Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 11:33 PM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

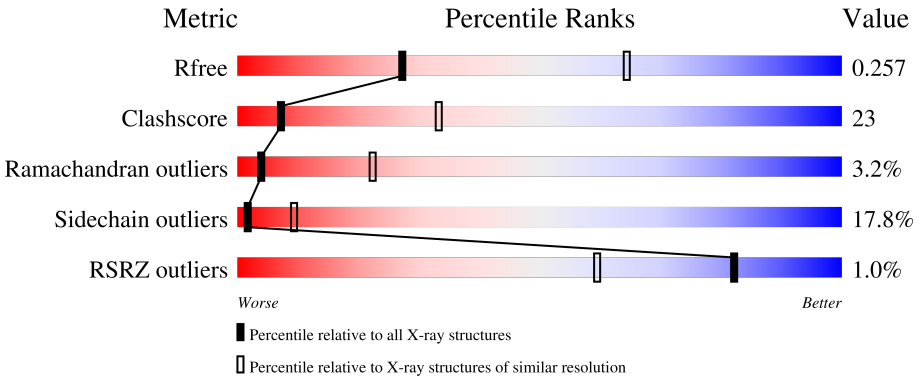
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 49% 31% 9% • 10%
1	B	1173	47% 31% 6% • 16%
1	C	1173	% 47% 32% 10% • 10%
1	D	1173	% 46% 30% 7% • 16%

2 Entry composition (i)

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

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

- Molecule 1 is a protein called Pyruvate carboxylase.

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

There are 96 discrepancies between the modelled and reference sequences:

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

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

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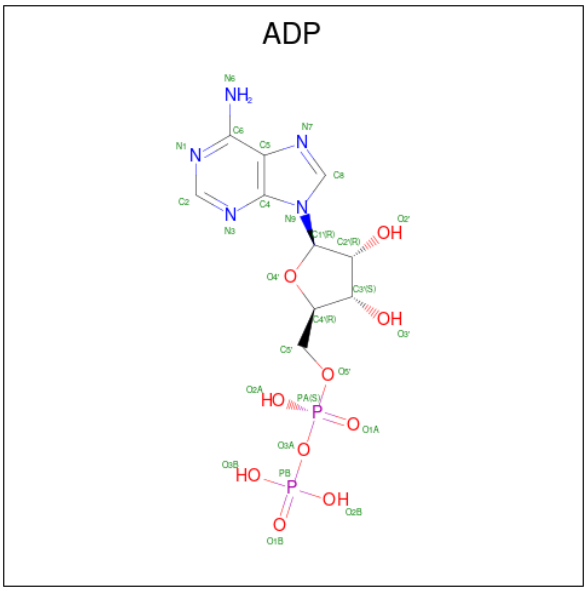
Chain	Residue	Modelled	Actual	Comment	Reference
C	26	PRO	-	expression tag	UNP Q99UY8
C	27	ARG	-	expression tag	UNP Q99UY8
C	28	GLY	-	expression tag	UNP Q99UY8
C	29	SER	-	expression tag	UNP Q99UY8
C	30	HIS	-	expression tag	UNP Q99UY8
C	31	MET	-	expression tag	UNP Q99UY8
C	32	ALA	-	expression tag	UNP Q99UY8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

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

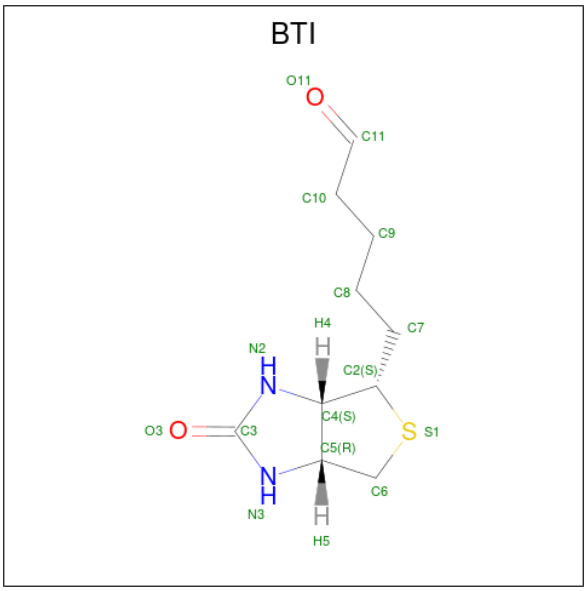


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 27 10 5 10 2	0	0

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

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

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



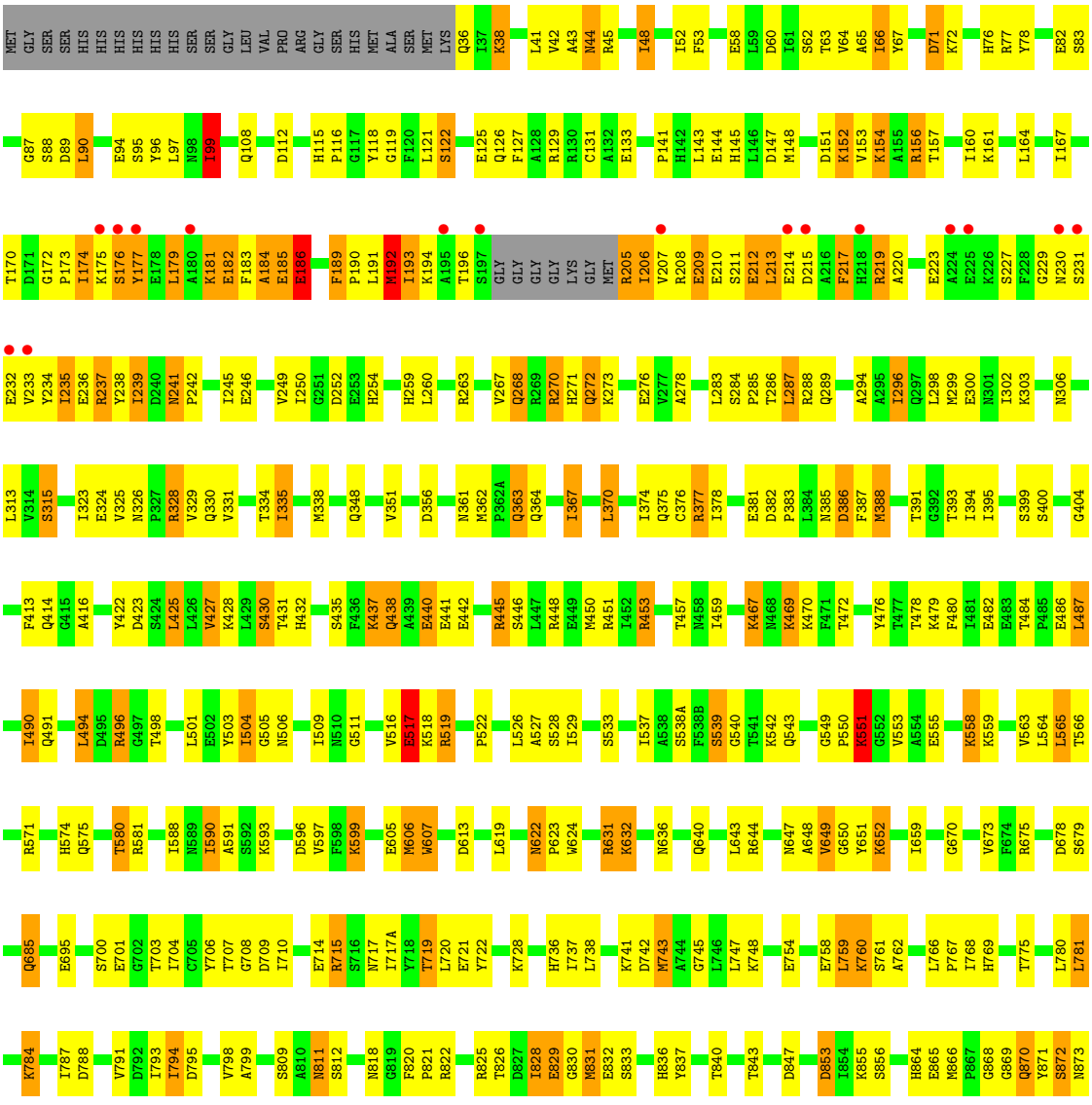
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	15	10	2	2	1	0	0

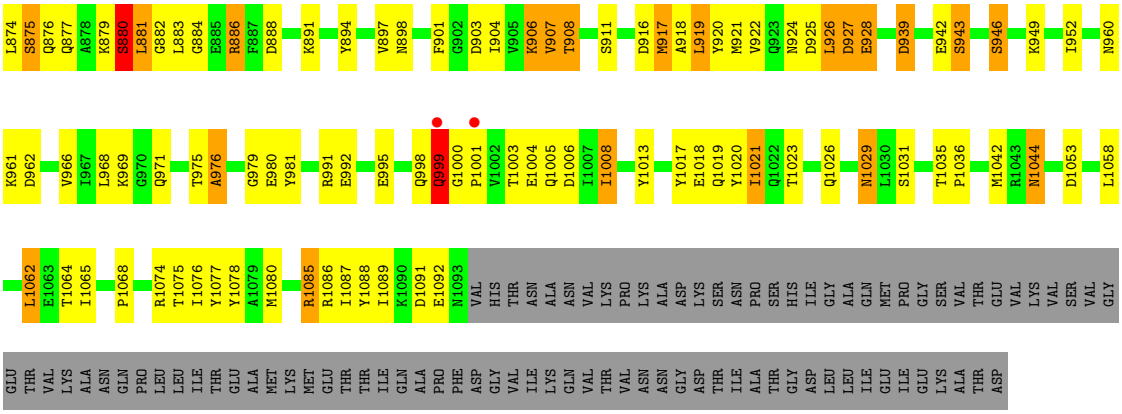
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

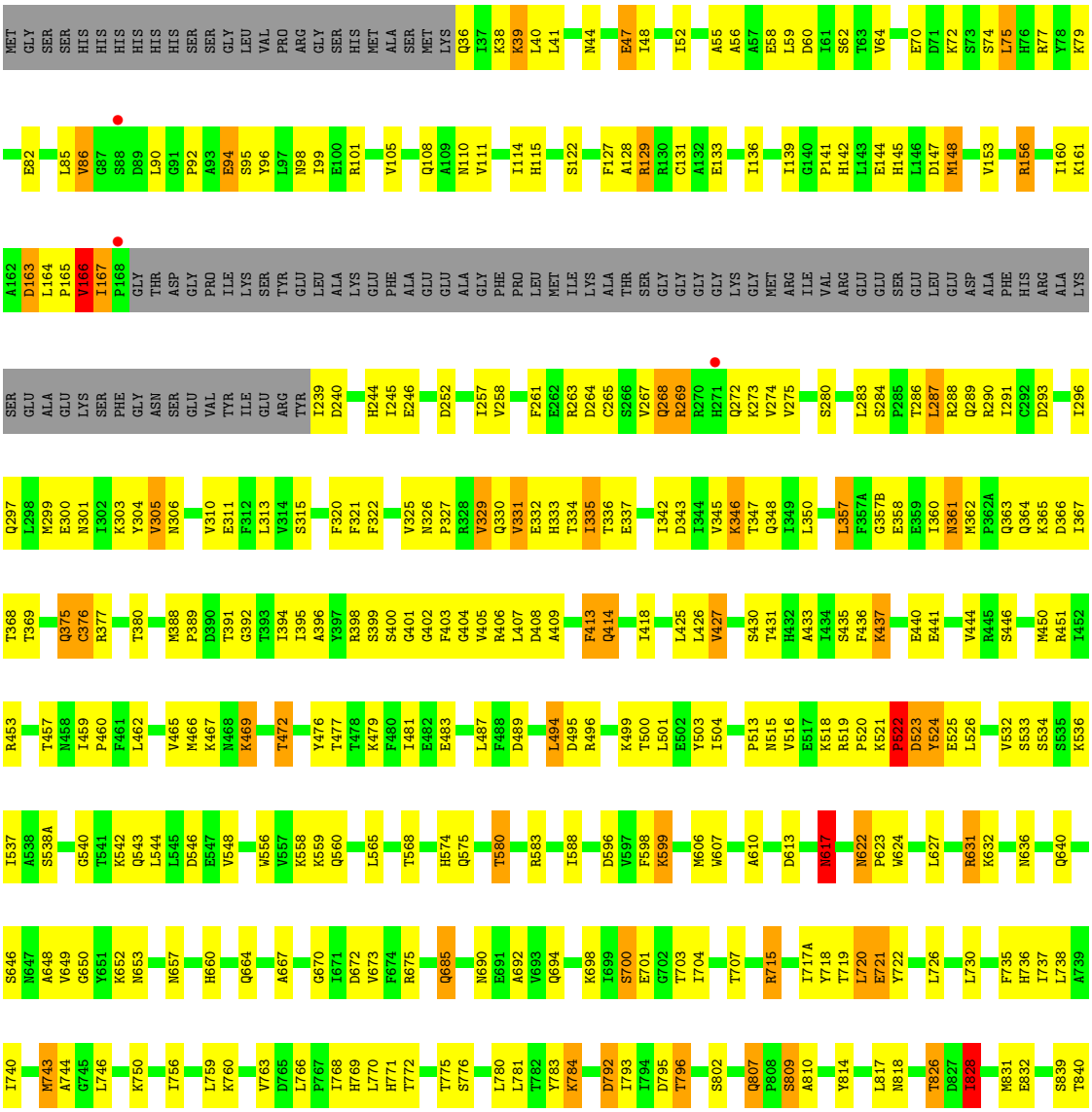
Chain A:

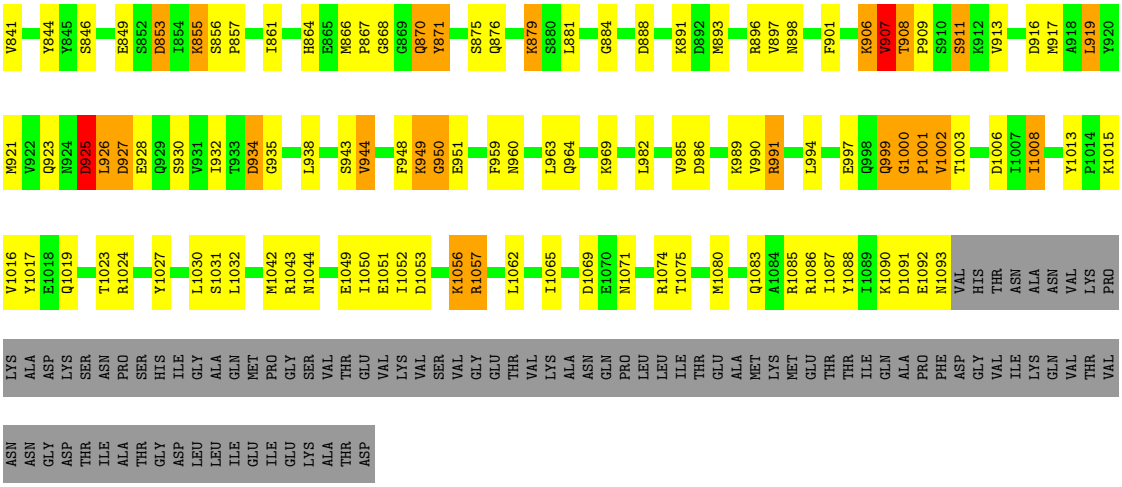




• Molecule 1: Pyruvate carboxylase

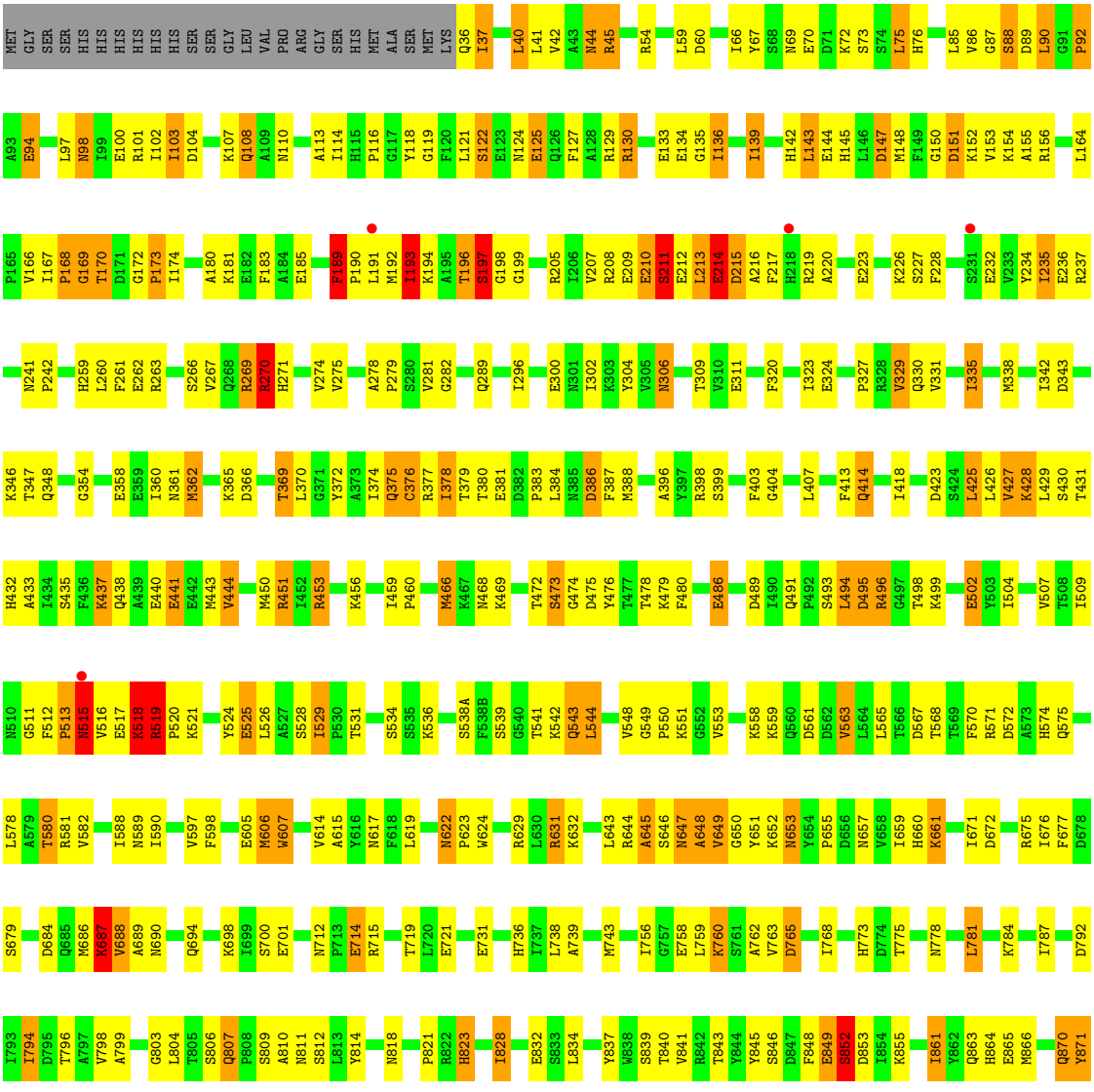
Chain B:

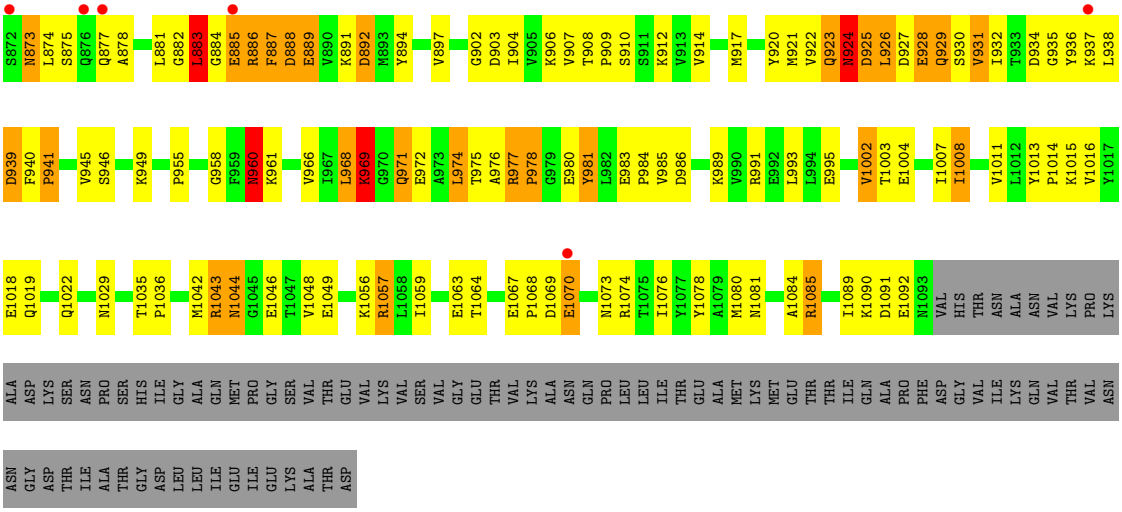




• Molecule 1: Pyruvate carboxylase

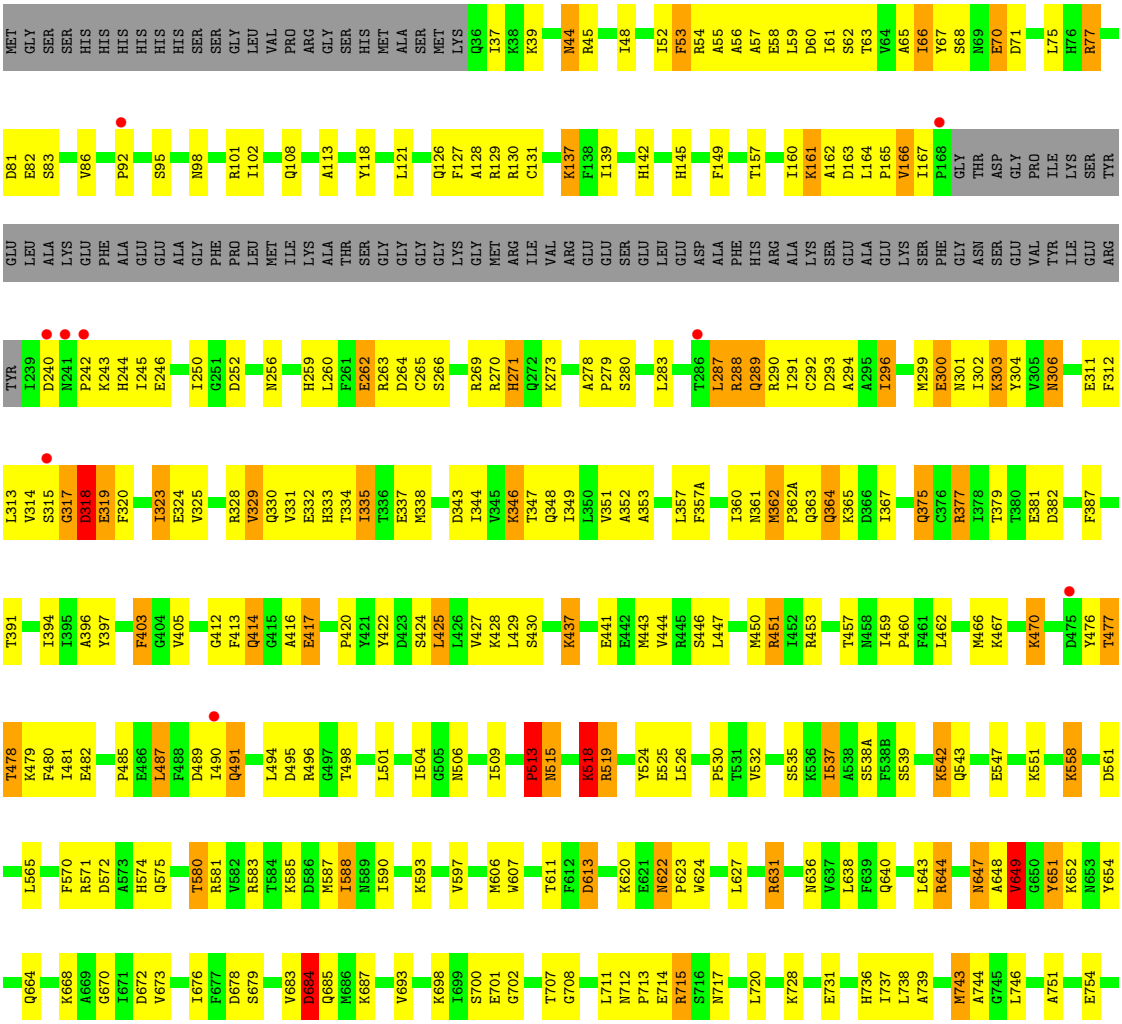
Chain C:

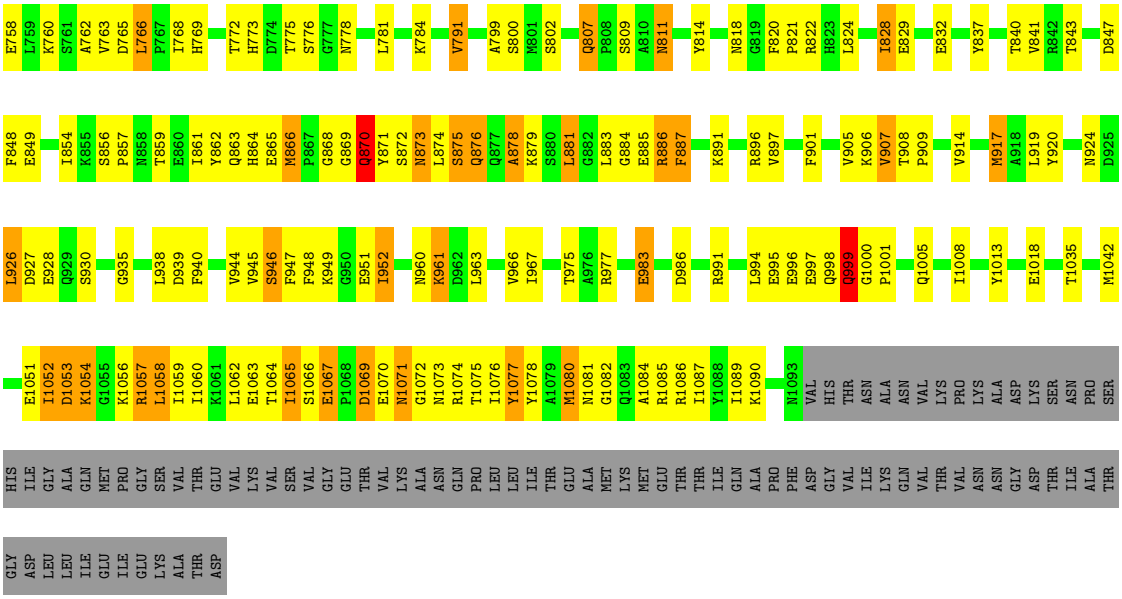




• Molecule 1: Pyruvate carboxylase

Chain D:




E758 L759 K760 S761 A762 V763 D765 L766 P767 I768 H769 T772 H773 D774 T775 S776 G777 N778 L781 K784 V791 A799 S800 M801 S802 Q807 P808 S809 A810 N811 Y814 N818 G819 F820 P821 R822 H823 L824 I828 E829 E832 Y837 T840 V841 R842 T843 D847
F848 E849 I854 K855 S856 P857 N858 T859 E860 I861 Y862 Q863 H864 E865 M866 P867 G868 G869 Q870 Y871 S872 N873 L874 S875 Q876 Q877 A878 K879 S880 L881 G882 L883 G884 E885 R886 F887 K891 R896 V897 F901 V905 K906 V907 T908 P909 V914 M917 A918 L919 Y920 N924 D925
L926 D927 E928 Q929 S930 G935 L938 D939 F940 V944 V945 S946 F947 F948 K949 G950 E951 I952 N960 K961 D962 L963 V966 I967 T975 A976 R977 E983 D986 R991 L994 E995 E996 E997 Q998 N999 G1000 P1001 Q1005 I1008 Y1013 E1018 T1035 M1042
E1051 I1052 D1053 K1054 G1055 K1056 R1057 L1058 I1059 I1060 K1061 L1062 E1063 T1064 I1065 S1066 E1067 P1068 D1069 E1070 N1071 G1072 N1073 R1074 T1075 I1076 Y1077 Y1078 A1079 M1080 N1081 G1082 Q1083 A1084 R1085 R1086 I1087 Y1088 I1089 K1090 N1093 VAL HIS THR ASN ALA ASN VAL LYS PRO LYS ALA ASP LYS SER ASN PRO SER
HIS ILE GLY ALA GLN MET PRO GLY SER VAL THR GLU VAL LYS VAL SER VAL GLY GLU THR VAL LYS ALA ASN GLN PRO LEU LEU ILE THR GLU ALA MET LYS MET GLU THR THR ILE GLN ALA PRO PHE ASP GLY VAL ILE LYS GLN VAL THR VAL ASN ASN GLY ASP THR ILE ALA THR
GLY ASP LEU LEU ILE GLU ILE GLU LYS ALA THR ASP

4 Data and refinement statistics (i)

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

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	0/8504	0.69	3/11500 (0.0%)
1	B	0.46	2/7990 (0.0%)	0.57	0/10811
1	C	0.53	5/8542 (0.1%)	0.61	3/11549 (0.0%)
1	D	0.59	2/7990 (0.0%)	0.68	4/10811 (0.0%)
All	All	0.55	9/33026 (0.0%)	0.64	10/44671 (0.0%)

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

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

All (9) bond length outliers are listed below:

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

All (10) bond angle outliers are listed below:

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

There are no chirality outliers.

All (9) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:GLY:H	1:B:543:GLN:NE2	1.88	0.71
1:D:53:PHE:HA	1:D:63:THR:HG21	1.72	0.71
1:B:640:GLN:HG3	1:B:673:VAL:HB	1.70	0.71
1:D:960:ASN:HB3	1:D:963:LEU:HB3	1.71	0.71
1:B:343:ASP:CG	1:B:346:LYS:HB2	2.11	0.71
1:B:1008:ILE:H	1:B:1008:ILE:CD1	2.04	0.71
1:D:518:LYS:HD2	1:D:518:LYS:C	2.11	0.71
1:B:306:ASN:OD1	1:B:348:GLN:HG3	1.91	0.71
1:D:453:ARG:HH12	1:D:495:ASP:HB3	1.55	0.71
1:B:477:THR:OG1	1:B:479:LYS:HB2	1.91	0.71
1:D:164:LEU:HD13	1:D:294:ALA:HB1	1.73	0.71
1:D:840:THR:O	1:D:843:THR:HB	1.90	0.71
1:B:144:GLU:O	1:B:148:MET:HB2	1.91	0.71
1:A:382:ASP:O	1:A:387:PHE:HA	1.90	0.71
1:B:898:ASN:HD22	1:B:906:LYS:HE3	1.56	0.71
1:A:164:LEU:HD22	1:A:294:ALA:HB1	1.72	0.71
1:D:391:THR:HG21	1:D:420:PRO:HB3	1.73	0.71
1:A:179:LEU:HG	1:A:217:PHE:HE2	1.56	0.70
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.24	0.70
1:A:632:LYS:NZ	1:A:632:LYS:HB2	2.06	0.70
1:C:259:HIS:O	1:C:260:LEU:HD23	1.91	0.70
1:A:622:ASN:HD22	1:A:624:TRP:H	1.38	0.70
1:C:525:GLU:OE2	1:C:525:GLU:HA	1.91	0.70
1:C:968:LEU:O	1:C:969:LYS:C	2.30	0.70
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.73	0.70
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.26	0.70
1:D:622:ASN:HD22	1:D:622:ASN:C	1.94	0.70
1:A:1000:GLY:H	1:A:1001:PRO:HD2	1.56	0.70
1:B:893:MET:O	1:B:897:VAL:HG23	1.92	0.70
1:C:166:VAL:HG12	1:C:167:ILE:H	1.55	0.70
1:A:173:PRO:HA	1:A:234:TYR:HB3	1.73	0.69
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.28	0.69
1:C:130:ARG:O	1:C:134:GLU:HG2	1.92	0.69
1:D:513:PRO:CD	4:D:1201:BTI:H11	2.20	0.69
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.75	0.69
1:B:363:GLN:OE1	1:B:363:GLN:HA	1.92	0.69
1:A:644:ARG:NH2	1:A:908:THR:CG2	2.56	0.69
1:D:142:HIS:HB2	1:D:145:HIS:HD2	1.56	0.69
1:A:191:LEU:O	1:A:238:TYR:HB2	1.92	0.69
1:B:395:ILE:HB	1:B:1086:ARG:HB2	1.74	0.69
1:B:494:LEU:HG	1:B:499:LYS:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:LEU:HB2	1:C:496:ARG:HH22	1.58	0.69
1:C:544:LEU:HD23	1:C:553:VAL:HG22	1.74	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.28	0.69
1:D:700:SER:H	1:D:736:HIS:HD2	1.39	0.69
1:A:254:HIS:CD2	1:A:356:ASP:HB2	2.27	0.68
1:B:275:VAL:HG21	1:B:466:MET:HE1	1.74	0.68
1:A:193:ILE:HG23	1:A:193:ILE:O	1.94	0.68
1:B:457:THR:OG1	1:B:459:ILE:HG12	1.93	0.68
1:D:334:THR:HA	1:D:337:GLU:HG3	1.74	0.68
1:B:704:ILE:N	1:B:704:ILE:HD13	2.06	0.68
1:D:580:THR:CG2	1:D:611:THR:HG22	2.23	0.68
1:B:770:LEU:HD12	1:B:771:HIS:N	2.08	0.68
1:D:542:LYS:HE2	1:D:631:ARG:NH2	2.09	0.68
1:C:92:PRO:HD2	1:C:94:GLU:OE2	1.94	0.68
1:C:864:HIS:CD2	1:C:866:MET:HG3	2.28	0.68
1:D:960:ASN:HD22	1:D:963:LEU:H	1.42	0.68
1:D:1071:ASN:HB3	1:D:1073:ASN:ND2	2.07	0.68
1:D:684:ASP:HA	1:D:687:LYS:HE2	1.75	0.68
1:D:1076:ILE:CD1	1:D:1089:ILE:HD13	2.23	0.68
1:A:254:HIS:HD2	1:A:356:ASP:HB2	1.58	0.67
1:A:144:GLU:O	1:A:148:MET:HB2	1.94	0.67
1:A:820:PHE:HB3	1:A:821:PRO:CD	2.24	0.67
1:C:144:GLU:O	1:C:148:MET:HB2	1.93	0.67
1:D:453:ARG:HH22	1:D:495:ASP:HB2	1.59	0.67
1:A:540:GLY:H	1:A:543:GLN:HE21	1.43	0.67
1:B:156:ARG:NH2	1:B:167:ILE:HG12	2.09	0.67
1:B:1085:ARG:HG3	1:B:1086:ARG:H	1.59	0.67
1:C:574:HIS:CD2	1:C:582:VAL:HB	2.30	0.67
1:A:90:LEU:HD22	1:A:95:SER:HA	1.76	0.67
1:A:709:ASP:OD1	1:A:748:LYS:NZ	2.26	0.67
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.24	0.67
1:A:949:LYS:HE3	1:A:971:GLN:OE1	1.95	0.67
1:D:252:ASP:HA	1:D:351:VAL:HG13	1.77	0.67
1:B:142:HIS:H	1:B:145:HIS:HD2	1.43	0.67
1:B:413:PHE:O	1:B:414:GLN:HB2	1.93	0.67
1:B:700:SER:N	1:B:736:HIS:HD2	1.93	0.67
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.42	0.67
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.76	0.67
1:B:41:LEU:HB2	1:B:111:VAL:HG21	1.76	0.67
1:C:269:ARG:HB2	1:C:269:ARG:HH11	1.59	0.67

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:HD12	1:C:86:VAL:HG21	1.83	0.60
1:A:425:LEU:HD12	1:A:425:LEU:C	2.22	0.60
1:D:39:LYS:HG3	1:D:62:SER:HB3	1.83	0.60
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.82	0.60
1:C:864:HIS:HD2	1:C:866:MET:H	1.48	0.60
1:B:263:ARG:HH21	1:B:330:GLN:HE21	1.49	0.60
1:B:744:ALA:HB3	1:B:746:LEU:HG	1.83	0.60
1:A:856:SER:OG	1:D:800:SER:HA	2.01	0.60
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.67	0.60
1:C:210:GLU:O	1:C:212:GLU:N	2.35	0.60
1:A:866:MET:HG2	1:A:894:TYR:CE2	2.36	0.60
1:C:118:TYR:CZ	1:C:331:VAL:HG22	2.36	0.60
1:C:926:LEU:HB3	1:C:930:SER:HB3	1.84	0.60
1:D:613:ASP:HB2	1:D:1013:TYR:CZ	2.37	0.60
1:A:383:PRO:HA	1:A:387:PHE:CE2	2.36	0.60
1:C:927:ASP:OD1	1:C:929:GLN:HG2	2.02	0.59
1:D:1076:ILE:HD11	1:D:1089:ILE:HD13	1.83	0.59
1:A:719:THR:O	1:A:722:TYR:N	2.34	0.59
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.60	0.59
1:C:261:PHE:CD1	1:C:369:THR:CG2	2.84	0.59
1:C:386:ASP:O	1:C:387:PHE:HB2	2.01	0.59
1:D:269:ARG:HG3	1:D:270:ARG:H	1.66	0.59
1:D:343:ASP:CG	1:D:346:LYS:HB2	2.21	0.59
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.83	0.59
1:A:1044:ASN:N	1:A:1044:ASN:ND2	2.50	0.59
1:B:469:LYS:H	1:B:469:LYS:HD3	1.67	0.59
1:C:269:ARG:HH11	1:C:269:ARG:CB	2.15	0.59
1:C:882:GLY:O	1:C:884:GLY:N	2.34	0.59
1:D:1076:ILE:HD13	1:D:1089:ILE:CD1	2.32	0.59
1:B:245:ILE:HG12	1:B:283:LEU:HD11	1.84	0.59
1:C:335:ILE:HD11	1:C:374:ILE:C	2.23	0.59
1:D:290:ARG:HE	1:D:320:PHE:HE1	1.50	0.59
1:D:349:ILE:O	1:D:349:ILE:CG2	2.50	0.59
1:D:558:LYS:HD2	1:D:765:ASP:O	2.02	0.59
1:A:52:ILE:HD12	1:A:115:HIS:CD2	2.37	0.59
1:C:494:LEU:HD23	1:C:496:ARG:HH21	1.67	0.59
1:C:870:GLN:O	1:C:870:GLN:CG	2.37	0.59
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.38	0.59
1:A:738:LEU:HD21	1:A:759:LEU:CD1	2.33	0.59
1:C:871:TYR:O	1:C:875:SER:HB2	2.03	0.59
1:D:278:ALA:HB2	1:D:335:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.84	0.59
1:A:254:HIS:HD2	1:A:356:ASP:CB	2.15	0.59
1:C:189:PHE:H	1:C:190:PRO:CD	2.16	0.59
1:C:1043:ARG:HD3	1:C:1046:GLU:HB2	1.85	0.59
1:A:413:PHE:CE2	1:A:416:ALA:HB2	2.38	0.58
1:B:763:VAL:C	1:B:766:LEU:H	2.06	0.58
1:C:41:LEU:C	1:C:41:LEU:HD23	2.23	0.58
1:A:209:GLU:HA	1:A:213:LEU:CD2	2.28	0.58
1:A:866:MET:CE	1:A:870:GLN:HG2	2.16	0.58
1:B:322:PHE:HE2	1:B:325:VAL:HG23	1.68	0.58
1:C:438:GLN:HA	1:C:441:GLU:CD	2.24	0.58
1:D:530:PRO:HB2	1:D:593:LYS:HD3	1.85	0.58
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.36	0.58
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.18	0.58
1:D:331:VAL:HG11	1:D:377:ARG:HD3	1.84	0.58
1:D:917:MET:HG2	1:D:944:VAL:CG2	2.27	0.58
1:A:313:LEU:HD22	1:A:323:ILE:CD1	2.33	0.58
1:A:921:MET:HG2	1:A:926:LEU:HB3	1.85	0.58
1:C:269:ARG:CG	1:C:270:ARG:H	2.17	0.58
1:B:413:PHE:O	1:B:414:GLN:CB	2.48	0.58
1:D:53:PHE:CZ	1:D:65:ALA:HB2	2.38	0.58
1:D:477:THR:C	1:D:479:LYS:H	2.05	0.58
1:D:644:ARG:NH1	1:D:908:THR:HG22	2.19	0.58
1:A:864:HIS:CD2	1:A:866:MET:CG	2.76	0.58
1:B:39:LYS:HG3	1:B:111:VAL:HA	1.84	0.58
1:B:437:LYS:HE3	1:B:437:LYS:CA	2.34	0.58
1:C:650:GLY:HA2	1:C:1013:TYR:HE1	1.65	0.58
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.85	0.58
1:D:828:ILE:O	1:D:832:GLU:HG2	2.02	0.58
1:A:273:LYS:HB3	1:A:276:GLU:OE2	2.04	0.58
1:B:332:GLU:HA	1:B:375:GLN:NE2	2.19	0.58
1:B:376:CYS:SG	1:B:462:LEU:HD13	2.43	0.58
1:B:406:ARG:NH1	1:D:403:PHE:HB2	2.19	0.58
1:C:572:ASP:HB3	1:C:807:GLN:NE2	2.19	0.58
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.68	0.58
1:A:644:ARG:HG2	1:A:647:ASN:OD1	2.02	0.58
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.58
1:C:205:ARG:NH1	1:C:223:GLU:OE1	2.36	0.58
1:C:940:PHE:HB3	1:C:941:PRO:HD2	1.86	0.58
1:A:296:ILE:O	1:A:300:GLU:HB2	2.04	0.58
1:B:999:GLN:HG2	1:B:1000:GLY:H	1.69	0.58

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	1:A:870:GLN:C	2.50	0.49
1:A:1020:TYR:CD2	1:A:1021:ILE:HD12	2.47	0.49
1:A:1087:ILE:CG2	1:A:1089:ILE:HD11	2.42	0.49
1:B:631:ARG:HG2	1:B:670:GLY:HA3	1.94	0.49
1:B:652:LYS:HG3	1:B:653:ASN:H	1.77	0.49
1:C:873:ASN:O	1:C:877:GLN:HG2	2.12	0.49
1:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.94	0.49
1:A:87:GLY:C	1:A:89:ASP:N	2.66	0.49
1:B:165:PRO:O	1:B:166:VAL:HG13	2.12	0.49
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.47	0.49
1:C:529:ILE:HG21	1:C:589:ASN:HB3	1.95	0.49
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.76	0.49
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.93	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:A:242:PRO:O	1:A:478:THR:HG23	2.13	0.49
1:B:704:ILE:HG12	1:B:738:LEU:HD11	1.94	0.49
1:B:879:LYS:HG3	1:B:884:GLY:HA3	1.95	0.49
1:B:574:HIS:CD2	1:B:580:THR:HA	2.48	0.49
1:B:701:GLU:OE2	1:B:737:ILE:CG2	2.59	0.49
1:C:114:ILE:HG13	1:C:136:ILE:CG2	2.43	0.49
1:C:136:ILE:N	1:C:136:ILE:CD1	2.69	0.49
1:C:597:VAL:HG11	1:C:834:LEU:HD12	1.95	0.49
1:D:873:ASN:ND2	1:D:873:ASN:H	2.07	0.49
1:A:820:PHE:HB3	1:A:821:PRO:HD2	1.94	0.49
1:B:763:VAL:HB	1:B:766:LEU:HB2	1.95	0.49
1:C:622:ASN:HD22	1:C:623:PRO:N	2.11	0.49
1:A:715:ARG:NH1	1:A:865:GLU:OE2	2.46	0.49
1:B:395:ILE:HG12	1:B:453:ARG:O	2.13	0.49
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.28	0.49
1:D:252:ASP:HA	1:D:351:VAL:CG1	2.43	0.49
1:D:728:LYS:HE2	1:D:762:ALA:HB1	1.95	0.49
1:D:917:MET:CG	1:D:944:VAL:CG2	2.89	0.49
1:A:71:ASP:OD2	1:A:422:TYR:CE1	2.65	0.48
1:B:99:ILE:HG23	1:B:127:PHE:HA	1.95	0.48
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.59	0.48
1:C:59:LEU:O	1:C:60:ASP:HB3	2.13	0.48
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.28	0.48
1:A:385:ASN:O	1:A:387:PHE:N	2.46	0.48
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.95	0.48
1:D:506:ASN:HD22	4:D:1201:BTI:H92	1.78	0.48
1:D:509:ILE:HD13	1:D:1074:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1053:ASP:O	1:D:1054:LYS:C	2.51	0.48
1:A:177:TYR:C	1:A:179:LEU:N	2.67	0.48
1:A:329:VAL:CG2	1:A:348:GLN:OE1	2.61	0.48
1:B:772:THR:HG22	1:B:783:TYR:CZ	2.48	0.48
1:C:191:LEU:HA	1:C:237:ARG:HA	1.95	0.48
1:C:615:ALA:HA	1:C:619:LEU:HB2	1.95	0.48
1:D:412:GLY:O	1:D:413:PHE:HB3	2.14	0.48
1:D:587:MET:HA	1:D:590:ILE:HD11	1.95	0.48
1:A:435:SER:OG	1:A:438:GLN:HB2	2.14	0.48
1:A:469:LYS:HD2	1:A:469:LYS:HA	1.58	0.48
1:A:784:LYS:HD3	1:A:784:LYS:O	2.12	0.48
1:B:258:VAL:HB	1:B:364:GLN:OE1	2.13	0.48
1:C:924:ASN:O	1:C:925:ASP:CB	2.60	0.48
1:D:397:TYR:HA	1:D:451:ARG:O	2.13	0.48
1:D:504:ILE:CG2	1:D:1042:MET:HG3	2.44	0.48
1:D:1071:ASN:HB3	1:D:1073:ASN:HD22	1.79	0.48
1:D:1089:ILE:CG2	1:D:1090:LYS:N	2.76	0.48
1:A:38:LYS:HB3	1:A:38:LYS:HE2	1.61	0.48
1:A:364:GLN:HA	1:A:367:ILE:HG13	1.94	0.48
1:B:565:LEU:HD11	1:B:598:PHE:HE2	1.79	0.48
1:B:802:SER:OG	1:B:809:SER:HB2	2.14	0.48
1:C:580:THR:HB	1:C:614:VAL:HG21	1.94	0.48
1:C:938:LEU:O	1:C:939:ASP:O	2.32	0.48
1:C:1019:GLN:HA	1:C:1022:GLN:NE2	2.28	0.48
1:D:590:ILE:HG13	1:D:837:TYR:CE2	2.48	0.48
1:A:78:TYR:CE2	1:C:1081:ASN:HA	2.49	0.48
1:B:287:LEU:O	1:B:291:ILE:HG13	2.14	0.48
1:C:152:LYS:HE2	1:C:324:GLU:OE2	2.13	0.48
1:C:278:ALA:CB	1:C:335:ILE:CG2	2.91	0.48
1:C:756:ILE:O	1:C:760:LYS:HB2	2.14	0.48
1:D:429:LEU:HD23	1:D:443:MET:SD	2.53	0.48
1:A:94:GLU:O	1:A:94:GLU:CG	2.58	0.48
1:A:871:TYR:HE1	1:A:891:LYS:CD	2.25	0.48
1:B:580:THR:HG21	1:B:610:ALA:HB3	1.96	0.48
1:C:360:ILE:O	1:C:362:MET:N	2.46	0.48
1:D:983:GLU:HA	1:D:983:GLU:OE2	2.13	0.48
1:D:1065:ILE:HG23	1:D:1076:ILE:HG13	1.95	0.48
1:A:791:VAL:O	1:A:822:ARG:NH2	2.37	0.48
1:A:1003:THR:HG22	1:A:1006:ASP:OD2	2.14	0.48
1:C:570:PHE:O	1:C:574:HIS:HE1	1.96	0.48
1:D:664:GLN:O	1:D:668:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LEU:HD12	1:D:165:PRO:HD2	1.96	0.48
1:B:284:SER:OG	1:B:287:LEU:HB2	2.14	0.48
1:C:213:LEU:C	1:C:215:ASP:N	2.67	0.48
1:D:118:TYR:CZ	1:D:331:VAL:HG22	2.49	0.48
1:A:156:ARG:NH1	1:A:167:ILE:O	2.47	0.47
1:A:313:LEU:CD2	1:A:323:ILE:HD11	2.39	0.47
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.96	0.47
1:C:438:GLN:HA	1:C:441:GLU:HG2	1.97	0.47
1:C:882:GLY:C	1:C:884:GLY:N	2.67	0.47
1:D:66:ILE:HB	1:D:86:VAL:HG23	1.96	0.47
1:D:896:ARG:HD2	1:D:928:GLU:OE2	2.13	0.47
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.95	0.47
1:D:1075:THR:HG22	1:D:1077:TYR:CE1	2.49	0.47
1:A:1003:THR:CG2	1:A:1006:ASP:H	2.24	0.47
1:B:1042:MET:HE1	1:B:1062:LEU:HB2	1.95	0.47
1:C:738:LEU:HD21	1:C:759:LEU:HD13	1.97	0.47
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.79	0.47
1:B:286:THR:O	1:B:290:ARG:CG	2.62	0.47
1:B:396:ALA:HB3	1:B:453:ARG:HB2	1.96	0.47
1:B:652:LYS:HG3	1:B:653:ASN:N	2.29	0.47
1:D:593:LYS:O	1:D:597:VAL:HG23	2.15	0.47
1:D:883:LEU:O	1:D:886:ARG:HG2	2.15	0.47
1:A:189:PHE:CE2	1:A:208:ARG:HD2	2.50	0.47
1:A:879:LYS:C	1:A:881:LEU:H	2.18	0.47
1:B:565:LEU:HD21	1:B:826:THR:CG2	2.44	0.47
1:C:381:GLU:O	1:C:383:PRO:HD3	2.15	0.47
1:C:644:ARG:HA	1:C:677:PHE:CE1	2.49	0.47
1:C:686:MET:O	1:C:687:LYS:C	2.53	0.47
1:D:720:LEU:HD21	1:D:758:GLU:CG	2.37	0.47
1:A:193:ILE:O	1:A:193:ILE:CG2	2.60	0.47
1:A:263:ARG:HH21	1:A:330:GLN:HE21	1.63	0.47
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.44	0.47
1:A:979:GLY:O	1:A:981:TYR:N	2.47	0.47
1:B:36:GLN:O	1:B:36:GLN:HG2	2.15	0.47
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.80	0.47
1:B:414:GLN:OE1	1:D:1082:GLY:O	2.32	0.47
1:B:519:ARG:CB	1:B:520:PRO:CD	2.90	0.47
1:B:556:TRP:O	1:B:560:GLN:NE2	2.43	0.47
1:B:740:ILE:HD11	1:B:759:LEU:CD1	2.44	0.47
1:B:864:HIS:HD2	1:B:866:MET:H	1.63	0.47
1:C:902:GLY:O	1:C:903:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.95	0.47
1:A:239:ILE:CD1	1:A:315:SER:HB3	2.44	0.47
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.97	0.47
1:B:59:LEU:HD22	1:B:350:LEU:HD21	1.97	0.47
1:B:394:ILE:O	1:B:414:GLN:O	2.33	0.47
1:C:130:ARG:NH1	1:C:133:GLU:OE1	2.47	0.47
1:C:814:TYR:CZ	1:C:828:ILE:HG13	2.49	0.47
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.47
1:D:760:LYS:CD	1:D:768:ILE:HD12	2.44	0.47
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.65	0.47
1:B:867:PRO:O	1:B:870:GLN:HB2	2.14	0.47
1:D:712:ASN:OD1	1:D:714:GLU:HG2	2.15	0.47
1:A:325:VAL:CG1	1:A:326:ASN:N	2.77	0.47
1:A:853:ASP:OD2	1:A:853:ASP:N	2.41	0.47
1:A:875:SER:C	1:A:877:GLN:N	2.68	0.47
1:A:879:LYS:O	1:A:881:LEU:N	2.48	0.47
1:A:979:GLY:C	1:A:981:TYR:H	2.18	0.47
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.70	0.47
1:C:606:MET:HE1	1:C:671:ILE:HD11	1.95	0.47
1:C:760:LYS:NZ	1:C:792:ASP:OD2	2.46	0.47
1:D:54:ARG:O	1:D:58:GLU:HG3	2.15	0.47
1:D:938:LEU:O	1:D:939:ASP:HB3	2.14	0.47
1:A:440:GLU:O	1:A:440:GLU:HG2	2.15	0.46
1:B:129:ARG:O	1:B:133:GLU:HG3	2.15	0.46
1:B:501:LEU:CD1	1:B:1085:ARG:HG2	2.45	0.46
1:D:565:LEU:HD23	1:D:824:LEU:HD11	1.96	0.46
1:B:465:VAL:HG22	1:B:487:LEU:CD2	2.45	0.46
1:B:540:GLY:N	1:B:543:GLN:HE21	2.06	0.46
1:C:407:LEU:HD21	1:C:429:LEU:HD13	1.96	0.46
1:D:343:ASP:OD2	1:D:343:ASP:C	2.54	0.46
1:D:477:THR:C	1:D:479:LYS:N	2.68	0.46
1:A:174:ILE:HB	1:A:179:LEU:HD13	1.97	0.46
1:A:968:LEU:O	1:A:969:LYS:C	2.53	0.46
1:B:459:ILE:N	1:B:460:PRO:HD2	2.30	0.46
1:C:866:MET:HG2	1:C:894:TYR:CE2	2.50	0.46
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.63	0.46
1:D:647:ASN:O	1:D:649:VAL:N	2.47	0.46
1:A:879:LYS:O	1:A:882:GLY:N	2.42	0.46
1:A:1035:THR:HB	1:A:1036:PRO:HD3	1.98	0.46
1:C:949:LYS:HD2	1:C:971:GLN:OE1	2.15	0.46
1:C:977:ARG:O	1:C:978:PRO:C	2.53	0.46

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG22	1:B:325:VAL:HG22	1.98	0.45
1:B:437:LYS:HE3	1:B:437:LYS:HA	1.97	0.45
1:B:1091:ASP:C	1:B:1093:ASN:N	2.69	0.45
1:C:473:SER:OG	1:C:474:GLY:N	2.49	0.45
1:A:53:PHE:CZ	1:A:65:ALA:HB2	2.52	0.45
1:A:211:SER:C	1:A:213:LEU:H	2.19	0.45
1:A:329:VAL:CG2	1:A:348:GLN:NE2	2.80	0.45
1:A:719:THR:O	1:A:720:LEU:C	2.54	0.45
1:A:870:GLN:OE1	1:A:911:SER:HB2	2.16	0.45
1:B:330:GLN:O	1:B:331:VAL:C	2.53	0.45
1:B:650:GLY:HA2	1:B:1013:TYR:CE1	2.51	0.45
1:C:995:GLU:CG	1:C:1002:VAL:CG2	2.86	0.45
1:D:245:ILE:O	1:D:312:PHE:HB2	2.16	0.45
1:A:208:ARG:HG3	1:A:208:ARG:O	2.16	0.45
1:A:453:ARG:HG3	1:A:453:ARG:NH1	2.31	0.45
1:A:565:LEU:HD23	1:A:565:LEU:C	2.33	0.45
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.26	0.45
1:C:98:ASN:C	1:C:98:ASN:HD22	2.19	0.45
1:C:837:TYR:CZ	1:C:841:VAL:HG21	2.52	0.45
1:A:94:GLU:HA	1:A:97:LEU:HD12	1.98	0.45
1:A:335:ILE:HD11	1:A:374:ILE:O	2.17	0.45
1:A:647:ASN:HA	1:A:659:ILE:HD11	1.99	0.45
1:A:704:ILE:HD12	1:A:738:LEU:HD11	1.99	0.45
1:B:391:THR:HG22	1:B:392:GLY:N	2.31	0.45
1:B:395:ILE:CG1	1:B:396:ALA:N	2.79	0.45
1:B:1032:LEU:HD13	1:B:1052:ILE:HA	1.99	0.45
1:C:864:HIS:CD2	1:C:866:MET:H	2.33	0.45
1:D:299:MET:HB3	1:D:304:TYR:HB3	1.99	0.45
1:D:337:GLU:HG2	1:D:344:ILE:CD1	2.46	0.45
1:A:43:ALA:HA	1:A:66:ILE:HD13	1.99	0.45
1:C:215:ASP:CB	1:C:219:ARG:HH22	2.29	0.45
1:C:304:TYR:OH	1:C:327:PRO:HA	2.16	0.45
1:C:690:ASN:O	1:C:694:GLN:HG2	2.16	0.45
1:D:738:LEU:HD12	1:D:739:ALA:N	2.32	0.45
1:B:481:ILE:HD12	1:B:481:ILE:H	1.82	0.45
1:C:380:THR:HG22	1:C:426:LEU:HD11	1.99	0.45
1:C:432:HIS:CG	1:C:433:ALA:N	2.84	0.45
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.81	0.45
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.51	0.45
1:A:237:ARG:NH1	1:A:237:ARG:CG	2.71	0.45
1:A:259:HIS:CD2	1:A:296:ILE:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:GLY:HA2	1:A:715:ARG:NH1	2.32	0.45
1:A:1065:ILE:N	1:A:1065:ILE:HD12	2.32	0.45
1:B:257:ILE:HD12	1:B:300:GLU:OE1	2.16	0.45
1:B:402:GLY:H	1:B:405:VAL:HG21	1.82	0.45
1:B:846:SER:HA	1:B:849:GLU:CG	2.46	0.45
1:C:512:PHE:C	1:C:512:PHE:CD2	2.90	0.45
1:C:1069:ASP:OD2	1:C:1073:ASN:O	2.34	0.45
1:A:975:THR:O	1:A:976:ALA:HB2	2.16	0.45
1:A:1017:TYR:CZ	1:A:1021:ILE:HD13	2.52	0.45
1:B:164:LEU:HB3	1:B:165:PRO:HD2	1.98	0.45
1:B:400:SER:OG	1:B:401:GLY:N	2.50	0.45
1:B:627:LEU:HD12	1:B:627:LEU:O	2.17	0.45
1:C:731:GLU:OE1	1:C:763:VAL:HB	2.17	0.45
1:D:331:VAL:HG12	1:D:375:GLN:HE22	1.82	0.45
1:A:259:HIS:C	1:A:260:LEU:HD23	2.37	0.45
1:A:533:SER:O	1:A:537:ILE:HG12	2.17	0.45
1:A:880:SER:O	1:A:880:SER:OG	2.34	0.45
1:A:1068:PRO:HD3	1:A:1074:ARG:HE	1.81	0.45
1:B:871:TYR:O	1:B:871:TYR:HD1	1.97	0.45
1:C:261:PHE:CD1	1:C:369:THR:HG22	2.52	0.45
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.35	0.45
1:D:245:ILE:HG21	1:D:283:LEU:HD11	1.99	0.45
1:D:1076:ILE:HD13	1:D:1089:ILE:HD13	1.93	0.45
1:A:65:ALA:O	1:A:83:SER:HA	2.17	0.45
1:A:90:LEU:HD21	1:A:94:GLU:HG3	2.00	0.45
1:A:181:LYS:O	1:A:182:GLU:HB3	2.17	0.45
1:A:643:LEU:CD1	1:A:648:ALA:HA	2.47	0.45
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.82	0.44
1:A:212:GLU:N	1:A:213:LEU:HD23	2.32	0.44
1:A:1058:LEU:HD22	1:A:1080:MET:SD	2.58	0.44
1:B:646:SER:HB3	1:B:685:GLN:NE2	2.26	0.44
1:C:145:HIS:HE1	1:C:302:ILE:O	1.99	0.44
1:C:524:TYR:CD2	1:C:843:THR:HG22	2.51	0.44
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.52	0.44
1:D:302:ILE:O	1:D:303:LYS:C	2.55	0.44
1:D:485:PRO:C	1:D:487:LEU:H	2.20	0.44
1:D:938:LEU:O	1:D:939:ASP:CB	2.62	0.44
1:B:239:ILE:CG2	1:B:313:LEU:HD21	2.47	0.44
1:B:960:ASN:HD22	1:B:963:LEU:H	1.65	0.44
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.32	0.44
1:C:807:GLN:H	1:C:807:GLN:HG2	1.62	0.44

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HD3	1:B:335:ILE:HG22	2.00	0.44
1:B:1049:GLU:C	1:B:1050:ILE:HG13	2.38	0.44
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.52	0.44
1:D:702:GLY:O	1:D:738:LEU:HD12	2.18	0.44
1:A:48:ILE:HG13	1:A:118:TYR:CE2	2.53	0.43
1:B:1080:MET:CE	1:B:1085:ARG:NH2	2.81	0.43
1:C:374:ILE:HG22	1:C:443:MET:CE	2.47	0.43
1:C:571:ARG:NH2	1:C:605:GLU:OE1	2.50	0.43
1:C:631:ARG:HD3	1:C:631:ARG:O	2.18	0.43
1:D:627:LEU:O	1:D:631:ARG:HB2	2.17	0.43
1:D:744:ALA:HB3	1:D:746:LEU:HG	1.99	0.43
1:D:818:ASN:N	1:D:818:ASN:HD22	2.15	0.43
1:D:917:MET:HE3	1:D:940:PHE:HD2	1.82	0.43
1:A:38:LYS:N	1:A:112:ASP:OD1	2.47	0.43
1:A:219:ARG:HA	1:A:219:ARG:NE	2.21	0.43
1:A:252:ASP:HA	1:A:351:VAL:HG13	2.00	0.43
1:A:563:VAL:HG11	1:A:794:ILE:HD12	1.98	0.43
1:B:521:LYS:HB3	1:B:1043:ARG:NH2	2.33	0.43
1:C:606:MET:HE1	1:C:671:ILE:HD12	2.00	0.43
1:C:798:VAL:O	1:C:799:ALA:C	2.57	0.43
1:D:264:ASP:HB2	1:D:280:SER:HA	1.99	0.43
1:D:1054:LYS:O	1:D:1054:LYS:HG3	2.18	0.43
1:A:239:ILE:CD1	1:A:315:SER:CB	2.95	0.43
1:A:799:ALA:N	1:A:811:ASN:ND2	2.67	0.43
1:B:59:LEU:O	1:B:60:ASP:HB2	2.18	0.43
1:B:814:TYR:CE2	1:B:828:ILE:HG21	2.53	0.43
1:B:891:LYS:HB2	1:B:891:LYS:HE3	1.85	0.43
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	2.00	0.43
1:D:814:TYR:CZ	1:D:828:ILE:HG13	2.54	0.43
1:A:820:PHE:HB3	1:A:821:PRO:HD3	1.99	0.43
1:A:866:MET:HE2	1:A:871:TYR:N	2.33	0.43
1:B:163:ASP:O	1:B:164:LEU:HD23	2.18	0.43
1:B:746:LEU:HA	1:B:746:LEU:HD23	1.74	0.43
1:C:563:VAL:HG23	1:C:823:HIS:O	2.18	0.43
1:C:643:LEU:HD23	1:C:676:ILE:HG12	1.99	0.43
1:C:715:ARG:HH21	1:C:865:GLU:CD	2.21	0.43
1:D:288:ARG:HA	1:D:291:ILE:HD12	2.00	0.43
1:A:706:TYR:O	1:A:743:MET:HE3	2.19	0.43
1:A:825:ARG:O	1:A:826:THR:HB	2.17	0.43
1:A:960:ASN:OD1	1:A:960:ASN:C	2.57	0.43
1:B:897:VAL:HG22	1:B:921:MET:HE3	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:GLU:OE1	1:B:1057:ARG:NH1	2.51	0.43
1:C:169:GLY:HA3	1:C:236:GLU:HA	2.00	0.43
1:C:193:ILE:CG1	1:C:235:ILE:HB	2.48	0.43
1:D:246:GLU:HB3	1:D:311:GLU:HA	2.00	0.43
1:D:640:GLN:HG3	1:D:673:VAL:CB	2.49	0.43
1:D:743:MET:CE	1:D:905:VAL:HG13	2.48	0.43
1:D:869:GLY:O	1:D:870:GLN:C	2.57	0.43
1:A:381:GLU:HA	1:A:388:MET:O	2.18	0.43
1:B:537:ILE:C	1:B:538(A):SER:H	2.22	0.43
1:B:1075:THR:HG1	1:B:1088:TYR:HE2	1.65	0.43
1:C:66:ILE:HB	1:C:86:VAL:CG2	2.49	0.43
1:C:358:GLU:OE1	1:C:358:GLU:HA	2.19	0.43
1:D:164:LEU:HA	1:D:165:PRO:HD2	1.89	0.43
1:D:1042:MET:HB2	1:D:1062:LEU:HD12	2.00	0.43
1:A:147:ASP:OD2	1:A:154:LYS:HE3	2.19	0.43
1:A:636:ASN:OD1	1:A:636:ASN:N	2.52	0.43
1:B:55:ALA:O	1:B:58:GLU:HB2	2.19	0.43
1:D:289:GLN:NE2	1:D:289:GLN:CA	2.76	0.43
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.84	0.43
1:D:891:LYS:HB2	1:D:891:LYS:HE2	1.78	0.43
1:B:994:LEU:HD23	1:B:994:LEU:HA	1.88	0.43
1:C:87:GLY:HA2	1:C:101:ARG:NH1	2.33	0.43
1:C:438:GLN:HA	1:C:441:GLU:CG	2.49	0.43
1:C:519:ARG:HG3	1:C:520:PRO:O	2.17	0.43
1:D:491:GLN:H	1:D:491:GLN:HG2	1.73	0.43
1:D:948:PHE:CD1	1:D:967:ILE:HD13	2.54	0.43
1:A:45:ARG:HA	1:A:76:HIS:CD2	2.54	0.43
1:A:563:VAL:HG21	1:A:787:ILE:HG12	2.01	0.43
1:A:747:LEU:O	1:A:747:LEU:HG	2.18	0.43
1:B:128:ALA:O	1:B:131:CYS:HB2	2.19	0.43
1:B:320:PHE:O	1:B:321:PHE:CD1	2.72	0.43
1:B:335:ILE:CG2	1:B:336:THR:N	2.77	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.19	0.43
1:C:543:GLN:H	1:C:543:GLN:HG2	1.59	0.43
1:D:479:LYS:HG2	1:D:482:GLU:OE2	2.19	0.43
1:D:837:TYR:CZ	1:D:841:VAL:HG21	2.53	0.43
1:D:1008:ILE:HD12	1:D:1008:ILE:HA	1.85	0.43
1:A:207:VAL:CG1	1:A:213:LEU:HD22	2.49	0.43
1:A:509:ILE:HD11	1:A:1065:ILE:HG21	2.00	0.43
1:B:368:THR:CG2	1:B:369:THR:N	2.81	0.43
1:B:817:LEU:O	1:B:818:ASN:C	2.58	0.43

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:GLN:O	1:D:547:GLU:HG2	2.20	0.42
1:D:613:ASP:HB2	1:D:1013:TYR:CE2	2.54	0.42
1:D:693:VAL:HG11	1:D:700:SER:HB3	2.00	0.42
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.23	0.41
1:C:67:TYR:O	1:C:85:LEU:HD12	2.20	0.41
1:C:495:ASP:HB2	1:C:499:LYS:HG3	2.02	0.41
1:C:1070:GLU:H	1:C:1070:GLU:HG3	1.60	0.41
1:D:129:ARG:O	1:D:131:CYS:N	2.53	0.41
1:D:331:VAL:HG13	1:D:428:LYS:HE2	2.02	0.41
1:D:638:LEU:HD22	1:D:672:ASP:HB3	2.02	0.41
1:D:946:SER:O	1:D:951:GLU:HB2	2.20	0.41
1:D:947:PHE:C	1:D:949:LYS:H	2.23	0.41
1:A:378:ILE:HB	1:A:427:VAL:HG23	2.02	0.41
1:A:706:TYR:O	1:A:743:MET:CE	2.67	0.41
1:A:798:VAL:O	1:A:799:ALA:C	2.59	0.41
1:B:380:THR:HG23	1:B:426:LEU:HD11	2.02	0.41
1:B:703:THR:C	1:B:704:ILE:HD13	2.40	0.41
1:C:1008:ILE:H	1:C:1008:ILE:HG13	1.65	0.41
1:D:679:SER:HA	1:D:907:VAL:CG2	2.49	0.41
1:D:731:GLU:HB2	1:D:766:LEU:HD22	2.03	0.41
1:A:250:ILE:HD11	1:A:260:LEU:HD11	2.03	0.41
1:A:780:LEU:O	1:A:781:LEU:C	2.57	0.41
1:B:360:ILE:O	1:B:361:ASN:C	2.58	0.41
1:B:719:THR:HG22	1:B:721:GLU:H	1.85	0.41
1:C:338:MET:CE	1:C:430:SER:CB	2.71	0.41
1:C:688:VAL:O	1:C:689:ALA:C	2.57	0.41
1:D:121:LEU:HB3	1:D:127:PHE:CD2	2.55	0.41
1:D:487:LEU:HD12	1:D:487:LEU:HA	1.83	0.41
1:A:826:THR:HG21	1:A:831:MET:CE	2.50	0.41
1:B:433:ALA:C	1:B:435:SER:H	2.23	0.41
1:B:925:ASP:O	1:B:926:LEU:HD13	2.21	0.41
1:C:119:GLY:N	1:C:122:SER:OG	2.52	0.41
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.91	0.41
1:C:403:PHE:O	1:C:404:GLY:C	2.58	0.41
1:C:809:SER:HB3	1:C:812:SER:HB2	2.03	0.41
1:C:1042:MET:HE1	1:C:1048:VAL:HB	2.02	0.41
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.86	0.41
1:A:832:GLU:O	1:A:836:HIS:CD2	2.74	0.41
1:A:942:GLU:O	1:A:946:SER:HB3	2.20	0.41
1:B:77:ARG:NH1	1:D:1059:ILE:CD1	2.83	0.41
1:B:265:CYS:O	1:B:268:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ARG:HA	1:B:715:ARG:HD2	1.83	0.41
1:C:278:ALA:HB2	1:C:335:ILE:CG2	2.50	0.41
1:C:837:TYR:CE2	1:C:841:VAL:HG21	2.55	0.41
1:C:1007:ILE:O	1:C:1011:VAL:HG23	2.20	0.41
1:D:683:VAL:O	1:D:685:GLN:N	2.53	0.41
1:D:743:MET:HG3	1:D:907:VAL:HG13	2.02	0.41
1:D:1065:ILE:HG22	1:D:1066:SER:N	2.35	0.41
1:A:501:LEU:HD22	1:A:1078:TYR:CD1	2.56	0.41
1:A:880:SER:O	1:A:881:LEU:HD23	2.21	0.41
1:A:888:ASP:OD1	1:A:888:ASP:N	2.53	0.41
1:A:1023:THR:O	1:A:1026:GLN:N	2.52	0.41
1:B:391:THR:CG2	1:B:392:GLY:N	2.83	0.41
1:B:398:ARG:HH22	1:B:1085:ARG:HE	1.68	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.01	0.41
1:C:154:LYS:O	1:C:155:ALA:C	2.58	0.41
1:C:444:VAL:CG2	1:C:466:MET:HB3	2.42	0.41
1:C:936:TYR:CZ	1:C:966:VAL:HG12	2.55	0.41
1:D:242:PRO:HB3	1:D:313:LEU:HG	2.03	0.41
1:A:593:LYS:O	1:A:597:VAL:HG23	2.21	0.41
1:A:1075:THR:HG22	1:A:1077:TYR:CE1	2.55	0.41
1:C:215:ASP:CB	1:C:219:ARG:NH2	2.84	0.41
1:C:565:LEU:HD22	1:C:598:PHE:HE2	1.85	0.41
1:C:955:PRO:HG2	1:C:958:GLY:CA	2.49	0.41
1:D:142:HIS:N	1:D:145:HIS:HD2	2.17	0.41
1:D:417:GLU:H	1:D:417:GLU:HG2	1.74	0.41
1:D:453:ARG:NH1	1:D:495:ASP:HB3	2.31	0.41
1:B:402:GLY:H	1:B:405:VAL:CG2	2.34	0.41
1:B:1069:ASP:OD2	1:B:1071:ASN:HB2	2.21	0.41
1:C:479:LYS:O	1:C:480:PHE:C	2.58	0.41
1:C:550:PRO:HD2	1:C:551:LYS:H	1.85	0.41
1:C:558:LYS:HD3	1:C:765:ASP:O	2.20	0.41
1:C:773:HIS:HA	1:C:806:SER:O	2.20	0.41
1:A:170:THR:HB	1:A:234:TYR:HB2	2.03	0.41
1:A:192:MET:HG3	1:A:193:ILE:N	2.35	0.41
1:A:246:GLU:OE1	1:A:330:GLN:NE2	2.48	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.71	0.41
1:A:924:ASN:HB2	1:A:926:LEU:HD22	2.02	0.41
1:B:101:ARG:O	1:B:105:VAL:HG23	2.20	0.41
1:B:908:THR:HG22	1:B:909:PRO:HA	2.03	0.41
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.77	0.41
1:C:486:GLU:O	1:C:486:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:ASN:HD22	1:C:624:TRP:N	2.11	0.41
1:C:758:GLU:O	1:C:762:ALA:HB2	2.20	0.41
1:C:1059:ILE:O	1:C:1080:MET:HA	2.21	0.41
1:C:1091:ASP:OD2	1:C:1092:GLU:N	2.54	0.41
1:D:712:ASN:HA	1:D:713:PRO:HD2	1.95	0.41
1:D:866:MET:CE	1:D:874:LEU:CD2	2.99	0.41
1:D:870:GLN:O	1:D:872:SER:N	2.53	0.41
1:D:883:LEU:O	1:D:886:ARG:N	2.53	0.41
1:D:908:THR:HA	1:D:909:PRO:HA	1.79	0.41
1:A:152:LYS:HD2	1:A:152:LYS:HA	1.75	0.41
1:B:525:GLU:HB3	1:B:840:THR:CG2	2.41	0.41
1:B:667:ALA:HB1	1:B:698:LYS:HE2	2.03	0.41
1:B:913:VAL:HG22	1:B:943:SER:O	2.21	0.41
1:B:991:ARG:NH1	1:B:1002:VAL:HG12	2.36	0.41
1:C:169:GLY:HA2	1:C:236:GLU:HA	2.03	0.41
1:C:219:ARG:HB2	1:C:219:ARG:HH11	1.86	0.41
1:C:370:LEU:O	1:C:432:HIS:HE1	2.04	0.41
1:C:440:GLU:HG3	1:C:472:THR:HG22	2.03	0.41
1:C:651:TYR:HD2	1:C:1013:TYR:CE2	2.38	0.41
1:D:296:ILE:O	1:D:296:ILE:HG23	2.21	0.41
1:D:414:GLN:HE21	1:D:414:GLN:HB3	1.74	0.41
1:D:1080:MET:O	1:D:1081:ASN:C	2.58	0.41
1:A:41:LEU:HD23	1:A:42:VAL:N	2.36	0.40
1:A:606:MET:HE3	1:A:607:TRP:HB2	2.01	0.40
1:B:56:ALA:O	1:B:59:LEU:N	2.55	0.40
1:B:780:LEU:HD13	1:C:778:ASN:HD21	1.85	0.40
1:B:867:PRO:O	1:B:868:GLY:C	2.59	0.40
1:D:570:PHE:HB2	1:D:606:MET:HB3	2.02	0.40
1:A:181:LYS:HE3	1:A:181:LYS:HA	2.03	0.40
1:A:206:ILE:H	1:A:206:ILE:HG13	1.59	0.40
1:A:717:ASN:HB3	1:A:717(A):ILE:HD12	2.03	0.40
1:A:873:ASN:C	1:A:875:SER:N	2.74	0.40
1:B:363:GLN:OE1	1:B:363:GLN:CA	2.64	0.40
1:B:406:ARG:N	1:B:430:SER:O	2.38	0.40
1:B:756:ILE:HD13	1:B:756:ILE:HA	1.94	0.40
1:B:1053:ASP:HB3	1:B:1056:LYS:HG3	2.03	0.40
1:C:517:GLU:HB3	1:C:519:ARG:NE	2.36	0.40
1:C:684:ASP:HA	1:C:687:LYS:HZ3	1.86	0.40
1:D:337:GLU:HG2	1:D:344:ILE:HD12	2.03	0.40
1:D:875:SER:OG	1:D:887:PHE:CE2	2.69	0.40
1:D:998:GLN:O	1:D:999:GLN:O	2.39	0.40

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

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

All (132) Ramachandran outliers are listed below:

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

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

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

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

5.3.2 Protein sidechains (i)

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

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

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

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

Mol	Chain	Res	Type
1	A	36	GLN

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

such sidechains are listed below:

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BTI	D	1201	-	16,16,16	1.78	2 (12%)	21,21,21	2.13	6 (28%)

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

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTI	D	1201	-	-	5/5/27/27	0/2/2/2
2	ADP	A	1201	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

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

All (9) bond angle outliers are listed below:

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

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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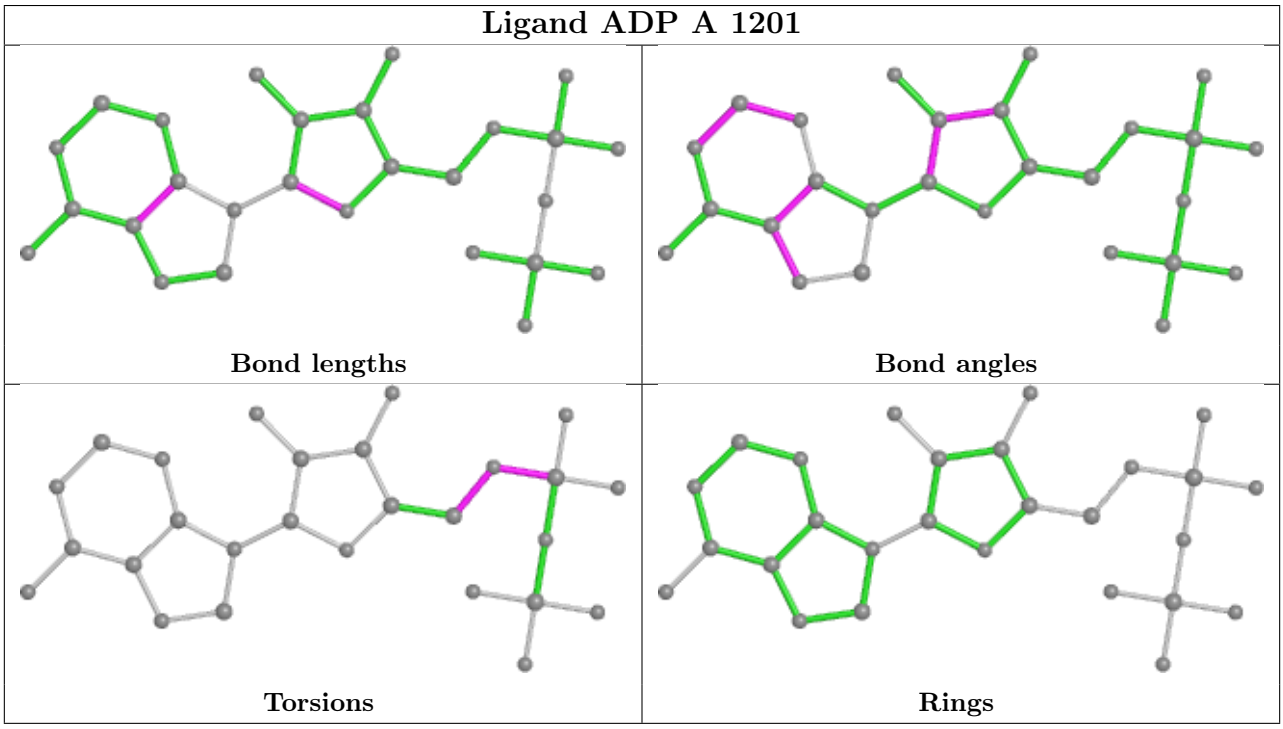
Mol	Chain	Res	Type	Atoms
4	D	1201	BTI	C2-C7-C8-C9
4	D	1201	BTI	C7-C8-C9-C10
2	A	1201	ADP	C5'-O5'-PA-O3A
2	A	1201	ADP	C4'-C5'-O5'-PA
2	A	1201	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

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

All (40) RSRZ outliers are listed below:

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

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BTI	D	1201	15/15	0.81	0.42	128,133,136,136	0
2	ADP	A	1201	27/27	0.87	0.20	108,112,144,146	0
3	MN	C	1201	1/1	0.97	0.29	105,105,105,105	0
3	MN	D	1202	1/1	0.97	0.18	79,79,79,79	0

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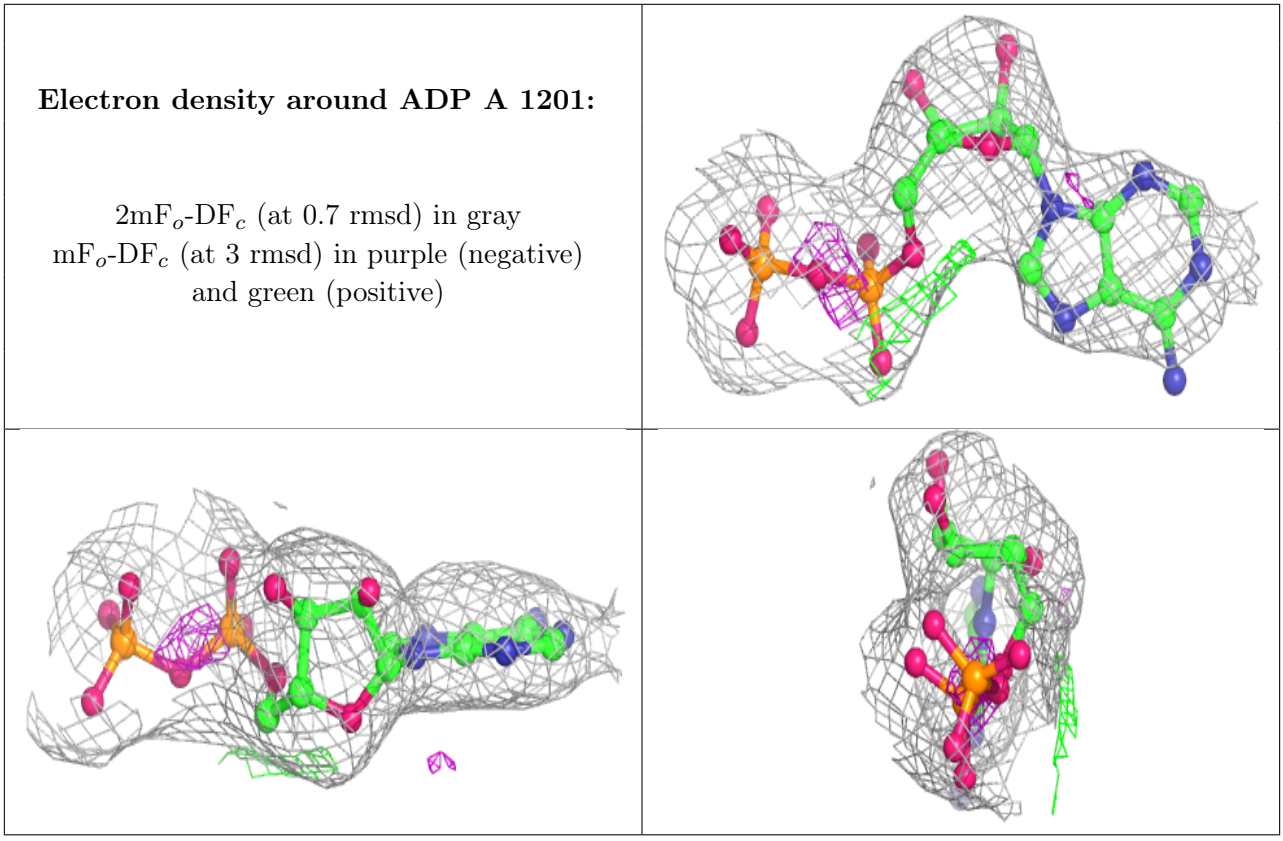
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	B	1201	1/1	0.97	0.18	108,108,108,108	0
3	MN	A	1202	1/1	0.98	0.30	83,83,83,83	0

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

Electron density around ADP A 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.