CD1	1:B:1085:ARG:HG2	2.45	0.46
1:D:565:LEU:HD23	1:D:824:LEU:HD11	1.96	0.46
1:B:465:VAL:HG22	1:B:487:LEU:CD2	2.45	0.46
1:B:540:GLY:N	1:B:543:GLN:HE21	2.06	0.46
1:C:407:LEU:HD21	1:C:429:LEU:HD13	1.96	0.46
1:D:343:ASP:C	1:D:343:ASP:OD2	2.54	0.46
1:D:477:THR:C	1:D:479:LYS:N	2.68	0.46
1:A:174:ILE:HB	1:A:179:LEU:HD13	1.97	0.46
1:A:968:LEU:O	1:A:969:LYS:C	2.53	0.46
1:B:459:ILE:N	1:B:460:PRO:HD2	2.30	0.46
1:C:866:MET:HG2	1:C:894:TYR:CE2	2.50	0.46
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.63	0.46
1:D:647:ASN:O	1:D:649:VAL:N	2.47	0.46
1:A:1035:THR:HB	1:A:1036:PRO:HD3	1.98	0.46
1:A:879:LYS:O	1:A:882:GLY:N	2.42	0.46
1:C:949:LYS:HD2	1:C:971:GLN:OE1	2.15	0.46
1:C:977:ARG:O	1:C:978:PRO:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:ILE:HD12	1:D:490:ILE:H	1.80	0.46
1:D:543:GLN:HE21	1:D:636:ASN:HA	1.76	0.46
1:A:551:LYS:HA	1:A:551:LYS:HE3	1.97	0.46
1:C:578:LEU:HD22	1:C:845:TYR:HB3	1.98	0.46
1:D:624:TRP:CD2	1:D:1005:GLN:HG2	2.51	0.46
1:A:503:TYR:O	1:A:505:GLY:N	2.49	0.46
1:B:268:GLN:HB3	1:B:273:LYS:HA	1.96	0.46
1:B:846:SER:HA	1:B:849:GLU:HG2	1.97	0.46
1:D:56:ALA:HB1	1:D:61:ILE:HB	1.98	0.46
1:D:56:ALA:O	1:D:59:LEU:N	2.38	0.46
1:D:874:LEU:O	1:D:887:PHE:HE1	1.99	0.46
1:A:840:THR:O	1:A:843:THR:HB	2.15	0.46
1:B:1065:ILE:CG2	1:B:1074:ARG:HD3	2.45	0.46
1:B:622:ASN:HD22	1:B:624:TRP:H	1.62	0.46
1:C:504:ILE:CG2	1:C:1042:MET:HG3	2.46	0.46
1:D:991:ARG:O	1:D:995:GLU:HB2	2.15	0.46
1:B:367:ILE:O	1:B:367:ILE:HG22	2.15	0.46
1:B:38:LYS:HA	1:B:38:LYS:HD2	1.76	0.46
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.97	0.46
1:B:896:ARG:HD2	1:B:928:GLU:OE2	2.15	0.46
1:C:568:THR:OG1	1:C:807:GLN:HG3	2.16	0.46
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.98	0.46
1:C:921:MET:O	1:C:926:LEU:N	2.47	0.46
1:D:149:PHE:CE2	1:D:325:VAL:HG21	2.51	0.46
1:D:66:ILE:HG13	1:D:86:VAL:HG21	1.97	0.46
1:D:708:GLY:HA2	1:D:715:ARG:NH1	2.30	0.46
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.46	0.46
1:A:395:ILE:HD12	1:A:1086:ARG:HB2	1.98	0.46
1:A:715:ARG:NE	1:A:715:ARG:O	2.47	0.46
1:D:828:ILE:HD12	1:D:829:GLU:H	1.80	0.46
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.45	0.46
1:A:870:GLN:O	1:A:871:TYR:C	2.52	0.46
1:B:331:VAL:HG23	1:B:332:GLU:OE2	2.15	0.46
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.98	0.46
1:C:431:THR:HG21	1:C:443:MET:HA	1.97	0.46
1:C:606:MET:CE	1:C:607:TRP:HB2	2.45	0.46
1:C:87:GLY:HA3	1:C:90:LEU:HB2	1.98	0.46
1:C:897:VAL:HG12	1:C:914:VAL:HG13	1.98	0.46
1:D:290:ARG:NE	1:D:320:PHE:HE1	2.13	0.46
1:D:872:SER:C	1:D:873:ASN:HD22	2.15	0.46
1:D:743:MET:HG3	1:D:907:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ASP:C	1:B:1093:ASN:N	2.69	0.45
1:B:310:VAL:HG22	1:B:325:VAL:HG22	1.98	0.45
1:B:437:LYS:HE3	1:B:437:LYS:HA	1.97	0.45
1:C:473:SER:OG	1:C:474:GLY:N	2.49	0.45
1:A:211:SER:C	1:A:213:LEU:H	2.19	0.45
1:A:329:VAL:CG2	1:A:348:GLN:NE2	2.80	0.45
1:A:53:PHE:CZ	1:A:65:ALA:HB2	2.52	0.45
1:A:719:THR:O	1:A:720:LEU:C	2.54	0.45
1:A:870:GLN:OE1	1:A:911:SER:HB2	2.16	0.45
1:B:330:GLN:O	1:B:331:VAL:C	2.53	0.45
1:B:650:GLY:HA2	1:B:1013:TYR:CE1	2.51	0.45
1:C:995:GLU:CG	1:C:1002:VAL:CG2	2.86	0.45
1:D:245:ILE:O	1:D:312:PHE:HB2	2.16	0.45
1:A:208:ARG:O	1:A:208:ARG:HG3	2.16	0.45
1:A:453:ARG:NH1	1:A:453:ARG:HG3	2.31	0.45
1:A:565:LEU:C	1:A:565:LEU:HD23	2.33	0.45
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.26	0.45
1:C:837:TYR:CZ	1:C:841:VAL:HG21	2.52	0.45
1:C:98:ASN:C	1:C:98:ASN:HD22	2.19	0.45
1:A:335:ILE:HD11	1:A:374:ILE:O	2.17	0.45
1:A:647:ASN:HA	1:A:659:ILE:HD11	1.99	0.45
1:A:704:ILE:HD12	1:A:738:LEU:HD11	1.99	0.45
1:A:94:GLU:HA	1:A:97:LEU:HD12	1.98	0.45
1:B:1032:LEU:HD13	1:B:1052:ILE:HA	1.99	0.45
1:B:391:THR:HG22	1:B:392:GLY:N	2.31	0.45
1:B:395:ILE:CG1	1:B:396:ALA:N	2.79	0.45
1:C:864:HIS:CD2	1:C:866:MET:H	2.33	0.45
1:D:299:MET:HB3	1:D:304:TYR:HB3	1.99	0.45
1:D:337:GLU:HG2	1:D:344:ILE:CD1	2.46	0.45
1:A:43:ALA:HA	1:A:66:ILE:HD13	1.99	0.45
1:C:215:ASP:CB	1:C:219:ARG:HH22	2.29	0.45
1:C:304:TYR:OH	1:C:327:PRO:HA	2.16	0.45
1:C:690:ASN:O	1:C:694:GLN:HG2	2.16	0.45
1:D:738:LEU:HD12	1:D:739:ALA:N	2.32	0.45
1:B:481:ILE:H	1:B:481:ILE:HD12	1.82	0.45
1:C:380:THR:HG22	1:C:426:LEU:HD11	1.99	0.45
1:C:432:HIS:CG	1:C:433:ALA:N	2.84	0.45
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.81	0.45
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.51	0.45
1:A:1065:ILE:N	1:A:1065:ILE:HD12	2.32	0.45
1:A:237:ARG:NH1	1:A:237:ARG:CG	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:HIS:CD2	1:A:296:ILE:HD13	2.52	0.45
1:A:708:GLY:HA2	1:A:715:ARG:NH1	2.32	0.45
1:B:257:ILE:HD12	1:B:300:GLU:OE1	2.16	0.45
1:B:402:GLY:H	1:B:405:VAL:HG21	1.82	0.45
1:B:846:SER:HA	1:B:849:GLU:CG	2.46	0.45
1:C:1069:ASP:OD2	1:C:1073:ASN:O	2.34	0.45
1:C:512:PHE:C	1:C:512:PHE:CD2	2.90	0.45
1:A:1017:TYR:CZ	1:A:1021:ILE:HD13	2.52	0.45
1:A:975:THR:O	1:A:976:ALA:HB2	2.16	0.45
1:B:164:LEU:HB3	1:B:165:PRO:HD2	1.98	0.45
1:B:400:SER:OG	1:B:401:GLY:N	2.50	0.45
1:B:627:LEU:HD12	1:B:627:LEU:O	2.17	0.45
1:C:731:GLU:OE1	1:C:763:VAL:HB	2.17	0.45
1:D:331:VAL:HG12	1:D:375:GLN:HE22	1.82	0.45
1:A:1068:PRO:HD3	1:A:1074:ARG:HE	1.81	0.45
1:A:259:HIS:C	1:A:260:LEU:HD23	2.37	0.45
1:A:533:SER:O	1:A:537:ILE:HG12	2.17	0.45
1:A:880:SER:OG	1:A:880:SER:O	2.34	0.45
1:B:871:TYR:HD1	1:B:871:TYR:O	1.97	0.45
1:C:261:PHE:CD1	1:C:369:THR:HG22	2.52	0.45
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.35	0.45
1:D:1076:ILE:HD13	1:D:1089:ILE:HD13	1.93	0.45
1:D:245:ILE:HG21	1:D:283:LEU:HD11	1.99	0.45
1:A:181:LYS:O	1:A:182:GLU:HB3	2.17	0.45
1:A:643:LEU:CD1	1:A:648:ALA:HA	2.47	0.45
1:A:65:ALA:O	1:A:83:SER:HA	2.17	0.45
1:A:90:LEU:HD21	1:A:94:GLU:HG3	2.00	0.45
1:A:1058:LEU:HD22	1:A:1080:MET:SD	2.58	0.44
1:A:212:GLU:N	1:A:213:LEU:HD23	2.32	0.44
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.82	0.44
1:B:646:SER:HB3	1:B:685:GLN:NE2	2.26	0.44
1:C:145:HIS:HE1	1:C:302:ILE:O	1.99	0.44
1:C:524:TYR:CD2	1:C:843:THR:HG22	2.51	0.44
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.52	0.44
1:D:302:ILE:O	1:D:303:LYS:C	2.55	0.44
1:D:485:PRO:C	1:D:487:LEU:H	2.20	0.44
1:D:938:LEU:O	1:D:939:ASP:CB	2.62	0.44
1:B:239:ILE:CG2	1:B:313:LEU:HD21	2.47	0.44
1:B:960:ASN:HD22	1:B:963:LEU:H	1.65	0.44
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.32	0.44
1:C:807:GLN:HG2	1:C:807:GLN:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ILE:O	1:D:300:GLU:CB	2.60	0.44
1:D:622:ASN:C	1:D:622:ASN:ND2	2.65	0.44
1:A:213:LEU:N	1:A:213:LEU:CD2	2.80	0.44
1:A:259:HIS:HD2	1:A:296:ILE:HD13	1.83	0.44
1:A:329:VAL:CG2	1:A:348:GLN:CD	2.86	0.44
1:B:522:PRO:C	1:B:524:TYR:N	2.69	0.44
1:B:796:THR:HB	1:B:810:ALA:HB2	1.98	0.44
1:C:1035:THR:N	1:C:1036:PRO:HD2	2.32	0.44
1:C:675:ARG:HA	1:C:701:GLU:HB3	2.00	0.44
1:D:526:LEU:HD23	1:D:526:LEU:HA	1.84	0.44
1:D:926:LEU:HD12	1:D:926:LEU:HA	1.84	0.44
1:A:920:TYR:CE1	1:A:939:ASP:O	2.71	0.44
1:B:907:VAL:O	1:B:911:SER:CB	2.48	0.44
1:C:217:PHE:CD2	1:C:217:PHE:C	2.91	0.44
1:C:622:ASN:ND2	1:C:624:TRP:N	2.60	0.44
1:B:261:PHE:HE1	1:B:367:ILE:O	2.00	0.44
1:B:403:PHE:HE2	1:D:337:GLU:HB3	1.83	0.44
1:C:631:ARG:HD3	1:C:631:ARG:HA	1.76	0.44
1:D:162:ALA:O	1:D:163:ASP:HB2	2.18	0.44
1:D:266:SER:HA	1:D:478:THR:HG22	2.00	0.44
1:D:772:THR:HG23	1:D:773:HIS:N	2.33	0.44
1:A:551:LYS:O	1:A:555:GLU:HG2	2.17	0.44
1:B:70:GLU:HG3	1:B:92:PRO:HB3	1.99	0.44
1:C:700:SER:H	1:C:736:HIS:CD2	2.29	0.44
1:D:68:SER:OG	1:D:422:TYR:OH	2.34	0.44
1:D:643:LEU:O	1:D:676:ILE:HA	2.18	0.44
1:A:179:LEU:CG	1:A:217:PHE:HE2	2.29	0.44
1:A:267:VAL:HG22	1:A:480:PHE:HD2	1.83	0.44
1:A:760:LYS:HG2	1:A:768:ILE:HD12	1.99	0.44
1:B:704:ILE:CD1	1:B:730:LEU:HD11	2.48	0.44
1:C:150:GLY:O	1:C:151:ASP:HB2	2.18	0.44
1:C:193:ILE:HG12	1:C:235:ILE:HB	2.00	0.44
1:C:518:LYS:O	1:C:519:ARG:O	2.36	0.44
1:D:588:ILE:HA	1:D:588:ILE:HD13	1.62	0.44
1:A:869:GLY:O	1:A:871:TYR:N	2.51	0.44
1:B:717(A):ILE:HB	1:B:718:TYR:CD1	2.52	0.44
1:D:328:ARG:HD3	1:D:329:VAL:O	2.18	0.44
1:D:935:GLY:CA	1:D:966:VAL:HG13	2.37	0.44
1:A:286:THR:O	1:A:289:GLN:N	2.51	0.44
1:A:490:ILE:HG13	1:A:490:ILE:H	1.37	0.44
1:A:87:GLY:O	1:A:89:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:GLU:C	1:B:1050:ILE:HG13	2.38	0.44
1:B:263:ARG:HD3	1:B:335:ILE:HG22	2.00	0.44
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.52	0.44
1:D:702:GLY:O	1:D:738:LEU:HD12	2.18	0.44
1:A:48:ILE:HG13	1:A:118:TYR:CE2	2.53	0.43
1:B:1080:MET:CE	1:B:1085:ARG:NH2	2.81	0.43
1:C:374:ILE:HG22	1:C:443:MET:CE	2.47	0.43
1:C:571:ARG:NH2	1:C:605:GLU:OE1	2.50	0.43
1:C:631:ARG:HD3	1:C:631:ARG:O	2.18	0.43
1:D:627:LEU:O	1:D:631:ARG:HB2	2.17	0.43
1:D:744:ALA:HB3	1:D:746:LEU:HG	1.99	0.43
1:D:818:ASN:N	1:D:818:ASN:HD22	2.15	0.43
1:D:917:MET:HE3	1:D:940:PHE:HD2	1.82	0.43
1:A:38:LYS:N	1:A:112:ASP:OD1	2.47	0.43
1:A:219:ARG:HA	1:A:219:ARG:NE	2.21	0.43
1:A:252:ASP:HA	1:A:351:VAL:HG13	2.00	0.43
1:A:563:VAL:HG11	1:A:794:ILE:HD12	1.98	0.43
1:B:521:LYS:HB3	1:B:1043:ARG:NH2	2.33	0.43
1:C:606:MET:HE1	1:C:671:ILE:HD12	2.00	0.43
1:C:798:VAL:O	1:C:799:ALA:C	2.57	0.43
1:D:1054:LYS:HG3	1:D:1054:LYS:O	2.18	0.43
1:D:264:ASP:HB2	1:D:280:SER:HA	1.99	0.43
1:A:239:ILE:CD1	1:A:315:SER:CB	2.95	0.43
1:A:799:ALA:N	1:A:811:ASN:ND2	2.67	0.43
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	2.00	0.43
1:B:59:LEU:O	1:B:60:ASP:HB2	2.18	0.43
1:B:814:TYR:CE2	1:B:828:ILE:HG21	2.53	0.43
1:B:891:LYS:HB2	1:B:891:LYS:HE3	1.85	0.43
1:D:814:TYR:CZ	1:D:828:ILE:HG13	2.54	0.43
1:A:820:PHE:HB3	1:A:821:PRO:HD3	1.99	0.43
1:A:866:MET:HE2	1:A:871:TYR:N	2.33	0.43
1:B:163:ASP:O	1:B:164:LEU:HD23	2.18	0.43
1:B:746:LEU:HA	1:B:746:LEU:HD23	1.74	0.43
1:C:643:LEU:HD23	1:C:676:ILE:HG12	1.99	0.43
1:C:715:ARG:HH21	1:C:865:GLU:CD	2.21	0.43
1:C:563:VAL:HG23	1:C:823:HIS:O	2.18	0.43
1:D:288:ARG:HA	1:D:291:ILE:HD12	2.00	0.43
1:A:706:TYR:O	1:A:743:MET:HE3	2.19	0.43
1:A:825:ARG:O	1:A:826:THR:HB	2.17	0.43
1:A:960:ASN:C	1:A:960:ASN:OD1	2.57	0.43
1:B:1051:GLU:OE1	1:B:1057:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:VAL:HG22	1:B:921:MET:HE3	1.95	0.43
1:C:169:GLY:HA3	1:C:236:GLU:HA	2.00	0.43
1:C:193:ILE:CG1	1:C:235:ILE:HB	2.48	0.43
1:D:246:GLU:HB3	1:D:311:GLU:HA	2.00	0.43
1:D:640:GLN:HG3	1:D:673:VAL:CB	2.49	0.43
1:D:743:MET:CE	1:D:905:VAL:HG13	2.48	0.43
1:D:869:GLY:O	1:D:870:GLN:C	2.57	0.43
1:A:381:GLU:HA	1:A:388:MET:O	2.18	0.43
1:B:1075:THR:HG1	1:B:1088:TYR:HE2	1.65	0.43
1:B:537:ILE:C	1:B:538(A):SER:H	2.22	0.43
1:C:358:GLU:HA	1:C:358:GLU:OE1	2.19	0.43
1:C:66:ILE:HB	1:C:86:VAL:CG2	2.49	0.43
1:D:1042:MET:HB2	1:D:1062:LEU:HD12	2.00	0.43
1:D:164:LEU:HA	1:D:165:PRO:HD2	1.89	0.43
1:A:147:ASP:OD2	1:A:154:LYS:HE3	2.19	0.43
1:A:636:ASN:OD1	1:A:636:ASN:N	2.52	0.43
1:B:55:ALA:O	1:B:58:GLU:HB2	2.19	0.43
1:D:289:GLN:NE2	1:D:289:GLN:CA	2.76	0.43
1:D:377:ARG:HH11	1:D:377:ARG:HG3	1.84	0.43
1:D:891:LYS:HB2	1:D:891:LYS:HE2	1.78	0.43
1:B:994:LEU:HD23	1:B:994:LEU:HA	1.88	0.43
1:C:87:GLY:HA2	1:C:101:ARG:NH1	2.33	0.43
1:C:438:GLN:HA	1:C:441:GLU:CG	2.49	0.43
1:C:519:ARG:HG3	1:C:520:PRO:O	2.17	0.43
1:D:491:GLN:HG2	1:D:491:GLN:H	1.73	0.43
1:D:948:PHE:CD1	1:D:967:ILE:HD13	2.54	0.43
1:A:45:ARG:HA	1:A:76:HIS:CD2	2.54	0.43
1:A:563:VAL:HG21	1:A:787:ILE:HG12	2.01	0.43
1:A:747:LEU:HG	1:A:747:LEU:O	2.18	0.43
1:B:128:ALA:O	1:B:131:CYS:HB2	2.19	0.43
1:B:320:PHE:O	1:B:321:PHE:CD1	2.72	0.43
1:B:335:ILE:CG2	1:B:336:THR:N	2.77	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.19	0.43
1:C:543:GLN:HG2	1:C:543:GLN:H	1.59	0.43
1:D:1008:ILE:HA	1:D:1008:ILE:HD12	1.85	0.43
1:D:479:LYS:HG2	1:D:482:GLU:OE2	2.19	0.43
1:D:837:TYR:CZ	1:D:841:VAL:HG21	2.53	0.43
1:A:509:ILE:HD11	1:A:1065:ILE:HG21	2.00	0.43
1:A:207:VAL:CG1	1:A:213:LEU:HD22	2.49	0.43
1:B:368:THR:CG2	1:B:369:THR:N	2.81	0.43
1:B:817:LEU:O	1:B:818:ASN:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:LEU:HD12	1:B:919:LEU:HA	1.87	0.43
1:B:881:LEU:HD21	1:B:923:GLN:OE1	2.19	0.43
1:C:311:GLU:HB2	1:C:324:GLU:HB3	2.01	0.43
1:C:396:ALA:HB3	1:C:453:ARG:HB2	2.00	0.43
1:C:655:PRO:HG2	1:C:985:VAL:HG23	2.01	0.43
1:D:743:MET:HE3	1:D:905:VAL:HG13	2.01	0.43
1:A:184:ALA:CB	1:A:185:GLU:OE2	2.60	0.42
1:A:487:LEU:HA	1:A:487:LEU:HD12	1.83	0.42
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.42
1:A:650:GLY:HA2	1:A:1013:TYR:CE1	2.53	0.42
1:B:831:MET:O	1:B:832:GLU:C	2.56	0.42
1:B:944:VAL:O	1:B:948:PHE:HD1	2.02	0.42
1:C:1014:PRO:O	1:C:1018:GLU:HG2	2.18	0.42
1:C:215:ASP:HB2	1:C:219:ARG:HH12	1.84	0.42
1:C:459:ILE:N	1:C:460:PRO:CD	2.82	0.42
1:D:1052:ILE:HG22	1:D:1053:ASP:N	2.24	0.42
1:D:314:VAL:HG12	1:D:314:VAL:O	2.19	0.42
1:D:437:LYS:HD3	1:D:441:GLU:OE1	2.19	0.42
1:D:647:ASN:C	1:D:647:ASN:HD22	2.22	0.42
1:D:994:LEU:O	1:D:998:GLN:HG3	2.19	0.42
1:A:818:ASN:HD22	1:A:818:ASN:N	2.16	0.42
1:A:869:GLY:O	1:A:872:SER:N	2.51	0.42
1:B:275:VAL:CG2	1:B:466:MET:HE3	2.38	0.42
1:B:814:TYR:OH	1:B:828:ILE:HG12	2.19	0.42
1:B:908:THR:HA	1:B:909:PRO:HA	1.69	0.42
1:A:445:ARG:CZ	1:C:54:ARG:HG2	2.48	0.42
1:C:908:THR:HA	1:C:909:PRO:HA	1.77	0.42
1:D:532:VAL:HG12	1:D:537:ILE:HD12	2.01	0.42
1:A:325:VAL:HG12	1:A:326:ASN:N	2.34	0.42
1:B:156:ARG:HH21	1:B:166:VAL:HB	1.84	0.42
1:B:481:ILE:N	1:B:481:ILE:HD12	2.34	0.42
1:C:940:PHE:HB3	1:C:941:PRO:CD	2.46	0.42
1:D:142:HIS:H	1:D:145:HIS:CD2	2.35	0.42
1:D:338:MET:CE	1:D:430:SER:HB3	2.49	0.42
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.33	0.42
1:D:67:TYR:CD1	1:D:77:ARG:HG3	2.55	0.42
1:A:278:ALA:CB	1:A:335:ILE:CG2	2.95	0.42
1:A:362:MET:HE2	1:A:362:MET:HB3	1.66	0.42
1:B:871:TYR:CD1	1:B:871:TYR:C	2.92	0.42
1:D:351:VAL:C	1:D:353:ALA:H	2.22	0.42
1:D:952:ILE:HA	1:D:952:ILE:HD12	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:O	1:A:793:ILE:HA	2.19	0.42
1:A:581:ARG:HD3	1:A:581:ARG:HA	1.77	0.42
1:B:1008:ILE:N	1:B:1008:ILE:CD1	2.72	0.42
1:B:245:ILE:CG2	1:B:246:GLU:N	2.82	0.42
1:B:631:ARG:HA	1:B:631:ARG:HD3	1.46	0.42
1:D:1089:ILE:HG22	1:D:1090:LYS:N	2.33	0.42
1:D:444:VAL:CG2	1:D:466:MET:HB2	2.49	0.42
1:D:470:LYS:HB3	1:D:480:PHE:HE1	1.85	0.42
1:D:481:ILE:HG22	1:D:482:GLU:N	2.34	0.42
1:D:583:ARG:NH1	1:D:1035:THR:HA	2.34	0.42
1:A:43:ALA:HA	1:A:66:ILE:HD11	2.01	0.42
1:A:651:TYR:CE1	1:A:652:LYS:HG2	2.54	0.42
1:A:991:ARG:HG3	1:A:995:GLU:HG3	2.01	0.42
1:B:613:ASP:O	1:B:617:ASN:HB2	2.18	0.42
1:B:960:ASN:HD22	1:B:963:LEU:HB3	1.84	0.42
1:D:65:ALA:O	1:D:83:SER:HA	2.19	0.42
1:A:231:SER:O	1:A:232:GLU:HG3	2.19	0.42
1:A:916:ASP:OD1	1:A:943:SER:OG	2.32	0.42
1:C:198:GLY:HA3	1:C:228:PHE:CE2	2.55	0.42
1:C:517:GLU:C	1:C:519:ARG:N	2.73	0.42
1:C:647:ASN:O	1:C:648:ALA:HB3	2.20	0.42
1:C:661:LYS:HZ1	1:C:1004:GLU:HB3	1.85	0.42
1:B:1044:ASN:OD1	1:D:1067:GLU:HG3	2.20	0.42
1:D:318:ASP:O	1:D:319:GLU:CB	2.67	0.42
1:D:470:LYS:HB3	1:D:480:PHE:CE1	2.54	0.42
1:A:457:THR:OG1	1:A:459:ILE:HD12	2.20	0.42
1:A:519:ARG:HD2	1:A:522:PRO:HG3	2.02	0.42
1:A:830:GLY:O	1:A:833:SER:HB3	2.20	0.42
1:C:567:ASP:HB2	1:C:598:PHE:CZ	2.55	0.42
1:D:364:GLN:OE1	1:D:364:GLN:O	2.37	0.42
1:A:871:TYR:CD2	1:A:871:TYR:C	2.92	0.42
1:A:873:ASN:O	1:A:875:SER:N	2.53	0.42
1:B:388:MET:HA	1:B:389:PRO:HD3	1.83	0.42
1:D:897:VAL:CG1	1:D:914:VAL:HG13	2.50	0.42
1:A:175:LYS:O	1:A:176:SER:C	2.59	0.42
1:A:879:LYS:C	1:A:881:LEU:N	2.74	0.42
1:B:72:LYS:O	1:B:77:ARG:HD3	2.19	0.42
1:C:191:LEU:HD23	1:C:237:ARG:CA	2.42	0.42
1:C:320:PHE:CD2	1:C:320:PHE:C	2.94	0.42
1:C:517:GLU:C	1:C:519:ARG:H	2.23	0.42
1:C:803:GLY:O	1:C:804:LEU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:GLN:O	1:D:547:GLU:HG2	2.20	0.42
1:D:613:ASP:HB2	1:D:1013:TYR:CE2	2.54	0.42
1:D:693:VAL:HG11	1:D:700:SER:HB3	2.00	0.42
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.23	0.41
1:C:1070:GLU:HG3	1:C:1070:GLU:H	1.60	0.41
1:C:495:ASP:HB2	1:C:499:LYS:HG3	2.02	0.41
1:C:67:TYR:O	1:C:85:LEU:HD12	2.20	0.41
1:D:129:ARG:O	1:D:131:CYS:N	2.53	0.41
1:D:331:VAL:HG13	1:D:428:LYS:HE2	2.02	0.41
1:D:638:LEU:HD22	1:D:672:ASP:HB3	2.02	0.41
1:D:946:SER:O	1:D:951:GLU:HB2	2.20	0.41
1:D:947:PHE:C	1:D:949:LYS:H	2.23	0.41
1:A:378:ILE:HB	1:A:427:VAL:HG23	2.02	0.41
1:A:706:TYR:O	1:A:743:MET:CE	2.67	0.41
1:A:798:VAL:O	1:A:799:ALA:C	2.59	0.41
1:B:380:THR:HG23	1:B:426:LEU:HD11	2.02	0.41
1:B:703:THR:C	1:B:704:ILE:HD13	2.40	0.41
1:C:1008:ILE:H	1:C:1008:ILE:HG13	1.65	0.41
1:D:679:SER:HA	1:D:907:VAL:CG2	2.49	0.41
1:D:731:GLU:HB2	1:D:766:LEU:HD22	2.03	0.41
1:A:250:ILE:HD11	1:A:260:LEU:HD11	2.03	0.41
1:A:780:LEU:O	1:A:781:LEU:C	2.57	0.41
1:B:360:ILE:O	1:B:361:ASN:C	2.58	0.41
1:B:719:THR:HG22	1:B:721:GLU:H	1.85	0.41
1:C:338:MET:CE	1:C:430:SER:CB	2.71	0.41
1:C:688:VAL:O	1:C:689:ALA:C	2.57	0.41
1:D:121:LEU:HB3	1:D:127:PHE:CD2	2.55	0.41
1:D:487:LEU:HA	1:D:487:LEU:HD12	1.83	0.41
1:A:826:THR:HG21	1:A:831:MET:CE	2.50	0.41
1:B:433:ALA:C	1:B:435:SER:H	2.23	0.41
1:B:925:ASP:O	1:B:926:LEU:HD13	2.21	0.41
1:C:1042:MET:HE1	1:C:1048:VAL:HB	2.02	0.41
1:C:119:GLY:N	1:C:122:SER:OG	2.52	0.41
1:C:384:LEU:HA	1:C:384:LEU:HD23	1.91	0.41
1:C:403:PHE:O	1:C:404:GLY:C	2.58	0.41
1:C:809:SER:HB3	1:C:812:SER:HB2	2.03	0.41
1:A:619:LEU:HA	1:A:619:LEU:HD23	1.86	0.41
1:A:832:GLU:O	1:A:836:HIS:CD2	2.74	0.41
1:A:942:GLU:O	1:A:946:SER:HB3	2.20	0.41
1:B:265:CYS:O	1:B:268:GLN:NE2	2.54	0.41
1:B:715:ARG:HA	1:B:715:ARG:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1007:ILE:O	1:C:1011:VAL:HG23	2.20	0.41
1:C:278:ALA:HB2	1:C:335:ILE:CG2	2.50	0.41
1:C:837:TYR:CE2	1:C:841:VAL:HG21	2.55	0.41
1:B:77:ARG:NH1	1:D:1059:ILE:CD1	2.83	0.41
1:D:1065:ILE:HG22	1:D:1066:SER:N	2.35	0.41
1:D:683:VAL:O	1:D:685:GLN:N	2.53	0.41
1:D:743:MET:HG3	1:D:907:VAL:HG13	2.02	0.41
1:A:1023:THR:O	1:A:1026:GLN:N	2.52	0.41
1:A:501:LEU:HD22	1:A:1078:TYR:CD1	2.56	0.41
1:A:880:SER:O	1:A:881:LEU:HD23	2.21	0.41
1:A:888:ASP:OD1	1:A:888:ASP:N	2.53	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.01	0.41
1:B:398:ARG:HH22	1:B:1085:ARG:HE	1.68	0.41
1:B:391:THR:CG2	1:B:392:GLY:N	2.83	0.41
1:C:154:LYS:O	1:C:155:ALA:C	2.58	0.41
1:C:444:VAL:CG2	1:C:466:MET:HB3	2.42	0.41
1:C:936:TYR:CZ	1:C:966:VAL:HG12	2.55	0.41
1:D:242:PRO:HB3	1:D:313:LEU:HG	2.03	0.41
1:A:1075:THR:HG22	1:A:1077:TYR:CE1	2.55	0.41
1:A:593:LYS:O	1:A:597:VAL:HG23	2.21	0.41
1:C:215:ASP:CB	1:C:219:ARG:NH2	2.84	0.41
1:C:565:LEU:HD22	1:C:598:PHE:HE2	1.85	0.41
1:C:955:PRO:HG2	1:C:958:GLY:CA	2.49	0.41
1:D:142:HIS:N	1:D:145:HIS:HD2	2.17	0.41
1:D:417:GLU:H	1:D:417:GLU:HG2	1.74	0.41
1:D:453:ARG:NH1	1:D:495:ASP:HB3	2.31	0.41
1:B:1069:ASP:OD2	1:B:1071:ASN:HB2	2.21	0.41
1:B:402:GLY:H	1:B:405:VAL:CG2	2.34	0.41
1:C:479:LYS:O	1:C:480:PHE:C	2.58	0.41
1:C:550:PRO:HD2	1:C:551:LYS:H	1.85	0.41
1:C:558:LYS:HD3	1:C:765:ASP:O	2.20	0.41
1:C:773:HIS:HA	1:C:806:SER:O	2.20	0.41
1:A:192:MET:HG3	1:A:193:ILE:N	2.35	0.41
1:A:170:THR:HB	1:A:234:TYR:HB2	2.03	0.41
1:A:246:GLU:OE1	1:A:330:GLN:NE2	2.48	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.71	0.41
1:A:924:ASN:HB2	1:A:926:LEU:HD22	2.02	0.41
1:B:908:THR:HG22	1:B:909:PRO:HA	2.03	0.41
1:C:1059:ILE:O	1:C:1080:MET:HA	2.21	0.41
1:C:1091:ASP:OD2	1:C:1092:GLU:N	2.54	0.41
1:C:296:ILE:HA	1:C:296:ILE:HD13	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLU:HG2	1:C:486:GLU:O	2.20	0.41
1:C:758:GLU:O	1:C:762:ALA:HB2	2.20	0.41
1:D:712:ASN:HA	1:D:713:PRO:HD2	1.95	0.41
1:D:866:MET:CE	1:D:874:LEU:CD2	2.99	0.41
1:D:870:GLN:O	1:D:872:SER:N	2.53	0.41
1:D:908:THR:HA	1:D:909:PRO:HA	1.79	0.41
1:B:101:ARG:O	1:B:105:VAL:HG23	2.20	0.41
1:C:622:ASN:HD22	1:C:624:TRP:N	2.11	0.41
1:D:883:LEU:O	1:D:886:ARG:N	2.53	0.41
1:A:152:LYS:HD2	1:A:152:LYS:HA	1.75	0.41
1:B:991:ARG:NH1	1:B:1002:VAL:HG12	2.36	0.41
1:B:525:GLU:HB3	1:B:840:THR:CG2	2.41	0.41
1:B:667:ALA:HB1	1:B:698:LYS:HE2	2.03	0.41
1:B:913:VAL:HG22	1:B:943:SER:O	2.21	0.41
1:C:219:ARG:HH11	1:C:219:ARG:HB2	1.86	0.41
1:C:169:GLY:HA2	1:C:236:GLU:HA	2.03	0.41
1:C:370:LEU:O	1:C:432:HIS:HE1	2.04	0.41
1:C:440:GLU:HG3	1:C:472:THR:HG22	2.03	0.41
1:C:651:TYR:HD2	1:C:1013:TYR:CE2	2.38	0.41
1:D:1080:MET:O	1:D:1081:ASN:C	2.58	0.41
1:D:296:ILE:HG23	1:D:296:ILE:O	2.21	0.41
1:D:414:GLN:HE21	1:D:414:GLN:HB3	1.74	0.41
1:A:41:LEU:HD23	1:A:42:VAL:N	2.36	0.40
1:A:606:MET:HE3	1:A:607:TRP:HB2	2.01	0.40
1:B:56:ALA:O	1:B:59:LEU:N	2.55	0.40
1:B:780:LEU:HD13	1:C:778:ASN:HD21	1.85	0.40
1:B:867:PRO:O	1:B:868:GLY:C	2.59	0.40
1:D:570:PHE:HB2	1:D:606:MET:HB3	2.02	0.40
1:A:181:LYS:HA	1:A:181:LYS:HE3	2.03	0.40
1:A:206:ILE:HG13	1:A:206:ILE:H	1.59	0.40
1:A:717:ASN:HB3	1:A:717(A):ILE:HD12	2.03	0.40
1:A:873:ASN:C	1:A:875:SER:N	2.74	0.40
1:B:1053:ASP:HB3	1:B:1056:LYS:HG3	2.03	0.40
1:B:363:GLN:CA	1:B:363:GLN:OE1	2.64	0.40
1:B:406:ARG:N	1:B:430:SER:O	2.38	0.40
1:B:756:ILE:HA	1:B:756:ILE:HD13	1.94	0.40
1:C:517:GLU:HB3	1:C:519:ARG:NE	2.36	0.40
1:C:684:ASP:HA	1:C:687:LYS:HZ3	1.86	0.40
1:D:337:GLU:HG2	1:D:344:ILE:HD12	2.03	0.40
1:D:875:SER:OG	1:D:887:PHE:CE2	2.69	0.40
1:D:998:GLN:O	1:D:999:GLN:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:HB3	1:A:400:SER:H	1.52	0.40
1:A:516:VAL:O	1:A:517:GLU:C	2.59	0.40
1:A:516:VAL:O	1:A:518:LYS:N	2.55	0.40
1:A:590:ILE:O	1:A:591:ALA:C	2.60	0.40
1:B:504:ILE:CG2	1:B:1042:MET:HG3	2.50	0.40
1:B:650:GLY:HA2	1:B:1013:TYR:CZ	2.57	0.40
1:C:721:GLU:N	1:C:721:GLU:OE1	2.52	0.40
1:C:87:GLY:C	1:C:89:ASP:N	2.74	0.40
1:D:1075:THR:HG22	1:D:1077:TYR:HE1	1.83	0.40
1:D:357:LEU:O	1:D:362:MET:HB2	2.21	0.40
1:A:812:SER:HB3	1:D:778:ASN:HD21	1.86	0.40
1:A:48:ILE:O	1:A:48:ILE:HD13	2.21	0.40
1:A:952:ILE:O	1:A:952:ILE:HG22	2.21	0.40
1:B:769:HIS:CE1	1:B:793:ILE:HG21	2.55	0.40
1:C:652:LYS:HG3	1:C:653:ASN:N	2.36	0.40
1:C:90:LEU:HD12	1:C:90:LEU:HA	1.90	0.40
1:D:142:HIS:O	1:D:145:HIS:HB2	2.21	0.40
1:D:250:ILE:HG21	1:D:347:THR:HG21	2.04	0.40
1:D:425:LEU:HD12	1:D:425:LEU:C	2.42	0.40
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.56	0.40
1:A:780:LEU:HD13	1:D:778:ASN:ND2	2.35	0.40
1:D:866:MET:CE	1:D:874:LEU:HD22	2.51	0.40
1:D:960:ASN:HD22	1:D:963:LEU:N	2.16	0.40
1:A:370:LEU:O	1:A:432:HIS:HE1	2.05	0.40
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.36	0.40
1:B:239:ILE:HG21	1:B:313:LEU:HD21	2.02	0.40
1:C:174:ILE:HG13	1:C:235:ILE:CG2	2.51	0.40
1:C:565:LEU:HD22	1:C:598:PHE:CE2	2.55	0.40
1:D:292:CYS:O	1:D:293:ASP:C	2.60	0.40
1:D:429:LEU:CD2	1:D:443:MET:SD	3.10	0.40
1:D:477:THR:HG23	1:D:479:LYS:HB2	2.02	0.40
1:D:52:ILE:O	1:D:55:ALA:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1048/1173 (89%)	907 (86%)	111 (11%)	30 (3%)	4	24
1	B	985/1173 (84%)	847 (86%)	117 (12%)	21 (2%)	7	33
1	C	1057/1173 (90%)	896 (85%)	113 (11%)	48 (4%)	2	14
1	D	985/1173 (84%)	842 (86%)	110 (11%)	33 (3%)	3	20
All	All	4075/4692 (87%)	3492 (86%)	451 (11%)	132 (3%)	4	22

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ALA
1	A	527	ALA
1	A	880	SER
1	A	999	GLN
1	B	94	GLU
1	B	95	SER
1	B	148	MET
1	B	166	VAL
1	B	414	GLN
1	B	522	PRO
1	B	523	ASP
1	B	950	GLY
1	B	1001	PRO
1	C	151	ASP
1	C	168	PRO
1	C	211	SER
1	C	214	GLU
1	C	515	ASN
1	C	645	ALA
1	C	687	LYS
1	C	852	SER
1	C	883	LEU
1	C	885	GLU
1	C	887	PHE
1	C	923	GLN
1	C	925	ASP
1	C	939	ASP
1	C	978	PRO

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Mol	Chain	Res	Type
1	C	1057	ARG
1	D	92	PRO
1	D	319	GLU
1	D	494	LEU
1	D	684	ASP
1	D	870	GLN
1	D	884	GLY
1	D	999	GLN
1	D	1084	ALA
1	A	99	ILE
1	A	177	TYR
1	A	182	GLU
1	A	220	ALA
1	A	517	GLU
1	A	649	VAL
1	A	868	GLY
1	A	870	GLN
1	A	876	GLN
1	A	976	ALA
1	B	147	ASP
1	B	495	ASP
1	B	648	ALA
1	C	92	PRO
1	C	169	GLY
1	C	197	SER
1	C	208	ARG
1	C	361	ASN
1	C	518	LYS
1	C	931	VAL
1	C	960	ASN
1	C	969	LYS
1	C	974	LEU
1	D	130	ARG
1	D	161	LYS
1	D	303	LYS
1	D	306	ASN
1	D	317	GLY
1	D	318	ASP
1	D	478	THR
1	D	515	ASN
1	D	854	ILE
1	D	1001	PRO

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Mol	Chain	Res	Type
1	A	88	SER
1	A	176	SER
1	A	223	GLU
1	A	270	ARG
1	A	386	ASP
1	A	551	LYS
1	A	874	LEU
1	A	884	GLY
1	C	88	SER
1	C	227	SER
1	C	270	ARG
1	C	648	ALA
1	C	935	GLY
1	D	271	HIS
1	D	414	GLN
1	D	648	ALA
1	D	876	GLN
1	D	886	ARG
1	A	186	GLU
1	A	192	MET
1	A	504	ILE
1	A	903	ASP
1	B	413	PHE
1	B	558	LYS
1	B	617	ASN
1	B	925	ASP
1	C	124	ASN
1	C	199	GLY
1	C	282	GLY
1	C	489	ASP
1	C	980	GLU
1	C	1084	ALA
1	D	518	LYS
1	A	511	GLY
1	A	550	PRO
1	A	980	GLU
1	B	907	VAL
1	B	1002	VAL
1	C	354	GLY
1	C	760	LYS
1	C	941	PRO
1	C	981	TYR

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Mol	Chain	Res	Type
1	D	53	PHE
1	D	70	GLU
1	D	878	ALA
1	A	229	GLY
1	B	86	VAL
1	C	519	ARG
1	C	924	ASN
1	D	160	ILE
1	D	649	VAL
1	B	1000	GLY
1	C	173	PRO
1	D	166	VAL
1	D	868	GLY
1	D	513	PRO
1	C	189	PHE
1	C	649	VAL
1	C	821	PRO
1	D	1052	ILE
1	B	828	ILE
1	C	932	ILE

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	908/1006 (90%)	730 (80%)	178 (20%)	1	7
1	B	856/1006 (85%)	721 (84%)	135 (16%)	2	12
1	C	910/1006 (90%)	721 (79%)	189 (21%)	1	5
1	D	856/1006 (85%)	728 (85%)	128 (15%)	3	14
All	All	3530/4024 (88%)	2900 (82%)	630 (18%)	2	9

All (630) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	44	ASN
1	A	48	ILE
1	A	60	ASP
1	A	62	SER
1	A	63	THR
1	A	66	ILE
1	A	71	ASP
1	A	72	LYS
1	A	77	ARG
1	A	90	LEU
1	A	99	ILE
1	A	108	GLN
1	A	122	SER
1	A	125	GLU
1	A	126	GLN
1	A	131	CYS
1	A	143	LEU
1	A	152	LYS
1	A	154	LYS
1	A	156	ARG
1	A	157	THR
1	A	160	ILE
1	A	161	LYS
1	A	179	LEU
1	A	181	LYS
1	A	185	GLU
1	A	186	GLU
1	A	189	PHE
1	A	192	MET
1	A	193	ILE
1	A	194	LYS
1	A	196	THR
1	A	205	ARG
1	A	206	ILE
1	A	209	GLU
1	A	210	GLU
1	A	212	GLU
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE
1	A	219	ARG

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Mol	Chain	Res	Type
1	A	227	SER
1	A	230	ASN
1	A	233	VAL
1	A	235	ILE
1	A	237	ARG
1	A	239	ILE
1	A	241	ASN
1	A	268	GLN
1	A	270	ARG
1	A	271	HIS
1	A	272	GLN
1	A	287	LEU
1	A	288	ARG
1	A	296	ILE
1	A	303	LYS
1	A	306	ASN
1	A	315	SER
1	A	328	ARG
1	A	331	VAL
1	A	335	ILE
1	A	361	ASN
1	A	363	GLN
1	A	367	ILE
1	A	370	LEU
1	A	376	CYS
1	A	377	ARG
1	A	386	ASP
1	A	388	MET
1	A	391	THR
1	A	393	THR
1	A	423	ASP
1	A	425	LEU
1	A	427	VAL
1	A	428	LYS
1	A	430	SER
1	A	437	LYS
1	A	438	GLN
1	A	440	GLU
1	A	445	ARG
1	A	451	ARG
1	A	453	ARG
1	A	467	LYS

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Mol	Chain	Res	Type
1	A	469	LYS
1	A	470	LYS
1	A	472	THR
1	A	479	LYS
1	A	482	GLU
1	A	486	GLU
1	A	487	LEU
1	A	490	ILE
1	A	491	GLN
1	A	494	LEU
1	A	496	ARG
1	A	506	ASN
1	A	517	GLU
1	A	519	ARG
1	A	526	LEU
1	A	528	SER
1	A	538(A)	SER
1	A	539	SER
1	A	542	LYS
1	A	551	LYS
1	A	558	LYS
1	A	559	LYS
1	A	565	LEU
1	A	566	THR
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	599	LYS
1	A	606	MET
1	A	607	TRP
1	A	613	ASP
1	A	622	ASN
1	A	631	ARG
1	A	632	LYS
1	A	649	VAL
1	A	652	LYS
1	A	685	GLN
1	A	695	GLU
1	A	707	THR
1	A	710	ILE
1	A	714	GLU
1	A	715	ARG

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Mol	Chain	Res	Type
1	A	719	THR
1	A	743	MET
1	A	754	GLU
1	A	759	LEU
1	A	760	LYS
1	A	761	SER
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	784	LYS
1	A	794	ILE
1	A	809	SER
1	A	811	ASN
1	A	828	ILE
1	A	829	GLU
1	A	831	MET
1	A	853	ASP
1	A	855	LYS
1	A	872	SER
1	A	875	SER
1	A	880	SER
1	A	881	LEU
1	A	886	ARG
1	A	904	ILE
1	A	906	LYS
1	A	907	VAL
1	A	908	THR
1	A	917	MET
1	A	919	LEU
1	A	925	ASP
1	A	926	LEU
1	A	927	ASP
1	A	928	GLU
1	A	939	ASP
1	A	943	SER
1	A	946	SER
1	A	961	LYS
1	A	962	ASP
1	A	966	VAL
1	A	992	GLU
1	A	999	GLN
1	A	1008	ILE

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Mol	Chain	Res	Type
1	A	1019	GLN
1	A	1021	ILE
1	A	1029	ASN
1	A	1031	SER
1	A	1044	ASN
1	A	1053	ASP
1	A	1062	LEU
1	A	1064	THR
1	A	1085	ARG
1	B	39	LYS
1	B	40	LEU
1	B	47	GLU
1	B	62	SER
1	B	74	SER
1	B	75	LEU
1	B	79	LYS
1	B	90	LEU
1	B	98	ASN
1	B	108	GLN
1	B	110	ASN
1	B	122	SER
1	B	129	ARG
1	B	153	VAL
1	B	156	ARG
1	B	160	ILE
1	B	161	LYS
1	B	163	ASP
1	B	166	VAL
1	B	167	ILE
1	B	240	ASP
1	B	268	GLN
1	B	269	ARG
1	B	287	LEU
1	B	288	ARG
1	B	296	ILE
1	B	299	MET
1	B	303	LYS
1	B	305	VAL
1	B	315	SER
1	B	329	VAL
1	B	331	VAL
1	B	335	ILE

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Mol	Chain	Res	Type
1	B	346	LYS
1	B	347	THR
1	B	357	LEU
1	B	358	GLU
1	B	361	ASN
1	B	365	LYS
1	B	366	ASP
1	B	375	GLN
1	B	376	CYS
1	B	399	SER
1	B	407	LEU
1	B	408	ASP
1	B	427	VAL
1	B	437	LYS
1	B	451	ARG
1	B	467	LYS
1	B	469	LYS
1	B	472	THR
1	B	489	ASP
1	B	494	LEU
1	B	496	ARG
1	B	500	THR
1	B	516	VAL
1	B	518	LYS
1	B	523	ASP
1	B	524	TYR
1	B	526	LEU
1	B	533	SER
1	B	534	SER
1	B	536	LYS
1	B	542	LYS
1	B	546	ASP
1	B	559	LYS
1	B	580	THR
1	B	588	ILE
1	B	599	LYS
1	B	606	MET
1	B	607	TRP
1	B	617	ASN
1	B	622	ASN
1	B	631	ARG
1	B	632	LYS

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Mol	Chain	Res	Type
1	B	649	VAL
1	B	657	ASN
1	B	664	GLN
1	B	685	GLN
1	B	700	SER
1	B	707	THR
1	B	715	ARG
1	B	720	LEU
1	B	721	GLU
1	B	743	MET
1	B	750	LYS
1	B	760	LYS
1	B	775	THR
1	B	781	LEU
1	B	784	LYS
1	B	792	ASP
1	B	796	THR
1	B	807	GLN
1	B	809	SER
1	B	826	THR
1	B	828	ILE
1	B	839	SER
1	B	853	ASP
1	B	855	LYS
1	B	870	GLN
1	B	871	TYR
1	B	875	SER
1	B	876	GLN
1	B	879	LYS
1	B	888	ASP
1	B	906	LYS
1	B	907	VAL
1	B	908	THR
1	B	911	SER
1	B	916	ASP
1	B	919	LEU
1	B	925	ASP
1	B	926	LEU
1	B	927	ASP
1	B	932	ILE
1	B	934	ASP
1	B	944	VAL

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Mol	Chain	Res	Type
1	B	949	LYS
1	B	969	LYS
1	B	982	LEU
1	B	985	VAL
1	B	991	ARG
1	B	997	GLU
1	B	999	GLN
1	B	1003	THR
1	B	1008	ILE
1	B	1015	LYS
1	B	1019	GLN
1	B	1023	THR
1	B	1024	ARG
1	B	1031	SER
1	B	1056	LYS
1	B	1057	ARG
1	B	1087	ILE
1	B	1090	LYS
1	C	36	GLN
1	C	37	ILE
1	C	40	LEU
1	C	44	ASN
1	C	45	ARG
1	C	70	GLU
1	C	73	SER
1	C	75	LEU
1	C	88	SER
1	C	90	LEU
1	C	94	GLU
1	C	97	LEU
1	C	98	ASN
1	C	100	GLU
1	C	103	ILE
1	C	108	GLN
1	C	110	ASN
1	C	122	SER
1	C	125	GLU
1	C	130	ARG
1	C	136	ILE
1	C	139	ILE
1	C	143	LEU
1	C	147	ASP

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Mol	Chain	Res	Type
1	C	164	LEU
1	C	170	THR
1	C	181	LYS
1	C	183	PHE
1	C	185	GLU
1	C	189	PHE
1	C	192	MET
1	C	193	ILE
1	C	196	THR
1	C	197	SER
1	C	210	GLU
1	C	211	SER
1	C	213	LEU
1	C	214	GLU
1	C	215	ASP
1	C	226	LYS
1	C	232	GLU
1	C	235	ILE
1	C	262	GLU
1	C	269	ARG
1	C	270	ARG
1	C	281	VAL
1	C	306	ASN
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	362	MET
1	C	365	LYS
1	C	366	ASP
1	C	369	THR
1	C	375	GLN
1	C	377	ARG
1	C	378	ILE
1	C	379	THR
1	C	386	ASP
1	C	388	MET
1	C	398	ARG
1	C	414	GLN
1	C	418	ILE
1	C	423	ASP
1	C	425	LEU
1	C	427	VAL

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Mol	Chain	Res	Type
1	C	428	LYS
1	C	435	SER
1	C	437	LYS
1	C	444	VAL
1	C	451	ARG
1	C	453	ARG
1	C	456	LYS
1	C	466	MET
1	C	468	ASN
1	C	469	LYS
1	C	473	SER
1	C	475	ASP
1	C	486	GLU
1	C	491	GLN
1	C	493	SER
1	C	494	LEU
1	C	495	ASP
1	C	496	ARG
1	C	502	GLU
1	C	509	ILE
1	C	515	ASN
1	C	516	VAL
1	C	518	LYS
1	C	519	ARG
1	C	521	LYS
1	C	525	GLU
1	C	526	LEU
1	C	528	SER
1	C	529	ILE
1	C	531	THR
1	C	534	SER
1	C	536	LYS
1	C	538(A)	SER
1	C	541	THR
1	C	542	LYS
1	C	543	GLN
1	C	544	LEU
1	C	559	LYS
1	C	561	ASP
1	C	563	VAL
1	C	580	THR
1	C	588	ILE

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Mol	Chain	Res	Type
1	C	606	MET
1	C	607	TRP
1	C	617	ASN
1	C	622	ASN
1	C	629	ARG
1	C	631	ARG
1	C	632	LYS
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	653	ASN
1	C	660	HIS
1	C	661	LYS
1	C	679	SER
1	C	687	LYS
1	C	688	VAL
1	C	714	GLU
1	C	719	THR
1	C	743	MET
1	C	765	ASP
1	C	781	LEU
1	C	784	LYS
1	C	794	ILE
1	C	807	GLN
1	C	818	ASN
1	C	823	HIS
1	C	828	ILE
1	C	839	SER
1	C	852	SER
1	C	853	ASP
1	C	855	LYS
1	C	861	ILE
1	C	863	GLN
1	C	870	GLN
1	C	871	TYR
1	C	873	ASN
1	C	881	LEU
1	C	883	LEU
1	C	886	ARG
1	C	887	PHE
1	C	888	ASP
1	C	889	GLU

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Mol	Chain	Res	Type
1	C	891	LYS
1	C	892	ASP
1	C	904	ILE
1	C	906	LYS
1	C	907	VAL
1	C	912	LYS
1	C	923	GLN
1	C	924	ASN
1	C	926	LEU
1	C	928	GLU
1	C	929	GLN
1	C	934	ASP
1	C	937	LYS
1	C	945	VAL
1	C	946	SER
1	C	960	ASN
1	C	961	LYS
1	C	968	LEU
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	974	LEU
1	C	975	THR
1	C	977	ARG
1	C	983	GLU
1	C	986	ASP
1	C	1002	VAL
1	C	1003	THR
1	C	1008	ILE
1	C	1015	LYS
1	C	1029	ASN
1	C	1043	ARG
1	C	1044	ASN
1	C	1049	GLU
1	C	1063	GLU
1	C	1064	THR
1	C	1070	GLU
1	C	1085	ARG
1	C	1090	LYS
1	D	37	ILE
1	D	44	ASN
1	D	60	ASP

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Mol	Chain	Res	Type
1	D	66	ILE
1	D	70	GLU
1	D	71	ASP
1	D	75	LEU
1	D	77	ARG
1	D	82	GLU
1	D	101	ARG
1	D	108	GLN
1	D	126	GLN
1	D	137	LYS
1	D	157	THR
1	D	161	LYS
1	D	166	VAL
1	D	240	ASP
1	D	262	GLU
1	D	271	HIS
1	D	273	LYS
1	D	287	LEU
1	D	288	ARG
1	D	289	GLN
1	D	296	ILE
1	D	300	GLU
1	D	306	ASN
1	D	318	ASP
1	D	323	ILE
1	D	329	VAL
1	D	335	ILE
1	D	346	LYS
1	D	361	ASN
1	D	362	MET
1	D	364	GLN
1	D	375	GLN
1	D	377	ARG
1	D	403	PHE
1	D	405	VAL
1	D	417	GLU
1	D	424	SER
1	D	425	LEU
1	D	427	VAL
1	D	437	LYS
1	D	451	ARG
1	D	457	THR

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Mol	Chain	Res	Type
1	D	467	LYS
1	D	470	LYS
1	D	476	TYR
1	D	477	THR
1	D	487	LEU
1	D	489	ASP
1	D	491	GLN
1	D	496	ARG
1	D	498	THR
1	D	518	LYS
1	D	519	ARG
1	D	525	GLU
1	D	535	SER
1	D	537	ILE
1	D	538(A)	SER
1	D	542	LYS
1	D	551	LYS
1	D	558	LYS
1	D	580	THR
1	D	585	LYS
1	D	588	ILE
1	D	607	TRP
1	D	613	ASP
1	D	620	LYS
1	D	622	ASN
1	D	631	ARG
1	D	644	ARG
1	D	647	ASN
1	D	649	VAL
1	D	684	ASP
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	754	GLU
1	D	763	VAL
1	D	766	LEU
1	D	775	THR
1	D	781	LEU
1	D	784	LYS
1	D	791	VAL
1	D	807	GLN
1	D	809	SER

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Mol	Chain	Res	Type
1	D	811	ASN
1	D	828	ILE
1	D	859	THR
1	D	863	GLN
1	D	866	MET
1	D	870	GLN
1	D	873	ASN
1	D	875	SER
1	D	881	LEU
1	D	885	GLU
1	D	887	PHE
1	D	906	LYS
1	D	907	VAL
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	945	VAL
1	D	946	SER
1	D	952	ILE
1	D	961	LYS
1	D	975	THR
1	D	977	ARG
1	D	983	GLU
1	D	996	GLU
1	D	999	GLN
1	D	1053	ASP
1	D	1054	LYS
1	D	1056	LYS
1	D	1057	ARG
1	D	1058	LEU
1	D	1064	THR
1	D	1065	ILE
1	D	1067	GLU
1	D	1069	ASP
1	D	1070	GLU
1	D	1071	ASN
1	D	1077	TYR
1	D	1080	MET
1	D	1085	ARG
1	D	1086	ARG
1	D	1087	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	108	GLN
1	A	142	HIS
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	268	GLN
1	A	301	ASN
1	A	326	ASN
1	A	330	GLN
1	A	432	HIS
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	617	ASN
1	A	622	ASN
1	A	660	HIS
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	873	ASN
1	A	877	GLN
1	A	898	ASN
1	A	999	GLN
1	A	1005	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1081	ASN
1	B	98	ASN
1	B	108	GLN
1	B	145	HIS
1	B	244	HIS
1	B	268	GLN
1	B	326	ASN
1	B	330	GLN

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	375	GLN
1	B	491	GLN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	660	HIS
1	B	685	GLN
1	B	717	ASN
1	B	736	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	898	ASN
1	B	960	ASN
1	B	998	GLN
1	B	999	GLN
1	B	1005	GLN
1	B	1019	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1071	ASN
1	B	1073	ASN
1	B	1093	ASN
1	C	36	GLN
1	C	44	ASN
1	C	108	GLN
1	C	145	HIS
1	C	230	ASN
1	C	241	ASN
1	C	271	HIS
1	C	326	ASN
1	C	330	GLN
1	C	375	GLN
1	C	464	ASN
1	C	506	ASN

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Mol	Chain	Res	Type
1	C	574	HIS
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	647	ASN
1	C	653	ASN
1	C	685	GLN
1	C	736	HIS
1	C	778	ASN
1	C	811	ASN
1	C	818	ASN
1	C	864	HIS
1	C	870	GLN
1	C	898	ASN
1	C	929	GLN
1	C	1005	GLN
1	C	1019	GLN
1	C	1022	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1083	GLN
1	D	44	ASN
1	D	126	GLN
1	D	145	HIS
1	D	241	ASN
1	D	244	HIS
1	D	268	GLN
1	D	289	GLN
1	D	301	ASN
1	D	326	ASN
1	D	330	GLN
1	D	363	GLN
1	D	364	GLN
1	D	375	GLN
1	D	414	GLN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	617	ASN
1	D	622	ASN
1	D	647	ASN

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Mol	Chain	Res	Type
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	864	HIS
1	D	873	ASN
1	D	929	GLN
1	D	960	ASN
1	D	999	GLN
1	D	1005	GLN
1	D	1025	ASN
1	D	1073	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	BTI	D	1201	-	16,16,16	1.78	2 (12%)	21,21,21	2.13	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	1201	-	24,29,29	1.02	2 (8%)	29,45,45	1.20	3 (10%)

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
4	BTI	D	1201	-	-	5/5/27/27	0/2/2/2
2	ADP	A	1201	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1201	BTI	O3-C3	5.17	1.34	1.23
4	D	1201	BTI	C2-S1	-4.08	1.76	1.82
2	A	1201	ADP	C5-C4	2.63	1.47	1.40
2	A	1201	ADP	O4'-C1'	2.02	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1201	BTI	C6-C5-N3	-4.99	106.68	113.03
4	D	1201	BTI	C5-C6-S1	4.55	110.21	106.31
4	D	1201	BTI	C2-C4-N2	-3.48	110.00	113.13
4	D	1201	BTI	C4-C2-S1	3.19	108.25	105.20
2	A	1201	ADP	N3-C2-N1	-2.85	124.22	128.68
4	D	1201	BTI	C6-S1-C2	2.81	95.65	89.89
2	A	1201	ADP	C4-C5-N7	-2.61	106.68	109.40
4	D	1201	BTI	N2-C3-N3	2.15	110.78	108.76
2	A	1201	ADP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O1A
4	D	1201	BTI	C11-C10-C9-C8
4	D	1201	BTI	S1-C2-C7-C8
4	D	1201	BTI	C4-C2-C7-C8

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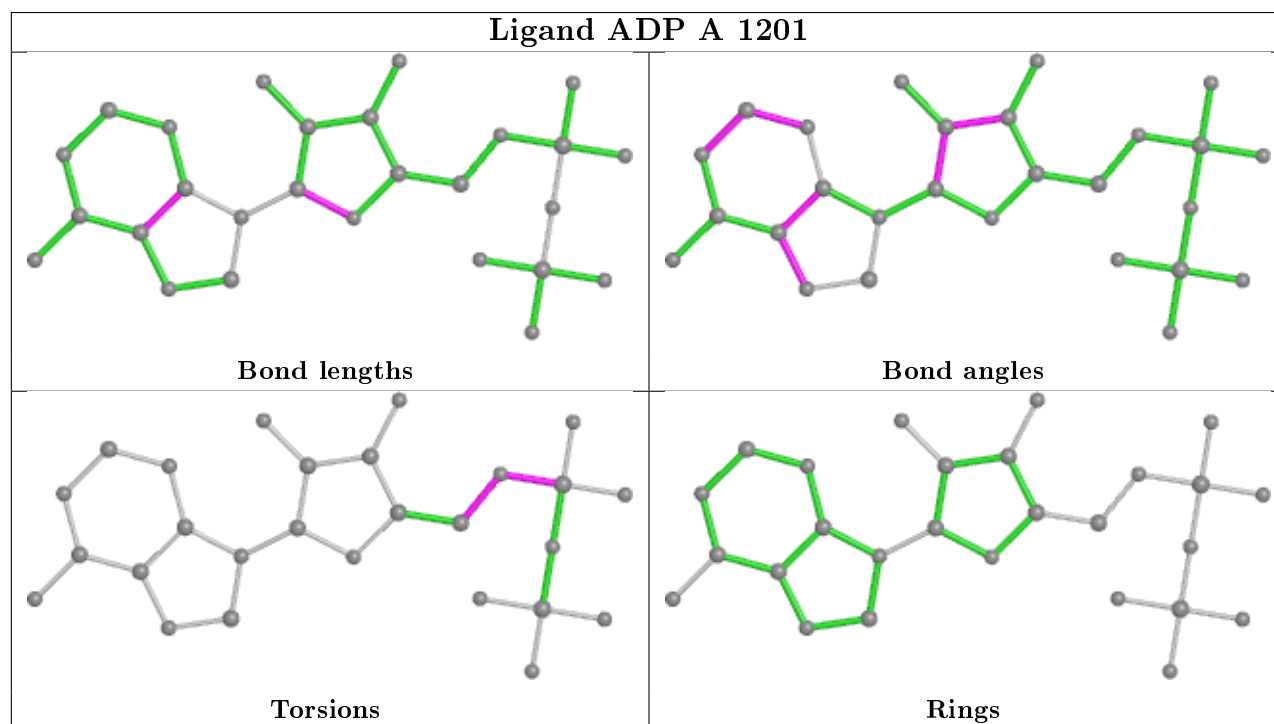
Mol	Chain	Res	Type	Atoms
4	D	1201	BTI	C2-C7-C8-C9
4	D	1201	BTI	C7-C8-C9-C10
2	A	1201	ADP	C5'-O5'-PA-O3A
2	A	1201	ADP	C4'-C5'-O5'-PA
2	A	1201	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1201	BTI	4	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1052/1173 (89%)	-0.55	18 (1%) 70 41	36, 75, 131, 167	0
1	B	989/1173 (84%)	-0.41	3 (0%) 94 84	59, 105, 154, 233	0
1	C	1059/1173 (90%)	-0.42	10 (0%) 84 63	56, 101, 150, 197	0
1	D	989/1173 (84%)	-0.52	9 (0%) 84 63	41, 82, 173, 267	0
All	All	4089/4692 (87%)	-0.47	40 (0%) 82 59	36, 93, 151, 267	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	240	ASP	4.4
1	D	241	ASN	4.0
1	A	224	ALA	3.7
1	A	176	SER	3.7
1	D	490	ILE	3.6
1	D	168	PRO	3.5
1	A	218	HIS	3.3
1	A	999	GLN	3.2
1	A	175	LYS	3.2
1	A	195	ALA	3.1
1	A	180	ALA	2.8
1	C	231	SER	2.8
1	D	475	ASP	2.8
1	C	937	LYS	2.7
1	C	218	HIS	2.7
1	A	214	GLU	2.7
1	A	232	GLU	2.6
1	B	168	PRO	2.6
1	A	231	SER	2.6
1	C	515	ASN	2.6
1	A	207	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	230	ASN	2.6
1	D	92	PRO	2.6
1	B	271	HIS	2.5
1	D	242	PRO	2.5
1	A	177	TYR	2.5
1	C	191	LEU	2.5
1	C	872	SER	2.4
1	C	876	GLN	2.4
1	D	315	SER	2.4
1	C	1070	GLU	2.3
1	A	197	SER	2.3
1	A	225	GLU	2.3
1	A	1001	PRO	2.2
1	D	286	THR	2.2
1	C	877	GLN	2.2
1	B	88	SER	2.1
1	C	885	GLU	2.1
1	A	215	ASP	2.1
1	A	233	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

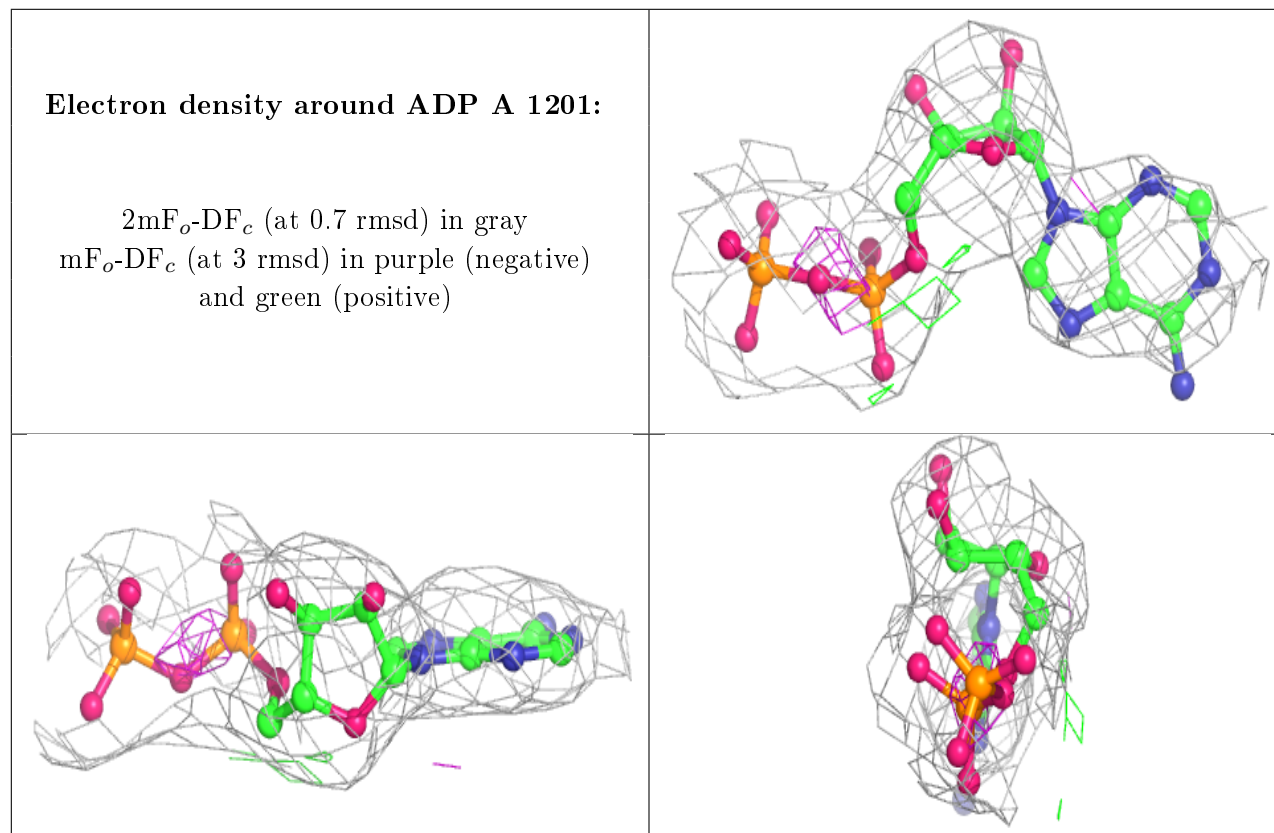
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BTI	D	1201	15/15	0.81	0.42	128,133,136,136	0
2	ADP	A	1201	27/27	0.87	0.20	108,112,144,146	0
3	MN	D	1202	1/1	0.97	0.18	79,79,79,79	0
3	MN	B	1201	1/1	0.97	0.18	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	C	1201	1/1	0.97	0.29	105,105,105,105	0
3	MN	A	1202	1/1	0.98	0.30	83,83,83,83	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.