



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 PM GMT

PDB ID : 4HNT
Title : crystal structure of F403A mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

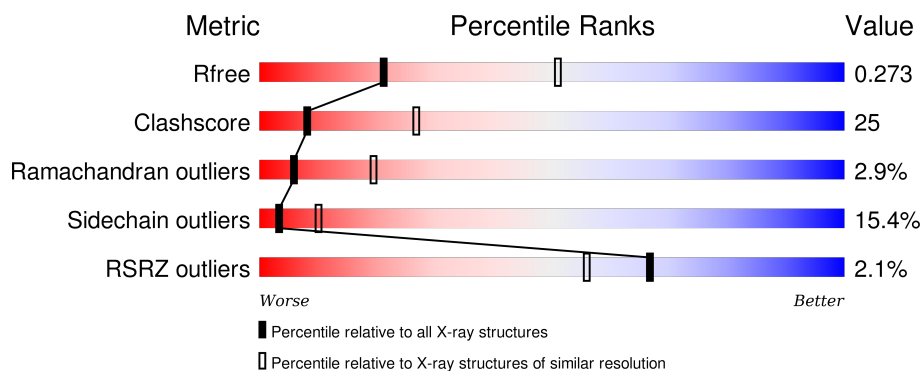
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 50% 32% 8% • 10%
1	B	1173	 2% 47% 30% 6% • 16%
1	C	1173	 2% 46% 35% 9% • 10%
1	D	1173	 % 48% 28% 8% 16%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTI	A	1203	-	-	-	X
4	BTI	B	1201	-	-	-	X
4	BTI	D	1201	-	-	-	X
5	ATP	C	1202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 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
			8336	5286	1404	1619	27			
1	B	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8373	5307	1412	1626	28			
1	D	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			

There are 92 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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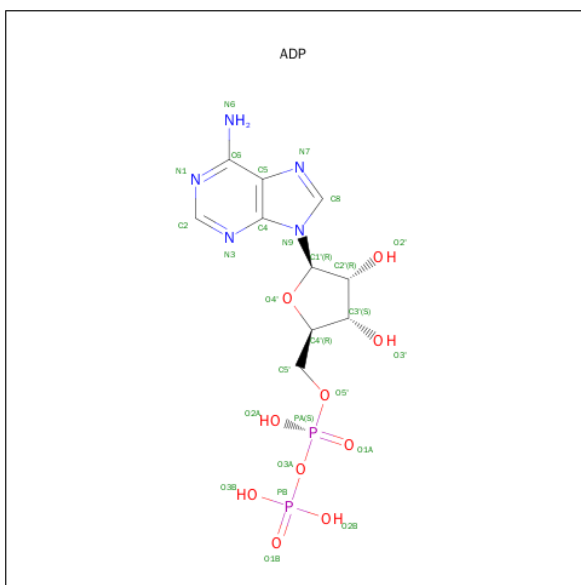
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
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
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
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

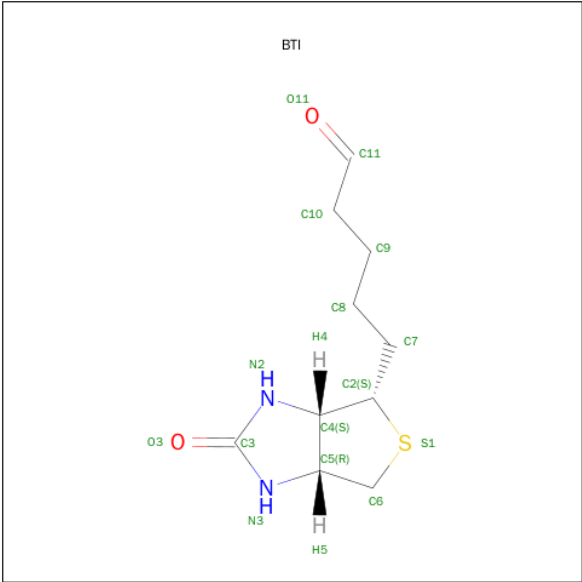


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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

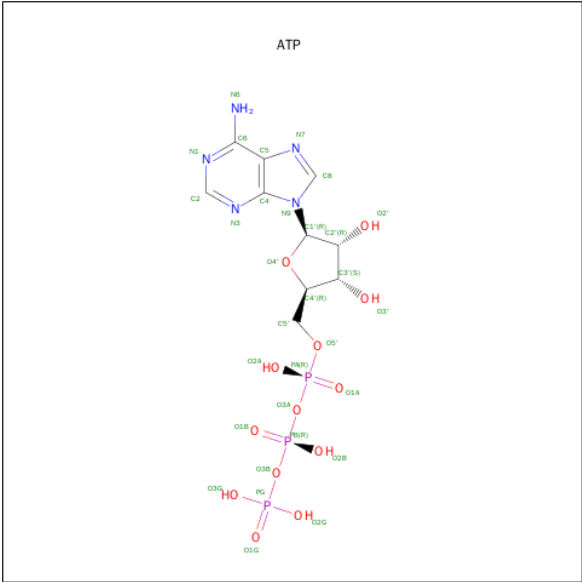
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- 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
4	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

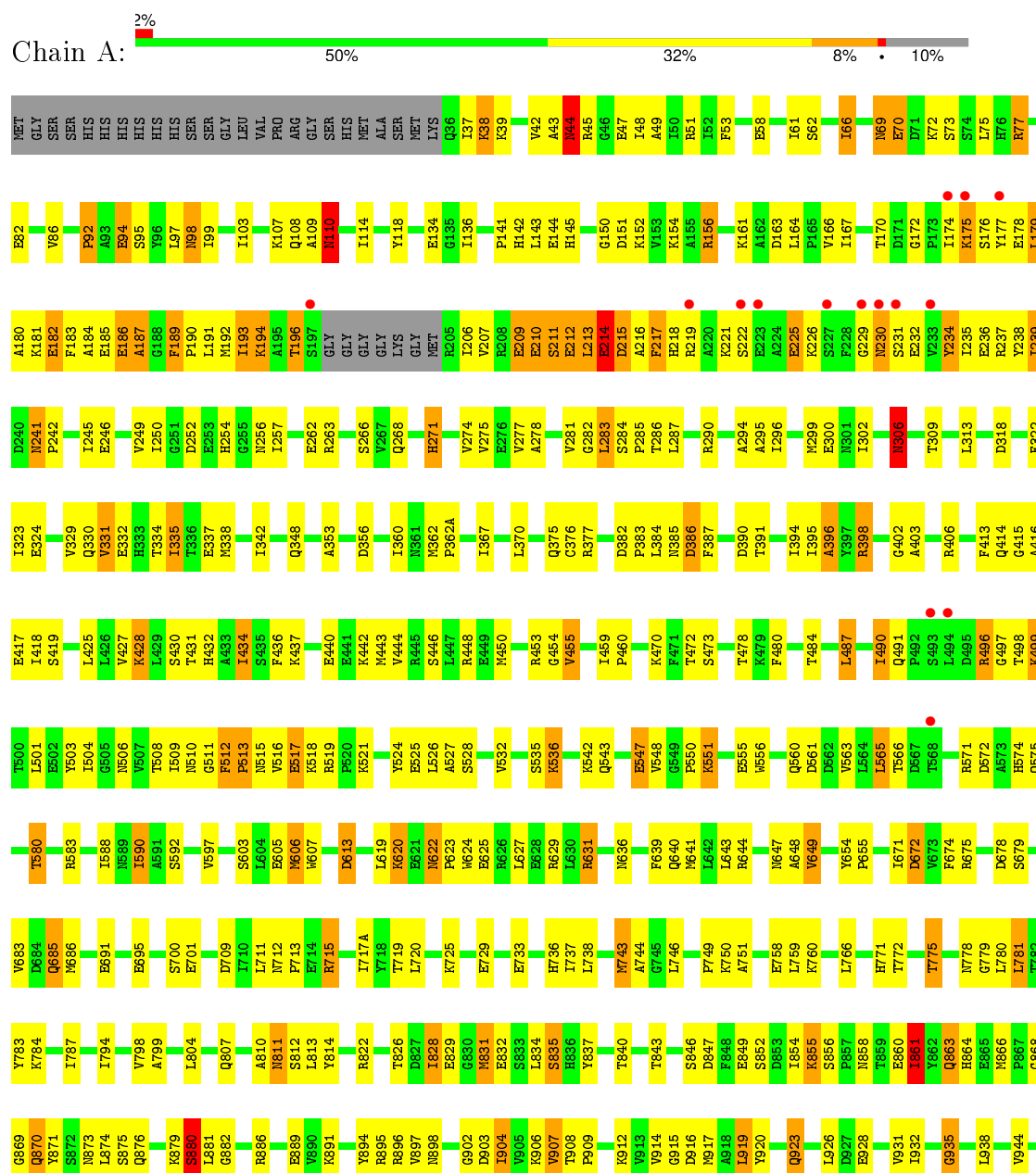


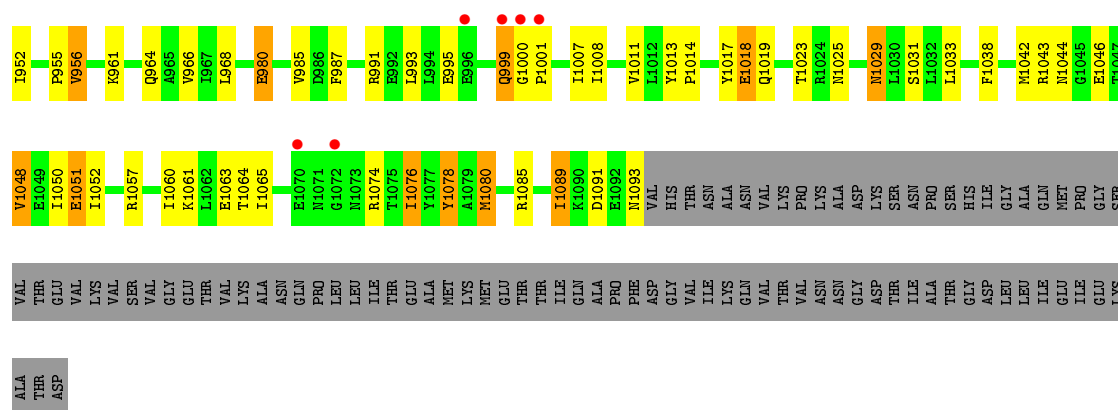
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

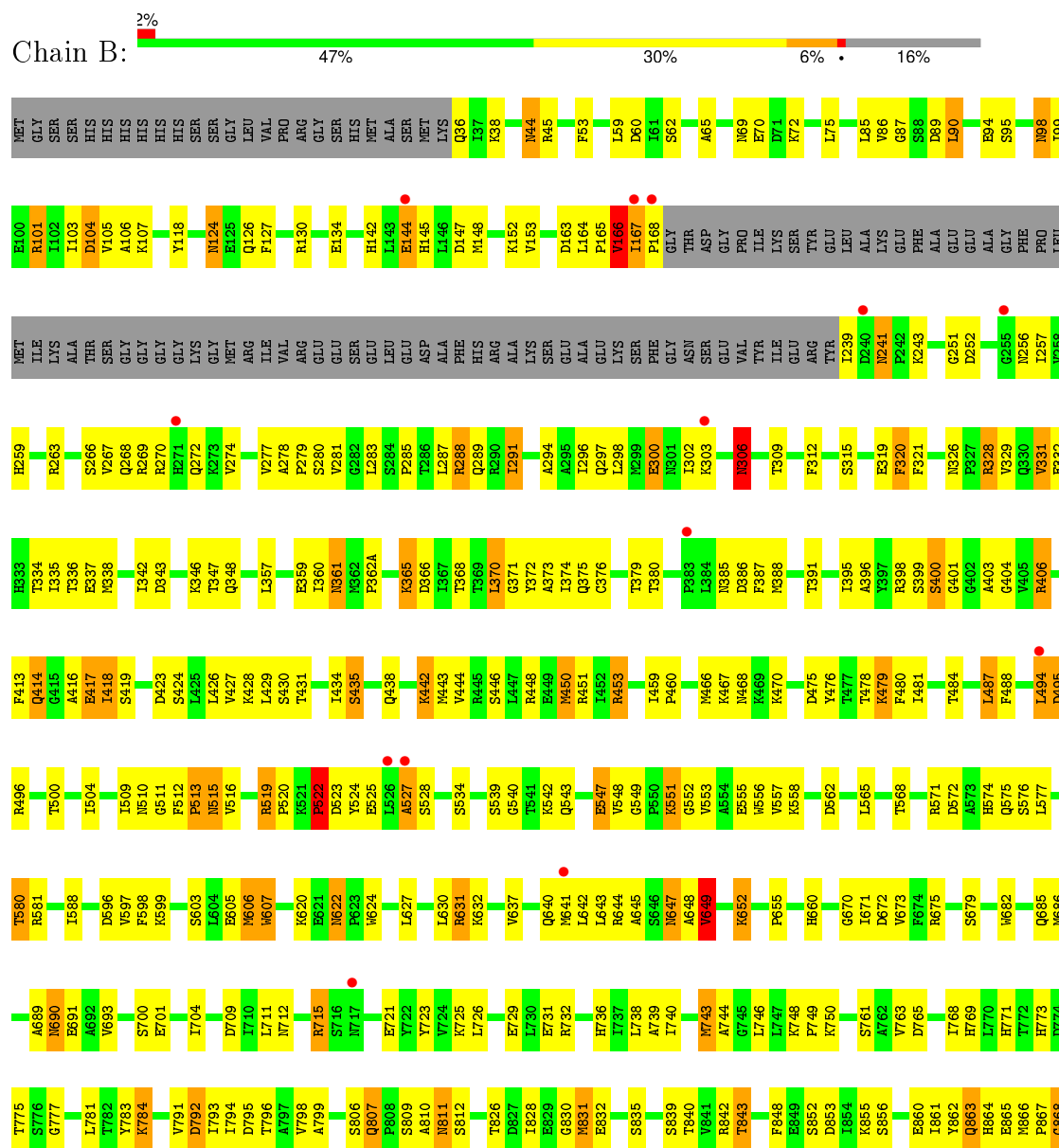
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

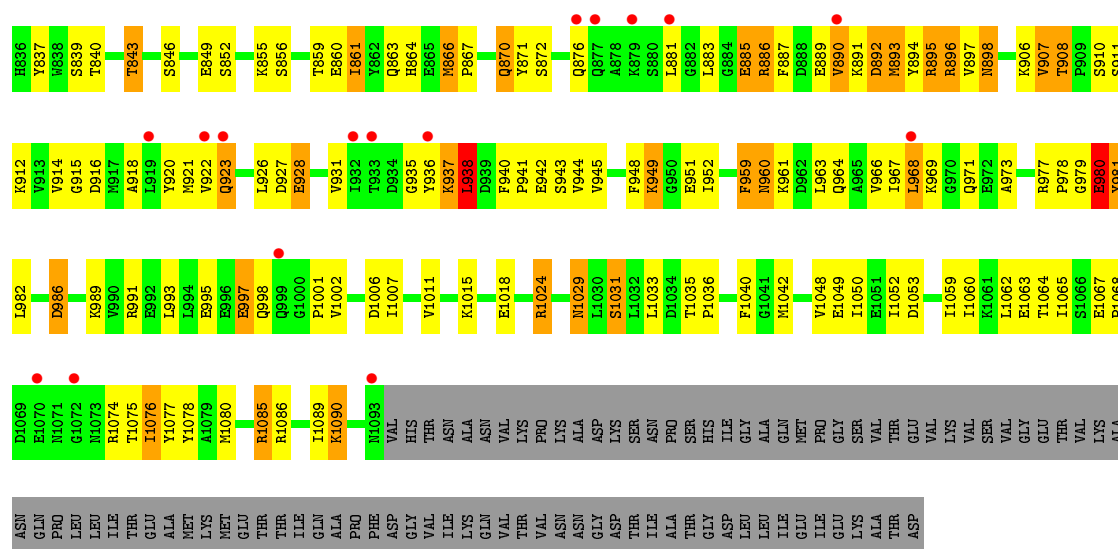
• Molecule 1: Pyruvate carboxylase



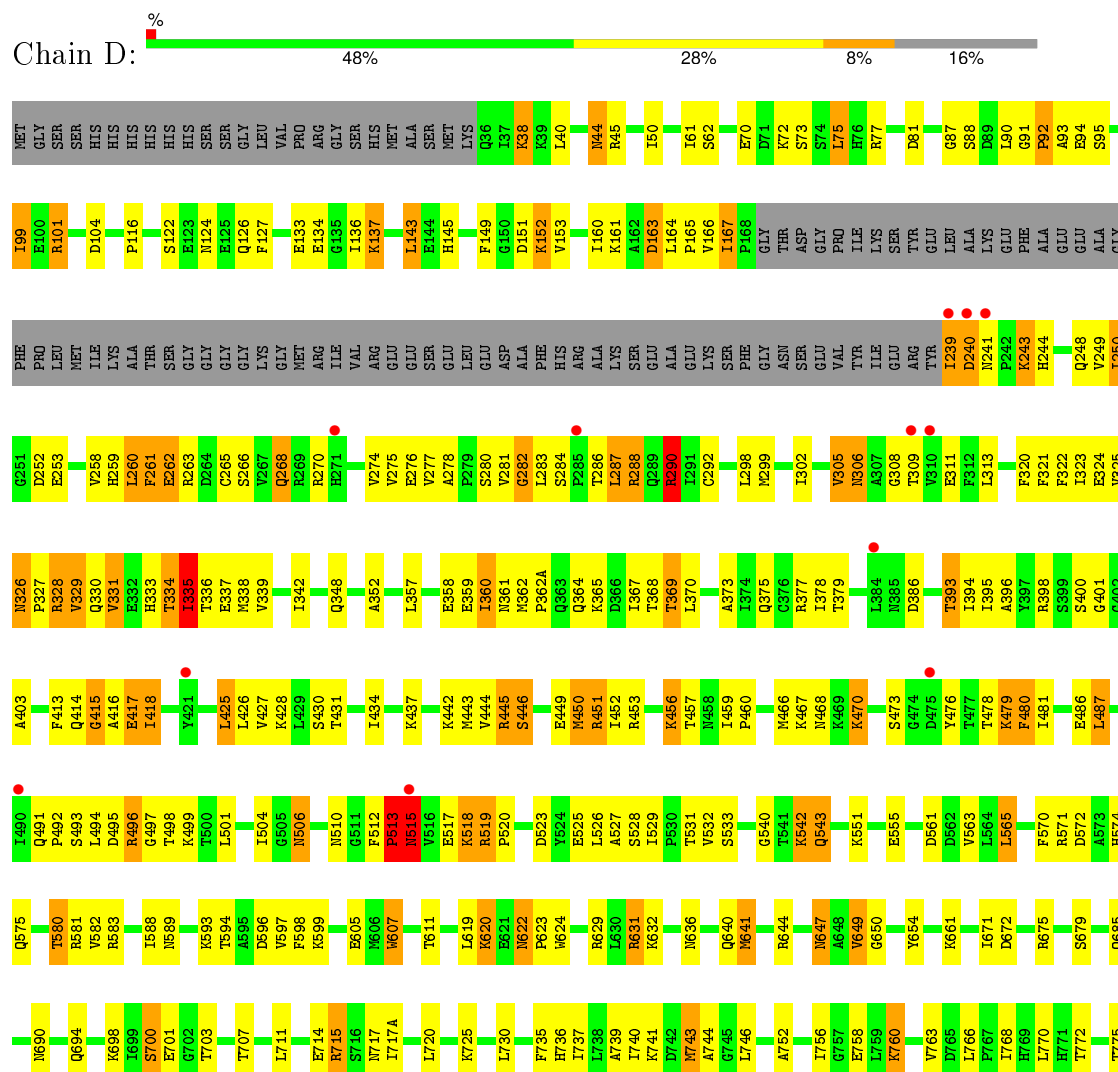


• Molecule 1: Pyruvate carboxylase





- Molecule 1: Pyruvate carboxylase



VAL	R1057	D939	H864	S776
GLY	I1060	F940	E865	
GLU	K1061	V944	M866	T782
THR	I1062	V945	G869	Y783
VAL	E1063	I952	Q870	K784
LYS	T1064	N957	Y871	Q785
ALA	D1069	N960	L874	A786
ASN	E1070	N963	S875	I787
GLN	N1071	L963	A878	V791
PRO	G1072	V966	K879	T796
LEU	N1073	I967	S880	A799
ILE	Y1078	I974	L881	S800
THR	A1079	R977	L883	L804
GLU	M1080	P978	G884	Q807
ALA	M1083	Y981	E885	A810
GLY	A1084	D886	R886	N811
THR	R1085	F887	D888	
THR	R1086	E988		Y814
ILE	I1087	R991	R896	Y815
GLN	Y1088	E995	V897	A816
ALA	I1089	E996	N898	L817
PRO	N1093	E1004	F899	F820
ASP	VAL	I1008	L900	P821
GLY	HIS	Y1013	F901	R822
THR	THR	P1014	I904	
VAL	ASN	R1015	V907	T828
ILE	ASN	V1016	T908	E829
LYS	ALA	THR	P909	Q830
GLN	ASN	ASN	S910	M831
VAL	VAL	ASN	S911	E832
THR	PRO	T1023	M917	
ASN	LYS	ALA	A918	H836
ASN	ALA	D1034	L919	
GLY	ASP	T1035	Y920	T843
ASP	LYS	P1036	M921	F844
THR	THR	M1042		Y845
ILE	ASN	R1043	N924	F848
ALA	PRO	N1044	D925	E849
THR	SER	M1045	L926	S852
GLY	HIS	G1046	D927	D853
ASP	ILE	GLY	E928	A854
LEU	GLY	THR	Q929	K855
LEU	ALA	THR	S930	S856
ILE	GLN	I1052	V931	P857
GLU	MET	D1053		
ILE	PRO	K1054		E860
GLU	GLY	G1055		L861
LYS	SER	VAL		Y862
LYS	THR	VAL		Q863
ASP	ASP			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23 Å 256.28 Å 126.69 Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 91.0 (29.79-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.279 0.207 , 0.273	Depositor DCC
R_{free} test set	7085 reflections (5.81%)	DCC
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.9	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 128487 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ATP, 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	0.68	1/8497 (0.0%)	0.73	1/11490 (0.0%)
1	B	0.63	4/7983 (0.1%)	0.66	3/10801 (0.0%)
1	C	0.65	4/8535 (0.0%)	0.68	4/11539 (0.0%)
1	D	0.66	5/7983 (0.1%)	0.70	2/10801 (0.0%)
All	All	0.65	14/32998 (0.0%)	0.69	10/44631 (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	6
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	18

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	14.00	1.80	1.52
1	B	936	TYR	C-N	11.65	1.60	1.34
1	C	513	PRO	C-N	10.85	1.58	1.34
1	C	515	ASN	N-CA	10.62	1.67	1.46
1	B	961	LYS	C-O	10.00	1.42	1.23
1	C	513	PRO	N-CA	8.86	1.62	1.47
1	D	290	ARG	CZ-NH1	8.75	1.44	1.33
1	A	513	PRO	CA-C	8.56	1.70	1.52
1	D	513	PRO	CA-C	7.66	1.68	1.52
1	D	515	ASN	N-CA	7.36	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	513	PRO	CA-C	7.18	1.67	1.52
1	D	513	PRO	C-N	6.20	1.48	1.34
1	D	513	PRO	N-CA	5.96	1.57	1.47
1	B	763	VAL	N-CA	5.78	1.57	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	C-N-CA	8.07	141.87	121.70
1	D	513	PRO	CA-C-N	7.87	134.51	117.20
1	C	513	PRO	CA-C-N	7.83	134.42	117.20
1	B	763	VAL	CA-C-N	7.35	133.38	117.20
1	C	513	PRO	N-CA-CB	-6.11	95.88	102.60
1	A	513	PRO	CA-C-N	6.09	130.60	117.20
1	B	763	VAL	O-C-N	-5.91	113.25	122.70
1	B	513	PRO	CA-C-N	5.68	129.69	117.20
1	C	513	PRO	O-C-N	-5.66	113.64	122.70
1	D	513	PRO	O-C-N	-5.57	113.78	122.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	150	GLY	Peptide
1	A	196	THR	Peptide
1	A	271	HIS	Peptide
1	A	415	GLY	Peptide
1	A	490	ILE	Peptide
1	B	522	PRO	Peptide
1	B	524	TYR	Peptide
1	B	936	TYR	Sidechain
1	C	150	GLY	Peptide
1	C	211	SER	Peptide
1	C	228	PHE	Peptide
1	C	262	GLU	Peptide
1	C	420	PRO	Peptide
1	C	493	SER	Peptide
1	C	494	LEU	Peptide
1	D	415	GLY	Peptide
1	D	416	ALA	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	8336	0	8249	430	0
1	B	7832	0	7767	352	0
1	C	8373	0	8287	456	0
1	D	7832	0	7767	376	0
2	A	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	16	4	0
4	B	15	0	16	4	0
4	D	15	0	16	3	0
5	C	31	0	12	10	0
All	All	32480	0	32142	1586	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 25.

All (1586) 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:C:515:ASN:N	1:C:515:ASN:CA	1.67	1.56
1:C:513:PRO:CA	1:C:513:PRO:C	1.80	1.47
1:D:607:TRP:HE3	1:D:641:MET:CE	1.51	1.23
1:C:918:ALA:O	1:C:922:VAL:HG23	1.39	1.22
1:B:403:ALA:O	1:B:442:LYS:HE2	1.42	1.18
1:C:334:THR:HB	1:C:406:ARG:NH1	1.59	1.17
1:C:893:MET:HA	1:C:896:ARG:CD	1.74	1.16
1:A:334:THR:HG22	1:A:406:ARG:HH12	1.06	1.16
1:A:413:PHE:CZ	1:A:416:ALA:HB2	1.82	1.14
1:C:1024:ARG:HG2	1:C:1024:ARG:HH11	1.02	1.14
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.00	1.12
1:C:396:ALA:HB3	1:C:453:ARG:HG3	1.27	1.11
1:D:607:TRP:CE3	1:D:641:MET:HE1	1.86	1.10
1:D:504:ILE:HG21	1:D:1042:MET:HE2	1.28	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:PHE:HB3	1:C:941:PRO:HD2	1.33	1.09
1:C:936:TYR:O	1:C:937:LYS:HG3	1.52	1.09
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.23	1.08
1:A:935:GLY:HA3	1:A:966:VAL:CG1	1.84	1.08
1:B:259:HIS:CD2	1:B:296:ILE:HD11	1.89	1.08
1:A:213:LEU:O	1:A:215:ASP:N	1.87	1.07
1:A:334:THR:CG2	1:A:406:ARG:HH12	1.68	1.06
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.36	1.06
1:D:268:GLN:O	1:D:481:ILE:HD12	1.55	1.06
1:D:607:TRP:HE3	1:D:641:MET:HE1	1.17	1.05
1:C:1085:ARG:HH11	1:C:1085:ARG:HG2	1.17	1.05
1:C:1029:ASN:HD21	1:C:1031:SER:HB2	1.16	1.05
1:D:607:TRP:CE3	1:D:641:MET:CE	2.40	1.05
1:C:167:ILE:HD12	1:C:167:ILE:H	1.23	1.03
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.41	1.03
1:C:377:ARG:HH11	1:C:377:ARG:CG	1.71	1.03
1:B:991:ARG:NH1	1:B:1002:VAL:O	1.92	1.03
1:C:192:MET:HE1	5:C:1202:ATP:C5	1.95	1.02
1:C:893:MET:HA	1:C:896:ARG:HD3	1.00	1.00
1:C:940:PHE:CB	1:C:944:VAL:HG11	1.92	1.00
1:B:338:MET:CE	1:B:430:SER:HB3	1.92	0.99
1:C:377:ARG:HG2	1:C:377:ARG:HH11	0.85	0.99
1:C:977:ARG:NH1	1:C:980:GLU:OE1	1.94	0.99
1:C:811:ASN:HD22	1:C:811:ASN:H	1.10	0.99
1:C:170:THR:HG22	1:C:171:ASP:H	1.27	0.98
1:D:496:ARG:HH11	1:D:496:ARG:HB3	1.26	0.98
1:A:935:GLY:HA3	1:A:966:VAL:HG11	1.45	0.98
1:A:334:THR:CG2	1:A:406:ARG:NH1	2.26	0.97
1:C:1085:ARG:HH11	1:C:1085:ARG:CG	1.78	0.97
1:B:700:SER:H	1:B:736:HIS:HD2	1.09	0.97
1:D:451:ARG:HG3	1:D:451:ARG:HH11	1.28	0.97
1:C:175:LYS:O	1:C:176:SER:O	1.83	0.97
1:C:377:ARG:HG2	1:C:377:ARG:NH1	1.68	0.97
1:B:338:MET:HE2	1:B:430:SER:HB3	1.47	0.97
1:A:179:LEU:H	1:A:179:LEU:HD23	1.26	0.96
1:C:44:ASN:HD22	1:C:45:ARG:H	0.96	0.96
1:A:156:ARG:HH11	1:A:156:ARG:HB3	1.31	0.95
1:D:357:LEU:O	1:D:362:MET:HB2	1.66	0.95
1:D:44:ASN:HD22	1:D:45:ARG:H	1.15	0.95
1:B:44:ASN:HD22	1:B:45:ARG:N	1.65	0.94
1:C:1085:ARG:NH1	1:C:1085:ARG:HG2	1.72	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:H	1:D:143:LEU:CD1	1.81	0.94
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.03	0.93
1:B:44:ASN:ND2	1:B:45:ARG:H	1.65	0.93
1:C:396:ALA:HA	1:C:414:GLN:HE22	1.31	0.93
1:C:893:MET:CA	1:C:896:ARG:HD3	1.95	0.93
1:C:895:ARG:HH11	1:C:895:ARG:CG	1.82	0.93
1:C:334:THR:CB	1:C:406:ARG:NH1	2.32	0.92
1:C:175:LYS:H	1:C:175:LYS:CD	1.82	0.92
1:C:1024:ARG:CG	1:C:1024:ARG:HH11	1.82	0.92
1:C:334:THR:HB	1:C:406:ARG:HH11	1.31	0.92
1:D:540:GLY:H	1:D:543:GLN:HE21	1.08	0.91
1:C:940:PHE:HB2	1:C:944:VAL:CG1	2.00	0.91
1:B:945:VAL:HG12	1:B:967:ILE:HG23	1.52	0.91
1:B:44:ASN:HD22	1:B:45:ARG:H	0.92	0.91
1:D:166:VAL:HG12	1:D:167:ILE:H	1.34	0.91
1:D:38:LYS:HE2	1:D:38:LYS:HA	1.51	0.90
1:D:494:LEU:HG	1:D:499:LYS:HE2	1.51	0.90
1:C:700:SER:H	1:C:736:HIS:HD2	1.03	0.90
1:A:334:THR:HB	1:A:406:ARG:NH1	1.85	0.90
1:C:1029:ASN:ND2	1:C:1031:SER:HB2	1.87	0.90
1:C:866:MET:HE2	1:C:871:TYR:HD1	1.35	0.89
1:C:895:ARG:HH11	1:C:895:ARG:HG3	1.35	0.89
1:B:288:ARG:CG	1:B:288:ARG:HH11	1.85	0.89
1:C:192:MET:HE1	5:C:1202:ATP:C6	2.08	0.89
1:A:44:ASN:HD22	1:A:45:ARG:H	1.19	0.89
1:C:1024:ARG:HG2	1:C:1024:ARG:NH1	1.81	0.89
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.54	0.89
1:A:334:THR:HB	1:A:406:ARG:HH11	1.37	0.88
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.03	0.88
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.53	0.88
1:C:949:LYS:HD3	1:C:951:GLU:OE1	1.73	0.88
1:B:288:ARG:NH1	1:B:288:ARG:HG3	1.82	0.88
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.37	0.88
1:A:334:THR:CB	1:A:406:ARG:NH1	2.38	0.87
1:B:864:HIS:HD2	1:B:866:MET:H	1.18	0.87
1:A:334:THR:HG22	1:A:406:ARG:NH1	1.87	0.86
1:A:398:ARG:HH11	1:A:398:ARG:CG	1.88	0.86
1:B:259:HIS:HD2	1:B:296:ILE:HD11	1.34	0.85
1:C:44:ASN:ND2	1:C:45:ARG:H	1.75	0.85
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.42	0.85
1:A:402:GLY:HA2	1:C:408:ASP:OD1	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:GLY:H	1:D:543:GLN:NE2	1.74	0.84
1:A:863:GLN:O	1:A:895:ARG:HD2	1.77	0.84
1:D:250:ILE:HD11	1:D:260:LEU:HD11	1.59	0.84
1:C:700:SER:H	1:C:736:HIS:CD2	1.94	0.84
1:B:798:VAL:HG12	1:B:831:MET:CE	2.07	0.84
1:B:606:MET:CE	1:B:607:TRP:HB2	2.07	0.84
1:D:811:ASN:H	1:D:811:ASN:HD22	1.23	0.84
1:B:543:GLN:O	1:B:547:GLU:HG2	1.77	0.83
1:B:999:GLN:HG2	1:B:1000:GLY:H	1.43	0.83
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.61	0.82
1:D:1053:ASP:HB2	1:D:1056:LYS:CD	2.08	0.82
1:C:198:GLY:HA3	1:C:228:PHE:HE2	1.43	0.82
1:B:539:SER:HA	1:B:543:GLN:HE21	1.42	0.82
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.42	0.82
1:B:338:MET:HE3	1:B:373:ALA:HB1	1.61	0.82
1:C:87:GLY:HA3	1:C:90:LEU:HD22	1.60	0.82
1:D:1053:ASP:HB2	1:D:1056:LYS:HD2	1.60	0.81
1:C:840:THR:O	1:C:843:THR:HB	1.80	0.81
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.10	0.81
1:C:890:VAL:O	1:C:891:LYS:HG3	1.79	0.81
1:C:334:THR:HG22	1:C:406:ARG:HH12	1.46	0.81
1:C:940:PHE:CB	1:C:944:VAL:CG1	2.56	0.81
1:C:152:LYS:H	1:C:196:THR:CG2	1.94	0.81
1:C:979:GLY:O	1:C:981:TYR:N	2.12	0.81
1:A:620:LYS:HG2	4:A:1203:BTI:H63	1.62	0.81
1:B:1066:SER:HB2	1:D:1064:THR:HG21	1.63	0.81
1:C:334:THR:CG2	1:C:406:ARG:HH12	1.94	0.81
1:D:143:LEU:H	1:D:143:LEU:HD12	1.46	0.81
1:D:166:VAL:HG12	1:D:167:ILE:N	1.96	0.81
1:C:39:LYS:HG3	1:C:62:SER:HB2	1.62	0.80
1:A:504:ILE:HD13	1:A:1042:MET:HE3	1.63	0.80
1:C:198:GLY:HA3	1:C:228:PHE:CE2	2.17	0.80
1:A:213:LEU:C	1:A:215:ASP:H	1.83	0.80
1:C:892:ASP:O	1:C:896:ARG:HD2	1.82	0.80
1:C:940:PHE:HB3	1:C:941:PRO:CD	2.12	0.80
1:A:290:ARG:NH2	1:A:318:ASP:O	2.13	0.80
1:A:77:ARG:HH11	1:A:77:ARG:CG	1.95	0.80
1:C:44:ASN:HD22	1:C:45:ARG:N	1.77	0.79
1:C:572:ASP:HB3	1:C:807:GLN:NE2	1.97	0.79
1:D:451:ARG:HG3	1:D:451:ARG:NH1	1.96	0.79
1:A:700:SER:H	1:A:736:HIS:HD2	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:THR:HG23	1:D:1085:ARG:HH22	1.47	0.79
1:B:396:ALA:HB3	1:B:453:ARG:HB2	1.65	0.79
1:A:622:ASN:ND2	1:A:624:TRP:H	1.81	0.79
1:D:504:ILE:HG21	1:D:1042:MET:CE	2.13	0.78
1:C:238:TYR:HD1	5:C:1202:ATP:C2	2.01	0.78
1:D:495:ASP:HB3	1:D:498:THR:HB	1.66	0.78
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.17	0.78
1:B:101:ARG:CG	1:B:101:ARG:HH11	1.96	0.78
1:D:513:PRO:O	1:D:515:ASN:HB2	1.82	0.78
1:C:1062:LEU:HD12	1:C:1078:TYR:CE2	2.18	0.78
1:B:306:ASN:OD1	1:B:348:GLN:HG2	1.83	0.78
1:A:176:SER:O	1:A:179:LEU:HB3	1.84	0.78
1:D:243:LYS:HZ3	1:D:243:LYS:HB3	1.47	0.77
1:C:921:MET:HA	1:C:926:LEU:HB2	1.67	0.77
1:C:87:GLY:HA3	1:C:90:LEU:CD2	2.15	0.77
1:A:98:ASN:C	1:A:98:ASN:HD22	1.88	0.77
1:C:893:MET:HE1	1:C:918:ALA:HA	1.67	0.77
1:C:167:ILE:HD12	1:C:167:ILE:N	1.99	0.77
1:A:1018:GLU:OE1	1:A:1018:GLU:HA	1.83	0.77
1:C:940:PHE:HB2	1:C:944:VAL:HG11	1.65	0.76
1:C:183:PHE:CD2	1:C:183:PHE:O	2.38	0.76
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.67	0.76
1:D:357:LEU:HA	1:D:360:ILE:HD12	1.65	0.76
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.66	0.76
1:D:259:HIS:H	1:D:364:GLN:HE22	1.32	0.76
1:B:864:HIS:CD2	1:B:866:MET:H	2.03	0.76
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.67	0.76
1:C:378:ILE:HG13	1:C:450:MET:HE1	1.67	0.76
1:D:143:LEU:N	1:D:143:LEU:HD12	2.00	0.76
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.67	0.76
1:D:866:MET:HE2	1:D:871:TYR:HA	1.68	0.76
1:C:188:GLY:HA3	1:C:237:ARG:HH22	1.51	0.76
1:D:337:GLU:HG2	1:D:342:ILE:O	1.85	0.75
1:C:918:ALA:O	1:C:922:VAL:CG2	2.29	0.75
1:A:189:PHE:HB3	1:A:190:PRO:CD	2.16	0.75
1:A:175:LYS:NZ	1:A:232:GLU:HG3	2.02	0.75
1:D:306:ASN:OD1	1:D:348:GLN:HG2	1.87	0.75
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.67	0.75
1:B:540:GLY:H	1:B:543:GLN:NE2	1.84	0.75
1:C:644:ARG:NH1	1:C:650:GLY:O	2.20	0.75
1:A:1060:ILE:HG12	1:A:1080:MET:HG3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:VAL:HG22	1:B:830:GLY:HA3	1.68	0.75
1:A:1042:MET:HE1	1:A:1048:VAL:HG12	1.67	0.75
1:A:1051:GLU:OE1	1:A:1057:ARG:NH2	2.20	0.75
1:C:912:LYS:O	1:C:916:ASP:N	2.19	0.75
1:D:298:LEU:O	1:D:302:ILE:HG13	1.87	0.75
1:D:506:ASN:ND2	1:D:510:ASN:HD22	1.85	0.74
1:A:167:ILE:HD11	1:A:323:ILE:HD11	1.69	0.74
1:D:840:THR:O	1:D:843:THR:HB	1.87	0.74
1:C:334:THR:CG2	1:C:406:ARG:NH1	2.49	0.74
1:C:326:ASN:ND2	1:C:330:GLN:OE1	2.20	0.74
1:C:530:PRO:HB2	1:C:593:LYS:HD3	1.70	0.74
1:C:178:GLU:O	1:C:182:GLU:HG3	1.88	0.74
1:C:494:LEU:HB2	1:C:496:ARG:NH1	2.03	0.74
1:B:1052:ILE:HG22	1:B:1052:ILE:O	1.87	0.74
1:A:991:ARG:O	1:A:995:GLU:HG3	1.88	0.74
1:A:590:ILE:HG13	1:A:837:TYR:CE2	2.21	0.74
1:D:917:MET:HG2	1:D:944:VAL:HG11	1.69	0.74
1:C:378:ILE:HG13	1:C:450:MET:CE	2.18	0.74
1:D:1047:THR:HG23	1:D:1061:LYS:HB2	1.70	0.73
1:D:278:ALA:HB2	1:D:335:ILE:HG23	1.69	0.73
1:C:238:TYR:CD1	5:C:1202:ATP:C2	2.76	0.73
1:A:620:LYS:HG3	1:A:1023:THR:HG21	1.71	0.73
1:C:910:SER:O	1:C:914:VAL:HG23	1.88	0.73
1:B:395:ILE:HG13	1:B:453:ARG:HB3	1.69	0.73
1:B:269:ARG:HG2	1:B:481:ILE:HG21	1.70	0.73
1:A:406:ARG:HH21	1:C:403:ALA:HB2	1.54	0.73
1:A:152:LYS:NZ	1:A:324:GLU:OE2	2.21	0.73
1:A:51:ARG:NH2	1:A:337:GLU:OE1	2.19	0.73
1:D:991:ARG:O	1:D:995:GLU:HG3	1.89	0.73
1:A:470:LYS:HB2	1:A:480:PHE:CE1	2.24	0.73
1:A:241:ASN:N	1:A:242:PRO:HD3	2.04	0.72
1:D:418:ILE:HD12	1:D:418:ILE:H	1.54	0.72
1:D:456:LYS:N	1:D:456:LYS:HD3	2.04	0.72
1:D:166:VAL:CG1	1:D:167:ILE:H	2.03	0.72
1:A:164:LEU:HD22	1:A:294:ALA:HB1	1.71	0.72
1:A:864:HIS:HD2	1:A:866:MET:H	1.38	0.72
1:A:896:ARG:HD2	1:A:928:GLU:OE2	1.89	0.72
1:A:206:ILE:HD11	1:A:238:TYR:CE1	2.24	0.71
1:B:338:MET:HE1	1:B:430:SER:HB3	1.70	0.71
1:C:811:ASN:HD22	1:C:811:ASN:N	1.84	0.71
1:B:279:PRO:HD2	1:B:372:TYR:HD2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:VAL:HG12	1:B:914:VAL:HG13	1.72	0.71
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.72	0.71
1:C:646:SER:HB2	1:C:685:GLN:HE22	1.53	0.71
1:D:444:VAL:HG23	1:D:466:MET:HB3	1.70	0.71
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.72	0.71
1:B:118:TYR:OH	1:B:331:VAL:HG13	1.90	0.71
1:D:917:MET:SD	1:D:921:MET:CE	2.79	0.71
1:B:145:HIS:HE1	1:B:302:ILE:O	1.72	0.71
1:C:200:GLY:C	1:C:202:LYS:H	1.92	0.71
1:B:1046:GLU:HG2	1:B:1047:THR:N	2.04	0.71
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.72	0.71
1:D:864:HIS:HD2	1:D:866:MET:H	1.36	0.71
1:B:259:HIS:HD2	1:B:296:ILE:CD1	2.02	0.71
1:A:217:PHE:CE2	1:A:221:LYS:HE3	2.26	0.71
1:B:142:HIS:H	1:B:145:HIS:HD2	1.38	0.71
1:D:116:PRO:HB2	1:D:122:SER:HA	1.72	0.71
1:D:339:VAL:O	1:D:369:THR:HA	1.90	0.71
1:A:413:PHE:CZ	1:A:416:ALA:CB	2.69	0.70
1:C:170:THR:HG22	1:C:171:ASP:N	2.04	0.70
1:A:44:ASN:HD22	1:A:45:ARG:N	1.87	0.70
1:A:516:VAL:O	1:A:516:VAL:HG12	1.89	0.70
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.88	0.70
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.56	0.70
1:C:175:LYS:H	1:C:175:LYS:HD3	1.53	0.70
1:C:574:HIS:CD2	1:C:582:VAL:HB	2.26	0.70
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.73	0.70
1:B:861:ILE:HG13	1:B:862:TYR:N	2.06	0.70
1:B:1052:ILE:HD11	1:B:1058:LEU:HG	1.74	0.70
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.26	0.70
1:B:577:LEU:HD13	1:B:842:ARG:NH2	2.06	0.70
1:A:644:ARG:HH11	1:A:909:PRO:HD3	1.56	0.70
1:D:540:GLY:N	1:D:543:GLN:HE21	1.87	0.70
1:C:437:LYS:HD3	1:C:437:LYS:H	1.57	0.70
1:C:504:ILE:HD13	1:C:1042:MET:CE	2.22	0.70
1:C:911:SER:O	1:C:915:GLY:N	2.18	0.70
1:B:744:ALA:HB3	1:B:746:LEU:HG	1.74	0.70
1:C:359:GLU:N	1:C:359:GLU:OE2	2.23	0.70
1:C:335:ILE:HD11	1:C:373:ALA:O	1.92	0.69
1:D:263:ARG:CD	1:D:335:ILE:HG21	2.23	0.69
1:D:358:GLU:HG2	1:D:359:GLU:OE2	1.92	0.69
1:A:898:ASN:HD21	1:A:904:ILE:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:ILE:CG2	1:D:1042:MET:HE2	2.17	0.69
1:C:940:PHE:CB	1:C:941:PRO:HD2	2.19	0.69
1:C:230:ASN:HD22	1:C:231:SER:N	1.90	0.69
1:B:571:ARG:HH11	1:B:575:GLN:NE2	1.91	0.69
1:A:691:GLU:O	1:A:695:GLU:HG3	1.92	0.69
1:A:338:MET:HE1	1:A:430:SER:HB2	1.73	0.69
1:B:927:ASP:OD2	1:B:927:ASP:N	2.25	0.69
1:D:607:TRP:HE3	1:D:641:MET:HE3	1.54	0.69
1:C:943:SER:OG	1:C:944:VAL:N	2.26	0.69
1:B:999:GLN:HG2	1:B:1000:GLY:N	2.07	0.69
1:A:513:PRO:O	1:A:515:ASN:HB2	1.93	0.69
1:A:499:LYS:HE3	1:A:1025:ASN:O	1.93	0.69
1:C:167:ILE:CD1	1:C:167:ILE:H	2.04	0.68
1:B:375:GLN:NE2	1:B:428:LYS:HD3	2.07	0.68
1:D:874:LEU:O	1:D:887:PHE:HE1	1.76	0.68
1:A:622:ASN:HD22	1:A:623:PRO:HD2	1.58	0.68
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.29	0.68
1:A:167:ILE:CD1	1:A:323:ILE:HD11	2.24	0.68
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.27	0.68
1:C:893:MET:O	1:C:897:VAL:N	2.22	0.68
1:C:156:ARG:NH2	1:C:170:THR:O	2.26	0.68
1:C:69:ASN:O	1:C:72:LYS:HG3	1.93	0.68
1:B:414:GLN:HG3	1:D:1084:ALA:HB2	1.74	0.68
1:C:396:ALA:CB	1:C:453:ARG:HG3	2.15	0.68
1:C:156:ARG:HG2	1:C:166:VAL:HG11	1.76	0.67
1:D:960:ASN:HD22	1:D:963:LEU:HB2	1.59	0.67
1:B:347:THR:HG23	1:B:360:ILE:HD13	1.77	0.67
1:D:263:ARG:HD3	1:D:335:ILE:CG2	2.24	0.67
1:C:200:GLY:O	1:C:202:LYS:N	2.26	0.67
1:A:840:THR:O	1:A:843:THR:HB	1.94	0.67
1:D:70:GLU:CD	1:D:70:GLU:H	1.96	0.67
1:C:926:LEU:CD1	1:C:938:LEU:HD11	2.25	0.67
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.59	0.67
1:A:194:LYS:NZ	1:A:236:GLU:OE1	2.24	0.67
1:D:543:GLN:HE22	1:D:636:ASN:HA	1.59	0.67
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.25	0.67
1:C:152:LYS:H	1:C:196:THR:HG23	1.58	0.67
1:B:98:ASN:C	1:B:98:ASN:HD22	1.98	0.67
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.93	0.67
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.75	0.67
1:D:362:MET:CE	1:D:367:ILE:HD11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:THR:HG23	1:D:1085:ARG:NH2	2.09	0.66
1:D:717(A):ILE:HG13	1:D:957:ASN:OD1	1.95	0.66
1:C:978:PRO:HA	1:C:981:TYR:CZ	2.30	0.66
1:C:328:ARG:HG3	1:C:329:VAL:O	1.96	0.66
1:D:828:ILE:O	1:D:832:GLU:HG2	1.96	0.66
1:D:338:MET:CE	1:D:430:SER:HB3	2.25	0.66
1:A:334:THR:HG21	1:A:428:LYS:HZ2	1.60	0.66
1:C:940:PHE:HB3	1:C:944:VAL:HG11	1.76	0.66
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.26	0.66
1:A:952:ILE:O	1:A:952:ILE:CG2	2.43	0.66
1:C:940:PHE:CG	1:C:944:VAL:HG11	2.30	0.66
1:D:917:MET:SD	1:D:921:MET:HE1	2.36	0.66
1:D:263:ARG:NH1	1:D:336:THR:OG1	2.28	0.66
1:B:413:PHE:HD1	1:B:414:GLN:HB3	1.60	0.66
1:C:261:PHE:HE1	1:C:367:ILE:HG22	1.61	0.66
1:D:756:ILE:HD12	1:D:786:ALA:HB1	1.77	0.66
1:C:385:ASN:O	1:C:387:PHE:N	2.28	0.66
1:B:268:GLN:HB3	1:B:272:GLN:O	1.95	0.66
1:B:796:THR:HB	1:B:810:ALA:HB2	1.78	0.66
1:C:192:MET:CE	5:C:1202:ATP:C6	2.79	0.65
1:D:44:ASN:ND2	1:D:45:ARG:H	1.92	0.65
1:C:646:SER:HB2	1:C:685:GLN:NE2	2.11	0.65
1:D:917:MET:SD	1:D:921:MET:HE3	2.37	0.65
1:C:39:LYS:HG3	1:C:62:SER:CB	2.27	0.65
1:C:398:ARG:HH11	1:C:398:ARG:HG3	1.62	0.65
1:A:206:ILE:CG2	1:A:207:VAL:N	2.60	0.65
1:B:99:ILE:HD12	1:B:99:ILE:H	1.62	0.65
1:C:396:ALA:HB3	1:C:453:ARG:CG	2.17	0.65
1:A:192:MET:HE1	1:A:238:TYR:CE1	2.32	0.65
1:C:811:ASN:H	1:C:811:ASN:ND2	1.89	0.65
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.61	0.65
1:B:380:THR:HG22	1:B:426:LEU:HD11	1.78	0.65
1:D:622:ASN:C	1:D:622:ASN:HD22	1.98	0.65
1:A:207:VAL:HA	1:A:212:GLU:OE2	1.96	0.65
1:B:927:ASP:HB2	1:B:929:GLN:H	1.61	0.65
1:D:445:ARG:HG2	1:D:445:ARG:O	1.97	0.65
1:C:175:LYS:CD	1:C:175:LYS:N	2.57	0.64
1:C:700:SER:N	1:C:736:HIS:HD2	1.87	0.64
1:B:268:GLN:CB	1:B:272:GLN:O	2.45	0.64
1:D:1087:ILE:HG22	1:D:1089:ILE:HD12	1.80	0.64
1:A:70:GLU:HG3	1:A:92:PRO:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PRO:O	1:C:174:ILE:HD12	1.97	0.64
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.32	0.64
1:B:548:VAL:HG23	1:B:552:GLY:HA3	1.79	0.64
1:B:1066:SER:CB	1:D:1064:THR:HG21	2.27	0.64
1:D:622:ASN:ND2	1:D:624:TRP:H	1.95	0.64
1:C:103:ILE:HG21	1:C:134:GLU:HG3	1.79	0.64
1:D:715:ARG:NH1	1:D:865:GLU:OE2	2.31	0.64
1:A:811:ASN:H	1:A:811:ASN:HD22	1.45	0.64
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.77	0.64
1:C:183:PHE:HD2	1:C:183:PHE:O	1.76	0.64
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.28	0.64
1:A:470:LYS:HB2	1:A:480:PHE:HE1	1.63	0.64
1:B:892:ASP:O	1:B:896:ARG:HG3	1.98	0.64
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.78	0.64
1:A:542:LYS:HE2	1:A:672:ASP:OD2	1.96	0.64
1:D:498:THR:CG2	1:D:1085:ARG:HH22	2.09	0.64
1:B:435:SER:HB3	1:B:438:GLN:HE21	1.63	0.64
1:D:394:ILE:HD11	1:D:426:LEU:HD21	1.79	0.64
1:A:613:ASP:HB2	1:A:1013:TYR:CZ	2.32	0.64
1:C:504:ILE:HD13	1:C:1042:MET:HE2	1.79	0.64
1:C:170:THR:CG2	1:C:171:ASP:H	2.08	0.64
1:C:41:LEU:HD22	1:C:114:ILE:HG12	1.79	0.64
1:D:685:GLN:OE1	1:D:978:PRO:HD2	1.98	0.64
1:B:647:ASN:O	1:B:649:VAL:N	2.30	0.64
1:D:986:ASP:OD2	1:D:988:GLU:HB2	1.97	0.64
1:A:179:LEU:HA	1:A:182:GLU:OE2	1.96	0.63
1:B:540:GLY:H	1:B:543:GLN:HE21	1.46	0.63
1:C:518:LYS:O	1:C:518:LYS:HG3	1.97	0.63
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.29	0.63
1:B:606:MET:HE1	1:B:607:TRP:HB2	1.80	0.63
1:A:881:LEU:HD13	1:A:923:GLN:HE22	1.62	0.63
1:D:594:THR:HG23	1:D:598:PHE:HD1	1.64	0.63
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.12	0.63
1:A:216:ALA:C	1:A:218:HIS:H	2.01	0.63
1:D:492:PRO:O	1:D:493:SER:OG	2.16	0.63
1:A:1018:GLU:OE1	1:A:1018:GLU:CA	2.46	0.63
1:D:622:ASN:HD22	1:D:623:PRO:N	1.97	0.63
1:C:794:ILE:HD12	1:C:796:THR:HG23	1.81	0.63
1:A:828:ILE:O	1:A:832:GLU:HG2	1.99	0.63
1:A:216:ALA:O	1:A:218:HIS:N	2.31	0.63
1:D:496:ARG:NH1	1:D:496:ARG:HB3	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:SER:O	1:A:179:LEU:HD22	1.98	0.63
1:C:760:LYS:HE3	1:C:790:GLY:O	1.99	0.63
1:B:952:ILE:HG22	1:B:952:ILE:O	1.98	0.63
1:D:518:LYS:O	1:D:518:LYS:HG3	1.99	0.63
1:D:259:HIS:H	1:D:364:GLN:NE2	1.95	0.63
1:A:362:MET:CE	1:A:367:ILE:HD11	2.29	0.63
1:B:69:ASN:HD22	1:B:72:LYS:HE3	1.64	0.63
1:C:357:LEU:O	1:C:362:MET:HB3	1.99	0.63
1:A:334:THR:HG21	1:A:428:LYS:NZ	2.13	0.62
1:A:44:ASN:ND2	1:A:45:ARG:H	1.95	0.62
1:A:781:LEU:HD13	1:D:816:ALA:HB1	1.80	0.62
1:C:515:ASN:N	1:C:515:ASN:HA	2.00	0.62
1:A:490:ILE:O	1:A:490:ILE:CD1	2.47	0.62
1:A:583:ARG:HG2	1:A:619:LEU:HD22	1.81	0.62
1:D:607:TRP:CZ3	1:D:641:MET:HE1	2.33	0.62
1:C:377:ARG:CG	1:C:377:ARG:NH1	2.43	0.62
1:D:364:GLN:HA	1:D:367:ILE:HD12	1.82	0.62
1:A:278:ALA:HB3	1:A:335:ILE:HG12	1.80	0.62
1:B:266:SER:O	1:B:478:THR:HA	1.99	0.62
1:D:565:LEU:C	1:D:565:LEU:HD12	2.19	0.62
1:B:860:GLU:O	1:B:863:GLN:HG2	1.99	0.62
1:A:775:THR:OG1	1:A:861:ILE:CD1	2.47	0.62
1:C:273:LYS:HB3	1:C:276:GLU:OE2	2.00	0.62
1:B:606:MET:HE3	1:B:607:TRP:HB2	1.80	0.62
1:B:539:SER:HA	1:B:543:GLN:NE2	2.12	0.62
1:A:700:SER:H	1:A:736:HIS:CD2	2.14	0.62
1:A:879:LYS:C	1:A:881:LEU:H	2.03	0.62
1:D:244:HIS:HD2	1:D:265:CYS:HB2	1.63	0.62
1:D:661:LYS:NZ	1:D:1004:GLU:OE2	2.25	0.62
1:B:620:LYS:HG3	4:B:1201:BTI:H63	1.81	0.62
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.47	0.62
1:B:413:PHE:CE2	1:B:416:ALA:HB2	2.35	0.62
1:C:867:PRO:HB2	1:C:870:GLN:HB3	1.80	0.62
1:A:547:GLU:OE2	1:A:547:GLU:HA	2.00	0.62
1:B:98:ASN:ND2	1:B:101:ARG:H	1.98	0.62
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.82	0.62
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.65	0.62
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.82	0.62
1:B:746:LEU:HD11	1:B:865:GLU:HG2	1.82	0.62
1:C:252:ASP:HB3	1:C:357:LEU:HB2	1.80	0.62
1:B:565:LEU:HD11	1:B:598:PHE:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:O	1:A:432:HIS:HE1	1.83	0.61
1:C:266:SER:O	1:C:478:THR:HA	2.00	0.61
1:B:320:PHE:N	1:B:320:PHE:CD1	2.67	0.61
1:A:406:ARG:HE	1:C:403:ALA:HA	1.65	0.61
1:A:935:GLY:CA	1:A:966:VAL:CG1	2.72	0.61
1:D:93:ALA:O	1:D:95:SER:N	2.33	0.61
1:D:151:ASP:O	1:D:153:VAL:N	2.33	0.61
1:D:143:LEU:H	1:D:143:LEU:HD13	1.64	0.61
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.82	0.61
1:C:519:ARG:HG2	1:C:520:PRO:O	2.00	0.61
1:A:403:ALA:HA	1:C:406:ARG:HH21	1.65	0.61
1:B:700:SER:H	1:B:736:HIS:CD2	2.01	0.61
1:C:675:ARG:HA	1:C:701:GLU:HB3	1.82	0.61
1:C:221:LYS:O	1:C:224:ALA:HB3	2.01	0.61
1:A:167:ILE:HB	1:A:236:GLU:OE2	2.01	0.61
1:A:644:ARG:NH1	1:A:909:PRO:HD3	2.16	0.61
1:D:281:VAL:O	1:D:283:LEU:N	2.33	0.61
1:A:563:VAL:HG21	1:A:787:ILE:HG12	1.81	0.61
1:B:644:ARG:HD3	1:B:909:PRO:HD3	1.81	0.61
1:A:37:ILE:HD12	1:A:353:ALA:HB2	1.82	0.61
1:D:1070:GLU:HG3	1:D:1071:ASN:N	2.14	0.61
1:A:210:GLU:O	1:A:212:GLU:N	2.28	0.61
1:C:1033:LEU:CD2	1:C:1050:ILE:HD13	2.31	0.61
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.83	0.61
1:C:243:LYS:HD3	1:C:476:TYR:O	2.01	0.61
1:A:999:GLN:HG2	1:A:1000:GLY:H	1.66	0.60
1:A:490:ILE:O	1:A:490:ILE:HD12	2.01	0.60
1:A:999:GLN:HG2	1:A:1000:GLY:N	2.16	0.60
1:D:647:ASN:C	1:D:647:ASN:HD22	2.03	0.60
1:B:338:MET:CE	1:B:430:SER:CB	2.75	0.60
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.34	0.60
1:D:335:ILE:CG2	1:D:336:THR:N	2.63	0.60
1:D:335:ILE:HG22	1:D:336:THR:N	2.15	0.60
1:B:337:GLU:HG2	1:B:342:ILE:O	2.01	0.60
1:A:605:GLU:HG3	1:A:640:GLN:HG2	1.83	0.60
1:B:101:ARG:CG	1:B:101:ARG:NH1	2.60	0.60
1:D:338:MET:HE2	1:D:430:SER:HB3	1.83	0.60
1:B:934:ASP:O	1:B:938:LEU:HG	2.00	0.60
1:C:141:PRO:HB2	1:C:145:HIS:HB2	1.83	0.60
1:D:641:MET:HB3	1:D:671:ILE:HD12	1.83	0.60
1:A:622:ASN:HD22	1:A:623:PRO:CD	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:GLU:HG2	1:B:1047:THR:H	1.64	0.60
1:C:69:ASN:OD1	1:C:69:ASN:N	2.34	0.60
1:A:444:VAL:O	1:A:448:ARG:HG3	2.01	0.60
1:D:690:ASN:O	1:D:694:GLN:HG2	2.02	0.60
1:A:192:MET:HE2	1:A:238:TYR:CD1	2.37	0.60
1:C:238:TYR:CD1	5:C:1202:ATP:H2	2.20	0.60
1:B:269:ARG:O	1:B:272:GLN:N	2.30	0.60
1:B:243:LYS:HG3	1:B:266:SER:OG	2.02	0.60
1:C:556:TRP:O	1:C:560:GLN:HG2	2.01	0.60
1:B:798:VAL:HG12	1:B:831:MET:HE2	1.83	0.60
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.15	0.60
1:C:323:ILE:HD11	5:C:1202:ATP:N7	2.17	0.59
1:D:278:ALA:HB2	1:D:335:ILE:CG2	2.32	0.59
1:D:960:ASN:HD22	1:D:963:LEU:H	1.49	0.59
1:B:917:MET:O	1:B:921:MET:HG2	2.01	0.59
1:D:885:GLU:OE2	1:D:885:GLU:HA	2.02	0.59
1:C:186:GLU:OE2	1:C:186:GLU:N	2.35	0.59
1:A:278:ALA:CB	1:A:335:ILE:HG12	2.31	0.59
1:A:509:ILE:HD12	1:A:1089:ILE:HG21	1.84	0.59
1:A:192:MET:CE	1:A:238:TYR:CD1	2.85	0.59
1:C:949:LYS:CD	1:C:951:GLU:OE1	2.48	0.59
1:B:606:MET:HE3	1:B:607:TRP:N	2.18	0.59
1:C:979:GLY:C	1:C:981:TYR:H	2.05	0.59
1:A:338:MET:CE	1:A:430:SER:HB2	2.32	0.59
1:B:167:ILE:HG13	1:B:168:PRO:HD3	1.85	0.59
1:A:897:VAL:HG12	1:A:914:VAL:HG13	1.83	0.59
1:C:1042:MET:HE1	1:C:1060:ILE:HG21	1.83	0.59
1:B:731:GLU:OE1	1:B:765:ASP:N	2.35	0.59
1:A:503:TYR:OH	1:A:1038:PHE:O	2.20	0.59
1:D:512:PHE:CZ	4:D:1201:BTI:H5	2.37	0.59
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.85	0.59
1:D:101:ARG:O	1:D:104:ASP:HB2	2.01	0.59
1:B:655:PRO:HG3	1:B:982:LEU:HB3	1.84	0.59
1:A:382:ASP:OD1	1:A:384:LEU:HD13	2.02	0.59
1:B:167:ILE:CG1	1:B:168:PRO:HD3	2.31	0.59
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.00	0.59
1:A:145:HIS:HE1	1:A:302:ILE:O	1.86	0.59
1:A:434:ILE:HG13	1:C:341:GLY:O	2.02	0.59
1:A:720:LEU:HD11	1:A:758:GLU:HG3	1.85	0.59
1:C:1068:PRO:HD3	1:C:1074:ARG:NH1	2.18	0.59
1:D:243:LYS:HZ3	1:D:243:LYS:CB	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:ILE:O	1:B:1052:ILE:CG2	2.49	0.59
1:B:955:PRO:HG2	1:B:958:GLY:O	2.02	0.59
1:C:193:ILE:HB	1:C:235:ILE:HB	1.84	0.59
1:A:179:LEU:CD2	1:A:179:LEU:H	2.02	0.59
1:D:811:ASN:H	1:D:811:ASN:ND2	1.94	0.59
1:D:263:ARG:HD3	1:D:335:ILE:HG22	1.85	0.59
1:A:362:MET:HE3	1:A:362:MET:CA	2.33	0.59
1:A:377:ARG:HB3	1:A:425:LEU:HD13	1.84	0.59
1:A:1033:LEU:HD23	1:A:1050:ILE:HG12	1.85	0.59
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.84	0.59
1:A:860:GLU:OE2	1:A:891:LYS:NZ	2.34	0.59
1:C:895:ARG:CG	1:C:895:ARG:NH1	2.49	0.58
1:B:380:THR:CG2	1:B:426:LEU:HD11	2.33	0.58
1:D:920:TYR:OH	1:D:938:LEU:O	2.21	0.58
1:B:898:ASN:ND2	1:B:906:LYS:HE3	2.17	0.58
1:C:434:ILE:HD12	1:C:435:SER:N	2.18	0.58
1:C:936:TYR:O	1:C:937:LYS:CG	2.39	0.58
1:C:886:ARG:HG2	1:C:889:GLU:OE1	2.03	0.58
1:A:506:ASN:OD1	4:A:1203:BTI:H92	2.03	0.58
1:C:175:LYS:H	1:C:175:LYS:HD2	1.65	0.58
1:C:267:VAL:HG22	1:C:480:PHE:HD2	1.68	0.58
1:D:679:SER:HA	1:D:907:VAL:HG23	1.84	0.58
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.60	0.58
1:C:517:GLU:O	1:C:519:ARG:N	2.36	0.58
1:C:866:MET:CE	1:C:871:TYR:HD1	2.14	0.58
1:A:181:LYS:HG2	1:A:185:GLU:OE2	2.03	0.58
1:B:864:HIS:HD2	1:B:866:MET:N	1.97	0.58
1:B:263:ARG:HD3	1:B:335:ILE:CG2	2.32	0.58
1:A:1029:ASN:HD22	1:A:1029:ASN:C	2.07	0.58
1:D:519:ARG:HB2	1:D:520:PRO:CD	2.34	0.58
1:A:590:ILE:H	1:A:590:ILE:HD12	1.68	0.58
1:B:279:PRO:HD2	1:B:372:TYR:CD2	2.37	0.58
1:A:142:HIS:H	1:A:145:HIS:HD2	1.51	0.58
1:D:249:VAL:HG22	1:D:308:GLY:O	2.03	0.58
1:A:641:MET:HE1	1:A:643:LEU:HD13	1.86	0.58
1:C:649:VAL:CG1	1:C:649:VAL:O	2.51	0.58
1:C:743:MET:CG	1:C:907:VAL:HG13	2.33	0.58
1:A:384:LEU:HG	1:A:490:ILE:CD1	2.33	0.58
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.68	0.58
1:A:622:ASN:C	1:A:622:ASN:HD22	2.06	0.58
1:A:194:LYS:HE2	2:A:1201:ADP:N7	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:H	1:C:196:THR:HG22	1.69	0.58
1:D:875:SER:OG	1:D:887:PHE:CE1	2.53	0.58
1:B:404:GLY:O	1:B:431:THR:HA	2.04	0.58
1:B:328:ARG:HD3	1:B:329:VAL:O	2.04	0.58
1:D:1034:ASP:OD1	1:D:1036:PRO:HD2	2.03	0.58
1:D:513:PRO:CD	4:D:1201:BTI:H4	2.34	0.58
1:C:434:ILE:HD12	1:C:435:SER:H	1.69	0.58
1:B:597:VAL:CG2	1:B:830:GLY:HA3	2.34	0.57
1:C:359:GLU:CD	1:C:359:GLU:H	2.07	0.57
1:B:124:ASN:C	1:B:124:ASN:OD1	2.42	0.57
1:B:588:ILE:HD13	1:B:630:LEU:HD23	1.86	0.57
1:A:572:ASP:HB3	1:A:807:GLN:HE22	1.68	0.57
1:A:622:ASN:HD21	1:A:624:TRP:HD1	1.49	0.57
1:D:243:LYS:HB3	1:D:243:LYS:NZ	2.06	0.57
1:C:1007:ILE:O	1:C:1011:VAL:HG23	2.03	0.57
1:C:846:SER:HA	1:C:849:GLU:HG2	1.84	0.57
1:A:180:ALA:O	1:A:183:PHE:N	2.31	0.57
1:C:936:TYR:HD1	1:C:966:VAL:HG12	1.69	0.57
1:B:338:MET:HE2	1:B:430:SER:CB	2.28	0.57
1:A:37:ILE:O	1:A:61:ILE:HG12	2.04	0.57
1:B:682:TRP:CE3	1:B:685:GLN:HG3	2.39	0.57
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.19	0.57
1:C:959:PHE:N	1:C:959:PHE:CD1	2.71	0.57
1:D:986:ASP:OD2	1:D:986:ASP:C	2.42	0.57
1:B:504:ILE:CG2	1:B:1042:MET:HG3	2.34	0.57
1:B:606:MET:C	1:B:606:MET:HE3	2.24	0.57
1:A:501:LEU:HB3	1:A:1078:TYR:CE1	2.40	0.57
1:D:542:LYS:C	1:D:542:LYS:HD3	2.25	0.57
1:A:192:MET:HE1	1:A:238:TYR:HE1	1.68	0.57
1:A:206:ILE:HD11	1:A:238:TYR:CZ	2.39	0.57
1:B:413:PHE:CD1	1:B:414:GLN:HB3	2.39	0.57
1:B:334:THR:HG22	1:B:406:ARG:NH2	2.18	0.57
1:B:860:GLU:HA	1:B:863:GLN:HE21	1.69	0.57
1:A:174:ILE:HD11	1:A:235:ILE:CG2	2.35	0.57
1:A:565:LEU:HD21	1:A:826:THR:HB	1.87	0.57
1:C:828:ILE:HD12	1:C:829:GLU:N	2.19	0.57
1:D:288:ARG:O	1:D:288:ARG:HG2	2.04	0.57
1:C:192:MET:HE1	5:C:1202:ATP:C4	2.40	0.57
1:D:622:ASN:C	1:D:622:ASN:ND2	2.58	0.57
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.69	0.57
1:C:357:LEU:HA	1:C:360:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLU:HG2	1:B:527:ALA:HB3	1.87	0.57
1:B:712:ASN:OD1	1:B:712:ASN:C	2.43	0.57
1:A:406:ARG:HH21	1:C:403:ALA:CB	2.17	0.56
1:A:180:ALA:O	1:A:184:ALA:N	2.33	0.56
1:C:961:LYS:O	1:C:964:GLN:N	2.38	0.56
1:A:103:ILE:HG21	1:A:134:GLU:HG3	1.87	0.56
1:A:206:ILE:HG22	1:A:207:VAL:N	2.19	0.56
1:B:332:GLU:N	1:B:332:GLU:OE1	2.37	0.56
1:D:362:MET:HE1	1:D:367:ILE:HD11	1.87	0.56
1:A:175:LYS:HZ2	1:A:232:GLU:HG3	1.68	0.56
1:B:272:GLN:HE21	1:B:274:VAL:HG22	1.71	0.56
1:B:59:LEU:O	1:B:60:ASP:HB2	2.06	0.56
1:A:446:SER:O	1:A:450:MET:HG2	2.06	0.56
1:D:260:LEU:HD22	1:D:342:ILE:HD13	1.88	0.56
1:B:525:GLU:HB3	1:B:840:THR:HG21	1.87	0.56
1:D:331:VAL:O	1:D:428:LYS:HE2	2.05	0.56
1:A:109:ALA:O	1:A:110:ASN:HB2	2.04	0.56
1:B:396:ALA:HB3	1:B:453:ARG:CB	2.35	0.56
1:C:986:ASP:OD1	1:C:989:LYS:HG3	2.06	0.56
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.54	0.56
1:B:403:ALA:C	1:B:442:LYS:HE2	2.23	0.56
1:D:799:ALA:H	1:D:811:ASN:ND2	2.03	0.56
1:C:641:MET:HE2	1:C:674:PHE:CE1	2.41	0.56
1:C:756:ILE:O	1:C:760:LYS:HB2	2.06	0.56
1:D:457:THR:OG1	1:D:459:ILE:HG13	2.05	0.56
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.88	0.56
1:D:330:GLN:O	1:D:333:HIS:ND1	2.30	0.56
1:A:631:ARG:NH2	1:A:672:ASP:OD1	2.39	0.56
1:A:98:ASN:C	1:A:98:ASN:ND2	2.56	0.55
1:A:382:ASP:O	1:A:387:PHE:N	2.38	0.55
1:A:396:ALA:HB3	1:A:453:ARG:HB2	1.88	0.55
1:B:504:ILE:HG21	1:B:1042:MET:HG3	1.87	0.55
1:C:200:GLY:C	1:C:202:LYS:N	2.59	0.55
1:B:414:GLN:HE22	1:D:1079:ALA:HB2	1.70	0.55
1:C:991:ARG:NH1	1:C:1002:VAL:O	2.31	0.55
1:D:252:ASP:O	1:D:305:VAL:HG22	2.05	0.55
1:D:866:MET:CE	1:D:871:TYR:HA	2.35	0.55
1:D:875:SER:OG	1:D:887:PHE:CZ	2.58	0.55
1:C:794:ILE:HD12	1:C:796:THR:CG2	2.36	0.55
1:C:679:SER:HB3	1:C:908:THR:O	2.06	0.55
1:B:379:THR:HG22	1:B:424:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:ASP:OD2	1:C:745:GLY:HA2	2.07	0.55
1:B:513:PRO:O	1:B:515:ASN:HB2	2.06	0.55
1:B:251:GLY:HA3	1:B:257:ILE:HG12	1.89	0.55
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.88	0.55
1:B:101:ARG:HG2	1:B:101:ARG:NH1	2.20	0.55
1:A:897:VAL:HG11	1:A:917:MET:HB3	1.88	0.55
1:A:641:MET:CE	1:A:643:LEU:HD13	2.37	0.55
1:C:396:ALA:CA	1:C:414:GLN:HE22	2.10	0.55
1:C:230:ASN:C	1:C:230:ASN:HD22	2.10	0.55
1:B:620:LYS:CG	4:B:1201:BTI:H63	2.37	0.55
1:C:960:ASN:O	1:C:963:LEU:HB3	2.06	0.55
1:D:752:ALA:HB2	1:D:782:THR:HG23	1.88	0.55
1:B:448:ARG:HH22	1:B:467:LYS:HD2	1.72	0.55
1:B:403:ALA:O	1:B:442:LYS:CE	2.35	0.55
1:C:494:LEU:HD22	1:C:494:LEU:H	1.71	0.55
1:D:263:ARG:HG2	1:D:335:ILE:HG21	1.88	0.55
1:B:577:LEU:HD13	1:B:842:ARG:HH22	1.71	0.55
1:A:1065:ILE:HG12	1:A:1076:ILE:HD13	1.89	0.55
1:D:263:ARG:HD3	1:D:335:ILE:HG21	1.86	0.55
1:C:142:HIS:H	1:C:145:HIS:HD2	1.54	0.55
1:B:771:HIS:HB2	1:B:795:ASP:OD2	2.07	0.55
1:B:924:ASN:HB2	1:B:926:LEU:HD21	1.88	0.55
1:C:313:LEU:HD22	1:C:323:ILE:HD12	1.88	0.54
1:A:991:ARG:HB2	1:A:1007:ILE:HD11	1.89	0.54
1:C:828:ILE:HD12	1:C:829:GLU:H	1.73	0.54
1:B:343:ASP:CG	1:B:346:LYS:HB2	2.28	0.54
1:B:1080:MET:O	1:B:1081:ASN:C	2.45	0.54
1:C:370:LEU:O	1:C:432:HIS:HE1	1.90	0.54
1:B:263:ARG:HG2	1:B:278:ALA:HB2	1.89	0.54
1:D:459:ILE:HB	1:D:460:PRO:HD3	1.88	0.54
1:C:867:PRO:HG3	1:C:906:LYS:O	2.08	0.54
1:B:334:THR:O	1:B:338:MET:HG3	2.07	0.54
1:A:194:LYS:HD2	1:A:234:TYR:OH	2.07	0.54
1:A:572:ASP:HB3	1:A:807:GLN:NE2	2.22	0.54
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.89	0.54
1:C:504:ILE:HD13	1:C:1042:MET:HE1	1.89	0.54
1:D:960:ASN:ND2	1:D:963:LEU:H	2.05	0.54
1:B:263:ARG:HD3	1:B:335:ILE:HG22	1.87	0.54
1:C:37:ILE:HG22	1:C:37:ILE:O	2.06	0.54
1:C:941:PRO:C	1:C:943:SER:H	2.11	0.54
1:A:216:ALA:C	1:A:218:HIS:N	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:LEU:HD13	1:D:362:MET:HG3	1.89	0.54
1:D:91:GLY:O	1:D:92:PRO:O	2.25	0.54
1:C:43:ALA:HA	1:C:66:ILE:HD11	1.89	0.54
1:C:539:SER:HA	1:C:543:GLN:HG3	1.89	0.54
1:A:334:THR:CG2	1:A:428:LYS:NZ	2.71	0.54
1:C:1042:MET:CE	1:C:1060:ILE:HG21	2.38	0.54
1:D:864:HIS:CD2	1:D:866:MET:HB2	2.43	0.54
1:C:770:LEU:HB3	1:C:794:ILE:HG22	1.89	0.54
1:D:262:GLU:OE2	1:D:262:GLU:N	2.33	0.54
1:B:144:GLU:O	1:B:148:MET:HB2	2.08	0.54
1:D:124:ASN:OD1	1:D:126:GLN:HB2	2.07	0.54
1:D:446:SER:O	1:D:450:MET:HG2	2.08	0.54
1:C:174:ILE:HG22	1:C:217:PHE:HE1	1.72	0.54
1:A:156:ARG:NH1	1:A:156:ARG:HB3	2.12	0.54
1:C:889:GLU:C	1:C:891:LYS:H	2.12	0.54
1:A:811:ASN:H	1:A:811:ASN:ND2	2.04	0.54
1:D:570:PHE:O	1:D:574:HIS:HE1	1.91	0.54
1:B:312:PHE:HA	1:B:321:PHE:O	2.08	0.54
1:B:252:ASP:OD1	1:B:256:ASN:HB2	2.08	0.54
1:A:186:GLU:O	1:A:187:ALA:HB2	2.08	0.54
1:D:717:ASN:HD22	1:D:717:ASN:N	2.06	0.54
1:A:501:LEU:HD11	1:A:1080:MET:HE2	1.90	0.53
1:A:266:SER:O	1:A:268:GLN:HG2	2.08	0.53
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.89	0.53
1:D:596:ASP:O	1:D:599:LYS:HG2	2.08	0.53
1:A:512:PHE:CZ	4:A:1203:BTI:H5	2.42	0.53
1:C:385:ASN:C	1:C:387:PHE:H	2.12	0.53
1:A:384:LEU:HD12	1:A:384:LEU:H	1.73	0.53
1:B:624:TRP:CZ2	1:B:1008:ILE:CD1	2.91	0.53
1:B:773:HIS:HA	1:B:806:SER:O	2.09	0.53
1:A:484:THR:HB	1:A:487:LEU:HD22	1.90	0.53
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.37	0.53
1:C:959:PHE:HD1	1:C:959:PHE:H	1.53	0.53
1:C:738:LEU:CD2	1:C:759:LEU:HD13	2.39	0.53
1:B:494:LEU:O	1:B:496:ARG:N	2.42	0.53
1:C:513:PRO:CB	1:C:513:PRO:C	2.74	0.53
1:C:224:ALA:HB3	1:C:231:SER:HB2	1.91	0.53
1:A:360:ILE:HG22	1:A:362:MET:H	1.73	0.53
1:D:661:LYS:HG2	1:D:1008:ILE:HD13	1.91	0.53
1:C:259:HIS:O	1:C:260:LEU:HD23	2.08	0.53
1:A:406:ARG:NH2	1:C:403:ALA:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:THR:OG1	1:A:861:ILE:HD13	2.07	0.53
1:C:145:HIS:HA	1:C:148:MET:HG2	1.91	0.53
1:A:701:GLU:HG3	1:A:737:ILE:HB	1.89	0.53
1:B:679:SER:O	1:B:905:VAL:HB	2.08	0.53
1:A:217:PHE:HE2	1:A:221:LYS:HE3	1.71	0.53
1:A:398:ARG:NH1	1:A:398:ARG:CG	2.59	0.53
1:D:145:HIS:HE1	1:D:302:ILE:O	1.92	0.53
1:B:89:ASP:OD1	1:B:90:LEU:HD12	2.09	0.53
1:C:551:LYS:O	1:C:555:GLU:HG2	2.08	0.53
1:A:874:LEU:HD11	1:A:919:LEU:CD2	2.39	0.53
1:A:413:PHE:HZ	1:A:416:ALA:HB2	1.61	0.53
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.73	0.53
1:C:192:MET:HB2	1:C:238:TYR:HB2	1.91	0.53
1:C:382:ASP:O	1:C:387:PHE:HA	2.08	0.53
1:B:924:ASN:HB2	1:B:926:LEU:CD2	2.39	0.53
1:B:495:ASP:O	1:B:496:ARG:C	2.47	0.53
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.73	0.53
1:B:945:VAL:HG12	1:B:967:ILE:CG2	2.32	0.53
1:A:194:LYS:HB3	1:A:234:TYR:CE2	2.44	0.53
1:B:840:THR:O	1:B:843:THR:HB	2.09	0.53
1:A:543:GLN:NE2	1:A:543:GLN:H	2.06	0.53
1:C:59:LEU:O	1:C:60:ASP:HB2	2.07	0.53
1:C:166:VAL:HG12	1:C:167:ILE:HD12	1.90	0.52
1:D:496:ARG:HH11	1:D:496:ARG:CB	2.12	0.52
1:D:513:PRO:O	1:D:515:ASN:CB	2.55	0.52
1:D:506:ASN:HD21	1:D:510:ASN:HD22	1.56	0.52
1:D:760:LYS:HG2	1:D:768:ILE:HD13	1.91	0.52
1:B:749:PRO:HG3	1:B:781:LEU:HB3	1.90	0.52
1:D:311:GLU:HG3	1:D:324:GLU:HG3	1.91	0.52
1:C:717:ASN:HD22	1:C:717(A):ILE:HG13	1.74	0.52
1:B:167:ILE:CG1	1:B:168:PRO:CD	2.87	0.52
1:D:519:ARG:HB2	1:D:520:PRO:HD2	1.91	0.52
1:D:451:ARG:HH11	1:D:451:ARG:CG	2.08	0.52
1:A:879:LYS:O	1:A:881:LEU:N	2.42	0.52
1:C:519:ARG:CG	1:C:520:PRO:O	2.57	0.52
1:D:284:SER:OG	1:D:287:LEU:HB2	2.09	0.52
1:A:625:GLU:O	1:A:629:ARG:HG3	2.09	0.52
1:A:849:GLU:O	1:A:852:SER:C	2.44	0.52
1:D:166:VAL:CG1	1:D:167:ILE:N	2.64	0.52
1:C:646:SER:O	1:C:653:ASN:HA	2.09	0.52
1:B:863:GLN:O	1:B:895:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:ALA:O	1:D:883:LEU:HB2	2.09	0.52
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.23	0.52
1:A:241:ASN:N	1:A:242:PRO:CD	2.72	0.52
1:D:571:ARG:HG2	1:D:611:THR:HG21	1.90	0.52
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.44	0.52
1:D:1043:ARG:O	1:D:1046:GLU:HB2	2.10	0.52
1:C:394:ILE:HD11	1:C:426:LEU:HD22	1.92	0.52
1:D:494:LEU:HG	1:D:499:LYS:CE	2.32	0.52
1:D:921:MET:HG2	1:D:926:LEU:HB3	1.91	0.52
1:D:594:THR:HG23	1:D:598:PHE:CD1	2.44	0.52
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.74	0.52
1:B:540:GLY:N	1:B:543:GLN:HE21	2.08	0.52
1:A:952:ILE:O	1:A:952:ILE:HG22	2.10	0.52
1:A:828:ILE:HD12	1:A:829:GLU:H	1.75	0.52
1:B:624:TRP:HZ2	1:B:1008:ILE:HD13	1.74	0.52
1:B:743:MET:SD	1:B:907:VAL:HG13	2.49	0.52
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.91	0.52
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.91	0.52
1:A:804:LEU:HD13	1:A:854:ILE:HG22	1.92	0.52
1:D:401:GLY:O	1:D:445:ARG:NH2	2.39	0.52
1:D:497:GLY:O	1:D:501:LEU:HG	2.10	0.52
1:B:644:ARG:HD2	1:B:647:ASN:OD1	2.09	0.52
1:C:1068:PRO:HD3	1:C:1074:ARG:CZ	2.40	0.52
1:A:655:PRO:HG2	1:A:985:VAL:HG23	1.92	0.52
1:A:114:ILE:HG13	1:A:136:ILE:HG21	1.92	0.52
1:A:622:ASN:ND2	1:A:623:PRO:HD2	2.24	0.52
1:C:641:MET:CE	1:C:674:PHE:CE1	2.93	0.52
1:D:593:LYS:O	1:D:597:VAL:HG23	2.09	0.52
1:A:47:GLU:OE1	1:A:428:LYS:HE3	2.10	0.52
1:B:927:ASP:OD2	1:B:930:SER:HB2	2.10	0.52
1:C:59:LEU:HD11	1:C:346:LYS:HG2	1.91	0.52
1:D:431:THR:OG1	1:D:443:MET:HB2	2.10	0.52
1:C:926:LEU:HD11	1:C:938:LEU:HD11	1.92	0.51
1:C:375:GLN:OE1	1:C:377:ARG:HD2	2.10	0.51
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.75	0.51
1:B:641:MET:HB3	1:B:671:ILE:HD12	1.92	0.51
1:A:192:MET:CE	1:A:238:TYR:HD1	2.22	0.51
1:D:1060:ILE:HG12	1:D:1080:MET:HG3	1.91	0.51
1:A:360:ILE:CG2	1:A:362:MET:HG2	2.40	0.51
1:D:313:LEU:O	1:D:320:PHE:HA	2.09	0.51
1:A:964:GLN:HG2	1:A:968:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.93	0.51
1:B:86:VAL:HG11	1:B:95:SER:O	2.10	0.51
1:A:331:VAL:HG12	1:A:428:LYS:HE2	1.92	0.51
1:D:513:PRO:HD2	4:D:1201:BTI:H4	1.91	0.51
1:D:263:ARG:CG	1:D:335:ILE:HG21	2.40	0.51
1:D:542:LYS:HE3	1:D:672:ASP:OD1	2.11	0.51
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.45	0.51
1:B:574:HIS:CD2	1:B:580:THR:HA	2.45	0.51
1:A:118:TYR:OH	1:A:331:VAL:HG13	2.10	0.51
1:D:495:ASP:HB3	1:D:498:THR:CB	2.37	0.51
1:D:832:GLU:O	1:D:836:HIS:CD2	2.64	0.51
1:D:605:GLU:HA	1:D:640:GLN:HB3	1.91	0.51
1:C:926:LEU:HD13	1:C:938:LEU:HD11	1.90	0.51
1:D:149:PHE:HZ	1:D:302:ILE:HD13	1.76	0.51
1:D:501:LEU:HD11	1:D:1080:MET:HE2	1.91	0.51
1:C:948:PHE:CD2	1:C:959:PHE:CD2	2.98	0.51
1:C:404:GLY:O	1:C:431:THR:HA	2.10	0.51
1:A:334:THR:CB	1:A:406:ARG:HH11	2.08	0.51
1:C:199:GLY:HA2	5:C:1202:ATP:O3B	2.10	0.51
1:D:811:ASN:N	1:D:811:ASN:ND2	2.56	0.51
1:A:524:TYR:HD2	1:A:843:THR:HG22	1.76	0.51
1:A:384:LEU:HG	1:A:490:ILE:HD11	1.92	0.51
1:A:521:LYS:NZ	1:A:1046:GLU:OE1	2.43	0.51
1:A:39:LYS:HE2	1:A:82:GLU:OE1	2.11	0.51
1:A:556:TRP:O	1:A:560:GLN:HG2	2.11	0.51
1:A:222:SER:O	1:A:226:LYS:HB2	2.10	0.51
1:C:1024:ARG:NH1	1:C:1024:ARG:CG	2.53	0.51
1:C:920:TYR:CE1	1:C:940:PHE:CD2	2.99	0.51
1:B:798:VAL:CG1	1:B:831:MET:CE	2.86	0.51
1:A:497:GLY:O	1:A:501:LEU:HG	2.11	0.51
1:D:418:ILE:HD12	1:D:418:ILE:N	2.23	0.51
1:D:449:GLU:O	1:D:450:MET:C	2.49	0.51
1:A:794:ILE:CD1	1:A:813:LEU:CD2	2.89	0.51
1:C:334:THR:CB	1:C:406:ARG:HH12	2.13	0.51
1:D:1056:LYS:O	1:D:1056:LYS:HG2	2.11	0.51
1:D:160:ILE:O	1:D:161:LYS:C	2.48	0.51
1:C:864:HIS:HD2	1:C:866:MET:H	1.57	0.51
1:C:921:MET:CA	1:C:926:LEU:HB2	2.40	0.51
1:B:395:ILE:N	1:B:453:ARG:O	2.34	0.51
1:C:989:LYS:O	1:C:993:LEU:HB2	2.10	0.51
1:C:173:PRO:C	1:C:174:ILE:HD12	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:SER:HA	1:B:478:THR:HG22	1.93	0.50
1:C:304:TYR:OH	1:C:307:ALA:O	2.16	0.50
1:B:917:MET:HG2	1:B:944:VAL:HG11	1.93	0.50
1:B:124:ASN:OD1	1:B:127:PHE:N	2.30	0.50
1:A:874:LEU:CD1	1:A:919:LEU:HD21	2.41	0.50
1:B:512:PHE:HB3	1:B:516:VAL:HB	1.92	0.50
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.93	0.50
1:C:334:THR:CB	1:C:406:ARG:HH11	2.09	0.50
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.40	0.50
1:A:775:THR:OG1	1:A:861:ILE:HD11	2.10	0.50
1:B:893:MET:HG2	1:B:921:MET:HB2	1.92	0.50
1:C:193:ILE:HG12	1:C:194:LYS:N	2.25	0.50
1:A:874:LEU:HD11	1:A:919:LEU:HD22	1.94	0.50
1:C:647:ASN:N	1:C:647:ASN:OD1	2.44	0.50
1:B:365:LYS:HB2	1:B:365:LYS:HZ3	1.75	0.50
1:B:811:ASN:H	1:B:811:ASN:HD22	1.59	0.50
1:C:376:CYS:SG	1:C:462:LEU:HD13	2.51	0.50
1:A:375:GLN:NE2	1:A:428:LYS:HZ3	2.10	0.50
1:D:679:SER:HA	1:D:907:VAL:CG2	2.42	0.50
1:D:740:ILE:HD13	1:D:740:ILE:N	2.27	0.50
1:C:1036:PRO:O	1:C:1040:PHE:HB2	2.10	0.50
1:C:1062:LEU:CD1	1:C:1078:TYR:CE2	2.92	0.50
1:B:165:PRO:O	1:B:166:VAL:HG13	2.11	0.50
1:D:425:LEU:HD12	1:D:425:LEU:C	2.31	0.50
1:B:571:ARG:HH21	1:B:605:GLU:CD	2.15	0.50
1:B:374:ILE:HG22	1:B:443:MET:CE	2.41	0.50
1:C:337:GLU:OE2	1:C:406:ARG:NH2	2.45	0.50
1:B:285:PRO:O	1:B:288:ARG:HG2	2.11	0.50
1:B:565:LEU:HD11	1:B:598:PHE:HE2	1.76	0.50
1:D:542:LYS:O	1:D:542:LYS:HD3	2.11	0.50
1:C:798:VAL:O	1:C:799:ALA:C	2.50	0.50
1:A:406:ARG:HH21	1:C:403:ALA:CA	2.24	0.50
1:B:332:GLU:HA	1:B:375:GLN:NE2	2.27	0.50
1:C:644:ARG:O	1:C:645:ALA:C	2.50	0.50
1:D:122:SER:HB2	1:D:328:ARG:HG2	1.94	0.50
1:A:799:ALA:H	1:A:811:ASN:ND2	2.08	0.50
1:B:647:ASN:HB3	1:B:652:LYS:O	2.12	0.50
1:D:62:SER:HA	1:D:81:ASP:OD1	2.12	0.50
1:C:1063:GLU:O	1:C:1064:THR:HG23	2.12	0.50
1:C:709:ASP:H	1:C:715:ARG:HG2	1.77	0.50
1:C:189:PHE:H	1:C:190:PRO:CD	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:861:ILE:HD11	1:C:866:MET:O	2.12	0.50
1:C:396:ALA:HA	1:C:414:GLN:NE2	2.13	0.50
1:A:866:MET:HG2	1:A:894:TYR:CE2	2.47	0.50
1:B:395:ILE:HD11	1:B:453:ARG:HG2	1.93	0.50
1:C:398:ARG:HG3	1:C:398:ARG:NH1	2.25	0.50
1:B:832:GLU:OE2	1:C:859:THR:OG1	2.28	0.50
1:B:385:ASN:CG	1:B:385:ASN:O	2.50	0.50
1:A:334:THR:OG1	1:A:375:GLN:NE2	2.44	0.49
1:D:746:LEU:HD11	1:D:865:GLU:HG2	1.93	0.49
1:B:294:ALA:O	1:B:297:GLN:HB3	2.11	0.49
1:C:1029:ASN:C	1:C:1029:ASN:HD22	2.14	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:C:219:ARG:O	1:C:223:GLU:HB2	2.13	0.49
1:A:42:VAL:HG23	1:A:53:PHE:HE2	1.77	0.49
1:D:167:ILE:HG23	1:D:321:PHE:CG	2.48	0.49
1:D:1053:ASP:HB2	1:D:1056:LYS:HD3	1.94	0.49
1:D:164:LEU:HG	1:D:165:PRO:HD2	1.95	0.49
1:C:386:ASP:O	1:C:387:PHE:HB2	2.11	0.49
1:C:891:LYS:HA	1:C:894:TYR:HB2	1.94	0.49
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.94	0.49
1:D:561:ASP:O	1:D:822:ARG:HD2	2.12	0.49
1:A:375:GLN:NE2	1:A:428:LYS:NZ	2.61	0.49
1:A:229:GLY:O	1:A:230:ASN:HB2	2.12	0.49
1:B:103:ILE:HG21	1:B:134:GLU:HG3	1.95	0.49
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.46	0.49
1:D:90:LEU:HB2	1:D:95:SER:OG	2.13	0.49
1:A:206:ILE:CD1	1:A:238:TYR:CE1	2.96	0.49
1:C:887:PHE:HA	1:C:890:VAL:HG23	1.95	0.49
1:B:867:PRO:O	1:B:868:GLY:C	2.51	0.49
1:C:399:SER:HB3	1:C:400:SER:H	1.47	0.49
1:B:1066:SER:HB2	1:D:1064:THR:CG2	2.39	0.49
1:A:375:GLN:HE22	1:A:428:LYS:NZ	2.11	0.49
1:A:454:GLY:O	1:A:455:VAL:HG22	2.12	0.49
1:A:69:ASN:HD22	1:A:72:LYS:HE3	1.77	0.49
1:A:239:ILE:O	1:A:239:ILE:HG13	2.13	0.49
1:B:581:ARG:HG3	1:B:848:PHE:CD2	2.48	0.49
1:B:991:ARG:NH1	1:B:1002:VAL:HG12	2.28	0.49
1:C:69:ASN:HD21	1:C:88:SER:HA	1.77	0.49
1:A:184:ALA:HA	1:A:191:LEU:HD11	1.94	0.49
1:A:69:ASN:ND2	1:A:72:LYS:HE3	2.27	0.49
1:C:680:LEU:HD11	1:C:952:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:LYS:HB2	1:B:951:GLU:HG3	1.94	0.49
1:C:687:LYS:O	1:C:691:GLU:HG3	2.13	0.49
1:A:334:THR:HG23	1:A:428:LYS:HZ1	1.78	0.48
1:B:999:GLN:NE2	1:B:1001:PRO:HG3	2.28	0.48
1:A:627:LEU:O	1:A:631:ARG:HB2	2.13	0.48
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.46	0.48
1:C:944:VAL:HG13	1:C:945:VAL:HG13	1.95	0.48
1:D:403:ALA:O	1:D:442:LYS:HD3	2.13	0.48
1:D:581:ARG:HG3	1:D:848:PHE:CG	2.47	0.48
1:C:968:LEU:O	1:C:969:LYS:C	2.51	0.48
1:C:704:ILE:HB	1:C:740:ILE:HD13	1.95	0.48
1:A:43:ALA:HA	1:A:66:ILE:HD11	1.95	0.48
1:C:1060:ILE:HG12	1:C:1080:MET:HG3	1.95	0.48
1:C:174:ILE:HG22	1:C:217:PHE:CE1	2.48	0.48
1:C:494:LEU:HB2	1:C:496:ARG:HH12	1.76	0.48
1:D:286:THR:O	1:D:290:ARG:HG3	2.14	0.48
1:B:948:PHE:HA	1:B:959:PHE:CE2	2.48	0.48
1:D:700:SER:H	1:D:736:HIS:HD2	1.62	0.48
1:B:300:GLU:HG2	1:B:300:GLU:O	2.12	0.48
1:C:895:ARG:HG2	1:C:895:ARG:NH1	2.25	0.48
1:C:948:PHE:CD2	1:C:959:PHE:HD2	2.31	0.48
1:B:103:ILE:O	1:B:107:LYS:HG3	2.14	0.48
1:D:413:PHE:O	1:D:415:GLY:N	2.46	0.48
1:B:542:LYS:HE3	1:B:631:ARG:NH2	2.28	0.48
1:B:542:LYS:HE2	1:B:672:ASP:OD2	2.14	0.48
1:D:338:MET:HE2	1:D:430:SER:CB	2.44	0.48
1:A:799:ALA:H	1:A:811:ASN:HD21	1.60	0.48
1:C:284:SER:OG	1:C:287:LEU:HB2	2.13	0.48
1:B:690:ASN:ND2	1:B:700:SER:OG	2.47	0.48
1:D:38:LYS:CE	1:D:38:LYS:HA	2.34	0.48
1:A:170:THR:HG22	1:A:172:GLY:O	2.13	0.48
1:B:711:LEU:HD11	1:B:750:LYS:HB3	1.95	0.48
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.96	0.48
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.94	0.48
1:A:332:GLU:HG2	1:A:332:GLU:O	2.13	0.48
1:D:38:LYS:HE2	1:D:38:LYS:CA	2.33	0.48
1:A:196:THR:HG22	1:A:232:GLU:O	2.14	0.48
1:C:1075:THR:HG22	1:C:1077:TYR:CE1	2.49	0.48
1:C:866:MET:HE2	1:C:871:TYR:CD1	2.28	0.48
1:C:378:ILE:HG13	1:C:450:MET:HE3	1.96	0.48
1:B:268:GLN:HA	1:B:274:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:ARG:NH2	1:D:908:THR:HB	2.29	0.48
1:C:259:HIS:C	1:C:260:LEU:HD23	2.34	0.48
1:C:253:GLU:HG2	1:C:305:VAL:HG11	1.95	0.48
1:C:883:LEU:HD11	1:C:923:GLN:HG2	1.96	0.48
1:C:281:VAL:HG12	1:C:282:GLY:N	2.29	0.48
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.96	0.48
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.12	0.48
1:C:811:ASN:ND2	1:C:811:ASN:N	2.51	0.48
1:C:1062:LEU:HD12	1:C:1078:TYR:CD2	2.48	0.48
1:D:431:THR:HG21	1:D:443:MET:HA	1.94	0.48
1:D:804:LEU:HD13	1:D:854:ILE:HG22	1.96	0.48
1:D:814:TYR:C	1:D:814:TYR:CD2	2.87	0.48
1:D:504:ILE:HD13	1:D:1042:MET:HE1	1.95	0.47
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.95	0.47
1:D:582:VAL:HA	1:D:845:TYR:CE2	2.49	0.47
1:D:309:THR:HB	1:D:326:ASN:HD22	1.79	0.47
1:C:931:VAL:HG13	1:C:931:VAL:O	2.14	0.47
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.47	0.47
1:C:332:GLU:HA	1:C:375:GLN:NE2	2.29	0.47
1:B:927:ASP:HB2	1:B:930:SER:H	1.79	0.47
1:B:99:ILE:HD12	1:B:99:ILE:N	2.28	0.47
1:A:384:LEU:N	1:A:384:LEU:HD12	2.29	0.47
1:D:679:SER:OG	1:D:909:PRO:HD2	2.14	0.47
1:C:649:VAL:HG13	1:C:649:VAL:O	2.14	0.47
1:C:667:ALA:HB1	1:C:698:LYS:HE3	1.94	0.47
1:A:964:GLN:HG2	1:A:968:LEU:CD1	2.44	0.47
1:A:42:VAL:CG2	1:A:53:PHE:CE2	2.97	0.47
1:B:960:ASN:HD22	1:B:963:LEU:HB3	1.79	0.47
1:B:309:THR:HB	1:B:326:ASN:HB2	1.96	0.47
1:C:390:ASP:OD1	1:C:456:LYS:HG2	2.14	0.47
1:C:334:THR:O	1:C:338:MET:HG3	2.15	0.47
1:A:403:ALA:CA	1:C:406:ARG:HH21	2.27	0.47
1:A:175:LYS:HZ1	1:A:232:GLU:HG3	1.78	0.47
1:A:241:ASN:H	1:A:242:PRO:HD3	1.79	0.47
1:D:244:HIS:N	1:D:266:SER:OG	2.46	0.47
1:A:178:GLU:HG2	1:A:181:LYS:HB2	1.96	0.47
1:C:224:ALA:O	1:C:228:PHE:HD1	1.98	0.47
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.63	0.47
1:D:152:LYS:HG2	1:D:152:LYS:O	2.15	0.47
1:A:178:GLU:HG2	1:A:178:GLU:O	2.14	0.47
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:ILE:HD13	1:D:791:VAL:HG23	1.97	0.47
1:C:149:PHE:O	1:C:151:ASP:N	2.42	0.47
1:B:799:ALA:H	1:B:811:ASN:ND2	2.13	0.47
1:A:1042:MET:HE1	1:A:1048:VAL:CG1	2.42	0.47
1:A:242:PRO:HD2	1:A:478:THR:OG1	2.14	0.47
1:A:516:VAL:O	1:A:517:GLU:C	2.51	0.47
1:D:756:ILE:HD11	1:D:770:LEU:HD22	1.97	0.47
1:D:1087:ILE:HG22	1:D:1089:ILE:CD1	2.43	0.47
1:A:70:GLU:CG	1:A:92:PRO:HB3	2.44	0.47
1:A:383:PRO:HA	1:A:387:PHE:CE2	2.49	0.47
1:B:641:MET:HE2	1:B:671:ILE:HG13	1.97	0.47
1:B:1087:ILE:HG22	1:B:1089:ILE:HD13	1.95	0.47
1:D:1069:ASP:OD1	1:D:1073:ASN:HB2	2.14	0.47
1:C:515:ASN:H	1:C:515:ASN:CA	2.06	0.47
1:C:926:LEU:HD13	1:C:938:LEU:CD1	2.44	0.47
1:C:701:GLU:HG2	1:C:739:ALA:HB2	1.97	0.47
1:B:167:ILE:HG12	1:B:168:PRO:CD	2.45	0.47
1:C:948:PHE:CE2	1:C:959:PHE:HD2	2.32	0.47
1:B:624:TRP:O	1:B:627:LEU:HB3	2.15	0.47
1:C:744:ALA:HB3	1:C:746:LEU:HG	1.97	0.47
1:B:104:ASP:O	1:B:105:VAL:C	2.53	0.47
1:A:1091:ASP:OD2	1:A:1093:ASN:HA	2.15	0.47
1:D:137:LYS:HD2	1:D:352:ALA:HB1	1.97	0.47
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.33	0.47
1:B:864:HIS:CD2	1:B:866:MET:HB2	2.50	0.47
1:C:652:LYS:HD3	1:C:653:ASN:O	2.15	0.47
1:C:41:LEU:HD23	1:C:41:LEU:C	2.34	0.47
1:C:357:LEU:O	1:C:362:MET:CB	2.62	0.47
1:B:565:LEU:HD21	1:B:826:THR:HB	1.96	0.47
1:D:908:THR:HA	1:D:909:PRO:HA	1.57	0.47
1:A:846:SER:HA	1:A:849:GLU:HG2	1.96	0.47
1:A:334:THR:CG2	1:A:428:LYS:HZ1	2.27	0.47
1:B:977:ARG:CZ	1:B:980:GLU:HG3	2.44	0.47
1:B:715:ARG:HD2	1:B:715:ARG:O	2.15	0.47
1:C:1085:ARG:NH1	1:C:1085:ARG:CG	2.44	0.47
1:B:620:LYS:NZ	4:B:1201:BTI:HN3	2.13	0.47
1:B:624:TRP:HZ2	1:B:1008:ILE:CD1	2.28	0.47
1:C:1065:ILE:HG12	1:C:1076:ILE:HG23	1.96	0.47
1:C:542:LYS:HD3	1:C:542:LYS:C	2.35	0.47
1:D:379:THR:O	1:D:457:THR:HB	2.14	0.46
1:D:532:VAL:HG21	1:D:596:ASP:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:PHE:CD2	1:B:964:GLN:HA	2.50	0.46
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.96	0.46
1:A:606:MET:CE	1:A:639:PHE:HB3	2.45	0.46
1:C:177:TYR:OH	1:C:181:LYS:HE3	2.15	0.46
1:C:936:TYR:HD1	1:C:966:VAL:CG1	2.28	0.46
1:D:1085:ARG:HG3	1:D:1085:ARG:HH11	1.79	0.46
1:A:674:PHE:N	1:A:674:PHE:CD2	2.83	0.46
1:D:323:ILE:HG22	1:D:324:GLU:HG2	1.97	0.46
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.46
1:B:596:ASP:O	1:B:599:LYS:HG2	2.15	0.46
1:D:927:ASP:HB3	1:D:930:SER:H	1.78	0.46
1:D:1054:LYS:HB3	1:D:1054:LYS:HE2	1.41	0.46
1:C:893:MET:HA	1:C:896:ARG:HD2	1.86	0.46
1:D:258:VAL:HG21	1:D:362:MET:CE	2.45	0.46
1:A:866:MET:HE1	1:A:871:TYR:HA	1.97	0.46
1:A:550:PRO:HB2	1:A:736:HIS:CE1	2.49	0.46
1:A:1078:TYR:HB2	1:A:1085:ARG:HB3	1.97	0.46
1:B:744:ALA:CB	1:B:746:LEU:HG	2.44	0.46
1:A:572:ASP:OD1	1:A:771:HIS:CE1	2.68	0.46
1:B:525:GLU:HG3	1:B:527:ALA:H	1.80	0.46
1:C:631:ARG:HG2	1:C:670:GLY:HA3	1.97	0.46
1:C:241:ASN:N	1:C:242:PRO:CD	2.77	0.46
1:B:459:ILE:HB	1:B:460:PRO:HD3	1.97	0.46
1:A:778:ASN:O	1:A:779:GLY:C	2.52	0.46
1:C:885:GLU:C	1:C:887:PHE:H	2.18	0.46
1:A:620:LYS:HD2	1:A:620:LYS:HA	1.53	0.46
1:A:729:GLU:O	1:A:733:GLU:HG2	2.15	0.46
1:A:551:LYS:HD3	1:A:551:LYS:HA	1.55	0.46
1:C:711:LEU:HD11	1:C:750:LYS:HB3	1.98	0.46
1:A:398:ARG:HG3	1:A:398:ARG:HH11	1.77	0.46
1:D:260:LEU:O	1:D:261:PHE:HB2	2.15	0.46
1:D:864:HIS:CD2	1:D:866:MET:H	2.25	0.46
1:D:527:ALA:HB2	1:D:840:THR:HG21	1.97	0.46
1:B:1052:ILE:O	1:B:1053:ASP:HB2	2.15	0.46
1:A:880:SER:O	1:A:881:LEU:HD23	2.16	0.46
1:A:42:VAL:HG23	1:A:53:PHE:CE2	2.51	0.46
1:B:572:ASP:HB3	1:B:807:GLN:NE2	2.31	0.46
1:A:622:ASN:HD22	1:A:623:PRO:N	2.13	0.46
1:C:570:PHE:O	1:C:574:HIS:HE1	1.98	0.46
1:B:620:LYS:HE2	1:B:1023:THR:OG1	2.16	0.46
1:C:1033:LEU:HD23	1:C:1050:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:H	1:A:145:HIS:CD2	2.31	0.46
1:A:641:MET:HE2	1:A:674:PHE:CE1	2.51	0.46
1:C:717:ASN:ND2	1:C:717(A):ILE:HG13	2.31	0.46
1:A:214:GLU:O	1:A:218:HIS:CD2	2.68	0.46
1:D:248:GLN:HG2	1:D:260:LEU:HD12	1.98	0.46
1:D:1044:ASN:ND2	1:D:1064:THR:HA	2.30	0.46
1:D:335:ILE:HG22	1:D:336:THR:H	1.79	0.46
1:C:606:MET:HE1	1:C:639:PHE:HB3	1.98	0.46
1:B:743:MET:HA	1:B:773:HIS:CD2	2.51	0.46
1:C:631:ARG:HD3	1:C:631:ARG:HA	1.53	0.46
1:A:772:THR:HG22	1:A:783:TYR:CE2	2.51	0.46
1:C:940:PHE:CB	1:C:941:PRO:CD	2.82	0.46
1:C:377:ARG:HD3	1:C:377:ARG:N	2.30	0.46
1:D:811:ASN:N	1:D:811:ASN:HD22	2.00	0.46
1:C:641:MET:HE3	1:C:674:PHE:CD1	2.50	0.46
1:C:382:ASP:OD1	1:C:384:LEU:HB2	2.15	0.46
1:A:879:LYS:C	1:A:881:LEU:N	2.68	0.46
1:C:347:THR:HG23	1:C:360:ILE:HD13	1.97	0.46
1:D:878:ALA:O	1:D:884:GLY:N	2.49	0.46
1:D:927:ASP:O	1:D:931:VAL:HG12	2.16	0.46
1:B:1001:PRO:HG2	1:B:1002:VAL:H	1.81	0.46
1:C:810:ALA:HB1	1:C:831:MET:CE	2.46	0.46
1:B:547:GLU:HB2	1:B:548:VAL:HG13	1.96	0.46
1:B:263:ARG:NH1	1:B:336:THR:OG1	2.49	0.46
1:A:277:VAL:C	1:A:335:ILE:HD11	2.36	0.46
1:A:555:GLU:OE2	1:A:555:GLU:HA	2.15	0.46
1:D:772:THR:HG22	1:D:783:TYR:CE2	2.51	0.46
1:C:526:LEU:HA	1:C:526:LEU:HD23	1.74	0.46
1:B:103:ILE:O	1:B:106:ALA:HB3	2.16	0.46
1:C:619:LEU:O	1:C:620:LYS:HB2	2.16	0.46
1:B:387:PHE:HE2	1:B:488:PHE:HE2	1.64	0.46
1:D:40:LEU:C	1:D:40:LEU:HD23	2.36	0.46
1:B:417:GLU:H	1:B:417:GLU:HG2	1.55	0.46
1:C:332:GLU:HA	1:C:375:GLN:HE22	1.81	0.45
1:A:1089:ILE:HG22	1:A:1089:ILE:O	2.15	0.45
1:A:377:ARG:HB3	1:A:425:LEU:CD1	2.45	0.45
1:C:813:LEU:O	1:C:814:TYR:C	2.53	0.45
1:B:748:LYS:HB3	1:B:749:PRO:HD2	1.98	0.45
1:C:704:ILE:HG21	1:C:723:TYR:HD2	1.81	0.45
1:D:900:LEU:HD13	1:D:928:GLU:HG3	1.97	0.45
1:C:1018:GLU:OE1	1:C:1018:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TYR:CE1	1:A:236:GLU:HG3	2.51	0.45
1:A:382:ASP:OD2	1:A:385:ASN:HB2	2.16	0.45
1:A:386:ASP:O	1:A:387:PHE:HB2	2.16	0.45
1:B:565:LEU:HD12	1:B:565:LEU:C	2.36	0.45
1:B:374:ILE:HG22	1:B:443:MET:HE3	1.98	0.45
1:C:798:VAL:CG1	1:C:835:SER:HA	2.46	0.45
1:A:418:ILE:HD12	1:A:418:ILE:N	2.31	0.45
1:D:512:PHE:CD2	1:D:512:PHE:C	2.90	0.45
1:D:917:MET:O	1:D:921:MET:HB2	2.16	0.45
1:A:524:TYR:HD2	1:A:843:THR:CG2	2.29	0.45
1:C:234:TYR:C	1:C:235:ILE:HG22	2.37	0.45
1:A:395:ILE:O	1:A:396:ALA:HB2	2.16	0.45
1:B:729:GLU:HG2	1:B:732:ARG:NH2	2.31	0.45
1:A:207:VAL:HG11	1:A:213:LEU:HD23	1.97	0.45
1:C:192:MET:HE3	1:C:192:MET:HB3	1.87	0.45
1:A:193:ILE:HG13	1:A:194:LYS:N	2.32	0.45
1:C:385:ASN:C	1:C:387:PHE:N	2.69	0.45
1:D:938:LEU:O	1:D:939:ASP:CB	2.63	0.45
1:C:1049:GLU:HG2	1:C:1059:ILE:HD13	1.98	0.45
1:A:920:TYR:OH	1:A:938:LEU:HB3	2.16	0.45
1:D:529:ILE:HD13	1:D:589:ASN:HB3	1.99	0.45
1:B:259:HIS:CD2	1:B:296:ILE:CD1	2.76	0.45
1:A:869:GLY:O	1:A:871:TYR:N	2.49	0.45
1:D:337:GLU:CG	1:D:342:ILE:O	2.60	0.45
1:B:689:ALA:O	1:B:693:VAL:HG23	2.16	0.45
1:D:305:VAL:O	1:D:306:ASN:CB	2.65	0.45
1:B:539:SER:CA	1:B:543:GLN:HE21	2.22	0.45
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.82	0.45
1:A:167:ILE:CD1	1:A:323:ILE:CD1	2.94	0.45
1:A:278:ALA:N	1:A:335:ILE:HD11	2.32	0.45
1:A:370:LEU:O	1:A:432:HIS:CE1	2.67	0.45
1:D:459:ILE:N	1:D:460:PRO:HD2	2.32	0.45
1:D:574:HIS:HD2	1:D:580:THR:HA	1.81	0.45
1:A:874:LEU:HD12	1:A:919:LEU:HD21	1.98	0.45
1:C:1049:GLU:HG2	1:C:1059:ILE:CD1	2.46	0.45
1:D:796:THR:HB	1:D:810:ALA:HB2	1.98	0.45
1:A:179:LEU:HD11	1:A:217:PHE:CE1	2.51	0.45
1:B:347:THR:O	1:B:348:GLN:C	2.52	0.45
1:B:302:ILE:O	1:B:303:LYS:HB2	2.17	0.45
1:D:262:GLU:OE1	1:D:288:ARG:NH1	2.50	0.45
1:B:715:ARG:HD2	1:B:715:ARG:C	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:THR:HG22	1:C:311:GLU:HG2	1.98	0.45
1:D:583:ARG:HG2	1:D:619:LEU:HD22	1.98	0.45
1:C:580:THR:HB	1:C:614:VAL:HG21	1.98	0.45
1:A:873:ASN:O	1:A:875:SER:N	2.49	0.45
1:A:192:MET:CE	1:A:238:TYR:CE1	3.00	0.45
1:D:871:TYR:CE1	1:D:891:LYS:HD3	2.52	0.45
1:B:631:ARG:HG2	1:B:670:GLY:HA3	1.99	0.45
1:C:267:VAL:HG22	1:C:480:PHE:CD2	2.51	0.45
1:A:174:ILE:HD11	1:A:235:ILE:HG22	1.99	0.45
1:C:738:LEU:HD21	1:C:759:LEU:HD13	1.98	0.45
1:C:129:ARG:HG3	1:C:143:LEU:CD1	2.46	0.45
1:A:459:ILE:O	1:A:460:PRO:C	2.54	0.45
1:C:443:MET:HG2	1:C:466:MET:SD	2.57	0.45
1:C:513:PRO:CA	1:C:513:PRO:O	2.53	0.45
1:C:437:LYS:CD	1:C:437:LYS:H	2.22	0.45
1:A:606:MET:CE	1:A:639:PHE:CD2	3.00	0.45
1:B:932:ILE:HG13	1:B:933:THR:N	2.32	0.45
1:A:431:THR:HG21	1:A:443:MET:HA	1.99	0.45
1:C:690:ASN:O	1:C:694:GLN:HG2	2.17	0.45
1:B:398:ARG:HD3	1:B:1083:GLN:HE21	1.82	0.45
1:C:440:GLU:HG3	1:C:472:THR:HG22	1.99	0.45
1:C:897:VAL:O	1:C:898:ASN:C	2.55	0.45
1:C:173:PRO:O	1:C:174:ILE:CD1	2.64	0.45
1:A:177:TYR:O	1:A:179:LEU:N	2.50	0.45
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.73	0.45
1:C:221:LYS:HG3	1:C:233:VAL:HG13	1.99	0.45
1:A:512:PHE:C	1:A:512:PHE:CD2	2.90	0.45
1:B:511:GLY:O	4:B:1201:BTI:H102	2.17	0.45
1:D:907:VAL:O	1:D:910:SER:N	2.49	0.45
1:B:251:GLY:HA2	1:B:257:ILE:HA	1.99	0.45
1:B:748:LYS:O	1:B:749:PRO:C	2.55	0.45
1:D:479:LYS:O	1:D:480:PHE:C	2.55	0.45
1:C:673:VAL:HG22	1:C:699:ILE:HB	1.98	0.45
1:C:99:ILE:HG23	1:C:127:PHE:HD1	1.82	0.45
1:A:245:ILE:HG13	1:A:283:LEU:HD11	1.99	0.45
1:D:898:ASN:ND2	1:D:904:ILE:H	2.15	0.45
1:A:179:LEU:HA	1:A:182:GLU:CD	2.37	0.44
1:D:259:HIS:N	1:D:364:GLN:HE22	2.05	0.44
1:D:167:ILE:HG23	1:D:321:PHE:CB	2.47	0.44
1:B:267:VAL:HG12	1:B:481:ILE:HD11	1.99	0.44
1:A:879:LYS:HB2	1:A:879:LYS:HE2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:PHE:O	1:C:666:SER:OG	2.29	0.44
1:C:162:ALA:HB2	1:C:301:ASN:HD22	1.82	0.44
1:A:508:THR:O	1:A:508:THR:HG22	2.17	0.44
1:A:156:ARG:HD2	1:A:166:VAL:HG11	1.99	0.44
1:D:325:VAL:O	1:D:327:PRO:HD3	2.18	0.44
1:D:944:VAL:O	1:D:945:VAL:C	2.54	0.44
1:B:571:ARG:HD2	1:B:571:ARG:C	2.38	0.44
1:A:338:MET:HE1	1:A:430:SER:CB	2.44	0.44
1:D:787:ILE:HD13	1:D:817:LEU:HD11	1.99	0.44
1:B:574:HIS:HD2	1:B:580:THR:HA	1.81	0.44
1:B:784:LYS:HE2	1:C:785:GLN:HE21	1.82	0.44
1:A:712:ASN:HA	1:A:713:PRO:HD3	1.83	0.44
1:D:134:GLU:HB2	1:D:136:ILE:HD12	1.99	0.44
1:C:892:ASP:O	1:C:896:ARG:CD	2.62	0.44
1:A:622:ASN:HD22	1:A:624:TRP:H	1.60	0.44
1:D:917:MET:CE	1:D:940:PHE:HD2	2.31	0.44
1:D:650:GLY:HA3	1:D:654:TYR:CE1	2.53	0.44
1:B:144:GLU:H	1:B:144:GLU:HG3	1.53	0.44
1:B:709:ASP:OD1	1:B:748:LYS:NZ	2.50	0.44
1:A:955:PRO:O	1:A:956:VAL:C	2.56	0.44
1:C:1029:ASN:C	1:C:1029:ASN:ND2	2.70	0.44
1:A:174:ILE:HD11	1:A:235:ILE:HG21	1.97	0.44
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.98	0.44
1:B:631:ARG:HA	1:B:631:ARG:HD3	1.50	0.44
1:B:167:ILE:HG12	1:B:168:PRO:HD2	1.99	0.44
1:C:191:LEU:HD13	1:C:235:ILE:HD11	2.00	0.44
1:C:717:ASN:C	1:C:717:ASN:HD22	2.20	0.44
1:A:873:ASN:C	1:A:875:SER:H	2.21	0.44
1:C:294:ALA:O	1:C:297:GLN:HB3	2.17	0.44
1:A:413:PHE:O	1:A:414:GLN:C	2.56	0.44
1:A:641:MET:HE3	1:A:674:PHE:CD1	2.53	0.44
1:C:960:ASN:O	1:C:961:LYS:C	2.56	0.44
1:A:99:ILE:O	1:A:103:ILE:HG12	2.17	0.44
1:A:1046:GLU:O	1:A:1061:LYS:HA	2.18	0.44
1:A:246:GLU:HB2	1:A:309:THR:CG2	2.48	0.44
1:B:603:SER:HA	1:B:637:VAL:HG12	1.99	0.44
1:B:792:ASP:N	1:B:792:ASP:OD2	2.51	0.44
1:C:188:GLY:HA3	1:C:237:ARG:NH2	2.28	0.44
1:C:964:GLN:NE2	1:C:973:ALA:HB2	2.32	0.44
1:A:275:VAL:HG22	1:A:376:CYS:HB3	1.98	0.44
1:D:717:ASN:HD22	1:D:717:ASN:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HD3	1:C:83:SER:OG	2.18	0.44
1:B:1077:TYR:OH	1:D:1063:GLU:HB3	2.17	0.44
1:D:828:ILE:HD12	1:D:829:GLU:N	2.33	0.44
1:B:682:TRP:HE3	1:B:685:GLN:HG3	1.81	0.44
1:B:912:LYS:NZ	1:B:916:ASP:OD1	2.48	0.44
1:C:1090:LYS:HB3	1:C:1090:LYS:HE3	1.56	0.44
1:C:775:THR:HG21	1:C:861:ILE:HG13	2.00	0.44
1:A:866:MET:CE	1:A:871:TYR:HA	2.47	0.44
1:B:277:VAL:HA	1:B:335:ILE:HD11	1.99	0.44
1:D:701:GLU:HG2	1:D:737:ILE:HB	2.00	0.44
1:A:886:ARG:O	1:A:889:GLU:N	2.45	0.44
1:B:429:LEU:HD22	1:B:450:MET:CE	2.48	0.44
1:B:556:TRP:O	1:B:557:VAL:C	2.56	0.44
1:B:361:ASN:HA	1:B:361:ASN:HD22	1.50	0.44
1:D:302:ILE:H	1:D:302:ILE:HG13	1.70	0.43
1:D:263:ARG:HG2	1:D:335:ILE:CG2	2.48	0.43
1:B:99:ILE:H	1:B:99:ILE:CD1	2.29	0.43
1:D:283:LEU:C	1:D:283:LEU:HD23	2.39	0.43
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.53	0.43
1:C:993:LEU:O	1:C:997:GLU:HG2	2.18	0.43
1:D:898:ASN:HD21	1:D:904:ILE:H	1.66	0.43
1:B:645:ALA:HB1	1:B:686:MET:HA	2.00	0.43
1:A:177:TYR:C	1:A:179:LEU:N	2.69	0.43
1:C:493:SER:HA	1:C:494:LEU:HD13	1.99	0.43
1:B:165:PRO:HB2	1:B:321:PHE:HD2	1.83	0.43
1:A:306:ASN:OD1	1:A:348:GLN:HG2	2.18	0.43
1:B:738:LEU:O	1:B:768:ILE:HA	2.19	0.43
1:B:375:GLN:HG3	1:B:430:SER:OG	2.18	0.43
1:C:225:GLU:HB3	1:C:231:SER:HB3	1.99	0.43
1:A:720:LEU:CD2	1:A:758:GLU:HG3	2.42	0.43
1:D:338:MET:HE1	1:D:430:SER:HB3	1.98	0.43
1:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.43
1:C:115:HIS:ND1	1:C:116:PRO:HD2	2.33	0.43
1:D:50:ILE:HD11	1:D:75:LEU:HB3	1.99	0.43
1:D:487:LEU:HD12	1:D:487:LEU:HA	1.82	0.43
1:C:565:LEU:HD12	1:C:824:LEU:HD21	2.00	0.43
1:A:225:GLU:HA	1:A:225:GLU:OE1	2.17	0.43
1:A:622:ASN:C	1:A:622:ASN:ND2	2.70	0.43
1:A:322:PHE:O	1:A:323:ILE:HD13	2.18	0.43
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.62	0.43
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLU:N	1:D:70:GLU:CD	2.69	0.43
1:A:858:ASN:ND2	1:A:860:GLU:H	2.17	0.43
1:A:1065:ILE:HG22	1:A:1074:ARG:HD3	2.00	0.43
1:D:61:ILE:HG22	1:D:62:SER:O	2.19	0.43
1:C:241:ASN:N	1:C:242:PRO:HD3	2.33	0.43
1:B:551:LYS:O	1:B:555:GLU:HG2	2.19	0.43
1:A:856:SER:OG	1:D:800:SER:HA	2.19	0.43
1:B:1042:MET:HE2	1:B:1078:TYR:HE2	1.84	0.43
1:D:494:LEU:CD2	1:D:496:ARG:HA	2.49	0.43
1:B:949:LYS:HE2	1:B:951:GLU:OE1	2.18	0.43
1:C:118:TYR:HA	1:C:122:SER:OG	2.19	0.43
1:B:1063:GLU:OE1	1:D:1086:ARG:NH1	2.51	0.43
1:A:561:ASP:O	1:A:822:ARG:HD2	2.19	0.43
1:C:937:LYS:O	1:C:938:LEU:HB2	2.17	0.43
1:D:259:HIS:NE2	1:D:292:CYS:HB3	2.34	0.43
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.51	0.43
1:B:704:ILE:CG2	1:B:726:LEU:HD23	2.40	0.43
1:D:164:LEU:HD22	1:D:298:LEU:HB2	2.01	0.43
1:A:470:LYS:CB	1:A:480:PHE:CE1	3.00	0.43
1:A:547:GLU:HB3	1:A:548:VAL:HG13	1.99	0.43
1:D:952:ILE:HA	1:D:952:ILE:HD12	1.87	0.43
1:C:43:ALA:HA	1:C:66:ILE:CD1	2.49	0.43
1:A:798:VAL:HG11	1:A:835:SER:N	2.34	0.43
1:A:711:LEU:HG	1:A:751:ALA:HB2	2.00	0.43
1:A:38:LYS:HE2	1:A:38:LYS:HB3	1.60	0.43
1:D:963:LEU:HD12	1:D:967:ILE:HD12	2.01	0.43
1:C:148:MET:HA	1:C:154:LYS:HD2	1.99	0.43
1:A:1065:ILE:CG2	1:A:1074:ARG:HD3	2.49	0.43
1:A:655:PRO:HG2	1:A:985:VAL:CG2	2.48	0.43
1:B:883:LEU:O	1:B:884:GLY:C	2.56	0.43
1:B:386:ASP:HB3	1:B:388:MET:HG3	2.01	0.43
1:A:715:ARG:HD2	1:A:715:ARG:HA	1.80	0.43
1:A:855:LYS:O	1:A:855:LYS:HG3	2.17	0.43
1:A:394:ILE:O	1:A:414:GLN:O	2.36	0.43
1:C:142:HIS:N	1:C:145:HIS:HD2	2.16	0.43
1:B:655:PRO:HD3	1:B:982:LEU:CD1	2.49	0.43
1:A:1029:ASN:ND2	1:A:1029:ASN:C	2.71	0.43
1:C:216:ALA:O	1:C:217:PHE:C	2.56	0.43
1:A:177:TYR:O	1:A:178:GLU:C	2.56	0.43
1:A:547:GLU:CA	1:A:547:GLU:OE2	2.66	0.43
1:C:129:ARG:HG3	1:C:143:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:VAL:HG21	1:D:476:TYR:OH	2.19	0.43
1:A:252:ASP:OD1	1:A:256:ASN:HB2	2.19	0.43
1:D:239:ILE:HD13	1:D:239:ILE:HA	1.82	0.43
1:A:118:TYR:C	1:A:118:TYR:CD1	2.91	0.42
1:D:871:TYR:HE1	1:D:891:LYS:HD3	1.84	0.42
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.53	0.42
1:C:347:THR:O	1:C:348:GLN:C	2.56	0.42
1:B:448:ARG:NH2	1:B:467:LYS:HD2	2.32	0.42
1:D:879:LYS:C	1:D:881:LEU:H	2.22	0.42
1:B:1048:VAL:HG12	1:B:1050:ILE:HD12	2.01	0.42
1:C:238:TYR:CE1	5:C:1202:ATP:H2	2.37	0.42
1:A:1017:TYR:O	1:A:1018:GLU:C	2.57	0.42
1:D:456:LYS:H	1:D:456:LYS:HD3	1.83	0.42
1:D:820:PHE:HB3	1:D:821:PRO:HD2	2.01	0.42
1:B:291:ILE:HG12	1:B:320:PHE:HD2	1.84	0.42
1:C:1002:VAL:HG13	1:C:1006:ASP:OD2	2.19	0.42
1:C:448:ARG:HH22	1:C:467:LYS:HE3	1.84	0.42
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.42
1:C:941:PRO:O	1:C:945:VAL:HG22	2.19	0.42
1:C:926:LEU:CD1	1:C:938:LEU:CD1	2.96	0.42
1:C:175:LYS:O	1:C:176:SER:C	2.49	0.42
1:C:501:LEU:HD22	1:C:1078:TYR:CE1	2.54	0.42
1:B:938:LEU:HA	1:B:938:LEU:HD23	1.79	0.42
1:D:879:LYS:HG2	1:D:884:GLY:HA3	2.01	0.42
1:A:417:GLU:C	1:A:418:ILE:HD12	2.40	0.42
1:D:796:THR:CB	1:D:810:ALA:HB2	2.49	0.42
1:C:661:LYS:O	1:C:664:GLN:HB2	2.20	0.42
1:C:780:LEU:HD23	1:C:780:LEU:HA	1.80	0.42
1:A:532:VAL:HG13	1:A:536:LYS:HD2	2.01	0.42
1:A:207:VAL:CG1	1:A:209:GLU:H	2.33	0.42
1:D:258:VAL:HB	1:D:364:GLN:NE2	2.34	0.42
1:A:506:ASN:ND2	1:A:510:ASN:HD22	2.18	0.42
1:A:952:ILE:O	1:A:952:ILE:HG23	2.17	0.42
1:D:93:ALA:C	1:D:95:SER:H	2.22	0.42
1:D:93:ALA:C	1:D:95:SER:N	2.73	0.42
1:D:378:ILE:HG23	1:D:459:ILE:HG12	2.00	0.42
1:B:85:LEU:HG	1:B:87:GLY:H	1.84	0.42
1:B:889:GLU:O	1:B:890:VAL:C	2.58	0.42
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.84	0.42
1:B:522:PRO:HB2	1:B:523:ASP:H	1.68	0.42
1:A:597:VAL:HG21	1:A:834:LEU:HG	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:LEU:HD11	1:A:812:SER:HB3	2.00	0.42
1:A:213:LEU:O	1:A:214:GLU:C	2.55	0.42
1:B:278:ALA:HA	1:B:279:PRO:HA	1.62	0.42
1:B:631:ARG:O	1:B:631:ARG:HD3	2.19	0.42
1:C:281:VAL:HG12	1:C:282:GLY:H	1.83	0.42
1:C:111:VAL:HG12	1:C:113:ALA:H	1.83	0.42
1:B:468:ASN:OD1	1:B:470:LYS:HB2	2.19	0.42
1:C:920:TYR:CE1	1:C:940:PHE:HD2	2.37	0.42
1:C:1080:MET:CE	1:C:1085:ARG:NH2	2.83	0.42
1:C:907:VAL:O	1:C:911:SER:OG	2.35	0.42
1:D:506:ASN:HD22	1:D:506:ASN:HA	1.64	0.42
1:A:382:ASP:OD1	1:A:384:LEU:CD1	2.67	0.42
1:D:909:PRO:HG2	1:D:952:ILE:HG13	2.01	0.42
1:B:443:MET:HG2	1:B:466:MET:CE	2.49	0.42
1:C:124:ASN:HB3	1:C:127:PHE:HB3	2.02	0.42
1:B:996:GLU:OE1	1:B:996:GLU:C	2.58	0.42
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.78	0.42
1:C:831:MET:O	1:C:832:GLU:C	2.58	0.42
1:C:572:ASP:HB3	1:C:807:GLN:HE21	1.80	0.42
1:D:870:GLN:O	1:D:871:TYR:C	2.57	0.42
1:C:383:PRO:HB3	1:C:387:PHE:CZ	2.54	0.42
1:B:655:PRO:HD3	1:B:982:LEU:HD13	2.00	0.42
1:B:124:ASN:OD1	1:B:126:GLN:N	2.53	0.42
1:B:551:LYS:HZ3	1:B:551:LYS:HB2	1.84	0.42
1:C:803:GLY:O	1:C:804:LEU:C	2.56	0.42
1:A:167:ILE:HD12	1:A:323:ILE:CD1	2.50	0.42
1:C:246:GLU:OE1	1:C:330:GLN:NE2	2.52	0.42
1:D:874:LEU:O	1:D:887:PHE:CE1	2.65	0.42
1:D:1087:ILE:HD13	1:D:1087:ILE:HA	1.86	0.42
1:C:794:ILE:CD1	1:C:796:THR:CG2	2.97	0.42
1:C:760:LYS:CE	1:C:790:GLY:O	2.67	0.42
1:A:384:LEU:H	1:A:384:LEU:CD1	2.33	0.42
1:B:291:ILE:HG12	1:B:320:PHE:CD2	2.55	0.42
1:B:783:TYR:O	1:B:784:LYS:C	2.56	0.42
1:A:246:GLU:O	1:A:262:GLU:HA	2.19	0.42
1:D:856:SER:HB3	1:D:857:PRO:HD2	2.00	0.42
1:D:730:LEU:O	1:D:735:PHE:HD1	2.02	0.42
1:C:39:LYS:HE3	1:C:82:GLU:OE2	2.20	0.42
1:B:69:ASN:O	1:B:72:LYS:HG3	2.19	0.42
1:D:572:ASP:HB3	1:D:807:GLN:HE21	1.83	0.42
1:B:251:GLY:HA3	1:B:257:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASN:ND2	1:C:510:ASN:HD22	2.18	0.42
1:A:912:LYS:NZ	1:A:916:ASP:OD1	2.45	0.42
1:C:336:THR:O	1:C:340:THR:HG23	2.19	0.42
1:C:896:ARG:NE	1:C:928:GLU:OE1	2.53	0.42
1:A:781:LEU:HD21	1:D:784:LYS:HG3	2.01	0.42
1:B:769:HIS:NE2	1:B:795:ASP:OD1	2.48	0.42
1:C:1077:TYR:N	1:C:1077:TYR:CD1	2.88	0.42
1:A:606:MET:HE2	1:A:639:PHE:CG	2.55	0.42
1:D:239:ILE:O	1:D:241:ASN:N	2.52	0.42
1:A:902:GLY:O	1:A:903:ASP:HB3	2.19	0.42
1:D:703:THR:CG2	1:D:741:LYS:HB2	2.48	0.42
1:B:130:ARG:HA	1:B:130:ARG:HD2	1.80	0.42
1:B:690:ASN:O	1:B:691:GLU:C	2.59	0.41
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.76	0.41
1:C:627:LEU:O	1:C:631:ARG:HB2	2.20	0.41
1:A:48:ILE:HG23	1:A:49:ALA:N	2.34	0.41
1:B:362(A):PRO:HB2	1:B:366:ASP:HB2	2.01	0.41
1:B:280:SER:OG	1:B:283:LEU:HG	2.20	0.41
1:A:219:ARG:O	1:A:219:ARG:HG2	2.19	0.41
1:A:898:ASN:ND2	1:A:904:ILE:H	2.12	0.41
1:D:828:ILE:HD12	1:D:829:GLU:H	1.85	0.41
1:A:362:MET:HE3	1:A:362(A):PRO:HD2	2.01	0.41
1:B:251:GLY:CA	1:B:257:ILE:HG23	2.50	0.41
1:A:225:GLU:OE2	1:A:231:SER:HB3	2.20	0.41
1:C:772:THR:HG22	1:C:783:TYR:CE2	2.55	0.41
1:D:860:GLU:O	1:D:863:GLN:HG2	2.19	0.41
1:A:744:ALA:HB3	1:A:746:LEU:HG	2.02	0.41
1:C:809:SER:HB3	1:C:812:SER:HB2	2.01	0.41
1:C:152:LYS:HG3	1:C:197:SER:H	1.84	0.41
1:C:979:GLY:O	1:C:982:LEU:N	2.52	0.41
1:B:98:ASN:C	1:B:98:ASN:ND2	2.70	0.41
1:C:59:LEU:HD22	1:C:350:LEU:HD21	2.02	0.41
1:A:254:HIS:HD2	1:A:356:ASP:OD2	2.02	0.41
1:B:370:LEU:HD22	1:D:370:LEU:HB3	2.02	0.41
1:C:469:LYS:HA	1:C:469:LYS:HD2	1.61	0.41
1:C:866:MET:HE3	1:C:870:GLN:HG2	2.02	0.41
1:A:211:SER:H	1:A:213:LEU:HD12	1.85	0.41
1:D:1035:THR:N	1:D:1036:PRO:CD	2.84	0.41
1:B:343:ASP:OD2	1:B:346:LYS:HB2	2.21	0.41
1:A:743:MET:CG	1:A:907:VAL:HG13	2.50	0.41
1:B:509:ILE:HG22	1:B:510:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:THR:HB	1:D:375:GLN:NE2	2.35	0.41
1:B:371:GLY:HA2	1:B:434:ILE:HA	2.02	0.41
1:D:276:GLU:OE2	1:D:377:ARG:NH1	2.50	0.41
1:D:322:PHE:CZ	1:D:325:VAL:HG23	2.56	0.41
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.85	0.41
1:A:605:GLU:HA	1:A:640:GLN:O	2.20	0.41
1:A:641:MET:HB3	1:A:671:ILE:HD12	2.03	0.41
1:A:915:GLY:O	1:A:919:LEU:HD22	2.20	0.41
1:A:810:ALA:HB1	1:A:831:MET:CE	2.50	0.41
1:A:390:ASP:HB3	1:A:455:VAL:HG12	2.01	0.41
1:B:949:LYS:O	1:B:974:LEU:HG	2.20	0.41
1:B:509:ILE:HD12	1:B:1076:ILE:HD11	2.01	0.41
1:C:752:ALA:HB2	1:C:782:THR:HG23	2.03	0.41
1:D:743:MET:HG2	1:D:744:ALA:N	2.34	0.41
1:B:400:SER:HB3	1:B:401:GLY:H	1.70	0.41
1:C:712:ASN:HA	1:C:713:PRO:HD2	1.97	0.41
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.23	0.41
1:C:170:THR:HG21	1:C:174:ILE:HD11	2.01	0.41
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.83	0.41
1:B:302:ILE:O	1:B:303:LYS:CB	2.68	0.41
1:D:563:VAL:CG2	1:D:787:ILE:HG12	2.49	0.41
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.20	0.41
1:A:987:PHE:HE2	1:A:1011:VAL:HG21	1.85	0.41
1:B:53:PHE:CZ	1:B:65:ALA:HB2	2.55	0.41
1:A:1052:ILE:O	1:A:1052:ILE:HG22	2.20	0.41
1:B:406:ARG:NH1	1:D:403:ALA:HA	2.36	0.41
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.51	0.41
1:A:382:ASP:O	1:A:387:PHE:HA	2.19	0.41
1:A:107:LYS:C	1:A:109:ALA:H	2.23	0.41
1:C:400:SER:H	1:C:407:LEU:HD11	1.86	0.41
1:D:893:MET:SD	1:D:896:ARG:NH2	2.94	0.41
1:C:898:ASN:HD22	1:C:906:LYS:HD3	1.86	0.41
1:A:375:GLN:HE22	1:A:428:LYS:HZ1	1.68	0.41
1:D:700:SER:H	1:D:736:HIS:CD2	2.38	0.41
1:D:413:PHE:C	1:D:415:GLY:N	2.74	0.41
1:B:784:LYS:HE2	1:C:785:GLN:NE2	2.36	0.41
1:B:642:LEU:HG	1:B:643:LEU:N	2.35	0.41
1:A:683:VAL:HA	1:A:686:MET:HG3	2.02	0.41
1:B:945:VAL:HA	1:B:967:ILE:CG2	2.50	0.41
1:B:799:ALA:HB3	1:B:835:SER:OG	2.20	0.41
1:B:701:GLU:HG2	1:B:739:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG12	1:C:373:ALA:HB3	2.03	0.41
1:B:952:ILE:CG2	1:B:952:ILE:O	2.68	0.41
1:D:565:LEU:C	1:D:565:LEU:CD1	2.89	0.41
1:D:650:GLY:HA3	1:D:654:TYR:HE1	1.86	0.41
1:C:991:ARG:O	1:C:995:GLU:HG2	2.21	0.41
1:D:574:HIS:CD2	1:D:580:THR:HA	2.56	0.41
1:A:66:ILE:HB	1:A:86:VAL:HG22	2.03	0.41
1:A:606:MET:HE2	1:A:639:PHE:HB3	2.03	0.41
1:D:927:ASP:H	1:D:930:SER:HB2	1.85	0.41
1:B:793:ILE:HG22	1:B:794:ILE:N	2.36	0.41
1:B:640:GLN:HG3	1:B:673:VAL:CG1	2.51	0.41
1:B:484:THR:HB	1:B:487:LEU:HD22	2.01	0.41
1:A:1063:GLU:OE2	1:C:1086:ARG:NH2	2.54	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.03	0.41
1:D:974:LEU:HB3	1:D:981:TYR:CE1	2.56	0.41
1:C:893:MET:O	1:C:897:VAL:HG23	2.21	0.41
1:B:338:MET:HE1	1:B:430:SER:CB	2.45	0.41
1:A:512:PHE:CD2	1:A:513:PRO:N	2.89	0.41
1:A:295:ALA:O	1:A:299:MET:HG2	2.21	0.41
1:C:549:GLY:O	1:C:553:VAL:HG23	2.20	0.41
1:B:881:LEU:HD22	1:B:923:GLN:NE2	2.35	0.41
1:A:980:GLU:OE1	1:A:980:GLU:O	2.39	0.41
1:D:588:ILE:HD12	1:D:588:ILE:HG23	1.83	0.41
1:D:711:LEU:HA	1:D:711:LEU:HD23	1.88	0.41
1:A:47:GLU:CD	1:A:428:LYS:HD2	2.41	0.40
1:B:798:VAL:O	1:B:799:ALA:C	2.59	0.40
1:B:577:LEU:HD13	1:B:842:ARG:CZ	2.51	0.40
1:A:498:THR:O	1:A:499:LYS:C	2.59	0.40
1:C:381:GLU:O	1:C:383:PRO:HD3	2.21	0.40
1:D:281:VAL:CG1	1:D:282:GLY:N	2.83	0.40
1:C:145:HIS:CE1	1:C:304:TYR:HA	2.56	0.40
1:A:170:THR:HG22	1:A:172:GLY:H	1.85	0.40
1:B:444:VAL:CG2	1:B:466:MET:HB3	2.52	0.40
1:C:189:PHE:N	1:C:190:PRO:CD	2.84	0.40
1:A:647:ASN:O	1:A:649:VAL:N	2.53	0.40
1:A:566:THR:HA	1:A:603:SER:O	2.21	0.40
1:A:296:ILE:O	1:A:300:GLU:HB2	2.21	0.40
1:C:729:GLU:O	1:C:733:GLU:HG2	2.21	0.40
1:C:268:GLN:HA	1:C:272:GLN:O	2.20	0.40
1:D:442:LYS:HE2	1:D:442:LYS:HB2	1.66	0.40
1:A:720:LEU:HD21	1:A:758:GLU:CG	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:869:GLY:O	1:D:870:GLN:C	2.59	0.40
1:D:149:PHE:HZ	1:D:302:ILE:CD1	2.34	0.40
1:D:921:MET:HG2	1:D:926:LEU:CB	2.51	0.40
1:B:908:THR:HG22	1:B:909:PRO:HA	2.03	0.40
1:C:350:LEU:O	1:C:355:ALA:HB3	2.21	0.40
1:C:189:PHE:H	1:C:190:PRO:HD2	1.86	0.40
1:D:927:ASP:HB2	1:D:930:SER:OG	2.20	0.40
1:B:777:GLY:O	1:C:780:LEU:HD12	2.21	0.40
1:D:468:ASN:HD22	1:D:470:LYS:H	1.69	0.40
1:A:281:VAL:HG21	1:A:436:PHE:CG	2.56	0.40
1:C:461:PHE:O	1:C:464:ASN:HB2	2.21	0.40
1:B:241:ASN:HA	1:B:479:LYS:HE2	2.03	0.40
1:B:549:GLY:O	1:B:553:VAL:HG23	2.22	0.40
1:B:164:LEU:HD11	1:B:298:LEU:HB2	2.02	0.40
1:C:1089:ILE:HA	1:C:1089:ILE:HD13	1.80	0.40
1:D:398:ARG:NH2	1:D:451:ARG:HE	2.19	0.40
1:A:511:GLY:O	4:A:1203:BTI:H103	2.20	0.40
1:C:911:SER:HG	1:C:911:SER:H	1.59	0.40
1:D:400:SER:OG	1:D:401:GLY:N	2.54	0.40
1:A:335:ILE:H	1:A:335:ILE:HG22	1.48	0.40
1:B:624:TRP:CZ2	1:B:1008:ILE:HD11	2.56	0.40
1:B:949:LYS:HG2	1:B:968:LEU:HD21	2.03	0.40
1:A:551:LYS:O	1:A:555:GLU:HG2	2.21	0.40
1:C:444:VAL:O	1:C:448:ARG:HG3	2.21	0.40
1:A:263:ARG:HH21	1:A:330:GLN:HE21	1.69	0.40
1:A:250:ILE:HG21	1:A:250:ILE:HD13	1.93	0.40
1:D:362:MET:HA	1:D:362(A):PRO:HD2	1.97	0.40
1:A:863:GLN:O	1:A:895:ARG:CD	2.61	0.40
1:A:622:ASN:O	1:A:623:PRO:C	2.60	0.40
1:A:337:GLU:HG2	1:A:342:ILE:O	2.21	0.40
1:C:641:MET:HB3	1:C:671:ILE:HD12	2.04	0.40
1:A:278:ALA:HB3	1:A:335:ILE:CG1	2.48	0.40
1:C:480:PHE:C	1:C:480:PHE:CD1	2.94	0.40
1:A:170:THR:HG21	1:A:174:ILE:HG23	2.03	0.40
1:B:624:TRP:CZ2	1:B:1008:ILE:HD13	2.53	0.40
1:C:995:GLU:O	1:C:998:GLN:O	2.39	0.40
1:C:691:GLU:O	1:C:695:GLU:HB2	2.21	0.40
1:C:180:ALA:O	1:C:181:LYS:C	2.60	0.40
1:A:647:ASN:HB2	1:A:654:TYR:HE1	1.85	0.40
1:B:418:ILE:HD12	1:B:419:SER:O	2.21	0.40
1:D:393:THR:HG23	1:D:417:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:CD	1:C:428:LYS:HE3	2.41	0.40
1:A:717(A):ILE:HD12	1:A:717(A):ILE:N	2.37	0.40
1:B:856:SER:OG	1:C:800:SER:HA	2.21	0.40
1:D:166:VAL:HG22	1:D:322:PHE:HB3	2.02	0.40
1:D:869:GLY:O	1:D:871:TYR:N	2.55	0.40
1:A:496:ARG:O	1:A:497:GLY:C	2.60	0.40
1:D:926:LEU:HD12	1:D:926:LEU:HA	1.91	0.40
1:D:924:ASN:CB	1:D:926:LEU:HD22	2.50	0.40
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.56	0.40
1:A:1029:ASN:ND2	1:A:1031:SER:H	2.20	0.40
1:D:373:ALA:HA	1:D:431:THR:O	2.22	0.40
1:D:739:ALA:C	1:D:740:ILE:HD13	2.42	0.40
1:A:606:MET:C	1:A:606:MET:SD	3.00	0.40
1:D:1083:GLN:HB3	1:D:1083:GLN:HE21	1.49	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%)	916 (87%)	102 (10%)	30 (3%)	6	19
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	7	25
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	4	14
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	6	21
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	6	19

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA

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Mol	Chain	Res	Type
1	A	211	SER
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE
1	A	230	ASN
1	A	396	ALA
1	A	709	ASP
1	A	870	GLN
1	A	880	SER
1	B	163	ASP
1	B	270	ARG
1	B	414	GLN
1	B	495	ASP
1	B	522	PRO
1	B	975	THR
1	C	176	SER
1	C	195	ALA
1	C	201	GLY
1	C	204	MET
1	C	214	GLU
1	C	215	ASP
1	C	386	ASP
1	C	518	LYS
1	C	649	VAL
1	C	886	ARG
1	C	890	VAL
1	C	980	GLU
1	D	92	PRO
1	D	152	LYS
1	D	240	ASP
1	D	515	ASN
1	D	870	GLN
1	A	499	LYS
1	A	527	ALA
1	A	648	ALA
1	A	861	ILE
1	B	166	VAL
1	B	528	SER
1	B	868	GLY
1	B	881	LEU
1	B	903	ASP
1	B	1001	PRO

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Mol	Chain	Res	Type
1	C	87	GLY
1	C	203	GLY
1	C	229	GLY
1	C	385	ASN
1	C	645	ALA
1	C	937	LYS
1	C	938	LEU
1	C	942	GLU
1	D	87	GLY
1	D	94	GLU
1	D	163	ASP
1	D	306	ASN
1	D	414	GLN
1	D	450	MET
1	D	649	VAL
1	D	799	ALA
1	D	884	GLY
1	D	888	ASP
1	A	94	GLU
1	A	517	GLU
1	B	475	ASP
1	B	1002	VAL
1	B	1081	ASN
1	C	151	ASP
1	C	197	SER
1	C	981	TYR
1	C	1053	ASP
1	D	334	THR
1	D	517	GLU
1	D	518	LYS
1	D	1069	ASP
1	A	44	ASN
1	A	209	GLU
1	A	882	GLY
1	B	306	ASN
1	B	648	ALA
1	B	649	VAL
1	B	1000	GLY
1	C	173	PRO
1	C	216	ALA
1	C	269	ARG
1	C	355	ALA

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Mol	Chain	Res	Type
1	C	821	PRO
1	D	133	GLU
1	D	261	PHE
1	D	480	PHE
1	D	513	PRO
1	B	527	ALA
1	B	1053	ASP
1	C	898	ASN
1	C	935	GLY
1	D	335	ILE
1	D	854	ILE
1	A	92	PRO
1	A	110	ASN
1	A	189	PHE
1	A	241	ASN
1	A	306	ASN
1	B	480	PHE
1	B	562	ASP
1	C	174	ILE
1	C	180	ALA
1	C	1001	PRO
1	A	1001	PRO
1	D	282	GLY
1	A	282	GLY
1	A	1014	PRO
1	B	890	VAL
1	C	189	PHE
1	A	868	GLY
1	C	291	ILE
1	C	327	PRO
1	A	956	VAL
1	C	168	PRO
1	A	935	GLY
1	D	1014	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	907/1005 (90%)	778 (86%)	129 (14%)	4	12
1	B	855/1005 (85%)	726 (85%)	129 (15%)	3	10
1	C	909/1005 (90%)	751 (83%)	158 (17%)	2	7
1	D	855/1005 (85%)	727 (85%)	128 (15%)	3	11
All	All	3526/4020 (88%)	2982 (85%)	544 (15%)	3	10

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	44	ASN
1	A	62	SER
1	A	66	ILE
1	A	69	ASN
1	A	70	GLU
1	A	73	SER
1	A	75	LEU
1	A	77	ARG
1	A	94	GLU
1	A	95	SER
1	A	97	LEU
1	A	98	ASN
1	A	108	GLN
1	A	110	ASN
1	A	143	LEU
1	A	144	GLU
1	A	156	ARG
1	A	161	LYS
1	A	163	ASP
1	A	175	LYS
1	A	179	LEU
1	A	182	GLU
1	A	186	GLU
1	A	193	ILE
1	A	194	LYS
1	A	210	GLU
1	A	212	GLU
1	A	214	GLU
1	A	215	ASP
1	A	225	GLU
1	A	234	TYR
1	A	237	ARG

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Mol	Chain	Res	Type
1	A	239	ILE
1	A	257	ILE
1	A	271	HIS
1	A	283	LEU
1	A	286	THR
1	A	287	LEU
1	A	306	ASN
1	A	313	LEU
1	A	329	VAL
1	A	331	VAL
1	A	335	ILE
1	A	386	ASP
1	A	391	THR
1	A	398	ARG
1	A	419	SER
1	A	427	VAL
1	A	428	LYS
1	A	434	ILE
1	A	437	LYS
1	A	440	GLU
1	A	442	LYS
1	A	455	VAL
1	A	472	THR
1	A	473	SER
1	A	487	LEU
1	A	491	GLN
1	A	496	ARG
1	A	512	PHE
1	A	518	LYS
1	A	525	GLU
1	A	526	LEU
1	A	528	SER
1	A	535	SER
1	A	536	LYS
1	A	547	GLU
1	A	551	LYS
1	A	565	LEU
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	592	SER
1	A	606	MET

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Mol	Chain	Res	Type
1	A	607	TRP
1	A	613	ASP
1	A	620	LYS
1	A	622	ASN
1	A	631	ARG
1	A	649	VAL
1	A	672	ASP
1	A	679	SER
1	A	685	GLN
1	A	715	ARG
1	A	719	THR
1	A	725	LYS
1	A	743	MET
1	A	750	LYS
1	A	760	LYS
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	784	LYS
1	A	811	ASN
1	A	828	ILE
1	A	831	MET
1	A	835	SER
1	A	855	LYS
1	A	861	ILE
1	A	863	GLN
1	A	870	GLN
1	A	876	GLN
1	A	880	SER
1	A	904	ILE
1	A	907	VAL
1	A	908	THR
1	A	919	LEU
1	A	923	GLN
1	A	926	LEU
1	A	931	VAL
1	A	932	ILE
1	A	944	VAL
1	A	961	LYS
1	A	980	GLU
1	A	993	LEU
1	A	999	GLN

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Mol	Chain	Res	Type
1	A	1008	ILE
1	A	1018	GLU
1	A	1019	GLN
1	A	1029	ASN
1	A	1043	ARG
1	A	1044	ASN
1	A	1048	VAL
1	A	1051	GLU
1	A	1064	THR
1	A	1076	ILE
1	A	1080	MET
1	A	1089	ILE
1	B	36	GLN
1	B	38	LYS
1	B	44	ASN
1	B	62	SER
1	B	70	GLU
1	B	75	LEU
1	B	90	LEU
1	B	94	GLU
1	B	98	ASN
1	B	101	ARG
1	B	104	ASP
1	B	124	ASN
1	B	144	GLU
1	B	147	ASP
1	B	152	LYS
1	B	153	VAL
1	B	166	VAL
1	B	167	ILE
1	B	239	ILE
1	B	241	ASN
1	B	281	VAL
1	B	287	LEU
1	B	288	ARG
1	B	289	GLN
1	B	291	ILE
1	B	300	GLU
1	B	306	ASN
1	B	315	SER
1	B	319	GLU
1	B	320	PHE

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Mol	Chain	Res	Type
1	B	328	ARG
1	B	331	VAL
1	B	357	LEU
1	B	359	GLU
1	B	361	ASN
1	B	365	LYS
1	B	368	THR
1	B	370	LEU
1	B	376	CYS
1	B	391	THR
1	B	399	SER
1	B	400	SER
1	B	406	ARG
1	B	417	GLU
1	B	418	ILE
1	B	423	ASP
1	B	427	VAL
1	B	435	SER
1	B	442	LYS
1	B	446	SER
1	B	450	MET
1	B	451	ARG
1	B	453	ARG
1	B	479	LYS
1	B	487	LEU
1	B	494	LEU
1	B	500	THR
1	B	515	ASN
1	B	519	ARG
1	B	534	SER
1	B	547	GLU
1	B	551	LYS
1	B	558	LYS
1	B	576	SER
1	B	580	THR
1	B	606	MET
1	B	607	TRP
1	B	622	ASN
1	B	631	ARG
1	B	632	LYS
1	B	647	ASN
1	B	649	VAL

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Mol	Chain	Res	Type
1	B	652	LYS
1	B	660	HIS
1	B	690	ASN
1	B	715	ARG
1	B	721	GLU
1	B	725	LYS
1	B	740	ILE
1	B	743	MET
1	B	761	SER
1	B	775	THR
1	B	784	LYS
1	B	791	VAL
1	B	792	ASP
1	B	807	GLN
1	B	809	SER
1	B	811	ASN
1	B	812	SER
1	B	828	ILE
1	B	831	MET
1	B	839	SER
1	B	843	THR
1	B	852	SER
1	B	853	ASP
1	B	855	LYS
1	B	863	GLN
1	B	871	TYR
1	B	872	SER
1	B	875	SER
1	B	876	GLN
1	B	879	LYS
1	B	880	SER
1	B	881	LEU
1	B	886	ARG
1	B	897	VAL
1	B	907	VAL
1	B	908	THR
1	B	919	LEU
1	B	927	ASP
1	B	929	GLN
1	B	930	SER
1	B	934	ASP
1	B	936	TYR

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Mol	Chain	Res	Type
1	B	938	LEU
1	B	939	ASP
1	B	942	GLU
1	B	944	VAL
1	B	949	LYS
1	B	957	ASN
1	B	962	ASP
1	B	963	LEU
1	B	991	ARG
1	B	1029	ASN
1	B	1057	ARG
1	B	1070	GLU
1	B	1071	ASN
1	B	1085	ARG
1	B	1089	ILE
1	C	44	ASN
1	C	45	ARG
1	C	69	ASN
1	C	70	GLU
1	C	75	LEU
1	C	77	ARG
1	C	86	VAL
1	C	90	LEU
1	C	97	LEU
1	C	98	ASN
1	C	100	GLU
1	C	101	ARG
1	C	110	ASN
1	C	112	ASP
1	C	123	GLU
1	C	142	HIS
1	C	144	GLU
1	C	151	ASP
1	C	154	LYS
1	C	156	ARG
1	C	166	VAL
1	C	167	ILE
1	C	171	ASP
1	C	175	LYS
1	C	178	GLU
1	C	179	LEU
1	C	192	MET

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Mol	Chain	Res	Type
1	C	193	ILE
1	C	194	LYS
1	C	202	LYS
1	C	205	ARG
1	C	208	ARG
1	C	209	GLU
1	C	210	GLU
1	C	215	ASP
1	C	219	ARG
1	C	223	GLU
1	C	225	GLU
1	C	230	ASN
1	C	232	GLU
1	C	234	TYR
1	C	235	ILE
1	C	237	ARG
1	C	253	GLU
1	C	257	ILE
1	C	262	GLU
1	C	269	ARG
1	C	280	SER
1	C	286	THR
1	C	287	LEU
1	C	288	ARG
1	C	306	ASN
1	C	315	SER
1	C	318	ASP
1	C	324	GLU
1	C	358	GLU
1	C	359	GLU
1	C	365	LYS
1	C	368	THR
1	C	377	ARG
1	C	384	LEU
1	C	386	ASP
1	C	391	THR
1	C	395	ILE
1	C	414	GLN
1	C	437	LYS
1	C	442	LYS
1	C	444	VAL
1	C	446	SER

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Mol	Chain	Res	Type
1	C	451	ARG
1	C	453	ARG
1	C	467	LYS
1	C	469	LYS
1	C	473	SER
1	C	491	GLN
1	C	493	SER
1	C	494	LEU
1	C	531	THR
1	C	533	SER
1	C	537	ILE
1	C	539	SER
1	C	543	GLN
1	C	545	LEU
1	C	547	GLU
1	C	559	LYS
1	C	563	VAL
1	C	589	ASN
1	C	606	MET
1	C	607	TRP
1	C	616	TYR
1	C	622	ASN
1	C	631	ARG
1	C	641	MET
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	652	LYS
1	C	660	HIS
1	C	661	LYS
1	C	680	LEU
1	C	695	GLU
1	C	707	THR
1	C	717	ASN
1	C	719	THR
1	C	725	LYS
1	C	743	MET
1	C	750	LYS
1	C	760	LYS
1	C	781	LEU
1	C	783	TYR
1	C	784	LYS

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Mol	Chain	Res	Type
1	C	807	GLN
1	C	811	ASN
1	C	833	SER
1	C	835	SER
1	C	839	SER
1	C	843	THR
1	C	852	SER
1	C	855	LYS
1	C	856	SER
1	C	860	GLU
1	C	861	ILE
1	C	863	GLN
1	C	866	MET
1	C	870	GLN
1	C	872	SER
1	C	876	GLN
1	C	881	LEU
1	C	885	GLU
1	C	892	ASP
1	C	893	MET
1	C	895	ARG
1	C	896	ARG
1	C	907	VAL
1	C	908	THR
1	C	923	GLN
1	C	927	ASP
1	C	928	GLU
1	C	938	LEU
1	C	949	LYS
1	C	959	PHE
1	C	960	ASN
1	C	967	ILE
1	C	968	LEU
1	C	971	GLN
1	C	980	GLU
1	C	986	ASP
1	C	997	GLU
1	C	1015	LYS
1	C	1024	ARG
1	C	1029	ASN
1	C	1031	SER
1	C	1048	VAL

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Mol	Chain	Res	Type
1	C	1052	ILE
1	C	1067	GLU
1	C	1076	ILE
1	C	1085	ARG
1	C	1090	LYS
1	D	38	LYS
1	D	44	ASN
1	D	72	LYS
1	D	73	SER
1	D	75	LEU
1	D	77	ARG
1	D	88	SER
1	D	99	ILE
1	D	101	ARG
1	D	137	LYS
1	D	143	LEU
1	D	163	ASP
1	D	167	ILE
1	D	239	ILE
1	D	240	ASP
1	D	243	LYS
1	D	250	ILE
1	D	253	GLU
1	D	260	LEU
1	D	262	GLU
1	D	268	GLN
1	D	270	ARG
1	D	280	SER
1	D	287	LEU
1	D	288	ARG
1	D	290	ARG
1	D	305	VAL
1	D	326	ASN
1	D	328	ARG
1	D	329	VAL
1	D	331	VAL
1	D	335	ILE
1	D	360	ILE
1	D	361	ASN
1	D	365	LYS
1	D	368	THR
1	D	369	THR

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Mol	Chain	Res	Type
1	D	386	ASP
1	D	393	THR
1	D	395	ILE
1	D	417	GLU
1	D	418	ILE
1	D	425	LEU
1	D	427	VAL
1	D	434	ILE
1	D	437	LYS
1	D	445	ARG
1	D	446	SER
1	D	451	ARG
1	D	452	ILE
1	D	456	LYS
1	D	467	LYS
1	D	470	LYS
1	D	473	SER
1	D	478	THR
1	D	479	LYS
1	D	486	GLU
1	D	487	LEU
1	D	491	GLN
1	D	496	ARG
1	D	506	ASN
1	D	513	PRO
1	D	519	ARG
1	D	523	ASP
1	D	525	GLU
1	D	526	LEU
1	D	528	SER
1	D	531	THR
1	D	533	SER
1	D	542	LYS
1	D	543	GLN
1	D	551	LYS
1	D	555	GLU
1	D	565	LEU
1	D	580	THR
1	D	607	TRP
1	D	620	LYS
1	D	622	ASN
1	D	629	ARG

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Mol	Chain	Res	Type
1	D	631	ARG
1	D	632	LYS
1	D	641	MET
1	D	647	ASN
1	D	649	VAL
1	D	700	SER
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	725	LYS
1	D	743	MET
1	D	760	LYS
1	D	763	VAL
1	D	766	LEU
1	D	775	THR
1	D	784	LYS
1	D	791	VAL
1	D	811	ASN
1	D	831	MET
1	D	839	SER
1	D	852	SER
1	D	853	ASP
1	D	856	SER
1	D	863	GLN
1	D	866	MET
1	D	870	GLN
1	D	885	GLU
1	D	886	ARG
1	D	907	VAL
1	D	908	THR
1	D	911	SER
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	927	ASP
1	D	944	VAL
1	D	952	ILE
1	D	963	LEU
1	D	977	ARG
1	D	996	GLU
1	D	1046	GLU
1	D	1052	ILE

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Mol	Chain	Res	Type
1	D	1054	LYS
1	D	1057	ARG
1	D	1061	LYS
1	D	1064	THR
1	D	1080	MET
1	D	1083	GLN
1	D	1085	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN
1	A	108	GLN
1	A	126	GLN
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	256	ASN
1	A	268	GLN
1	A	330	GLN
1	A	375	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	622	ASN
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	898	ASN
1	A	923	GLN
1	A	1005	GLN
1	A	1025	ASN

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Mol	Chain	Res	Type
1	A	1029	ASN
1	A	1044	ASN
1	B	36	GLN
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	145	HIS
1	B	256	ASN
1	B	272	GLN
1	B	301	ASN
1	B	326	ASN
1	B	330	GLN
1	B	361	ASN
1	B	363	GLN
1	B	375	GLN
1	B	432	HIS
1	B	438	GLN
1	B	515	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	622	ASN
1	B	690	ASN
1	B	736	HIS
1	B	778	ASN
1	B	811	ASN
1	B	863	GLN
1	B	864	HIS
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	998	GLN
1	B	1005	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1073	ASN
1	B	1083	GLN
1	C	44	ASN
1	C	98	ASN

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Mol	Chain	Res	Type
1	C	110	ASN
1	C	142	HIS
1	C	145	HIS
1	C	230	ASN
1	C	289	GLN
1	C	301	ASN
1	C	326	ASN
1	C	330	GLN
1	C	414	GLN
1	C	464	ASN
1	C	506	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	685	GLN
1	C	694	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	785	GLN
1	C	807	GLN
1	C	811	ASN
1	C	818	ASN
1	C	863	GLN
1	C	864	HIS
1	C	876	GLN
1	C	877	GLN
1	C	898	ASN
1	C	923	GLN
1	C	964	GLN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1093	ASN
1	D	44	ASN
1	D	145	HIS
1	D	244	HIS
1	D	256	ASN
1	D	301	ASN

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	330	GLN
1	D	348	GLN
1	D	364	GLN
1	D	375	GLN
1	D	432	HIS
1	D	468	ASN
1	D	491	GLN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	807	GLN
1	D	811	ASN
1	D	818	ASN
1	D	864	HIS
1	D	877	GLN
1	D	898	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1025	ASN
1	D	1083	GLN

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

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
2	ADP	A	1201	-	22,29,29	1.07	2 (9%)	27,45,45	2.10	5 (18%)
4	BTI	A	1203	-	14,16,16	1.89	2 (14%)	13,21,21	1.51	3 (23%)
4	BTI	B	1201	-	14,16,16	1.82	3 (21%)	13,21,21	1.42	2 (15%)
5	ATP	C	1202	-	24,33,33	1.06	2 (8%)	31,52,52	2.14	5 (16%)
4	BTI	D	1201	-	14,16,16	1.83	2 (14%)	13,21,21	1.50	2 (15%)

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
2	ADP	A	1201	-	-	0/12/32/32	0/3/3/3
4	BTI	A	1203	-	-	0/5/27/27	0/2/2/2
4	BTI	B	1201	-	-	0/5/27/27	0/2/2/2
5	ATP	C	1202	-	-	0/18/38/38	0/3/3/3
4	BTI	D	1201	-	-	0/5/27/27	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	C2-S1	-3.61	1.76	1.82
4	D	1201	BTI	C2-S1	-3.32	1.77	1.82
4	B	1201	BTI	C2-S1	-2.97	1.77	1.82
4	B	1201	BTI	C3-N2	-2.08	1.32	1.35
2	A	1201	ADP	O4'-C1'	2.46	1.44	1.41
5	C	1202	ATP	O4'-C1'	2.69	1.44	1.41
2	A	1201	ADP	C5-C4	3.07	1.47	1.40
5	C	1202	ATP	C5-C4	3.25	1.47	1.40
4	D	1201	BTI	O3-C3	5.02	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1201	BTI	O3-C3	5.23	1.34	1.23
4	A	1203	BTI	O3-C3	5.25	1.34	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	N3-C2-N1	-7.22	123.36	128.89
5	C	1202	ATP	C2'-C1'-N9	-6.70	104.06	114.29
5	C	1202	ATP	N3-C2-N1	-6.24	124.12	128.89
5	C	1202	ATP	PA-O3A-PB	-4.64	119.71	132.73
2	A	1201	ADP	C2'-C1'-N9	-4.27	107.77	114.29
5	C	1202	ATP	C4-C5-N7	-3.09	106.64	109.48
5	C	1202	ATP	PB-O3B-PG	-2.84	123.16	132.67
2	A	1201	ADP	C4-C5-N7	-2.81	106.89	109.48
4	B	1201	BTI	O3-C3-N2	-2.59	122.89	125.90
2	A	1201	ADP	PA-O3A-PB	-2.59	123.98	132.67
4	A	1203	BTI	C5-N3-C3	-2.33	110.74	112.49
4	D	1201	BTI	C8-C7-C2	-2.23	108.52	113.70
4	A	1203	BTI	O3-C3-N3	-2.07	123.50	125.90
2	A	1201	ADP	O3B-PB-O2B	2.23	115.86	107.38
4	A	1203	BTI	N2-C3-N3	2.72	110.76	108.88
4	B	1201	BTI	N2-C3-N3	3.04	110.98	108.88
4	D	1201	BTI	N2-C3-N3	3.64	111.39	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ADP	1	0
4	A	1203	BTI	4	0
4	B	1201	BTI	4	0
5	C	1202	ATP	10	0
4	D	1201	BTI	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.25	21 (1%) 68 58	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.16	25 (2%) 61 48	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.11	26 (2%) 61 48	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.22	13 (1%) 79 71	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.18	85 (2%) 67 56	47, 80, 125, 178	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	SER	5.2
1	A	229	GLY	4.7
1	A	233	VAL	4.6
1	D	490	ILE	4.6
1	D	240	ASP	4.3
1	A	177	TYR	3.7
1	C	877	GLN	3.7
1	B	168	PRO	3.7
1	C	936	TYR	3.7
1	D	285	PRO	3.6
1	C	1093	ASN	3.4
1	A	230	ASN	3.4
1	A	223	GLU	3.3
1	D	475	ASP	3.2
1	C	881	LEU	3.1
1	B	526	LEU	3.1
1	D	271	HIS	3.1
1	C	890	VAL	3.1
1	C	1070	GLU	3.1
1	C	282	GLY	3.0
1	C	876	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	LYS	2.9
1	A	1001	PRO	2.9
1	D	310	VAL	2.9
1	D	239	ILE	2.9
1	C	492	PRO	2.9
1	A	1000	GLY	2.8
1	B	527	ALA	2.8
1	A	197	SER	2.8
1	B	1093	ASN	2.8
1	C	922	VAL	2.8
1	A	1072	GLY	2.8
1	C	999	GLN	2.7
1	D	421	TYR	2.7
1	A	222	SER	2.7
1	C	515	ASN	2.7
1	C	879	LYS	2.7
1	A	999	GLN	2.7
1	D	515	ASN	2.6
1	C	932	ILE	2.5
1	A	219	ARG	2.5
1	C	516	VAL	2.5
1	C	919	LEU	2.5
1	B	271	HIS	2.5
1	A	227	SER	2.5
1	B	255	GLY	2.5
1	B	1072	GLY	2.5
1	B	167	ILE	2.5
1	B	882	GLY	2.5
1	C	717	ASN	2.5
1	B	1071	ASN	2.4
1	A	493	SER	2.4
1	B	975	THR	2.4
1	B	1091	ASP	2.4
1	B	1070	GLU	2.3
1	C	933	THR	2.3
1	B	717	ASN	2.3
1	A	174	ILE	2.3
1	B	144	GLU	2.3
1	C	285	PRO	2.3
1	C	177	TYR	2.3
1	C	739	ALA	2.3
1	C	230	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1072	GLY	2.3
1	B	240	ASP	2.2
1	B	641	MET	2.2
1	A	996	GLU	2.2
1	B	494	LEU	2.2
1	A	1070	GLU	2.2
1	B	999	GLN	2.1
1	C	968	LEU	2.1
1	D	309	THR	2.1
1	D	384	LEU	2.1
1	B	303	LYS	2.1
1	B	880	SER	2.1
1	C	923	GLN	2.1
1	B	383	PRO	2.1
1	B	881	LEU	2.1
1	C	741	LYS	2.1
1	B	1092	GLU	2.0
1	A	494	LEU	2.0
1	D	241	ASN	2.0
1	B	1000	GLY	2.0
1	A	568	THR	2.0
1	D	1070	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	BTI	A	1203	15/15	0.93	0.30	3.03	92,99,104,105	0
4	BTI	B	1201	15/15	0.91	0.33	2.30	105,109,114,115	0
4	BTI	D	1201	15/15	0.92	0.29	2.30	105,109,113,116	0
3	MN	C	1201	1/1	0.98	0.27	0.04	76,76,76,76	0
3	MN	D	1202	1/1	0.99	0.19	-0.14	74,74,74,74	0
3	MN	B	1202	1/1	0.97	0.19	-0.33	82,82,82,82	0
2	ADP	A	1201	27/27	0.89	0.18	-0.36	86,91,110,110	0
3	MN	A	1202	1/1	0.99	0.20	-0.42	74,74,74,74	0
5	ATP	C	1202	31/31	0.94	0.16	-0.65	102,108,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.