



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 PM UTC

PDB ID : 4HNT / pdb_00004hnt
Title : crystal structure of F403A mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<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

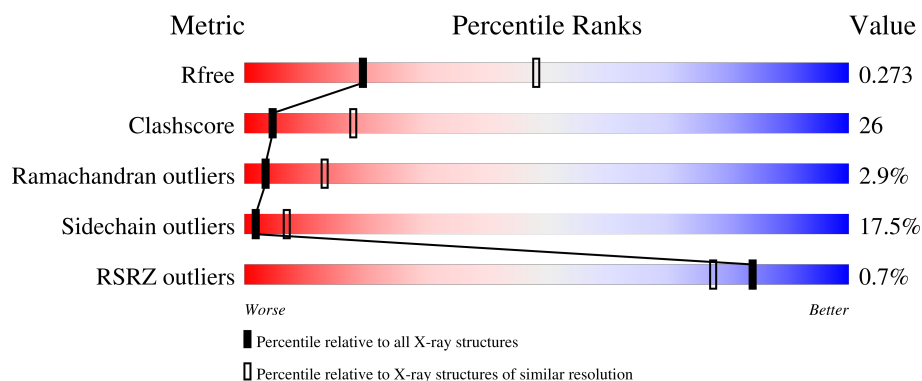
1 Overall quality at a glance

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	
1	B	1173	
1	C	1173	
1	D	1173	

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
5	ATP	C	1202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8336	5286	1404	1619	27			
1	B	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8373	5307	1412	1626	28			
1	D	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			

There are 92 discrepancies between the modelled and reference sequences:

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

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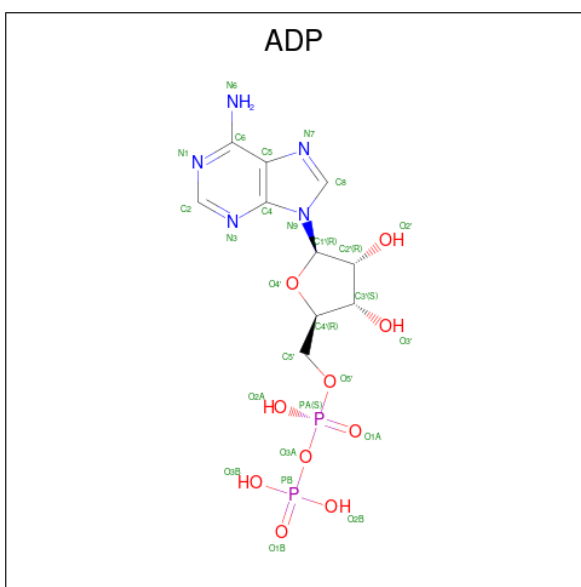
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag	UNP Q99UY8
B	15	HIS	-	expression tag	UNP Q99UY8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

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

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

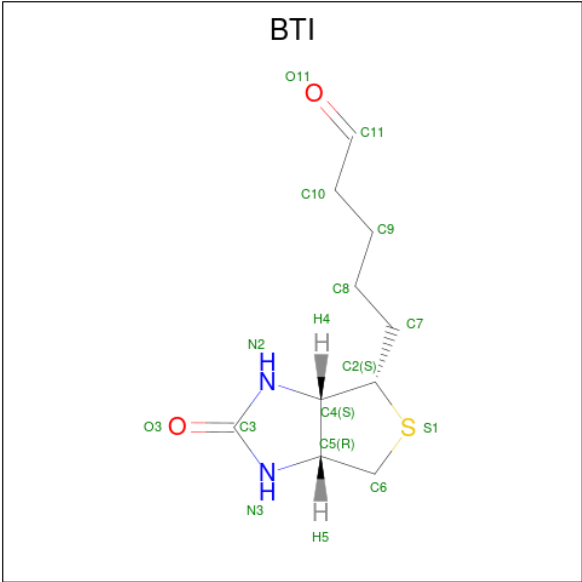


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

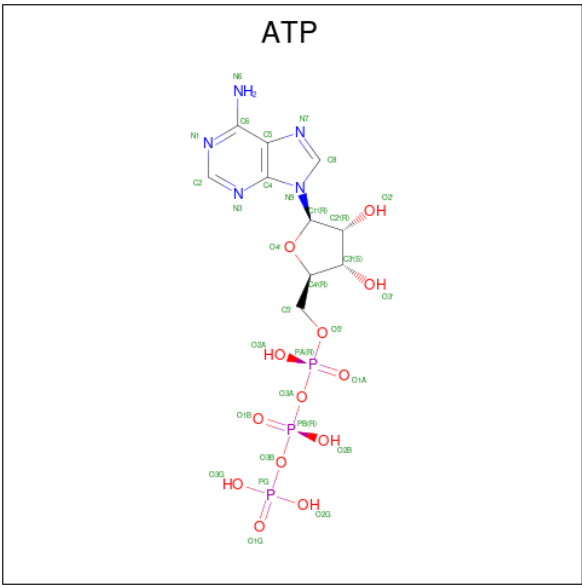
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0

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

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

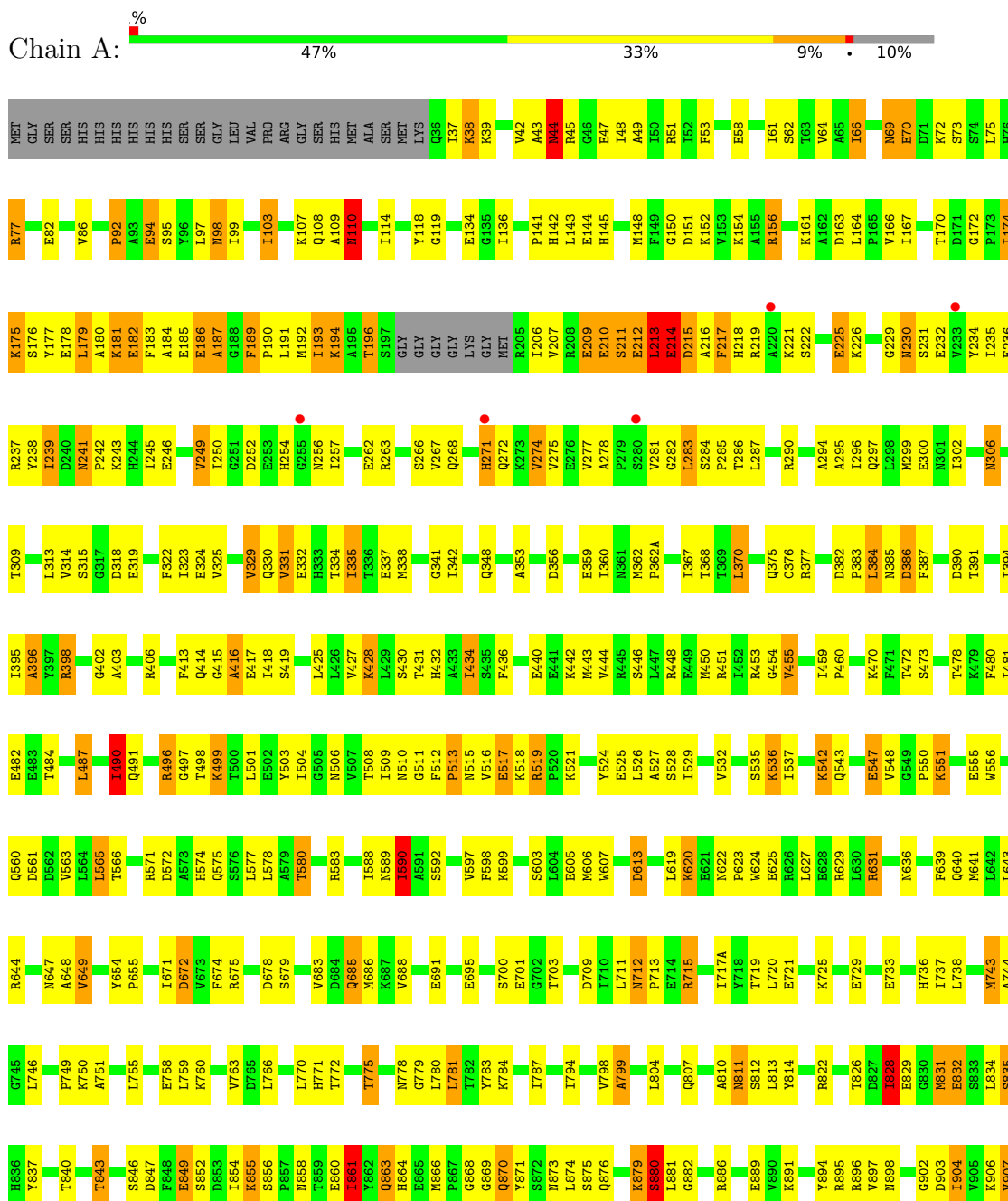


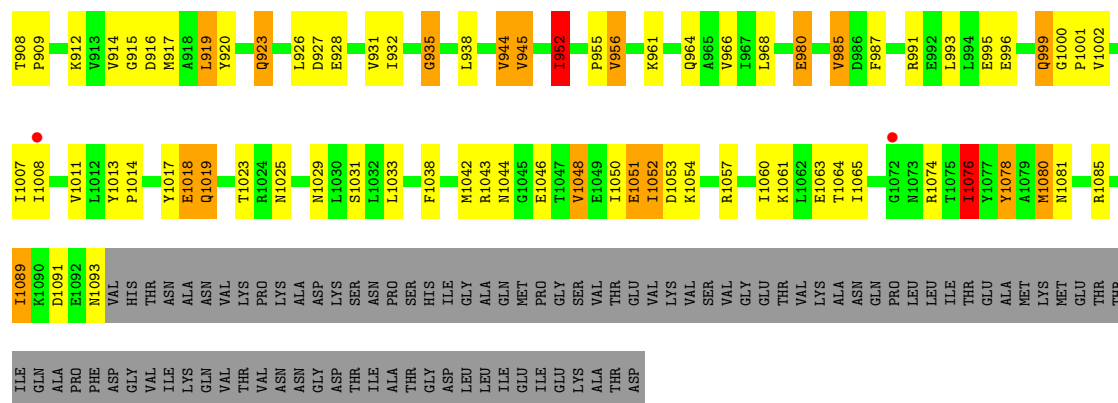
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

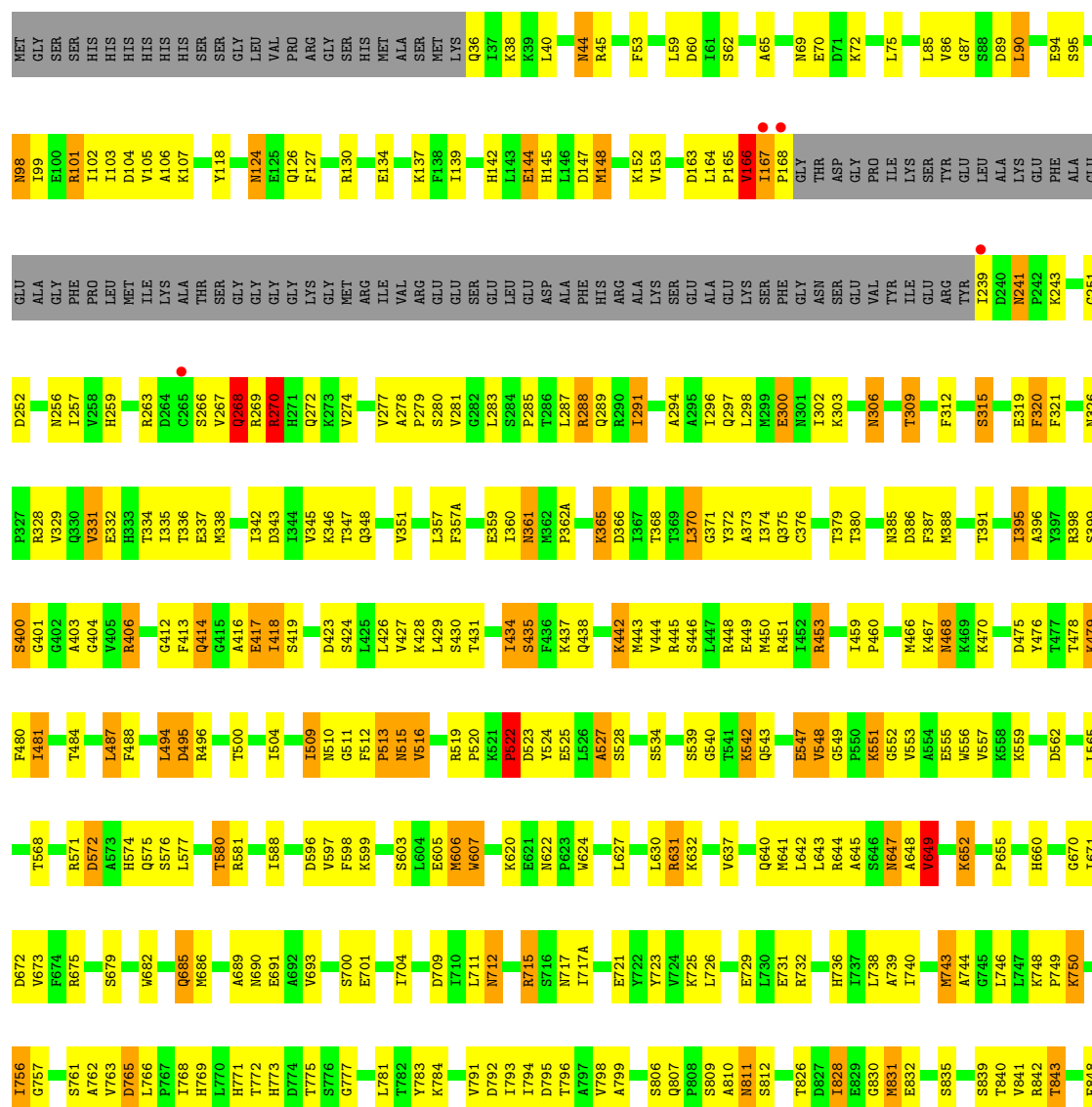
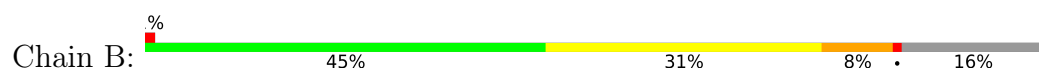
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

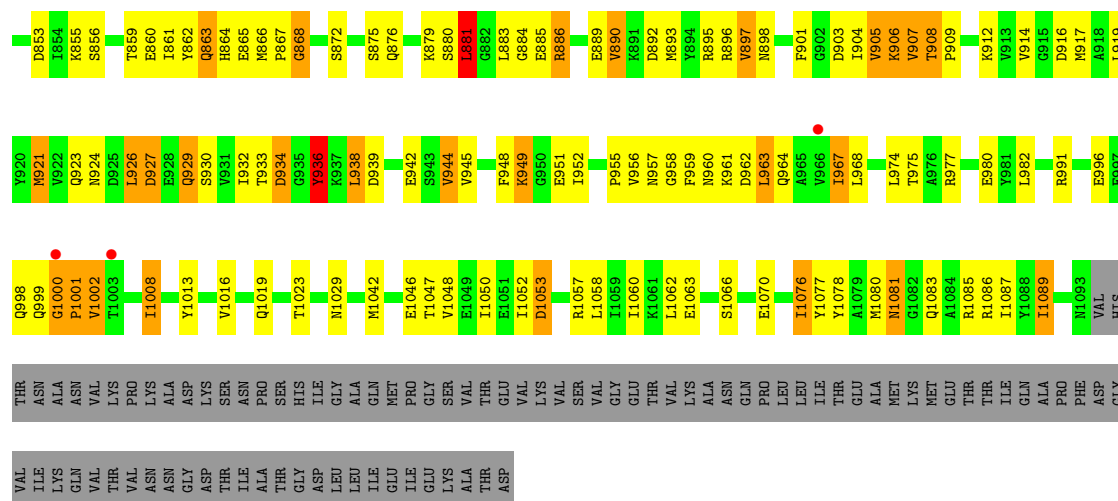
• Molecule 1: Pyruvate carboxylase



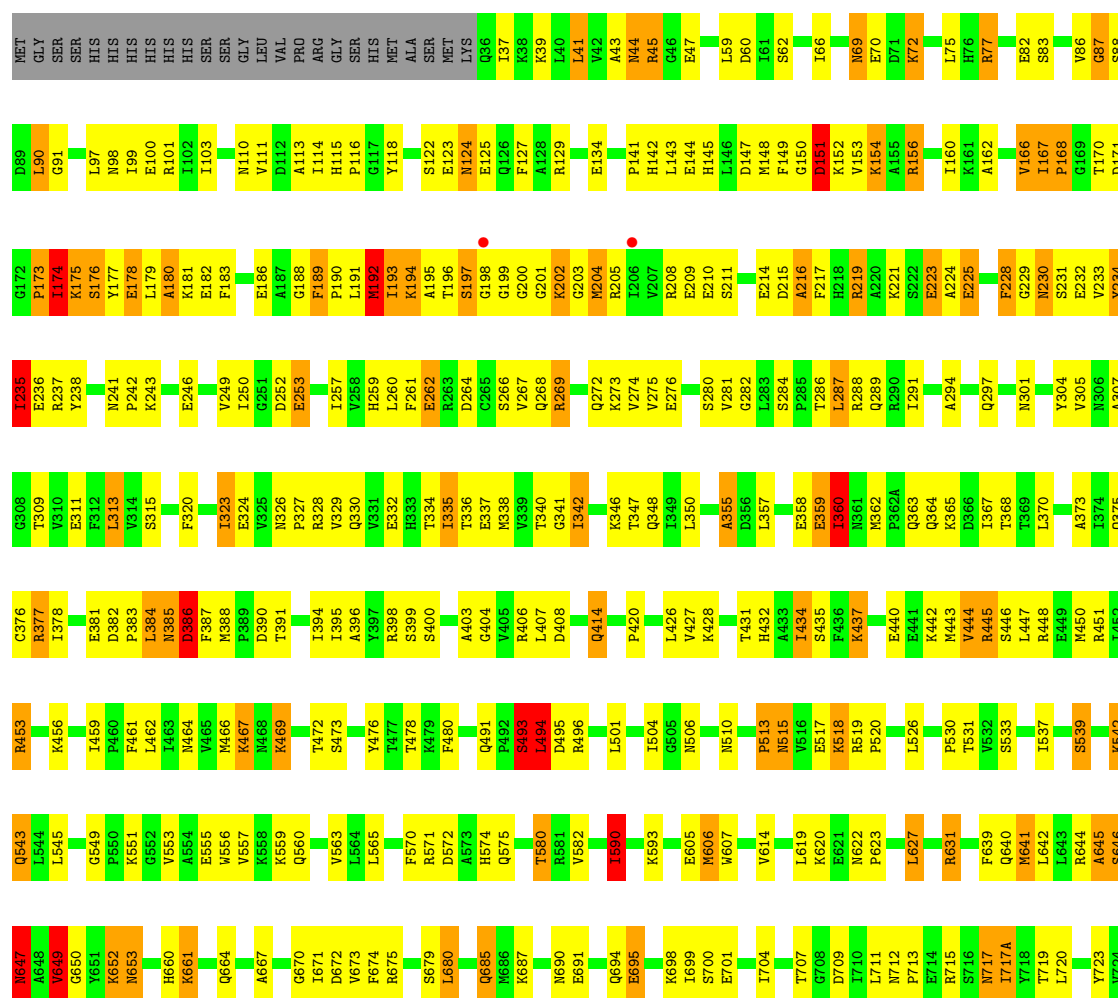


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase





ASN	ASN	GLY	ASP	THR	ILE	ALA	THR	THR	GLY	ASP	LEU	LEU	ALA	GLN	MET	GLU	ILE	GLU	PRO	GLY	GLY	LYS	VAL	THR	THR	GLN	ASN	VAL	THR	VAL	ASN	GLN	ASN	PRO	PRO	PHE	ASP	GLY	THR	VAL	ILE	LYS	GLN	VAL	THR	VAL					
P1014	K1015	V1016	T1023	D1034	T1035	P1036	M1042	R1043	N1044	G1045	E1046	T1047	I1052	D1053	K1054	G1055	K1056	R1057	I1060	K1061	L1062	E1063	T1064	I1065	D1069	E1070	N1071	G1072	N1073	Y1078	A1079	M1080	Q1083	A1084	R1085	R1086	I1087	Y1088	I1089	K1090	N1093	VAL	HIS	THR	VAL	ILE	LYS	GLN	VAL	THR	VAL
L919	Y920	M921	N924	D925	L926	D927	E928	Q929	S930	V931	G935	L938	D939	F940	Y944	V945	I952	N957	N960	L963	V966	I967	L974	P978	Y981	E982	E983	D986	F987	E988	R991	E995	E996	G1000	P1001	V1002	T1003	E1004	I1008	Y1013											
F848	E849	S852	D853	I854	K855	S856	P857	E860	I861	Y862	Q863	H864	E865	M866	G869	Y871	S872	N873	L874	S875	Q876	Q877	A878	K879	S880	L881	G882	L883	G884	E885	R886	F887	D888	K891	D892	M893	R896	V897	N898	F899	L900	F901	G902	D903	I904	V907	T908	P909	S910	S911	M917
V763	D765	L766	P767	I768	H769	L770	H771	T772	T775	S776	T782	Y783	K784	I699	S700	E701	G702	T703	T707	L711	E714	R715	S716	N717	I717A	L720	K725	L730	F735	H736	I737	L738	A739	I740	K741	D742	M743	A744	G745	L746	K750	A751	A752	I756	G757	E758	L759	Y654			
K661	I671	D672	R675	S679	Q685	M690	Q694	K698	S699	S700	E701	G702	T703	T707	L711	E714	R715	S716	N717	I717A	L720	K725	L730	F735	H736	I737	L738	A739	I740	K741	D742	M743	A744	G745	L746	K750	A751	A752	I756	G757	E758	L759	Y654								
D567	F570	R571	D572	A573	H574	Q575	T580	R581	V582	R583	I588	N589	I590	K593	T594	A595	D596	F597	F598	K599	E605	M606	W607	T611	M617	F618	L619	K620	E621	N622	P623	W624	R629	L630	R631	K632	N636	Q640	M641	R644	N647	A648	V649	G650	Y654						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23Å 256.28Å 126.69Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 90.9 (30.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.209 , 0.279 0.207 , 0.273	Depositor DCC
R_{free} test set	7085 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

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

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: ATP, MN, ADP, BTI

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	0.85	11/8497 (0.1%)	1.02	28/11490 (0.2%)
1	B	0.82	11/7983 (0.1%)	0.96	23/10801 (0.2%)
1	C	0.84	9/8535 (0.1%)	0.98	15/11539 (0.1%)
1	D	0.83	12/7983 (0.2%)	1.01	24/10801 (0.2%)
All	All	0.84	43/32998 (0.1%)	0.99	90/44631 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	18

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	20.03	1.80	1.52
1	B	936	TYR	C-N	19.07	1.60	1.33
1	C	513	PRO	C-N	18.08	1.58	1.33
1	B	961	LYS	C-O	15.87	1.42	1.24
1	C	515	ASN	N-CA	13.83	1.67	1.46
1	B	513	PRO	CA-C	13.50	1.67	1.52
1	A	513	PRO	CA-C	12.38	1.70	1.52
1	C	513	PRO	N-CA	11.71	1.62	1.47
1	D	515	ASN	N-CA	11.53	1.61	1.46
1	D	513	PRO	CA-C	11.10	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	513	PRO	C-N	10.44	1.48	1.33
1	B	763	VAL	N-CA	10.35	1.57	1.46
1	A	315	SER	CA-C	9.22	1.64	1.53
1	C	849	GLU	CA-C	8.63	1.63	1.52
1	D	290	ARG	CZ-NH1	8.34	1.44	1.32
1	D	513	PRO	N-CA	7.86	1.57	1.47
1	B	936	TYR	N-CA	7.79	1.56	1.46
1	A	513	PRO	C-N	7.75	1.44	1.33
1	B	763	VAL	CA-C	7.42	1.61	1.52
1	A	590	ILE	CA-CB	7.24	1.63	1.54
1	D	763	VAL	CA-C	7.12	1.61	1.52
1	B	515	ASN	N-CA	7.07	1.54	1.46
1	D	315	SER	CA-C	6.17	1.60	1.53
1	B	513	PRO	C-N	6.16	1.41	1.33
1	D	515	ASN	CA-C	6.11	1.60	1.52
1	A	849	GLU	N-CA	6.07	1.53	1.46
1	C	763	VAL	N-CA	6.03	1.53	1.46
1	A	513	PRO	N-CA	5.86	1.54	1.47
1	C	762	ALA	C-N	5.86	1.41	1.33
1	D	290	ARG	NE-CZ	5.77	1.39	1.33
1	A	175	LYS	CA-C	5.55	1.56	1.52
1	A	315	SER	N-CA	5.54	1.53	1.46
1	B	936	TYR	CA-CB	5.53	1.62	1.53
1	A	763	VAL	C-N	5.51	1.42	1.33
1	B	315	SER	N-CA	5.44	1.53	1.46
1	D	952	ILE	CA-CB	5.39	1.60	1.54
1	D	763	VAL	N-CA	5.37	1.52	1.46
1	C	160	ILE	C-N	5.30	1.41	1.33
1	D	507	VAL	CA-CB	-5.24	1.48	1.54
1	B	765	ASP	N-CA	5.13	1.52	1.46
1	A	274	VAL	CA-CB	-5.12	1.49	1.55
1	C	848	PHE	C-N	-5.11	1.26	1.33
1	A	799	ALA	CA-CB	-5.01	1.45	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	CA-C-N	13.85	141.87	122.07
1	C	513	PRO	C-N-CA	13.85	141.87	122.07
1	D	515	ASN	CA-CB-CG	10.39	122.99	112.60
1	B	763	VAL	O-C-N	-9.11	113.25	123.00
1	D	938	LEU	N-CA-C	8.95	122.70	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	952	ILE	N-CA-C	-8.91	104.23	112.43
1	D	271	HIS	N-CA-C	-7.91	101.40	113.89
1	D	944	VAL	N-CA-C	7.86	117.91	110.53
1	C	515	ASN	CA-CB-CG	7.58	120.18	112.60
1	A	828	ILE	CB-CA-C	-7.51	102.18	112.24
1	C	513	PRO	N-CA-CB	-7.02	95.88	103.25
1	B	513	PRO	CA-C-O	-6.96	113.96	121.27
1	C	235	ILE	N-CA-C	6.88	117.69	108.27
1	B	961	LYS	CA-C-O	6.86	128.02	120.82
1	B	763	VAL	CA-C-O	-6.82	113.37	121.28
1	C	495	ASP	N-CA-C	6.78	119.79	109.62
1	C	513	PRO	O-C-N	-6.67	113.64	122.64
1	A	952	ILE	CB-CA-C	-6.63	103.46	110.62
1	D	513	PRO	O-C-N	-6.56	113.78	122.64
1	D	590	ILE	CB-CA-C	-6.51	102.96	111.88
1	A	952	ILE	N-CA-C	-6.47	106.94	113.47
1	A	416	ALA	N-CA-C	6.40	118.79	110.53
1	D	1000	GLY	CA-C-N	6.39	127.83	119.84
1	D	1000	GLY	C-N-CA	6.39	127.83	119.84
1	B	763	VAL	CA-C-N	-6.33	110.06	121.14
1	B	763	VAL	C-N-CA	-6.33	110.06	121.14
1	A	688	VAL	N-CA-C	6.33	116.49	110.42
1	B	828	ILE	CB-CA-C	-6.24	104.01	111.81
1	C	647	ASN	N-CA-C	-6.11	106.47	114.04
1	B	513	PRO	O-C-N	-6.09	116.34	122.98
1	A	272	GLN	N-CA-C	6.01	118.92	108.76
1	A	529	ILE	CA-C-N	5.97	126.17	119.90
1	A	529	ILE	C-N-CA	5.97	126.17	119.90
1	C	360	ILE	N-CA-C	5.96	116.75	110.72
1	A	565	LEU	N-CA-C	5.95	118.89	109.50
1	A	1076	ILE	N-CA-C	5.92	116.71	108.89
1	A	64	VAL	N-CA-C	5.91	116.38	108.11
1	B	268	GLN	N-CA-C	5.88	118.34	109.23
1	A	119	GLY	N-CA-C	5.86	119.85	113.58
1	A	314	VAL	O-C-N	-5.80	117.09	123.18
1	A	849	GLU	CA-C-N	-5.79	112.31	120.82
1	A	849	GLU	C-N-CA	-5.79	112.31	120.82
1	A	175	LYS	N-CA-C	5.74	119.74	111.02
1	D	967	ILE	N-CA-C	5.72	116.36	110.82
1	B	412	GLY	N-CA-C	5.71	119.31	111.54
1	D	529	ILE	CA-C-N	5.68	126.00	119.92
1	D	529	ILE	C-N-CA	5.68	126.00	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	VAL	N-CA-C	5.68	116.03	107.80
1	A	513	PRO	O-C-N	-5.67	114.99	122.64
1	D	617	ASN	N-CA-C	5.66	117.31	111.03
1	B	772	THR	N-CA-C	5.64	117.36	108.96
1	B	762	ALA	O-C-N	-5.60	114.98	122.49
1	A	770	LEU	N-CA-C	5.57	117.60	108.52
1	A	1052	ILE	CB-CA-C	-5.55	104.94	111.94
1	B	572	ASP	N-CA-C	5.55	117.33	111.28
1	A	832	GLU	N-CA-C	-5.54	105.40	111.82
1	D	489	ASP	N-CA-C	5.48	117.73	109.23
1	D	589	ASN	N-CA-C	5.47	117.95	111.33
1	C	124	ASN	N-CA-C	5.46	118.38	107.62
1	C	590	ILE	CB-CA-C	-5.46	104.99	111.65
1	A	329	VAL	CB-CA-C	-5.45	102.35	111.29
1	A	537	ILE	N-CA-C	5.44	115.64	110.42
1	D	515	ASN	CA-C-N	5.44	131.00	122.84
1	D	515	ASN	C-N-CA	5.44	131.00	122.84
1	A	849	GLU	N-CA-C	5.42	118.09	109.96
1	B	904	ILE	N-CA-C	5.42	116.65	108.96
1	D	1035	THR	CA-C-N	-5.38	114.12	119.56
1	D	1035	THR	C-N-CA	-5.38	114.12	119.56
1	D	314	VAL	N-CA-C	5.37	115.32	107.37
1	B	1060	ILE	N-CA-C	5.37	115.58	107.75
1	B	468	ASN	N-CA-C	5.36	117.95	109.96
1	C	91	GLY	CA-C-N	5.34	125.16	119.28
1	C	91	GLY	C-N-CA	5.34	125.16	119.28
1	D	267	VAL	CB-CA-C	-5.31	107.27	113.22
1	A	589	ASN	N-CA-C	5.31	117.06	111.28
1	B	445	ARG	N-CA-C	-5.28	105.21	110.97
1	B	166	VAL	N-CA-C	5.28	120.31	109.34
1	D	832	GLU	N-CA-C	-5.23	105.75	111.82
1	D	459	ILE	CA-C-N	5.22	125.27	119.32
1	D	459	ILE	C-N-CA	5.22	125.27	119.32
1	A	849	GLU	CB-CA-C	-5.20	101.58	109.89
1	B	148	MET	N-CA-C	-5.17	105.54	111.07
1	A	712	ASN	CA-C-N	5.16	124.82	119.56
1	A	712	ASN	C-N-CA	5.16	124.82	119.56
1	C	192	MET	N-CA-C	5.14	116.97	108.13
1	A	763	VAL	N-CA-C	5.12	115.86	108.48
1	B	712	ASN	N-CA-C	5.12	116.83	109.04
1	B	961	LYS	O-C-N	-5.09	116.82	122.07
1	B	905	VAL	CB-CA-C	-5.07	105.14	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	515	ASN	N-CA-C	5.05	118.41	111.54

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	150	GLY	Peptide
1	A	196	THR	Peptide
1	A	271	HIS	Peptide
1	A	415	GLY	Peptide
1	A	490	ILE	Peptide
1	B	522	PRO	Peptide
1	B	524	TYR	Peptide
1	B	936	TYR	Sidechain
1	C	150	GLY	Peptide
1	C	211	SER	Peptide
1	C	228	PHE	Peptide
1	C	262	GLU	Peptide
1	C	420	PRO	Peptide
1	C	493	SER	Peptide
1	C	494	LEU	Peptide
1	D	415	GLY	Peptide
1	D	416	ALA	Peptide

5.2 Too-close contacts [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	8336	0	8249	455	0
1	B	7832	0	7767	368	0
1	C	8373	0	8287	477	0
1	D	7832	0	7767	400	0
2	A	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	15	0	16	4	0
4	B	15	0	16	4	0
4	D	15	0	16	3	0
5	C	31	0	12	10	0
All	All	32480	0	32142	1671	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 26.

All (1671) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASN:N	1:C:515:ASN:CA	1.67	1.56
1:C:513:PRO:C	1:C:513:PRO:CA	1.80	1.52
1:D:607:TRP:HE3	1:D:641:MET:CE	1.51	1.23
1:C:918:ALA:O	1:C:922:VAL:HG23	1.39	1.22
1:B:403:ALA:O	1:B:442:LYS:HE2	1.42	1.18
1:C:334:THR:HB	1:C:406:ARG:NH1	1.59	1.17
1:A:334:THR:HG22	1:A:406:ARG:HH12	1.06	1.16
1:C:893:MET:HA	1:C:896:ARG:CD	1.74	1.16
1:A:413:PHE:CZ	1:A:416:ALA:HB2	1.82	1.14
1:C:1024:ARG:HH11	1:C:1024:ARG:HG2	1.02	1.14
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.00	1.12
1:C:396:ALA:HB3	1:C:453:ARG:HG3	1.27	1.11
1:C:940:PHE:HB3	1:C:941:PRO:HD2	1.33	1.09
1:C:936:TYR:O	1:C:937:LYS:HG3	1.52	1.09
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.23	1.08
1:A:935:GLY:HA3	1:A:966:VAL:CG1	1.84	1.08
1:B:259:HIS:CD2	1:B:296:ILE:HD11	1.89	1.08
1:C:504:ILE:HD13	1:C:1042:MET:HE2	1.35	1.07
1:A:213:LEU:O	1:A:215:ASP:N	1.87	1.07
1:D:607:TRP:CE3	1:D:641:MET:HE1	1.90	1.07
1:A:334:THR:CG2	1:A:406:ARG:HH12	1.68	1.06
1:D:268:GLN:O	1:D:481:ILE:HD12	1.55	1.06
1:C:1085:ARG:HG2	1:C:1085:ARG:HH11	1.17	1.05
1:C:1029:ASN:HD21	1:C:1031:SER:HB2	1.16	1.05
1:D:607:TRP:CE3	1:D:641:MET:CE	2.40	1.05
1:C:167:ILE:HD12	1:C:167:ILE:H	1.23	1.03
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.41	1.03
1:B:991:ARG:NH1	1:B:1002:VAL:O	1.92	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:HH11	1:C:377:ARG:CG	1.71	1.03
1:A:504:ILE:HD13	1:A:1042:MET:HE3	1.37	1.02
1:C:378:ILE:HG13	1:C:450:MET:HE1	1.37	1.01
1:C:893:MET:HA	1:C:896:ARG:HD3	1.00	1.00
1:C:940:PHE:CB	1:C:944:VAL:HG11	1.92	1.00
1:B:338:MET:CE	1:B:430:SER:HB3	1.92	0.99
1:C:377:ARG:HH11	1:C:377:ARG:HG2	0.85	0.99
1:C:1042:MET:HE1	1:C:1060:ILE:HG21	1.44	0.99
1:C:977:ARG:NH1	1:C:980:GLU:OE1	1.94	0.99
1:C:811:ASN:HD22	1:C:811:ASN:H	1.10	0.99
1:C:170:THR:HG22	1:C:171:ASP:H	1.27	0.98
1:C:192:MET:HE1	5:C:1202:ATP:C5	1.99	0.98
1:D:496:ARG:HH11	1:D:496:ARG:HB3	1.26	0.98
1:A:935:GLY:HA3	1:A:966:VAL:HG11	1.45	0.98
1:A:334:THR:CG2	1:A:406:ARG:NH1	2.26	0.97
1:B:700:SER:H	1:B:736:HIS:HD2	1.09	0.97
1:C:1085:ARG:HH11	1:C:1085:ARG:CG	1.78	0.97
1:D:607:TRP:HE3	1:D:641:MET:HE1	1.24	0.97
1:D:451:ARG:HG3	1:D:451:ARG:HH11	1.28	0.97
1:C:175:LYS:O	1:C:176:SER:O	1.83	0.97
1:C:377:ARG:HG2	1:C:377:ARG:NH1	1.68	0.97
1:A:179:LEU:HD23	1:A:179:LEU:H	1.26	0.96
1:C:44:ASN:HD22	1:C:45:ARG:H	0.96	0.96
1:A:156:ARG:HH11	1:A:156:ARG:HB3	1.31	0.95
1:D:357:LEU:O	1:D:362:MET:HB2	1.66	0.95
1:D:44:ASN:HD22	1:D:45:ARG:H	1.15	0.95
1:B:44:ASN:HD22	1:B:45:ARG:N	1.65	0.94
1:A:192:MET:HE2	1:A:238:TYR:CD1	2.02	0.94
1:D:866:MET:HE2	1:D:871:TYR:HA	1.47	0.94
1:C:1085:ARG:HG2	1:C:1085:ARG:NH1	1.72	0.94
1:D:143:LEU:H	1:D:143:LEU:CD1	1.81	0.94
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.03	0.93
1:B:44:ASN:ND2	1:B:45:ARG:H	1.65	0.93
1:C:396:ALA:HA	1:C:414:GLN:HE22	1.31	0.93
1:C:893:MET:CA	1:C:896:ARG:HD3	1.95	0.93
1:C:895:ARG:HH11	1:C:895:ARG:CG	1.82	0.93
1:C:334:THR:CB	1:C:406:ARG:NH1	2.32	0.92
1:C:175:LYS:CD	1:C:175:LYS:H	1.82	0.92
1:C:192:MET:HE1	5:C:1202:ATP:C6	2.05	0.92
1:C:1024:ARG:HH11	1:C:1024:ARG:CG	1.82	0.92
1:C:334:THR:HB	1:C:406:ARG:HH11	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:GLY:H	1:D:543:GLN:HE21	1.08	0.91
1:C:940:PHE:HB2	1:C:944:VAL:CG1	2.00	0.91
1:B:945:VAL:HG12	1:B:967:ILE:HG23	1.52	0.91
1:B:44:ASN:HD22	1:B:45:ARG:H	0.92	0.91
1:D:166:VAL:HG12	1:D:167:ILE:H	1.34	0.91
1:D:917:MET:SD	1:D:921:MET:HE3	2.11	0.90
1:D:38:LYS:HA	1:D:38:LYS:HE2	1.51	0.90
1:D:494:LEU:HG	1:D:499:LYS:HE2	1.51	0.90
1:C:700:SER:H	1:C:736:HIS:HD2	1.03	0.90
1:A:334:THR:HB	1:A:406:ARG:NH1	1.85	0.90
1:C:1029:ASN:ND2	1:C:1031:SER:HB2	1.87	0.90
1:C:895:ARG:HH11	1:C:895:ARG:HG3	1.35	0.89
1:B:288:ARG:HH11	1:B:288:ARG:CG	1.85	0.89
1:A:44:ASN:HD22	1:A:45:ARG:H	1.19	0.89
1:C:1024:ARG:HG2	1:C:1024:ARG:NH1	1.81	0.89
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.54	0.89
1:A:334:THR:HB	1:A:406:ARG:HH11	1.37	0.88
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.53	0.88
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.03	0.88
1:C:949:LYS:HD3	1:C:951:GLU:OE1	1.73	0.88
1:B:288:ARG:HG3	1:B:288:ARG:NH1	1.82	0.88
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.37	0.88
1:D:501:LEU:HD11	1:D:1080:MET:HE2	1.54	0.87
1:A:334:THR:CB	1:A:406:ARG:NH1	2.38	0.87
1:B:864:HIS:HD2	1:B:866:MET:H	1.18	0.87
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.55	0.86
1:A:334:THR:HG22	1:A:406:ARG:NH1	1.87	0.86
1:A:398:ARG:HH11	1:A:398:ARG:CG	1.88	0.86
1:A:641:MET:HE3	1:A:643:LEU:HD13	1.57	0.85
1:B:259:HIS:HD2	1:B:296:ILE:HD11	1.34	0.85
1:B:338:MET:HE2	1:B:430:SER:HB3	1.57	0.85
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.42	0.85
1:C:44:ASN:ND2	1:C:45:ARG:H	1.75	0.85
1:A:213:LEU:C	1:A:215:ASP:H	1.83	0.84
1:C:1042:MET:HE1	1:C:1060:ILE:CG2	2.06	0.84
1:A:402:GLY:HA2	1:C:408:ASP:OD1	1.77	0.84
1:D:540:GLY:H	1:D:543:GLN:NE2	1.74	0.84
1:A:863:GLN:O	1:A:895:ARG:HD2	1.77	0.84
1:D:250:ILE:HD11	1:D:260:LEU:HD11	1.59	0.84
1:B:606:MET:CE	1:B:607:TRP:HB2	2.07	0.84
1:B:798:VAL:HG12	1:B:831:MET:CE	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:SER:H	1:C:736:HIS:CD2	1.94	0.84
1:D:811:ASN:H	1:D:811:ASN:HD22	1.23	0.84
1:B:543:GLN:O	1:B:547:GLU:HG2	1.77	0.83
1:B:999:GLN:HG2	1:B:1000:GLY:H	1.43	0.83
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.61	0.82
1:D:1053:ASP:HB2	1:D:1056:LYS:CD	2.08	0.82
1:B:338:MET:HE1	1:B:430:SER:HB3	1.60	0.82
1:C:198:GLY:HA3	1:C:228:PHE:HE2	1.43	0.82
1:B:539:SER:HA	1:B:543:GLN:HE21	1.42	0.82
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.42	0.82
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.42	0.82
1:C:87:GLY:HA3	1:C:90:LEU:HD22	1.60	0.82
1:C:840:THR:O	1:C:843:THR:HB	1.80	0.81
1:C:890:VAL:O	1:C:891:LYS:HG3	1.79	0.81
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.10	0.81
1:D:1053:ASP:HB2	1:D:1056:LYS:HD2	1.60	0.81
1:A:98:ASN:C	1:A:98:ASN:HD22	1.88	0.81
1:C:152:LYS:H	1:C:196:THR:CG2	1.94	0.81
1:C:334:THR:HG22	1:C:406:ARG:HH12	1.46	0.81
1:C:940:PHE:CB	1:C:944:VAL:CG1	2.56	0.81
1:C:979:GLY:O	1:C:981:TYR:N	2.12	0.81
1:A:620:LYS:HG2	4:A:1203:BTI:H63	1.62	0.81
1:B:338:MET:HE3	1:B:373:ALA:HB1	1.61	0.81
1:B:1066:SER:HB2	1:D:1064:THR:HG21	1.63	0.81
1:B:606:MET:HE1	1:B:607:TRP:HB2	1.63	0.81
1:C:334:THR:CG2	1:C:406:ARG:HH12	1.94	0.81
1:D:143:LEU:H	1:D:143:LEU:HD12	1.46	0.81
1:D:607:TRP:HE3	1:D:641:MET:HE3	1.44	0.81
1:C:39:LYS:HG3	1:C:62:SER:HB2	1.62	0.80
1:C:198:GLY:HA3	1:C:228:PHE:CE2	2.17	0.80
1:A:290:ARG:NH2	1:A:318:ASP:O	2.13	0.80
1:C:892:ASP:O	1:C:896:ARG:HD2	1.82	0.80
1:C:940:PHE:HB3	1:C:941:PRO:CD	2.12	0.80
1:A:77:ARG:HH11	1:A:77:ARG:CG	1.95	0.80
1:D:338:MET:HE1	1:D:430:SER:HB3	1.64	0.80
1:C:44:ASN:HD22	1:C:45:ARG:N	1.77	0.79
1:C:572:ASP:HB3	1:C:807:GLN:NE2	1.97	0.79
1:A:700:SER:H	1:A:736:HIS:HD2	1.30	0.79
1:D:451:ARG:HG3	1:D:451:ARG:NH1	1.96	0.79
1:B:396:ALA:HB3	1:B:453:ARG:HB2	1.65	0.79
1:D:498:THR:HG23	1:D:1085:ARG:HH22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ASN:ND2	1:A:624:TRP:H	1.81	0.79
1:D:504:ILE:HG21	1:D:1042:MET:CE	2.13	0.78
1:A:606:MET:HE2	1:A:639:PHE:CD2	2.17	0.78
1:C:200:GLY:C	1:C:202:LYS:H	1.92	0.78
1:A:641:MET:HE2	1:A:674:PHE:CE1	2.19	0.78
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.17	0.78
1:B:101:ARG:CG	1:B:101:ARG:HH11	1.96	0.78
1:B:306:ASN:OD1	1:B:348:GLN:HG2	1.83	0.78
1:C:238:TYR:HD1	5:C:1202:ATP:C2	2.01	0.78
1:C:1062:LEU:HD12	1:C:1078:TYR:CE2	2.18	0.78
1:D:495:ASP:HB3	1:D:498:THR:HB	1.66	0.78
1:A:176:SER:O	1:A:179:LEU:HB3	1.84	0.78
1:D:243:LYS:HZ3	1:D:243:LYS:HB3	1.47	0.77
1:B:429:LEU:HD22	1:B:450:MET:HE3	1.66	0.77
1:C:921:MET:HA	1:C:926:LEU:HB2	1.67	0.77
1:D:513:PRO:O	1:D:515:ASN:HB2	1.82	0.77
1:C:87:GLY:HA3	1:C:90:LEU:CD2	2.15	0.77
1:A:1018:GLU:OE1	1:A:1018:GLU:HA	1.83	0.77
1:C:167:ILE:HD12	1:C:167:ILE:N	1.99	0.77
1:C:866:MET:HE2	1:C:871:TYR:HD1	1.47	0.77
1:C:183:PHE:CD2	1:C:183:PHE:O	2.38	0.76
1:C:940:PHE:HB2	1:C:944:VAL:HG11	1.65	0.76
1:D:504:ILE:HD13	1:D:1042:MET:HE2	1.65	0.76
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.67	0.76
1:D:357:LEU:HA	1:D:360:ILE:HD12	1.65	0.76
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.66	0.76
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.67	0.76
1:B:864:HIS:CD2	1:B:866:MET:H	2.03	0.76
1:D:259:HIS:H	1:D:364:GLN:HE22	1.32	0.76
1:D:143:LEU:HD12	1:D:143:LEU:N	2.00	0.76
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.67	0.76
1:C:188:GLY:HA3	1:C:237:ARG:HH22	1.51	0.76
1:D:337:GLU:HG2	1:D:342:ILE:O	1.85	0.75
1:A:175:LYS:NZ	1:A:232:GLU:HG3	2.02	0.75
1:A:189:PHE:HB3	1:A:190:PRO:CD	2.16	0.75
1:C:918:ALA:O	1:C:922:VAL:CG2	2.29	0.75
1:D:306:ASN:OD1	1:D:348:GLN:HG2	1.87	0.75
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.67	0.75
1:B:540:GLY:H	1:B:543:GLN:NE2	1.84	0.75
1:C:644:ARG:NH1	1:C:650:GLY:O	2.20	0.75
1:A:1060:ILE:HG12	1:A:1080:MET:HG3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:VAL:HG22	1:B:830:GLY:HA3	1.68	0.75
1:C:893:MET:HE1	1:C:918:ALA:HA	1.69	0.75
1:A:1051:GLU:OE1	1:A:1057:ARG:NH2	2.20	0.75
1:B:443:MET:HG2	1:B:466:MET:HE3	1.68	0.75
1:C:912:LYS:O	1:C:916:ASP:N	2.19	0.75
1:D:298:LEU:O	1:D:302:ILE:HG13	1.87	0.75
1:D:506:ASN:ND2	1:D:510:ASN:HD22	1.85	0.74
1:A:167:ILE:HD11	1:A:323:ILE:HD11	1.69	0.74
1:D:840:THR:O	1:D:843:THR:HB	1.87	0.74
1:C:326:ASN:ND2	1:C:330:GLN:OE1	2.20	0.74
1:C:334:THR:CG2	1:C:406:ARG:NH1	2.49	0.74
1:C:178:GLU:O	1:C:182:GLU:HG3	1.88	0.74
1:C:530:PRO:HB2	1:C:593:LYS:HD3	1.70	0.74
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.68	0.74
1:A:991:ARG:O	1:A:995:GLU:HG3	1.88	0.74
1:B:1052:ILE:HG22	1:B:1052:ILE:O	1.87	0.74
1:C:494:LEU:HB2	1:C:496:ARG:NH1	2.03	0.74
1:A:590:ILE:HG13	1:A:837:TYR:CE2	2.21	0.74
1:D:917:MET:HG2	1:D:944:VAL:HG11	1.69	0.74
1:D:166:VAL:HG12	1:D:167:ILE:N	1.96	0.74
1:D:1047:THR:HG23	1:D:1061:LYS:HB2	1.70	0.73
1:D:278:ALA:HB2	1:D:335:ILE:HG23	1.69	0.73
1:A:620:LYS:HG3	1:A:1023:THR:HG21	1.71	0.73
1:C:238:TYR:CD1	5:C:1202:ATP:C2	2.76	0.73
1:C:910:SER:O	1:C:914:VAL:HG23	1.88	0.73
1:C:275:VAL:HG11	1:C:466:MET:HE1	1.71	0.73
1:B:269:ARG:HG2	1:B:481:ILE:HG21	1.70	0.73
1:B:395:ILE:HG13	1:B:453:ARG:HB3	1.69	0.73
1:A:406:ARG:HH21	1:C:403:ALA:HB2	1.54	0.73
1:A:51:ARG:NH2	1:A:337:GLU:OE1	2.19	0.73
1:A:152:LYS:NZ	1:A:324:GLU:OE2	2.21	0.73
1:D:991:ARG:O	1:D:995:GLU:HG3	1.89	0.73
1:A:338:MET:HE1	1:A:430:SER:HB2	1.70	0.73
1:A:470:LYS:HB2	1:A:480:PHE:CE1	2.24	0.73
1:A:241:ASN:N	1:A:242:PRO:HD3	2.04	0.72
1:D:418:ILE:HD12	1:D:418:ILE:H	1.54	0.72
1:D:456:LYS:HD3	1:D:456:LYS:N	2.04	0.72
1:D:166:VAL:CG1	1:D:167:ILE:H	2.03	0.72
1:A:164:LEU:HD22	1:A:294:ALA:HB1	1.71	0.72
1:A:864:HIS:HD2	1:A:866:MET:H	1.38	0.72
1:A:896:ARG:HD2	1:A:928:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLU:CD	1:D:70:GLU:H	1.96	0.72
1:A:206:ILE:HD11	1:A:238:TYR:CE1	2.24	0.71
1:C:811:ASN:HD22	1:C:811:ASN:N	1.84	0.71
1:B:98:ASN:C	1:B:98:ASN:HD22	1.98	0.71
1:B:279:PRO:HD2	1:B:372:TYR:HD2	1.56	0.71
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.72	0.71
1:B:897:VAL:HG12	1:B:914:VAL:HG13	1.72	0.71
1:C:646:SER:HB2	1:C:685:GLN:HE22	1.53	0.71
1:D:444:VAL:HG23	1:D:466:MET:HB3	1.70	0.71
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.72	0.71
1:B:118:TYR:OH	1:B:331:VAL:HG13	1.90	0.71
1:B:145:HIS:HE1	1:B:302:ILE:O	1.72	0.71
1:B:1046:GLU:HG2	1:B:1047:THR:N	2.04	0.71
1:D:362:MET:HE1	1:D:367:ILE:HD11	1.73	0.71
1:A:606:MET:HE2	1:A:639:PHE:CG	2.26	0.71
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.72	0.71
1:D:864:HIS:HD2	1:D:866:MET:H	1.36	0.71
1:A:217:PHE:CE2	1:A:221:LYS:HE3	2.26	0.71
1:B:142:HIS:H	1:B:145:HIS:HD2	1.38	0.71
1:B:259:HIS:HD2	1:B:296:ILE:CD1	2.02	0.71
1:D:116:PRO:HB2	1:D:122:SER:HA	1.72	0.71
1:D:339:VAL:O	1:D:369:THR:HA	1.90	0.71
1:D:504:ILE:HG21	1:D:1042:MET:HE2	1.70	0.71
1:A:413:PHE:CZ	1:A:416:ALA:CB	2.69	0.70
1:A:44:ASN:HD22	1:A:45:ARG:N	1.87	0.70
1:A:516:VAL:HG12	1:A:516:VAL:O	1.89	0.70
1:C:170:THR:HG22	1:C:171:ASP:N	2.04	0.70
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.88	0.70
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.56	0.70
1:C:175:LYS:H	1:C:175:LYS:HD3	1.53	0.70
1:C:574:HIS:CD2	1:C:582:VAL:HB	2.26	0.70
1:B:861:ILE:HG13	1:B:862:TYR:N	2.06	0.70
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.73	0.70
1:B:1052:ILE:HD11	1:B:1058:LEU:HG	1.74	0.70
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.26	0.70
1:A:644:ARG:HH11	1:A:909:PRO:HD3	1.56	0.70
1:B:577:LEU:HD13	1:B:842:ARG:NH2	2.06	0.70
1:C:437:LYS:H	1:C:437:LYS:HD3	1.57	0.70
1:D:540:GLY:N	1:D:543:GLN:HE21	1.87	0.70
1:B:744:ALA:HB3	1:B:746:LEU:HG	1.74	0.70
1:C:359:GLU:OE2	1:C:359:GLU:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:SER:O	1:C:915:GLY:N	2.18	0.70
1:C:335:ILE:HD11	1:C:373:ALA:O	1.92	0.69
1:A:898:ASN:HD21	1:A:904:ILE:H	1.40	0.69
1:D:263:ARG:CD	1:D:335:ILE:HG21	2.23	0.69
1:D:358:GLU:HG2	1:D:359:GLU:OE2	1.92	0.69
1:D:917:MET:SD	1:D:921:MET:CE	2.79	0.69
1:C:378:ILE:HG13	1:C:450:MET:CE	2.18	0.69
1:B:571:ARG:HH11	1:B:575:GLN:NE2	1.91	0.69
1:C:230:ASN:HD22	1:C:231:SER:N	1.90	0.69
1:C:940:PHE:CB	1:C:941:PRO:HD2	2.19	0.69
1:A:691:GLU:O	1:A:695:GLU:HG3	1.92	0.69
1:B:927:ASP:OD2	1:B:927:ASP:N	2.25	0.69
1:A:499:LYS:HE3	1:A:1025:ASN:O	1.93	0.69
1:B:999:GLN:HG2	1:B:1000:GLY:N	2.07	0.69
1:D:622:ASN:C	1:D:622:ASN:HD22	1.98	0.69
1:C:167:ILE:H	1:C:167:ILE:CD1	2.04	0.68
1:B:375:GLN:NE2	1:B:428:LYS:HD3	2.07	0.68
1:D:874:LEU:O	1:D:887:PHE:HE1	1.76	0.68
1:A:622:ASN:HD22	1:A:623:PRO:HD2	1.58	0.68
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.29	0.68
1:A:167:ILE:CD1	1:A:323:ILE:HD11	2.24	0.68
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.27	0.68
1:A:216:ALA:C	1:A:218:HIS:H	2.01	0.68
1:B:414:GLN:HG3	1:D:1084:ALA:HB2	1.74	0.68
1:C:69:ASN:O	1:C:72:LYS:HG3	1.93	0.68
1:C:156:ARG:NH2	1:C:170:THR:O	2.26	0.68
1:C:893:MET:O	1:C:897:VAL:N	2.22	0.68
1:C:396:ALA:CB	1:C:453:ARG:HG3	2.15	0.68
1:C:943:SER:OG	1:C:944:VAL:N	2.26	0.68
1:C:156:ARG:HG2	1:C:166:VAL:HG11	1.76	0.67
1:D:960:ASN:HD22	1:D:963:LEU:HB2	1.59	0.67
1:B:347:THR:HG23	1:B:360:ILE:HD13	1.77	0.67
1:D:263:ARG:HD3	1:D:335:ILE:CG2	2.24	0.67
1:A:840:THR:O	1:A:843:THR:HB	1.94	0.67
1:C:200:GLY:O	1:C:202:LYS:N	2.26	0.67
1:A:194:LYS:NZ	1:A:236:GLU:OE1	2.24	0.67
1:A:513:PRO:O	1:A:515:ASN:HB2	1.93	0.67
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.59	0.67
1:C:926:LEU:CD1	1:C:938:LEU:HD11	2.25	0.67
1:D:565:LEU:C	1:D:565:LEU:HD12	2.19	0.67
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:H	1:C:196:THR:HG23	1.58	0.67
1:D:543:GLN:HE22	1:D:636:ASN:HA	1.59	0.67
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.93	0.67
1:A:879:LYS:C	1:A:881:LEU:H	2.03	0.67
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.75	0.67
1:D:362:MET:CE	1:D:367:ILE:HD11	2.24	0.67
1:D:498:THR:HG23	1:D:1085:ARG:NH2	2.09	0.66
1:D:717(A):ILE:HG13	1:D:957:ASN:OD1	1.95	0.66
1:C:328:ARG:HG3	1:C:329:VAL:O	1.96	0.66
1:C:978:PRO:HA	1:C:981:TYR:CZ	2.30	0.66
1:D:338:MET:CE	1:D:430:SER:HB3	2.25	0.66
1:D:828:ILE:O	1:D:832:GLU:HG2	1.96	0.66
1:A:952:ILE:CG2	1:A:952:ILE:O	2.43	0.66
1:C:940:PHE:HB3	1:C:944:VAL:HG11	1.76	0.66
1:B:413:PHE:HD1	1:B:414:GLN:HB3	1.60	0.66
1:C:261:PHE:HE1	1:C:367:ILE:HG22	1.61	0.66
1:C:940:PHE:CG	1:C:944:VAL:HG11	2.30	0.66
1:D:263:ARG:NH1	1:D:336:THR:OG1	2.28	0.66
1:C:385:ASN:O	1:C:387:PHE:N	2.28	0.66
1:D:756:ILE:HD12	1:D:786:ALA:HB1	1.77	0.66
1:B:268:GLN:HB3	1:B:272:GLN:O	1.95	0.66
1:B:796:THR:HB	1:B:810:ALA:HB2	1.78	0.66
1:C:641:MET:HE3	1:C:674:PHE:CD1	2.32	0.65
1:C:192:MET:CE	5:C:1202:ATP:C6	2.79	0.65
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.27	0.65
1:D:44:ASN:ND2	1:D:45:ARG:H	1.92	0.65
1:D:647:ASN:HD22	1:D:647:ASN:C	2.03	0.65
1:C:646:SER:HB2	1:C:685:GLN:NE2	2.11	0.65
1:D:258:VAL:HG21	1:D:362:MET:HE2	1.79	0.65
1:C:39:LYS:HG3	1:C:62:SER:CB	2.27	0.65
1:C:398:ARG:HG3	1:C:398:ARG:HH11	1.62	0.65
1:A:206:ILE:CG2	1:A:207:VAL:N	2.60	0.65
1:B:99:ILE:H	1:B:99:ILE:HD12	1.62	0.65
1:D:299:MET:HE2	1:D:310:VAL:HG22	1.78	0.65
1:B:380:THR:HG22	1:B:426:LEU:HD11	1.78	0.65
1:C:396:ALA:HB3	1:C:453:ARG:CG	2.17	0.65
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.61	0.65
1:C:811:ASN:H	1:C:811:ASN:ND2	1.89	0.65
1:A:207:VAL:HA	1:A:212:GLU:OE2	1.96	0.65
1:A:1042:MET:HE2	1:A:1048:VAL:CG1	2.26	0.65
1:B:927:ASP:HB2	1:B:929:GLN:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ARG:HG2	1:D:445:ARG:O	1.97	0.65
1:D:826:THR:HG21	1:D:831:MET:HE1	1.78	0.65
1:A:70:GLU:HG3	1:A:92:PRO:HB3	1.80	0.64
1:B:268:GLN:CB	1:B:272:GLN:O	2.45	0.64
1:C:175:LYS:CD	1:C:175:LYS:N	2.57	0.64
1:C:700:SER:N	1:C:736:HIS:HD2	1.87	0.64
1:D:1087:ILE:HG22	1:D:1089:ILE:HD12	1.80	0.64
1:C:173:PRO:O	1:C:174:ILE:HD12	1.97	0.64
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.32	0.64
1:A:811:ASN:HD22	1:A:811:ASN:H	1.45	0.64
1:B:548:VAL:HG23	1:B:552:GLY:HA3	1.79	0.64
1:B:1066:SER:CB	1:D:1064:THR:HG21	2.27	0.64
1:C:103:ILE:HG21	1:C:134:GLU:HG3	1.79	0.64
1:C:979:GLY:C	1:C:981:TYR:H	2.05	0.64
1:D:622:ASN:ND2	1:D:624:TRP:H	1.95	0.64
1:D:715:ARG:NH1	1:D:865:GLU:OE2	2.31	0.64
1:A:470:LYS:HB2	1:A:480:PHE:HE1	1.63	0.64
1:B:892:ASP:O	1:B:896:ARG:HG3	1.98	0.64
1:C:183:PHE:O	1:C:183:PHE:HD2	1.76	0.64
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.28	0.64
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.77	0.64
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.78	0.64
1:A:542:LYS:HE2	1:A:672:ASP:OD2	1.96	0.64
1:A:613:ASP:HB2	1:A:1013:TYR:CZ	2.32	0.64
1:B:435:SER:HB3	1:B:438:GLN:HE21	1.63	0.64
1:D:394:ILE:HD11	1:D:426:LEU:HD21	1.79	0.64
1:D:498:THR:CG2	1:D:1085:ARG:HH22	2.09	0.64
1:B:647:ASN:O	1:B:649:VAL:N	2.30	0.64
1:C:41:LEU:HD22	1:C:114:ILE:HG12	1.79	0.64
1:C:170:THR:CG2	1:C:171:ASP:H	2.08	0.64
1:D:685:GLN:OE1	1:D:978:PRO:HD2	1.98	0.64
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.79	0.64
1:D:986:ASP:OD2	1:D:988:GLU:HB2	1.97	0.64
1:A:179:LEU:HA	1:A:182:GLU:OE2	1.96	0.63
1:B:540:GLY:H	1:B:543:GLN:HE21	1.46	0.63
1:C:518:LYS:O	1:C:518:LYS:HG3	1.97	0.63
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.29	0.63
1:A:881:LEU:HD13	1:A:923:GLN:HE22	1.62	0.63
1:D:594:THR:HG23	1:D:598:PHE:HD1	1.64	0.63
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.12	0.63
1:A:334:THR:HG21	1:A:428:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ILE:O	1:A:832:GLU:HG2	1.99	0.63
1:A:1018:GLU:OE1	1:A:1018:GLU:CA	2.46	0.63
1:C:794:ILE:HD12	1:C:796:THR:HG23	1.81	0.63
1:D:622:ASN:HD22	1:D:623:PRO:N	1.97	0.63
1:A:176:SER:O	1:A:179:LEU:HD22	1.98	0.63
1:A:216:ALA:O	1:A:218:HIS:N	2.31	0.63
1:B:952:ILE:HG22	1:B:952:ILE:O	1.98	0.63
1:C:760:LYS:HE3	1:C:790:GLY:O	1.99	0.63
1:D:496:ARG:HB3	1:D:496:ARG:NH1	2.08	0.63
1:D:518:LYS:HG3	1:D:518:LYS:O	1.99	0.63
1:A:362:MET:CE	1:A:367:ILE:HD11	2.29	0.63
1:B:69:ASN:HD22	1:B:72:LYS:HE3	1.64	0.63
1:C:357:LEU:O	1:C:362:MET:HB3	1.99	0.63
1:D:259:HIS:H	1:D:364:GLN:NE2	1.95	0.63
1:A:44:ASN:ND2	1:A:45:ARG:H	1.95	0.62
1:A:781:LEU:HD13	1:D:816:ALA:HB1	1.80	0.62
1:C:504:ILE:HD13	1:C:1042:MET:CE	2.22	0.62
1:A:490:ILE:CD1	1:A:490:ILE:O	2.47	0.62
1:A:583:ARG:HG2	1:A:619:LEU:HD22	1.81	0.62
1:A:622:ASN:HD22	1:A:622:ASN:C	2.06	0.62
1:C:515:ASN:N	1:C:515:ASN:HA	2.00	0.62
1:A:278:ALA:HB3	1:A:335:ILE:HG12	1.80	0.62
1:B:266:SER:O	1:B:478:THR:HA	1.99	0.62
1:C:377:ARG:CG	1:C:377:ARG:NH1	2.43	0.62
1:D:364:GLN:HA	1:D:367:ILE:HD12	1.82	0.62
1:A:775:THR:OG1	1:A:861:ILE:CD1	2.47	0.62
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.07	0.62
1:B:124:ASN:OD1	1:B:124:ASN:C	2.42	0.62
1:B:860:GLU:O	1:B:863:GLN:HG2	1.99	0.62
1:C:273:LYS:HB3	1:C:276:GLU:OE2	2.00	0.62
1:C:359:GLU:H	1:C:359:GLU:CD	2.07	0.62
1:A:700:SER:H	1:A:736:HIS:CD2	2.14	0.62
1:B:539:SER:HA	1:B:543:GLN:NE2	2.12	0.62
1:B:620:LYS:HG3	4:B:1201:BTI:H63	1.81	0.62
1:D:244:HIS:HD2	1:D:265:CYS:HB2	1.63	0.62
1:D:661:LYS:NZ	1:D:1004:GLU:OE2	2.25	0.62
1:B:413:PHE:CE2	1:B:416:ALA:HB2	2.35	0.62
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.47	0.62
1:A:547:GLU:OE2	1:A:547:GLU:HA	2.00	0.62
1:C:867:PRO:HB2	1:C:870:GLN:HB3	1.80	0.62
1:D:986:ASP:OD2	1:D:986:ASP:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.82	0.62
1:B:98:ASN:ND2	1:B:101:ARG:H	1.98	0.62
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.65	0.62
1:B:746:LEU:HD11	1:B:865:GLU:HG2	1.82	0.62
1:C:252:ASP:HB3	1:C:357:LEU:HB2	1.80	0.62
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.82	0.62
1:A:1042:MET:HE2	1:A:1048:VAL:HG11	1.81	0.62
1:B:565:LEU:HD11	1:B:598:PHE:CE2	2.35	0.62
1:A:370:LEU:O	1:A:432:HIS:HE1	1.83	0.61
1:B:320:PHE:N	1:B:320:PHE:CD1	2.67	0.61
1:C:266:SER:O	1:C:478:THR:HA	2.00	0.61
1:A:406:ARG:HE	1:C:403:ALA:HA	1.65	0.61
1:A:935:GLY:CA	1:A:966:VAL:CG1	2.72	0.61
1:D:93:ALA:O	1:D:95:SER:N	2.33	0.61
1:B:712:ASN:OD1	1:B:712:ASN:C	2.43	0.61
1:D:151:ASP:O	1:D:153:VAL:N	2.33	0.61
1:C:519:ARG:HG2	1:C:520:PRO:O	2.00	0.61
1:D:143:LEU:H	1:D:143:LEU:HD13	1.64	0.61
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.82	0.61
1:A:403:ALA:HA	1:C:406:ARG:HH21	1.65	0.61
1:B:700:SER:H	1:B:736:HIS:CD2	2.01	0.61
1:C:675:ARG:HA	1:C:701:GLU:HB3	1.82	0.61
1:A:167:ILE:HB	1:A:236:GLU:OE2	2.01	0.61
1:A:563:VAL:HG21	1:A:787:ILE:HG12	1.81	0.61
1:A:644:ARG:NH1	1:A:909:PRO:HD3	2.16	0.61
1:C:221:LYS:O	1:C:224:ALA:HB3	2.01	0.61
1:D:281:VAL:O	1:D:283:LEU:N	2.33	0.61
1:A:37:ILE:HD12	1:A:353:ALA:HB2	1.82	0.61
1:B:644:ARG:HD3	1:B:909:PRO:HD3	1.81	0.61
1:D:542:LYS:HD3	1:D:542:LYS:C	2.25	0.61
1:D:1070:GLU:HG3	1:D:1071:ASN:N	2.14	0.61
1:A:210:GLU:O	1:A:212:GLU:N	2.28	0.61
1:C:1033:LEU:CD2	1:C:1050:ILE:HD13	2.31	0.61
1:C:243:LYS:HD3	1:C:476:TYR:O	2.01	0.61
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.83	0.61
1:A:999:GLN:HG2	1:A:1000:GLY:H	1.66	0.60
1:A:490:ILE:O	1:A:490:ILE:HD12	2.01	0.60
1:A:999:GLN:HG2	1:A:1000:GLY:N	2.16	0.60
1:D:622:ASN:C	1:D:622:ASN:ND2	2.58	0.60
1:B:338:MET:CE	1:B:430:SER:CB	2.75	0.60
1:B:403:ALA:C	1:B:442:LYS:HE2	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ILE:CG2	1:D:336:THR:N	2.63	0.60
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.34	0.60
1:C:606:MET:HE3	1:C:606:MET:H	1.66	0.60
1:D:335:ILE:HG22	1:D:336:THR:N	2.15	0.60
1:A:605:GLU:HG3	1:A:640:GLN:HG2	1.83	0.60
1:B:337:GLU:HG2	1:B:342:ILE:O	2.01	0.60
1:B:101:ARG:CG	1:B:101:ARG:NH1	2.60	0.60
1:B:934:ASP:O	1:B:938:LEU:HG	2.00	0.60
1:C:141:PRO:HB2	1:C:145:HIS:HB2	1.83	0.60
1:A:622:ASN:HD22	1:A:623:PRO:CD	2.14	0.60
1:D:641:MET:HB3	1:D:671:ILE:HD12	1.83	0.60
1:A:444:VAL:O	1:A:448:ARG:HG3	2.01	0.60
1:B:1046:GLU:HG2	1:B:1047:THR:H	1.64	0.60
1:C:69:ASN:OD1	1:C:69:ASN:N	2.34	0.60
1:D:690:ASN:O	1:D:694:GLN:HG2	2.02	0.60
1:B:243:LYS:HG3	1:B:266:SER:OG	2.02	0.60
1:B:269:ARG:O	1:B:272:GLN:N	2.30	0.60
1:C:238:TYR:CD1	5:C:1202:ATP:H2	2.20	0.60
1:C:556:TRP:O	1:C:560:GLN:HG2	2.01	0.60
1:A:334:THR:HG21	1:A:428:LYS:HZ2	1.66	0.60
1:C:866:MET:CE	1:C:871:TYR:HD1	2.14	0.60
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.15	0.60
1:B:917:MET:O	1:B:921:MET:HG2	2.01	0.59
1:C:186:GLU:N	1:C:186:GLU:OE2	2.35	0.59
1:C:323:ILE:HD11	5:C:1202:ATP:N7	2.17	0.59
1:D:278:ALA:HB2	1:D:335:ILE:CG2	2.32	0.59
1:D:885:GLU:OE2	1:D:885:GLU:HA	2.02	0.59
1:D:960:ASN:HD22	1:D:963:LEU:H	1.49	0.59
1:A:278:ALA:CB	1:A:335:ILE:HG12	2.31	0.59
1:A:509:ILE:HD12	1:A:1089:ILE:HG21	1.84	0.59
1:C:230:ASN:HD22	1:C:230:ASN:C	2.10	0.59
1:C:304:TYR:OH	1:C:307:ALA:O	2.16	0.59
1:A:338:MET:CE	1:A:430:SER:HB2	2.32	0.59
1:A:897:VAL:HG12	1:A:914:VAL:HG13	1.83	0.59
1:B:167:ILE:HG13	1:B:168:PRO:HD3	1.85	0.59
1:B:606:MET:C	1:B:606:MET:HE3	2.28	0.59
1:C:949:LYS:CD	1:C:951:GLU:OE1	2.48	0.59
1:A:503:TYR:OH	1:A:1038:PHE:O	2.20	0.59
1:B:731:GLU:OE1	1:B:765:ASP:N	2.35	0.59
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.85	0.59
1:B:655:PRO:HG3	1:B:982:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:MET:O	1:B:1081:ASN:C	2.45	0.59
1:D:101:ARG:O	1:D:104:ASP:HB2	2.01	0.59
1:D:512:PHE:CZ	4:D:1201:BTI:H5	2.37	0.59
1:A:145:HIS:HE1	1:A:302:ILE:O	1.86	0.59
1:A:382:ASP:OD1	1:A:384:LEU:HD13	2.02	0.59
1:A:434:ILE:HG13	1:C:341:GLY:O	2.02	0.59
1:B:167:ILE:CG1	1:B:168:PRO:HD3	2.31	0.59
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.00	0.59
1:A:720:LEU:HD11	1:A:758:GLU:HG3	1.85	0.59
1:B:343:ASP:CG	1:B:346:LYS:HB2	2.28	0.59
1:C:1068:PRO:HD3	1:C:1074:ARG:NH1	2.18	0.59
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.33	0.59
1:B:1052:ILE:O	1:B:1052:ILE:CG2	2.49	0.59
1:D:243:LYS:HZ3	1:D:243:LYS:CB	2.08	0.59
1:A:622:ASN:HD21	1:A:624:TRP:CD1	2.21	0.59
1:B:955:PRO:HG2	1:B:958:GLY:O	2.02	0.59
1:C:193:ILE:HB	1:C:235:ILE:HB	1.84	0.59
1:A:175:LYS:HZ1	1:A:232:GLU:HG3	1.68	0.59
1:A:179:LEU:H	1:A:179:LEU:CD2	2.02	0.59
1:A:216:ALA:C	1:A:218:HIS:N	2.59	0.59
1:A:362:MET:HE3	1:A:362:MET:CA	2.33	0.59
1:A:377:ARG:HB3	1:A:425:LEU:HD13	1.84	0.59
1:A:1033:LEU:HD23	1:A:1050:ILE:HG12	1.85	0.59
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.84	0.59
1:D:263:ARG:HD3	1:D:335:ILE:HG22	1.85	0.59
1:D:811:ASN:H	1:D:811:ASN:ND2	1.94	0.59
1:B:380:THR:CG2	1:B:426:LEU:HD11	2.33	0.58
1:B:898:ASN:ND2	1:B:906:LYS:HE3	2.17	0.58
1:C:434:ILE:HD12	1:C:435:SER:N	2.18	0.58
1:C:895:ARG:CG	1:C:895:ARG:NH1	2.49	0.58
1:D:920:TYR:OH	1:D:938:LEU:O	2.21	0.58
1:A:506:ASN:OD1	4:A:1203:BTI:H92	2.03	0.58
1:C:886:ARG:HG2	1:C:889:GLU:OE1	2.03	0.58
1:C:936:TYR:O	1:C:937:LYS:CG	2.39	0.58
1:C:941:PRO:C	1:C:943:SER:H	2.11	0.58
1:C:175:LYS:H	1:C:175:LYS:HD2	1.65	0.58
1:C:267:VAL:HG22	1:C:480:PHE:HD2	1.68	0.58
1:D:679:SER:HA	1:D:907:VAL:HG23	1.84	0.58
1:A:77:ARG:CG	1:A:77:ARG:NH1	2.60	0.58
1:C:517:GLU:O	1:C:519:ARG:N	2.36	0.58
1:C:889:GLU:C	1:C:891:LYS:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HG2	1:A:185:GLU:OE2	2.03	0.58
1:B:263:ARG:HD3	1:B:335:ILE:CG2	2.32	0.58
1:B:864:HIS:HD2	1:B:866:MET:N	1.97	0.58
1:D:519:ARG:HB2	1:D:520:PRO:CD	2.34	0.58
1:A:142:HIS:H	1:A:145:HIS:HD2	1.51	0.58
1:A:590:ILE:HD12	1:A:590:ILE:H	1.68	0.58
1:B:279:PRO:HD2	1:B:372:TYR:CD2	2.37	0.58
1:C:385:ASN:C	1:C:387:PHE:H	2.12	0.58
1:C:649:VAL:O	1:C:649:VAL:CG1	2.51	0.58
1:D:249:VAL:HG22	1:D:308:GLY:O	2.03	0.58
1:A:384:LEU:HG	1:A:490:ILE:CD1	2.33	0.58
1:A:606:MET:HE2	1:A:639:PHE:HB3	1.84	0.58
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.68	0.58
1:C:743:MET:CG	1:C:907:VAL:HG13	2.33	0.58
1:A:194:LYS:HE2	2:A:1201:ADP:N7	2.19	0.58
1:A:501:LEU:HD11	1:A:1080:MET:HE2	1.85	0.58
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.34	0.58
1:B:328:ARG:HD3	1:B:329:VAL:O	2.04	0.58
1:B:404:GLY:O	1:B:431:THR:HA	2.04	0.58
1:C:152:LYS:H	1:C:196:THR:HG22	1.69	0.58
1:D:875:SER:OG	1:D:887:PHE:CE1	2.53	0.58
1:D:1034:ASP:OD1	1:D:1036:PRO:HD2	2.03	0.58
1:C:434:ILE:HD12	1:C:435:SER:H	1.69	0.58
1:D:513:PRO:CD	4:D:1201:BTI:H4	2.34	0.58
1:A:572:ASP:HB3	1:A:807:GLN:HE22	1.68	0.57
1:B:588:ILE:HD13	1:B:630:LEU:HD23	1.86	0.57
1:B:597:VAL:CG2	1:B:830:GLY:HA3	2.34	0.57
1:A:180:ALA:O	1:A:183:PHE:N	2.31	0.57
1:A:622:ASN:HD21	1:A:624:TRP:HD1	1.49	0.57
1:C:846:SER:HA	1:C:849:GLU:HG2	1.84	0.57
1:C:1007:ILE:O	1:C:1011:VAL:HG23	2.03	0.57
1:C:1080:MET:HE1	1:C:1085:ARG:NH2	2.19	0.57
1:D:243:LYS:HB3	1:D:243:LYS:NZ	2.06	0.57
1:A:37:ILE:O	1:A:61:ILE:HG12	2.04	0.57
1:B:495:ASP:O	1:B:496:ARG:C	2.47	0.57
1:B:682:TRP:CE3	1:B:685:GLN:HG3	2.39	0.57
1:C:936:TYR:HD1	1:C:966:VAL:HG12	1.69	0.57
1:C:959:PHE:CD1	1:C:959:PHE:N	2.71	0.57
1:D:492:PRO:O	1:D:493:SER:OG	2.16	0.57
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.19	0.57
1:A:501:LEU:HB3	1:A:1078:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:CG2	1:B:1042:MET:HG3	2.34	0.57
1:C:513:PRO:C	1:C:513:PRO:CB	2.74	0.57
1:A:206:ILE:HD11	1:A:238:TYR:CZ	2.39	0.57
1:B:413:PHE:CD1	1:B:414:GLN:HB3	2.39	0.57
1:A:174:ILE:HD11	1:A:235:ILE:CG2	2.35	0.57
1:A:565:LEU:HD21	1:A:826:THR:HB	1.87	0.57
1:A:810:ALA:CB	1:A:831:MET:HE1	2.29	0.57
1:B:334:THR:HG22	1:B:406:ARG:NH2	2.18	0.57
1:B:860:GLU:HA	1:B:863:GLN:HE21	1.69	0.57
1:C:828:ILE:HD12	1:C:829:GLU:N	2.19	0.57
1:D:288:ARG:HG2	1:D:288:ARG:O	2.04	0.57
1:B:525:GLU:HG2	1:B:527:ALA:HB3	1.87	0.57
1:C:357:LEU:HA	1:C:360:ILE:HD12	1.87	0.57
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.69	0.57
1:A:103:ILE:HG21	1:A:134:GLU:HG3	1.87	0.56
1:A:180:ALA:O	1:A:184:ALA:N	2.33	0.56
1:A:406:ARG:HH21	1:C:403:ALA:CB	2.17	0.56
1:C:961:LYS:O	1:C:964:GLN:N	2.38	0.56
1:D:504:ILE:HG21	1:D:1042:MET:HE3	1.83	0.56
1:A:446:SER:O	1:A:450:MET:HG2	2.06	0.56
1:B:59:LEU:O	1:B:60:ASP:HB2	2.06	0.56
1:B:272:GLN:HE21	1:B:274:VAL:HG22	1.71	0.56
1:B:332:GLU:N	1:B:332:GLU:OE1	2.37	0.56
1:B:338:MET:HE1	1:B:430:SER:CB	2.34	0.56
1:B:798:VAL:HG12	1:B:831:MET:HE2	1.86	0.56
1:A:375:GLN:NE2	1:A:428:LYS:HZ3	2.03	0.56
1:B:525:GLU:HB3	1:B:840:THR:HG21	1.87	0.56
1:D:260:LEU:HD22	1:D:342:ILE:HD13	1.88	0.56
1:D:331:VAL:O	1:D:428:LYS:HE2	2.05	0.56
1:A:109:ALA:O	1:A:110:ASN:HB2	2.04	0.56
1:A:860:GLU:OE2	1:A:891:LYS:NZ	2.34	0.56
1:B:396:ALA:HB3	1:B:453:ARG:CB	2.35	0.56
1:A:206:ILE:HG22	1:A:207:VAL:N	2.19	0.56
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.54	0.56
1:C:986:ASP:OD1	1:C:989:LYS:HG3	2.06	0.56
1:A:849:GLU:O	1:A:852:SER:C	2.44	0.56
1:C:756:ILE:O	1:C:760:LYS:HB2	2.06	0.56
1:D:457:THR:OG1	1:D:459:ILE:HG13	2.05	0.56
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.88	0.56
1:D:799:ALA:H	1:D:811:ASN:ND2	2.03	0.56
1:A:631:ARG:NH2	1:A:672:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:ASN:C	1:C:1029:ASN:HD22	2.14	0.56
1:D:330:GLN:O	1:D:333:HIS:ND1	2.30	0.56
1:D:449:GLU:O	1:D:450:MET:C	2.49	0.56
1:A:382:ASP:O	1:A:387:PHE:N	2.38	0.55
1:A:396:ALA:HB3	1:A:453:ARG:HB2	1.88	0.55
1:D:160:ILE:O	1:D:161:LYS:C	2.48	0.55
1:B:414:GLN:HE22	1:D:1079:ALA:HB2	1.70	0.55
1:B:504:ILE:HG21	1:B:1042:MET:HG3	1.87	0.55
1:C:991:ARG:NH1	1:C:1002:VAL:O	2.31	0.55
1:A:98:ASN:C	1:A:98:ASN:ND2	2.56	0.55
1:B:379:THR:HG22	1:B:424:SER:O	2.07	0.55
1:C:173:PRO:C	1:C:174:ILE:HD12	2.32	0.55
1:C:679:SER:HB3	1:C:908:THR:O	2.06	0.55
1:C:794:ILE:HD12	1:C:796:THR:CG2	2.36	0.55
1:D:252:ASP:O	1:D:305:VAL:HG22	2.05	0.55
1:D:875:SER:OG	1:D:887:PHE:CZ	2.58	0.55
1:C:742:ASP:OD2	1:C:745:GLY:HA2	2.07	0.55
1:A:334:THR:HG23	1:A:428:LYS:HZ1	1.72	0.55
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.88	0.55
1:B:251:GLY:HA3	1:B:257:ILE:HG12	1.89	0.55
1:B:513:PRO:O	1:B:515:ASN:HB2	2.06	0.55
1:A:897:VAL:HG11	1:A:917:MET:HB3	1.88	0.55
1:B:101:ARG:NH1	1:B:101:ARG:HG2	2.20	0.55
1:D:425:LEU:C	1:D:425:LEU:HD12	2.31	0.55
1:B:448:ARG:HH22	1:B:467:LYS:HD2	1.72	0.55
1:B:620:LYS:CG	4:B:1201:BTI:H63	2.37	0.55
1:C:396:ALA:CA	1:C:414:GLN:HE22	2.10	0.55
1:C:960:ASN:O	1:C:963:LEU:HB3	2.06	0.55
1:D:334:THR:HG22	1:D:338:MET:HE2	1.88	0.55
1:D:752:ALA:HB2	1:D:782:THR:HG23	1.88	0.55
1:A:1065:ILE:HG12	1:A:1076:ILE:HD13	1.89	0.55
1:B:403:ALA:O	1:B:442:LYS:CE	2.35	0.55
1:B:571:ARG:HH21	1:B:605:GLU:CD	2.15	0.55
1:B:577:LEU:HD13	1:B:842:ARG:HH22	1.71	0.55
1:C:494:LEU:H	1:C:494:LEU:HD22	1.71	0.55
1:D:263:ARG:HG2	1:D:335:ILE:HG21	1.88	0.55
1:B:771:HIS:HB2	1:B:795:ASP:OD2	2.07	0.55
1:B:924:ASN:HB2	1:B:926:LEU:HD21	1.88	0.55
1:C:142:HIS:H	1:C:145:HIS:HD2	1.54	0.55
1:D:263:ARG:HD3	1:D:335:ILE:HG21	1.86	0.55
1:A:991:ARG:HB2	1:A:1007:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LEU:HD22	1:C:323:ILE:HD12	1.88	0.54
1:C:370:LEU:O	1:C:432:HIS:HE1	1.90	0.54
1:C:644:ARG:O	1:C:645:ALA:C	2.50	0.54
1:C:828:ILE:HD12	1:C:829:GLU:H	1.73	0.54
1:A:606:MET:HE2	1:A:639:PHE:CB	2.37	0.54
1:B:263:ARG:HG2	1:B:278:ALA:HB2	1.89	0.54
1:B:385:ASN:CG	1:B:385:ASN:O	2.50	0.54
1:C:798:VAL:O	1:C:799:ALA:C	2.50	0.54
1:D:459:ILE:HB	1:D:460:PRO:HD3	1.88	0.54
1:A:194:LYS:HD2	1:A:234:TYR:OH	2.07	0.54
1:A:572:ASP:HB3	1:A:807:GLN:NE2	2.22	0.54
1:B:334:THR:O	1:B:338:MET:HG3	2.07	0.54
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.89	0.54
1:C:867:PRO:HG3	1:C:906:LYS:O	2.08	0.54
1:D:960:ASN:ND2	1:D:963:LEU:H	2.05	0.54
1:B:263:ARG:HD3	1:B:335:ILE:HG22	1.87	0.54
1:C:37:ILE:HG22	1:C:37:ILE:O	2.06	0.54
1:C:43:ALA:HA	1:C:66:ILE:HD11	1.89	0.54
1:C:539:SER:HA	1:C:543:GLN:HG3	1.89	0.54
1:D:91:GLY:O	1:D:92:PRO:O	2.25	0.54
1:D:357:LEU:HD13	1:D:362:MET:HG3	1.89	0.54
1:A:334:THR:CG2	1:A:428:LYS:NZ	2.71	0.54
1:B:144:GLU:O	1:B:148:MET:HB2	2.08	0.54
1:B:867:PRO:O	1:B:868:GLY:C	2.51	0.54
1:C:770:LEU:HB3	1:C:794:ILE:HG22	1.89	0.54
1:D:124:ASN:OD1	1:D:126:GLN:HB2	2.07	0.54
1:D:262:GLU:OE2	1:D:262:GLU:N	2.33	0.54
1:D:446:SER:O	1:D:450:MET:HG2	2.08	0.54
1:D:607:TRP:CZ3	1:D:641:MET:HE1	2.39	0.54
1:D:864:HIS:CD2	1:D:866:MET:HB2	2.43	0.54
1:A:156:ARG:HB3	1:A:156:ARG:NH1	2.12	0.54
1:A:186:GLU:O	1:A:187:ALA:HB2	2.08	0.54
1:B:252:ASP:OD1	1:B:256:ASN:HB2	2.08	0.54
1:B:312:PHE:HA	1:B:321:PHE:O	2.08	0.54
1:C:174:ILE:HG22	1:C:217:PHE:HE1	1.72	0.54
1:D:570:PHE:O	1:D:574:HIS:HE1	1.91	0.54
1:D:717:ASN:N	1:D:717:ASN:HD22	2.06	0.54
1:A:266:SER:O	1:A:268:GLN:HG2	2.08	0.53
1:A:334:THR:CG2	1:A:428:LYS:HZ1	2.21	0.53
1:D:596:ASP:O	1:D:599:LYS:HG2	2.08	0.53
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:H	1:A:384:LEU:HD12	1.73	0.53
1:A:484:THR:HB	1:A:487:LEU:HD22	1.90	0.53
1:A:512:PHE:CZ	4:A:1203:BTI:H5	2.42	0.53
1:B:624:TRP:CZ2	1:B:1008:ILE:CD1	2.91	0.53
1:B:773:HIS:HA	1:B:806:SER:O	2.09	0.53
1:A:338:MET:HE1	1:A:430:SER:CB	2.38	0.53
1:C:204:MET:HE1	5:C:1202:ATP:O1A	2.07	0.53
1:C:738:LEU:CD2	1:C:759:LEU:HD13	2.39	0.53
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.37	0.53
1:C:959:PHE:H	1:C:959:PHE:HD1	1.53	0.53
1:B:494:LEU:O	1:B:496:ARG:N	2.42	0.53
1:C:513:PRO:C	1:C:513:PRO:HA	2.17	0.53
1:C:968:LEU:O	1:C:969:LYS:C	2.51	0.53
1:A:360:ILE:HG22	1:A:362:MET:H	1.73	0.53
1:C:224:ALA:HB3	1:C:231:SER:HB2	1.91	0.53
1:C:259:HIS:O	1:C:260:LEU:HD23	2.08	0.53
1:D:661:LYS:HG2	1:D:1008:ILE:HD13	1.91	0.53
1:A:406:ARG:NH2	1:C:403:ALA:HB2	2.23	0.53
1:A:775:THR:OG1	1:A:861:ILE:HD13	2.07	0.53
1:C:145:HIS:HA	1:C:148:MET:HG2	1.91	0.53
1:A:701:GLU:HG3	1:A:737:ILE:HB	1.89	0.53
1:B:679:SER:O	1:B:905:VAL:HB	2.08	0.53
1:A:217:PHE:HE2	1:A:221:LYS:HE3	1.71	0.53
1:A:398:ARG:CG	1:A:398:ARG:NH1	2.59	0.53
1:A:874:LEU:HD11	1:A:919:LEU:CD2	2.39	0.53
1:B:89:ASP:OD1	1:B:90:LEU:HD12	2.09	0.53
1:C:551:LYS:O	1:C:555:GLU:HG2	2.08	0.53
1:D:145:HIS:HE1	1:D:302:ILE:O	1.92	0.53
1:A:413:PHE:HZ	1:A:416:ALA:HB2	1.61	0.53
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.73	0.53
1:B:924:ASN:HB2	1:B:926:LEU:CD2	2.39	0.53
1:C:192:MET:HB2	1:C:238:TYR:HB2	1.91	0.53
1:C:382:ASP:O	1:C:387:PHE:HA	2.08	0.53
1:A:194:LYS:HB3	1:A:234:TYR:CE2	2.44	0.53
1:A:543:GLN:H	1:A:543:GLN:NE2	2.06	0.53
1:B:840:THR:O	1:B:843:THR:HB	2.09	0.53
1:B:945:VAL:HG12	1:B:967:ILE:CG2	2.32	0.53
1:C:59:LEU:O	1:C:60:ASP:HB2	2.07	0.53
1:B:749:PRO:HG3	1:B:781:LEU:HB3	1.90	0.52
1:C:166:VAL:HG12	1:C:167:ILE:HD12	1.90	0.52
1:C:717:ASN:HD22	1:C:717(A):ILE:HG13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:GLU:HG3	1:D:324:GLU:HG3	1.91	0.52
1:D:496:ARG:HH11	1:D:496:ARG:CB	2.12	0.52
1:D:506:ASN:HD21	1:D:510:ASN:HD22	1.56	0.52
1:D:513:PRO:O	1:D:515:ASN:CB	2.55	0.52
1:D:760:LYS:HG2	1:D:768:ILE:HD13	1.91	0.52
1:D:814:TYR:C	1:D:814:TYR:CD2	2.87	0.52
1:A:192:MET:HE2	1:A:238:TYR:CE1	2.45	0.52
1:B:167:ILE:CG1	1:B:168:PRO:CD	2.87	0.52
1:C:175:LYS:O	1:C:176:SER:C	2.49	0.52
1:D:519:ARG:HB2	1:D:520:PRO:HD2	1.91	0.52
1:A:625:GLU:O	1:A:629:ARG:HG3	2.09	0.52
1:A:879:LYS:O	1:A:881:LEU:N	2.42	0.52
1:C:259:HIS:C	1:C:260:LEU:HD23	2.34	0.52
1:C:519:ARG:CG	1:C:520:PRO:O	2.57	0.52
1:D:284:SER:OG	1:D:287:LEU:HB2	2.09	0.52
1:D:451:ARG:HH11	1:D:451:ARG:CG	2.08	0.52
1:B:863:GLN:O	1:B:895:ARG:HG3	2.09	0.52
1:C:646:SER:O	1:C:653:ASN:HA	2.09	0.52
1:D:166:VAL:CG1	1:D:167:ILE:N	2.64	0.52
1:D:878:ALA:O	1:D:883:LEU:HB2	2.09	0.52
1:A:241:ASN:N	1:A:242:PRO:CD	2.72	0.52
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.23	0.52
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.44	0.52
1:C:394:ILE:HD11	1:C:426:LEU:HD22	1.92	0.52
1:D:571:ARG:HG2	1:D:611:THR:HG21	1.90	0.52
1:D:1043:ARG:O	1:D:1046:GLU:HB2	2.10	0.52
1:A:192:MET:CE	1:A:238:TYR:CD1	2.85	0.52
1:B:606:MET:HE3	1:B:607:TRP:N	2.24	0.52
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.74	0.52
1:D:494:LEU:HG	1:D:499:LYS:CE	2.32	0.52
1:D:594:THR:HG23	1:D:598:PHE:CD1	2.44	0.52
1:D:921:MET:HG2	1:D:926:LEU:HB3	1.91	0.52
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.91	0.52
1:A:804:LEU:HD13	1:A:854:ILE:HG22	1.92	0.52
1:A:828:ILE:HD12	1:A:829:GLU:H	1.75	0.52
1:A:952:ILE:O	1:A:952:ILE:HG22	2.10	0.52
1:B:540:GLY:N	1:B:543:GLN:HE21	2.08	0.52
1:B:624:TRP:HZ2	1:B:1008:ILE:HD13	1.74	0.52
1:B:743:MET:SD	1:B:907:VAL:HG13	2.49	0.52
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.91	0.52
1:A:114:ILE:HG13	1:A:136:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PRO:HG2	1:A:985:VAL:HG23	1.92	0.52
1:B:644:ARG:HD2	1:B:647:ASN:OD1	2.09	0.52
1:C:1068:PRO:HD3	1:C:1074:ARG:CZ	2.40	0.52
1:D:401:GLY:O	1:D:445:ARG:NH2	2.39	0.52
1:D:497:GLY:O	1:D:501:LEU:HG	2.10	0.52
1:A:622:ASN:ND2	1:A:623:PRO:HD2	2.24	0.52
1:B:104:ASP:O	1:B:105:VAL:C	2.53	0.52
1:C:641:MET:CE	1:C:674:PHE:CE1	2.93	0.52
1:D:593:LYS:O	1:D:597:VAL:HG23	2.09	0.52
1:A:47:GLU:OE1	1:A:428:LYS:HE3	2.10	0.52
1:B:927:ASP:OD2	1:B:930:SER:HB2	2.10	0.52
1:C:59:LEU:HD11	1:C:346:LYS:HG2	1.91	0.52
1:C:641:MET:HE3	1:C:674:PHE:CE1	2.45	0.52
1:C:885:GLU:C	1:C:887:PHE:H	2.18	0.52
1:D:431:THR:OG1	1:D:443:MET:HB2	2.10	0.52
1:A:516:VAL:O	1:A:517:GLU:C	2.51	0.51
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.75	0.51
1:B:641:MET:HB3	1:B:671:ILE:HD12	1.92	0.51
1:C:41:LEU:C	1:C:41:LEU:HD23	2.34	0.51
1:C:375:GLN:OE1	1:C:377:ARG:HD2	2.10	0.51
1:C:926:LEU:HD11	1:C:938:LEU:HD11	1.92	0.51
1:A:360:ILE:CG2	1:A:362:MET:HG2	2.40	0.51
1:A:964:GLN:HG2	1:A:968:LEU:HD11	1.93	0.51
1:D:313:LEU:O	1:D:320:PHE:HA	2.09	0.51
1:D:1060:ILE:HG12	1:D:1080:MET:HG3	1.91	0.51
1:B:86:VAL:HG11	1:B:95:SER:O	2.10	0.51
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.93	0.51
1:A:331:VAL:HG12	1:A:428:LYS:HE2	1.92	0.51
1:B:574:HIS:CD2	1:B:580:THR:HA	2.45	0.51
1:C:542:LYS:HD3	1:C:542:LYS:C	2.35	0.51
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.45	0.51
1:D:263:ARG:CG	1:D:335:ILE:HG21	2.40	0.51
1:D:513:PRO:HD2	4:D:1201:BTI:H4	1.91	0.51
1:D:542:LYS:HE3	1:D:672:ASP:OD1	2.11	0.51
1:A:118:TYR:OH	1:A:331:VAL:HG13	2.10	0.51
1:D:495:ASP:HB3	1:D:498:THR:CB	2.37	0.51
1:D:605:GLU:HA	1:D:640:GLN:HB3	1.91	0.51
1:D:832:GLU:O	1:D:836:HIS:CD2	2.64	0.51
1:A:210:GLU:C	1:A:212:GLU:H	2.18	0.51
1:A:778:ASN:O	1:A:779:GLY:C	2.52	0.51
1:C:404:GLY:O	1:C:431:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:LEU:HD13	1:C:938:LEU:HD11	1.90	0.51
1:C:948:PHE:CD2	1:C:959:PHE:CD2	2.98	0.51
1:D:149:PHE:HZ	1:D:302:ILE:HD13	1.76	0.51
1:A:39:LYS:HE2	1:A:82:GLU:OE1	2.11	0.51
1:A:222:SER:O	1:A:226:LYS:HB2	2.10	0.51
1:A:334:THR:CB	1:A:406:ARG:HH11	2.08	0.51
1:A:384:LEU:HG	1:A:490:ILE:HD11	1.92	0.51
1:A:521:LYS:NZ	1:A:1046:GLU:OE1	2.43	0.51
1:A:524:TYR:HD2	1:A:843:THR:HG22	1.76	0.51
1:A:556:TRP:O	1:A:560:GLN:HG2	2.11	0.51
1:C:199:GLY:HA2	5:C:1202:ATP:O3B	2.10	0.51
1:D:811:ASN:ND2	1:D:811:ASN:N	2.56	0.51
1:A:497:GLY:O	1:A:501:LEU:HG	2.11	0.51
1:A:641:MET:CE	1:A:643:LEU:HD13	2.37	0.51
1:A:794:ILE:CD1	1:A:813:LEU:CD2	2.89	0.51
1:B:798:VAL:CG1	1:B:831:MET:CE	2.86	0.51
1:C:920:TYR:CE1	1:C:940:PHE:CD2	2.99	0.51
1:C:1024:ARG:CG	1:C:1024:ARG:NH1	2.53	0.51
1:D:418:ILE:HD12	1:D:418:ILE:N	2.23	0.51
1:C:334:THR:CB	1:C:406:ARG:HH12	2.13	0.51
1:D:1056:LYS:HG2	1:D:1056:LYS:O	2.11	0.51
1:B:395:ILE:N	1:B:453:ARG:O	2.34	0.51
1:C:864:HIS:HD2	1:C:866:MET:H	1.57	0.51
1:C:921:MET:CA	1:C:926:LEU:HB2	2.40	0.51
1:C:989:LYS:O	1:C:993:LEU:HB2	2.10	0.51
1:A:874:LEU:CD1	1:A:919:LEU:HD21	2.41	0.50
1:B:124:ASN:OD1	1:B:127:PHE:N	2.30	0.50
1:B:266:SER:HA	1:B:478:THR:HG22	1.93	0.50
1:B:512:PHE:HB3	1:B:516:VAL:HB	1.92	0.50
1:B:917:MET:HG2	1:B:944:VAL:HG11	1.93	0.50
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.40	0.50
1:A:775:THR:OG1	1:A:861:ILE:HD11	2.10	0.50
1:A:811:ASN:H	1:A:811:ASN:ND2	2.04	0.50
1:A:874:LEU:HD11	1:A:919:LEU:HD22	1.94	0.50
1:B:365:LYS:HZ3	1:B:365:LYS:HB2	1.75	0.50
1:B:893:MET:HG2	1:B:921:MET:HB2	1.92	0.50
1:C:193:ILE:HG12	1:C:194:LYS:N	2.25	0.50
1:C:334:THR:CB	1:C:406:ARG:HH11	2.09	0.50
1:C:647:ASN:OD1	1:C:647:ASN:N	2.44	0.50
1:A:277:VAL:C	1:A:335:ILE:HD11	2.36	0.50
1:B:811:ASN:H	1:B:811:ASN:HD22	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:CYS:SG	1:C:462:LEU:HD13	2.51	0.50
1:D:40:LEU:C	1:D:40:LEU:HD23	2.36	0.50
1:A:879:LYS:C	1:A:881:LEU:N	2.68	0.50
1:C:813:LEU:O	1:C:814:TYR:C	2.53	0.50
1:C:1036:PRO:O	1:C:1040:PHE:HB2	2.10	0.50
1:D:679:SER:HA	1:D:907:VAL:CG2	2.42	0.50
1:D:740:ILE:N	1:D:740:ILE:HD13	2.27	0.50
1:B:165:PRO:O	1:B:166:VAL:HG13	2.11	0.50
1:B:565:LEU:C	1:B:565:LEU:HD12	2.36	0.50
1:C:1062:LEU:CD1	1:C:1078:TYR:CE2	2.92	0.50
1:B:374:ILE:HG22	1:B:443:MET:CE	2.41	0.50
1:D:512:PHE:C	1:D:512:PHE:CD2	2.90	0.50
1:B:285:PRO:O	1:B:288:ARG:HG2	2.11	0.50
1:B:565:LEU:HD11	1:B:598:PHE:HE2	1.76	0.50
1:C:337:GLU:OE2	1:C:406:ARG:NH2	2.45	0.50
1:D:542:LYS:HD3	1:D:542:LYS:O	2.11	0.50
1:A:406:ARG:HH21	1:C:403:ALA:CA	2.24	0.50
1:A:799:ALA:H	1:A:811:ASN:ND2	2.08	0.50
1:B:332:GLU:HA	1:B:375:GLN:NE2	2.27	0.50
1:B:647:ASN:HB3	1:B:652:LYS:O	2.12	0.50
1:C:189:PHE:H	1:C:190:PRO:CD	2.24	0.50
1:C:385:ASN:C	1:C:387:PHE:N	2.69	0.50
1:C:709:ASP:H	1:C:715:ARG:HG2	1.77	0.50
1:C:1063:GLU:O	1:C:1064:THR:HG23	2.12	0.50
1:D:62:SER:HA	1:D:81:ASP:OD1	2.12	0.50
1:D:122:SER:HB2	1:D:328:ARG:HG2	1.94	0.50
1:D:362:MET:HE1	1:D:367:ILE:CD1	2.41	0.50
1:A:866:MET:HG2	1:A:894:TYR:CE2	2.47	0.50
1:B:395:ILE:HD11	1:B:453:ARG:HG2	1.93	0.50
1:B:832:GLU:OE2	1:C:859:THR:OG1	2.28	0.50
1:C:396:ALA:HA	1:C:414:GLN:NE2	2.13	0.50
1:C:398:ARG:HG3	1:C:398:ARG:NH1	2.25	0.50
1:C:861:ILE:HD11	1:C:866:MET:O	2.12	0.50
1:A:334:THR:OG1	1:A:375:GLN:NE2	2.44	0.49
1:B:294:ALA:O	1:B:297:GLN:HB3	2.11	0.49
1:B:347:THR:O	1:B:348:GLN:C	2.52	0.49
1:C:866:MET:HE3	1:C:870:GLN:HG2	1.94	0.49
1:D:746:LEU:HD11	1:D:865:GLU:HG2	1.93	0.49
1:A:42:VAL:HG23	1:A:53:PHE:HE2	1.77	0.49
1:A:459:ILE:O	1:A:460:PRO:C	2.54	0.49
1:C:219:ARG:O	1:C:223:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:MET:HE3	1:C:640:GLN:O	2.12	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:B:748:LYS:O	1:B:749:PRO:C	2.55	0.49
1:C:897:VAL:O	1:C:898:ASN:C	2.55	0.49
1:D:164:LEU:HG	1:D:165:PRO:HD2	1.95	0.49
1:D:167:ILE:HG23	1:D:321:PHE:CG	2.48	0.49
1:D:1053:ASP:HB2	1:D:1056:LYS:HD3	1.94	0.49
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.94	0.49
1:C:891:LYS:HA	1:C:894:TYR:HB2	1.94	0.49
1:D:479:LYS:O	1:D:480:PHE:C	2.55	0.49
1:D:561:ASP:O	1:D:822:ARG:HD2	2.12	0.49
1:A:179:LEU:HA	1:A:182:GLU:CD	2.37	0.49
1:A:229:GLY:O	1:A:230:ASN:HB2	2.12	0.49
1:A:375:GLN:NE2	1:A:428:LYS:NZ	2.61	0.49
1:A:512:PHE:C	1:A:512:PHE:CD2	2.90	0.49
1:B:103:ILE:HG21	1:B:134:GLU:HG3	1.95	0.49
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.46	0.49
1:B:571:ARG:C	1:B:571:ARG:HD2	2.38	0.49
1:C:234:TYR:C	1:C:235:ILE:HG22	2.37	0.49
1:D:90:LEU:HB2	1:D:95:SER:OG	2.13	0.49
1:D:944:VAL:O	1:D:945:VAL:C	2.54	0.49
1:A:206:ILE:CD1	1:A:238:TYR:CE1	2.96	0.49
1:A:955:PRO:O	1:A:956:VAL:C	2.56	0.49
1:C:386:ASP:O	1:C:387:PHE:HB2	2.11	0.49
1:C:399:SER:HB3	1:C:400:SER:H	1.47	0.49
1:C:887:PHE:HA	1:C:890:VAL:HG23	1.95	0.49
1:B:1066:SER:HB2	1:D:1064:THR:CG2	2.39	0.49
1:A:69:ASN:HD22	1:A:72:LYS:HE3	1.77	0.49
1:A:239:ILE:O	1:A:239:ILE:HG13	2.13	0.49
1:A:375:GLN:HE22	1:A:428:LYS:NZ	2.11	0.49
1:A:454:GLY:O	1:A:455:VAL:HG22	2.12	0.49
1:B:98:ASN:C	1:B:98:ASN:ND2	2.70	0.49
1:B:581:ARG:HG3	1:B:848:PHE:CD2	2.48	0.49
1:A:69:ASN:ND2	1:A:72:LYS:HE3	2.27	0.49
1:A:184:ALA:HA	1:A:191:LEU:HD11	1.94	0.49
1:A:413:PHE:O	1:A:414:GLN:C	2.56	0.49
1:B:949:LYS:HB2	1:B:951:GLU:HG3	1.94	0.49
1:B:991:ARG:NH1	1:B:1002:VAL:HG12	2.28	0.49
1:C:69:ASN:HD21	1:C:88:SER:HA	1.77	0.49
1:C:680:LEU:HD11	1:C:952:ILE:HG22	1.94	0.49
1:C:687:LYS:O	1:C:691:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:ASN:HD22	1:C:717:ASN:C	2.20	0.49
1:C:960:ASN:O	1:C:961:LYS:C	2.56	0.49
1:A:627:LEU:O	1:A:631:ARG:HB2	2.13	0.48
1:B:999:GLN:NE2	1:B:1001:PRO:HG3	2.28	0.48
1:C:641:MET:HE3	1:C:674:PHE:HD1	1.76	0.48
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.46	0.48
1:C:944:VAL:HG13	1:C:945:VAL:HG13	1.95	0.48
1:C:1029:ASN:ND2	1:C:1029:ASN:C	2.70	0.48
1:D:403:ALA:O	1:D:442:LYS:HD3	2.13	0.48
1:D:581:ARG:HG3	1:D:848:PHE:CG	2.47	0.48
1:A:43:ALA:HA	1:A:66:ILE:HD11	1.95	0.48
1:B:556:TRP:O	1:B:557:VAL:C	2.56	0.48
1:C:704:ILE:HB	1:C:740:ILE:HD13	1.95	0.48
1:B:606:MET:HE3	1:B:606:MET:H	1.79	0.48
1:B:948:PHE:HA	1:B:959:PHE:CE2	2.48	0.48
1:C:174:ILE:HG22	1:C:217:PHE:CE1	2.48	0.48
1:C:494:LEU:HB2	1:C:496:ARG:HH12	1.76	0.48
1:C:1060:ILE:HG12	1:C:1080:MET:HG3	1.95	0.48
1:D:283:LEU:C	1:D:283:LEU:HD23	2.39	0.48
1:D:286:THR:O	1:D:290:ARG:HG3	2.14	0.48
1:D:700:SER:H	1:D:736:HIS:HD2	1.62	0.48
1:B:103:ILE:O	1:B:107:LYS:HG3	2.14	0.48
1:C:895:ARG:NH1	1:C:895:ARG:HG2	2.25	0.48
1:C:948:PHE:CD2	1:C:959:PHE:HD2	2.31	0.48
1:D:413:PHE:O	1:D:415:GLY:N	2.46	0.48
1:A:799:ALA:H	1:A:811:ASN:HD21	1.60	0.48
1:A:873:ASN:C	1:A:875:SER:H	2.21	0.48
1:B:542:LYS:HE2	1:B:672:ASP:OD2	2.14	0.48
1:B:542:LYS:HE3	1:B:631:ARG:NH2	2.28	0.48
1:C:284:SER:OG	1:C:287:LEU:HB2	2.13	0.48
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.96	0.48
1:A:170:THR:HG22	1:A:172:GLY:O	2.13	0.48
1:A:177:TYR:C	1:A:179:LEU:N	2.69	0.48
1:A:332:GLU:O	1:A:332:GLU:HG2	2.13	0.48
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.94	0.48
1:B:690:ASN:ND2	1:B:700:SER:OG	2.47	0.48
1:B:711:LEU:HD11	1:B:750:LYS:HB3	1.95	0.48
1:D:38:LYS:HA	1:D:38:LYS:CE	2.34	0.48
1:A:196:THR:HG22	1:A:232:GLU:O	2.14	0.48
1:B:374:ILE:HG22	1:B:443:MET:HE3	1.95	0.48
1:C:1075:THR:HG22	1:C:1077:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LYS:HE2	1:D:38:LYS:CA	2.33	0.48
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.96	0.48
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.12	0.48
1:B:268:GLN:HA	1:B:274:VAL:HG23	1.95	0.48
1:C:253:GLU:HG2	1:C:305:VAL:HG11	1.95	0.48
1:C:281:VAL:HG12	1:C:282:GLY:N	2.29	0.48
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.95	0.48
1:C:883:LEU:HD11	1:C:923:GLN:HG2	1.96	0.48
1:D:644:ARG:NH2	1:D:908:THR:HB	2.29	0.48
1:C:811:ASN:N	1:C:811:ASN:ND2	2.51	0.48
1:C:1062:LEU:HD12	1:C:1078:TYR:CD2	2.48	0.48
1:D:70:GLU:CD	1:D:70:GLU:N	2.69	0.48
1:D:431:THR:HG21	1:D:443:MET:HA	1.94	0.48
1:D:804:LEU:HD13	1:D:854:ILE:HG22	1.96	0.48
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.95	0.47
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.47	0.47
1:B:883:LEU:O	1:B:884:GLY:C	2.56	0.47
1:C:931:VAL:HG13	1:C:931:VAL:O	2.14	0.47
1:D:309:THR:HB	1:D:326:ASN:HD22	1.79	0.47
1:D:582:VAL:HA	1:D:845:TYR:CE2	2.49	0.47
1:A:42:VAL:CG2	1:A:53:PHE:CE2	2.97	0.47
1:A:384:LEU:HD12	1:A:384:LEU:N	2.29	0.47
1:A:964:GLN:HG2	1:A:968:LEU:CD1	2.44	0.47
1:B:99:ILE:HD12	1:B:99:ILE:N	2.28	0.47
1:B:309:THR:HB	1:B:326:ASN:HB2	1.96	0.47
1:B:927:ASP:HB2	1:B:930:SER:H	1.79	0.47
1:B:960:ASN:HD22	1:B:963:LEU:HB3	1.79	0.47
1:C:332:GLU:HA	1:C:375:GLN:NE2	2.29	0.47
1:C:390:ASP:OD1	1:C:456:LYS:HG2	2.14	0.47
1:C:649:VAL:O	1:C:649:VAL:HG13	2.14	0.47
1:C:667:ALA:HB1	1:C:698:LYS:HE3	1.94	0.47
1:D:679:SER:OG	1:D:909:PRO:HD2	2.14	0.47
1:D:879:LYS:C	1:D:881:LEU:H	2.22	0.47
1:D:1042:MET:HE1	1:D:1060:ILE:HG21	1.96	0.47
1:A:177:TYR:O	1:A:178:GLU:C	2.56	0.47
1:A:241:ASN:H	1:A:242:PRO:HD3	1.79	0.47
1:A:403:ALA:CA	1:C:406:ARG:HH21	2.27	0.47
1:C:216:ALA:O	1:C:217:PHE:C	2.56	0.47
1:C:334:THR:O	1:C:338:MET:HG3	2.15	0.47
1:D:244:HIS:N	1:D:266:SER:OG	2.46	0.47
1:A:118:TYR:CD1	1:A:118:TYR:C	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:HG2	1:A:181:LYS:HB2	1.96	0.47
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.63	0.47
1:C:224:ALA:O	1:C:228:PHE:HD1	1.98	0.47
1:D:152:LYS:O	1:D:152:LYS:HG2	2.15	0.47
1:A:178:GLU:HG2	1:A:178:GLU:O	2.14	0.47
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.26	0.47
1:A:1017:TYR:O	1:A:1018:GLU:C	2.57	0.47
1:C:149:PHE:O	1:C:151:ASP:N	2.42	0.47
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.95	0.47
1:D:756:ILE:HD13	1:D:791:VAL:HG23	1.97	0.47
1:A:70:GLU:CG	1:A:92:PRO:HB3	2.44	0.47
1:A:242:PRO:HD2	1:A:478:THR:OG1	2.14	0.47
1:A:383:PRO:HA	1:A:387:PHE:CE2	2.49	0.47
1:A:417:GLU:C	1:A:418:ILE:HD12	2.40	0.47
1:B:799:ALA:H	1:B:811:ASN:ND2	2.13	0.47
1:B:889:GLU:O	1:B:890:VAL:C	2.58	0.47
1:B:1087:ILE:HG22	1:B:1089:ILE:HD13	1.95	0.47
1:D:756:ILE:HD11	1:D:770:LEU:HD22	1.97	0.47
1:D:1069:ASP:OD1	1:D:1073:ASN:HB2	2.14	0.47
1:D:1087:ILE:HG22	1:D:1089:ILE:CD1	2.43	0.47
1:A:213:LEU:O	1:A:214:GLU:C	2.55	0.47
1:A:1091:ASP:OD2	1:A:1093:ASN:HA	2.15	0.47
1:B:167:ILE:HG12	1:B:168:PRO:CD	2.45	0.47
1:B:338:MET:HE2	1:B:430:SER:CB	2.39	0.47
1:B:624:TRP:O	1:B:627:LEU:HB3	2.15	0.47
1:B:715:ARG:HD2	1:B:715:ARG:C	2.32	0.47
1:B:996:GLU:C	1:B:996:GLU:OE1	2.58	0.47
1:C:515:ASN:CA	1:C:515:ASN:H	2.06	0.47
1:C:701:GLU:HG2	1:C:739:ALA:HB2	1.97	0.47
1:C:744:ALA:HB3	1:C:746:LEU:HG	1.97	0.47
1:C:926:LEU:HD13	1:C:938:LEU:CD1	2.44	0.47
1:C:948:PHE:CE2	1:C:959:PHE:HD2	2.32	0.47
1:D:93:ALA:C	1:D:95:SER:H	2.22	0.47
1:D:137:LYS:HD2	1:D:352:ALA:HB1	1.97	0.47
1:A:846:SER:HA	1:A:849:GLU:HG2	1.96	0.47
1:B:565:LEU:HD21	1:B:826:THR:HB	1.96	0.47
1:B:864:HIS:CD2	1:B:866:MET:HB2	2.50	0.47
1:C:357:LEU:O	1:C:362:MET:CB	2.62	0.47
1:C:652:LYS:HD3	1:C:653:ASN:O	2.15	0.47
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.33	0.47
1:D:606:MET:HE2	1:D:606:MET:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:908:THR:HA	1:D:909:PRO:HA	1.57	0.47
1:B:300:GLU:O	1:B:300:GLU:HG2	2.12	0.47
1:B:641:MET:HE2	1:B:671:ILE:HG13	1.97	0.47
1:B:715:ARG:HD2	1:B:715:ARG:O	2.15	0.47
1:B:977:ARG:CZ	1:B:980:GLU:HG3	2.44	0.47
1:C:803:GLY:O	1:C:804:LEU:C	2.56	0.47
1:C:831:MET:O	1:C:832:GLU:C	2.58	0.47
1:D:870:GLN:O	1:D:871:TYR:C	2.57	0.47
1:B:620:LYS:NZ	4:B:1201:BTI:HN3	2.13	0.47
1:B:624:TRP:HZ2	1:B:1008:ILE:CD1	2.28	0.47
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.23	0.47
1:C:1065:ILE:HG12	1:C:1076:ILE:HG23	1.96	0.47
1:C:1085:ARG:CG	1:C:1085:ARG:NH1	2.44	0.47
1:D:93:ALA:C	1:D:95:SER:N	2.73	0.47
1:A:606:MET:CE	1:A:639:PHE:HB3	2.45	0.46
1:B:948:PHE:CD2	1:B:964:GLN:HA	2.50	0.46
1:C:177:TYR:OH	1:C:181:LYS:HE3	2.15	0.46
1:D:379:THR:O	1:D:457:THR:HB	2.14	0.46
1:D:532:VAL:HG21	1:D:596:ASP:CB	2.45	0.46
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.96	0.46
1:A:674:PHE:N	1:A:674:PHE:CD2	2.83	0.46
1:B:596:ASP:O	1:B:599:LYS:HG2	2.15	0.46
1:C:936:TYR:HD1	1:C:966:VAL:CG1	2.28	0.46
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.46
1:D:323:ILE:HG22	1:D:324:GLU:HG2	1.97	0.46
1:D:927:ASP:HB3	1:D:930:SER:H	1.78	0.46
1:D:1054:LYS:HB3	1:D:1054:LYS:HE2	1.41	0.46
1:D:1085:ARG:HH11	1:D:1085:ARG:HG3	1.79	0.46
1:A:550:PRO:HB2	1:A:736:HIS:CE1	2.49	0.46
1:A:572:ASP:OD1	1:A:771:HIS:CE1	2.68	0.46
1:A:1078:TYR:HB2	1:A:1085:ARG:HB3	1.97	0.46
1:B:459:ILE:HB	1:B:460:PRO:HD3	1.97	0.46
1:B:525:GLU:HG3	1:B:527:ALA:H	1.80	0.46
1:B:690:ASN:O	1:B:691:GLU:C	2.59	0.46
1:B:744:ALA:CB	1:B:746:LEU:HG	2.44	0.46
1:B:783:TYR:O	1:B:784:LYS:C	2.56	0.46
1:C:241:ASN:N	1:C:242:PRO:CD	2.77	0.46
1:C:347:THR:O	1:C:348:GLN:C	2.56	0.46
1:C:631:ARG:HG2	1:C:670:GLY:HA3	1.97	0.46
1:C:893:MET:HA	1:C:896:ARG:HD2	1.86	0.46
1:C:917:MET:HE3	1:C:921:MET:SD	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:VAL:HG21	1:D:362:MET:CE	2.45	0.46
1:A:551:LYS:HD3	1:A:551:LYS:HA	1.55	0.46
1:A:620:LYS:HD2	1:A:620:LYS:HA	1.53	0.46
1:A:729:GLU:O	1:A:733:GLU:HG2	2.15	0.46
1:C:711:LEU:HD11	1:C:750:LYS:HB3	1.98	0.46
1:A:42:VAL:HG23	1:A:53:PHE:CE2	2.51	0.46
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.77	0.46
1:A:880:SER:O	1:A:881:LEU:HD23	2.16	0.46
1:B:572:ASP:HB3	1:B:807:GLN:NE2	2.31	0.46
1:B:1052:ILE:O	1:B:1053:ASP:HB2	2.15	0.46
1:D:260:LEU:O	1:D:261:PHE:HB2	2.15	0.46
1:D:527:ALA:HB2	1:D:840:THR:HG21	1.97	0.46
1:D:607:TRP:CE3	1:D:641:MET:HE3	2.34	0.46
1:D:864:HIS:CD2	1:D:866:MET:H	2.25	0.46
1:A:142:HIS:H	1:A:145:HIS:CD2	2.31	0.46
1:A:622:ASN:HD22	1:A:623:PRO:N	2.13	0.46
1:B:620:LYS:HE2	1:B:1023:THR:OG1	2.16	0.46
1:C:570:PHE:O	1:C:574:HIS:HE1	1.98	0.46
1:C:717:ASN:ND2	1:C:717(A):ILE:HG13	2.31	0.46
1:C:1033:LEU:HD23	1:C:1050:ILE:HD13	1.97	0.46
1:A:214:GLU:O	1:A:218:HIS:CD2	2.68	0.46
1:A:772:THR:HG22	1:A:783:TYR:CE2	2.51	0.46
1:B:743:MET:HA	1:B:773:HIS:CD2	2.51	0.46
1:C:47:GLU:CD	1:C:428:LYS:HE3	2.41	0.46
1:C:631:ARG:HD3	1:C:631:ARG:HA	1.53	0.46
1:D:248:GLN:HG2	1:D:260:LEU:HD12	1.98	0.46
1:D:335:ILE:HG22	1:D:336:THR:H	1.79	0.46
1:D:1044:ASN:ND2	1:D:1064:THR:HA	2.30	0.46
1:A:192:MET:CE	1:A:238:TYR:HD1	2.22	0.46
1:C:347:THR:HG23	1:C:360:ILE:HD13	1.97	0.46
1:C:377:ARG:HD3	1:C:377:ARG:N	2.30	0.46
1:C:382:ASP:OD1	1:C:384:LEU:HB2	2.15	0.46
1:C:940:PHE:CB	1:C:941:PRO:CD	2.82	0.46
1:D:811:ASN:HD22	1:D:811:ASN:N	2.00	0.46
1:D:878:ALA:O	1:D:884:GLY:N	2.49	0.46
1:D:927:ASP:O	1:D:931:VAL:HG12	2.16	0.46
1:A:555:GLU:OE2	1:A:555:GLU:HA	2.15	0.46
1:A:1029:ASN:C	1:A:1029:ASN:ND2	2.71	0.46
1:B:263:ARG:NH1	1:B:336:THR:OG1	2.49	0.46
1:B:547:GLU:HB2	1:B:548:VAL:HG13	1.96	0.46
1:B:1001:PRO:HG2	1:B:1002:VAL:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:LEU:HD23	1:C:526:LEU:HA	1.74	0.46
1:C:810:ALA:HB1	1:C:831:MET:CE	2.46	0.46
1:D:772:THR:HG22	1:D:783:TYR:CE2	2.51	0.46
1:B:103:ILE:O	1:B:106:ALA:HB3	2.16	0.46
1:B:387:PHE:HE2	1:B:488:PHE:HE2	1.64	0.46
1:B:417:GLU:H	1:B:417:GLU:HG2	1.55	0.46
1:D:565:LEU:C	1:D:565:LEU:CD1	2.89	0.46
1:A:377:ARG:HB3	1:A:425:LEU:CD1	2.45	0.45
1:A:1089:ILE:O	1:A:1089:ILE:HG22	2.15	0.45
1:B:748:LYS:HB3	1:B:749:PRO:HD2	1.98	0.45
1:C:332:GLU:HA	1:C:375:GLN:HE22	1.81	0.45
1:C:704:ILE:HG21	1:C:723:TYR:HD2	1.81	0.45
1:C:1018:GLU:OE1	1:C:1018:GLU:HA	2.16	0.45
1:D:900:LEU:HD13	1:D:928:GLU:HG3	1.97	0.45
1:A:234:TYR:CE1	1:A:236:GLU:HG3	2.51	0.45
1:A:382:ASP:OD2	1:A:385:ASN:HB2	2.16	0.45
1:A:386:ASP:O	1:A:387:PHE:HB2	2.16	0.45
1:A:418:ILE:HD12	1:A:418:ILE:N	2.31	0.45
1:C:798:VAL:CG1	1:C:835:SER:HA	2.46	0.45
1:A:395:ILE:O	1:A:396:ALA:HB2	2.16	0.45
1:A:524:TYR:HD2	1:A:843:THR:CG2	2.29	0.45
1:B:729:GLU:HG2	1:B:732:ARG:NH2	2.31	0.45
1:D:917:MET:O	1:D:921:MET:HB2	2.16	0.45
1:A:47:GLU:CD	1:A:428:LYS:HD2	2.41	0.45
1:A:193:ILE:HG13	1:A:194:LYS:N	2.32	0.45
1:A:207:VAL:HG11	1:A:213:LEU:HD23	1.97	0.45
1:A:920:TYR:OH	1:A:938:LEU:HB3	2.16	0.45
1:C:1049:GLU:HG2	1:C:1059:ILE:HD13	1.98	0.45
1:D:529:ILE:HD13	1:D:589:ASN:HB3	1.99	0.45
1:D:938:LEU:O	1:D:939:ASP:CB	2.63	0.45
1:A:869:GLY:O	1:A:871:TYR:N	2.49	0.45
1:B:259:HIS:CD2	1:B:296:ILE:CD1	2.76	0.45
1:B:689:ALA:O	1:B:693:VAL:HG23	2.16	0.45
1:D:337:GLU:CG	1:D:342:ILE:O	2.60	0.45
1:A:107:LYS:C	1:A:109:ALA:H	2.23	0.45
1:A:167:ILE:CD1	1:A:323:ILE:CD1	2.94	0.45
1:A:278:ALA:N	1:A:335:ILE:HD11	2.32	0.45
1:A:370:LEU:O	1:A:432:HIS:CE1	2.67	0.45
1:A:874:LEU:HD12	1:A:919:LEU:HD21	1.98	0.45
1:A:1042:MET:CE	1:A:1048:VAL:HG12	2.47	0.45
1:B:539:SER:CA	1:B:543:GLN:HE21	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.82	0.45
1:C:480:PHE:CD1	1:C:480:PHE:C	2.94	0.45
1:C:619:LEU:O	1:C:620:LYS:HB2	2.16	0.45
1:C:1049:GLU:HG2	1:C:1059:ILE:CD1	2.46	0.45
1:D:305:VAL:O	1:D:306:ASN:CB	2.65	0.45
1:D:459:ILE:N	1:D:460:PRO:HD2	2.32	0.45
1:D:574:HIS:HD2	1:D:580:THR:HA	1.81	0.45
1:D:796:THR:HB	1:D:810:ALA:HB2	1.98	0.45
1:A:179:LEU:HD11	1:A:217:PHE:CE1	2.51	0.45
1:A:622:ASN:O	1:A:623:PRO:C	2.60	0.45
1:A:873:ASN:O	1:A:875:SER:N	2.49	0.45
1:B:302:ILE:O	1:B:303:LYS:HB2	2.17	0.45
1:C:180:ALA:O	1:C:181:LYS:C	2.60	0.45
1:C:309:THR:HG22	1:C:311:GLU:HG2	1.98	0.45
1:C:580:THR:HB	1:C:614:VAL:HG21	1.98	0.45
1:D:262:GLU:OE1	1:D:288:ARG:NH1	2.50	0.45
1:D:583:ARG:HG2	1:D:619:LEU:HD22	1.98	0.45
1:A:174:ILE:HD11	1:A:235:ILE:HG22	1.99	0.45
1:A:192:MET:CE	1:A:238:TYR:CE1	3.00	0.45
1:A:496:ARG:O	1:A:497:GLY:C	2.60	0.45
1:A:606:MET:SD	1:A:606:MET:C	3.00	0.45
1:A:622:ASN:ND2	1:A:622:ASN:C	2.70	0.45
1:B:631:ARG:HG2	1:B:670:GLY:HA3	1.99	0.45
1:C:129:ARG:HG3	1:C:143:LEU:CD1	2.46	0.45
1:C:267:VAL:HG22	1:C:480:PHE:CD2	2.51	0.45
1:C:443:MET:HG2	1:C:466:MET:SD	2.57	0.45
1:C:738:LEU:HD21	1:C:759:LEU:HD13	1.98	0.45
1:C:979:GLY:C	1:C:981:TYR:N	2.70	0.45
1:D:869:GLY:O	1:D:870:GLN:C	2.59	0.45
1:D:871:TYR:CE1	1:D:891:LYS:HD3	2.52	0.45
1:A:431:THR:HG21	1:A:443:MET:HA	1.99	0.45
1:B:269:ARG:O	1:B:270:ARG:C	2.60	0.45
1:B:398:ARG:HD3	1:B:1083:GLN:HE21	1.82	0.45
1:B:932:ILE:HG13	1:B:933:THR:N	2.32	0.45
1:C:437:LYS:H	1:C:437:LYS:CD	2.22	0.45
1:C:440:GLU:HG3	1:C:472:THR:HG22	1.99	0.45
1:C:690:ASN:O	1:C:694:GLN:HG2	2.17	0.45
1:C:1080:MET:HE1	1:C:1085:ARG:HH21	1.82	0.45
1:D:739:ALA:C	1:D:740:ILE:HD13	2.42	0.45
1:A:177:TYR:O	1:A:179:LEU:N	2.50	0.45
1:A:245:ILE:HG13	1:A:283:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.73	0.45
1:B:251:GLY:HA2	1:B:257:ILE:HA	1.99	0.45
1:B:511:GLY:O	4:B:1201:BTI:H102	2.17	0.45
1:C:99:ILE:HG23	1:C:127:PHE:HD1	1.82	0.45
1:C:173:PRO:O	1:C:174:ILE:CD1	2.64	0.45
1:C:221:LYS:HG3	1:C:233:VAL:HG13	1.99	0.45
1:C:673:VAL:HG22	1:C:699:ILE:HB	1.98	0.45
1:D:898:ASN:ND2	1:D:904:ILE:H	2.15	0.45
1:D:907:VAL:O	1:D:910:SER:N	2.49	0.45
1:A:508:THR:HG22	1:A:508:THR:O	2.17	0.44
1:A:641:MET:HE2	1:A:674:PHE:CD1	2.50	0.44
1:A:873:ASN:C	1:A:875:SER:N	2.75	0.44
1:A:879:LYS:HB2	1:A:879:LYS:HE2	1.66	0.44
1:B:98:ASN:CG	1:B:101:ARG:HB2	2.42	0.44
1:B:267:VAL:HG12	1:B:481:ILE:HD11	1.99	0.44
1:C:162:ALA:HB2	1:C:301:ASN:HD22	1.82	0.44
1:D:167:ILE:HG23	1:D:321:PHE:CB	2.47	0.44
1:D:259:HIS:N	1:D:364:GLN:HE22	2.05	0.44
1:A:156:ARG:HD2	1:A:166:VAL:HG11	1.99	0.44
1:A:252:ASP:CG	1:A:256:ASN:HB2	2.42	0.44
1:A:322:PHE:C	1:A:323:ILE:HD13	2.43	0.44
1:A:712:ASN:HA	1:A:713:PRO:HD3	1.83	0.44
1:A:826:THR:HG21	1:A:831:MET:HE2	1.99	0.44
1:B:40:LEU:C	1:B:40:LEU:HD23	2.42	0.44
1:B:574:HIS:HD2	1:B:580:THR:HA	1.81	0.44
1:B:784:LYS:HE2	1:C:785:GLN:HE21	1.82	0.44
1:B:798:VAL:O	1:B:799:ALA:C	2.59	0.44
1:C:320:PHE:C	1:C:320:PHE:CD2	2.94	0.44
1:D:134:GLU:HB2	1:D:136:ILE:HD12	1.99	0.44
1:D:325:VAL:O	1:D:327:PRO:HD3	2.18	0.44
1:D:647:ASN:C	1:D:647:ASN:ND2	2.74	0.44
1:D:787:ILE:HD13	1:D:817:LEU:HD11	1.99	0.44
1:A:622:ASN:HD22	1:A:624:TRP:H	1.60	0.44
1:A:1042:MET:HE2	1:A:1048:VAL:HG12	2.00	0.44
1:B:144:GLU:H	1:B:144:GLU:HG3	1.53	0.44
1:B:709:ASP:OD1	1:B:748:LYS:NZ	2.50	0.44
1:C:892:ASP:O	1:C:896:ARG:CD	2.62	0.44
1:D:333:HIS:O	1:D:334:THR:C	2.60	0.44
1:D:650:GLY:HA3	1:D:654:TYR:CE1	2.53	0.44
1:D:917:MET:CE	1:D:940:PHE:HD2	2.31	0.44
1:A:174:ILE:HD11	1:A:235:ILE:HG21	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:THR:O	1:A:499:LYS:C	2.59	0.44
1:C:736:HIS:C	1:C:737:ILE:HG13	2.43	0.44
1:C:1042:MET:HE1	1:C:1060:ILE:HG22	1.97	0.44
1:D:1042:MET:HE1	1:D:1060:ILE:CG2	2.47	0.44
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.98	0.44
1:B:167:ILE:HG12	1:B:168:PRO:HD2	1.99	0.44
1:B:631:ARG:HA	1:B:631:ARG:HD3	1.50	0.44
1:C:191:LEU:HD13	1:C:235:ILE:HD11	2.00	0.44
1:C:294:ALA:O	1:C:297:GLN:HB3	2.17	0.44
1:A:99:ILE:O	1:A:103:ILE:HG12	2.17	0.44
1:A:246:GLU:HB2	1:A:309:THR:CG2	2.48	0.44
1:A:1046:GLU:O	1:A:1061:LYS:HA	2.18	0.44
1:B:603:SER:HA	1:B:637:VAL:HG12	1.99	0.44
1:B:792:ASP:OD2	1:B:792:ASP:N	2.51	0.44
1:C:890:VAL:C	1:C:891:LYS:HG3	2.41	0.44
1:A:275:VAL:HG22	1:A:376:CYS:HB3	1.98	0.44
1:B:1077:TYR:OH	1:D:1063:GLU:HB3	2.17	0.44
1:C:77:ARG:HD3	1:C:83:SER:OG	2.18	0.44
1:C:188:GLY:HA3	1:C:237:ARG:NH2	2.28	0.44
1:C:964:GLN:NE2	1:C:973:ALA:HB2	2.32	0.44
1:D:717:ASN:HD22	1:D:717:ASN:H	1.65	0.44
1:B:682:TRP:HE3	1:B:685:GLN:HG3	1.81	0.44
1:B:912:LYS:NZ	1:B:916:ASP:OD1	2.48	0.44
1:C:1090:LYS:HB3	1:C:1090:LYS:HE3	1.56	0.44
1:D:246:GLU:OE2	1:D:273:LYS:NZ	2.44	0.44
1:D:828:ILE:HD12	1:D:829:GLU:N	2.33	0.44
1:A:866:MET:CE	1:A:871:TYR:HA	2.47	0.44
1:A:886:ARG:O	1:A:889:GLU:N	2.45	0.44
1:B:277:VAL:HA	1:B:335:ILE:HD11	1.99	0.44
1:B:361:ASN:HD22	1:B:361:ASN:HA	1.50	0.44
1:C:775:THR:HG21	1:C:861:ILE:HG13	2.00	0.44
1:D:701:GLU:HG2	1:D:737:ILE:HB	2.00	0.44
1:D:875:SER:C	1:D:877:GLN:H	2.25	0.44
1:B:99:ILE:H	1:B:99:ILE:CD1	2.29	0.43
1:B:645:ALA:HB1	1:B:686:MET:HA	2.00	0.43
1:C:167:ILE:O	1:C:168:PRO:C	2.61	0.43
1:C:192:MET:HE3	1:C:192:MET:HB3	1.54	0.43
1:C:993:LEU:O	1:C:997:GLU:HG2	2.18	0.43
1:D:263:ARG:HG2	1:D:335:ILE:CG2	2.48	0.43
1:D:302:ILE:HG13	1:D:302:ILE:H	1.70	0.43
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:ASN:HD21	1:D:904:ILE:H	1.66	0.43
1:A:306:ASN:OD1	1:A:348:GLN:HG2	2.18	0.43
1:B:165:PRO:HB2	1:B:321:PHE:HD2	1.83	0.43
1:B:738:LEU:O	1:B:768:ILE:HA	2.19	0.43
1:B:798:VAL:HG12	1:B:831:MET:HE1	1.95	0.43
1:C:493:SER:HA	1:C:494:LEU:HD13	1.99	0.43
1:D:413:PHE:C	1:D:415:GLY:N	2.74	0.43
1:A:720:LEU:CD2	1:A:758:GLU:HG3	2.42	0.43
1:B:375:GLN:HG3	1:B:430:SER:OG	2.18	0.43
1:C:115:HIS:ND1	1:C:116:PRO:HD2	2.33	0.43
1:C:225:GLU:HB3	1:C:231:SER:HB3	1.99	0.43
1:C:565:LEU:HD12	1:C:824:LEU:HD21	2.00	0.43
1:C:941:PRO:C	1:C:943:SER:N	2.75	0.43
1:D:50:ILE:HD11	1:D:75:LEU:HB3	1.99	0.43
1:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.43
1:D:487:LEU:HD12	1:D:487:LEU:HA	1.82	0.43
1:D:516:VAL:O	1:D:517:GLU:C	2.60	0.43
1:A:322:PHE:O	1:A:323:ILE:HD13	2.18	0.43
1:A:856:SER:OG	1:D:800:SER:HA	2.19	0.43
1:A:858:ASN:ND2	1:A:860:GLU:H	2.17	0.43
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.33	0.43
1:A:1065:ILE:HG22	1:A:1074:ARG:HD3	2.00	0.43
1:B:551:LYS:O	1:B:555:GLU:HG2	2.19	0.43
1:C:241:ASN:N	1:C:242:PRO:HD3	2.33	0.43
1:D:61:ILE:HG22	1:D:62:SER:O	2.19	0.43
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.62	0.43
1:A:481:ILE:O	1:A:482:GLU:C	2.61	0.43
1:A:561:ASP:O	1:A:822:ARG:HD2	2.19	0.43
1:B:949:LYS:HE2	1:B:951:GLU:OE1	2.18	0.43
1:B:1042:MET:HE2	1:B:1078:TYR:HE2	1.84	0.43
1:B:1063:GLU:OE1	1:D:1086:ARG:NH1	2.51	0.43
1:C:118:TYR:HA	1:C:122:SER:OG	2.19	0.43
1:D:494:LEU:CD2	1:D:496:ARG:HA	2.49	0.43
1:D:542:LYS:HB2	1:D:636:ASN:C	2.44	0.43
1:A:148:MET:HE3	1:A:148:MET:HB2	1.87	0.43
1:A:1018:GLU:O	1:A:1019:GLN:C	2.61	0.43
1:B:509:ILE:HG22	1:B:510:ASN:CG	2.43	0.43
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.51	0.43
1:C:937:LYS:O	1:C:938:LEU:HB2	2.17	0.43
1:D:259:HIS:NE2	1:D:292:CYS:HB3	2.34	0.43
1:D:570:PHE:C	1:D:574:HIS:HE1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HB3	1:A:38:LYS:HE2	1.60	0.43
1:A:470:LYS:CB	1:A:480:PHE:CE1	3.00	0.43
1:A:547:GLU:HB3	1:A:548:VAL:HG13	1.99	0.43
1:A:711:LEU:HG	1:A:751:ALA:HB2	2.00	0.43
1:A:798:VAL:HG11	1:A:835:SER:N	2.34	0.43
1:B:704:ILE:CG2	1:B:726:LEU:HD23	2.40	0.43
1:C:43:ALA:HA	1:C:66:ILE:CD1	2.49	0.43
1:D:151:ASP:C	1:D:153:VAL:H	2.25	0.43
1:D:164:LEU:HD22	1:D:298:LEU:HB2	2.01	0.43
1:D:952:ILE:HD12	1:D:952:ILE:HA	1.87	0.43
1:D:1069:ASP:OD2	1:D:1069:ASP:C	2.61	0.43
1:A:341:GLY:C	1:A:342:ILE:HD12	2.44	0.43
1:A:655:PRO:HG2	1:A:985:VAL:CG2	2.48	0.43
1:A:715:ARG:HA	1:A:715:ARG:HD2	1.80	0.43
1:A:855:LYS:O	1:A:855:LYS:HG3	2.17	0.43
1:A:1065:ILE:CG2	1:A:1074:ARG:HD3	2.49	0.43
1:B:386:ASP:HB3	1:B:388:MET:HG3	2.01	0.43
1:B:885:GLU:C	1:B:886:ARG:HG3	2.44	0.43
1:C:148:MET:HA	1:C:154:LYS:HD2	1.99	0.43
1:D:963:LEU:HD12	1:D:967:ILE:HD12	2.01	0.43
1:A:394:ILE:O	1:A:414:GLN:O	2.36	0.43
1:B:302:ILE:C	1:B:303:LYS:HG3	2.44	0.43
1:B:655:PRO:HD3	1:B:982:LEU:CD1	2.49	0.43
1:C:142:HIS:N	1:C:145:HIS:HD2	2.16	0.43
1:A:252:ASP:OD1	1:A:256:ASN:HB2	2.19	0.43
1:A:547:GLU:OE2	1:A:547:GLU:CA	2.66	0.43
1:C:129:ARG:HG3	1:C:143:LEU:HD13	2.00	0.43
1:D:239:ILE:HD13	1:D:239:ILE:HA	1.82	0.43
1:D:277:VAL:HG21	1:D:476:TYR:OH	2.19	0.43
1:A:641:MET:HE2	1:A:674:PHE:HE1	1.73	0.42
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.53	0.42
1:B:448:ARG:NH2	1:B:467:LYS:HD2	2.32	0.42
1:B:1048:VAL:HG12	1:B:1050:ILE:HD12	2.01	0.42
1:D:871:TYR:HE1	1:D:891:LYS:HD3	1.84	0.42
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.42
1:B:291:ILE:HG12	1:B:320:PHE:HD2	1.84	0.42
1:B:955:PRO:O	1:B:956:VAL:C	2.62	0.42
1:C:238:TYR:CE1	5:C:1202:ATP:H2	2.37	0.42
1:C:448:ARG:HH22	1:C:467:LYS:HE3	1.84	0.42
1:C:1002:VAL:HG13	1:C:1006:ASP:OD2	2.19	0.42
1:D:456:LYS:HD3	1:D:456:LYS:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:820:PHE:HB3	1:D:821:PRO:HD2	2.01	0.42
1:A:192:MET:HE3	2:A:1201:ADP:C5	2.55	0.42
1:A:532:VAL:HG13	1:A:536:LYS:HD2	2.01	0.42
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.79	0.42
1:C:501:LEU:HD22	1:C:1078:TYR:CE1	2.54	0.42
1:C:661:LYS:O	1:C:664:GLN:HB2	2.20	0.42
1:C:780:LEU:HD23	1:C:780:LEU:HA	1.80	0.42
1:C:926:LEU:CD1	1:C:938:LEU:CD1	2.96	0.42
1:C:941:PRO:O	1:C:945:VAL:HG22	2.19	0.42
1:D:472:THR:C	1:D:474:GLY:N	2.77	0.42
1:D:631:ARG:C	1:D:631:ARG:HD3	2.41	0.42
1:D:796:THR:CB	1:D:810:ALA:HB2	2.49	0.42
1:D:879:LYS:HG2	1:D:884:GLY:HA3	2.01	0.42
1:A:207:VAL:CG1	1:A:209:GLU:H	2.33	0.42
1:A:506:ASN:ND2	1:A:510:ASN:HD22	2.18	0.42
1:A:597:VAL:HG21	1:A:834:LEU:HG	1.99	0.42
1:A:780:LEU:HD11	1:A:812:SER:HB3	2.00	0.42
1:A:952:ILE:O	1:A:952:ILE:HG23	2.17	0.42
1:B:85:LEU:HG	1:B:87:GLY:H	1.84	0.42
1:B:522:PRO:HB2	1:B:523:ASP:H	1.68	0.42
1:C:194:LYS:NZ	1:C:236:GLU:OE2	2.51	0.42
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.84	0.42
1:D:258:VAL:HB	1:D:364:GLN:NE2	2.34	0.42
1:D:378:ILE:HG23	1:D:459:ILE:HG12	2.00	0.42
1:D:413:PHE:C	1:D:415:GLY:H	2.27	0.42
1:D:866:MET:HE3	1:D:874:LEU:HD22	2.01	0.42
1:B:278:ALA:HA	1:B:279:PRO:HA	1.62	0.42
1:B:468:ASN:OD1	1:B:470:LYS:HB2	2.19	0.42
1:B:631:ARG:HD3	1:B:631:ARG:O	2.19	0.42
1:C:111:VAL:HG12	1:C:113:ALA:H	1.83	0.42
1:C:281:VAL:HG12	1:C:282:GLY:H	1.83	0.42
1:C:571:ARG:HH21	1:C:605:GLU:CD	2.27	0.42
1:A:382:ASP:OD1	1:A:384:LEU:CD1	2.67	0.42
1:C:124:ASN:HB3	1:C:127:PHE:HB3	2.02	0.42
1:C:447:LEU:HA	1:C:447:LEU:HD23	1.78	0.42
1:C:907:VAL:O	1:C:911:SER:OG	2.35	0.42
1:C:920:TYR:CE1	1:C:940:PHE:HD2	2.37	0.42
1:C:1080:MET:CE	1:C:1085:ARG:NH2	2.83	0.42
1:D:506:ASN:HD22	1:D:506:ASN:HA	1.64	0.42
1:D:909:PRO:HG2	1:D:952:ILE:HG13	2.01	0.42
1:A:384:LEU:C	1:A:386:ASP:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:OD1	1:B:126:GLN:N	2.53	0.42
1:B:655:PRO:HD3	1:B:982:LEU:HD13	2.00	0.42
1:C:383:PRO:HB3	1:C:387:PHE:CZ	2.54	0.42
1:C:572:ASP:HB3	1:C:807:GLN:HE21	1.80	0.42
1:A:167:ILE:HD12	1:A:323:ILE:CD1	2.50	0.42
1:A:246:GLU:O	1:A:262:GLU:HA	2.19	0.42
1:A:384:LEU:H	1:A:384:LEU:CD1	2.33	0.42
1:B:291:ILE:HG12	1:B:320:PHE:CD2	2.55	0.42
1:C:246:GLU:OE1	1:C:330:GLN:NE2	2.52	0.42
1:C:760:LYS:CE	1:C:790:GLY:O	2.67	0.42
1:C:794:ILE:CD1	1:C:796:THR:CG2	2.97	0.42
1:D:606:MET:SD	1:D:606:MET:C	3.03	0.42
1:D:730:LEU:O	1:D:735:PHE:HD1	2.02	0.42
1:D:856:SER:HB3	1:D:857:PRO:HD2	2.00	0.42
1:D:874:LEU:O	1:D:887:PHE:CE1	2.65	0.42
1:D:1087:ILE:HD13	1:D:1087:ILE:HA	1.86	0.42
1:A:912:LYS:NZ	1:A:916:ASP:OD1	2.45	0.42
1:A:1080:MET:O	1:A:1081:ASN:C	2.63	0.42
1:B:69:ASN:O	1:B:72:LYS:HG3	2.19	0.42
1:B:251:GLY:HA3	1:B:257:ILE:HG23	2.02	0.42
1:C:39:LYS:HE3	1:C:82:GLU:OE2	2.20	0.42
1:C:336:THR:O	1:C:340:THR:HG23	2.19	0.42
1:C:342:ILE:HG12	1:C:362:MET:HE1	2.01	0.42
1:C:506:ASN:ND2	1:C:510:ASN:HD22	2.18	0.42
1:D:572:ASP:HB3	1:D:807:GLN:HE21	1.83	0.42
1:A:503:TYR:O	1:A:504:ILE:C	2.60	0.42
1:A:781:LEU:HD21	1:D:784:LYS:HG3	2.01	0.42
1:A:902:GLY:O	1:A:903:ASP:HB3	2.19	0.42
1:B:130:ARG:HA	1:B:130:ARG:HD2	1.80	0.42
1:B:413:PHE:O	1:B:414:GLN:C	2.62	0.42
1:B:769:HIS:NE2	1:B:795:ASP:OD1	2.48	0.42
1:C:125:GLU:CD	1:C:147:ASP:HB2	2.45	0.42
1:C:810:ALA:O	1:C:811:ASN:C	2.61	0.42
1:C:896:ARG:NE	1:C:928:GLU:OE1	2.53	0.42
1:C:1077:TYR:N	1:C:1077:TYR:CD1	2.88	0.42
1:D:239:ILE:O	1:D:241:ASN:N	2.52	0.42
1:D:703:THR:CG2	1:D:741:LYS:HB2	2.48	0.42
1:A:48:ILE:HG23	1:A:49:ALA:N	2.34	0.41
1:A:196:THR:HG21	1:A:230:ASN:CG	2.45	0.41
1:A:219:ARG:O	1:A:219:ARG:HG2	2.19	0.41
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LEU:C	1:A:578:LEU:HG	2.44	0.41
1:A:598:PHE:O	1:A:599:LYS:C	2.63	0.41
1:A:944:VAL:O	1:A:945:VAL:C	2.63	0.41
1:B:280:SER:OG	1:B:283:LEU:HG	2.20	0.41
1:B:362(A):PRO:HB2	1:B:366:ASP:HB2	2.01	0.41
1:C:627:LEU:O	1:C:631:ARG:HB2	2.20	0.41
1:C:893:MET:HE3	1:C:893:MET:HB2	1.96	0.41
1:A:175:LYS:HZ2	1:A:232:GLU:HG3	1.79	0.41
1:A:225:GLU:OE2	1:A:231:SER:HB3	2.20	0.41
1:A:362:MET:HE3	1:A:362(A):PRO:HD2	2.01	0.41
1:A:744:ALA:HB3	1:A:746:LEU:HG	2.02	0.41
1:A:898:ASN:ND2	1:A:904:ILE:H	2.12	0.41
1:B:251:GLY:CA	1:B:257:ILE:HG23	2.50	0.41
1:B:756:ILE:O	1:B:757:GLY:C	2.61	0.41
1:C:772:THR:HG22	1:C:783:TYR:CE2	2.55	0.41
1:C:809:SER:HB3	1:C:812:SER:HB2	2.01	0.41
1:D:828:ILE:HD12	1:D:829:GLU:H	1.85	0.41
1:D:860:GLU:O	1:D:863:GLN:HG2	2.19	0.41
1:A:254:HIS:HD2	1:A:356:ASP:OD2	2.02	0.41
1:B:370:LEU:HD22	1:D:370:LEU:HB3	2.02	0.41
1:B:606:MET:HE3	1:B:607:TRP:HB2	1.97	0.41
1:C:59:LEU:HD22	1:C:350:LEU:HD21	2.02	0.41
1:C:152:LYS:HG3	1:C:197:SER:H	1.84	0.41
1:C:469:LYS:HD2	1:C:469:LYS:HA	1.61	0.41
1:C:979:GLY:O	1:C:982:LEU:N	2.52	0.41
1:A:211:SER:H	1:A:213:LEU:HD12	1.85	0.41
1:A:743:MET:CG	1:A:907:VAL:HG13	2.50	0.41
1:B:343:ASP:OD2	1:B:346:LYS:HB2	2.21	0.41
1:B:371:GLY:HA2	1:B:434:ILE:HA	2.02	0.41
1:B:509:ILE:HG22	1:B:510:ASN:OD1	2.20	0.41
1:B:631:ARG:HD3	1:B:631:ARG:C	2.38	0.41
1:D:276:GLU:OE2	1:D:377:ARG:NH1	2.50	0.41
1:D:334:THR:HB	1:D:375:GLN:NE2	2.35	0.41
1:D:872:SER:C	1:D:874:LEU:H	2.29	0.41
1:D:1035:THR:N	1:D:1036:PRO:CD	2.84	0.41
1:A:390:ASP:HB3	1:A:455:VAL:HG12	2.01	0.41
1:A:605:GLU:HA	1:A:640:GLN:O	2.20	0.41
1:A:641:MET:HB3	1:A:671:ILE:HD12	2.03	0.41
1:A:915:GLY:O	1:A:919:LEU:HD22	2.20	0.41
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.85	0.41
1:B:400:SER:HB3	1:B:401:GLY:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ILE:HD12	1:B:1076:ILE:HD11	2.01	0.41
1:B:859:THR:OG1	1:C:832:GLU:OE2	2.33	0.41
1:B:949:LYS:O	1:B:974:LEU:HG	2.20	0.41
1:C:712:ASN:HA	1:C:713:PRO:HD2	1.97	0.41
1:C:752:ALA:HB2	1:C:782:THR:HG23	2.03	0.41
1:C:870:GLN:O	1:C:871:TYR:C	2.62	0.41
1:C:870:GLN:CD	1:C:874:LEU:HD22	2.46	0.41
1:D:322:PHE:CZ	1:D:325:VAL:HG23	2.56	0.41
1:D:743:MET:HG2	1:D:744:ALA:N	2.34	0.41
1:A:152:LYS:HD3	1:A:152:LYS:HA	1.83	0.41
1:A:296:ILE:O	1:A:297:GLN:C	2.63	0.41
1:A:987:PHE:HE2	1:A:1011:VAL:HG21	1.85	0.41
1:A:1052:ILE:O	1:A:1052:ILE:HG22	2.20	0.41
1:B:53:PHE:CZ	1:B:65:ALA:HB2	2.55	0.41
1:B:302:ILE:O	1:B:303:LYS:CB	2.68	0.41
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.20	0.41
1:C:170:THR:HG21	1:C:174:ILE:HD11	2.01	0.41
1:D:563:VAL:CG2	1:D:787:ILE:HG12	2.49	0.41
1:A:382:ASP:O	1:A:387:PHE:HA	2.19	0.41
1:B:406:ARG:NH1	1:D:403:ALA:HA	2.36	0.41
1:C:400:SER:H	1:C:407:LEU:HD11	1.86	0.41
1:D:893:MET:SD	1:D:896:ARG:NH2	2.94	0.41
1:A:683:VAL:HA	1:A:686:MET:HG3	2.02	0.41
1:B:642:LEU:HG	1:B:643:LEU:N	2.35	0.41
1:B:784:LYS:HE2	1:C:785:GLN:NE2	2.36	0.41
1:B:1029:ASN:C	1:B:1029:ASN:ND2	2.76	0.41
1:C:898:ASN:HD22	1:C:906:LYS:HD3	1.86	0.41
1:D:700:SER:H	1:D:736:HIS:CD2	2.38	0.41
1:A:66:ILE:HB	1:A:86:VAL:HG22	2.03	0.41
1:A:1063:GLU:OE2	1:C:1086:ARG:NH2	2.54	0.41
1:B:484:THR:HB	1:B:487:LEU:HD22	2.01	0.41
1:B:640:GLN:HG3	1:B:673:VAL:CG1	2.51	0.41
1:B:701:GLU:HG2	1:B:739:ALA:HB2	2.03	0.41
1:B:793:ILE:HG22	1:B:794:ILE:N	2.36	0.41
1:B:799:ALA:HB3	1:B:835:SER:OG	2.20	0.41
1:B:945:VAL:HA	1:B:967:ILE:CG2	2.50	0.41
1:B:952:ILE:O	1:B:952:ILE:CG2	2.68	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.03	0.41
1:C:335:ILE:HG12	1:C:373:ALA:HB3	2.03	0.41
1:C:991:ARG:O	1:C:995:GLU:HG2	2.21	0.41
1:D:574:HIS:CD2	1:D:580:THR:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:GLY:HA3	1:D:654:TYR:HE1	1.86	0.41
1:D:927:ASP:H	1:D:930:SER:HB2	1.85	0.41
1:D:974:LEU:HB3	1:D:981:TYR:CE1	2.56	0.41
1:A:295:ALA:O	1:A:299:MET:HG2	2.21	0.41
1:A:512:PHE:CD2	1:A:513:PRO:N	2.89	0.41
1:A:980:GLU:O	1:A:980:GLU:OE1	2.39	0.41
1:B:841:VAL:C	1:B:843:THR:H	2.29	0.41
1:B:881:LEU:HD22	1:B:923:GLN:NE2	2.35	0.41
1:C:549:GLY:O	1:C:553:VAL:HG23	2.20	0.41
1:C:893:MET:O	1:C:897:VAL:HG23	2.21	0.41
1:D:275:VAL:HG11	1:D:466:MET:HE1	2.03	0.41
1:D:512:PHE:O	1:D:513:PRO:C	2.64	0.41
1:D:588:ILE:HD12	1:D:588:ILE:HG23	1.83	0.41
1:D:711:LEU:HD23	1:D:711:LEU:HA	1.88	0.41
1:A:170:THR:HG22	1:A:172:GLY:H	1.85	0.40
1:A:296:ILE:O	1:A:300:GLU:HB2	2.21	0.40
1:A:566:THR:HA	1:A:603:SER:O	2.21	0.40
1:A:647:ASN:O	1:A:649:VAL:N	2.53	0.40
1:B:444:VAL:CG2	1:B:466:MET:HB3	2.52	0.40
1:B:577:LEU:HD13	1:B:842:ARG:CZ	2.51	0.40
1:B:717:ASN:C	1:B:717(A):ILE:HD12	2.46	0.40
1:C:145:HIS:CE1	1:C:304:TYR:HA	2.56	0.40
1:C:189:PHE:N	1:C:190:PRO:CD	2.84	0.40
1:C:264:ASP:OD2	1:C:266:SER:OG	2.33	0.40
1:C:268:GLN:HA	1:C:272:GLN:O	2.20	0.40
1:C:381:GLU:O	1:C:383:PRO:HD3	2.21	0.40
1:C:729:GLU:O	1:C:733:GLU:HG2	2.21	0.40
1:C:866:MET:HE2	1:C:866:MET:HB3	2.02	0.40
1:D:281:VAL:CG1	1:D:282:GLY:N	2.83	0.40
1:A:281:VAL:HG21	1:A:436:PHE:CG	2.56	0.40
1:A:720:LEU:HD21	1:A:758:GLU:CG	2.44	0.40
1:A:927:ASP:OD1	1:A:927:ASP:C	2.64	0.40
1:B:164:LEU:HD11	1:B:298:LEU:HB2	2.02	0.40
1:B:241:ASN:HA	1:B:479:LYS:HE2	2.03	0.40
1:B:549:GLY:O	1:B:553:VAL:HG23	2.22	0.40
1:B:777:GLY:O	1:C:780:LEU:HD12	2.21	0.40
1:B:908:THR:HG22	1:B:909:PRO:HA	2.03	0.40
1:C:189:PHE:H	1:C:190:PRO:HD2	1.86	0.40
1:C:350:LEU:O	1:C:355:ALA:HB3	2.21	0.40
1:C:461:PHE:O	1:C:464:ASN:HB2	2.21	0.40
1:C:1089:ILE:HD13	1:C:1089:ILE:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:HZ	1:D:302:ILE:CD1	2.34	0.40
1:D:442:LYS:HE2	1:D:442:LYS:HB2	1.66	0.40
1:D:468:ASN:HD22	1:D:470:LYS:H	1.69	0.40
1:D:641:MET:HB2	1:D:641:MET:HE2	1.80	0.40
1:D:921:MET:HG2	1:D:926:LEU:CB	2.51	0.40
1:D:927:ASP:HB2	1:D:930:SER:OG	2.20	0.40
1:A:250:ILE:HD13	1:A:250:ILE:HG21	1.93	0.40
1:A:263:ARG:HH21	1:A:330:GLN:HE21	1.69	0.40
1:A:335:ILE:H	1:A:335:ILE:HG22	1.48	0.40
1:A:511:GLY:O	4:A:1203:BTI:H103	2.20	0.40
1:A:551:LYS:O	1:A:555:GLU:HG2	2.21	0.40
1:B:624:TRP:CZ2	1:B:1008:ILE:HD11	2.56	0.40
1:B:949:LYS:HG2	1:B:968:LEU:HD21	2.03	0.40
1:C:444:VAL:O	1:C:448:ARG:HG3	2.21	0.40
1:C:911:SER:H	1:C:911:SER:HG	1.59	0.40
1:D:398:ARG:NH2	1:D:451:ARG:HE	2.19	0.40
1:D:400:SER:OG	1:D:401:GLY:N	2.54	0.40
1:A:170:THR:HG21	1:A:174:ILE:HG23	2.03	0.40
1:A:278:ALA:HB3	1:A:335:ILE:CG1	2.48	0.40
1:A:337:GLU:HG2	1:A:342:ILE:O	2.21	0.40
1:A:647:ASN:HB2	1:A:654:TYR:HE1	1.85	0.40
1:A:712:ASN:OD1	1:A:712:ASN:C	2.64	0.40
1:A:717(A):ILE:HD12	1:A:717(A):ILE:N	2.37	0.40
1:A:863:GLN:O	1:A:895:ARG:CD	2.61	0.40
1:A:1053:ASP:O	1:A:1054:LYS:C	2.65	0.40
1:B:418:ILE:HD12	1:B:419:SER:O	2.21	0.40
1:B:624:TRP:CZ2	1:B:1008:ILE:HD13	2.53	0.40
1:B:715:ARG:HH12	1:B:865:GLU:CD	2.28	0.40
1:B:856:SER:OG	1:C:800:SER:HA	2.21	0.40
1:C:641:MET:HB3	1:C:671:ILE:HD12	2.04	0.40
1:C:691:GLU:O	1:C:695:GLU:HB2	2.21	0.40
1:C:995:GLU:O	1:C:998:GLN:O	2.39	0.40
1:D:362:MET:HA	1:D:362(A):PRO:HD2	1.97	0.40
1:D:393:THR:HG23	1:D:417:GLU:OE1	2.21	0.40
1:A:866:MET:HE1	1:A:871:TYR:HA	2.03	0.40
1:A:1029:ASN:ND2	1:A:1031:SER:H	2.20	0.40
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.56	0.40
1:D:166:VAL:HG22	1:D:322:PHE:HB3	2.02	0.40
1:D:358:GLU:CD	1:D:358:GLU:H	2.28	0.40
1:D:373:ALA:HA	1:D:431:THR:O	2.22	0.40
1:D:869:GLY:O	1:D:871:TYR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:924:ASN:CB	1:D:926:LEU:HD22	2.50	0.40
1:D:926:LEU:HD12	1:D:926:LEU:HA	1.91	0.40
1:D:1083:GLN:HE21	1:D:1083:GLN:HB3	1.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1048/1173 (89%)	916 (87%)	102 (10%)	30 (3%)	3	13
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	4	17
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	2	10
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	4	15
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	3	13

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	211	SER
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE
1	A	230	ASN
1	A	396	ALA
1	A	709	ASP
1	A	870	GLN
1	A	880	SER
1	B	163	ASP
1	B	270	ARG

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Mol	Chain	Res	Type
1	B	414	GLN
1	B	495	ASP
1	B	522	PRO
1	B	975	THR
1	C	176	SER
1	C	195	ALA
1	C	201	GLY
1	C	204	MET
1	C	214	GLU
1	C	215	ASP
1	C	386	ASP
1	C	518	LYS
1	C	649	VAL
1	C	886	ARG
1	C	890	VAL
1	C	980	GLU
1	D	92	PRO
1	D	152	LYS
1	D	240	ASP
1	D	515	ASN
1	D	870	GLN
1	A	499	LYS
1	A	527	ALA
1	A	648	ALA
1	A	861	ILE
1	B	166	VAL
1	B	528	SER
1	B	868	GLY
1	B	881	LEU
1	B	903	ASP
1	B	1001	PRO
1	C	87	GLY
1	C	203	GLY
1	C	229	GLY
1	C	385	ASN
1	C	645	ALA
1	C	937	LYS
1	C	938	LEU
1	C	942	GLU
1	D	87	GLY
1	D	94	GLU
1	D	163	ASP

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Mol	Chain	Res	Type
1	D	306	ASN
1	D	414	GLN
1	D	450	MET
1	D	649	VAL
1	D	799	ALA
1	D	884	GLY
1	D	888	ASP
1	A	94	GLU
1	A	517	GLU
1	B	475	ASP
1	B	1002	VAL
1	B	1081	ASN
1	C	151	ASP
1	C	197	SER
1	C	981	TYR
1	C	1053	ASP
1	D	334	THR
1	D	517	GLU
1	D	518	LYS
1	D	1069	ASP
1	A	44	ASN
1	A	209	GLU
1	A	882	GLY
1	B	306	ASN
1	B	648	ALA
1	B	649	VAL
1	B	1000	GLY
1	C	173	PRO
1	C	216	ALA
1	C	269	ARG
1	C	355	ALA
1	C	821	PRO
1	D	133	GLU
1	D	261	PHE
1	D	480	PHE
1	D	513	PRO
1	B	527	ALA
1	B	1053	ASP
1	C	898	ASN
1	C	935	GLY
1	D	335	ILE
1	D	854	ILE

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Mol	Chain	Res	Type
1	A	92	PRO
1	A	110	ASN
1	A	189	PHE
1	A	241	ASN
1	A	306	ASN
1	B	480	PHE
1	B	562	ASP
1	C	174	ILE
1	C	180	ALA
1	C	1001	PRO
1	A	1001	PRO
1	D	282	GLY
1	A	282	GLY
1	A	1014	PRO
1	B	890	VAL
1	C	189	PHE
1	A	868	GLY
1	C	291	ILE
1	C	327	PRO
1	A	956	VAL
1	C	168	PRO
1	A	935	GLY
1	D	1014	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	907/1005 (90%)	760 (84%)	147 (16%)	2	8
1	B	855/1005 (85%)	714 (84%)	141 (16%)	2	8
1	C	909/1005 (90%)	725 (80%)	184 (20%)	1	4
1	D	855/1005 (85%)	711 (83%)	144 (17%)	2	8
All	All	3526/4020 (88%)	2910 (82%)	616 (18%)	2	7

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	44	ASN
1	A	62	SER
1	A	66	ILE
1	A	69	ASN
1	A	70	GLU
1	A	73	SER
1	A	75	LEU
1	A	77	ARG
1	A	94	GLU
1	A	95	SER
1	A	97	LEU
1	A	98	ASN
1	A	103	ILE
1	A	108	GLN
1	A	110	ASN
1	A	143	LEU
1	A	144	GLU
1	A	156	ARG
1	A	161	LYS
1	A	163	ASP
1	A	174	ILE
1	A	179	LEU
1	A	181	LYS
1	A	182	GLU
1	A	186	GLU
1	A	193	ILE
1	A	194	LYS
1	A	210	GLU
1	A	212	GLU
1	A	213	LEU
1	A	214	GLU
1	A	215	ASP
1	A	225	GLU
1	A	237	ARG
1	A	239	ILE
1	A	243	LYS
1	A	249	VAL
1	A	257	ILE
1	A	267	VAL
1	A	271	HIS
1	A	283	LEU
1	A	286	THR

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	313	LEU
1	A	319	GLU
1	A	325	VAL
1	A	329	VAL
1	A	331	VAL
1	A	335	ILE
1	A	359	GLU
1	A	368	THR
1	A	370	LEU
1	A	384	LEU
1	A	386	ASP
1	A	391	THR
1	A	398	ARG
1	A	419	SER
1	A	427	VAL
1	A	428	LYS
1	A	434	ILE
1	A	440	GLU
1	A	442	LYS
1	A	451	ARG
1	A	455	VAL
1	A	472	THR
1	A	473	SER
1	A	487	LEU
1	A	490	ILE
1	A	491	GLN
1	A	496	ARG
1	A	518	LYS
1	A	519	ARG
1	A	525	GLU
1	A	526	LEU
1	A	528	SER
1	A	535	SER
1	A	536	LYS
1	A	542	LYS
1	A	547	GLU
1	A	551	LYS
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	592	SER

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Mol	Chain	Res	Type
1	A	607	TRP
1	A	613	ASP
1	A	620	LYS
1	A	631	ARG
1	A	649	VAL
1	A	672	ASP
1	A	679	SER
1	A	685	GLN
1	A	703	THR
1	A	715	ARG
1	A	719	THR
1	A	721	GLU
1	A	725	LYS
1	A	743	MET
1	A	750	LYS
1	A	755	LEU
1	A	760	LYS
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	784	LYS
1	A	811	ASN
1	A	828	ILE
1	A	831	MET
1	A	835	SER
1	A	843	THR
1	A	855	LYS
1	A	861	ILE
1	A	863	GLN
1	A	870	GLN
1	A	876	GLN
1	A	879	LYS
1	A	880	SER
1	A	904	ILE
1	A	907	VAL
1	A	908	THR
1	A	919	LEU
1	A	923	GLN
1	A	926	LEU
1	A	931	VAL
1	A	932	ILE
1	A	944	VAL

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Mol	Chain	Res	Type
1	A	945	VAL
1	A	952	ILE
1	A	961	LYS
1	A	980	GLU
1	A	985	VAL
1	A	993	LEU
1	A	996	GLU
1	A	999	GLN
1	A	1002	VAL
1	A	1008	ILE
1	A	1018	GLU
1	A	1019	GLN
1	A	1043	ARG
1	A	1044	ASN
1	A	1048	VAL
1	A	1051	GLU
1	A	1064	THR
1	A	1076	ILE
1	A	1080	MET
1	A	1089	ILE
1	B	36	GLN
1	B	38	LYS
1	B	44	ASN
1	B	62	SER
1	B	70	GLU
1	B	75	LEU
1	B	90	LEU
1	B	94	GLU
1	B	98	ASN
1	B	101	ARG
1	B	102	ILE
1	B	124	ASN
1	B	137	LYS
1	B	139	ILE
1	B	144	GLU
1	B	147	ASP
1	B	152	LYS
1	B	153	VAL
1	B	166	VAL
1	B	167	ILE
1	B	239	ILE
1	B	241	ASN

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Mol	Chain	Res	Type
1	B	268	GLN
1	B	270	ARG
1	B	281	VAL
1	B	287	LEU
1	B	288	ARG
1	B	289	GLN
1	B	291	ILE
1	B	300	GLU
1	B	309	THR
1	B	315	SER
1	B	319	GLU
1	B	320	PHE
1	B	331	VAL
1	B	345	VAL
1	B	351	VAL
1	B	357	LEU
1	B	357(A)	PHE
1	B	359	GLU
1	B	361	ASN
1	B	365	LYS
1	B	368	THR
1	B	370	LEU
1	B	376	CYS
1	B	391	THR
1	B	395	ILE
1	B	399	SER
1	B	400	SER
1	B	406	ARG
1	B	417	GLU
1	B	418	ILE
1	B	423	ASP
1	B	427	VAL
1	B	434	ILE
1	B	435	SER
1	B	437	LYS
1	B	442	LYS
1	B	446	SER
1	B	449	GLU
1	B	451	ARG
1	B	453	ARG
1	B	479	LYS
1	B	481	ILE

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Mol	Chain	Res	Type
1	B	487	LEU
1	B	494	LEU
1	B	500	THR
1	B	509	ILE
1	B	534	SER
1	B	542	LYS
1	B	547	GLU
1	B	548	VAL
1	B	551	LYS
1	B	559	LYS
1	B	576	SER
1	B	580	THR
1	B	606	MET
1	B	607	TRP
1	B	631	ARG
1	B	632	LYS
1	B	647	ASN
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS
1	B	685	GLN
1	B	715	ARG
1	B	721	GLU
1	B	725	LYS
1	B	740	ILE
1	B	743	MET
1	B	750	LYS
1	B	756	ILE
1	B	761	SER
1	B	766	LEU
1	B	775	THR
1	B	791	VAL
1	B	809	SER
1	B	811	ASN
1	B	812	SER
1	B	828	ILE
1	B	831	MET
1	B	839	SER
1	B	843	THR
1	B	853	ASP
1	B	855	LYS
1	B	863	GLN

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Mol	Chain	Res	Type
1	B	872	SER
1	B	875	SER
1	B	876	GLN
1	B	879	LYS
1	B	880	SER
1	B	881	LEU
1	B	886	ARG
1	B	897	VAL
1	B	906	LYS
1	B	907	VAL
1	B	908	THR
1	B	919	LEU
1	B	921	MET
1	B	926	LEU
1	B	927	ASP
1	B	929	GLN
1	B	934	ASP
1	B	936	TYR
1	B	938	LEU
1	B	939	ASP
1	B	942	GLU
1	B	944	VAL
1	B	949	LYS
1	B	957	ASN
1	B	962	ASP
1	B	963	LEU
1	B	967	ILE
1	B	998	GLN
1	B	1008	ILE
1	B	1019	GLN
1	B	1057	ARG
1	B	1070	GLU
1	B	1076	ILE
1	B	1085	ARG
1	B	1089	ILE
1	C	41	LEU
1	C	44	ASN
1	C	45	ARG
1	C	69	ASN
1	C	70	GLU
1	C	72	LYS
1	C	75	LEU

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Mol	Chain	Res	Type
1	C	77	ARG
1	C	86	VAL
1	C	90	LEU
1	C	97	LEU
1	C	98	ASN
1	C	100	GLU
1	C	101	ARG
1	C	110	ASN
1	C	123	GLU
1	C	144	GLU
1	C	151	ASP
1	C	153	VAL
1	C	154	LYS
1	C	156	ARG
1	C	166	VAL
1	C	167	ILE
1	C	174	ILE
1	C	175	LYS
1	C	178	GLU
1	C	179	LEU
1	C	192	MET
1	C	193	ILE
1	C	194	LYS
1	C	202	LYS
1	C	205	ARG
1	C	208	ARG
1	C	209	GLU
1	C	210	GLU
1	C	219	ARG
1	C	223	GLU
1	C	225	GLU
1	C	230	ASN
1	C	232	GLU
1	C	234	TYR
1	C	235	ILE
1	C	249	VAL
1	C	250	ILE
1	C	253	GLU
1	C	257	ILE
1	C	262	GLU
1	C	269	ARG
1	C	280	SER

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Mol	Chain	Res	Type
1	C	286	THR
1	C	287	LEU
1	C	288	ARG
1	C	289	GLN
1	C	313	LEU
1	C	315	SER
1	C	323	ILE
1	C	324	GLU
1	C	335	ILE
1	C	342	ILE
1	C	358	GLU
1	C	359	GLU
1	C	360	ILE
1	C	363	GLN
1	C	365	LYS
1	C	368	THR
1	C	377	ARG
1	C	384	LEU
1	C	386	ASP
1	C	388	MET
1	C	391	THR
1	C	395	ILE
1	C	414	GLN
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	442	LYS
1	C	444	VAL
1	C	445	ARG
1	C	446	SER
1	C	451	ARG
1	C	453	ARG
1	C	459	ILE
1	C	467	LYS
1	C	469	LYS
1	C	473	SER
1	C	491	GLN
1	C	493	SER
1	C	494	LEU
1	C	531	THR
1	C	533	SER
1	C	537	ILE

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Mol	Chain	Res	Type
1	C	539	SER
1	C	542	LYS
1	C	543	GLN
1	C	545	LEU
1	C	557	VAL
1	C	559	LYS
1	C	563	VAL
1	C	580	THR
1	C	590	ILE
1	C	606	MET
1	C	607	TRP
1	C	627	LEU
1	C	631	ARG
1	C	641	MET
1	C	642	LEU
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	652	LYS
1	C	653	ASN
1	C	660	HIS
1	C	661	LYS
1	C	680	LEU
1	C	685	GLN
1	C	695	GLU
1	C	707	THR
1	C	717	ASN
1	C	717(A)	ILE
1	C	719	THR
1	C	720	LEU
1	C	725	LYS
1	C	726	LEU
1	C	743	MET
1	C	750	LYS
1	C	760	LYS
1	C	781	LEU
1	C	783	TYR
1	C	784	LYS
1	C	807	GLN
1	C	811	ASN
1	C	828	ILE
1	C	833	SER

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Mol	Chain	Res	Type
1	C	835	SER
1	C	839	SER
1	C	843	THR
1	C	852	SER
1	C	854	ILE
1	C	855	LYS
1	C	856	SER
1	C	861	ILE
1	C	863	GLN
1	C	866	MET
1	C	870	GLN
1	C	876	GLN
1	C	879	LYS
1	C	881	LEU
1	C	885	GLU
1	C	892	ASP
1	C	893	MET
1	C	895	ARG
1	C	896	ARG
1	C	907	VAL
1	C	908	THR
1	C	911	SER
1	C	914	VAL
1	C	923	GLN
1	C	927	ASP
1	C	928	GLU
1	C	938	LEU
1	C	949	LYS
1	C	952	ILE
1	C	959	PHE
1	C	960	ASN
1	C	967	ILE
1	C	968	LEU
1	C	971	GLN
1	C	980	GLU
1	C	986	ASP
1	C	997	GLU
1	C	1008	ILE
1	C	1015	LYS
1	C	1021	ILE
1	C	1023	THR
1	C	1024	ARG

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Mol	Chain	Res	Type
1	C	1031	SER
1	C	1048	VAL
1	C	1052	ILE
1	C	1062	LEU
1	C	1067	GLU
1	C	1076	ILE
1	C	1085	ARG
1	C	1089	ILE
1	C	1090	LYS
1	D	37	ILE
1	D	38	LYS
1	D	44	ASN
1	D	70	GLU
1	D	72	LYS
1	D	73	SER
1	D	75	LEU
1	D	77	ARG
1	D	79	LYS
1	D	88	SER
1	D	99	ILE
1	D	101	ARG
1	D	137	LYS
1	D	143	LEU
1	D	144	GLU
1	D	163	ASP
1	D	167	ILE
1	D	239	ILE
1	D	240	ASP
1	D	243	LYS
1	D	250	ILE
1	D	253	GLU
1	D	260	LEU
1	D	262	GLU
1	D	268	GLN
1	D	270	ARG
1	D	280	SER
1	D	287	LEU
1	D	290	ARG
1	D	302	ILE
1	D	305	VAL
1	D	306	ASN
1	D	310	VAL

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Mol	Chain	Res	Type
1	D	326	ASN
1	D	329	VAL
1	D	331	VAL
1	D	335	ILE
1	D	358	GLU
1	D	360	ILE
1	D	361	ASN
1	D	365	LYS
1	D	368	THR
1	D	369	THR
1	D	378	ILE
1	D	393	THR
1	D	395	ILE
1	D	417	GLU
1	D	418	ILE
1	D	425	LEU
1	D	427	VAL
1	D	434	ILE
1	D	437	LYS
1	D	442	LYS
1	D	444	VAL
1	D	445	ARG
1	D	446	SER
1	D	451	ARG
1	D	452	ILE
1	D	456	LYS
1	D	467	LYS
1	D	470	LYS
1	D	473	SER
1	D	478	THR
1	D	479	LYS
1	D	486	GLU
1	D	487	LEU
1	D	491	GLN
1	D	496	ARG
1	D	506	ASN
1	D	519	ARG
1	D	523	ASP
1	D	525	GLU
1	D	526	LEU
1	D	528	SER
1	D	531	THR

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Mol	Chain	Res	Type
1	D	533	SER
1	D	542	LYS
1	D	543	GLN
1	D	551	LYS
1	D	555	GLU
1	D	565	LEU
1	D	566	THR
1	D	580	THR
1	D	590	ILE
1	D	607	TRP
1	D	620	LYS
1	D	629	ARG
1	D	631	ARG
1	D	632	LYS
1	D	641	MET
1	D	647	ASN
1	D	649	VAL
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	725	LYS
1	D	743	MET
1	D	750	LYS
1	D	756	ILE
1	D	760	LYS
1	D	763	VAL
1	D	766	LEU
1	D	775	THR
1	D	784	LYS
1	D	791	VAL
1	D	811	ASN
1	D	828	ILE
1	D	831	MET
1	D	839	SER
1	D	843	THR
1	D	852	SER
1	D	853	ASP
1	D	854	ILE
1	D	855	LYS
1	D	856	SER
1	D	863	GLN
1	D	866	MET

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Mol	Chain	Res	Type
1	D	870	GLN
1	D	885	GLU
1	D	907	VAL
1	D	908	THR
1	D	911	SER
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	927	ASP
1	D	944	VAL
1	D	945	VAL
1	D	952	ILE
1	D	963	LEU
1	D	983	GLU
1	D	996	GLU
1	D	1002	VAL
1	D	1046	GLU
1	D	1052	ILE
1	D	1054	LYS
1	D	1057	ARG
1	D	1064	THR
1	D	1065	ILE
1	D	1080	MET
1	D	1083	GLN
1	D	1085	ARG
1	D	1089	ILE
1	D	1090	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN
1	A	108	GLN
1	A	126	GLN
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	297	GLN
1	A	375	GLN
1	A	432	HIS

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Mol	Chain	Res	Type
1	A	506	ASN
1	A	543	GLN
1	A	575	GLN
1	A	589	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	863	GLN
1	A	864	HIS
1	A	877	GLN
1	A	898	ASN
1	A	923	GLN
1	A	1005	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	B	36	GLN
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	126	GLN
1	B	145	HIS
1	B	254	HIS
1	B	256	ASN
1	B	272	GLN
1	B	301	ASN
1	B	361	ASN
1	B	363	GLN
1	B	375	GLN
1	B	432	HIS
1	B	438	GLN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	622	ASN
1	B	690	ASN
1	B	694	GLN

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Mol	Chain	Res	Type
1	B	736	HIS
1	B	778	ASN
1	B	785	GLN
1	B	811	ASN
1	B	863	GLN
1	B	864	HIS
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	998	GLN
1	B	1005	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1071	ASN
1	B	1073	ASN
1	C	44	ASN
1	C	98	ASN
1	C	110	ASN
1	C	145	HIS
1	C	218	HIS
1	C	230	ASN
1	C	268	GLN
1	C	289	GLN
1	C	301	ASN
1	C	326	ASN
1	C	330	GLN
1	C	414	GLN
1	C	432	HIS
1	C	464	ASN
1	C	506	ASN
1	C	515	ASN
1	C	574	HIS
1	C	575	GLN
1	C	617	ASN
1	C	622	ASN
1	C	685	GLN
1	C	694	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	785	GLN

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Mol	Chain	Res	Type
1	C	807	GLN
1	C	811	ASN
1	C	818	ASN
1	C	858	ASN
1	C	863	GLN
1	C	864	HIS
1	C	873	ASN
1	C	876	GLN
1	C	877	GLN
1	C	898	ASN
1	C	923	GLN
1	C	924	ASN
1	C	954	GLN
1	C	964	GLN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	D	44	ASN
1	D	69	ASN
1	D	145	HIS
1	D	244	HIS
1	D	256	ASN
1	D	326	ASN
1	D	330	GLN
1	D	363	GLN
1	D	364	GLN
1	D	375	GLN
1	D	432	HIS
1	D	468	ASN
1	D	491	GLN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	807	GLN

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Mol	Chain	Res	Type
1	D	811	ASN
1	D	818	ASN
1	D	858	ASN
1	D	864	HIS
1	D	898	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1025	ASN
1	D	1026	GLN
1	D	1083	GLN
1	D	1093	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BTI	D	1201	-	15,16,16	1.67	2 (13%)	20,21,21	1.89	4 (20%)
4	BTI	B	1201	-	15,16,16	1.65	2 (13%)	20,21,21	2.28	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BTI	A	1203	-	15,16,16	1.73	2 (13%)	20,21,21	1.75	3 (15%)
5	ATP	C	1202	-	32,33,33	1.55	6 (18%)	48,52,52	1.75	10 (20%)
2	ADP	A	1201	-	28,29,29	1.62	5 (17%)	43,45,45	1.88	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTI	D	1201	-	-	2/6/27/27	0/2/2/2
4	BTI	B	1201	-	-	4/6/27/27	0/2/2/2
4	BTI	A	1203	-	-	4/6/27/27	0/2/2/2
5	ATP	C	1202	-	-	3/22/38/38	0/3/3/3
2	ADP	A	1201	-	-	7/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	O3-C3	5.05	1.34	1.23
4	B	1201	BTI	O3-C3	5.02	1.34	1.23
5	C	1202	ATP	C5-C4	4.90	1.47	1.39
4	D	1201	BTI	O3-C3	4.83	1.33	1.23
2	A	1201	ADP	C5-C4	4.67	1.47	1.39
2	A	1201	ADP	PA-O3A	4.36	1.64	1.59
5	C	1202	ATP	PB-O3B	4.31	1.64	1.59
4	A	1203	BTI	C2-S1	-3.66	1.76	1.82
4	D	1201	BTI	C2-S1	-3.38	1.77	1.82
4	B	1201	BTI	C2-S1	-3.02	1.77	1.82
2	A	1201	ADP	C5-C6	2.74	1.48	1.41
5	C	1202	ATP	C5-C6	2.60	1.48	1.41
2	A	1201	ADP	C5-N7	-2.56	1.34	1.39
5	C	1202	ATP	C8-N7	2.47	1.36	1.31
5	C	1202	ATP	C5-N7	-2.10	1.35	1.39
5	C	1202	ATP	PB-O3A	2.10	1.61	1.59
2	A	1201	ADP	C8-N7	2.02	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	-7.48	105.42	113.34
2	A	1201	ADP	C5-C4-N3	-5.93	118.55	126.72
5	C	1202	ATP	C5-C4-N3	-5.64	118.95	126.72
4	D	1201	BTI	C2-C4-N2	-5.24	107.80	113.34
4	B	1201	BTI	C6-C5-N3	-4.96	106.80	113.18
4	A	1203	BTI	C6-C5-N3	-4.95	106.80	113.18
4	D	1201	BTI	C6-C5-N3	-4.72	107.10	113.18
2	A	1201	ADP	N3-C4-N9	4.66	135.09	127.17
5	C	1202	ATP	N3-C4-N9	4.44	134.72	127.17
2	A	1201	ADP	C2-N3-C4	3.75	120.98	111.83
5	C	1202	ATP	C2'-C1'-N9	-3.72	104.06	113.30
5	C	1202	ATP	C4-C5-N7	-3.45	106.64	110.58
2	A	1201	ADP	N3-C2-N1	-3.45	123.36	128.58
5	C	1202	ATP	C2-N3-C4	3.43	120.20	111.83
4	A	1203	BTI	C5-C6-S1	3.26	110.56	106.06
2	A	1201	ADP	C4-C5-N7	-3.22	106.89	110.58
5	C	1202	ATP	N3-C2-N1	-2.95	124.12	128.58
5	C	1202	ATP	C5-N7-C8	2.58	107.51	103.45
4	B	1201	BTI	C4-C2-S1	2.56	107.94	105.03
5	C	1202	ATP	C4-N9-C8	2.56	108.42	105.74
4	D	1201	BTI	C8-C7-C2	-2.40	108.52	114.04
2	A	1201	ADP	C3'-C2'-C1'	2.38	105.96	101.46
2	A	1201	ADP	C5-N7-C8	2.35	107.15	103.45
2	A	1201	ADP	C2'-C1'-N9	-2.23	107.77	113.30
4	D	1201	BTI	N2-C3-N3	2.20	111.39	108.85
5	C	1202	ATP	C6-C5-N7	2.17	136.27	132.09
2	A	1201	ADP	O3B-PB-O2B	2.15	115.86	107.80
2	A	1201	ADP	O4'-C1'-N9	2.15	112.21	108.09
4	B	1201	BTI	O3-C3-N2	-2.09	122.89	125.89
2	A	1201	ADP	C2-N1-C6	2.08	122.15	118.73
2	A	1201	ADP	C2'-C3'-C4'	2.08	106.63	102.61
4	A	1203	BTI	C4-C2-S1	2.03	107.34	105.03
5	C	1202	ATP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O1A
2	A	1201	ADP	C5'-O5'-PA-O2A
4	A	1203	BTI	C11-C10-C9-C8
4	A	1203	BTI	S1-C2-C7-C8
4	A	1203	BTI	C4-C2-C7-C8

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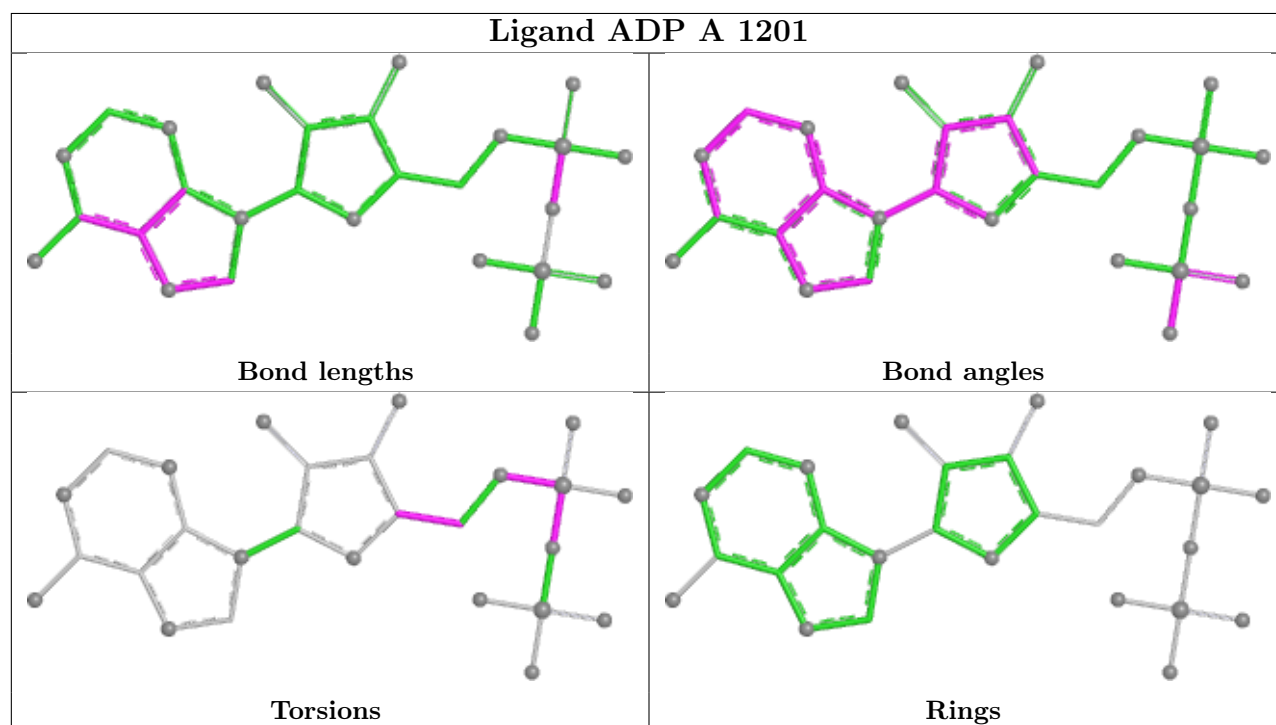
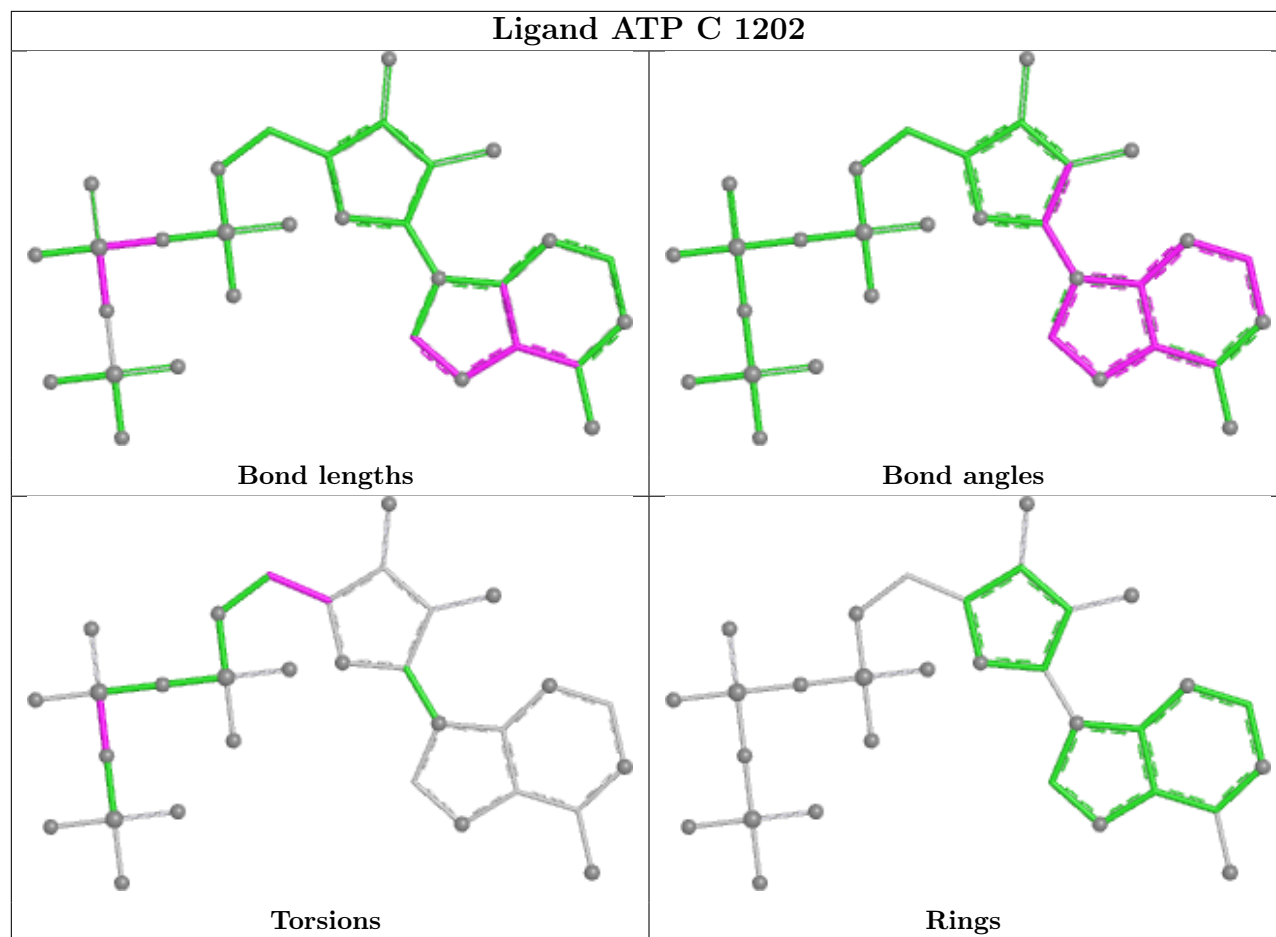
Mol	Chain	Res	Type	Atoms
4	B	1201	BTI	C9-C10-C11-O11
4	B	1201	BTI	S1-C2-C7-C8
4	D	1201	BTI	C9-C10-C11-O11
5	C	1202	ATP	O4'-C4'-C5'-O5'
5	C	1202	ATP	C3'-C4'-C5'-O5'
2	A	1201	ADP	C3'-C4'-C5'-O5'
2	A	1201	ADP	O4'-C4'-C5'-O5'
4	A	1203	BTI	C7-C8-C9-C10
4	B	1201	BTI	C4-C2-C7-C8
5	C	1202	ATP	PG-O3B-PB-O1B
4	B	1201	BTI	C11-C10-C9-C8
2	A	1201	ADP	C5'-O5'-PA-O3A
4	D	1201	BTI	C2-C7-C8-C9
2	A	1201	ADP	PB-O3A-PA-O1A
2	A	1201	ADP	PB-O3A-PA-O2A

There are no ring outliers.

5 monomers are involved in 23 short contacts:

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	936:TYR	C	937:LYS	N	1.60

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1052/1173 (89%)	-0.25	7 (0%) 84 77	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.19	7 (0%) 84 77	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.14	9 (0%) 82 75	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.24	6 (0%) 85 80	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.21	29 (0%) 84 77	47, 80, 125, 178	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	915	GLY	5.5
1	A	233	VAL	4.4
1	C	935	GLY	4.1
1	C	198	GLY	3.6
1	B	167	ILE	3.6
1	B	168	PRO	3.3
1	A	220	ALA	3.1
1	C	206	ILE	2.8
1	C	932	ILE	2.7
1	A	271	HIS	2.7
1	B	1003	THR	2.7
1	B	239	ILE	2.7
1	C	887	PHE	2.6
1	D	567	ASP	2.6
1	B	265	CYS	2.4
1	D	307	ALA	2.3
1	D	490	ILE	2.2
1	C	892	ASP	2.2
1	D	515	ASN	2.2
1	C	944	VAL	2.2
1	A	255	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	317	GLY	2.1
1	B	966	VAL	2.1
1	D	903	ASP	2.1
1	A	1008	ILE	2.1
1	A	280	SER	2.1
1	A	1072	GLY	2.0
1	C	982	LEU	2.0
1	B	1000	GLY	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](#)

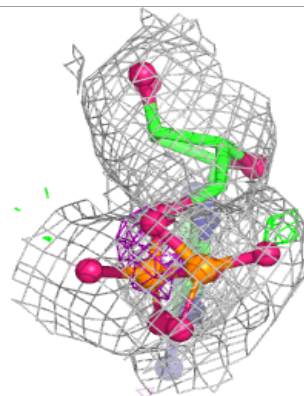
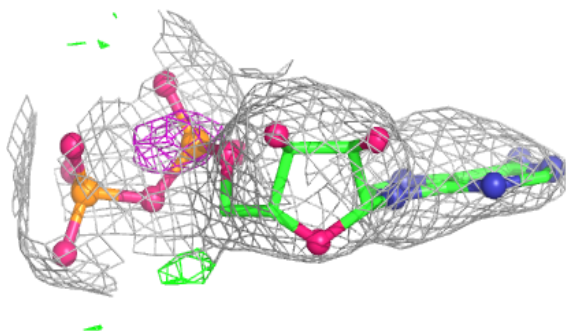
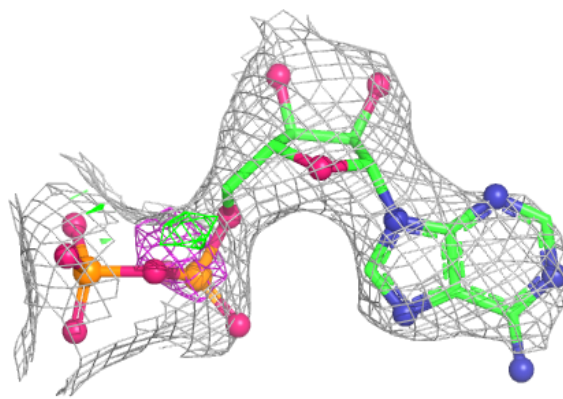
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	1201	27/27	0.85	0.10	86,91,110,110	0
4	BTI	B	1201	15/15	0.88	0.12	105,109,114,115	0
4	BTI	A	1203	15/15	0.89	0.12	92,99,104,105	0
4	BTI	D	1201	15/15	0.90	0.11	105,109,113,116	0
5	ATP	C	1202	31/31	0.90	0.09	102,108,115,115	0
3	MN	B	1202	1/1	0.96	0.05	82,82,82,82	0
3	MN	C	1201	1/1	0.98	0.08	76,76,76,76	0
3	MN	D	1202	1/1	0.98	0.04	74,74,74,74	0
3	MN	A	1202	1/1	0.98	0.04	74,74,74,74	0

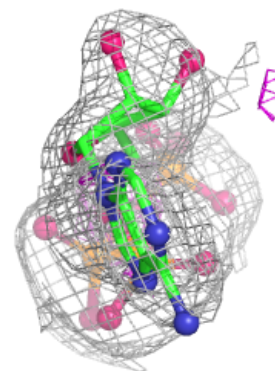
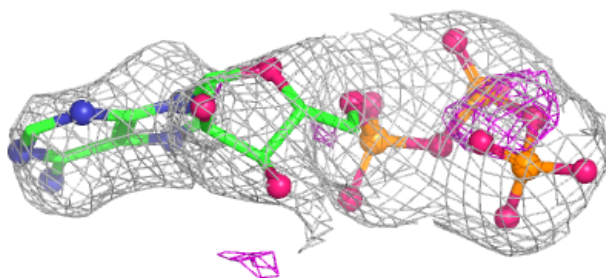
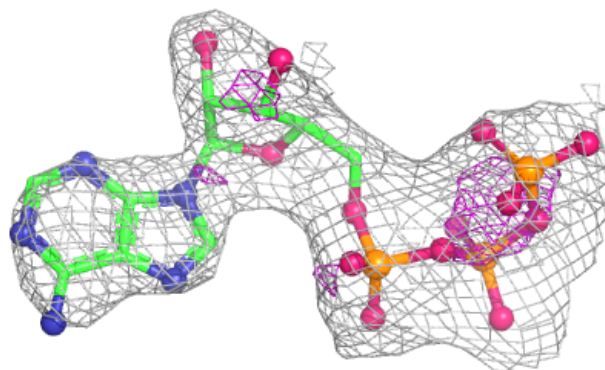
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP C 1202:**

$2mF_o - DF_c$ (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.