



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:29 AM UTC

PDB ID : 4HNV / pdb_00004hnv
Title : Crystal structure of R54E mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

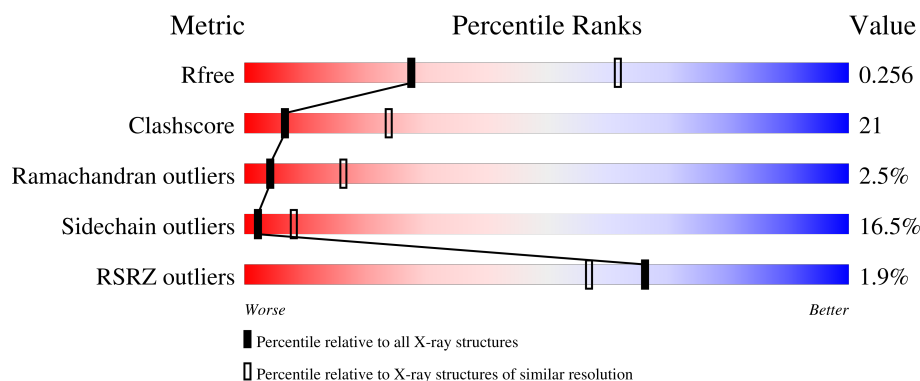
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1173	% 57% 31% 8% • •
1	B	1173	2% 48% 31% 8% • 12%
1	C	1173	2% 52% 30% 8% • 9%
1	D	1173	% 55% 28% 7% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTI	B	1201	-	-	X	-
4	BTI	B	1202	-	-	X	-
6	CL	D	1201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34066 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	1133	Total	C	N	O	S	0	0	0
			8938	5663	1502	1743	30			
1	B	1033	Total	C	N	O	S	0	0	0
			8155	5169	1375	1583	28			
1	C	1067	Total	C	N	O	S	0	0	0
			8439	5349	1418	1642	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8411	5333	1413	1636	29			

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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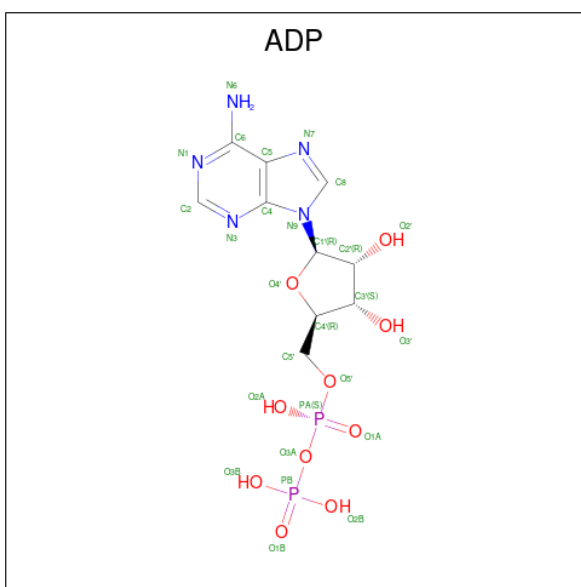
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
A	54	GLU	ARG	engineered mutation	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag	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	54	GLU	ARG	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	54	GLU	ARG	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	54	GLU	ARG	engineered mutation	UNP Q99UY8

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

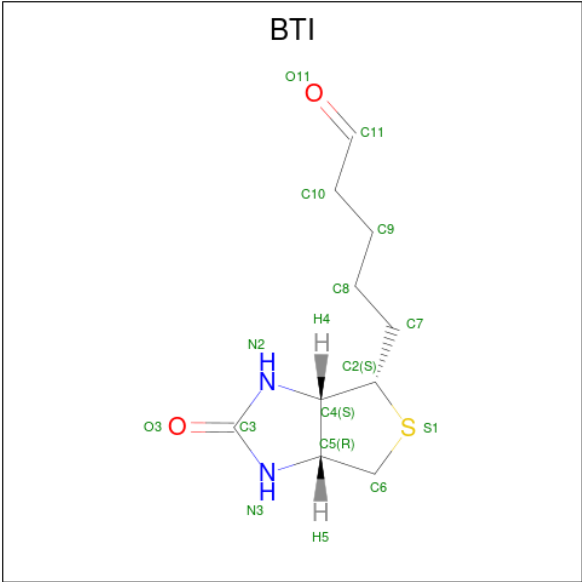


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

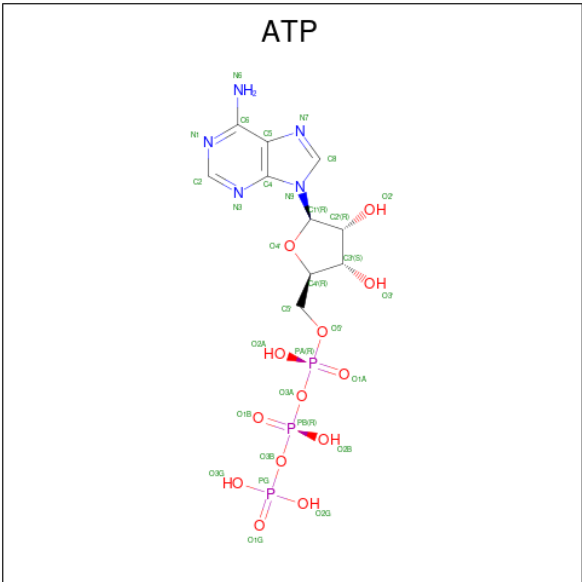
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn		
			1	1	0	0
3	B	1	Total	Mn		
			1	1	0	0
3	C	1	Total	Mn		
			1	1	0	0
3	D	1	Total	Mn		
			1	1	0	0

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



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

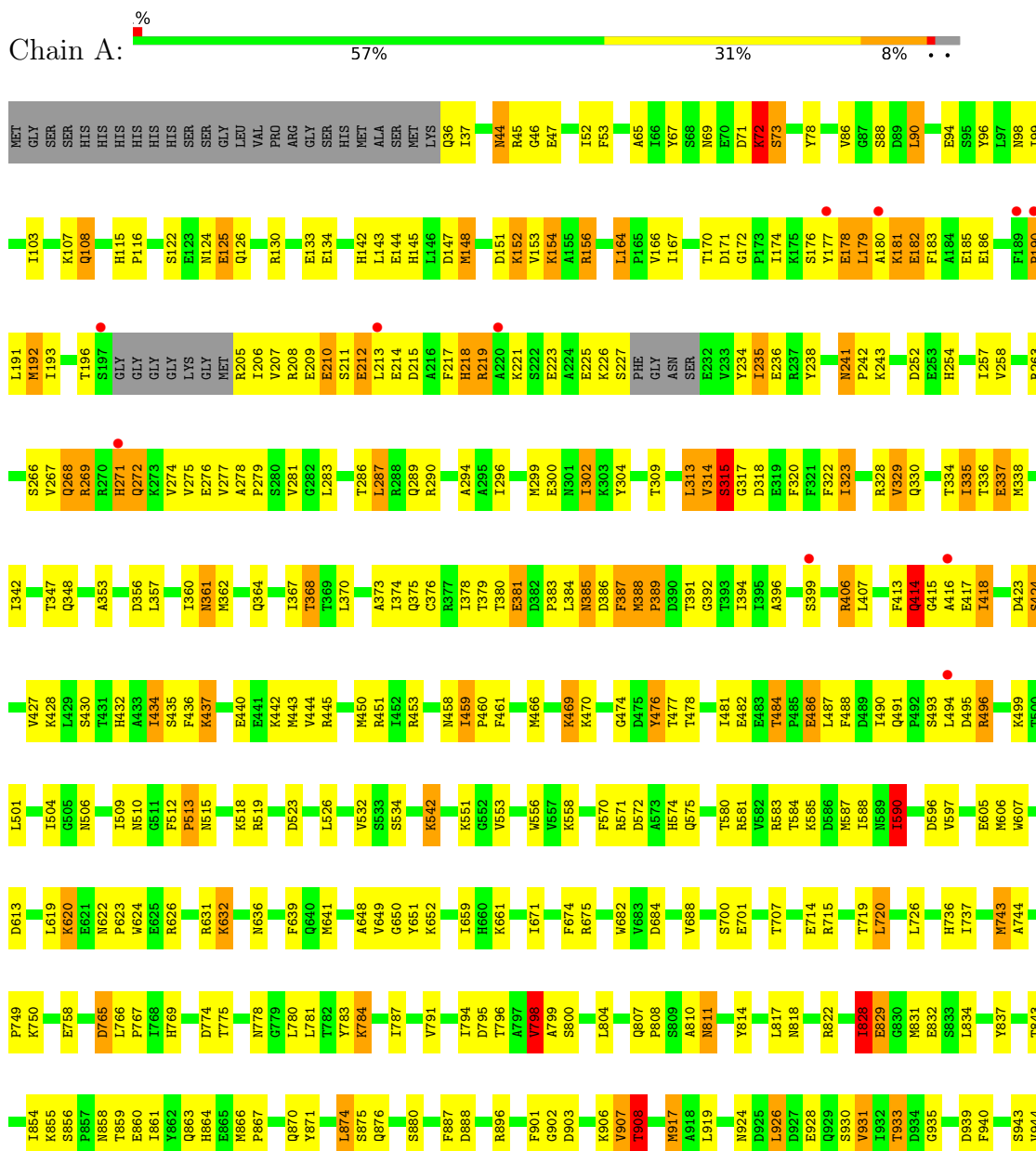
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

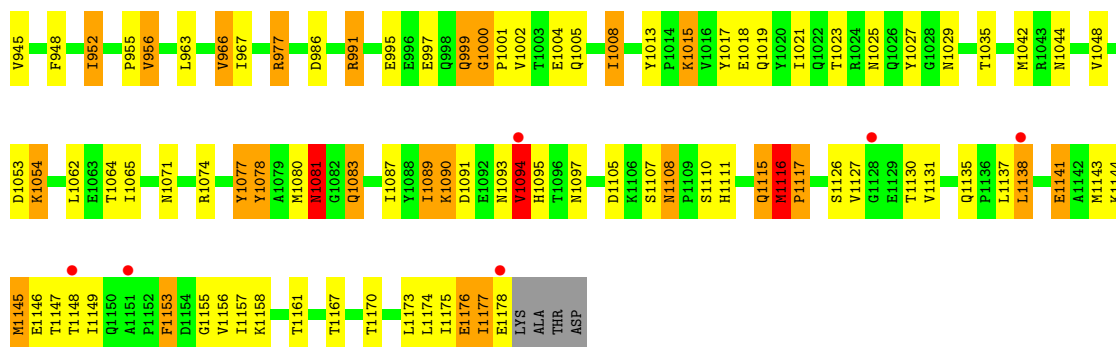
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

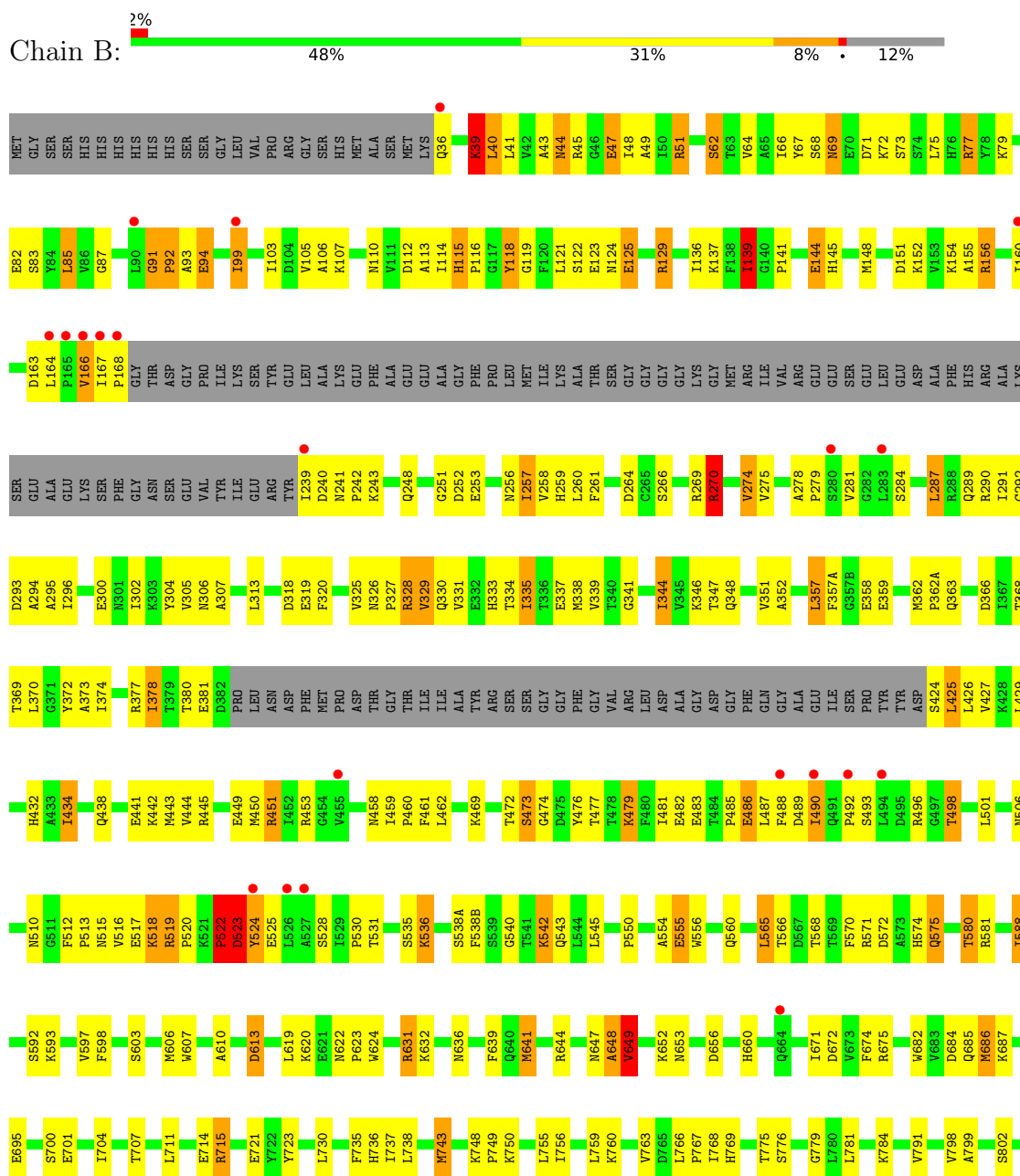
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

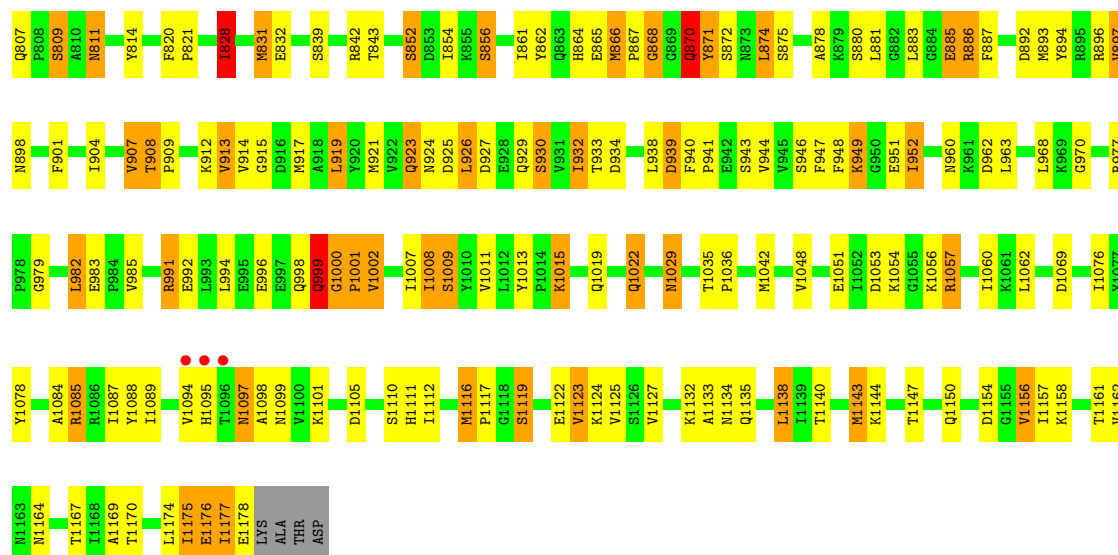
• Molecule 1: Pyruvate carboxylase



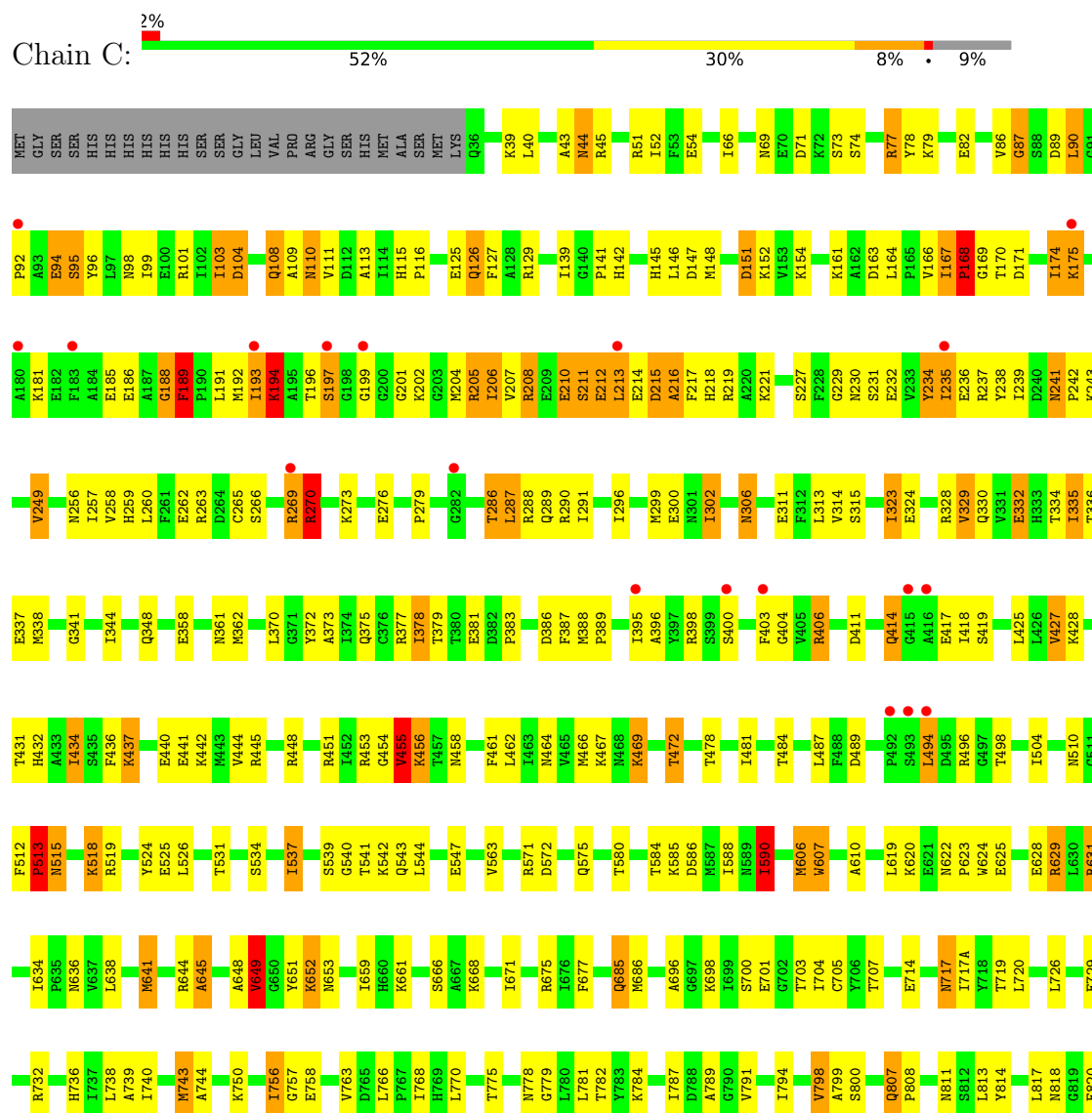


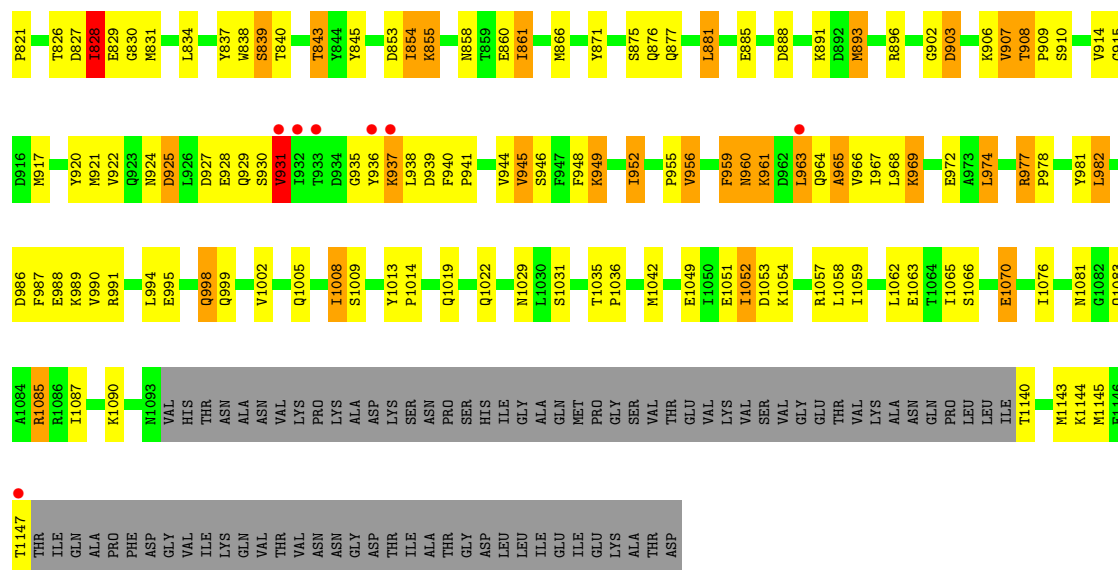
• Molecule 1: Pyruvate carboxylase



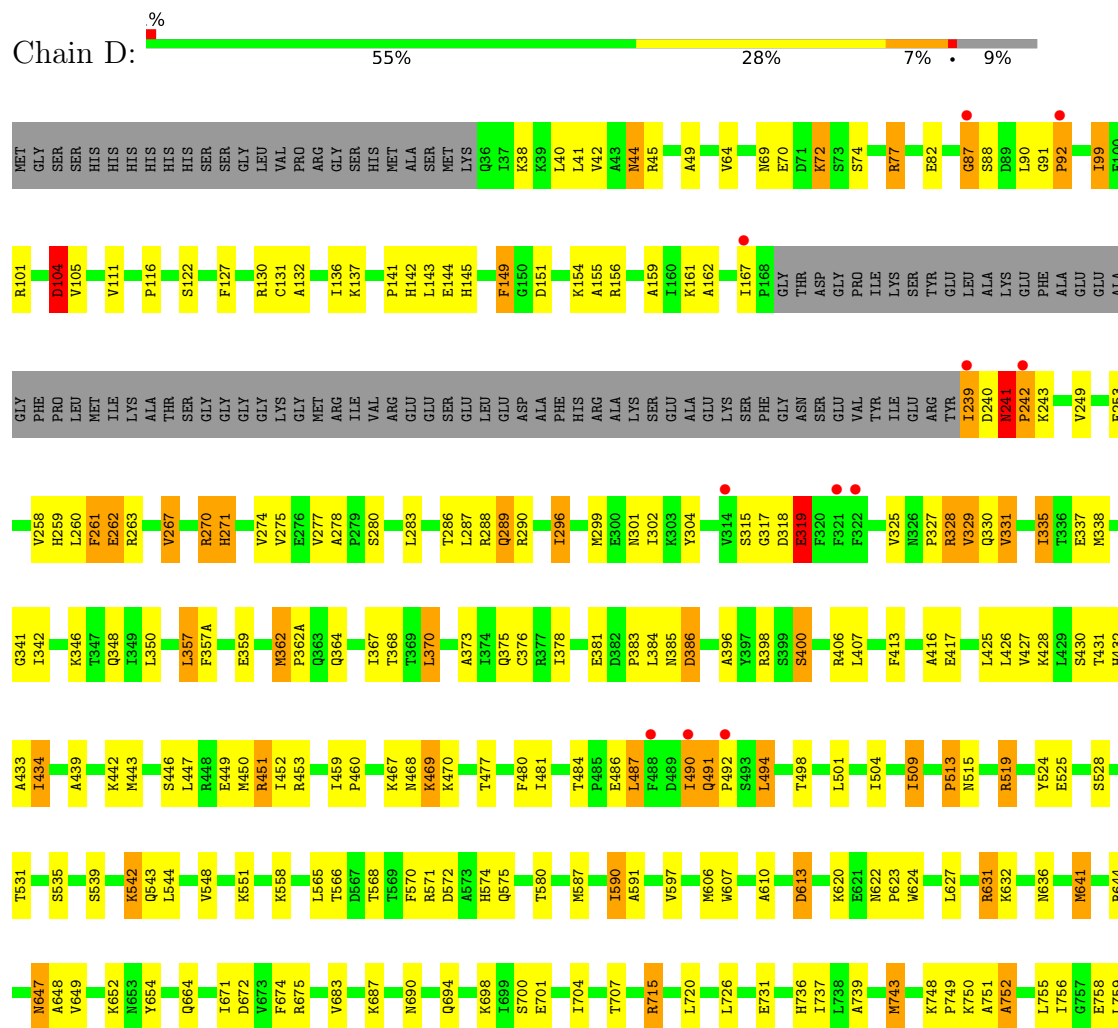


• Molecule 1: Pyruvate carboxylase





- Molecule 1: Pyruvate carboxylase



K760	S852	I932	K1054	Q1135
D853	D853	G935	G1055	L1138
V763	I854		K1056	
D765	K855	L938	R1057	E1141
P766	S856	D939	I1058	
P767		F940	I1059	K1144
I768	Q863	P941	I1060	
H769	H864		K1061	T1147
L770	E865	V944	L1062	T1148
H771	M866	V945	E1063	I1149
	P867		T1064	Q1150
D774	G868	K949	I1065	A1151
T775	Q869	G950	S1066	P1152
	Q870	E951	E1067	F1153
L780	Y871	I952	P1068	D1154
L781	S872		D1069	G1155
T782	N873	N960	E1070	V1156
Y783	L874	K961	E1071	I1157
K784	S875	D962	I1076	K1158
	Q876	L963	Y1077	Q1159
V791	Q877	Q964	Y1078	V1160
	A878	A965	A1079	T1161
D795	K879	V966	M1080	V1162
	S880			N1163
V798	L881	L974	R1085	
A799		P978	I1089	T1167
S800	G884		K1090	
L804	F887	D986		L1173
	M893		N1093	L1174
Q807	Y894	E996	VAL	I1175
M811	R895	E997	HIS	E1176
	R896	Q998	THR	I1177
Y814	V897	Q999	ASN	E1178
	N898	G1000	ALA	LYS
N818		P1001	ASN	ALA
	F901	V1002	VAL	THR
R823	G902		K1101	ASP
	D903	Y1013	P1102	
T826		P1014	K1103	
D827	V907	K1015	A1104	
I828	T908	V1016	D1105	
E829	P909		K1106	
G830		Q1019	S1107	
M831	R912		N1108	
E832		T1023	P1109	
	M917		S1110	
S835	A918	M1042	H1111	
H836	I919	R1043	Q1115	
Y837	Y920	N1044		V1123
W838	M921	G1045	V1127	
S839	V922	E1046		
T840		T1047		
	D925	V1048		
T843	L926	E1049		
	E927	I1050	V1131	
D847	E928	E1051	K1132	
F848	I1052	I1052	A1133	
E849	V931	D1053	N1134	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.43Å 256.74Å 127.05Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.80) 93.0 (30.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.256	Depositor DCC
R_{free} test set	7149 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34066	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ATP, 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	0.72	2/9106 (0.0%)	0.96	28/12319 (0.2%)
1	B	0.63	4/8305 (0.0%)	0.90	9/11239 (0.1%)
1	C	0.69	6/8601 (0.1%)	0.92	16/11625 (0.1%)
1	D	0.71	5/8569 (0.1%)	0.94	17/11596 (0.1%)
All	All	0.69	17/34581 (0.0%)	0.93	70/46779 (0.1%)

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	4
1	B	0	3
1	D	0	2
All	All	0	9

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	11.64	1.69	1.52
1	D	513	PRO	CA-C	9.25	1.63	1.52
1	C	763	VAL	N-CA	9.23	1.56	1.46
1	D	849	GLU	N-CA	7.16	1.55	1.45
1	C	515	ASN	N-CA	6.59	1.56	1.46
1	A	315	SER	N-CA	6.57	1.54	1.45
1	C	513	PRO	C-N	6.52	1.42	1.33
1	A	314	VAL	C-N	6.35	1.43	1.33
1	C	513	PRO	N-CA	6.20	1.55	1.47
1	D	513	PRO	N-CA	6.06	1.54	1.47
1	B	763	VAL	C-N	5.81	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	763	VAL	N-CA	5.62	1.52	1.46
1	C	763	VAL	CA-C	5.61	1.59	1.52
1	B	1094	VAL	CA-CB	5.50	1.60	1.55
1	B	763	VAL	N-CA	5.42	1.52	1.46
1	B	763	VAL	CA-C	5.40	1.59	1.52
1	D	945	VAL	CA-CB	5.08	1.60	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	THR	CA-C-N	-7.38	110.86	119.05
1	A	1035	THR	C-N-CA	-7.38	110.86	119.05
1	A	314	VAL	O-C-N	-7.17	115.33	123.07
1	A	828	ILE	CB-CA-C	-7.05	102.49	112.22
1	C	828	ILE	CB-CA-C	-6.87	103.00	111.87
1	A	513	PRO	CA-C-N	-6.82	112.91	124.31
1	A	513	PRO	C-N-CA	-6.82	112.91	124.31
1	A	315	SER	CA-C-O	-6.63	113.35	121.11
1	D	849	GLU	CA-C-O	-6.40	114.83	121.87
1	D	319	GLU	N-CA-C	6.32	118.68	108.32
1	B	866	MET	CA-C-N	6.28	127.15	120.11
1	B	866	MET	C-N-CA	6.28	127.15	120.11
1	A	513	PRO	CA-C-O	-6.24	114.52	121.32
1	C	315	SER	CA-C-N	6.14	133.44	121.41
1	C	315	SER	C-N-CA	6.14	133.44	121.41
1	A	388	MET	CA-C-N	6.04	127.39	119.84
1	A	388	MET	C-N-CA	6.04	127.39	119.84
1	C	189	PHE	CA-C-N	-6.03	112.30	119.84
1	C	189	PHE	C-N-CA	-6.03	112.30	119.84
1	B	1007	ILE	N-CA-C	6.03	116.77	110.62
1	A	876	GLN	N-CA-C	-6.01	104.81	111.36
1	D	513	PRO	N-CA-C	5.98	121.01	111.26
1	C	977	ARG	CA-C-N	5.95	125.43	119.24
1	C	977	ARG	C-N-CA	5.95	125.43	119.24
1	D	849	GLU	CA-C-N	-5.92	110.13	122.03
1	D	849	GLU	C-N-CA	-5.92	110.13	122.03
1	B	115	HIS	CA-C-N	5.92	125.54	119.56
1	B	115	HIS	C-N-CA	5.92	125.54	119.56
1	C	139	ILE	N-CA-C	5.92	112.54	106.21
1	B	870	GLN	N-CA-C	5.87	123.29	110.80
1	D	766	LEU	CA-C-N	-5.84	114.24	120.03
1	D	766	LEU	C-N-CA	-5.84	114.24	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	798	VAL	CB-CA-C	-5.82	103.24	111.28
1	D	632	LYS	N-CA-C	-5.82	105.02	111.36
1	A	931	VAL	N-CA-C	-5.81	104.85	110.72
1	A	1021	ILE	N-CA-C	5.73	116.47	110.62
1	A	590	ILE	CB-CA-C	-5.72	104.85	112.46
1	A	459	ILE	CA-C-N	-5.71	113.73	119.56
1	A	459	ILE	C-N-CA	-5.71	113.73	119.56
1	A	908	THR	N-CA-C	-5.67	102.60	109.57
1	D	572	ASP	N-CA-C	5.59	118.14	111.71
1	C	590	ILE	CB-CA-C	-5.58	105.04	112.46
1	C	515	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	1108	ASN	CA-C-N	5.54	125.22	119.56
1	A	1108	ASN	C-N-CA	5.54	125.22	119.56
1	B	828	ILE	CB-CA-C	-5.51	104.92	111.97
1	A	1116	MET	N-CA-C	5.48	112.95	108.07
1	A	364	GLN	N-CA-C	5.38	117.57	111.11
1	C	513	PRO	CA-C-N	5.38	130.49	122.74
1	C	513	PRO	C-N-CA	5.38	130.49	122.74
1	A	484	THR	CA-C-N	5.38	125.71	119.47
1	A	484	THR	C-N-CA	5.38	125.71	119.47
1	C	315	SER	O-C-N	5.37	129.51	123.28
1	D	271	HIS	N-CA-C	-5.36	106.42	113.17
1	A	418	ILE	N-CA-C	5.34	115.58	108.11
1	D	849	GLU	O-C-N	-5.29	116.56	122.75
1	D	1159	GLN	N-CA-C	5.29	117.11	109.07
1	C	69	ASN	N-CA-C	5.28	117.45	111.11
1	A	315	SER	O-C-N	-5.26	116.77	123.24
1	D	763	VAL	N-CA-C	5.24	117.60	108.90
1	D	828	ILE	CB-CA-C	-5.20	105.23	112.04
1	A	368	THR	CB-CA-C	-5.15	101.78	112.44
1	C	314	VAL	N-CA-C	5.12	115.49	108.12
1	A	952	ILE	N-CA-C	-5.10	106.95	113.22
1	D	687	LYS	N-CA-C	5.09	117.50	111.33
1	B	39	LYS	N-CA-C	5.07	117.42	108.75
1	C	194	LYS	N-CA-C	5.03	116.72	109.07
1	D	318	ASP	N-CA-C	-5.02	104.12	111.30
1	D	752	ALA	N-CA-C	-5.02	105.89	111.36
1	B	139	ILE	N-CA-C	5.00	111.56	106.21

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	1080	MET	Peptide
1	A	271	HIS	Peptide
1	A	494	LEU	Peptide
1	B	522	PRO	Peptide
1	B	92	PRO	Peptide
1	B	94	GLU	Peptide
1	D	1110	SER	Peptide
1	D	270	ARG	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	8938	0	8865	393	0
1	B	8155	0	8127	373	0
1	C	8439	0	8345	389	0
1	D	8411	0	8357	337	0
2	A	27	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	30	0	32	17	0
4	C	15	0	16	1	0
4	D	15	0	16	5	0
5	C	31	0	12	6	0
6	D	1	0	0	3	0
All	All	34066	0	33782	1457	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 21.

All (1457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1144:LYS:NZ	4:D:1202:BTI:H11	1.21	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:LYS:NZ	4:B:1202:BTI:C11	1.74	1.46
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.66	1.29
1:C:1144:LYS:NZ	4:D:1202:BTI:C11	1.91	1.29
1:C:1144:LYS:HZ1	4:D:1202:BTI:C11	1.44	1.29
1:B:1144:LYS:NZ	4:B:1202:BTI:H11	1.40	1.25
1:A:1144:LYS:NZ	4:B:1201:BTI:C11	2.00	1.23
1:A:1144:LYS:NZ	4:B:1201:BTI:H11	1.57	1.16
1:C:260:LEU:HD21	1:C:362:MET:HE1	1.29	1.14
1:C:260:LEU:HD21	1:C:362:MET:CE	1.79	1.13
1:A:156:ARG:HD2	1:A:166:VAL:HG11	1.32	1.12
1:B:1144:LYS:HZ3	4:B:1202:BTI:C11	1.39	1.11
1:B:434:ILE:HD12	1:B:434:ILE:H	1.06	1.11
1:A:1144:LYS:HZ3	4:B:1201:BTI:H11	0.94	1.11
1:A:176:SER:O	1:A:179:LEU:HD22	1.51	1.10
1:C:960:ASN:HB2	1:C:963:LEU:HD23	1.31	1.10
1:A:156:ARG:HH11	1:A:156:ARG:HB3	1.08	1.08
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.26	1.07
1:D:357:LEU:O	1:D:362:MET:HB2	1.55	1.07
1:D:999:GLN:HG2	1:D:1000:GLY:N	1.58	1.07
1:D:999:GLN:CG	1:D:1000:GLY:H	1.67	1.06
1:C:960:ASN:CB	1:C:963:LEU:HD23	1.86	1.05
1:B:1085:ARG:HG2	1:B:1085:ARG:HH11	0.93	1.05
1:C:498:THR:OG1	1:C:1085:ARG:NH2	1.89	1.03
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.20	1.03
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.21	1.03
1:B:137:LYS:HE3	1:B:352:ALA:O	1.58	1.02
1:B:1144:LYS:HZ1	4:B:1202:BTI:C11	1.48	1.02
1:B:1085:ARG:HG2	1:B:1085:ARG:NH1	1.61	1.02
1:A:504:ILE:HG21	1:A:1042:MET:HE2	1.41	1.01
1:A:179:LEU:HD23	1:A:179:LEU:H	1.22	1.01
1:A:434:ILE:H	1:A:434:ILE:HD12	1.25	1.01
1:A:1144:LYS:HZ3	4:B:1201:BTI:C11	1.62	1.00
1:D:960:ASN:ND2	1:D:963:LEU:H	1.58	1.00
1:C:44:ASN:HD22	1:C:45:ARG:H	1.07	1.00
1:D:490:ILE:O	1:D:492:PRO:HD3	1.59	1.00
1:C:828:ILE:HD12	1:C:828:ILE:H	1.27	1.00
4:C:1203:BTI:O11	1:D:1144:LYS:NZ	1.94	1.00
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.41	0.99
1:C:677:PHE:HA	1:C:686:MET:HE3	1.43	0.98
1:A:156:ARG:HH11	1:A:156:ARG:CB	1.75	0.98
1:C:653:ASN:HD21	1:C:685:GLN:HE22	1.10	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD11	1:A:490:ILE:HD11	1.00	0.98
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.26	0.98
1:D:44:ASN:HD22	1:D:45:ARG:H	0.98	0.97
1:C:700:SER:H	1:C:736:HIS:HD2	1.12	0.97
1:A:384:LEU:CD1	1:A:490:ILE:HD11	1.93	0.95
1:C:398:ARG:NE	1:C:1083:GLN:HG2	1.81	0.95
1:A:606:MET:HE2	1:A:639:PHE:HB3	1.44	0.95
1:A:44:ASN:HD22	1:A:45:ARG:H	0.96	0.94
1:D:504:ILE:HD13	1:D:1042:MET:HE3	1.49	0.94
1:B:1085:ARG:HH11	1:B:1085:ARG:CG	1.80	0.94
1:B:44:ASN:HD22	1:B:45:ARG:H	0.98	0.93
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.04	0.93
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.51	0.92
1:A:469:LYS:HD2	1:A:469:LYS:N	1.85	0.92
1:D:287:LEU:HD11	1:D:317:GLY:O	1.68	0.91
1:D:700:SER:H	1:D:736:HIS:HD2	1.17	0.91
1:A:1144:LYS:HZ1	4:B:1201:BTI:C11	1.71	0.91
1:D:879:LYS:HG2	1:D:884:GLY:HA3	1.52	0.91
1:D:864:HIS:CD2	1:D:866:MET:HG3	2.06	0.91
1:C:398:ARG:HE	1:C:1083:GLN:HG2	1.32	0.90
1:D:644:ARG:HH21	1:D:908:THR:HB	1.36	0.90
1:C:454:GLY:O	1:C:455:VAL:HG13	1.70	0.90
1:A:641:MET:HE3	1:A:674:PHE:CD1	2.06	0.89
1:B:44:ASN:HD22	1:B:45:ARG:N	1.70	0.89
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.54	0.89
1:C:1051:GLU:HG3	1:C:1057:ARG:NH2	1.88	0.89
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.06	0.89
1:D:259:HIS:H	1:D:364:GLN:HE22	1.21	0.89
1:B:378:ILE:HG13	1:B:427:VAL:HG23	1.54	0.89
1:D:338:MET:HE2	1:D:430:SER:HB3	1.55	0.89
1:A:700:SER:H	1:A:736:HIS:HD2	1.20	0.88
1:D:999:GLN:HE21	1:D:1001:PRO:HD2	1.38	0.88
1:D:960:ASN:HD22	1:D:963:LEU:H	1.20	0.88
1:A:254:HIS:HD2	1:A:356:ASP:OD2	1.57	0.88
1:A:1115:GLN:CD	1:A:1115:GLN:H	1.79	0.88
1:A:156:ARG:HD2	1:A:166:VAL:CG1	2.03	0.88
1:C:960:ASN:HB2	1:C:963:LEU:CD2	2.03	0.88
1:B:575:GLN:HB2	1:B:580:THR:HG23	1.57	0.87
1:A:181:LYS:O	1:A:185:GLU:HG3	1.72	0.87
1:A:406:ARG:HH11	1:A:406:ARG:CG	1.85	0.87
1:B:897:VAL:CG1	1:B:914:VAL:HG13	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:HIS:HD2	1:B:866:MET:H	1.22	0.87
1:D:873:ASN:HD22	1:D:873:ASN:H	1.20	0.87
1:C:191:LEU:HB3	1:C:235:ILE:HD11	1.57	0.86
1:A:384:LEU:HD11	1:A:490:ILE:CD1	1.97	0.86
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.06	0.86
1:C:263:ARG:HH21	1:C:330:GLN:NE2	1.72	0.86
1:D:1069:ASP:OD2	1:D:1071:ASN:N	2.08	0.86
1:B:329:VAL:HG13	1:B:348:GLN:NE2	1.90	0.86
1:C:840:THR:O	1:C:843:THR:HB	1.76	0.85
1:B:44:ASN:ND2	1:B:45:ARG:H	1.74	0.85
1:B:434:ILE:HD12	1:B:434:ILE:N	1.89	0.85
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.38	0.85
1:A:622:ASN:ND2	1:A:624:TRP:H	1.74	0.85
1:B:1144:LYS:HZ1	4:B:1202:BTI:H11	0.69	0.85
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.58	0.85
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.58	0.85
1:C:1049:GLU:HG2	1:C:1059:ILE:HD12	1.55	0.85
1:D:509:ILE:HD13	1:D:1089:ILE:HG21	1.59	0.85
1:A:174:ILE:HD12	1:A:179:LEU:HB2	1.57	0.85
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.57	0.85
1:A:219:ARG:O	1:A:223:GLU:HB2	1.77	0.84
1:A:315:SER:O	1:A:317:GLY:C	2.20	0.84
1:D:1108:ASN:HB3	1:D:1109:PRO:HD3	1.58	0.84
1:B:897:VAL:HG12	1:B:914:VAL:HG13	1.59	0.84
1:A:558:LYS:HE2	1:A:765:ASP:O	1.77	0.84
1:B:241:ASN:HD22	1:B:477:THR:HG21	1.43	0.83
1:D:338:MET:CE	1:D:430:SER:HB3	2.09	0.83
1:C:504:ILE:HD13	1:C:1042:MET:CE	2.08	0.83
1:B:434:ILE:HG13	1:D:341:GLY:O	1.79	0.83
1:A:1145:MET:CE	1:A:1145:MET:HA	2.09	0.83
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.45	0.82
1:C:44:ASN:ND2	1:C:45:ARG:H	1.77	0.82
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.44	0.82
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.58	0.82
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.44	0.82
1:C:700:SER:H	1:C:736:HIS:CD2	1.98	0.82
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.62	0.82
1:A:641:MET:CE	1:A:674:PHE:CE1	2.62	0.81
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.14	0.81
1:B:434:ILE:H	1:B:434:ILE:CD1	1.85	0.81
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:ILE:HD12	1:C:828:ILE:N	1.94	0.81
1:D:840:THR:O	1:D:843:THR:HB	1.78	0.81
1:C:217:PHE:O	1:C:221:LYS:HB2	1.81	0.81
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.27	0.81
1:A:223:GLU:HA	1:A:226:LYS:HB3	1.63	0.81
1:D:641:MET:HE3	1:D:674:PHE:CD1	2.15	0.81
1:D:647:ASN:HD22	1:D:647:ASN:C	1.88	0.81
1:A:176:SER:O	1:A:179:LEU:CD2	2.29	0.80
1:B:47:GLU:CD	1:B:47:GLU:H	1.87	0.80
5:C:1202:ATP:O1G	5:C:1202:ATP:O3A	1.98	0.80
1:A:379:THR:HG22	1:A:424:SER:O	1.79	0.80
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.64	0.80
1:D:999:GLN:HG2	1:D:1000:GLY:H	0.75	0.80
1:C:152:LYS:NZ	5:C:1202:ATP:O1A	2.14	0.80
1:A:156:ARG:HB3	1:A:156:ARG:NH1	1.93	0.80
1:A:864:HIS:CD2	1:A:866:MET:CG	2.59	0.80
1:D:864:HIS:HD2	1:D:866:MET:H	1.30	0.80
1:C:196:THR:HG22	1:C:196:THR:O	1.82	0.80
1:C:306:ASN:OD1	1:C:348:GLN:HG2	1.82	0.80
1:D:44:ASN:HD22	1:D:45:ARG:N	1.80	0.80
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.80	0.79
1:C:1144:LYS:HZ3	4:D:1202:BTI:C11	1.74	0.79
1:B:811:ASN:H	1:B:811:ASN:HD22	1.30	0.79
1:B:570:PHE:O	1:B:574:HIS:HE1	1.66	0.79
1:B:506:ASN:ND2	1:B:510:ASN:HD22	1.81	0.78
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.66	0.78
1:A:362:MET:CE	1:A:367:ILE:HD11	2.12	0.78
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.13	0.78
1:B:1095:HIS:HB3	1:B:1098:ALA:HB3	1.66	0.78
1:C:221:LYS:NZ	1:C:231:SER:O	2.17	0.78
1:D:470:LYS:HE2	1:D:470:LYS:HA	1.66	0.78
1:B:1110:SER:HB2	1:B:1177:ILE:O	1.83	0.78
1:C:269:ARG:HG3	1:C:270:ARG:H	1.48	0.78
1:D:917:MET:HA	1:D:917:MET:HE2	1.66	0.78
1:C:87:GLY:HA3	1:C:90:LEU:HD22	1.66	0.78
1:C:196:THR:O	1:C:197:SER:HB3	1.84	0.78
1:D:1111:HIS:HB3	1:D:1173:LEU:CD1	2.13	0.77
1:B:606:MET:HE2	1:B:639:PHE:HB3	1.65	0.77
1:D:362:MET:HE1	1:D:367:ILE:HD11	1.65	0.77
1:B:291:ILE:HG12	1:B:320:PHE:HD2	1.49	0.77
1:A:179:LEU:H	1:A:179:LEU:CD2	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLU:OE1	1:C:466:MET:HB3	1.82	0.77
1:A:44:ASN:HD22	1:A:45:ARG:N	1.79	0.76
1:A:858:ASN:ND2	1:A:860:GLU:H	1.82	0.76
1:D:620:LYS:HE2	1:D:1023:THR:OG1	1.85	0.76
1:D:1108:ASN:HB3	1:D:1109:PRO:CD	2.16	0.76
1:A:800:SER:HA	1:D:856:SER:OG	1.86	0.76
1:C:396:ALA:HB3	1:C:453:ARG:HH11	1.49	0.76
1:B:686:MET:HE2	1:B:730:LEU:HD21	1.66	0.75
1:C:206:ILE:HD11	1:C:208:ARG:HE	1.51	0.75
1:A:496:ARG:HB3	1:A:496:ARG:HH11	1.52	0.75
1:A:864:HIS:HD2	1:A:866:MET:H	1.33	0.75
1:C:469:LYS:HE3	1:C:469:LYS:HA	1.67	0.75
1:D:504:ILE:HD13	1:D:1042:MET:CE	2.15	0.75
1:A:445:ARG:NH1	1:C:54:GLU:HG2	2.02	0.75
1:D:259:HIS:H	1:D:364:GLN:NE2	1.83	0.75
1:D:337:GLU:HG2	1:D:342:ILE:O	1.87	0.75
1:B:1122:GLU:HA	1:B:1164:ASN:OD1	1.85	0.74
1:C:269:ARG:HB2	1:C:269:ARG:HH11	1.51	0.74
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.00	0.74
1:C:1051:GLU:HG3	1:C:1057:ARG:HH22	1.53	0.74
1:D:622:ASN:ND2	1:D:624:TRP:H	1.85	0.74
1:B:913:VAL:HG11	1:B:947:PHE:HB2	1.68	0.74
1:A:999:GLN:HG2	1:A:1000:GLY:H	1.52	0.73
1:B:68:SER:O	1:B:85:LEU:HD12	1.88	0.73
1:C:677:PHE:HA	1:C:686:MET:CE	2.18	0.73
1:C:504:ILE:CG2	1:C:1042:MET:HE3	2.14	0.73
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.70	0.73
1:C:337:GLU:HG2	1:C:344:ILE:HD12	1.70	0.73
1:D:77:ARG:HH11	1:D:77:ARG:CG	1.97	0.73
1:D:240:ASP:O	1:D:241:ASN:HB2	1.87	0.73
1:D:999:GLN:HE21	1:D:1001:PRO:CD	2.00	0.73
1:C:44:ASN:HD22	1:C:45:ARG:N	1.85	0.73
1:D:398:ARG:HH21	1:D:451:ARG:HD2	1.54	0.73
1:D:335:ILE:HG12	1:D:373:ALA:HB3	1.71	0.73
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.70	0.73
1:A:622:ASN:HD22	1:A:622:ASN:C	1.94	0.73
1:A:142:HIS:H	1:A:145:HIS:HD2	1.37	0.72
1:A:177:TYR:O	1:A:178:GLU:C	2.32	0.72
1:B:445:ARG:O	1:B:449:GLU:HG3	1.89	0.72
1:A:107:LYS:HD2	1:A:134:GLU:OE1	1.88	0.72
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HA	1:B:338:MET:HE2	1.71	0.72
1:D:941:PRO:O	1:D:944:VAL:HG12	1.88	0.72
1:A:606:MET:HE2	1:A:639:PHE:CB	2.20	0.72
1:C:437:LYS:O	1:C:441:GLU:HG3	1.89	0.72
1:B:828:ILE:HD12	1:B:828:ILE:N	2.05	0.72
1:C:572:ASP:HB3	1:C:807:GLN:NE2	2.04	0.72
1:A:1081:ASN:HB3	1:C:78:TYR:CE2	2.25	0.72
1:B:253:GLU:HG3	1:B:305:VAL:HG11	1.70	0.72
1:D:44:ASN:ND2	1:D:45:ARG:H	1.82	0.72
1:A:235:ILE:HG13	1:A:236:GLU:H	1.55	0.71
1:C:937:LYS:HD3	1:D:1152:PRO:CB	2.21	0.71
1:C:175:LYS:H	1:C:175:LYS:HD2	1.53	0.71
1:A:406:ARG:HD2	1:A:407:LEU:N	2.04	0.71
1:C:263:ARG:NH2	1:C:330:GLN:HE21	1.87	0.71
1:C:188:GLY:HA3	1:C:237:ARG:HH22	1.55	0.71
1:D:575:GLN:NE2	1:D:610:ALA:H	1.87	0.71
1:A:434:ILE:HD12	1:A:434:ILE:N	2.04	0.71
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.55	0.71
1:A:513:PRO:O	1:A:515:ASN:HB2	1.90	0.71
1:A:924:ASN:HB2	1:A:926:LEU:HD22	1.73	0.71
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.09	0.71
1:C:145:HIS:HE1	1:C:302:ILE:O	1.73	0.71
1:A:156:ARG:CD	1:A:166:VAL:HG11	2.18	0.70
1:A:1093:ASN:O	1:A:1094:VAL:HB	1.90	0.70
1:B:99:ILE:H	1:B:99:ILE:HD12	1.57	0.70
1:C:820:PHE:HB3	1:C:821:PRO:CD	2.21	0.70
1:C:1144:LYS:HZ3	4:D:1202:BTI:H11	0.83	0.70
1:B:927:ASP:H	1:B:930:SER:HB2	1.56	0.70
1:B:934:ASP:O	1:B:938:LEU:HG	1.90	0.70
1:D:784:LYS:HE3	6:D:1201:CL:CL	2.28	0.70
1:B:125:GLU:CD	1:B:125:GLU:H	2.00	0.70
1:B:568:THR:OG1	1:B:807:GLN:HG3	1.92	0.70
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.05	0.70
1:C:494:LEU:H	1:C:494:LEU:HD22	1.57	0.69
1:D:941:PRO:HD2	1:D:944:VAL:HG11	1.74	0.69
1:A:44:ASN:ND2	1:A:45:ARG:H	1.81	0.69
1:A:263:ARG:HH21	1:A:330:GLN:NE2	1.89	0.69
1:A:406:ARG:HH12	1:C:403:PHE:HB2	1.55	0.69
1:D:142:HIS:HB3	1:D:144:GLU:OE1	1.91	0.69
1:D:828:ILE:HD12	1:D:828:ILE:N	2.07	0.69
1:C:338:MET:CE	1:C:373:ALA:HB1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LYS:HE3	1:B:264:ASP:OD1	1.92	0.69
1:D:509:ILE:HD13	1:D:1089:ILE:CG2	2.21	0.69
1:A:47:GLU:CD	1:A:428:LYS:HE2	2.17	0.69
1:D:87:GLY:HA3	1:D:90:LEU:HG	1.75	0.69
1:A:413:PHE:CE1	1:A:416:ALA:HB3	2.27	0.69
1:C:1029:ASN:C	1:C:1029:ASN:HD22	2.01	0.69
1:B:1101:LYS:HE2	1:B:1162:VAL:HG12	1.75	0.69
1:C:191:LEU:HB3	1:C:235:ILE:CD1	2.23	0.69
1:C:201:GLY:HA2	1:C:204:MET:HE3	1.75	0.69
1:B:261:PHE:CE1	1:B:368:THR:HA	2.28	0.68
1:B:927:ASP:N	1:B:930:SER:HB2	2.08	0.68
1:B:141:PRO:HB2	1:B:145:HIS:CB	2.23	0.68
1:C:978:PRO:HA	1:C:981:TYR:CE2	2.28	0.68
1:B:575:GLN:HE22	1:B:610:ALA:H	1.41	0.68
1:C:269:ARG:HG3	1:C:270:ARG:N	2.07	0.68
1:A:396:ALA:HB3	1:A:453:ARG:HB2	1.76	0.68
1:B:291:ILE:CG1	1:B:320:PHE:HD2	2.07	0.68
1:C:991:ARG:O	1:C:995:GLU:HG3	1.93	0.68
1:A:1146:GLU:O	1:A:1147:THR:HG23	1.94	0.68
1:B:329:VAL:HG13	1:B:348:GLN:HE22	1.57	0.68
1:C:210:GLU:O	1:C:211:SER:CB	2.41	0.68
1:A:235:ILE:HG13	1:A:236:GLU:N	2.06	0.68
1:B:1174:LEU:C	1:B:1175:ILE:HG12	2.19	0.68
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.77	0.68
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.76	0.67
1:C:866:MET:HE1	1:C:891:LYS:HG2	1.77	0.67
1:A:700:SER:H	1:A:736:HIS:CD2	2.07	0.67
1:C:866:MET:HE3	1:C:871:TYR:CD1	2.28	0.67
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.23	0.67
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.77	0.67
1:D:286:THR:O	1:D:290:ARG:HG3	1.94	0.67
1:A:622:ASN:HD22	1:A:624:TRP:H	1.42	0.67
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.42	0.67
1:B:555:GLU:OE1	1:B:555:GLU:HA	1.94	0.67
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.76	0.67
1:C:167:ILE:HG23	1:C:239:ILE:HD11	1.76	0.67
1:C:1029:ASN:ND2	1:C:1031:SER:H	1.92	0.67
1:D:1049:GLU:HG2	1:D:1059:ILE:HD13	1.75	0.67
1:A:1044:ASN:HA	1:A:1062:LEU:HD23	1.77	0.67
1:A:1115:GLN:H	1:A:1115:GLN:NE2	1.93	0.67
1:C:258:VAL:HG21	1:C:362:MET:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:HB	1:D:242:PRO:HG3	1.76	0.67
1:A:406:ARG:NH1	1:C:403:PHE:HB2	2.09	0.67
1:A:811:ASN:HD22	1:A:811:ASN:H	1.40	0.67
1:B:556:TRP:O	1:B:560:GLN:HG2	1.94	0.67
1:B:700:SER:H	1:B:736:HIS:HD2	1.40	0.67
1:D:641:MET:CE	1:D:674:PHE:CE1	2.78	0.67
1:C:653:ASN:HD21	1:C:685:GLN:NE2	1.90	0.67
1:B:40:LEU:C	1:B:40:LEU:HD23	2.19	0.67
1:B:370:LEU:HD21	1:D:341:GLY:HA3	1.76	0.67
1:C:700:SER:N	1:C:736:HIS:HD2	1.91	0.67
1:C:1049:GLU:HG2	1:C:1059:ILE:CD1	2.24	0.67
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.75	0.66
1:C:89:ASP:HB3	1:C:101:ARG:HH12	1.60	0.66
1:A:651:TYR:CE1	1:A:652:LYS:HG3	2.30	0.66
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.31	0.66
1:D:909:PRO:HG2	1:D:952:ILE:HG13	1.77	0.66
1:D:1108:ASN:CB	1:D:1109:PRO:HD3	2.23	0.66
1:A:499:LYS:NZ	1:A:1025:ASN:O	2.26	0.66
1:A:177:TYR:O	1:A:179:LEU:N	2.28	0.66
1:B:927:ASP:HB3	1:B:929:GLN:H	1.60	0.66
1:B:940:PHE:HB3	1:B:944:VAL:HG11	1.77	0.66
1:C:398:ARG:HE	1:C:1083:GLN:CG	2.04	0.66
1:A:215:ASP:O	1:A:218:HIS:HB2	1.95	0.66
1:B:451:ARG:HG2	1:B:453:ARG:HH21	1.61	0.66
1:A:156:ARG:CB	1:A:156:ARG:NH1	2.56	0.66
1:A:242:PRO:O	1:A:477:THR:HB	1.96	0.66
1:B:251:GLY:HA2	1:B:256:ASN:O	1.95	0.65
1:B:828:ILE:HD12	1:B:828:ILE:H	1.59	0.65
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.10	0.65
1:D:1044:ASN:HD22	1:D:1062:LEU:HD23	1.61	0.65
1:B:291:ILE:HG12	1:B:320:PHE:CD2	2.29	0.65
1:C:866:MET:HE3	1:C:871:TYR:CE1	2.32	0.65
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.79	0.65
1:A:1145:MET:HA	1:A:1145:MET:HE2	1.77	0.65
1:C:504:ILE:HD13	1:C:1042:MET:HE1	1.79	0.65
1:A:1145:MET:HA	1:A:1145:MET:HE3	1.76	0.65
1:B:144:GLU:O	1:B:148:MET:HB2	1.96	0.65
1:C:338:MET:HE3	1:C:373:ALA:CB	2.25	0.65
1:A:98:ASN:C	1:A:98:ASN:HD22	2.04	0.65
1:C:960:ASN:HB3	1:C:963:LEU:HD23	1.79	0.65
1:D:644:ARG:NH2	1:D:908:THR:HB	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASP:C	1:B:136:ILE:HG23	2.21	0.65
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.78	0.65
1:B:1000:GLY:H	1:B:1001:PRO:HD2	1.60	0.65
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.05	0.65
1:C:396:ALA:CB	1:C:453:ARG:NH1	2.60	0.65
1:D:400:SER:O	1:D:407:LEU:HD11	1.96	0.64
1:D:1062:LEU:HD12	1:D:1078:TYR:CE2	2.32	0.64
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.79	0.64
1:B:909:PRO:O	1:B:913:VAL:HG23	1.96	0.64
1:C:732:ARG:HG3	1:C:732:ARG:HH11	1.62	0.64
1:B:570:PHE:O	1:B:574:HIS:CE1	2.50	0.64
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.78	0.64
1:C:539:SER:HA	1:C:543:GLN:HG3	1.78	0.64
1:D:853:ASP:OD2	1:D:853:ASP:N	2.27	0.64
1:B:1156:VAL:HG23	1:B:1178:GLU:HB2	1.80	0.64
1:C:215:ASP:HB3	1:C:219:ARG:HG3	1.79	0.64
1:A:381:GLU:HG2	1:A:387:PHE:O	1.98	0.64
1:B:99:ILE:O	1:B:103:ILE:HD12	1.98	0.64
1:D:72:LYS:O	1:D:77:ARG:CD	2.46	0.64
1:A:142:HIS:H	1:A:145:HIS:CD2	2.15	0.64
1:A:176:SER:O	1:A:179:LEU:HB3	1.98	0.64
1:B:338:MET:CE	1:B:373:ALA:HB1	2.28	0.64
1:C:335:ILE:HA	1:C:338:MET:HE2	1.80	0.64
1:C:411:ASP:HB3	1:C:418:ILE:HG22	1.80	0.64
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.33	0.63
1:A:620:LYS:CG	1:A:1023:THR:HG21	2.28	0.63
1:D:72:LYS:O	1:D:77:ARG:NE	2.31	0.63
1:A:338:MET:HE3	1:A:373:ALA:HB1	1.80	0.63
1:A:501:LEU:HD13	1:A:1078:TYR:CD1	2.33	0.63
1:A:828:ILE:HD12	1:A:829:GLU:H	1.63	0.63
1:C:142:HIS:H	1:C:145:HIS:HD2	1.46	0.63
1:D:259:HIS:N	1:D:364:GLN:HE22	1.93	0.63
1:D:869:GLY:O	1:D:871:TYR:N	2.31	0.63
1:C:917:MET:O	1:C:921:MET:HG3	1.97	0.63
1:A:1131:VAL:HG12	1:A:1135:GLN:NE2	2.14	0.63
1:B:341:GLY:O	1:D:434:ILE:HG12	1.99	0.63
1:D:895:ARG:O	1:D:898:ASN:HB3	1.99	0.63
1:B:641:MET:HE3	1:B:674:PHE:CD1	2.34	0.63
1:C:606:MET:CE	1:C:607:TRP:HB2	2.28	0.63
1:C:458:ASN:ND2	1:C:462:LEU:HD11	2.14	0.63
1:B:864:HIS:CD2	1:B:866:MET:H	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:MET:HG2	1:B:926:LEU:CB	2.29	0.62
1:B:960:ASN:HB3	1:B:963:LEU:HB3	1.80	0.62
1:D:141:PRO:HG3	1:D:304:TYR:OH	1.99	0.62
1:B:912:LYS:NZ	1:B:943:SER:HB3	2.14	0.62
1:C:496:ARG:H	1:C:496:ARG:HD3	1.64	0.62
1:B:39:LYS:HD2	1:B:110:ASN:O	1.99	0.62
1:C:677:PHE:CA	1:C:686:MET:HE3	2.24	0.62
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.30	0.62
1:A:243:LYS:NZ	1:A:474:GLY:O	2.32	0.62
1:D:870:GLN:O	1:D:871:TYR:C	2.42	0.62
1:D:866:MET:CE	1:D:871:TYR:HA	2.29	0.62
1:A:192:MET:CE	1:A:238:TYR:HD1	2.10	0.62
1:A:496:ARG:HB3	1:A:496:ARG:NH1	2.14	0.62
1:B:861:ILE:HG13	1:B:862:TYR:N	2.14	0.62
1:A:1158:LYS:HB3	1:A:1176:GLU:HB3	1.81	0.62
1:B:606:MET:HE2	1:B:639:PHE:CB	2.29	0.62
1:C:649:VAL:HG13	1:C:649:VAL:O	2.00	0.62
1:D:91:GLY:O	1:D:92:PRO:O	2.18	0.62
1:C:189:PHE:HD2	1:C:189:PHE:O	1.82	0.62
1:A:124:ASN:OD1	1:A:126:GLN:HB2	2.00	0.62
1:A:361:ASN:HB3	1:C:434:ILE:HD13	1.82	0.62
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.52	0.62
1:C:396:ALA:CB	1:C:453:ARG:HH11	2.13	0.62
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.31	0.62
1:A:177:TYR:C	1:A:179:LEU:N	2.58	0.61
1:A:37:ILE:HD12	1:A:353:ALA:HB2	1.81	0.61
1:A:53:PHE:CZ	1:A:65:ALA:HB2	2.35	0.61
1:A:210:GLU:C	1:A:212:GLU:H	2.08	0.61
1:A:864:HIS:NE2	1:A:866:MET:HG3	2.14	0.61
1:A:866:MET:HE1	1:A:874:LEU:HD22	1.80	0.61
1:B:927:ASP:CB	1:B:930:SER:H	2.12	0.61
1:C:1029:ASN:C	1:C:1029:ASN:ND2	2.57	0.61
1:A:406:ARG:HD2	1:A:406:ARG:C	2.24	0.61
1:D:570:PHE:O	1:D:574:HIS:HE1	1.82	0.61
1:D:743:MET:HG3	1:D:907:VAL:CG1	2.30	0.61
1:B:339:VAL:O	1:B:369:THR:HA	2.00	0.61
1:C:738:LEU:HD23	1:C:768:ILE:HG12	1.81	0.61
1:A:225:GLU:OE2	1:A:225:GLU:HA	2.01	0.61
1:D:260:LEU:O	1:D:261:PHE:HB2	2.01	0.61
1:A:1110:SER:O	1:A:1177:ILE:HD12	2.00	0.61
1:A:1144:LYS:CE	4:B:1201:BTI:H11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ILE:O	1:B:492:PRO:HD3	2.01	0.61
1:A:241:ASN:HD22	1:A:477:THR:HG21	1.64	0.60
1:A:434:ILE:H	1:A:434:ILE:CD1	2.00	0.60
1:D:960:ASN:HD22	1:D:963:LEU:N	1.97	0.60
1:B:1144:LYS:CE	4:B:1202:BTI:C11	2.74	0.60
1:D:864:HIS:HD2	1:D:866:MET:HG3	1.66	0.60
1:C:448:ARG:HH22	1:C:467:LYS:NZ	1.99	0.60
1:A:661:LYS:NZ	1:A:1004:GLU:OE2	2.28	0.60
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.82	0.60
1:D:1067:GLU:OE1	1:D:1067:GLU:HA	2.02	0.60
1:C:86:VAL:HG12	1:C:86:VAL:O	2.00	0.60
1:C:436:PHE:HE2	1:C:472:THR:HA	1.66	0.60
1:C:931:VAL:HA	1:C:935:GLY:H	1.67	0.60
1:D:375:GLN:HG2	1:D:376:CYS:N	2.16	0.60
1:B:927:ASP:HB2	1:B:930:SER:HB2	1.82	0.60
1:C:411:ASP:HB3	1:C:418:ILE:CG2	2.32	0.60
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.83	0.60
1:A:1081:ASN:HB2	1:C:78:TYR:CG	2.36	0.60
1:B:424:SER:O	1:B:425:LEU:C	2.44	0.60
1:D:880:SER:O	1:D:881:LEU:HD23	2.02	0.60
1:A:180:ALA:O	1:A:183:PHE:N	2.27	0.60
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.84	0.60
1:D:1069:ASP:OD2	1:D:1069:ASP:C	2.45	0.60
1:D:1111:HIS:HB3	1:D:1173:LEU:HD13	1.84	0.60
1:B:555:GLU:OE1	1:B:555:GLU:CA	2.49	0.60
1:C:624:TRP:O	1:C:628:GLU:HG3	2.02	0.60
1:C:828:ILE:H	1:C:828:ILE:CD1	1.96	0.60
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.53	0.59
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.32	0.59
1:D:587:MET:O	1:D:590:ILE:HD12	2.02	0.59
1:A:156:ARG:CD	1:A:166:VAL:CG1	2.76	0.59
1:A:902:GLY:O	1:A:903:ASP:HB3	2.01	0.59
1:A:1105:ASP:H	1:A:1111:HIS:HD2	1.50	0.59
1:B:593:LYS:O	1:B:597:VAL:HG23	2.02	0.59
1:C:893:MET:HG3	1:C:922:VAL:HG23	1.84	0.59
1:A:180:ALA:O	1:A:181:LYS:C	2.44	0.59
1:C:205:ARG:HB2	1:C:205:ARG:HH11	1.67	0.59
1:C:71:ASP:OD2	1:C:96:TYR:OH	2.17	0.59
1:D:504:ILE:HG21	1:D:1042:MET:HE3	1.84	0.59
1:D:999:GLN:NE2	1:D:1001:PRO:HD2	2.14	0.59
1:D:1109:PRO:HG2	1:D:1111:HIS:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:SER:O	1:D:319:GLU:HB3	2.03	0.59
1:B:519:ARG:HB2	1:B:520:PRO:HD3	1.84	0.59
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.85	0.59
1:C:396:ALA:HB1	1:C:453:ARG:NH1	2.18	0.59
1:C:960:ASN:O	1:C:961:LYS:C	2.45	0.59
1:A:214:GLU:HB3	1:A:215:ASP:OD1	2.03	0.59
1:A:1015:LYS:HE2	1:A:1019:GLN:NE2	2.17	0.59
1:B:338:MET:HE3	1:B:373:ALA:HB1	1.84	0.59
1:B:622:ASN:ND2	1:B:624:TRP:H	2.01	0.59
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.11	0.58
1:C:937:LYS:HD3	1:D:1152:PRO:HB3	1.84	0.58
1:D:874:LEU:O	1:D:887:PHE:HE1	1.85	0.58
1:A:277:VAL:HG11	1:A:436:PHE:CE1	2.38	0.58
1:A:948:PHE:CD1	1:A:967:ILE:HD12	2.38	0.58
1:C:213:LEU:HD12	1:C:213:LEU:O	2.03	0.58
1:C:276:GLU:O	1:C:335:ILE:HD11	2.03	0.58
1:D:575:GLN:HE22	1:D:610:ALA:H	1.50	0.58
1:A:144:GLU:O	1:A:148:MET:HB3	2.04	0.58
1:A:210:GLU:O	1:A:212:GLU:N	2.37	0.58
1:B:114:ILE:O	1:B:139:ILE:HG13	2.04	0.58
1:D:877:GLN:O	1:D:881:LEU:HG	2.03	0.58
1:A:641:MET:CE	1:A:674:PHE:HE1	2.17	0.58
1:A:800:SER:HA	1:D:856:SER:HG	1.68	0.58
1:B:429:LEU:O	1:B:443:MET:HE1	2.03	0.58
1:C:323:ILE:HG22	1:C:324:GLU:N	2.18	0.58
1:B:99:ILE:H	1:B:99:ILE:CD1	2.12	0.58
1:D:40:LEU:CD2	1:D:42:VAL:HG23	2.34	0.58
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.49	0.58
1:D:544:LEU:O	1:D:548:VAL:HG22	2.04	0.58
1:D:896:ARG:HD2	1:D:928:GLU:OE2	2.03	0.58
1:D:1161:THR:O	1:D:1162:VAL:HG13	2.04	0.58
1:C:378:ILE:HD13	1:C:378:ILE:N	2.19	0.58
1:A:1115:GLN:HE22	1:A:1149:ILE:HD11	1.69	0.58
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.69	0.58
1:C:98:ASN:C	1:C:98:ASN:HD22	2.12	0.58
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.85	0.57
1:A:622:ASN:ND2	1:A:624:TRP:N	2.49	0.57
1:B:167:ILE:HG23	1:B:168:PRO:HD2	1.86	0.57
1:A:254:HIS:CD2	1:A:356:ASP:OD2	2.49	0.57
1:A:328:ARG:HD2	1:A:329:VAL:O	2.04	0.57
1:B:1116:MET:CB	1:B:1117:PRO:HD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ILE:HG13	1:D:450:MET:CE	2.34	0.57
1:C:740:ILE:HB	1:C:770:LEU:HD12	1.87	0.57
1:A:179:LEU:HD11	1:A:217:PHE:CZ	2.38	0.57
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.26	0.57
1:D:700:SER:H	1:D:736:HIS:CD2	2.09	0.57
1:C:196:THR:O	1:C:197:SER:CB	2.52	0.57
1:D:828:ILE:O	1:D:832:GLU:HG2	2.05	0.57
1:A:631:ARG:O	1:A:631:ARG:HD3	2.04	0.57
1:B:451:ARG:HG2	1:B:453:ARG:NH2	2.19	0.57
1:D:400:SER:HB3	1:D:449:GLU:CD	2.29	0.57
1:D:826:THR:HG21	1:D:831:MET:HE1	1.86	0.57
1:B:41:LEU:HD22	1:B:114:ILE:HG12	1.85	0.57
1:B:253:GLU:HG3	1:B:305:VAL:CG1	2.35	0.57
1:D:142:HIS:H	1:D:145:HIS:HD2	1.51	0.57
1:D:690:ASN:O	1:D:694:GLN:HG2	2.05	0.57
1:A:116:PRO:HB2	1:A:122:SER:HA	1.86	0.57
1:A:1064:THR:HG22	1:A:1065:ILE:N	2.19	0.57
1:B:543:GLN:H	1:B:543:GLN:NE2	2.03	0.57
1:C:675:ARG:HA	1:C:701:GLU:HB3	1.86	0.57
1:D:960:ASN:ND2	1:D:963:LEU:N	2.42	0.57
1:A:52:ILE:HD13	1:A:115:HIS:CG	2.40	0.57
1:B:325:VAL:O	1:B:327:PRO:HD3	2.05	0.57
1:D:873:ASN:H	1:D:873:ASN:ND2	1.94	0.57
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.40	0.56
1:C:732:ARG:HG3	1:C:732:ARG:NH1	2.20	0.56
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.69	0.56
1:D:1127:VAL:O	1:D:1157:ILE:O	2.23	0.56
1:B:334:THR:HA	1:B:337:GLU:OE2	2.05	0.56
1:B:370:LEU:O	1:B:432:HIS:HE1	1.89	0.56
1:B:513:PRO:O	1:B:515:ASN:HB2	2.05	0.56
1:B:738:LEU:HD23	1:B:768:ILE:HG13	1.87	0.56
1:B:921:MET:HG2	1:B:926:LEU:HB3	1.87	0.56
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.87	0.56
1:C:871:TYR:HE1	1:C:891:LYS:HD3	1.70	0.56
1:C:964:GLN:O	1:C:965:ALA:C	2.48	0.56
1:A:125:GLU:CD	1:A:125:GLU:H	2.14	0.56
1:A:67:TYR:O	1:A:86:VAL:HG23	2.05	0.56
1:A:386:ASP:O	1:A:387:PHE:HB2	2.04	0.56
1:A:1081:ASN:CB	1:C:78:TYR:CD2	2.88	0.56
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.56
1:D:149:PHE:HA	1:D:155:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:ALA:H	1:D:811:ASN:ND2	2.04	0.56
1:D:1015:LYS:O	1:D:1019:GLN:HG3	2.06	0.56
1:A:512:PHE:CD2	1:A:513:PRO:HD2	2.41	0.56
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.88	0.56
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.87	0.56
1:A:1110:SER:HB3	1:A:1176:GLU:HG2	1.87	0.56
1:B:1053:ASP:HB3	1:B:1056:LYS:HG2	1.86	0.56
1:B:1116:MET:HB3	1:B:1117:PRO:HD2	1.87	0.56
1:C:286:THR:O	1:C:290:ARG:HG3	2.06	0.56
1:C:937:LYS:HD3	1:D:1152:PRO:HB2	1.88	0.56
1:D:381:GLU:O	1:D:383:PRO:HD3	2.06	0.56
1:C:191:LEU:CB	1:C:235:ILE:HD11	2.32	0.56
1:C:215:ASP:O	1:C:216:ALA:C	2.49	0.56
1:C:652:LYS:HA	1:C:952:ILE:CD1	2.35	0.56
1:A:90:LEU:CD1	1:A:98:ASN:HB2	2.36	0.56
1:A:275:VAL:HG22	1:A:376:CYS:HB3	1.87	0.56
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.35	0.56
1:B:501:LEU:HB3	1:B:1078:TYR:CE1	2.41	0.56
1:C:644:ARG:O	1:C:645:ALA:C	2.49	0.56
1:C:1008:ILE:HD12	1:C:1009:SER:H	1.71	0.56
1:A:192:MET:HE3	2:A:1201:ADP:C6	2.41	0.56
1:A:866:MET:CE	1:A:870:GLN:HG2	2.36	0.56
1:C:311:GLU:OE2	5:C:1202:ATP:O1G	2.24	0.56
1:B:40:LEU:HA	1:B:113:ALA:O	2.07	0.55
1:C:238:TYR:CE1	5:C:1202:ATP:C2	2.94	0.55
1:D:468:ASN:OD1	1:D:469:LYS:N	2.40	0.55
1:B:71:ASP:C	1:B:73:SER:H	2.14	0.55
1:B:450:MET:HE3	1:B:450:MET:HA	1.87	0.55
1:C:404:GLY:HA3	1:C:442:LYS:HE2	1.88	0.55
1:B:287:LEU:HD22	1:B:287:LEU:O	2.06	0.55
1:B:445:ARG:NH1	1:B:449:GLU:OE1	2.39	0.55
1:C:927:ASP:OD1	1:C:929:GLN:HG2	2.05	0.55
1:D:864:HIS:CD2	1:D:866:MET:H	2.18	0.55
1:D:920:TYR:OH	1:D:938:LEU:O	2.25	0.55
1:D:1111:HIS:HB3	1:D:1173:LEU:HD11	1.87	0.55
1:A:622:ASN:HD21	1:A:624:TRP:HB2	1.71	0.55
1:B:374:ILE:HG22	1:B:443:MET:HE3	1.88	0.55
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.37	0.55
1:B:870:GLN:C	1:B:872:SER:H	2.15	0.55
1:C:206:ILE:HG13	1:C:206:ILE:O	2.05	0.55
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.40	0.55
1:B:923:GLN:HG3	1:B:923:GLN:O	2.06	0.55
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.42	0.55
1:B:71:ASP:C	1:B:73:SER:N	2.64	0.55
1:C:358:GLU:OE1	1:C:358:GLU:HA	2.05	0.55
1:C:456:LYS:HD3	1:C:456:LYS:N	2.22	0.55
1:A:313:LEU:HD22	1:A:323:ILE:HG13	1.88	0.55
1:B:67:TYR:CD1	1:B:77:ARG:HG3	2.42	0.55
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.06	0.55
1:B:252:ASP:OD1	1:B:357:LEU:N	2.40	0.55
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.72	0.55
1:D:524:TYR:CD2	1:D:843:THR:CG2	2.90	0.55
1:A:296:ILE:O	1:A:300:GLU:HB2	2.07	0.55
1:A:864:HIS:CD2	1:A:866:MET:H	2.19	0.55
1:A:935:GLY:HA3	1:A:966:VAL:CG1	2.36	0.55
1:D:641:MET:HE2	1:D:671:ILE:HG21	1.89	0.55
1:C:425:LEU:C	1:C:425:LEU:HD23	2.32	0.54
1:D:335:ILE:HD11	1:D:373:ALA:O	2.07	0.54
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.40	0.54
1:A:1115:GLN:OE1	1:A:1116:MET:HE3	2.06	0.54
1:B:438:GLN:HA	1:B:441:GLU:HG2	1.89	0.54
1:D:1135:GLN:O	1:D:1150:GLN:HA	2.08	0.54
1:A:1137:LEU:O	1:A:1138:LEU:HB2	2.07	0.54
1:D:384:LEU:HD21	1:D:490:ILE:HG23	1.89	0.54
1:D:814:TYR:CZ	1:D:828:ILE:HG13	2.43	0.54
1:A:1145:MET:HG3	1:B:515:ASN:OD1	2.07	0.54
1:B:1144:LYS:NZ	4:B:1202:BTI:O11	2.29	0.54
1:C:170:THR:HG21	1:C:174:ILE:HD11	1.90	0.54
1:C:1005:GLN:O	1:C:1008:ILE:HD12	2.07	0.54
1:A:268:GLN:HB3	1:A:272:GLN:O	2.08	0.54
1:A:443:MET:HG2	1:A:466:MET:HE3	1.90	0.54
1:C:238:TYR:CD1	5:C:1202:ATP:C2	2.96	0.54
1:D:1123:VAL:HG12	1:D:1163:ASN:O	2.07	0.54
1:A:606:MET:CE	1:A:639:PHE:HB3	2.29	0.54
1:C:717:ASN:HD22	1:C:717:ASN:C	2.14	0.54
1:C:930:SER:O	1:C:931:VAL:HG23	2.06	0.54
1:D:385:ASN:O	1:D:386:ASP:HB2	2.08	0.54
1:A:515:ASN:HA	1:B:1143:MET:HG3	1.88	0.54
1:A:1015:LYS:HE2	1:A:1019:GLN:HE22	1.73	0.54
1:B:1053:ASP:HB3	1:B:1056:LYS:CG	2.38	0.54
1:D:811:ASN:H	1:D:811:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG12	1:A:209:GLU:H	1.73	0.54
1:A:335:ILE:HD11	1:A:374:ILE:C	2.33	0.54
1:B:40:LEU:C	1:B:40:LEU:CD2	2.81	0.54
1:B:434:ILE:CG1	1:D:341:GLY:O	2.53	0.54
1:B:814:TYR:CZ	1:B:828:ILE:HG13	2.43	0.54
1:C:174:ILE:HG22	1:C:217:PHE:HE1	1.73	0.54
1:C:330:GLN:HB3	1:C:332:GLU:OE2	2.08	0.54
1:D:622:ASN:HD22	1:D:623:PRO:N	2.06	0.54
1:A:179:LEU:HD21	1:A:217:PHE:CE2	2.43	0.54
1:A:413:PHE:HE1	1:A:416:ALA:HB3	1.73	0.53
1:B:1132:LYS:HA	1:B:1154:ASP:OD1	2.09	0.53
1:D:1105:ASP:HB3	1:D:1109:PRO:HD2	1.90	0.53
1:A:1081:ASN:HB3	1:C:78:TYR:CD2	2.43	0.53
1:B:932:ILE:HG13	1:B:933:THR:N	2.23	0.53
1:D:743:MET:CG	1:D:907:VAL:HG13	2.37	0.53
1:A:178:GLU:HG3	1:A:181:LYS:HB2	1.91	0.53
1:C:370:LEU:O	1:C:432:HIS:HE1	1.91	0.53
1:B:472:THR:C	1:B:474:GLY:N	2.65	0.53
1:C:193:ILE:C	1:C:193:ILE:HD13	2.33	0.53
1:C:696:ALA:O	1:C:698:LYS:HG2	2.09	0.53
1:C:949:LYS:HE3	1:C:974:LEU:HG	1.90	0.53
1:D:622:ASN:HD22	1:D:622:ASN:C	2.16	0.53
1:D:866:MET:HE2	1:D:871:TYR:HA	1.89	0.53
1:A:309:THR:HG21	1:A:330:GLN:HE22	1.73	0.53
1:C:924:ASN:O	1:C:925:ASP:C	2.52	0.53
1:D:77:ARG:HG3	1:D:77:ARG:NH1	2.08	0.53
1:D:704:ILE:HG12	1:D:726:LEU:HD23	1.89	0.53
1:A:210:GLU:C	1:A:212:GLU:N	2.66	0.53
1:B:335:ILE:HD11	1:B:374:ILE:CA	2.39	0.53
1:B:545:LEU:HD11	1:B:550:PRO:HD3	1.90	0.53
1:C:606:MET:HE3	1:C:607:TRP:HB2	1.90	0.53
1:A:335:ILE:HD11	1:A:375:GLN:N	2.23	0.53
1:A:385:ASN:ND2	1:A:388:MET:HE3	2.24	0.53
1:B:695:GLU:O	1:B:695:GLU:HG2	2.07	0.53
1:C:169:GLY:CA	1:C:236:GLU:HA	2.39	0.53
1:C:265:CYS:HB3	1:C:273:LYS:HD3	1.89	0.53
1:D:151:ASP:HB3	1:D:154:LYS:HG3	1.90	0.53
1:B:472:THR:O	1:B:474:GLY:N	2.41	0.53
1:B:1053:ASP:HB3	1:B:1056:LYS:CD	2.38	0.53
1:C:111:VAL:HG12	1:C:113:ALA:H	1.74	0.53
1:C:234:TYR:H	1:C:234:TYR:HD2	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG11	1:A:436:PHE:HE1	1.73	0.53
1:A:179:LEU:O	1:A:182:GLU:HG2	2.09	0.53
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.44	0.53
1:B:337:GLU:HG2	1:B:344:ILE:HD12	1.91	0.53
1:B:871:TYR:O	1:B:871:TYR:CD1	2.62	0.53
1:C:826:THR:OG1	1:C:827:ASP:N	2.40	0.53
1:D:104:ASP:O	1:D:105:VAL:C	2.52	0.53
1:A:337:GLU:HB3	1:A:342:ILE:O	2.09	0.52
1:C:398:ARG:NH1	1:C:451:ARG:NH1	2.57	0.52
1:A:1117:PRO:HD3	1:A:1170:THR:OG1	2.09	0.52
1:C:811:ASN:HD22	1:C:811:ASN:H	1.55	0.52
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.23	0.52
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.44	0.52
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.74	0.52
1:A:458:ASN:O	1:A:461:PHE:HB3	2.09	0.52
1:B:335:ILE:HG12	1:B:373:ALA:CB	2.40	0.52
1:B:338:MET:HE3	1:B:373:ALA:CB	2.39	0.52
1:B:572:ASP:HB3	1:B:807:GLN:HE21	1.73	0.52
1:C:323:ILE:HG22	1:C:324:GLU:H	1.73	0.52
1:A:263:ARG:HH21	1:A:330:GLN:HE22	1.57	0.52
1:C:188:GLY:HA3	1:C:237:ARG:NH2	2.23	0.52
1:B:575:GLN:NE2	1:B:610:ALA:H	2.06	0.52
1:B:927:ASP:HB2	1:B:930:SER:H	1.73	0.52
1:C:337:GLU:CG	1:C:344:ILE:HD12	2.39	0.52
1:C:504:ILE:HD13	1:C:1042:MET:HE3	1.92	0.52
1:C:644:ARG:CZ	1:C:908:THR:HG21	2.38	0.52
1:C:756:ILE:HG22	1:C:789:ALA:HB1	1.90	0.52
1:C:955:PRO:O	1:C:956:VAL:C	2.52	0.52
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.43	0.52
1:D:509:ILE:CD1	1:D:1089:ILE:HG21	2.34	0.52
1:D:1159:GLN:NE2	1:D:1176:GLU:OE1	2.30	0.52
1:A:414:GLN:HE21	1:A:414:GLN:CA	2.22	0.52
1:B:105:VAL:O	1:B:106:ALA:C	2.52	0.52
1:B:921:MET:HG2	1:B:926:LEU:HB2	1.90	0.52
1:C:296:ILE:O	1:C:300:GLU:HB2	2.09	0.52
1:D:749:PRO:HG3	1:D:781:LEU:HB3	1.91	0.52
1:D:952:ILE:CG2	1:D:952:ILE:O	2.58	0.52
1:B:137:LYS:CE	1:B:352:ALA:O	2.47	0.52
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.56	0.52
1:B:871:TYR:O	1:B:871:TYR:HD1	1.93	0.52
1:B:1176:GLU:C	1:B:1177:ILE:HD13	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HG22	1:C:217:PHE:CE1	2.44	0.52
1:C:652:LYS:HA	1:C:952:ILE:HD11	1.91	0.52
1:D:263:ARG:NH2	1:D:330:GLN:HE21	2.08	0.52
1:A:991:ARG:O	1:A:995:GLU:HG3	2.10	0.52
1:B:144:GLU:O	1:B:148:MET:N	2.41	0.52
1:B:1097:ASN:H	1:B:1097:ASN:HD22	1.57	0.52
1:C:798:VAL:O	1:C:799:ALA:C	2.53	0.52
1:C:896:ARG:HB3	1:C:928:GLU:OE2	2.10	0.52
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.07	0.52
1:B:363:GLN:HB2	1:B:366:ASP:OD2	2.10	0.52
1:B:1087:ILE:HG22	1:B:1088:TYR:N	2.24	0.52
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.58	0.52
1:C:649:VAL:O	1:C:649:VAL:CG1	2.58	0.52
1:B:145:HIS:HE1	1:B:302:ILE:O	1.93	0.52
1:B:820:PHE:HB3	1:B:821:PRO:HD2	1.91	0.52
1:C:606:MET:HE1	1:C:671:ILE:HD11	1.90	0.52
1:A:580:THR:HG22	1:A:580:THR:O	2.10	0.51
1:B:358:GLU:OE2	1:B:358:GLU:HA	2.10	0.51
1:D:1042:MET:HE2	1:D:1048:VAL:HG11	1.92	0.51
1:D:1069:ASP:OD2	1:D:1070:GLU:N	2.43	0.51
1:B:1053:ASP:CG	1:B:1054:LYS:H	2.19	0.51
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.25	0.51
1:C:206:ILE:HD11	1:C:208:ARG:NE	2.24	0.51
1:C:940:PHE:HB3	1:C:944:VAL:HG11	1.92	0.51
1:D:370:LEU:O	1:D:432:HIS:HE1	1.92	0.51
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.57	0.51
1:A:688:VAL:HG21	1:A:977:ARG:NH2	2.26	0.51
1:A:513:PRO:O	1:A:515:ASN:CB	2.50	0.51
1:A:622:ASN:HD22	1:A:623:PRO:N	2.08	0.51
1:A:631:ARG:HD3	1:A:631:ARG:C	2.34	0.51
1:A:796:THR:HB	1:A:810:ALA:HB2	1.91	0.51
1:B:893:MET:CE	1:B:896:ARG:HH21	2.24	0.51
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.45	0.51
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.94	0.51
1:C:775:THR:CG2	1:C:861:ILE:HG13	2.41	0.51
1:C:814:TYR:CZ	1:C:828:ILE:HG13	2.45	0.51
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.18	0.51
1:B:620:LYS:HG2	4:B:1201:BTI:H63	1.93	0.51
1:B:701:GLU:OE2	1:B:769:HIS:ND1	2.44	0.51
1:B:991:ARG:HG3	1:B:992:GLU:N	2.24	0.51
1:D:671:ILE:O	1:D:698:LYS:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HD12	1:A:323:ILE:HD11	1.92	0.51
1:A:451:ARG:NH1	1:A:495:ASP:OD2	2.41	0.51
1:C:192:MET:HG3	1:C:206:ILE:HG22	1.92	0.51
1:C:893:MET:HG3	1:C:922:VAL:CG2	2.40	0.51
1:D:263:ARG:HG2	1:D:278:ALA:HB2	1.91	0.51
1:A:650:GLY:HA2	1:A:1013:TYR:CE1	2.46	0.51
1:B:269:ARG:O	1:B:270:ARG:C	2.53	0.51
1:B:897:VAL:HG11	1:B:914:VAL:HG13	1.86	0.51
1:B:1133:ALA:O	1:B:1134:ASN:HB2	2.10	0.51
1:C:938:LEU:HA	1:D:1115:GLN:HE22	1.76	0.51
1:D:597:VAL:HG22	1:D:830:GLY:HA3	1.93	0.51
1:A:896:ARG:NH1	1:A:928:GLU:OE1	2.44	0.51
1:B:802:SER:OG	1:B:809:SER:HB2	2.11	0.51
1:B:1000:GLY:N	1:B:1001:PRO:HD2	2.26	0.51
1:C:43:ALA:HA	1:C:66:ILE:HD11	1.92	0.51
1:C:194:LYS:HD2	1:C:234:TYR:CZ	2.46	0.51
1:C:959:PHE:N	1:C:959:PHE:CD1	2.78	0.51
1:D:74:SER:O	1:D:77:ARG:HB3	2.11	0.51
1:D:784:LYS:CE	6:D:1201:CL:CL	2.96	0.51
1:B:144:GLU:O	1:B:148:MET:CB	2.58	0.51
1:C:115:HIS:ND1	1:C:116:PRO:HD2	2.26	0.51
1:C:210:GLU:O	1:C:211:SER:HB3	2.11	0.51
1:D:542:LYS:HE3	1:D:672:ASP:OD1	2.10	0.51
1:A:572:ASP:HB3	1:A:807:GLN:NE2	2.25	0.51
1:A:622:ASN:ND2	1:A:622:ASN:C	2.64	0.51
1:C:90:LEU:HB3	1:C:95:SER:HB2	1.93	0.51
1:D:338:MET:HE1	1:D:430:SER:HB3	1.89	0.51
1:D:470:LYS:HB2	1:D:480:PHE:HE1	1.76	0.51
1:D:960:ASN:HD22	1:D:963:LEU:CB	2.23	0.51
1:A:166:VAL:CG1	1:A:167:ILE:N	2.74	0.50
1:A:257:ILE:HG22	1:A:296:ILE:CD1	2.41	0.50
1:A:553:VAL:O	1:A:556:TRP:HB3	2.11	0.50
1:B:711:LEU:HD11	1:B:750:LYS:HB3	1.93	0.50
1:C:703:THR:HG22	1:C:704:ILE:N	2.26	0.50
1:D:143:LEU:HD12	1:D:143:LEU:H	1.77	0.50
1:D:524:TYR:HD2	1:D:843:THR:CG2	2.24	0.50
1:D:1101:LYS:O	1:D:1102:PRO:C	2.54	0.50
1:A:71:ASP:O	1:A:72:LYS:C	2.54	0.50
1:B:40:LEU:HD23	1:B:41:LEU:N	2.27	0.50
1:B:370:LEU:HD21	1:D:341:GLY:CA	2.39	0.50
1:B:748:LYS:HB3	1:B:749:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:ILE:H	1:B:828:ILE:CD1	2.14	0.50
1:C:496:ARG:CD	1:C:496:ARG:N	2.75	0.50
1:D:413:PHE:CZ	1:D:416:ALA:HB2	2.46	0.50
1:D:622:ASN:ND2	1:D:622:ASN:C	2.66	0.50
1:A:179:LEU:HD23	1:A:179:LEU:N	2.07	0.50
1:B:121:LEU:O	1:B:124:ASN:HB3	2.10	0.50
1:B:530:PRO:HB2	1:B:593:LYS:HD3	1.94	0.50
1:B:856:SER:OG	1:C:800:SER:HA	2.12	0.50
1:B:912:LYS:HZ2	1:B:943:SER:HB3	1.76	0.50
1:C:77:ARG:HD3	1:C:78:TYR:CD2	2.47	0.50
1:A:828:ILE:O	1:A:832:GLU:HG2	2.11	0.50
1:C:820:PHE:HB3	1:C:821:PRO:HD3	1.91	0.50
1:A:622:ASN:ND2	1:A:624:TRP:HB2	2.27	0.50
1:C:181:LYS:O	1:C:185:GLU:HG2	2.11	0.50
1:B:335:ILE:HG12	1:B:373:ALA:HB1	1.93	0.50
1:D:328:ARG:HD3	1:D:329:VAL:O	2.11	0.50
1:B:118:TYR:CE2	1:B:331:VAL:HA	2.46	0.50
1:B:897:VAL:HG22	1:B:921:MET:HE1	1.93	0.50
1:C:51:ARG:HD3	1:C:406:ARG:HH12	1.77	0.50
1:C:99:ILE:O	1:C:103:ILE:HD12	2.12	0.50
1:C:1143:MET:O	1:C:1144:LYS:HB2	2.11	0.50
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.93	0.50
1:B:1095:HIS:CB	1:B:1098:ALA:HB3	2.40	0.50
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.09	0.50
1:C:813:LEU:O	1:C:814:TYR:C	2.53	0.50
1:B:498:THR:HG23	1:B:1085:ARG:HH22	1.77	0.50
1:B:522:PRO:C	1:B:524:TYR:N	2.69	0.50
1:B:682:TRP:CE3	1:B:685:GLN:HG2	2.47	0.50
1:C:1065:ILE:HG12	1:C:1076:ILE:HG12	1.94	0.50
1:D:770:LEU:HD12	1:D:771:HIS:H	1.76	0.50
1:D:871:TYR:CE1	1:D:887:PHE:HE2	2.29	0.50
1:B:568:THR:OG1	1:B:807:GLN:CG	2.58	0.49
1:B:867:PRO:O	1:B:868:GLY:C	2.54	0.49
1:A:902:GLY:O	1:A:903:ASP:CB	2.61	0.49
1:B:472:THR:C	1:B:474:GLY:H	2.20	0.49
1:C:563:VAL:HG21	1:C:787:ILE:HG12	1.93	0.49
1:C:893:MET:HE1	1:C:921:MET:SD	2.52	0.49
1:C:641:MET:HB3	1:C:671:ILE:HD12	1.95	0.49
1:A:871:TYR:CD1	1:A:871:TYR:O	2.65	0.49
1:B:755:LEU:O	1:B:759:LEU:HG	2.11	0.49
1:C:1005:GLN:HA	1:C:1008:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HD3	1:A:272:GLN:OE1	2.12	0.49
1:C:461:PHE:CE1	1:C:487:LEU:HB3	2.48	0.49
1:D:141:PRO:HB2	1:D:145:HIS:HB2	1.94	0.49
1:D:490:ILE:O	1:D:492:PRO:CD	2.48	0.49
1:A:380:THR:H	1:A:424:SER:HG	1.61	0.49
1:A:811:ASN:HD22	1:A:811:ASN:N	2.09	0.49
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.47	0.49
1:B:307:ALA:HB3	1:B:348:GLN:HE21	1.78	0.49
1:B:425:LEU:C	1:B:425:LEU:HD23	2.37	0.49
1:B:542:LYS:HE2	1:B:631:ARG:NH2	2.26	0.49
1:C:90:LEU:HD11	1:C:98:ASN:OD1	2.13	0.49
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.95	0.49
1:C:739:ALA:C	1:C:740:ILE:HD13	2.37	0.49
1:C:939:ASP:O	1:D:1147:THR:CG2	2.60	0.49
1:D:1153:PHE:O	1:D:1154:ASP:HB2	2.13	0.49
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.27	0.49
1:A:858:ASN:C	1:A:858:ASN:HD22	2.20	0.49
1:B:115:HIS:NE2	1:B:348:GLN:OE1	2.45	0.49
1:B:715:ARG:HD2	1:B:715:ARG:O	2.13	0.49
1:B:927:ASP:HB2	1:B:930:SER:CB	2.42	0.49
1:C:71:ASP:O	1:C:73:SER:N	2.46	0.49
1:D:918:ALA:O	1:D:922:VAL:HG23	2.12	0.49
1:D:998:GLN:O	1:D:999:GLN:O	2.31	0.49
1:D:1105:ASP:HB3	1:D:1109:PRO:CD	2.42	0.49
1:A:509:ILE:HD12	1:A:1089:ILE:HG21	1.94	0.49
1:B:43:ALA:HB3	1:B:116:PRO:HA	1.95	0.49
1:B:641:MET:CE	1:B:674:PHE:CE1	2.92	0.49
1:A:90:LEU:HD11	1:A:98:ASN:HB2	1.94	0.49
1:B:294:ALA:O	1:B:295:ALA:C	2.55	0.49
1:B:842:ARG:CZ	1:C:855:LYS:HE2	2.43	0.49
1:B:949:LYS:HG2	1:B:968:LEU:HD21	1.95	0.49
1:C:986:ASP:CG	1:C:989:LYS:HG3	2.38	0.49
1:C:991:ARG:HG3	1:C:995:GLU:HG3	1.95	0.49
1:D:262:GLU:OE2	1:D:288:ARG:HG3	2.13	0.49
1:A:98:ASN:C	1:A:98:ASN:ND2	2.70	0.49
1:A:783:TYR:O	1:A:787:ILE:HG13	2.12	0.49
1:B:333:HIS:O	1:B:334:THR:C	2.55	0.49
1:B:606:MET:HE2	1:B:639:PHE:CG	2.48	0.49
1:B:1112:ILE:CD1	1:B:1177:ILE:HD11	2.43	0.49
1:C:152:LYS:HG3	1:C:197:SER:HA	1.94	0.49
1:C:544:LEU:O	1:C:547:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.48	0.49
1:C:828:ILE:O	1:C:829:GLU:C	2.54	0.49
1:D:241:ASN:HD22	1:D:477:THR:HB	1.77	0.49
1:B:156:ARG:NH2	1:B:167:ILE:HG13	2.28	0.48
1:B:798:VAL:O	1:B:799:ALA:C	2.54	0.48
1:B:1169:ALA:O	1:B:1170:THR:C	2.54	0.48
1:C:931:VAL:HA	1:C:935:GLY:N	2.28	0.48
1:C:969:LYS:HE2	1:C:969:LYS:HA	1.94	0.48
1:A:632:LYS:HB3	1:A:632:LYS:HE2	1.57	0.48
1:B:1022:GLN:HA	1:B:1022:GLN:NE2	2.28	0.48
1:B:1101:LYS:HD2	1:B:1161:THR:HG22	1.95	0.48
1:D:675:ARG:HH22	1:D:795:ASP:CG	2.21	0.48
1:D:748:LYS:O	1:D:751:ALA:HB3	2.13	0.48
1:A:174:ILE:HG13	1:A:174:ILE:O	2.13	0.48
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.95	0.48
1:A:1071:ASN:O	1:A:1090:LYS:HE2	2.13	0.48
1:B:485:PRO:HD2	1:B:486:GLU:OE1	2.14	0.48
1:B:811:ASN:HD22	1:B:811:ASN:N	2.03	0.48
1:C:381:GLU:O	1:C:383:PRO:HD3	2.13	0.48
1:D:622:ASN:ND2	1:D:623:PRO:HD2	2.22	0.48
1:C:259:HIS:HB3	1:C:296:ILE:HD11	1.95	0.48
1:D:239:ILE:O	1:D:242:PRO:HD3	2.14	0.48
1:A:1064:THR:CG2	1:A:1065:ILE:N	2.76	0.48
1:A:1077:TYR:N	1:A:1077:TYR:CD1	2.81	0.48
1:B:1053:ASP:CG	1:B:1054:LYS:N	2.72	0.48
1:A:144:GLU:CD	1:A:144:GLU:H	2.22	0.48
1:A:299:MET:HE3	1:A:304:TYR:CG	2.48	0.48
1:A:784:LYS:HE3	6:D:1201:CL:CL	2.50	0.48
1:B:656:ASP:OD1	1:B:977:ARG:NH2	2.47	0.48
1:B:915:GLY:O	1:B:919:LEU:HD22	2.14	0.48
1:C:269:ARG:HB2	1:C:269:ARG:NH1	2.26	0.48
1:C:866:MET:HE3	1:C:871:TYR:HD1	1.79	0.48
1:D:142:HIS:O	1:D:143:LEU:C	2.55	0.48
1:A:380:THR:N	1:A:424:SER:OG	2.38	0.48
1:C:166:VAL:HG12	1:C:167:ILE:N	2.28	0.48
1:C:167:ILE:HD12	1:C:167:ILE:H	1.77	0.48
1:C:572:ASP:CB	1:C:807:GLN:HE22	2.22	0.48
1:A:778:ASN:ND2	1:D:780:LEU:HD13	2.29	0.48
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.48
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.49	0.48
1:C:496:ARG:HD3	1:C:496:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:THR:CG2	1:C:704:ILE:N	2.77	0.48
1:D:156:ARG:O	1:D:159:ALA:HB3	2.13	0.48
1:D:683:VAL:HG23	1:D:726:LEU:HD11	1.94	0.48
1:A:991:ARG:HG3	1:A:995:GLU:HG3	1.95	0.48
1:B:129:ARG:HH11	1:B:129:ARG:CB	2.27	0.48
1:C:986:ASP:OD1	1:C:988:GLU:HB2	2.14	0.48
1:D:40:LEU:HD21	1:D:42:VAL:HG23	1.95	0.48
1:A:130:ARG:NH1	1:A:133:GLU:OE1	2.43	0.48
1:B:125:GLU:CD	1:B:125:GLU:N	2.70	0.48
1:B:450:MET:HE3	1:B:450:MET:CA	2.43	0.48
1:C:235:ILE:HG13	1:C:236:GLU:N	2.27	0.48
1:D:77:ARG:CG	1:D:77:ARG:NH1	2.68	0.48
1:D:385:ASN:O	1:D:386:ASP:CB	2.60	0.48
1:A:1108:ASN:OD1	1:A:1108:ASN:C	2.56	0.47
1:C:775:THR:HG21	1:C:861:ILE:HG13	1.96	0.47
1:C:1144:LYS:HE2	1:D:513:PRO:HD3	1.95	0.47
1:D:286:THR:HG22	1:D:290:ARG:HD3	1.96	0.47
1:B:700:SER:HG	1:B:735:PHE:HD2	1.59	0.47
1:B:870:GLN:NE2	1:B:874:LEU:HD13	2.28	0.47
1:C:328:ARG:HG3	1:C:329:VAL:O	2.14	0.47
1:D:287:LEU:CD1	1:D:317:GLY:O	2.54	0.47
1:D:484:THR:HB	1:D:487:LEU:HD22	1.96	0.47
1:D:590:ILE:O	1:D:591:ALA:C	2.58	0.47
1:D:869:GLY:O	1:D:870:GLN:C	2.57	0.47
1:A:176:SER:O	1:A:179:LEU:CB	2.62	0.47
1:A:798:VAL:O	1:A:799:ALA:C	2.57	0.47
1:C:87:GLY:HA3	1:C:90:LEU:CD2	2.40	0.47
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.80	0.47
1:D:262:GLU:OE2	1:D:288:ARG:NH1	2.46	0.47
1:A:744:ALA:HB2	1:A:867:PRO:HA	1.96	0.47
1:C:631:ARG:C	1:C:631:ARG:HD3	2.35	0.47
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.11	0.47
1:A:99:ILE:O	1:A:103:ILE:HG12	2.13	0.47
1:A:856:SER:OG	1:D:800:SER:HA	2.14	0.47
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.97	0.47
1:A:512:PHE:CG	1:A:513:PRO:HD2	2.49	0.47
1:B:1161:THR:HG22	1:B:1161:THR:O	2.15	0.47
1:C:743:MET:CG	1:C:907:VAL:HG13	2.45	0.47
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.47	0.47
1:D:902:GLY:O	1:D:903:ASP:HB3	2.14	0.47
1:D:1158:LYS:HB2	1:D:1176:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:O	1:A:432:HIS:HE1	1.97	0.47
1:B:1001:PRO:HB2	1:B:1002:VAL:H	1.47	0.47
1:C:141:PRO:HB2	1:C:145:HIS:HB2	1.96	0.47
1:C:189:PHE:O	1:C:189:PHE:CD2	2.66	0.47
1:D:470:LYS:HE2	1:D:470:LYS:CA	2.42	0.47
1:D:620:LYS:HE2	1:D:1023:THR:HG1	1.78	0.47
1:A:156:ARG:NH2	1:A:170:THR:O	2.48	0.47
1:A:252:ASP:HB3	1:A:357:LEU:HG	1.97	0.47
1:B:91:GLY:O	1:B:93:ALA:N	2.47	0.47
1:B:878:ALA:HB1	1:B:883:LEU:HB2	1.97	0.47
1:B:913:VAL:HG13	1:B:943:SER:HB2	1.97	0.47
1:C:194:LYS:HD2	1:C:234:TYR:OH	2.15	0.47
1:C:586:ASP:OD1	1:C:845:TYR:OH	2.25	0.47
1:C:720:LEU:HD21	1:C:758:GLU:HG3	1.96	0.47
1:C:828:ILE:C	1:C:830:GLY:N	2.70	0.47
1:D:446:SER:O	1:D:450:MET:HG2	2.15	0.47
1:A:45:ARG:HD2	1:A:96:TYR:CE1	2.50	0.47
1:A:71:ASP:O	1:A:73:SER:N	2.47	0.47
1:A:263:ARG:NH2	1:A:330:GLN:NE2	2.58	0.47
1:A:413:PHE:CZ	1:A:416:ALA:HB3	2.49	0.47
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.33	0.47
1:C:211:SER:C	1:C:213:LEU:N	2.71	0.47
1:C:414:GLN:HG3	1:C:414:GLN:O	2.15	0.47
1:D:116:PRO:HB2	1:D:122:SER:HA	1.96	0.47
1:D:755:LEU:O	1:D:759:LEU:HG	2.14	0.47
1:D:1050:ILE:HB	1:D:1058:LEU:HB3	1.97	0.47
1:B:129:ARG:HH11	1:B:129:ARG:HB2	1.80	0.46
1:B:606:MET:HE2	1:B:639:PHE:CD2	2.50	0.46
1:B:644:ARG:HD2	1:B:647:ASN:OD1	2.15	0.46
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.50	0.46
1:C:373:ALA:HA	1:C:431:THR:O	2.15	0.46
1:C:768:ILE:HG22	1:C:791:VAL:HG23	1.96	0.46
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.50	0.46
1:A:461:PHE:HE1	1:A:488:PHE:CE2	2.33	0.46
1:A:999:GLN:CG	1:A:1000:GLY:H	2.21	0.46
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.80	0.46
1:C:210:GLU:O	1:C:211:SER:HB2	2.14	0.46
1:D:41:LEU:HB2	1:D:111:VAL:HG21	1.97	0.46
1:A:481:ILE:O	1:A:482:GLU:C	2.57	0.46
1:C:287:LEU:HD22	1:C:291:ILE:HD11	1.98	0.46
1:C:936:TYR:HE2	1:C:966:VAL:CG1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.06	0.46
1:D:431:THR:HG21	1:D:443:MET:HA	1.98	0.46
1:D:647:ASN:C	1:D:647:ASN:ND2	2.59	0.46
1:A:1127:VAL:HG13	1:A:1158:LYS:O	2.14	0.46
1:B:811:ASN:N	1:B:811:ASN:ND2	2.63	0.46
1:D:325:VAL:HG12	1:D:327:PRO:HD3	1.97	0.46
1:B:715:ARG:HH12	1:B:865:GLU:CD	2.23	0.46
1:C:540:GLY:HA3	1:C:636:ASN:O	2.15	0.46
1:C:705:CYS:HB3	1:C:743:MET:SD	2.55	0.46
1:D:866:MET:CE	1:D:870:GLN:HB3	2.46	0.46
1:D:1103:LYS:HB2	1:D:1104:ALA:H	1.61	0.46
1:A:486:GLU:C	1:A:488:PHE:H	2.24	0.46
1:A:1144:LYS:O	1:A:1145:MET:HE3	2.16	0.46
1:C:196:THR:O	1:C:196:THR:CG2	2.53	0.46
1:C:249:VAL:HG21	1:C:299:MET:HG3	1.98	0.46
1:C:584:THR:O	1:C:585:LYS:C	2.56	0.46
1:D:798:VAL:O	1:D:799:ALA:C	2.57	0.46
1:D:799:ALA:HB3	1:D:835:SER:OG	2.16	0.46
1:D:998:GLN:O	1:D:999:GLN:C	2.58	0.46
1:A:152:LYS:HB3	1:A:234:TYR:CE2	2.51	0.46
1:A:192:MET:HE3	2:A:1201:ADP:C5	2.51	0.46
1:A:570:PHE:O	1:A:574:HIS:HE1	1.99	0.46
1:A:597:VAL:HG21	1:A:834:LEU:HG	1.96	0.46
1:B:41:LEU:CD2	1:B:114:ILE:HG12	2.46	0.46
1:B:248:GLN:HB3	1:B:260:LEU:HB2	1.98	0.46
1:B:909:PRO:HG2	1:B:952:ILE:HG12	1.97	0.46
1:C:148:MET:SD	1:C:302:ILE:HG21	2.55	0.46
1:C:269:ARG:CG	1:C:270:ARG:H	2.24	0.46
1:A:46:GLY:O	1:A:47:GLU:C	2.59	0.46
1:A:130:ARG:HD2	1:A:133:GLU:OE1	2.15	0.46
1:A:166:VAL:HG12	1:A:167:ILE:N	2.30	0.46
1:B:828:ILE:O	1:B:832:GLU:HG2	2.15	0.46
1:C:52:ILE:HD13	1:C:115:HIS:CG	2.50	0.46
1:C:986:ASP:O	1:C:990:VAL:HG23	2.15	0.46
1:D:986:ASP:OD2	1:D:986:ASP:C	2.57	0.46
1:A:153:VAL:O	1:A:154:LYS:C	2.59	0.46
1:A:164:LEU:HD13	1:A:294:ALA:HB1	1.97	0.46
1:A:180:ALA:O	1:A:182:GLU:N	2.49	0.46
1:A:1141:GLU:HA	1:A:1145:MET:O	2.16	0.46
1:B:479:LYS:O	1:B:483:GLU:HG2	2.16	0.46
1:B:512:PHE:HB3	1:B:516:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ASP:HB3	1:B:930:SER:H	1.80	0.46
1:B:1116:MET:CB	1:B:1117:PRO:CD	2.93	0.46
1:C:141:PRO:HG2	1:C:146:LEU:HD11	1.97	0.46
1:A:47:GLU:OE2	1:A:428:LYS:HE2	2.16	0.46
1:A:558:LYS:CE	1:A:765:ASP:O	2.57	0.46
1:A:796:THR:CB	1:A:810:ALA:HB2	2.46	0.46
1:A:858:ASN:HD21	1:A:860:GLU:H	1.60	0.46
1:B:426:LEU:O	1:B:427:VAL:HG13	2.17	0.46
1:B:715:ARG:HD2	1:B:715:ARG:C	2.40	0.46
1:C:241:ASN:N	1:C:242:PRO:CD	2.78	0.46
1:D:329:VAL:CG2	1:D:348:GLN:HE22	2.10	0.46
1:B:240:ASP:C	1:B:242:PRO:HD3	2.42	0.45
1:C:403:PHE:O	1:C:442:LYS:HE3	2.15	0.45
1:C:677:PHE:HB3	1:C:703:THR:HB	1.97	0.45
1:D:378:ILE:HG23	1:D:459:ILE:HG13	1.97	0.45
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.52	0.45
1:D:917:MET:HA	1:D:917:MET:CE	2.41	0.45
1:A:414:GLN:HE21	1:A:414:GLN:HA	1.81	0.45
1:B:1062:LEU:HD11	1:B:1076:ILE:HG23	1.98	0.45
1:B:1124:LYS:C	1:B:1125:VAL:HG13	2.42	0.45
1:C:175:LYS:H	1:C:175:LYS:CD	2.27	0.45
1:C:641:MET:HE3	1:C:666:SER:HB3	1.97	0.45
1:C:854:ILE:H	1:C:854:ILE:HG13	1.60	0.45
1:D:396:ALA:HB3	1:D:453:ARG:CG	2.46	0.45
1:B:252:ASP:HA	1:B:351:VAL:HG13	1.98	0.45
1:B:326:ASN:ND2	1:B:330:GLN:NE2	2.65	0.45
1:B:641:MET:HE2	1:B:671:ILE:HG21	1.98	0.45
1:B:653:ASN:ND2	1:B:951:GLU:O	2.41	0.45
1:B:1135:GLN:O	1:B:1150:GLN:HA	2.17	0.45
1:D:715:ARG:HH12	1:D:865:GLU:CD	2.22	0.45
1:D:872:SER:O	1:D:875:SER:HB2	2.16	0.45
1:D:875:SER:OG	1:D:887:PHE:CZ	2.65	0.45
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.82	0.45
1:B:852:SER:HG	1:B:854:ILE:H	1.62	0.45
1:B:994:LEU:O	1:B:998:GLN:HG3	2.15	0.45
1:B:1008:ILE:HD12	1:B:1009:SER:N	2.31	0.45
1:C:375:GLN:CD	1:C:428:LYS:HD3	2.41	0.45
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.98	0.45
1:A:1161:THR:OG1	1:A:1173:LEU:O	2.33	0.45
1:B:924:ASN:O	1:B:925:ASP:HB2	2.16	0.45
1:C:71:ASP:C	1:C:73:SER:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:CD2	1:C:362:MET:CE	2.73	0.45
1:C:939:ASP:O	1:D:1147:THR:HG21	2.17	0.45
1:A:778:ASN:HD22	1:D:780:LEU:HD13	1.81	0.45
1:B:979:GLY:HA2	1:B:982:LEU:HD12	1.98	0.45
1:B:1123:VAL:HA	1:B:1138:LEU:HD12	1.98	0.45
1:C:948:PHE:CD2	1:C:964:GLN:HB2	2.52	0.45
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.48	0.45
1:B:64:VAL:HG22	1:B:82:GLU:HB2	1.98	0.45
1:B:252:ASP:OD1	1:B:357:LEU:HB2	2.16	0.45
1:C:398:ARG:HH21	1:C:1083:GLN:HB3	1.80	0.45
1:C:524:TYR:CD2	1:C:843:THR:CG2	3.00	0.45
1:C:820:PHE:HB3	1:C:821:PRO:HD2	1.98	0.45
1:D:259:HIS:HD2	1:D:261:PHE:H	1.65	0.45
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.99	0.45
1:D:752:ALA:HB2	1:D:782:THR:HG23	1.97	0.45
1:A:190:PRO:O	1:A:191:LEU:HD23	2.17	0.45
1:A:267:VAL:HG12	1:A:274:VAL:HB	1.99	0.45
1:A:277:VAL:CG1	1:A:436:PHE:HE1	2.29	0.45
1:A:322:PHE:O	1:A:323:ILE:HD13	2.17	0.45
1:A:1053:ASP:O	1:A:1054:LYS:C	2.60	0.45
1:C:625:GLU:O	1:C:629:ARG:HG3	2.17	0.45
1:D:145:HIS:HE1	1:D:302:ILE:O	2.00	0.45
1:D:494:LEU:N	1:D:494:LEU:HD23	2.31	0.45
1:D:613:ASP:HB2	1:D:1013:TYR:CZ	2.52	0.45
1:D:814:TYR:CE2	1:D:828:ILE:HG13	2.52	0.45
1:A:108:GLN:O	1:A:108:GLN:HG2	2.17	0.45
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.81	0.45
1:B:565:LEU:C	1:B:565:LEU:HD12	2.42	0.45
1:B:999:GLN:HG2	1:B:1001:PRO:HD2	1.99	0.45
1:C:386:ASP:O	1:C:387:PHE:HB2	2.17	0.45
1:D:131:CYS:O	1:D:132:ALA:C	2.57	0.45
1:D:1060:ILE:HG12	1:D:1080:MET:HG3	1.98	0.45
1:B:686:MET:HE2	1:B:730:LEU:CD2	2.42	0.45
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.98	0.45
1:B:946:SER:O	1:B:947:PHE:C	2.60	0.45
1:D:99:ILE:HG23	1:D:127:PHE:CD1	2.51	0.45
1:D:641:MET:CE	1:D:674:PHE:HE1	2.28	0.45
1:A:219:ARG:O	1:A:223:GLU:CB	2.59	0.44
1:A:356:ASP:O	1:A:357:LEU:C	2.60	0.44
2:A:1201:ADP:O1A	2:A:1201:ADP:O1B	2.35	0.44
1:B:811:ASN:H	1:B:811:ASN:ND2	2.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:LYS:HD2	1:C:987:PHE:CZ	2.52	0.44
1:C:907:VAL:O	1:C:910:SER:N	2.50	0.44
1:D:484:THR:HG22	1:D:486:GLU:HG2	1.98	0.44
1:A:1156:VAL:HG22	1:A:1178:GLU:HB2	1.97	0.44
1:C:323:ILE:HD13	1:C:323:ILE:HA	1.58	0.44
1:B:68:SER:OG	1:B:69:ASN:N	2.49	0.44
1:B:118:TYR:HD1	1:B:118:TYR:O	2.01	0.44
1:C:170:THR:HG22	1:C:171:ASP:N	2.32	0.44
1:D:267:VAL:HG12	1:D:481:ILE:HD11	1.98	0.44
1:D:270:ARG:HB3	1:D:271:HIS:H	1.65	0.44
1:D:1042:MET:HB3	1:D:1046:GLU:OE2	2.17	0.44
1:A:581:ARG:HA	1:A:581:ARG:HD3	1.62	0.44
1:A:650:GLY:HA2	1:A:1013:TYR:CZ	2.52	0.44
1:B:768:ILE:HG22	1:B:791:VAL:HG23	2.00	0.44
1:C:440:GLU:CD	1:C:466:MET:O	2.60	0.44
1:D:952:ILE:HD12	1:D:952:ILE:HA	1.74	0.44
1:A:268:GLN:HA	1:A:274:VAL:HG23	2.00	0.44
1:B:828:ILE:N	1:B:828:ILE:CD1	2.70	0.44
1:B:927:ASP:HB3	1:B:929:GLN:N	2.31	0.44
1:B:1127:VAL:HG13	1:B:1158:LYS:O	2.18	0.44
1:C:404:GLY:O	1:C:431:THR:HA	2.17	0.44
1:C:756:ILE:HG22	1:C:757:GLY:N	2.33	0.44
1:D:64:VAL:HG22	1:D:82:GLU:HB2	1.99	0.44
1:D:433:ALA:H	1:D:439:ALA:HB2	1.82	0.44
1:D:494:LEU:HD23	1:D:494:LEU:H	1.83	0.44
1:A:71:ASP:C	1:A:73:SER:N	2.74	0.44
1:B:540:GLY:H	1:B:543:GLN:NE2	2.15	0.44
1:B:893:MET:O	1:B:894:TYR:C	2.60	0.44
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.53	0.44
1:D:433:ALA:HB2	1:D:442:LYS:NZ	2.32	0.44
1:D:731:GLU:OE2	1:D:763:VAL:HG12	2.18	0.44
1:D:1044:ASN:HA	1:D:1062:LEU:HD23	1.99	0.44
1:A:435:SER:OG	1:A:437:LYS:HG2	2.17	0.44
1:A:1174:LEU:C	1:A:1175:ILE:HG12	2.42	0.44
1:B:368:THR:OG1	1:B:369:THR:N	2.50	0.44
1:B:1087:ILE:CG2	1:B:1088:TYR:N	2.81	0.44
1:C:169:GLY:HA3	1:C:236:GLU:HB3	2.00	0.44
1:D:304:TYR:OH	1:D:327:PRO:HA	2.18	0.44
1:D:760:LYS:HG2	1:D:768:ILE:HD12	2.00	0.44
1:A:170:THR:HB	1:A:172:GLY:O	2.18	0.44
1:A:952:ILE:O	1:A:952:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ARG:C	1:B:571:ARG:HD2	2.42	0.44
1:B:647:ASN:O	1:B:648:ALA:HB3	2.18	0.44
1:C:71:ASP:C	1:C:73:SER:N	2.73	0.44
1:D:378:ILE:HG23	1:D:459:ILE:CG1	2.47	0.44
1:A:347:THR:HG23	1:A:360:ILE:HG12	2.00	0.44
1:A:392:GLY:O	1:A:418:ILE:N	2.50	0.44
1:B:893:MET:HE1	1:B:896:ARG:HH21	1.82	0.44
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.82	0.44
1:B:944:VAL:O	1:B:948:PHE:HD1	2.01	0.44
1:C:541:THR:OG1	1:C:638:LEU:HG	2.18	0.44
1:C:964:GLN:O	1:C:967:ILE:N	2.34	0.44
1:D:130:ARG:HD2	1:D:130:ARG:HA	1.82	0.44
1:D:568:THR:OG1	1:D:807:GLN:HG3	2.17	0.44
1:D:941:PRO:HD2	1:D:944:VAL:CG1	2.47	0.44
1:A:381:GLU:O	1:A:383:PRO:HD3	2.17	0.43
1:A:384:LEU:H	1:A:384:LEU:HD12	1.82	0.43
1:B:239:ILE:O	1:B:239:ILE:HG22	2.17	0.43
1:B:519:ARG:CB	1:B:520:PRO:CD	2.96	0.43
1:C:71:ASP:O	1:C:74:SER:N	2.37	0.43
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.66	0.43
1:D:40:LEU:C	1:D:40:LEU:HD23	2.43	0.43
1:D:866:MET:HE3	1:D:870:GLN:HB3	2.00	0.43
1:D:951:GLU:O	1:D:952:ILE:HD13	2.17	0.43
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.04	0.43
1:A:506:ASN:ND2	1:A:510:ASN:HD22	2.16	0.43
1:A:1087:ILE:HG22	1:A:1089:ILE:HD12	2.00	0.43
1:B:885:GLU:C	1:B:887:PHE:H	2.25	0.43
1:C:756:ILE:HG22	1:C:789:ALA:CB	2.48	0.43
1:C:920:TYR:OH	1:C:938:LEU:O	2.34	0.43
1:D:999:GLN:CG	1:D:1000:GLY:N	2.42	0.43
1:A:322:PHE:CD1	1:A:322:PHE:C	2.96	0.43
1:A:532:VAL:HG21	1:A:596:ASP:HB2	2.00	0.43
1:A:1077:TYR:N	1:A:1077:TYR:HD1	2.16	0.43
1:B:66:ILE:HG13	1:B:66:ILE:O	2.18	0.43
1:B:647:ASN:O	1:B:649:VAL:N	2.46	0.43
1:C:323:ILE:CG2	1:C:324:GLU:N	2.81	0.43
1:C:456:LYS:HD3	1:C:456:LYS:H	1.83	0.43
1:C:462:LEU:O	1:C:466:MET:HG2	2.18	0.43
1:C:941:PRO:O	1:C:945:VAL:HG13	2.18	0.43
1:C:941:PRO:O	1:C:944:VAL:HG12	2.19	0.43
1:C:981:TYR:CE1	1:C:982:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:HIS:ND1	1:A:1176:GLU:HG3	2.33	0.43
1:B:898:ASN:ND2	1:B:904:ILE:H	2.16	0.43
1:C:817:LEU:O	1:C:818:ASN:C	2.61	0.43
1:D:40:LEU:HD21	1:D:42:VAL:CG2	2.48	0.43
1:B:1042:MET:HE1	1:B:1060:ILE:HG22	2.00	0.43
1:C:378:ILE:HG12	1:C:427:VAL:HG23	2.00	0.43
1:C:931:VAL:CA	1:C:935:GLY:H	2.29	0.43
1:D:470:LYS:HB2	1:D:480:PHE:CE1	2.53	0.43
1:D:879:LYS:C	1:D:881:LEU:H	2.27	0.43
1:A:266:SER:O	1:A:478:THR:HA	2.18	0.43
1:A:299:MET:HE3	1:A:304:TYR:CD1	2.53	0.43
1:A:571:ARG:NH2	1:A:605:GLU:OE2	2.46	0.43
1:A:986:ASP:OD1	1:A:986:ASP:C	2.62	0.43
1:A:1153:PHE:HE1	1:A:1177:ILE:HB	1.83	0.43
1:B:536:LYS:HE3	1:B:536:LYS:HB3	1.81	0.43
1:B:613:ASP:HB2	1:B:1013:TYR:CZ	2.52	0.43
1:B:799:ALA:H	1:B:811:ASN:ND2	2.15	0.43
1:C:188:GLY:CA	1:C:237:ARG:HH22	2.29	0.43
1:C:940:PHE:HB3	1:C:944:VAL:HG13	2.00	0.43
1:D:818:ASN:N	1:D:818:ASN:HD22	2.15	0.43
1:C:994:LEU:O	1:C:998:GLN:HB2	2.19	0.43
1:A:509:ILE:HD12	1:A:1089:ILE:CG2	2.49	0.43
1:B:1051:GLU:OE1	1:B:1057:ARG:CZ	2.66	0.43
1:C:104:ASP:O	1:C:108:GLN:OE1	2.35	0.43
1:C:641:MET:CE	1:C:666:SER:HB3	2.48	0.43
1:C:651:TYR:O	1:C:952:ILE:HD11	2.19	0.43
1:C:977:ARG:HA	1:C:978:PRO:HD3	1.83	0.43
1:D:491:GLN:O	1:D:492:PRO:C	2.61	0.43
1:D:1132:LYS:O	1:D:1151:ALA:CB	2.66	0.43
1:A:620:LYS:HG3	1:A:1023:THR:HG21	2.01	0.43
1:C:39:LYS:NZ	1:C:109:ALA:O	2.45	0.43
1:C:141:PRO:HG2	1:C:146:LEU:CD1	2.49	0.43
1:A:571:ARG:HH11	1:A:575:GLN:HE22	1.65	0.43
1:A:955:PRO:O	1:A:956:VAL:C	2.62	0.43
1:A:1115:GLN:C	1:A:1116:MET:HG3	2.44	0.43
1:B:51:ARG:CG	1:B:51:ARG:HH11	2.31	0.43
1:B:51:ARG:CG	1:B:51:ARG:NH1	2.81	0.43
1:B:106:ALA:O	1:B:107:LYS:C	2.62	0.43
1:C:287:LEU:HD22	1:C:291:ILE:CD1	2.48	0.43
1:C:375:GLN:HE22	1:C:428:LYS:HD3	1.81	0.43
1:C:877:GLN:O	1:C:881:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1132:LYS:O	1:D:1151:ALA:HB3	2.19	0.43
1:A:1008:ILE:HD12	1:A:1008:ILE:N	2.34	0.42
1:B:99:ILE:HD12	1:B:99:ILE:N	2.30	0.42
1:B:261:PHE:HE1	1:B:368:THR:HA	1.82	0.42
1:B:335:ILE:HD11	1:B:374:ILE:HA	2.00	0.42
1:B:738:LEU:HD21	1:B:759:LEU:HD13	2.01	0.42
1:C:234:TYR:N	1:C:234:TYR:CD2	2.87	0.42
1:C:814:TYR:CE2	1:C:828:ILE:CG1	3.02	0.42
1:D:513:PRO:O	1:D:515:ASN:HB2	2.19	0.42
1:D:739:ALA:HA	1:D:769:HIS:O	2.19	0.42
1:D:866:MET:HE1	1:D:871:TYR:HA	1.99	0.42
1:A:90:LEU:HD13	1:A:94:GLU:HG3	2.00	0.42
1:A:459:ILE:O	1:A:460:PRO:C	2.60	0.42
1:B:892:ASP:O	1:B:896:ARG:HG3	2.20	0.42
1:C:215:ASP:O	1:C:218:HIS:N	2.48	0.42
1:C:256:ASN:C	1:C:257:ILE:HG13	2.42	0.42
1:C:512:PHE:CG	1:C:513:PRO:HD2	2.54	0.42
1:C:624:TRP:HB3	1:C:1005:GLN:NE2	2.34	0.42
1:D:1159:GLN:CG	1:D:1176:GLU:HG2	2.50	0.42
1:D:1159:GLN:HG3	1:D:1176:GLU:HG2	2.00	0.42
1:A:486:GLU:CD	1:A:486:GLU:H	2.26	0.42
1:A:930:SER:HA	1:A:933:THR:HB	2.01	0.42
1:B:39:LYS:HA	1:B:62:SER:O	2.20	0.42
1:B:886:ARG:H	1:B:886:ARG:HG3	1.59	0.42
1:B:893:MET:HE3	1:B:921:MET:HB3	2.00	0.42
1:C:744:ALA:O	1:C:861:ILE:HD12	2.20	0.42
1:C:920:TYR:OH	1:C:938:LEU:HB3	2.20	0.42
1:D:142:HIS:CB	1:D:144:GLU:OE1	2.63	0.42
1:A:241:ASN:N	1:A:242:PRO:HD3	2.35	0.42
1:A:470:LYS:NZ	1:A:484:THR:HG23	2.35	0.42
1:A:641:MET:HE3	1:A:674:PHE:HD1	1.74	0.42
1:A:682:TRP:CZ3	1:A:977:ARG:HB2	2.54	0.42
1:A:1064:THR:OG1	1:C:1066:SER:HB3	2.19	0.42
1:B:622:ASN:HD22	1:B:623:PRO:CD	2.31	0.42
1:B:1015:LYS:HA	1:B:1015:LYS:HD3	1.78	0.42
1:C:192:MET:HE2	1:C:192:MET:HB3	1.87	0.42
1:C:619:LEU:O	1:C:620:LYS:C	2.62	0.42
1:D:167:ILE:H	1:D:167:ILE:HG13	1.68	0.42
1:D:241:ASN:H	1:D:242:PRO:HD3	1.84	0.42
1:D:375:GLN:CG	1:D:376:CYS:N	2.82	0.42
1:D:459:ILE:HB	1:D:460:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:MET:CE	1:A:430:SER:HB3	2.49	0.42
1:A:542:LYS:HB2	1:A:636:ASN:C	2.43	0.42
1:A:866:MET:HE2	1:A:870:GLN:HG2	2.01	0.42
1:B:1144:LYS:CE	4:B:1202:BTI:O11	2.67	0.42
1:C:167:ILE:HA	1:C:168:PRO:HD2	1.92	0.42
1:C:266:SER:O	1:C:478:THR:HA	2.19	0.42
1:C:936:TYR:HD2	1:C:936:TYR:HA	1.72	0.42
1:C:964:GLN:O	1:C:966:VAL:N	2.53	0.42
1:A:179:LEU:O	1:A:182:GLU:CG	2.68	0.42
1:A:817:LEU:O	1:A:818:ASN:C	2.62	0.42
1:B:347:THR:O	1:B:348:GLN:C	2.62	0.42
1:B:522:PRO:HB2	1:B:523:ASP:H	1.76	0.42
1:C:948:PHE:CD1	1:C:967:ILE:HD12	2.55	0.42
1:D:770:LEU:HD12	1:D:771:HIS:N	2.35	0.42
1:A:287:LEU:HD21	1:A:318:ASP:O	2.19	0.42
1:A:583:ARG:HG2	1:A:619:LEU:HD22	2.00	0.42
1:B:48:ILE:HG23	1:B:49:ALA:N	2.35	0.42
1:B:155:ALA:O	1:B:156:ARG:C	2.61	0.42
1:B:296:ILE:O	1:B:300:GLU:HB2	2.19	0.42
1:B:644:ARG:HH11	1:B:647:ASN:CG	2.28	0.42
1:B:878:ALA:O	1:B:883:LEU:N	2.40	0.42
1:B:1095:HIS:CG	1:B:1098:ALA:HB3	2.55	0.42
1:D:908:THR:HA	1:D:909:PRO:HA	1.66	0.42
1:D:921:MET:HE2	1:D:931:VAL:HG21	2.02	0.42
1:A:379:THR:N	1:A:458:ASN:OD1	2.42	0.42
1:A:381:GLU:HG2	1:A:387:PHE:HB3	2.00	0.42
1:B:1144:LYS:HZ3	4:B:1202:BTI:C10	2.22	0.42
1:C:40:LEU:HD23	1:C:40:LEU:C	2.44	0.42
1:C:151:ASP:C	1:C:151:ASP:OD1	2.61	0.42
1:C:335:ILE:HG22	1:C:336:THR:N	2.35	0.42
1:D:964:GLN:O	1:D:965:ALA:C	2.62	0.42
1:D:1085:ARG:HH11	1:D:1085:ARG:CG	2.33	0.42
1:B:588:ILE:HD13	1:B:588:ILE:HA	1.81	0.42
1:B:927:ASP:H	1:B:930:SER:CB	2.30	0.42
1:C:39:LYS:NZ	1:C:82:GLU:OE2	2.49	0.42
1:C:590:ILE:HG12	1:C:837:TYR:CD2	2.55	0.42
1:C:631:ARG:NH1	1:C:634:ILE:O	2.53	0.42
1:A:436:PHE:O	1:A:437:LYS:C	2.62	0.42
1:A:791:VAL:O	1:A:822:ARG:NH2	2.38	0.42
1:A:1138:LEU:HD22	1:A:1175:ILE:HD11	2.01	0.42
1:B:472:THR:O	1:B:473:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:NH1	1:C:71:ASP:OD1	2.53	0.42
1:C:1008:ILE:HD12	1:C:1009:SER:N	2.34	0.42
1:D:289:GLN:HE21	1:D:289:GLN:HA	1.85	0.42
1:D:811:ASN:ND2	1:D:811:ASN:H	2.17	0.42
1:D:1134:ASN:N	1:D:1151:ALA:HB3	2.34	0.42
1:A:780:LEU:O	1:A:781:LEU:C	2.62	0.41
1:A:940:PHE:CD1	1:A:967:ILE:HA	2.55	0.41
1:A:1029:ASN:C	1:A:1029:ASN:ND2	2.78	0.41
1:B:256:ASN:C	1:B:257:ILE:HG12	2.44	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.87	0.41
1:C:199:GLY:HA2	5:C:1202:ATP:O1B	2.20	0.41
1:C:909:PRO:HG2	1:C:952:ILE:HG13	2.02	0.41
1:D:42:VAL:HG11	1:D:49:ALA:HA	2.02	0.41
1:D:873:ASN:C	1:D:875:SER:H	2.28	0.41
1:A:78:TYR:CE2	1:C:1081:ASN:HA	2.54	0.41
1:A:145:HIS:HE1	1:A:302:ILE:O	2.02	0.41
1:A:334:THR:O	1:A:338:MET:HG3	2.20	0.41
1:A:907:VAL:O	1:A:908:THR:C	2.63	0.41
1:A:1017:TYR:O	1:A:1018:GLU:C	2.64	0.41
1:B:335:ILE:HD11	1:B:374:ILE:C	2.45	0.41
1:B:983:GLU:HA	1:B:983:GLU:OE1	2.19	0.41
1:B:1000:GLY:N	1:B:1001:PRO:CD	2.75	0.41
1:B:1069:ASP:O	1:B:1099:ASN:HB3	2.20	0.41
1:C:164:LEU:O	1:C:166:VAL:HG23	2.20	0.41
1:C:167:ILE:H	1:C:167:ILE:CD1	2.30	0.41
1:C:311:GLU:O	1:C:323:ILE:HB	2.20	0.41
1:C:939:ASP:OD1	1:D:1149:ILE:HG12	2.19	0.41
1:D:342:ILE:HD12	1:D:342:ILE:N	2.35	0.41
1:A:243:LYS:NZ	1:A:476:TYR:O	2.51	0.41
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.35	0.41
1:B:241:ASN:N	1:B:242:PRO:CD	2.83	0.41
1:C:126:GLN:O	1:C:127:PHE:C	2.63	0.41
1:C:358:GLU:OE1	1:C:358:GLU:CA	2.68	0.41
1:C:902:GLY:O	1:C:903:ASP:HB3	2.20	0.41
1:B:290:ARG:HB3	1:B:320:PHE:HE2	1.86	0.41
1:B:737:ILE:HG23	1:B:767:PRO:O	2.21	0.41
1:C:215:ASP:HB3	1:C:219:ARG:CG	2.50	0.41
1:C:540:GLY:H	1:C:543:GLN:HG2	1.85	0.41
1:C:1029:ASN:HD22	1:C:1031:SER:H	1.68	0.41
1:D:565:LEU:C	1:D:565:LEU:HD12	2.46	0.41
1:D:828:ILE:HD12	1:D:829:GLU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1108:ASN:CB	1:D:1109:PRO:CD	2.89	0.41
1:A:286:THR:O	1:A:290:ARG:HG3	2.21	0.41
1:A:1064:THR:OG1	1:C:1066:SER:CB	2.69	0.41
1:B:438:GLN:HG2	1:D:346:LYS:NZ	2.36	0.41
1:B:512:PHE:CD2	1:B:513:PRO:HD2	2.55	0.41
1:B:572:ASP:HB3	1:B:807:GLN:NE2	2.36	0.41
1:B:620:LYS:CG	4:B:1201:BTI:H63	2.50	0.41
1:C:652:LYS:HD3	1:C:653:ASN:O	2.20	0.41
1:C:858:ASN:OD1	1:C:860:GLU:HB2	2.21	0.41
1:D:69:ASN:O	1:D:72:LYS:HB2	2.21	0.41
1:D:378:ILE:O	1:D:426:LEU:HB2	2.21	0.41
1:D:701:GLU:HG2	1:D:737:ILE:HB	2.02	0.41
1:D:774:ASP:C	1:D:804:LEU:O	2.64	0.41
1:D:893:MET:O	1:D:897:VAL:HG23	2.21	0.41
1:A:263:ARG:NH1	1:A:336:THR:OG1	2.46	0.41
1:A:272:GLN:HE21	1:A:272:GLN:HB2	1.62	0.41
1:A:434:ILE:HG13	1:C:341:GLY:O	2.21	0.41
1:A:866:MET:HE2	1:A:866:MET:HB3	1.83	0.41
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.84	0.41
1:B:462:LEU:HD23	1:B:462:LEU:HA	1.82	0.41
1:C:914:VAL:O	1:C:915:GLY:C	2.64	0.41
1:D:641:MET:HE3	1:D:674:PHE:HE1	1.74	0.41
1:A:597:VAL:HG11	1:A:831:MET:HG2	2.03	0.41
1:B:479:LYS:HB3	1:B:483:GLU:OE2	2.20	0.41
1:B:581:ARG:O	1:B:619:LEU:HD21	2.20	0.41
1:B:1035:THR:HB	1:B:1036:PRO:HD3	2.01	0.41
1:C:90:LEU:CB	1:C:95:SER:HB2	2.51	0.41
1:C:212:GLU:H	1:C:212:GLU:HG3	1.49	0.41
1:C:534:SER:O	1:C:537:ILE:HB	2.21	0.41
1:D:259:HIS:HB3	1:D:296:ILE:HD13	2.03	0.41
1:A:192:MET:CE	1:A:238:TYR:CD1	2.97	0.41
1:A:268:GLN:O	1:A:481:ILE:HD12	2.21	0.41
1:A:278:ALA:HA	1:A:279:PRO:C	2.41	0.41
1:A:459:ILE:C	1:A:461:PHE:N	2.78	0.41
1:A:858:ASN:HD22	1:A:859:THR:N	2.19	0.41
1:A:948:PHE:CD1	1:A:967:ILE:CD1	3.04	0.41
1:A:948:PHE:CZ	1:A:963:LEU:HD23	2.56	0.41
1:A:1143:MET:O	1:B:513:PRO:HA	2.21	0.41
1:B:151:ASP:HB3	1:B:154:LYS:H	1.86	0.41
1:B:304:TYR:OH	1:B:327:PRO:HA	2.20	0.41
1:B:305:VAL:O	1:B:306:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HD2	1:B:329:VAL:O	2.21	0.41
1:B:459:ILE:N	1:B:460:PRO:HD2	2.36	0.41
1:B:498:THR:HG23	1:B:1085:ARG:NH2	2.36	0.41
1:B:641:MET:HE2	1:B:671:ILE:HG13	2.02	0.41
1:B:908:THR:HA	1:B:909:PRO:HA	1.67	0.41
1:C:192:MET:HE3	1:C:194:LYS:HB3	2.02	0.41
1:C:622:ASN:ND2	1:C:623:PRO:HD2	2.25	0.41
1:C:807:GLN:CB	1:C:808:PRO:CD	2.98	0.41
1:C:995:GLU:O	1:C:999:GLN:HA	2.21	0.41
1:D:606:MET:HE1	1:D:627:LEU:HD13	2.03	0.41
1:D:941:PRO:O	1:D:944:VAL:CG1	2.64	0.41
1:D:999:GLN:HE21	1:D:1001:PRO:N	2.18	0.41
1:A:1155:GLY:HA3	1:A:1177:ILE:HG22	2.01	0.41
1:B:598:PHE:CZ	1:B:831:MET:HE1	2.55	0.41
1:C:437:LYS:CD	1:C:437:LYS:H	2.33	0.41
1:C:1052:ILE:O	1:C:1053:ASP:HB2	2.21	0.41
1:D:277:VAL:HA	1:D:335:ILE:HD11	2.03	0.41
1:D:447:LEU:O	1:D:450:MET:HB2	2.20	0.41
1:D:864:HIS:CD2	1:D:866:MET:CG	2.93	0.41
1:D:1151:ALA:HA	1:D:1152:PRO:HD2	1.90	0.41
1:D:1153:PHE:HB3	1:D:1154:ASP:H	1.47	0.41
1:A:206:ILE:HD12	1:A:206:ILE:H	1.86	0.40
1:A:314:VAL:HG22	1:A:320:PHE:HB3	2.03	0.40
1:A:499:LYS:HB3	1:A:1027:TYR:HA	2.03	0.40
1:A:584:THR:O	1:A:585:LYS:C	2.64	0.40
1:A:875:SER:HA	1:A:887:PHE:CE1	2.56	0.40
1:B:278:ALA:CB	1:B:335:ILE:HG23	2.51	0.40
1:B:279:PRO:HD2	1:B:372:TYR:CD2	2.56	0.40
1:B:554:ALA:O	1:B:555:GLU:C	2.63	0.40
1:A:313:LEU:HD22	1:A:323:ILE:CG1	2.51	0.40
1:A:587:MET:SD	1:A:626:ARG:HD3	2.60	0.40
1:A:774:ASP:C	1:A:804:LEU:O	2.65	0.40
1:A:783:TYR:CE1	1:A:808:PRO:HG2	2.57	0.40
1:A:810:ALA:CB	1:A:831:MET:HE1	2.48	0.40
1:B:545:LEU:CD1	1:B:550:PRO:HD3	2.51	0.40
1:B:1119:SER:O	1:B:1140:THR:HA	2.21	0.40
1:C:379:THR:C	1:C:381:GLU:H	2.29	0.40
1:C:575:GLN:NE2	1:C:610:ALA:H	2.18	0.40
1:C:952:ILE:HD12	1:C:952:ILE:HA	1.76	0.40
1:D:41:LEU:HD23	1:D:42:VAL:N	2.37	0.40
1:A:388:MET:HA	1:A:389:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:MET:CG	1:A:907:VAL:HG13	2.46	0.40
1:A:999:GLN:HG2	1:A:1000:GLY:N	2.27	0.40
1:A:1083:GLN:HE21	1:A:1083:GLN:HB3	1.65	0.40
1:B:259:HIS:O	1:B:260:LEU:HD23	2.20	0.40
1:B:458:ASN:O	1:B:461:PHE:HB3	2.21	0.40
1:C:968:LEU:O	1:C:969:LYS:C	2.63	0.40
1:D:396:ALA:HB3	1:D:453:ARG:HG3	2.03	0.40
1:A:399:SER:HB2	1:A:407:LEU:HD13	2.02	0.40
1:A:486:GLU:C	1:A:488:PHE:N	2.78	0.40
1:B:566:THR:HG23	1:B:603:SER:OG	2.22	0.40
1:C:778:ASN:O	1:C:779:GLY:C	2.63	0.40
1:D:938:LEU:HD23	1:D:938:LEU:HA	1.74	0.40
1:D:974:LEU:HD13	1:D:978:PRO:HA	2.03	0.40
1:A:659:ILE:H	1:A:659:ILE:HG12	1.74	0.40
1:B:119:GLY:N	1:B:122:SER:OG	2.54	0.40
1:B:606:MET:CE	1:B:639:PHE:HB3	2.43	0.40
1:C:590:ILE:HD12	1:C:590:ILE:C	2.47	0.40
1:C:814:TYR:CZ	1:C:828:ILE:CG1	3.05	0.40
1:C:838:TRP:O	1:C:839:SER:C	2.61	0.40
1:C:1013:TYR:O	1:C:1014:PRO:C	2.64	0.40
1:D:1065:ILE:HG12	1:D:1076:ILE:HG12	2.03	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	1127/1173 (96%)	1022 (91%)	81 (7%)	24 (2%)	5	20
1	B	1027/1173 (88%)	906 (88%)	92 (9%)	29 (3%)	4	14
1	C	1063/1173 (91%)	926 (87%)	105 (10%)	32 (3%)	3	12
1	D	1061/1173 (90%)	947 (89%)	90 (8%)	24 (2%)	5	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4278/4692 (91%)	3801 (89%)	368 (9%)	109 (2%)	4 16

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	181	LYS
1	A	211	SER
1	A	956	VAL
1	A	1094	VAL
1	A	1095	HIS
1	A	1138	LEU
1	B	270	ARG
1	B	868	GLY
1	B	870	GLN
1	B	1001	PRO
1	C	92	PRO
1	C	168	PRO
1	C	211	SER
1	C	270	ARG
1	C	518	LYS
1	C	937	LYS
1	C	956	VAL
1	D	92	PRO
1	D	241	ASN
1	D	870	GLN
1	D	880	SER
1	D	999	GLN
1	D	1103	LYS
1	D	1108	ASN
1	D	1154	ASP
1	A	72	LYS
1	A	385	ASN
1	A	387	PHE
1	A	389	PRO
1	A	414	GLN
1	A	648	ALA
1	A	1081	ASN
1	B	87	GLY
1	B	91	GLY
1	B	163	ASP
1	B	166	VAL

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Mol	Chain	Res	Type
1	B	425	LEU
1	B	522	PRO
1	B	649	VAL
1	B	779	GLY
1	B	871	TYR
1	B	999	GLN
1	B	1002	VAL
1	C	87	GLY
1	C	188	GLY
1	C	197	SER
1	C	216	ALA
1	C	306	ASN
1	C	455	VAL
1	C	903	ASP
1	C	931	VAL
1	C	965	ALA
1	D	87	GLY
1	D	261	PHE
1	D	868	GLY
1	D	1052	ILE
1	D	1106	LYS
1	A	999	GLN
1	A	1001	PRO
1	A	1117	PRO
1	B	328	ARG
1	B	518	LYS
1	B	939	ASP
1	B	941	PRO
1	B	1000	GLY
1	C	189	PHE
1	C	645	ALA
1	C	648	ALA
1	C	1070	GLU
1	A	210	GLU
1	A	424	SER
1	B	69	ASN
1	B	72	LYS
1	B	473	SER
1	B	523	ASP
1	C	125	GLU
1	C	215	ASP
1	C	229	GLY

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Mol	Chain	Res	Type
1	C	925	ASP
1	D	386	ASP
1	D	648	ALA
1	D	869	GLY
1	A	190	PRO
1	A	221	LYS
1	A	476	TYR
1	B	519	ARG
1	B	648	ALA
1	C	94	GLU
1	C	214	GLU
1	C	961	LYS
1	D	104	ASP
1	D	491	GLN
1	D	854	ILE
1	D	903	ASP
1	D	939	ASP
1	A	415	GLY
1	B	1084	ALA
1	C	110	ASN
1	C	186	GLU
1	D	242	PRO
1	B	92	PRO
1	D	1014	PRO
1	B	970	GLY
1	D	331	VAL
1	A	1000	GLY
1	C	513	PRO
1	C	389	PRO
1	C	649	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	977/1006 (97%)	826 (84%)	151 (16%)	2 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	897/1006 (89%)	736 (82%)	161 (18%)	2	6
1	C	917/1006 (91%)	754 (82%)	163 (18%)	2	6
1	D	922/1006 (92%)	783 (85%)	139 (15%)	3	10
All	All	3713/4024 (92%)	3099 (84%)	614 (16%)	2	8

All (614) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	44	ASN
1	A	69	ASN
1	A	72	LYS
1	A	73	SER
1	A	88	SER
1	A	90	LEU
1	A	108	GLN
1	A	125	GLU
1	A	143	LEU
1	A	147	ASP
1	A	148	MET
1	A	152	LYS
1	A	154	LYS
1	A	156	ARG
1	A	164	LEU
1	A	171	ASP
1	A	179	LEU
1	A	182	GLU
1	A	186	GLU
1	A	192	MET
1	A	193	ILE
1	A	196	THR
1	A	205	ARG
1	A	208	ARG
1	A	212	GLU
1	A	213	LEU
1	A	218	HIS
1	A	219	ARG
1	A	227	SER
1	A	235	ILE
1	A	241	ASN
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	269	ARG
1	A	271	HIS
1	A	272	GLN
1	A	276	GLU
1	A	281	VAL
1	A	283	LEU
1	A	287	LEU
1	A	289	GLN
1	A	302	ILE
1	A	313	LEU
1	A	315	SER
1	A	323	ILE
1	A	329	VAL
1	A	335	ILE
1	A	337	GLU
1	A	361	ASN
1	A	368	THR
1	A	378	ILE
1	A	381	GLU
1	A	391	THR
1	A	406	ARG
1	A	414	GLN
1	A	417	GLU
1	A	423	ASP
1	A	427	VAL
1	A	434	ILE
1	A	437	LYS
1	A	440	GLU
1	A	442	LYS
1	A	444	VAL
1	A	450	MET
1	A	469	LYS
1	A	486	GLU
1	A	487	LEU
1	A	491	GLN
1	A	493	SER
1	A	496	ARG
1	A	518	LYS
1	A	519	ARG
1	A	523	ASP
1	A	526	LEU
1	A	534	SER

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Mol	Chain	Res	Type
1	A	542	LYS
1	A	551	LYS
1	A	588	ILE
1	A	590	ILE
1	A	607	TRP
1	A	613	ASP
1	A	620	LYS
1	A	632	LYS
1	A	649	VAL
1	A	684	ASP
1	A	707	THR
1	A	714	GLU
1	A	715	ARG
1	A	719	THR
1	A	720	LEU
1	A	726	LEU
1	A	743	MET
1	A	750	LYS
1	A	765	ASP
1	A	766	LEU
1	A	775	THR
1	A	784	LYS
1	A	794	ILE
1	A	798	VAL
1	A	811	ASN
1	A	828	ILE
1	A	829	GLU
1	A	843	THR
1	A	854	ILE
1	A	855	LYS
1	A	861	ILE
1	A	863	GLN
1	A	874	LEU
1	A	880	SER
1	A	888	ASP
1	A	906	LYS
1	A	907	VAL
1	A	908	THR
1	A	917	MET
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL

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Mol	Chain	Res	Type
1	A	933	THR
1	A	939	ASP
1	A	943	SER
1	A	944	VAL
1	A	945	VAL
1	A	966	VAL
1	A	977	ARG
1	A	991	ARG
1	A	997	GLU
1	A	1002	VAL
1	A	1008	ILE
1	A	1015	LYS
1	A	1048	VAL
1	A	1054	LYS
1	A	1077	TYR
1	A	1081	ASN
1	A	1083	GLN
1	A	1089	ILE
1	A	1090	LYS
1	A	1094	VAL
1	A	1097	ASN
1	A	1107	SER
1	A	1115	GLN
1	A	1116	MET
1	A	1126	SER
1	A	1130	THR
1	A	1141	GLU
1	A	1145	MET
1	A	1148	THR
1	A	1153	PHE
1	A	1157	ILE
1	A	1167	THR
1	A	1176	GLU
1	A	1177	ILE
1	B	36	GLN
1	B	39	LYS
1	B	40	LEU
1	B	44	ASN
1	B	47	GLU
1	B	51	ARG
1	B	62	SER
1	B	75	LEU

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Mol	Chain	Res	Type
1	B	77	ARG
1	B	83	SER
1	B	85	LEU
1	B	94	GLU
1	B	99	ILE
1	B	118	TYR
1	B	123	GLU
1	B	125	GLU
1	B	129	ARG
1	B	139	ILE
1	B	144	GLU
1	B	152	LYS
1	B	156	ARG
1	B	160	ILE
1	B	164	LEU
1	B	166	VAL
1	B	257	ILE
1	B	258	VAL
1	B	270	ARG
1	B	274	VAL
1	B	281	VAL
1	B	284	SER
1	B	287	LEU
1	B	289	GLN
1	B	292	CYS
1	B	293	ASP
1	B	313	LEU
1	B	318	ASP
1	B	319	GLU
1	B	329	VAL
1	B	335	ILE
1	B	344	ILE
1	B	346	LYS
1	B	357	LEU
1	B	357(A)	PHE
1	B	359	GLU
1	B	377	ARG
1	B	378	ILE
1	B	380	THR
1	B	381	GLU
1	B	434	ILE
1	B	442	LYS

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Mol	Chain	Res	Type
1	B	444	VAL
1	B	451	ARG
1	B	469	LYS
1	B	479	LYS
1	B	481	ILE
1	B	482	GLU
1	B	486	GLU
1	B	487	LEU
1	B	488	PHE
1	B	489	ASP
1	B	490	ILE
1	B	493	SER
1	B	496	ARG
1	B	498	THR
1	B	517	GLU
1	B	518	LYS
1	B	523	ASP
1	B	524	TYR
1	B	525	GLU
1	B	528	SER
1	B	531	THR
1	B	535	SER
1	B	536	LYS
1	B	538(A)	SER
1	B	538(B)	PHE
1	B	542	LYS
1	B	555	GLU
1	B	565	LEU
1	B	575	GLN
1	B	580	THR
1	B	588	ILE
1	B	592	SER
1	B	607	TRP
1	B	613	ASP
1	B	631	ARG
1	B	632	LYS
1	B	641	MET
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS
1	B	684	ASP
1	B	686	MET

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Mol	Chain	Res	Type
1	B	687	LYS
1	B	707	THR
1	B	714	GLU
1	B	715	ARG
1	B	721	GLU
1	B	743	MET
1	B	756	ILE
1	B	760	LYS
1	B	766	LEU
1	B	775	THR
1	B	781	LEU
1	B	784	LYS
1	B	809	SER
1	B	811	ASN
1	B	828	ILE
1	B	831	MET
1	B	839	SER
1	B	843	THR
1	B	852	SER
1	B	856	SER
1	B	870	GLN
1	B	874	LEU
1	B	875	SER
1	B	880	SER
1	B	881	LEU
1	B	885	GLU
1	B	886	ARG
1	B	897	VAL
1	B	907	VAL
1	B	908	THR
1	B	913	VAL
1	B	919	LEU
1	B	923	GLN
1	B	926	LEU
1	B	930	SER
1	B	932	ILE
1	B	939	ASP
1	B	949	LYS
1	B	952	ILE
1	B	962	ASP
1	B	982	LEU
1	B	985	VAL

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Mol	Chain	Res	Type
1	B	991	ARG
1	B	996	GLU
1	B	999	GLN
1	B	1008	ILE
1	B	1009	SER
1	B	1011	VAL
1	B	1015	LYS
1	B	1019	GLN
1	B	1022	GLN
1	B	1029	ASN
1	B	1048	VAL
1	B	1057	ARG
1	B	1085	ARG
1	B	1089	ILE
1	B	1097	ASN
1	B	1116	MET
1	B	1119	SER
1	B	1123	VAL
1	B	1138	LEU
1	B	1143	MET
1	B	1147	THR
1	B	1156	VAL
1	B	1157	ILE
1	B	1167	THR
1	B	1175	ILE
1	B	1176	GLU
1	B	1177	ILE
1	C	44	ASN
1	C	77	ARG
1	C	79	LYS
1	C	90	LEU
1	C	94	GLU
1	C	95	SER
1	C	103	ILE
1	C	104	ASP
1	C	108	GLN
1	C	110	ASN
1	C	126	GLN
1	C	129	ARG
1	C	147	ASP
1	C	151	ASP
1	C	154	LYS

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Mol	Chain	Res	Type
1	C	161	LYS
1	C	163	ASP
1	C	167	ILE
1	C	168	PRO
1	C	174	ILE
1	C	175	LYS
1	C	193	ILE
1	C	194	LYS
1	C	202	LYS
1	C	205	ARG
1	C	206	ILE
1	C	207	VAL
1	C	208	ARG
1	C	210	GLU
1	C	212	GLU
1	C	213	LEU
1	C	227	SER
1	C	230	ASN
1	C	232	GLU
1	C	234	TYR
1	C	235	ILE
1	C	241	ASN
1	C	243	LYS
1	C	249	VAL
1	C	262	GLU
1	C	269	ARG
1	C	270	ARG
1	C	286	THR
1	C	287	LEU
1	C	288	ARG
1	C	289	GLN
1	C	302	ILE
1	C	313	LEU
1	C	323	ILE
1	C	329	VAL
1	C	332	GLU
1	C	334	THR
1	C	335	ILE
1	C	361	ASN
1	C	377	ARG
1	C	378	ILE
1	C	388	MET

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Mol	Chain	Res	Type
1	C	395	ILE
1	C	400	SER
1	C	406	ARG
1	C	414	GLN
1	C	417	GLU
1	C	419	SER
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	444	VAL
1	C	445	ARG
1	C	455	VAL
1	C	456	LYS
1	C	464	ASN
1	C	469	LYS
1	C	472	THR
1	C	481	ILE
1	C	484	THR
1	C	489	ASP
1	C	494	LEU
1	C	510	ASN
1	C	515	ASN
1	C	518	LYS
1	C	519	ARG
1	C	525	GLU
1	C	526	LEU
1	C	531	THR
1	C	537	ILE
1	C	542	LYS
1	C	580	THR
1	C	588	ILE
1	C	590	ILE
1	C	606	MET
1	C	607	TRP
1	C	629	ARG
1	C	631	ARG
1	C	641	MET
1	C	649	VAL
1	C	652	LYS
1	C	659	ILE
1	C	668	LYS
1	C	685	GLN

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Mol	Chain	Res	Type
1	C	707	THR
1	C	714	GLU
1	C	717	ASN
1	C	717(A)	ILE
1	C	719	THR
1	C	726	LEU
1	C	729	GLU
1	C	743	MET
1	C	750	LYS
1	C	756	ILE
1	C	766	LEU
1	C	781	LEU
1	C	782	THR
1	C	784	LYS
1	C	794	ILE
1	C	798	VAL
1	C	807	GLN
1	C	828	ILE
1	C	831	MET
1	C	834	LEU
1	C	839	SER
1	C	843	THR
1	C	853	ASP
1	C	854	ILE
1	C	855	LYS
1	C	861	ILE
1	C	875	SER
1	C	876	GLN
1	C	881	LEU
1	C	885	GLU
1	C	888	ASP
1	C	893	MET
1	C	906	LYS
1	C	907	VAL
1	C	908	THR
1	C	931	VAL
1	C	945	VAL
1	C	946	SER
1	C	949	LYS
1	C	952	ILE
1	C	959	PHE
1	C	960	ASN

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Mol	Chain	Res	Type
1	C	963	LEU
1	C	969	LYS
1	C	972	GLU
1	C	974	LEU
1	C	982	LEU
1	C	998	GLN
1	C	1002	VAL
1	C	1008	ILE
1	C	1019	GLN
1	C	1022	GLN
1	C	1052	ILE
1	C	1054	LYS
1	C	1058	LEU
1	C	1062	LEU
1	C	1063	GLU
1	C	1070	GLU
1	C	1085	ARG
1	C	1087	ILE
1	C	1090	LYS
1	C	1140	THR
1	C	1145	MET
1	C	1147	THR
1	D	38	LYS
1	D	44	ASN
1	D	70	GLU
1	D	72	LYS
1	D	77	ARG
1	D	88	SER
1	D	99	ILE
1	D	101	ARG
1	D	104	ASP
1	D	136	ILE
1	D	137	LYS
1	D	149	PHE
1	D	161	LYS
1	D	239	ILE
1	D	241	ASN
1	D	243	LYS
1	D	253	GLU
1	D	258	VAL
1	D	262	GLU
1	D	267	VAL

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Mol	Chain	Res	Type
1	D	280	SER
1	D	283	LEU
1	D	289	GLN
1	D	296	ILE
1	D	319	GLU
1	D	328	ARG
1	D	329	VAL
1	D	331	VAL
1	D	335	ILE
1	D	357	LEU
1	D	357(A)	PHE
1	D	362	MET
1	D	362(A)	PRO
1	D	368	THR
1	D	370	LEU
1	D	400	SER
1	D	406	ARG
1	D	417	GLU
1	D	425	LEU
1	D	427	VAL
1	D	428	LYS
1	D	434	ILE
1	D	451	ARG
1	D	452	ILE
1	D	467	LYS
1	D	469	LYS
1	D	487	LEU
1	D	490	ILE
1	D	494	LEU
1	D	509	ILE
1	D	519	ARG
1	D	525	GLU
1	D	528	SER
1	D	531	THR
1	D	535	SER
1	D	539	SER
1	D	542	LYS
1	D	551	LYS
1	D	558	LYS
1	D	566	THR
1	D	580	THR
1	D	590	ILE

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Mol	Chain	Res	Type
1	D	607	TRP
1	D	613	ASP
1	D	631	ARG
1	D	641	MET
1	D	647	ASN
1	D	649	VAL
1	D	652	LYS
1	D	664	GLN
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	750	LYS
1	D	756	ILE
1	D	766	LEU
1	D	775	THR
1	D	781	LEU
1	D	784	LYS
1	D	791	VAL
1	D	798	VAL
1	D	807	GLN
1	D	811	ASN
1	D	828	ILE
1	D	831	MET
1	D	835	SER
1	D	839	SER
1	D	843	THR
1	D	853	ASP
1	D	856	SER
1	D	863	GLN
1	D	873	ASN
1	D	879	LYS
1	D	881	LEU
1	D	907	VAL
1	D	908	THR
1	D	912	LYS
1	D	917	MET
1	D	925	ASP
1	D	926	LEU
1	D	931	VAL
1	D	932	ILE
1	D	945	VAL
1	D	949	LYS

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Mol	Chain	Res	Type
1	D	952	ILE
1	D	961	LYS
1	D	996	GLU
1	D	999	GLN
1	D	1002	VAL
1	D	1016	VAL
1	D	1042	MET
1	D	1048	VAL
1	D	1052	ILE
1	D	1054	LYS
1	D	1056	LYS
1	D	1057	ARG
1	D	1062	LEU
1	D	1064	THR
1	D	1070	GLU
1	D	1085	ARG
1	D	1090	LYS
1	D	1093	ASN
1	D	1103	LYS
1	D	1105	ASP
1	D	1123	VAL
1	D	1131	VAL
1	D	1138	LEU
1	D	1141	GLU
1	D	1147	THR
1	D	1148	THR
1	D	1153	PHE
1	D	1156	VAL
1	D	1161	THR
1	D	1162	VAL
1	D	1167	THR
1	D	1174	LEU
1	D	1175	ILE
1	D	1177	ILE
1	D	1178	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	326	ASN
1	A	330	GLN
1	A	333	HIS
1	A	375	GLN
1	A	414	GLN
1	A	432	HIS
1	A	491	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	622	ASN
1	A	664	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	1005	GLN
1	A	1019	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1071	ASN
1	A	1081	ASN
1	A	1083	GLN
1	A	1111	HIS
1	A	1150	GLN
1	B	36	GLN
1	B	44	ASN
1	B	108	GLN
1	B	110	ASN
1	B	145	HIS
1	B	241	ASN
1	B	256	ASN
1	B	272	GLN
1	B	326	ASN

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Mol	Chain	Res	Type
1	B	330	GLN
1	B	432	HIS
1	B	506	ASN
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	736	HIS
1	B	778	ASN
1	B	807	GLN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	898	ASN
1	B	924	ASN
1	B	957	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1022	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1073	ASN
1	B	1097	ASN
1	B	1111	HIS
1	C	44	ASN
1	C	69	ASN
1	C	108	GLN
1	C	145	HIS
1	C	326	ASN
1	C	330	GLN
1	C	432	HIS
1	C	464	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN

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Mol	Chain	Res	Type
1	C	685	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN
1	C	818	ASN
1	C	870	GLN
1	C	873	ASN
1	C	877	GLN
1	C	898	ASN
1	C	998	GLN
1	C	1005	GLN
1	C	1019	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1073	ASN
1	C	1083	GLN
1	C	1093	ASN
1	D	44	ASN
1	D	69	ASN
1	D	108	GLN
1	D	142	HIS
1	D	145	HIS
1	D	241	ASN
1	D	244	HIS
1	D	256	ASN
1	D	259	HIS
1	D	289	GLN
1	D	301	ASN
1	D	330	GLN
1	D	348	GLN
1	D	364	GLN
1	D	506	ASN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	617	ASN
1	D	622	ASN
1	D	647	ASN
1	D	736	HIS
1	D	778	ASN

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Mol	Chain	Res	Type
1	D	811	ASN
1	D	818	ASN
1	D	823	HIS
1	D	858	ASN
1	D	863	GLN
1	D	864	HIS
1	D	873	ASN
1	D	898	ASN
1	D	954	GLN
1	D	960	ASN
1	D	999	GLN
1	D	1005	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1073	ASN
1	D	1081	ASN
1	D	1111	HIS
1	D	1115	GLN
1	D	1150	GLN
1	D	1164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	C	1203	-	15,16,16	1.71	2 (13%)	20,21,21	2.13	3 (15%)
4	BTI	B	1202	-	15,16,16	1.77	2 (13%)	20,21,21	2.11	4 (20%)
2	ADP	A	1201	-	28,29,29	1.42	4 (14%)	43,45,45	1.78	10 (23%)
5	ATP	C	1202	-	32,33,33	1.41	5 (15%)	48,52,52	1.71	9 (18%)
4	BTI	B	1201	-	15,16,16	1.74	2 (13%)	20,21,21	2.38	4 (20%)
4	BTI	D	1202	-	15,16,16	1.79	2 (13%)	20,21,21	1.92	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTI	C	1203	-	-	4/6/27/27	0/2/2/2
4	BTI	B	1202	-	-	3/6/27/27	0/2/2/2
2	ADP	A	1201	-	-	4/16/32/32	0/3/3/3
5	ATP	C	1202	-	-	5/22/38/38	0/3/3/3
4	BTI	B	1201	-	-	2/6/27/27	0/2/2/2
4	BTI	D	1202	-	-	4/6/27/27	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1201	BTI	O3-C3	5.46	1.35	1.23
2	A	1201	ADP	C5-C4	4.70	1.47	1.39
5	C	1202	ATP	C5-C4	4.70	1.47	1.39
4	B	1202	BTI	O3-C3	4.67	1.33	1.23
4	C	1203	BTI	O3-C3	4.61	1.33	1.23
4	D	1202	BTI	O3-C3	4.57	1.33	1.23
4	D	1202	BTI	C2-S1	-4.30	1.75	1.82
4	B	1202	BTI	C2-S1	-4.12	1.76	1.82
4	C	1203	BTI	C2-S1	-3.72	1.76	1.82
5	C	1202	ATP	PB-O3B	3.05	1.62	1.59
4	B	1201	BTI	C2-S1	-3.02	1.77	1.82
2	A	1201	ADP	C5-C6	2.64	1.48	1.41
5	C	1202	ATP	C5-C6	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ADP	C8-N7	2.45	1.36	1.31
5	C	1202	ATP	C5-N7	-2.27	1.34	1.39
2	A	1201	ADP	C5-N7	-2.26	1.35	1.39
5	C	1202	ATP	C8-N7	2.11	1.35	1.31

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	BTI	C2-C4-N2	-8.11	104.75	113.34
4	D	1202	BTI	C2-C4-N2	-6.38	106.59	113.34
4	C	1203	BTI	C2-C4-N2	-5.93	107.07	113.34
4	C	1203	BTI	C6-C5-N3	-5.87	105.61	113.18
2	A	1201	ADP	C5-C4-N3	-5.70	118.86	126.72
4	B	1202	BTI	C6-C5-N3	-5.54	106.04	113.18
5	C	1202	ATP	C5-C4-N3	-5.45	119.22	126.72
4	B	1202	BTI	C2-C4-N2	-5.43	107.59	113.34
4	B	1201	BTI	C6-C5-N3	-4.87	106.90	113.18
5	C	1202	ATP	N3-C4-N9	4.64	135.06	127.17
2	A	1201	ADP	N3-C4-N9	4.29	134.46	127.17
4	D	1202	BTI	C6-C5-N3	-3.72	108.39	113.18
2	A	1201	ADP	C2-N3-C4	3.63	120.70	111.83
5	C	1202	ATP	C2-N3-C4	3.62	120.67	111.83
2	A	1201	ADP	C4-C5-N7	-3.45	106.63	110.58
5	C	1202	ATP	N3-C2-N1	-3.44	123.38	128.58
2	A	1201	ADP	N3-C2-N1	-3.22	123.72	128.58
4	B	1202	BTI	C8-C7-C2	-3.09	106.95	114.04
5	C	1202	ATP	C4-C5-N7	-2.84	107.34	110.58
5	C	1202	ATP	C4-N9-C8	2.79	108.67	105.74
4	D	1202	BTI	C8-C7-C2	-2.66	107.93	114.04
4	C	1203	BTI	C4-C2-S1	2.64	108.03	105.03
2	A	1201	ADP	C5-N7-C8	2.45	107.29	103.45
4	B	1202	BTI	N2-C3-N3	2.39	111.61	108.85
2	A	1201	ADP	O3B-PB-O2B	2.36	116.63	107.80
2	A	1201	ADP	C6-C5-N7	2.27	136.46	132.09
4	B	1201	BTI	C5-C6-S1	2.23	109.14	106.06
4	B	1201	BTI	C4-C2-S1	2.22	107.55	105.03
5	C	1202	ATP	C2'-C1'-N9	-2.19	107.86	113.30
5	C	1202	ATP	C5-N7-C8	2.16	106.84	103.45
2	A	1201	ADP	O4'-C1'-N9	2.16	112.23	108.09
2	A	1201	ADP	C4-N9-C8	2.13	107.97	105.74
5	C	1202	ATP	C2-N1-C6	2.06	122.12	118.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O2A
4	B	1202	BTI	S1-C2-C7-C8
4	B	1202	BTI	C4-C2-C7-C8
4	C	1203	BTI	C9-C10-C11-O11
4	C	1203	BTI	S1-C2-C7-C8
4	C	1203	BTI	C4-C2-C7-C8
4	D	1202	BTI	C9-C10-C11-O11
4	D	1202	BTI	S1-C2-C7-C8
4	D	1202	BTI	C4-C2-C7-C8
5	C	1202	ATP	O4'-C4'-C5'-O5'
5	C	1202	ATP	C3'-C4'-C5'-O5'
4	B	1201	BTI	S1-C2-C7-C8
4	B	1201	BTI	C4-C2-C7-C8
5	C	1202	ATP	PB-O3B-PG-O2G
4	B	1202	BTI	C11-C10-C9-C8
2	A	1201	ADP	C5'-O5'-PA-O1A
2	A	1201	ADP	C5'-O5'-PA-O3A
4	D	1202	BTI	C7-C8-C9-C10
5	C	1202	ATP	PG-O3B-PB-O3A
4	C	1203	BTI	C7-C8-C9-C10
2	A	1201	ADP	PB-O3A-PA-O2A
5	C	1202	ATP	PG-O3B-PB-O2B

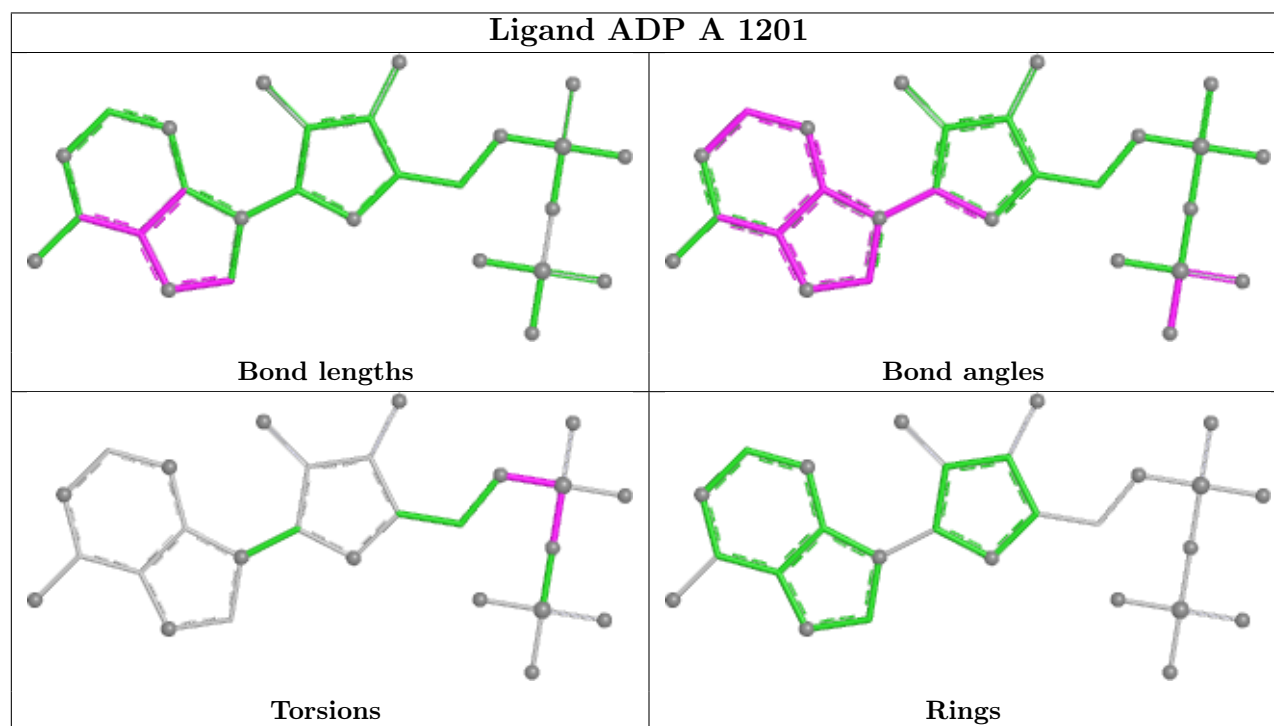
There are no ring outliers.

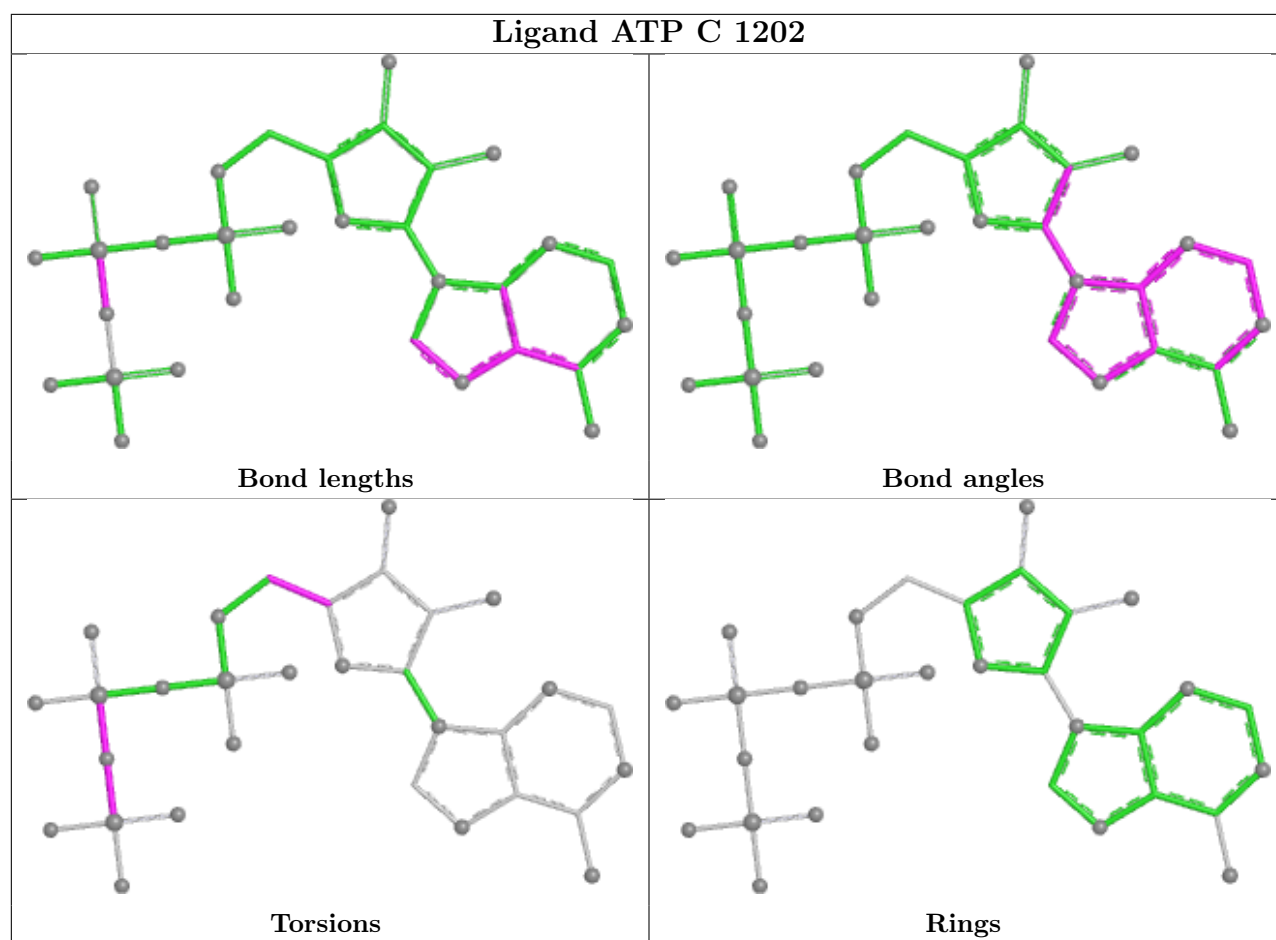
6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	BTI	1	0
4	B	1202	BTI	9	0
2	A	1201	ADP	3	0
5	C	1202	ATP	6	0
4	B	1201	BTI	8	0
4	D	1202	BTI	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1133/1173 (96%)	-0.38	17 (1%) 72 63	23, 51, 104, 136	0
1	B	1033/1173 (88%)	-0.17	24 (2%) 61 51	31, 65, 130, 216	0
1	C	1067/1173 (90%)	-0.19	26 (2%) 59 49	36, 62, 108, 133	0
1	D	1067/1173 (90%)	-0.36	15 (1%) 73 64	21, 57, 115, 174	0
All	All	4300/4692 (91%)	-0.28	82 (1%) 66 57	21, 59, 114, 216	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	ILE	4.9
1	D	92	PRO	4.3
1	C	933	THR	4.1
1	A	271	HIS	4.0
1	B	1095	HIS	3.9
1	A	213	LEU	3.8
1	B	1094	VAL	3.8
1	D	490	ILE	3.8
1	A	180	ALA	3.7
1	B	526	LEU	3.6
1	C	931	VAL	3.3
1	D	492	PRO	3.3
1	A	416	ALA	3.3
1	B	455	VAL	3.3
1	A	1094	VAL	3.2
1	D	314	VAL	3.2
1	B	524	TYR	3.2
1	C	395	ILE	3.2
1	C	1147	THR	3.2
1	C	180	ALA	3.1
1	C	92	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	494	LEU	3.1
1	B	1096	THR	3.1
1	C	269	ARG	3.0
1	C	932	ILE	3.0
1	D	1153	PHE	2.9
1	B	494	LEU	2.9
1	B	90	LEU	2.9
1	B	283	LEU	2.9
1	B	168	PRO	2.9
1	B	488	PHE	2.9
1	B	490	ILE	2.8
1	C	416	ALA	2.8
1	B	164	LEU	2.8
1	A	399	SER	2.7
1	C	936	TYR	2.7
1	B	492	PRO	2.7
1	B	166	VAL	2.6
1	A	1148	THR	2.6
1	A	197	SER	2.6
1	A	1128	GLY	2.6
1	C	235	ILE	2.6
1	C	494	LEU	2.5
1	C	963	LEU	2.5
1	B	160	ILE	2.5
1	C	415	GLY	2.5
1	C	403	PHE	2.5
1	B	527	ALA	2.5
1	A	190	PRO	2.5
1	A	220	ALA	2.5
1	C	183	PHE	2.4
1	D	322	PHE	2.4
1	D	167	ILE	2.4
1	C	400	SER	2.4
1	B	664	GLN	2.4
1	A	1138	LEU	2.3
1	B	280	SER	2.3
1	D	823	HIS	2.3
1	D	1093	ASN	2.3
1	A	189	PHE	2.2
1	D	488	PHE	2.2
1	B	239	ILE	2.2
1	C	492	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	282	GLY	2.2
1	C	937	LYS	2.2
1	B	99	ILE	2.2
1	D	239	ILE	2.2
1	B	36	GLN	2.2
1	C	175	LYS	2.2
1	D	87	GLY	2.2
1	C	213	LEU	2.2
1	C	193	ILE	2.1
1	C	493	SER	2.1
1	C	199	GLY	2.1
1	B	165	PRO	2.1
1	A	1178	GLU	2.1
1	A	177	TYR	2.1
1	C	197	SER	2.0
1	D	321	PHE	2.0
1	D	242	PRO	2.0
1	D	1174	LEU	2.0
1	A	1151	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	1201	27/27	0.87	0.10	75,82,96,97	0
5	ATP	C	1202	31/31	0.91	0.09	69,72,104,105	0
3	MN	D	1203	1/1	0.96	0.05	85,85,85,85	0
4	BTI	B	1201	15/15	0.96	0.09	56,59,61,64	0

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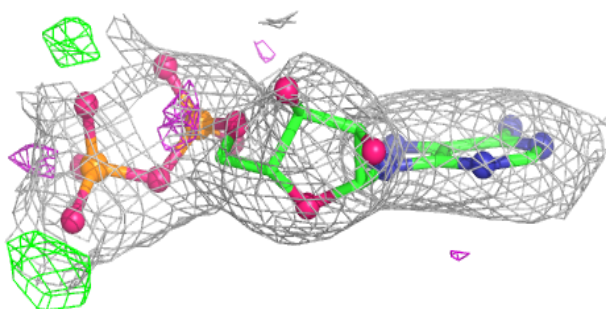
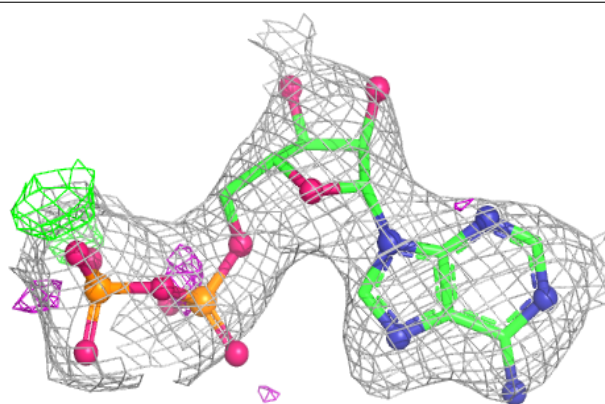
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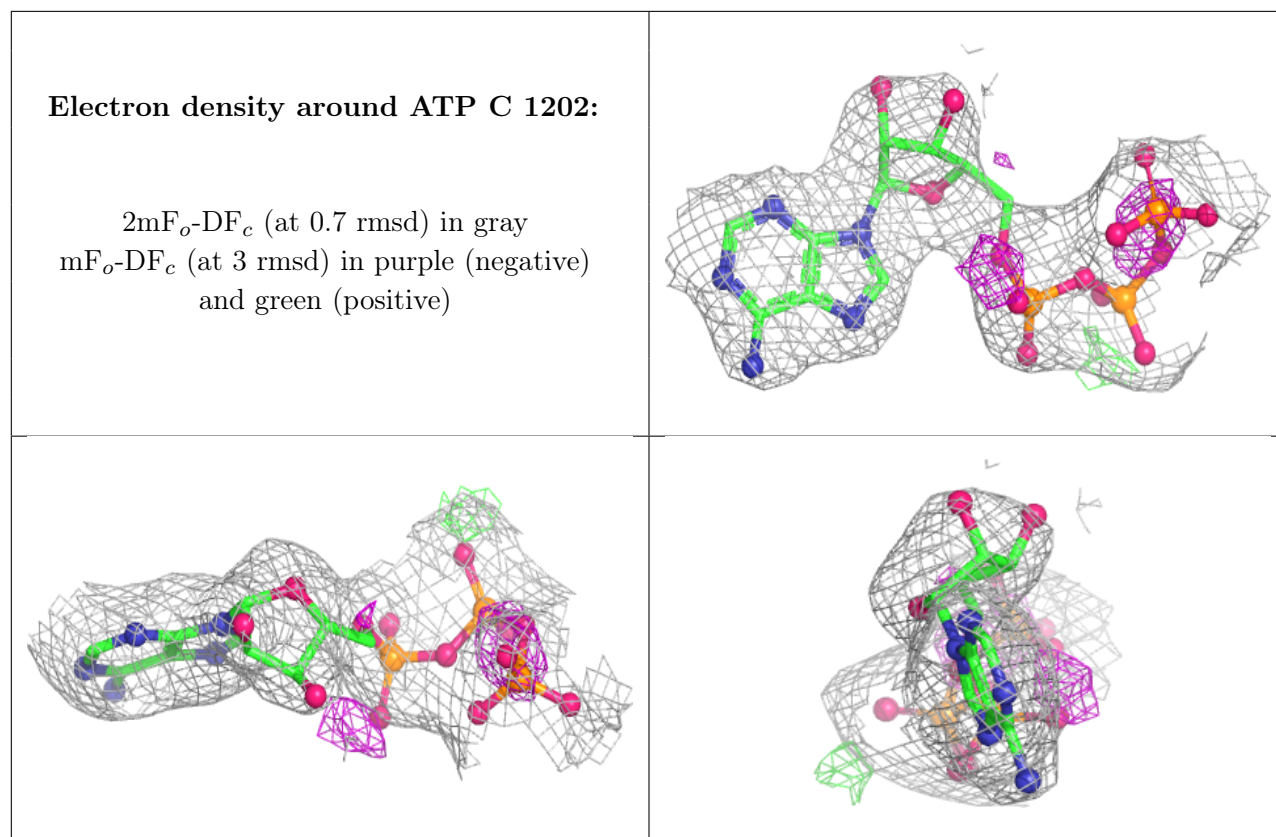
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BTI	C	1203	15/15	0.96	0.07	55,59,61,63	0
3	MN	A	1202	1/1	0.96	0.06	94,94,94,94	0
4	BTI	D	1202	15/15	0.97	0.07	46,50,51,52	0
3	MN	B	1203	1/1	0.98	0.03	83,83,83,83	0
3	MN	C	1201	1/1	0.98	0.10	55,55,55,55	0
4	BTI	B	1202	15/15	0.98	0.05	31,40,44,50	0
6	CL	D	1201	1/1	0.98	0.06	45,45,45,45	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.