



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:23 AM UTC

PDB ID : 4HNU / pdb_00004hnu
Title : crystal structure of K442E mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

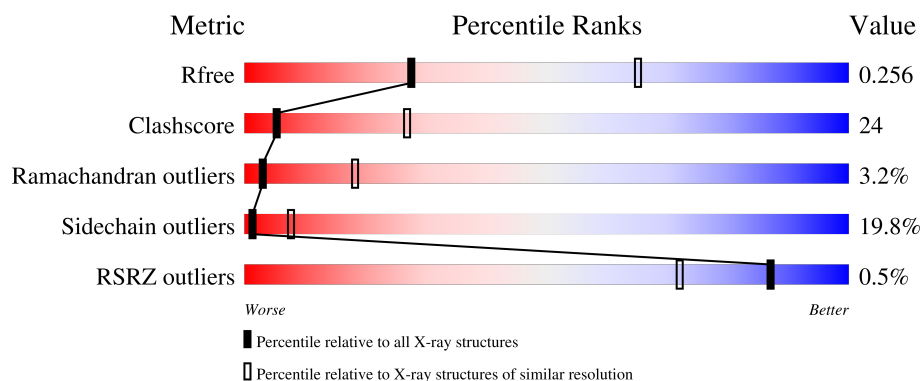
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 46% 33% 10% • 10%
1	B	1173	44% 32% 7% • 16%
1	C	1173	% 45% 34% 10% • 10%
1	D	1173	45% 30% 9% • 16%

2 Entry composition

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

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

- Molecule 1 is a protein called Pyruvate carboxylase.

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

There are 96 discrepancies between the modelled and reference sequences:

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

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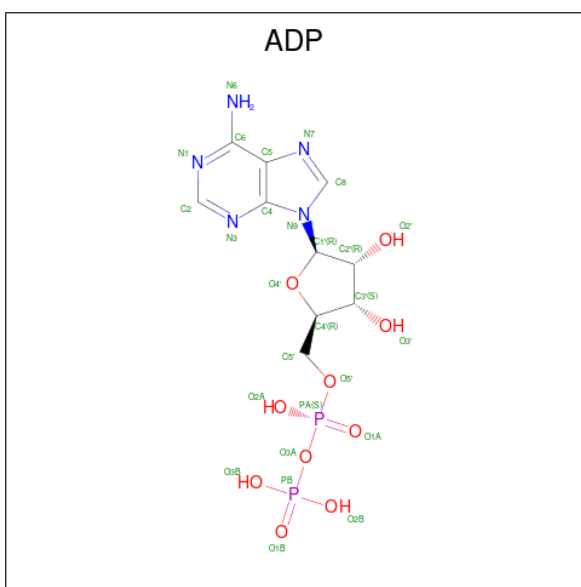
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	expression tag	UNP Q99UY8
A	33	SER	-	expression tag	UNP Q99UY8
A	442	GLU	LYS	engineered mutation	UNP Q99UY8
B	11	MET	-	expression tag	UNP Q99UY8
B	12	GLY	-	expression tag	UNP Q99UY8
B	13	SER	-	expression tag	UNP Q99UY8
B	14	SER	-	expression tag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

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

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

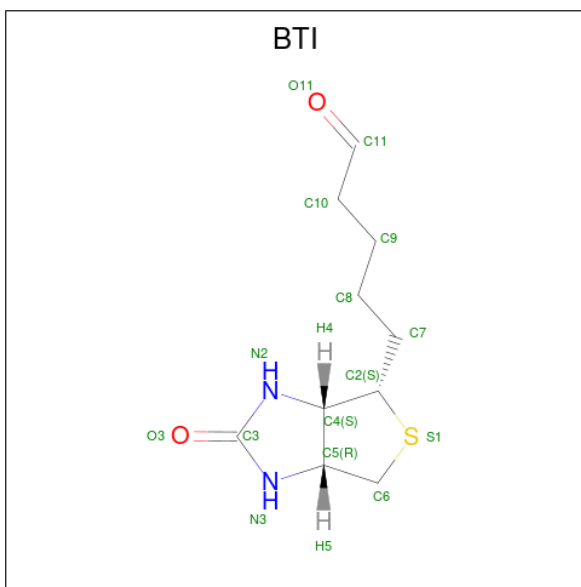


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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

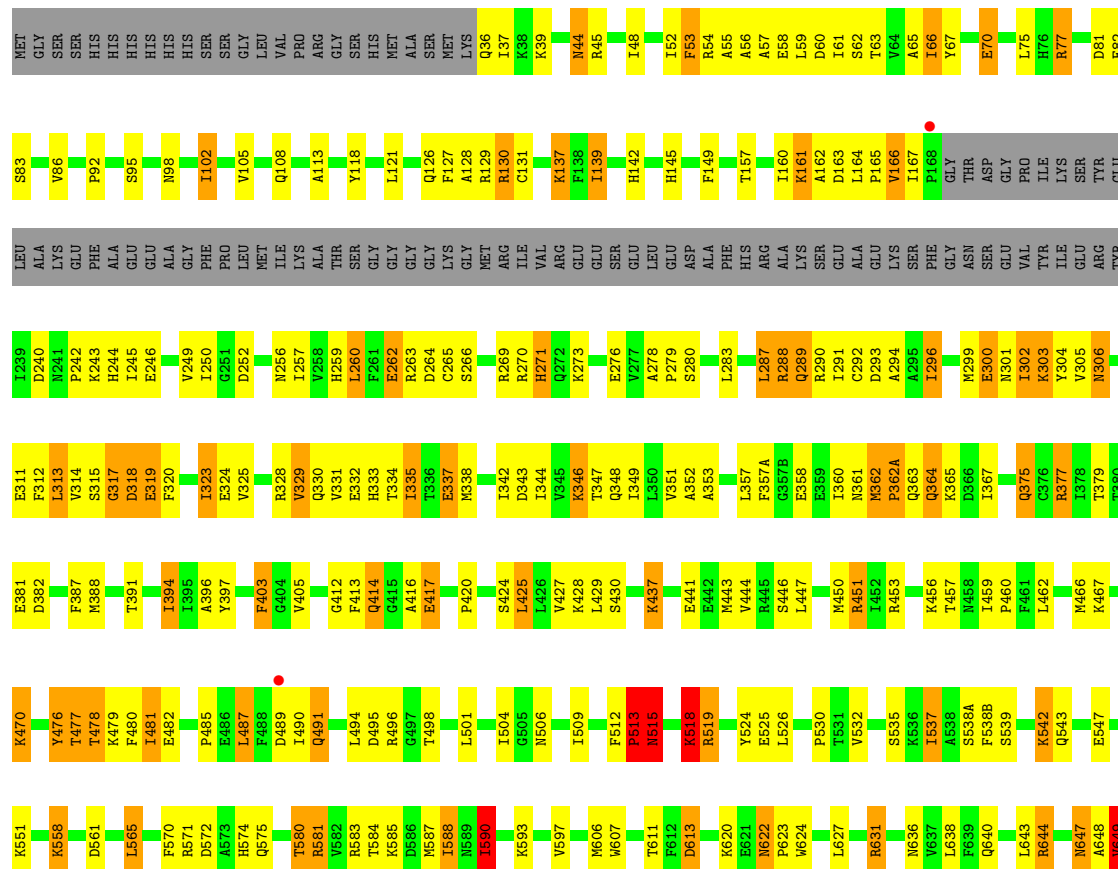
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

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





PHE	ASP	GLY	VAL	ILE	LYS	GLN	VAL	THR	VAL	ASN	ASN	VAL	VAL	THR	ASN	ALA	THR	ALA	ASP	GLY	ASN	ASP	THR	ILE	ILE	ALA	THR	GLY	ASP	LEU	LEU	ILE	ILE	GLU	ILE	GLU	LYS	ALA	THR	ASP										
W1093	VAL	HIS	THR	ASN	ALA	ASN	VAL	VAL	LYS	PRO	ASN	PRO	THR	THR	ALA	THR	THR	GLY	ASP	LEU	LEU	ILE	ILE	PRO	GLY	GLY	VAL	VAL	SER	VAL	THR	GLU	VAL	LYS	LYS	ALA	ALA	THR	PRO											
E997	Q998	Q999	G1000	P1001	Q1005	T1008	Y1013	P1014	E1018	T1035	M1042	E1051	I1052	D1053	K1054	G1055	K1056	R1057	L1058	I1059	I1060	K1061	L1062	E1063	T1064	I1065	S1066	E1067	P1068	D1069	E1070	N1071	G1072	N1073	R1074	T1075	I1076	Y1077	Y1078	M1080	N1081	G1082	Q1083	A1084	R1085	R1086	I1087	Y1088	K1090	
F901	V905	K906	V907	T908	P909	V914	M917	A918	L919	Y920	N924	D925	L926	D927	E928	Q929	S930	G935	L938	D939	F940	V944	V945	S946	F947	F948	K949	G950	E951	I952	N960	K961	D962	L963	V966	I967	T975	A976	R977	E983	D986	R991	L994	E995	E996					
L824	T828	E829	E832	Y837	T840	V841	R842	T843	D847	F848	E849	I854	K855	S856	P857	N858	T859	E860	I861	Q862	Q863	H864	E865	N866	P867	Q868	G869	Q870	S871	S872	N873	L874	S875	Q876	Q877	A878	K879	S880	L881	G882	L883	G884	E885	R886	F887	K891	Y894	R895	V896	V897
A739	M743	A744	G745	L746	K750	A751	E754	E758	L759	K760	S761	A762	V763	D765	L766	P767	I768	H769	T772	H773	D774	T775	S776	G777	N778	L781	T782	Y783	K784	V791	V798	A799	S800	N801	S802	Q807	P808	S809	A810	N811	S812	L813	Y814	N818	Q819	F820	P821	R822	H823	
G650	Y651	K652	K653	Y654	Q664	K668	A669	G670	I671	D672	V673	I676	F677	D678	S679	V683	D684	Q685	N686	K687	V688	V693	K698	T699	S700	E701	G702	T707	G708	L711	N712	P713	E714	S715	N717	I717A	L720	E721	Y722	K725	K728	E731	H736	I737	L738					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.57Å 258.52Å 126.90Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.00) 98.3 (30.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.256	Depositor DCC
R_{free} test set	5851 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32443	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	4/8504 (0.0%)	0.97	14/11500 (0.1%)
1	B	0.61	6/7990 (0.1%)	0.87	14/10811 (0.1%)
1	C	0.67	8/8542 (0.1%)	0.90	14/11549 (0.1%)
1	D	0.76	7/7990 (0.1%)	0.97	28/10811 (0.3%)
All	All	0.70	25/33026 (0.1%)	0.93	70/44671 (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	3
1	B	0	2
1	C	0	1
1	D	0	3
All	All	0	9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	SER	CA-C	11.33	1.66	1.53
1	B	513	PRO	CA-C	11.04	1.66	1.52
1	C	515	ASN	N-CA	10.26	1.59	1.46
1	C	513	PRO	CA-C	8.95	1.65	1.52
1	C	849	GLU	N-CA	8.88	1.57	1.46
1	B	513	PRO	C-N	8.19	1.45	1.33
1	D	513	PRO	CA-C	8.13	1.64	1.52
1	C	849	GLU	CA-C	8.13	1.64	1.52
1	B	515	ASN	N-CA	7.68	1.58	1.46
1	A	441	GLU	CA-C	-7.16	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	763	VAL	CA-C	7.16	1.61	1.52
1	C	765	ASP	N-CA	7.08	1.55	1.46
1	B	763	VAL	CA-C	6.88	1.60	1.52
1	D	513	PRO	N-CA	6.45	1.55	1.47
1	D	849	GLU	N-CA	6.39	1.54	1.45
1	C	763	VAL	C-N	6.30	1.43	1.33
1	C	513	PRO	C-N	6.19	1.42	1.33
1	A	513	PRO	CA-C	6.01	1.60	1.52
1	B	512	PHE	C-N	5.78	1.40	1.33
1	D	765	ASP	N-CA	5.77	1.53	1.46
1	A	440	GLU	C-N	-5.72	1.25	1.33
1	D	315	SER	C-N	5.50	1.41	1.33
1	A	763	VAL	N-CA	5.17	1.52	1.46
1	B	849	GLU	CA-C	5.07	1.59	1.52
1	D	513	PRO	C-N	5.02	1.40	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	765	ASP	N-CA-C	-11.76	100.50	112.97
1	D	952	ILE	N-CA-C	-10.32	103.30	113.20
1	D	977	ARG	CA-C-N	8.83	128.47	119.82
1	D	977	ARG	C-N-CA	8.83	128.47	119.82
1	D	849	GLU	CA-C-N	-7.91	108.81	121.86
1	D	849	GLU	C-N-CA	-7.91	108.81	121.86
1	D	1000	GLY	CA-C-N	7.81	129.60	119.84
1	D	1000	GLY	C-N-CA	7.81	129.60	119.84
1	D	315	SER	N-CA-C	7.76	121.46	110.68
1	C	512	PHE	CA-C-N	-7.49	110.48	119.84
1	C	512	PHE	C-N-CA	-7.49	110.48	119.84
1	C	849	GLU	N-CA-C	7.44	121.05	109.96
1	C	509	ILE	N-CA-C	7.35	117.88	111.56
1	A	828	ILE	CB-CA-C	-7.11	102.86	111.97
1	D	315	SER	N-CA-CB	-7.01	101.61	110.45
1	C	513	PRO	N-CA-CB	-6.85	96.05	103.25
1	C	513	PRO	CA-N-CD	6.85	121.59	112.00
1	B	512	PHE	CA-C-N	6.75	127.16	119.93
1	B	512	PHE	C-N-CA	6.75	127.16	119.93
1	C	828	ILE	CB-CA-C	-6.62	103.35	112.02
1	A	382	ASP	CA-C-N	6.57	125.80	118.97
1	A	382	ASP	C-N-CA	6.57	125.80	118.97
1	B	513	PRO	CA-C-N	6.56	131.92	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	PRO	C-N-CA	6.56	131.92	122.35
1	D	763	VAL	CA-C-N	6.54	132.59	121.14
1	D	763	VAL	C-N-CA	6.54	132.59	121.14
1	D	513	PRO	N-CA-C	6.49	125.85	112.47
1	A	441	GLU	CA-C-O	6.48	127.90	120.00
1	B	167	ILE	N-CA-C	6.36	115.55	108.05
1	B	91	GLY	CA-C-N	6.33	125.75	118.85
1	B	91	GLY	C-N-CA	6.33	125.75	118.85
1	D	812	SER	N-CA-C	-6.32	104.26	112.23
1	A	703	THR	N-CA-C	6.32	118.71	108.41
1	D	849	GLU	O-C-N	-6.27	115.88	122.96
1	C	654	TYR	CA-C-N	6.22	126.19	119.78
1	C	654	TYR	C-N-CA	6.22	126.19	119.78
1	A	441	GLU	O-C-N	6.03	131.15	122.28
1	A	416	ALA	N-CA-C	5.91	117.92	110.24
1	A	548	VAL	N-CA-C	5.90	117.77	112.17
1	D	849	GLU	CA-C-O	-5.86	114.73	121.47
1	D	515	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	831	MET	N-CA-C	5.71	118.24	111.33
1	D	512	PHE	CA-C-N	5.64	126.89	119.84
1	D	512	PHE	C-N-CA	5.64	126.89	119.84
1	D	848	PHE	O-C-N	-5.60	115.47	122.35
1	C	427	VAL	CB-CA-C	-5.58	101.06	110.71
1	D	828	ILE	N-CA-CB	5.55	118.09	110.54
1	D	832	GLU	N-CA-C	-5.53	105.17	111.14
1	B	1007	ILE	N-CA-C	5.51	116.57	111.45
1	B	164	LEU	CA-C-N	5.48	125.47	120.21
1	B	164	LEU	C-N-CA	5.48	125.47	120.21
1	A	314	VAL	N-CA-C	5.46	115.97	107.28
1	C	826	THR	N-CA-C	5.46	116.83	108.42
1	A	820	PHE	CA-C-N	5.42	124.61	118.97
1	A	820	PHE	C-N-CA	5.42	124.61	118.97
1	D	938	LEU	N-CA-C	5.38	120.49	113.88
1	B	166	VAL	N-CA-C	5.27	120.31	109.34
1	B	904	ILE	N-CA-C	5.26	116.72	109.46
1	C	1002	VAL	N-CA-C	5.25	113.94	106.53
1	C	206	ILE	N-CA-C	5.21	114.81	106.88
1	C	481	ILE	N-CA-C	5.20	115.35	110.30
1	D	590	ILE	CB-CA-C	-5.19	104.77	111.88
1	D	565	LEU	N-CA-C	5.17	118.02	109.85
1	B	39	LYS	N-CA-C	5.14	117.19	109.23
1	D	828	ILE	CB-CA-C	-5.11	105.25	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	688	VAL	N-CA-C	5.07	115.28	110.42
1	D	766	LEU	CA-C-N	-5.06	115.02	120.03
1	D	766	LEU	C-N-CA	-5.06	115.02	120.03
1	A	763	VAL	N-CA-C	5.03	116.95	108.81
1	A	1086	ARG	N-CA-C	5.03	116.59	108.34

There are no chirality outliers.

All (9) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8342	0	8246	420	0
1	B	7838	0	7764	358	0
1	C	8379	0	8284	412	0
1	D	7838	0	7764	388	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	15	0	16	4	0
All	All	32443	0	32086	1560	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 24.

All (1560) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:LYS:HD2	1:D:961:LYS:N	1.59	1.14
1:C:437:LYS:H	1:C:437:LYS:HD3	0.98	1.13
1:D:961:LYS:H	1:D:961:LYS:CD	1.59	1.12
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.84	1.11
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.03	1.11
1:B:275:VAL:HG21	1:B:466:MET:HE1	1.28	1.10
1:D:999:GLN:HG2	1:D:1000:GLY:N	1.58	1.09
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.34	1.09
1:A:866:MET:HE3	1:A:870:GLN:HG2	1.25	1.08
1:C:156:ARG:NH2	1:C:170:THR:O	1.85	1.08
1:C:338:MET:CE	1:C:430:SER:HB3	1.85	1.06
1:C:870:GLN:HG3	1:C:870:GLN:O	1.50	1.05
1:D:513:PRO:HD3	4:D:1201:BTI:H11	1.39	1.05
1:C:874:LEU:HD23	1:C:874:LEU:O	1.57	1.04
1:D:413:PHE:CE2	1:D:416:ALA:HB2	1.93	1.03
1:C:437:LYS:HD3	1:C:437:LYS:N	1.61	1.03
1:C:438:GLN:HG2	1:C:441:GLU:OE1	1.58	1.03
1:B:907:VAL:O	1:B:911:SER:HB3	1.58	1.02
1:A:883:LEU:HD22	1:A:886:ARG:NH1	1.75	1.02
1:C:828:ILE:HD12	1:C:828:ILE:H	1.21	1.02
1:D:917:MET:HG2	1:D:944:VAL:HG21	1.40	1.02
1:A:883:LEU:HD22	1:A:886:ARG:HH12	1.26	1.01
1:C:338:MET:HE2	1:C:430:SER:HB3	1.43	1.00
1:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.42	1.00
1:D:999:GLN:CG	1:D:1000:GLY:H	1.75	0.99
1:A:338:MET:CE	1:A:430:SER:HB2	1.93	0.98
1:D:999:GLN:HG2	1:D:1000:GLY:H	0.82	0.97
1:D:873:ASN:N	1:D:873:ASN:HD22	1.58	0.97
1:D:256:ASN:O	1:D:357:LEU:HD21	1.64	0.97
1:C:451:ARG:HG2	1:C:451:ARG:NH1	1.77	0.96
1:A:44:ASN:HD22	1:A:45:ARG:H	1.05	0.96
1:D:811:ASN:H	1:D:811:ASN:HD22	0.99	0.96
1:D:44:ASN:HD22	1:D:45:ARG:H	1.09	0.96
1:A:245:ILE:HD13	1:A:283:LEU:HD11	1.48	0.95
1:C:494:LEU:HB2	1:C:496:ARG:NH2	1.81	0.95
1:A:237:ARG:HG2	1:A:237:ARG:HH11	1.29	0.95
1:C:437:LYS:H	1:C:437:LYS:CD	1.77	0.95
1:A:209:GLU:HA	1:A:213:LEU:HD21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:ILE:HD12	1:C:1089:ILE:CD1	1.98	0.94
1:C:995:GLU:HG3	1:C:1002:VAL:HG21	1.47	0.93
1:D:811:ASN:HD22	1:D:811:ASN:N	1.67	0.92
1:A:338:MET:HE2	1:A:430:SER:HB2	1.51	0.92
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.08	0.92
1:B:897:VAL:HG22	1:B:921:MET:HE3	1.51	0.92
1:A:864:HIS:HD2	1:A:866:MET:H	1.17	0.91
1:B:275:VAL:HG21	1:B:466:MET:CE	1.99	0.91
1:A:706:TYR:O	1:A:743:MET:HE1	1.71	0.90
1:C:196:THR:O	1:C:197:SER:HB2	1.71	0.90
1:D:961:LYS:HD2	1:D:961:LYS:H	0.74	0.90
1:B:704:ILE:HD11	1:B:730:LEU:HD12	1.52	0.90
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.07	0.89
1:B:47:GLU:HG3	1:B:48:ILE:N	1.84	0.89
1:A:338:MET:CE	1:A:430:SER:CB	2.51	0.89
1:D:513:PRO:O	1:D:515:ASN:HB2	1.71	0.89
1:B:1008:ILE:HD13	1:B:1008:ILE:H	1.34	0.88
1:C:995:GLU:CG	1:C:1002:VAL:HG21	2.03	0.87
1:C:44:ASN:ND2	1:C:45:ARG:H	1.73	0.87
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.56	0.87
1:C:44:ASN:HD22	1:C:45:ARG:N	1.73	0.87
1:C:878:ALA:HA	1:C:883:LEU:HD12	1.56	0.87
1:A:700:SER:H	1:A:736:HIS:HD2	1.13	0.87
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.54	0.87
1:B:999:GLN:HE21	1:B:1001:PRO:HG3	1.40	0.86
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.06	0.86
1:C:44:ASN:HD22	1:C:45:ARG:H	0.88	0.86
1:C:306:ASN:OD1	1:C:348:GLN:HG2	1.75	0.85
1:A:335:ILE:HD11	1:A:374:ILE:C	2.01	0.85
1:A:622:ASN:ND2	1:A:624:TRP:H	1.74	0.85
1:A:998:GLN:HB3	1:A:999:GLN:HE21	1.39	0.85
1:C:849:GLU:O	1:C:852:SER:O	1.93	0.85
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.59	0.84
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.59	0.84
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.57	0.84
1:C:1076:ILE:HD12	1:C:1089:ILE:HD13	1.59	0.84
1:D:44:ASN:HD22	1:D:45:ARG:N	1.74	0.84
1:D:333:HIS:CD2	1:D:337:GLU:OE2	2.30	0.84
1:A:313:LEU:HD22	1:A:323:ILE:HD11	1.60	0.84
1:A:1018:GLU:OE1	1:A:1018:GLU:HA	1.76	0.84
1:A:338:MET:HE2	1:A:430:SER:CB	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:922:VAL:C	1:C:924:ASN:H	1.85	0.83
1:B:853:ASP:O	1:B:855:LYS:HD3	1.78	0.83
1:C:69:ASN:O	1:C:72:LYS:HG3	1.79	0.83
1:A:484:THR:HB	1:A:487:LEU:HD22	1.60	0.83
1:B:329:VAL:HG22	1:B:348:GLN:HE22	1.42	0.83
1:C:191:LEU:HD13	1:C:235:ILE:HD11	1.60	0.83
1:B:700:SER:H	1:B:736:HIS:HD2	1.23	0.83
1:A:811:ASN:HD22	1:A:811:ASN:H	1.22	0.83
1:A:219:ARG:HE	1:A:219:ARG:HA	1.44	0.83
1:C:451:ARG:HH11	1:C:451:ARG:CG	1.90	0.82
1:D:263:ARG:NH2	1:D:330:GLN:HE21	1.77	0.82
1:A:118:TYR:HB2	1:A:328:ARG:HH11	1.42	0.82
1:A:883:LEU:CD2	1:A:886:ARG:HH12	1.91	0.82
1:C:142:HIS:H	1:C:145:HIS:HD2	1.28	0.82
1:A:381:GLU:O	1:A:383:PRO:HD3	1.79	0.82
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.78	0.81
1:A:1042:MET:HE3	1:A:1062:LEU:HB2	1.63	0.81
1:C:269:ARG:HG3	1:C:270:ARG:H	1.45	0.81
1:D:44:ASN:ND2	1:D:45:ARG:H	1.77	0.81
1:B:47:GLU:HG3	1:B:48:ILE:H	1.43	0.81
1:D:864:HIS:HD2	1:D:866:MET:H	1.29	0.81
1:A:632:LYS:CB	1:A:632:LYS:NZ	2.44	0.81
1:A:382:ASP:OD2	1:A:385:ASN:HB3	1.81	0.81
1:C:278:ALA:HB3	1:C:335:ILE:HG23	1.62	0.81
1:A:184:ALA:HB1	1:A:185:GLU:OE2	1.81	0.80
1:B:239:ILE:HG22	1:B:239:ILE:O	1.82	0.80
1:A:118:TYR:HB2	1:A:328:ARG:NH1	1.96	0.80
1:C:438:GLN:HA	1:C:441:GLU:OE1	1.81	0.80
1:C:650:GLY:HA2	1:C:1013:TYR:CE1	2.17	0.80
1:C:571:ARG:NH1	1:C:575:GLN:OE1	2.15	0.80
1:B:395:ILE:HD12	1:B:1086:ARG:O	1.83	0.79
1:A:866:MET:HE2	1:A:871:TYR:HA	1.64	0.79
1:C:1056:LYS:O	1:C:1057:ARG:HB3	1.82	0.79
1:A:1044:ASN:N	1:A:1044:ASN:HD22	1.78	0.79
1:A:338:MET:HE1	1:A:430:SER:HB2	1.65	0.79
1:A:811:ASN:H	1:A:811:ASN:ND2	1.78	0.79
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.65	0.79
1:A:883:LEU:CD2	1:A:886:ARG:NH1	2.45	0.79
1:C:235:ILE:HG12	1:C:235:ILE:O	1.82	0.79
1:C:920:TYR:O	1:C:924:ASN:HB2	1.82	0.79
1:D:296:ILE:O	1:D:300:GLU:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LYS:HG3	1:C:781:LEU:HD21	1.65	0.79
1:C:444:VAL:HG23	1:C:466:MET:HB3	1.64	0.79
1:B:646:SER:HB3	1:B:685:GLN:HE22	1.48	0.78
1:C:502:GLU:OE1	1:C:502:GLU:HA	1.82	0.78
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.62	0.78
1:B:525:GLU:HB3	1:B:840:THR:HG23	1.64	0.78
1:D:289:GLN:NE2	1:D:289:GLN:HA	1.98	0.78
1:A:268:GLN:HB2	1:A:272:GLN:O	1.83	0.78
1:B:540:GLY:H	1:B:543:GLN:HE21	1.29	0.78
1:B:897:VAL:HG22	1:B:921:MET:CE	2.13	0.78
1:C:136:ILE:N	1:C:136:ILE:HD13	1.97	0.78
1:C:216:ALA:O	1:C:220:ALA:HB3	1.84	0.78
1:D:873:ASN:N	1:D:873:ASN:ND2	2.25	0.78
1:C:622:ASN:ND2	1:C:624:TRP:H	1.81	0.78
1:A:640:GLN:HG3	1:A:673:VAL:HB	1.64	0.78
1:A:1044:ASN:HD22	1:A:1044:ASN:H	1.31	0.77
1:D:349:ILE:O	1:D:349:ILE:HG22	1.83	0.77
1:A:48:ILE:O	1:A:52:ILE:HG12	1.85	0.77
1:C:191:LEU:HD23	1:C:237:ARG:HA	1.65	0.77
1:D:622:ASN:HD22	1:D:623:PRO:N	1.83	0.77
1:D:1052:ILE:HG22	1:D:1053:ASP:H	1.50	0.77
1:C:921:MET:HA	1:C:926:LEU:HD12	1.65	0.77
1:C:437:LYS:N	1:C:437:LYS:CD	2.39	0.76
1:A:1003:THR:HG23	1:A:1006:ASP:H	1.50	0.76
1:C:338:MET:HE2	1:C:430:SER:CB	2.16	0.76
1:B:343:ASP:CG	1:B:346:LYS:HB2	2.11	0.76
1:C:828:ILE:H	1:C:828:ILE:CD1	1.92	0.76
1:D:518:LYS:HD2	1:D:518:LYS:C	2.11	0.76
1:B:606:MET:HE2	1:B:639:PHE:HB3	1.68	0.76
1:C:153:VAL:HG21	1:C:173:PRO:HD3	1.66	0.76
1:D:447:LEU:HD11	1:D:462:LEU:HB3	1.66	0.76
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.68	0.75
1:C:396:ALA:HA	1:C:414:GLN:OE1	1.86	0.75
1:C:738:LEU:HD23	1:C:768:ILE:HG12	1.68	0.75
1:A:866:MET:CE	1:A:871:TYR:HA	2.17	0.75
1:C:125:GLU:OE2	1:C:147:ASP:HB2	1.85	0.75
1:C:168:PRO:HG2	1:C:237:ARG:HD3	1.68	0.75
1:B:704:ILE:HD11	1:B:730:LEU:CD1	2.17	0.75
1:C:968:LEU:O	1:C:969:LYS:C	2.30	0.75
1:D:142:HIS:HB2	1:D:145:HIS:CD2	2.21	0.75
1:A:145:HIS:HE1	1:A:302:ILE:O	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:O	1:C:215:ASP:N	2.20	0.75
1:B:44:ASN:ND2	1:B:48:ILE:HG21	2.02	0.75
1:C:712:ASN:OD1	1:C:714:GLU:HG3	1.86	0.75
1:A:259:HIS:HB3	1:A:296:ILE:CD1	2.17	0.74
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.52	0.74
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.20	0.74
1:A:700:SER:H	1:A:736:HIS:CD2	2.03	0.74
1:C:189:PHE:HB3	1:C:209:GLU:HA	1.69	0.74
1:D:746:LEU:HD11	1:D:865:GLU:HG2	1.70	0.74
1:D:917:MET:CG	1:D:944:VAL:HG21	2.17	0.74
1:B:1008:ILE:HD13	1:B:1008:ILE:N	2.02	0.73
1:C:129:ARG:HB2	1:C:143:LEU:HD11	1.70	0.73
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.18	0.73
1:A:235:ILE:HG13	1:A:236:GLU:N	2.01	0.73
1:B:338:MET:HE1	1:B:430:SER:HB3	1.69	0.73
1:A:170:THR:HG22	1:A:172:GLY:O	1.88	0.73
1:A:828:ILE:HD12	1:A:829:GLU:H	1.52	0.73
1:B:719:THR:H	1:B:722:TYR:HB3	1.53	0.73
1:C:622:ASN:HD22	1:C:624:TRP:H	1.36	0.73
1:D:622:ASN:HD22	1:D:622:ASN:C	1.94	0.73
1:C:922:VAL:O	1:C:924:ASN:N	2.22	0.73
1:B:959:PHE:CD1	1:B:964:GLN:NE2	2.57	0.73
1:C:1067:GLU:HA	1:C:1074:ARG:HH21	1.52	0.73
1:D:513:PRO:O	1:D:515:ASN:CB	2.36	0.73
1:D:501:LEU:HD13	1:D:1078:TYR:CD1	2.24	0.73
1:A:94:GLU:O	1:A:94:GLU:HG3	1.87	0.73
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.71	0.73
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.24	0.72
1:C:103:ILE:O	1:C:107:LYS:HG3	1.89	0.72
1:D:622:ASN:ND2	1:D:624:TRP:H	1.87	0.72
1:C:1067:GLU:OE1	1:C:1074:ARG:NH2	2.21	0.72
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.19	0.72
1:B:898:ASN:ND2	1:B:906:LYS:HE3	2.04	0.72
1:B:927:ASP:HB2	1:B:930:SER:OG	1.90	0.72
1:C:828:ILE:HD12	1:C:828:ILE:N	2.03	0.72
1:A:239:ILE:HD11	1:A:315:SER:CB	2.19	0.72
1:A:565:LEU:HD23	1:A:565:LEU:O	1.90	0.72
1:A:237:ARG:HG2	1:A:237:ARG:NH1	2.03	0.72
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.25	0.72
1:A:404:GLY:HA3	1:A:442:GLU:OE1	1.90	0.72
1:B:700:SER:H	1:B:736:HIS:CD2	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG21	1:A:173:PRO:HD3	1.72	0.71
1:B:540:GLY:H	1:B:543:GLN:NE2	1.88	0.71
1:D:53:PHE:HA	1:D:63:THR:HG21	1.72	0.71
1:B:640:GLN:HG3	1:B:673:VAL:HB	1.70	0.71
1:D:960:ASN:HB3	1:D:963:LEU:HB3	1.71	0.71
1:B:1008:ILE:H	1:B:1008:ILE:CD1	2.04	0.71
1:A:1029:ASN:C	1:A:1029:ASN:HD22	1.99	0.71
1:B:306:ASN:OD1	1:B:348:GLN:HG3	1.91	0.71
1:D:453:ARG:HH12	1:D:495:ASP:HB3	1.55	0.71
1:B:477:THR:OG1	1:B:479:LYS:HB2	1.91	0.71
1:D:164:LEU:HD13	1:D:294:ALA:HB1	1.73	0.71
1:D:840:THR:O	1:D:843:THR:HB	1.90	0.71
1:B:144:GLU:O	1:B:148:MET:HB2	1.91	0.71
1:A:382:ASP:O	1:A:387:PHE:HA	1.90	0.71
1:B:898:ASN:HD22	1:B:906:LYS:HE3	1.56	0.71
1:A:164:LEU:HD22	1:A:294:ALA:HB1	1.72	0.71
1:A:338:MET:HE1	1:A:430:SER:CB	2.20	0.71
1:A:606:MET:HE2	1:A:639:PHE:HB3	1.72	0.71
1:D:391:THR:HG21	1:D:420:PRO:HB3	1.73	0.71
1:A:179:LEU:HG	1:A:217:PHE:HE2	1.56	0.70
1:A:519:ARG:NH2	1:A:847:ASP:OD2	2.24	0.70
1:A:632:LYS:NZ	1:A:632:LYS:HB2	2.06	0.70
1:C:259:HIS:O	1:C:260:LEU:HD23	1.91	0.70
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.22	0.70
1:A:622:ASN:HD22	1:A:624:TRP:H	1.38	0.70
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.73	0.70
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.26	0.70
1:A:1000:GLY:H	1:A:1001:PRO:HD2	1.56	0.70
1:B:893:MET:O	1:B:897:VAL:HG23	1.92	0.70
1:C:166:VAL:HG12	1:C:167:ILE:H	1.55	0.70
1:A:173:PRO:HA	1:A:234:TYR:HB3	1.73	0.69
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.28	0.69
1:C:130:ARG:O	1:C:134:GLU:HG2	1.92	0.69
1:C:882:GLY:C	1:C:884:GLY:H	2.00	0.69
1:D:513:PRO:CD	4:D:1201:BTI:H11	2.20	0.69
1:A:590:ILE:CG1	1:A:837:TYR:CE2	2.75	0.69
1:B:363:GLN:OE1	1:B:363:GLN:HA	1.92	0.69
1:A:644:ARG:NH2	1:A:908:THR:CG2	2.56	0.69
1:D:142:HIS:HB2	1:D:145:HIS:HD2	1.56	0.69
1:A:191:LEU:O	1:A:238:TYR:HB2	1.92	0.69
1:B:395:ILE:HB	1:B:1086:ARG:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HG	1:B:499:LYS:HE2	1.73	0.69
1:C:494:LEU:HB2	1:C:496:ARG:HH22	1.58	0.69
1:C:544:LEU:HD23	1:C:553:VAL:HG22	1.74	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:C:525:GLU:OE2	1:C:525:GLU:HA	1.91	0.69
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.57	0.69
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.28	0.69
1:D:700:SER:H	1:D:736:HIS:HD2	1.39	0.69
1:A:254:HIS:CD2	1:A:356:ASP:HB2	2.27	0.68
1:A:193:ILE:HG23	1:A:193:ILE:O	1.94	0.68
1:B:457:THR:OG1	1:B:459:ILE:HG12	1.93	0.68
1:D:334:THR:HA	1:D:337:GLU:HG3	1.74	0.68
1:B:704:ILE:N	1:B:704:ILE:HD13	2.06	0.68
1:C:622:ASN:HD22	1:C:622:ASN:C	2.02	0.68
1:D:580:THR:CG2	1:D:611:THR:HG22	2.23	0.68
1:B:770:LEU:HD12	1:B:771:HIS:N	2.08	0.68
1:D:542:LYS:HE2	1:D:631:ARG:NH2	2.09	0.68
1:C:92:PRO:HD2	1:C:94:GLU:OE2	1.94	0.68
1:C:864:HIS:CD2	1:C:866:MET:HG3	2.28	0.68
1:D:870:GLN:O	1:D:871:TYR:C	2.36	0.68
1:C:849:GLU:C	1:C:852:SER:O	2.36	0.68
1:A:866:MET:HE3	1:A:870:GLN:CG	2.13	0.68
1:D:960:ASN:HD22	1:D:963:LEU:H	1.42	0.68
1:D:1071:ASN:HB3	1:D:1073:ASN:ND2	2.07	0.68
1:D:684:ASP:HA	1:D:687:LYS:HE2	1.75	0.68
1:D:1076:ILE:CD1	1:D:1089:ILE:HD13	2.23	0.68
1:A:254:HIS:HD2	1:A:356:ASP:HB2	1.58	0.67
1:A:144:GLU:O	1:A:148:MET:HB2	1.94	0.67
1:A:820:PHE:HB3	1:A:821:PRO:CD	2.24	0.67
1:C:144:GLU:O	1:C:148:MET:HB2	1.93	0.67
1:D:453:ARG:HH22	1:D:495:ASP:HB2	1.59	0.67
1:A:540:GLY:H	1:A:543:GLN:HE21	1.43	0.67
1:B:156:ARG:NH2	1:B:167:ILE:HG12	2.09	0.67
1:B:1085:ARG:HG3	1:B:1086:ARG:H	1.59	0.67
1:C:574:HIS:CD2	1:C:582:VAL:HB	2.30	0.67
1:A:90:LEU:HD22	1:A:95:SER:HA	1.76	0.67
1:A:709:ASP:OD1	1:A:748:LYS:NZ	2.26	0.67
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.24	0.67
1:A:949:LYS:HE3	1:A:971:GLN:OE1	1.95	0.67
1:D:252:ASP:HA	1:D:351:VAL:HG13	1.77	0.67
1:B:142:HIS:H	1:B:145:HIS:HD2	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PHE:O	1:B:414:GLN:HB2	1.93	0.67
1:B:700:SER:N	1:B:736:HIS:HD2	1.93	0.67
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.42	0.67
1:A:284:SER:HB2	1:A:285:PRO:HD2	1.76	0.67
1:B:41:LEU:HB2	1:B:111:VAL:HG21	1.76	0.67
1:C:269:ARG:HB2	1:C:269:ARG:HH11	1.59	0.67
1:C:539:SER:HA	1:C:543:GLN:HG3	1.77	0.67
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.76	0.66
1:D:999:GLN:CG	1:D:1000:GLY:N	2.43	0.66
1:C:104:ASP:O	1:C:108:GLN:NE2	2.28	0.66
1:A:44:ASN:HD22	1:A:45:ARG:N	1.88	0.66
1:C:849:GLU:O	1:C:852:SER:C	2.38	0.66
1:C:494:LEU:HB2	1:C:496:ARG:HH21	1.56	0.66
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.10	0.66
1:C:116:PRO:HB2	1:C:122:SER:HA	1.78	0.66
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.94	0.66
1:D:864:HIS:CD2	1:D:866:MET:H	2.14	0.66
1:A:338:MET:CE	1:A:430:SER:HB3	2.25	0.66
1:A:644:ARG:NH2	1:A:908:THR:HG21	2.11	0.66
1:B:64:VAL:HG22	1:B:82:GLU:HG3	1.77	0.66
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.78	0.66
1:A:87:GLY:C	1:A:89:ASP:H	2.04	0.65
1:A:205:ARG:HE	1:A:205:ARG:N	1.94	0.65
1:B:334:THR:HG22	1:B:406:ARG:NH2	2.11	0.65
1:B:1085:ARG:HG3	1:B:1086:ARG:N	2.10	0.65
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.60	0.65
1:C:811:ASN:HD22	1:C:811:ASN:H	1.43	0.65
1:C:1043:ARG:HH11	1:C:1043:ARG:HB3	1.62	0.65
1:D:332:GLU:HA	1:D:375:GLN:HE21	1.62	0.65
1:D:881:LEU:HD23	1:D:881:LEU:N	2.11	0.65
1:B:459:ILE:HB	1:B:460:PRO:CD	2.27	0.65
1:C:329:VAL:HG22	1:C:348:GLN:HE22	1.61	0.65
1:A:425:LEU:HD12	1:A:425:LEU:C	2.22	0.65
1:A:632:LYS:HB3	1:A:632:LYS:HZ3	1.61	0.65
1:B:503:TYR:HB2	1:B:1027:TYR:CD2	2.31	0.65
1:A:363:GLN:HA	1:A:363:GLN:NE2	2.11	0.65
1:C:438:GLN:O	1:C:441:GLU:HG2	1.96	0.65
1:C:910:SER:O	1:C:914:VAL:HG23	1.97	0.65
1:C:991:ARG:NH1	1:C:1002:VAL:O	2.30	0.65
1:A:99:ILE:HD13	1:A:127:PHE:HB2	1.78	0.64
1:B:771:HIS:HB2	1:B:795:ASP:OD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:VAL:CG2	1:B:921:MET:HE3	2.26	0.64
1:D:870:GLN:O	1:D:873:ASN:N	2.30	0.64
1:A:632:LYS:HB2	1:A:632:LYS:HZ2	1.61	0.64
1:D:920:TYR:OH	1:D:938:LEU:O	2.16	0.64
1:C:700:SER:H	1:C:736:HIS:HD2	1.45	0.64
1:B:479:LYS:O	1:B:483:GLU:HG2	1.98	0.64
1:C:335:ILE:HD11	1:C:374:ILE:C	2.23	0.64
1:D:343:ASP:CG	1:D:346:LYS:HB2	2.21	0.64
1:A:679:SER:HB2	1:A:908:THR:O	1.98	0.64
1:B:622:ASN:ND2	1:B:624:TRP:H	1.95	0.64
1:A:145:HIS:CE1	1:A:302:ILE:O	2.50	0.64
1:B:701:GLU:OE2	1:B:737:ILE:HG21	1.97	0.64
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.80	0.64
1:D:262:GLU:OE2	1:D:279:PRO:HB3	1.98	0.64
1:D:811:ASN:N	1:D:811:ASN:ND2	2.36	0.64
1:A:241:ASN:N	1:A:242:PRO:HD3	2.12	0.64
1:A:377:ARG:HG2	1:A:425:LEU:HD22	1.79	0.64
1:A:1087:ILE:HG22	1:A:1089:ILE:HD11	1.79	0.64
1:A:918:ALA:O	1:A:922:VAL:HG23	1.98	0.63
1:C:114:ILE:HG13	1:C:136:ILE:HG21	1.80	0.63
1:C:241:ASN:N	1:C:242:PRO:HD3	2.11	0.63
1:C:438:GLN:HA	1:C:441:GLU:CD	2.24	0.63
1:D:394:ILE:HG22	1:D:394:ILE:O	1.97	0.63
1:C:495:ASP:HB3	1:C:498:THR:HB	1.79	0.63
1:C:1076:ILE:CD1	1:C:1089:ILE:HD13	2.29	0.63
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.78	0.63
1:B:763:VAL:C	1:B:766:LEU:H	2.06	0.63
1:D:477:THR:C	1:D:479:LYS:H	2.05	0.63
1:D:98:ASN:O	1:D:102:ILE:HD12	1.98	0.63
1:B:311:GLU:OE1	1:B:326:ASN:ND2	2.32	0.63
1:C:41:LEU:C	1:C:41:LEU:HD23	2.23	0.63
1:D:453:ARG:HH22	1:D:495:ASP:CB	2.11	0.63
1:C:884:GLY:O	1:C:885:GLU:HB2	1.99	0.62
1:A:213:LEU:N	1:A:213:LEU:HD23	2.13	0.62
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.81	0.62
1:A:329:VAL:HG21	1:A:348:GLN:OE1	1.99	0.62
1:A:743:MET:HE2	1:A:743:MET:H	1.64	0.62
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.63	0.62
1:C:189:PHE:H	1:C:190:PRO:HD3	1.65	0.62
1:D:382:ASP:O	1:D:387:PHE:HA	1.99	0.62
1:B:792:ASP:OD2	1:B:792:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LEU:HD22	1:D:291:ILE:HD11	1.80	0.62
1:A:245:ILE:HD13	1:A:283:LEU:CD1	2.27	0.62
1:A:632:LYS:NZ	1:A:632:LYS:HB3	2.14	0.62
1:B:864:HIS:CD2	1:B:866:MET:HG3	2.35	0.62
1:A:622:ASN:HD22	1:A:622:ASN:C	2.06	0.62
1:C:142:HIS:N	1:C:145:HIS:HD2	1.98	0.62
1:C:278:ALA:CB	1:C:335:ILE:HG23	2.28	0.62
1:D:1069:ASP:O	1:D:1072:GLY:N	2.32	0.62
1:A:239:ILE:HD11	1:A:315:SER:HB2	1.81	0.62
1:A:503:TYR:O	1:A:504:ILE:C	2.42	0.62
1:A:540:GLY:N	1:A:543:GLN:HE21	1.97	0.62
1:A:927:ASP:OD2	1:A:928:GLU:N	2.33	0.62
1:B:306:ASN:OD1	1:B:348:GLN:CG	2.48	0.62
1:B:459:ILE:HB	1:B:460:PRO:HD3	1.80	0.62
1:C:494:LEU:CD2	1:C:496:ARG:HH21	2.13	0.62
1:A:239:ILE:HD11	1:A:315:SER:HB3	1.81	0.62
1:B:409:ALA:HA	1:B:427:VAL:HG12	1.80	0.62
1:D:570:PHE:O	1:D:574:HIS:HE1	1.82	0.62
1:D:1052:ILE:O	1:D:1053:ASP:C	2.40	0.62
1:A:394:ILE:O	1:A:414:GLN:O	2.18	0.61
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.82	0.61
1:A:728:LYS:HE2	1:A:762:ALA:HB1	1.82	0.61
1:D:289:GLN:HA	1:D:289:GLN:HE21	1.64	0.61
1:D:587:MET:O	1:D:590:ILE:HD12	2.00	0.61
1:B:263:ARG:HH21	1:B:330:GLN:NE2	1.97	0.61
1:C:296:ILE:O	1:C:300:GLU:HB2	1.99	0.61
1:B:437:LYS:O	1:B:441:GLU:HG2	1.99	0.61
1:C:87:GLY:O	1:C:90:LEU:N	2.28	0.61
1:B:52:ILE:HD13	1:B:345:VAL:HG11	1.82	0.61
1:D:1076:ILE:CD1	1:D:1089:ILE:CD1	2.79	0.61
1:A:571:ARG:HH11	1:A:575:GLN:NE2	1.98	0.61
1:B:264:ASP:HB2	1:B:280:SER:HB2	1.82	0.61
1:B:286:THR:O	1:B:290:ARG:HG3	2.01	0.61
1:C:499:LYS:O	1:C:502:GLU:HB2	2.00	0.61
1:A:67:TYR:HA	1:A:96:TYR:OH	2.01	0.61
1:B:465:VAL:HG22	1:B:487:LEU:HD23	1.82	0.61
1:C:269:ARG:HB2	1:C:269:ARG:NH1	2.15	0.61
1:C:874:LEU:O	1:C:874:LEU:CD2	2.41	0.61
1:C:1078:TYR:HB2	1:C:1085:ARG:O	2.00	0.61
1:B:738:LEU:HD23	1:B:768:ILE:HD13	1.82	0.61
1:D:317:GLY:O	1:D:318:ASP:C	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357(A):PHE:HE2	1:D:363:GLN:HA	1.65	0.61
1:A:192:MET:CE	1:A:238:TYR:HD1	2.14	0.61
1:D:866:MET:HE3	1:D:894:TYR:CD1	2.35	0.61
1:A:906:LYS:HZ3	1:A:906:LYS:HB2	1.66	0.60
1:A:1044:ASN:H	1:A:1044:ASN:ND2	1.98	0.60
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.65	0.60
1:C:375:GLN:HG3	1:C:376:CYS:N	2.16	0.60
1:C:443:MET:HG2	1:C:466:MET:HE3	1.83	0.60
1:D:606:MET:HE2	1:D:606:MET:O	2.00	0.60
1:B:156:ARG:HH21	1:B:167:ILE:HG12	1.65	0.60
1:C:66:ILE:HD12	1:C:86:VAL:HG21	1.83	0.60
1:D:866:MET:HE2	1:D:874:LEU:HD22	1.83	0.60
1:A:875:SER:C	1:A:877:GLN:H	2.08	0.60
1:C:210:GLU:C	1:C:212:GLU:H	2.10	0.60
1:D:39:LYS:HG3	1:D:62:SER:HB3	1.83	0.60
1:D:799:ALA:O	1:D:802:SER:OG	2.19	0.60
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.82	0.60
1:C:864:HIS:HD2	1:C:866:MET:H	1.48	0.60
1:B:263:ARG:HH21	1:B:330:GLN:HE21	1.49	0.60
1:B:744:ALA:HB3	1:B:746:LEU:HG	1.83	0.60
1:A:856:SER:OG	1:D:800:SER:HA	2.01	0.60
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.67	0.60
1:C:210:GLU:O	1:C:212:GLU:N	2.35	0.60
1:A:866:MET:HG2	1:A:894:TYR:CE2	2.36	0.60
1:C:118:TYR:CZ	1:C:331:VAL:HG22	2.36	0.60
1:C:213:LEU:C	1:C:215:ASP:H	2.09	0.60
1:C:926:LEU:HB3	1:C:930:SER:HB3	1.84	0.60
1:D:613:ASP:HB2	1:D:1013:TYR:CZ	2.37	0.60
1:A:383:PRO:HA	1:A:387:PHE:CE2	2.36	0.60
1:C:927:ASP:OD1	1:C:929:GLN:HG2	2.02	0.59
1:D:1076:ILE:HD11	1:D:1089:ILE:HD13	1.83	0.59
1:A:719:THR:O	1:A:722:TYR:N	2.34	0.59
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.60	0.59
1:C:261:PHE:CD1	1:C:369:THR:CG2	2.84	0.59
1:C:338:MET:CE	1:C:430:SER:CB	2.71	0.59
1:C:386:ASP:O	1:C:387:PHE:HB2	2.01	0.59
1:D:269:ARG:HG3	1:D:270:ARG:H	1.66	0.59
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.83	0.59
1:A:1044:ASN:N	1:A:1044:ASN:ND2	2.50	0.59
1:B:469:LYS:H	1:B:469:LYS:HD3	1.67	0.59
1:B:622:ASN:C	1:B:622:ASN:HD22	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HH11	1:C:269:ARG:CB	2.15	0.59
1:C:882:GLY:O	1:C:884:GLY:N	2.34	0.59
1:D:1076:ILE:HD13	1:D:1089:ILE:CD1	2.32	0.59
1:A:866:MET:HE2	1:A:871:TYR:CA	2.32	0.59
1:B:86:VAL:HG12	1:B:86:VAL:O	2.01	0.59
1:B:245:ILE:HG12	1:B:283:LEU:HD11	1.84	0.59
1:C:135:GLY:C	1:C:136:ILE:HD13	2.27	0.59
1:D:290:ARG:HE	1:D:320:PHE:HE1	1.50	0.59
1:D:349:ILE:O	1:D:349:ILE:CG2	2.50	0.59
1:D:558:LYS:HD2	1:D:765:ASP:O	2.02	0.59
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.31	0.59
1:C:425:LEU:HD12	1:C:425:LEU:C	2.28	0.59
1:A:52:ILE:HD12	1:A:115:HIS:CD2	2.37	0.59
1:C:494:LEU:HD23	1:C:496:ARG:HH21	1.67	0.59
1:C:870:GLN:O	1:C:870:GLN:CG	2.37	0.59
1:A:1088:TYR:C	1:A:1089:ILE:HD12	2.27	0.59
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.38	0.59
1:A:738:LEU:HD21	1:A:759:LEU:CD1	2.33	0.59
1:C:374:ILE:HG22	1:C:443:MET:HE3	1.84	0.59
1:C:871:TYR:O	1:C:875:SER:HB2	2.03	0.59
1:D:278:ALA:HB2	1:D:335:ILE:HG23	1.85	0.59
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.84	0.59
1:A:254:HIS:HD2	1:A:356:ASP:CB	2.15	0.59
1:C:189:PHE:H	1:C:190:PRO:CD	2.16	0.59
1:C:1043:ARG:HD3	1:C:1046:GLU:HB2	1.85	0.59
1:A:413:PHE:CE2	1:A:416:ALA:HB2	2.38	0.58
1:A:209:GLU:HA	1:A:213:LEU:CD2	2.28	0.58
1:A:866:MET:CE	1:A:870:GLN:HG2	2.16	0.58
1:B:322:PHE:HE2	1:B:325:VAL:HG23	1.68	0.58
1:D:530:PRO:HB2	1:D:593:LYS:HD3	1.85	0.58
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.36	0.58
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.18	0.58
1:D:331:VAL:HG11	1:D:377:ARG:HD3	1.84	0.58
1:D:917:MET:HG2	1:D:944:VAL:CG2	2.27	0.58
1:A:313:LEU:HD22	1:A:323:ILE:CD1	2.33	0.58
1:A:921:MET:HG2	1:A:926:LEU:HB3	1.85	0.58
1:C:269:ARG:CG	1:C:270:ARG:H	2.17	0.58
1:B:413:PHE:O	1:B:414:GLN:CB	2.48	0.58
1:D:53:PHE:CZ	1:D:65:ALA:HB2	2.38	0.58
1:D:644:ARG:NH1	1:D:908:THR:HG22	2.19	0.58
1:A:864:HIS:CD2	1:A:866:MET:CG	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:HG3	1:B:111:VAL:HA	1.84	0.58
1:B:437:LYS:HE3	1:B:437:LYS:CA	2.34	0.58
1:C:650:GLY:HA2	1:C:1013:TYR:HE1	1.65	0.58
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.85	0.58
1:D:828:ILE:O	1:D:832:GLU:HG2	2.02	0.58
1:A:273:LYS:HB3	1:A:276:GLU:OE2	2.04	0.58
1:B:332:GLU:HA	1:B:375:GLN:NE2	2.19	0.58
1:B:376:CYS:SG	1:B:462:LEU:HD13	2.43	0.58
1:B:406:ARG:NH1	1:D:403:PHE:HB2	2.19	0.58
1:B:1091:ASP:C	1:B:1093:ASN:H	2.11	0.58
1:C:572:ASP:HB3	1:C:807:GLN:NE2	2.19	0.58
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.68	0.58
1:A:644:ARG:HG2	1:A:647:ASN:OD1	2.02	0.58
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.58
1:C:205:ARG:NH1	1:C:223:GLU:OE1	2.36	0.58
1:C:940:PHE:HB3	1:C:941:PRO:HD2	1.86	0.58
1:A:296:ILE:O	1:A:300:GLU:HB2	2.04	0.58
1:B:999:GLN:HG2	1:B:1000:GLY:H	1.69	0.58
1:D:243:LYS:O	1:D:245:ILE:HG12	2.03	0.58
1:D:580:THR:HG22	1:D:611:THR:HG22	1.86	0.58
1:A:799:ALA:H	1:A:811:ASN:ND2	2.02	0.57
1:C:794:ILE:HD12	1:C:796:THR:HG23	1.86	0.57
1:D:622:ASN:ND2	1:D:624:TRP:N	2.52	0.57
1:A:590:ILE:HG12	1:A:837:TYR:CD2	2.39	0.57
1:A:871:TYR:HE1	1:A:891:LYS:HD2	1.68	0.57
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.85	0.57
1:D:791:VAL:O	1:D:822:ARG:NH2	2.36	0.57
1:A:400:SER:CB	1:A:446:SER:HB2	2.35	0.57
1:B:949:LYS:O	1:B:950:GLY:C	2.47	0.57
1:C:494:LEU:HD23	1:C:496:ARG:NH2	2.20	0.57
1:D:413:PHE:CD2	1:D:416:ALA:HB2	2.39	0.57
1:D:861:ILE:HG13	1:D:862:TYR:N	2.18	0.57
1:B:917:MET:HE2	1:B:944:VAL:HG21	1.85	0.57
1:B:949:LYS:O	1:B:951:GLU:N	2.37	0.57
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.36	0.57
1:B:544:LEU:O	1:B:548:VAL:HG22	2.05	0.57
1:B:770:LEU:HD12	1:B:771:HIS:H	1.68	0.57
1:C:121:LEU:HB3	1:C:127:PHE:CD2	2.39	0.57
1:C:989:LYS:O	1:C:993:LEU:HB2	2.04	0.57
1:D:640:GLN:HG3	1:D:673:VAL:CG1	2.34	0.57
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:GLY:O	1:C:553:VAL:HG23	2.03	0.57
1:C:960:ASN:OD1	1:C:960:ASN:N	2.37	0.57
1:A:239:ILE:O	1:A:239:ILE:HG13	2.03	0.57
1:B:335:ILE:HG22	1:B:336:THR:N	2.20	0.57
1:B:740:ILE:HD11	1:B:759:LEU:HD12	1.87	0.57
1:B:986:ASP:OD1	1:B:989:LYS:HG3	2.04	0.57
1:C:113:ALA:HB1	1:C:139:ILE:HD11	1.86	0.57
1:C:378:ILE:N	1:C:378:ILE:CD1	2.68	0.57
1:C:1019:GLN:HA	1:C:1022:GLN:HE21	1.70	0.57
1:D:128:ALA:O	1:D:131:CYS:HB2	2.05	0.57
1:A:509:ILE:CD1	1:A:1065:ILE:HG21	2.35	0.57
1:C:517:GLU:O	1:C:519:ARG:N	2.37	0.57
1:C:75:LEU:HG	1:C:413:PHE:CD2	2.40	0.57
1:A:267:VAL:HG23	1:A:476:TYR:CE2	2.40	0.56
1:B:329:VAL:HG22	1:B:348:GLN:NE2	2.14	0.56
1:C:701:GLU:HG2	1:C:739:ALA:HB2	1.87	0.56
1:C:917:MET:O	1:C:921:MET:HG3	2.04	0.56
1:C:938:LEU:O	1:C:939:ASP:C	2.48	0.56
1:D:997:GLU:OE2	1:D:1018:GLU:OE1	2.23	0.56
1:A:1029:ASN:C	1:A:1029:ASN:ND2	2.58	0.56
1:C:571:ARG:HH21	1:C:605:GLU:CD	2.13	0.56
1:A:641:MET:HE3	1:A:674:PHE:CD1	2.39	0.56
1:A:826:THR:HG21	1:A:831:MET:HE2	1.88	0.56
1:B:320:PHE:C	1:B:321:PHE:CD1	2.84	0.56
1:B:406:ARG:CZ	1:D:403:PHE:HB2	2.36	0.56
1:C:955:PRO:HG2	1:C:958:GLY:HA2	1.86	0.56
1:D:362(A):PRO:HB2	1:D:367:ILE:HG13	1.87	0.56
1:A:429:LEU:HD22	1:A:450:MET:HE3	1.88	0.56
1:A:119:GLY:N	1:A:122:SER:OG	2.38	0.56
1:A:129:ARG:O	1:A:133:GLU:HG3	2.06	0.56
1:A:362:MET:CE	1:A:367:ILE:HD11	2.35	0.56
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.39	0.56
1:C:98:ASN:O	1:C:102:ILE:HD12	2.05	0.56
1:D:363:GLN:HG3	1:D:365:LYS:HG3	1.87	0.56
1:D:446:SER:O	1:D:450:MET:HG2	2.05	0.56
1:A:118:TYR:CB	1:A:328:ARG:HH11	2.14	0.56
1:C:37:ILE:CD1	1:C:113:ALA:HB2	2.35	0.56
1:C:270:ARG:HH11	1:C:271:HIS:CD2	2.24	0.56
1:D:1077:TYR:N	1:D:1077:TYR:HD1	2.04	0.56
1:B:77:ARG:HH12	1:D:1059:ILE:CD1	2.18	0.56
1:C:544:LEU:O	1:C:548:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:THR:OG1	1:D:381:GLU:HB2	2.05	0.56
1:D:581:ARG:HD2	1:D:848:PHE:CE2	2.40	0.56
1:A:44:ASN:ND2	1:A:45:ARG:H	1.88	0.56
1:A:446:SER:O	1:A:450:MET:HG3	2.05	0.56
1:B:999:GLN:HG2	1:B:1000:GLY:N	2.21	0.56
1:C:343:ASP:OD2	1:C:346:LYS:HB2	2.06	0.56
1:C:878:ALA:HA	1:C:883:LEU:CD1	2.31	0.56
1:B:299:MET:HE1	1:B:325:VAL:HG11	1.87	0.56
1:B:322:PHE:CE2	1:B:325:VAL:HG23	2.40	0.56
1:C:215:ASP:HB3	1:C:219:ARG:HH22	1.71	0.56
1:C:1068:PRO:HD3	1:C:1074:ARG:NE	2.21	0.56
1:D:62:SER:HA	1:D:81:ASP:OD1	2.05	0.56
1:D:760:LYS:HD3	1:D:768:ILE:HD12	1.88	0.56
1:A:437:LYS:H	1:A:437:LYS:CD	2.18	0.56
1:C:207:VAL:HG12	1:C:207:VAL:O	2.04	0.56
1:C:657:ASN:OD1	1:C:984:PRO:HA	2.06	0.56
1:D:746:LEU:CD1	1:D:865:GLU:HG2	2.36	0.56
1:A:121:LEU:HB3	1:A:127:PHE:CD2	2.41	0.55
1:C:166:VAL:HG12	1:C:167:ILE:N	2.21	0.55
1:C:347:THR:HG23	1:C:360:ILE:HD13	1.88	0.55
1:C:920:TYR:OH	1:C:938:LEU:HG	2.06	0.55
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.29	0.55
1:D:590:ILE:CG1	1:D:837:TYR:CE2	2.90	0.55
1:B:705:CYS:HB3	1:B:743:MET:HE1	1.87	0.55
1:C:606:MET:HE1	1:C:671:ILE:HD12	1.87	0.55
1:D:1077:TYR:N	1:D:1077:TYR:CD1	2.74	0.55
1:A:596:ASP:O	1:A:599:LYS:HG2	2.06	0.55
1:C:194:LYS:HD3	1:C:236:GLU:OE2	2.06	0.55
1:C:1043:ARG:HH11	1:C:1043:ARG:CB	2.19	0.55
1:B:269:ARG:O	1:B:272:GLN:HB2	2.06	0.55
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.53	0.55
1:B:289:GLN:O	1:B:293:ASP:HB2	2.07	0.55
1:B:871:TYR:O	1:B:871:TYR:CD1	2.60	0.55
1:D:259:HIS:C	1:D:260:LEU:HD23	2.31	0.55
1:A:743:MET:HE2	1:A:743:MET:N	2.21	0.55
1:C:378:ILE:N	1:C:378:ILE:HD12	2.22	0.55
1:C:513:PRO:O	1:C:515:ASN:HB2	2.07	0.55
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.72	0.55
1:A:897:VAL:HG21	1:A:917:MET:HB3	1.89	0.55
1:B:142:HIS:H	1:B:145:HIS:CD2	2.25	0.55
1:D:381:GLU:HG2	1:D:387:PHE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:O	1:D:53:PHE:C	2.50	0.55
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.89	0.55
1:A:334:THR:HG21	1:A:430:SER:OG	2.06	0.55
1:B:622:ASN:HD22	1:B:623:PRO:N	2.04	0.55
1:D:701:GLU:OE2	1:D:769:HIS:ND1	2.36	0.55
1:B:55:ALA:HA	1:B:58:GLU:OE1	2.07	0.55
1:C:811:ASN:H	1:C:811:ASN:ND2	2.04	0.55
1:D:142:HIS:H	1:D:145:HIS:HD2	1.53	0.55
1:A:335:ILE:HD13	1:A:375:GLN:HB2	1.87	0.54
1:B:329:VAL:CG2	1:B:348:GLN:HE22	2.18	0.54
1:D:56:ALA:O	1:D:57:ALA:C	2.49	0.54
1:D:113:ALA:HB1	1:D:139:ILE:HD11	1.88	0.54
1:A:784:LYS:HD3	1:A:784:LYS:C	2.32	0.54
1:B:48:ILE:O	1:B:52:ILE:HG12	2.08	0.54
1:B:864:HIS:HD2	1:B:866:MET:HG3	1.72	0.54
1:D:717:ASN:HD22	1:D:717:ASN:H	1.55	0.54
1:A:504:ILE:CG2	1:A:1042:MET:HG3	2.37	0.54
1:B:333:HIS:O	1:B:334:THR:C	2.51	0.54
1:B:719:THR:HG22	1:B:720:LEU:N	2.21	0.54
1:B:934:ASP:O	1:B:938:LEU:HG	2.07	0.54
1:C:622:ASN:HD21	1:C:624:TRP:CD1	2.24	0.54
1:D:244:HIS:HD2	1:D:265:CYS:HB2	1.72	0.54
1:A:828:ILE:HD12	1:A:829:GLU:N	2.21	0.54
1:A:864:HIS:CG	1:A:866:MET:HG3	2.40	0.54
1:B:1093:ASN:O	1:B:1093:ASN:ND2	2.41	0.54
1:D:86:VAL:HG11	1:D:95:SER:O	2.08	0.54
1:D:986:ASP:OD2	1:D:986:ASP:C	2.48	0.54
1:B:47:GLU:CG	1:B:48:ILE:N	2.63	0.54
1:D:283:LEU:HD22	1:D:287:LEU:HD13	1.88	0.54
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.70	0.54
1:A:869:GLY:O	1:A:870:GLN:C	2.50	0.54
1:D:927:ASP:HB3	1:D:930:SER:OG	2.08	0.54
1:A:87:GLY:C	1:A:89:ASP:N	2.66	0.54
1:B:690:ASN:O	1:B:694:GLN:HG2	2.08	0.54
1:C:886:ARG:O	1:C:888:ASP:N	2.41	0.54
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.43	0.54
1:A:43:ALA:HA	1:A:66:ILE:CD1	2.38	0.54
1:B:357:LEU:O	1:B:362:MET:HB3	2.08	0.54
1:B:780:LEU:HD13	1:C:778:ASN:ND2	2.23	0.54
1:C:45:ARG:HA	1:C:76:HIS:CD2	2.43	0.54
1:D:622:ASN:C	1:D:622:ASN:ND2	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.88	0.54
1:B:114:ILE:HG13	1:B:136:ILE:HG21	1.90	0.54
1:C:329:VAL:HG22	1:C:348:GLN:NE2	2.23	0.54
1:C:507:VAL:HA	1:C:511:GLY:O	2.07	0.54
1:C:796:THR:HB	1:C:810:ALA:HB2	1.89	0.54
1:A:555:GLU:O	1:A:558:LYS:HG3	2.06	0.54
1:B:252:ASP:HB3	1:B:357:LEU:HD23	1.90	0.54
1:B:394:ILE:HG13	1:B:418:ILE:HD13	1.90	0.54
1:B:927:ASP:H	1:B:930:SER:HB2	1.73	0.54
1:B:959:PHE:HD1	1:B:964:GLN:NE2	2.05	0.54
1:C:270:ARG:HH11	1:C:271:HIS:HD2	1.55	0.53
1:D:743:MET:HE1	1:D:905:VAL:HG13	1.90	0.53
1:D:1075:THR:CG2	1:D:1077:TYR:HE1	2.21	0.53
1:A:58:GLU:HB3	1:C:441:GLU:HG3	1.91	0.53
1:A:263:ARG:HG2	1:A:278:ALA:HB2	1.90	0.53
1:B:337:GLU:HG2	1:B:342:ILE:O	2.08	0.53
1:B:999:GLN:NE2	1:B:1001:PRO:HG3	2.19	0.53
1:C:342:ILE:HG13	1:C:362:MET:HE1	1.89	0.53
1:C:864:HIS:HD2	1:C:866:MET:HG3	1.72	0.53
1:D:278:ALA:CB	1:D:335:ILE:HG23	2.38	0.53
1:A:498:THR:HG23	1:A:1085:ARG:HH12	1.74	0.53
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.41	0.53
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.90	0.53
1:C:438:GLN:CG	1:C:441:GLU:OE1	2.43	0.53
1:C:645:ALA:N	1:C:677:PHE:O	2.39	0.53
1:D:866:MET:HE2	1:D:874:LEU:CD2	2.39	0.53
1:D:1065:ILE:HG22	1:D:1066:SER:H	1.72	0.53
1:B:398:ARG:HH22	1:B:1085:ARG:HH21	1.54	0.53
1:D:506:ASN:ND2	4:D:1201:BTI:H92	2.23	0.53
1:D:876:GLN:O	1:D:879:LYS:N	2.33	0.53
1:D:1053:ASP:O	1:D:1054:LYS:C	2.51	0.53
1:C:840:THR:O	1:C:843:THR:HB	2.09	0.53
1:C:1076:ILE:HD12	1:C:1089:ILE:HD11	1.88	0.53
1:D:318:ASP:O	1:D:319:GLU:HB2	2.08	0.53
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.90	0.53
1:A:811:ASN:HD22	1:A:811:ASN:N	2.01	0.53
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.91	0.53
1:B:866:MET:HB3	1:B:870:GLN:HB3	1.91	0.53
1:C:170:THR:HB	1:C:172:GLY:O	2.07	0.53
1:C:647:ASN:ND2	1:C:652:LYS:O	2.40	0.53
1:C:1044:ASN:HD22	1:C:1044:ASN:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ARG:HH22	1:D:847:ASP:CG	2.16	0.53
1:A:644:ARG:NH2	1:A:908:THR:HG22	2.24	0.53
1:B:94:GLU:O	1:B:96:TYR:N	2.41	0.53
1:C:215:ASP:HB3	1:C:219:ARG:NH2	2.23	0.53
1:C:338:MET:HE1	1:C:430:SER:HB3	1.87	0.53
1:D:640:GLN:HG3	1:D:673:VAL:HB	1.89	0.53
1:A:284:SER:OG	1:A:287:LEU:HB2	2.09	0.53
1:B:141:PRO:HA	1:B:305:VAL:HG12	1.91	0.53
1:B:398:ARG:NH2	1:B:1085:ARG:HE	2.07	0.53
1:B:704:ILE:CD1	1:B:730:LEU:CD1	2.85	0.53
1:C:266:SER:O	1:C:478:THR:HA	2.09	0.53
1:A:565:LEU:HD23	1:A:565:LEU:C	2.33	0.53
1:B:504:ILE:HG21	1:B:1042:MET:HG3	1.91	0.53
1:D:622:ASN:HD21	1:D:624:TRP:H	1.56	0.53
1:A:719:THR:O	1:A:721:GLU:N	2.43	0.53
1:D:413:PHE:CZ	1:D:416:ALA:HB2	2.44	0.53
1:B:267:VAL:HG22	1:B:476:TYR:CE2	2.44	0.52
1:C:928:GLU:O	1:C:931:VAL:HG12	2.09	0.52
1:D:539:SER:HA	1:D:543:GLN:HG3	1.91	0.52
1:A:174:ILE:HD12	1:A:179:LEU:HD12	1.90	0.52
1:A:189:PHE:CD2	1:A:208:ARG:HD2	2.44	0.52
1:A:1089:ILE:HD12	1:A:1089:ILE:N	2.24	0.52
1:B:436:PHE:HE2	1:B:472:THR:HA	1.74	0.52
1:B:532:VAL:HB	1:B:537:ILE:HD11	1.89	0.52
1:B:730:LEU:HD22	1:B:735:PHE:CE1	2.44	0.52
1:C:213:LEU:C	1:C:215:ASP:N	2.67	0.52
1:D:342:ILE:HG21	1:D:362:MET:HE2	1.91	0.52
1:A:703:THR:HG21	1:A:741:LYS:HB2	1.90	0.52
1:A:631:ARG:HG2	1:A:670:GLY:HA3	1.92	0.52
1:A:799:ALA:H	1:A:811:ASN:HD21	1.56	0.52
1:B:660:HIS:CD2	1:B:692:ALA:HB2	2.45	0.52
1:C:648:ALA:HB2	1:C:659:ILE:HD12	1.90	0.52
1:C:799:ALA:H	1:C:811:ASN:ND2	2.07	0.52
1:D:323:ILE:HG22	1:D:324:GLU:HG2	1.91	0.52
1:D:897:VAL:HG12	1:D:914:VAL:HG13	1.92	0.52
1:A:144:GLU:O	1:A:148:MET:HE3	2.10	0.52
1:A:152:LYS:CE	1:A:324:GLU:HB3	2.40	0.52
1:A:283:LEU:CD2	1:A:287:LEU:HD13	2.38	0.52
1:B:841:VAL:O	1:B:844:TYR:HB2	2.09	0.52
1:C:866:MET:HG2	1:C:894:TYR:CZ	2.44	0.52
1:D:447:LEU:CD1	1:D:462:LEU:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:O	1:A:431:THR:HA	2.09	0.52
1:A:622:ASN:HD22	1:A:623:PRO:N	2.08	0.52
1:D:357:LEU:HA	1:D:360:ILE:HD12	1.91	0.52
1:A:539:SER:HB2	1:A:543:GLN:HG2	1.90	0.52
1:A:742:ASP:OD2	1:A:745:GLY:HA2	2.10	0.52
1:C:686:MET:O	1:C:687:LYS:C	2.53	0.52
1:C:810:ALA:HB1	1:C:831:MET:HE1	1.92	0.52
1:D:48:ILE:O	1:D:52:ILE:HD12	2.09	0.52
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.92	0.52
1:A:241:ASN:N	1:A:242:PRO:CD	2.72	0.52
1:A:437:LYS:H	1:A:437:LYS:HD2	1.75	0.52
1:A:879:LYS:C	1:A:881:LEU:H	2.18	0.52
1:B:743:MET:SD	1:B:743:MET:N	2.75	0.52
1:C:289:GLN:OE1	1:C:289:GLN:HA	2.09	0.52
1:A:448:ARG:HH22	1:A:467:LYS:HE2	1.74	0.52
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.25	0.52
1:D:711:LEU:HG	1:D:751:ALA:HB2	1.90	0.52
1:C:814:TYR:CZ	1:C:828:ILE:CG1	2.93	0.52
1:D:477:THR:C	1:D:479:LYS:N	2.68	0.52
1:D:717:ASN:HD22	1:D:717:ASN:N	2.08	0.52
1:D:252:ASP:OD2	1:D:256:ASN:N	2.42	0.51
1:D:878:ALA:O	1:D:883:LEU:HB2	2.09	0.51
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.92	0.51
1:A:494:LEU:HD22	1:A:496:ARG:HH22	1.74	0.51
1:A:979:GLY:C	1:A:981:TYR:H	2.18	0.51
1:D:137:LYS:HD2	1:D:352:ALA:HB1	1.92	0.51
1:D:524:TYR:HD2	1:D:843:THR:HG22	1.76	0.51
1:B:401:GLY:O	1:D:54:ARG:NH1	2.43	0.51
1:C:169:GLY:CA	1:C:236:GLU:HA	2.40	0.51
1:C:563:VAL:HG11	1:C:787:ILE:HG12	1.93	0.51
1:D:357(A):PHE:CE2	1:D:363:GLN:HA	2.44	0.51
1:A:501:LEU:HD11	1:A:1080:MET:HE2	1.93	0.51
1:C:874:LEU:O	1:C:878:ALA:HB2	2.10	0.51
1:D:290:ARG:HG3	1:D:290:ARG:HH11	1.74	0.51
1:A:116:PRO:HB2	1:A:122:SER:HA	1.92	0.51
1:D:343:ASP:OD2	1:D:343:ASP:C	2.54	0.51
1:D:581:ARG:HG3	1:D:848:PHE:CD2	2.46	0.51
1:A:64:VAL:HG22	1:A:82:GLU:HB2	1.91	0.51
1:A:183:PHE:O	1:A:186:GLU:CG	2.58	0.51
1:A:549:GLY:O	1:A:553:VAL:HG23	2.11	0.51
1:A:968:LEU:O	1:A:969:LYS:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:HH22	1:B:1085:ARG:NH2	2.09	0.51
1:B:446:SER:O	1:B:450:MET:HG3	2.10	0.51
1:B:881:LEU:CD2	1:B:923:GLN:OE1	2.59	0.51
1:C:211:SER:O	1:C:214:GLU:HB2	2.11	0.51
1:C:495:ASP:CB	1:C:498:THR:HB	2.40	0.51
1:C:1080:MET:HE1	1:C:1085:ARG:HH21	1.74	0.51
1:C:41:LEU:HD23	1:C:42:VAL:N	2.26	0.51
1:C:977:ARG:O	1:C:978:PRO:C	2.53	0.51
1:D:1051:GLU:OE2	1:D:1057:ARG:NH1	2.44	0.51
1:A:875:SER:C	1:A:877:GLN:N	2.68	0.51
1:B:377:ARG:HG2	1:B:425:LEU:CD1	2.40	0.51
1:B:743:MET:HE3	1:B:907:VAL:HG22	1.93	0.51
1:B:986:ASP:O	1:B:990:VAL:HG23	2.11	0.51
1:C:338:MET:HE1	1:C:430:SER:C	2.36	0.51
1:D:574:HIS:CD2	1:D:580:THR:HA	2.46	0.51
1:D:651:TYR:CZ	1:D:652:LYS:HD3	2.46	0.51
1:A:1076:ILE:HG13	1:A:1089:ILE:HD13	1.93	0.51
1:B:85:LEU:HD12	1:B:86:VAL:H	1.74	0.51
1:B:115:HIS:HB2	1:B:139:ILE:HD12	1.93	0.51
1:C:98:ASN:C	1:C:98:ASN:HD22	2.19	0.51
1:C:170:THR:HB	1:C:172:GLY:H	1.76	0.51
1:C:652:LYS:HG3	1:C:653:ASN:H	1.76	0.51
1:A:877:GLN:NE2	1:A:919:LEU:CD2	2.74	0.51
1:A:540:GLY:H	1:A:543:GLN:NE2	2.06	0.50
1:B:85:LEU:HD12	1:B:86:VAL:N	2.26	0.50
1:B:304:TYR:OH	1:B:327:PRO:HA	2.10	0.50
1:B:440:GLU:O	1:B:444:VAL:HG23	2.10	0.50
1:A:870:GLN:O	1:A:871:TYR:C	2.52	0.50
1:B:75:LEU:HG	1:B:413:PHE:CD2	2.47	0.50
1:C:189:PHE:N	1:C:190:PRO:CD	2.74	0.50
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.46	0.50
1:D:872:SER:C	1:D:873:ASN:HD22	2.15	0.50
1:D:874:LEU:O	1:D:887:PHE:CE1	2.64	0.50
1:C:267:VAL:HG23	1:C:476:TYR:CE2	2.47	0.50
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.47	0.50
1:C:1004:GLU:HA	1:C:1007:ILE:HG13	1.93	0.50
1:D:1042:MET:HE2	1:D:1078:TYR:HE2	1.76	0.50
1:B:1006:ASP:HB3	1:B:1017:TYR:OH	2.11	0.50
1:B:1086:ARG:NH2	1:D:1063:GLU:OE1	2.44	0.50
1:B:1091:ASP:C	1:B:1093:ASN:N	2.69	0.50
1:A:211:SER:C	1:A:213:LEU:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:SER:CB	1:A:543:GLN:HG2	2.42	0.50
1:A:719:THR:O	1:A:720:LEU:C	2.54	0.50
1:B:330:GLN:O	1:B:331:VAL:C	2.53	0.50
1:C:375:GLN:HE22	1:C:428:LYS:HD3	1.77	0.50
1:C:775:THR:HG21	1:C:861:ILE:HG13	1.93	0.50
1:D:738:LEU:HD12	1:D:739:ALA:H	1.77	0.50
1:B:404:GLY:O	1:B:431:THR:HA	2.11	0.50
1:B:856:SER:CB	1:B:857:PRO:HD2	2.41	0.50
1:C:924:ASN:O	1:C:925:ASP:HB2	2.11	0.50
1:D:678:ASP:OD2	1:D:685:GLN:NE2	2.44	0.50
1:C:40:LEU:HD12	1:C:113:ALA:HB3	1.94	0.50
1:C:234:TYR:CE1	1:C:236:GLU:HG3	2.47	0.50
1:D:477:THR:O	1:D:479:LYS:N	2.45	0.50
1:D:856:SER:HB2	1:D:857:PRO:HD2	1.94	0.50
1:A:170:THR:OG1	1:A:235:ILE:HG23	2.11	0.50
1:A:259:HIS:HB3	1:A:296:ILE:HD12	1.94	0.50
1:B:297:GLN:O	1:B:301:ASN:HB2	2.12	0.50
1:B:377:ARG:HG2	1:B:425:LEU:HD11	1.94	0.50
1:A:504:ILE:HG21	1:A:1042:MET:HG3	1.93	0.50
1:A:1087:ILE:HG22	1:A:1089:ILE:CD1	2.42	0.50
1:B:583:ARG:NH2	1:B:1030:LEU:O	2.44	0.50
1:B:596:ASP:O	1:B:599:LYS:HG2	2.12	0.50
1:A:177:TYR:C	1:A:179:LEU:N	2.67	0.49
1:B:398:ARG:NE	1:B:1083:GLN:HB3	2.25	0.49
1:B:575:GLN:NE2	1:B:610:ALA:H	2.10	0.49
1:B:652:LYS:CG	1:B:653:ASN:N	2.75	0.49
1:C:512:PHE:C	1:C:512:PHE:CD2	2.90	0.49
1:C:606:MET:HE1	1:C:671:ILE:HD11	1.92	0.49
1:C:889:GLU:HA	1:C:892:ASP:OD1	2.11	0.49
1:A:529:ILE:HD12	1:A:837:TYR:HE1	1.77	0.49
1:A:991:ARG:NH1	1:A:1004:GLU:OE1	2.39	0.49
1:B:287:LEU:HD22	1:B:291:ILE:HD11	1.94	0.49
1:B:1092:GLU:O	1:B:1093:ASN:HB3	2.12	0.49
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.94	0.49
1:D:164:LEU:HD13	1:D:294:ALA:CB	2.40	0.49
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.27	0.49
1:D:561:ASP:O	1:D:822:ARG:HD2	2.12	0.49
1:A:259:HIS:C	1:A:260:LEU:HD23	2.37	0.49
1:A:338:MET:HE1	1:A:430:SER:C	2.37	0.49
1:A:877:GLN:NE2	1:A:919:LEU:HD23	2.25	0.49
1:B:44:ASN:ND2	1:B:48:ILE:CG2	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PRO:HB2	1:B:145:HIS:CD2	2.46	0.49
1:B:565:LEU:HD21	1:B:826:THR:HG21	1.95	0.49
1:C:130:ARG:CZ	1:C:130:ARG:HB3	2.41	0.49
1:C:846:SER:HA	1:C:849:GLU:HG2	1.95	0.49
1:C:976:ALA:HB3	1:C:981:TYR:HE2	1.76	0.49
1:A:1020:TYR:CD2	1:A:1021:ILE:HD12	2.47	0.49
1:A:1087:ILE:CG2	1:A:1089:ILE:HD11	2.42	0.49
1:B:631:ARG:HG2	1:B:670:GLY:HA3	1.94	0.49
1:B:652:LYS:HG3	1:B:653:ASN:H	1.77	0.49
1:C:873:ASN:O	1:C:877:GLN:HG2	2.12	0.49
1:C:882:GLY:C	1:C:884:GLY:N	2.67	0.49
1:B:165:PRO:O	1:B:166:VAL:HG13	2.12	0.49
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.47	0.49
1:C:529:ILE:HG21	1:C:589:ASN:HB3	1.95	0.49
1:D:302:ILE:O	1:D:303:LYS:C	2.55	0.49
1:D:485:PRO:C	1:D:487:LEU:H	2.20	0.49
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.76	0.49
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.93	0.49
1:D:459:ILE:N	1:D:460:PRO:CD	2.75	0.49
1:A:242:PRO:O	1:A:478:THR:HG23	2.13	0.49
1:A:329:VAL:CG2	1:A:348:GLN:CD	2.86	0.49
1:B:522:PRO:C	1:B:524:TYR:N	2.69	0.49
1:B:704:ILE:HG12	1:B:738:LEU:HD11	1.94	0.49
1:B:879:LYS:HG3	1:B:884:GLY:HA3	1.95	0.49
1:B:574:HIS:CD2	1:B:580:THR:HA	2.48	0.49
1:B:701:GLU:OE2	1:B:737:ILE:CG2	2.59	0.49
1:C:114:ILE:HG13	1:C:136:ILE:CG2	2.43	0.49
1:C:136:ILE:N	1:C:136:ILE:CD1	2.69	0.49
1:C:217:PHE:C	1:C:217:PHE:CD2	2.91	0.49
1:C:597:VAL:HG11	1:C:834:LEU:HD12	1.95	0.49
1:D:811:ASN:H	1:D:811:ASN:ND2	1.79	0.49
1:D:873:ASN:ND2	1:D:873:ASN:H	2.07	0.49
1:A:820:PHE:HB3	1:A:821:PRO:HD2	1.94	0.49
1:B:338:MET:HE1	1:B:430:SER:CB	2.41	0.49
1:B:763:VAL:HB	1:B:766:LEU:HB2	1.95	0.49
1:A:715:ARG:NH1	1:A:865:GLU:OE2	2.46	0.49
1:B:395:ILE:HG12	1:B:453:ARG:O	2.13	0.49
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.28	0.49
1:D:252:ASP:HA	1:D:351:VAL:CG1	2.43	0.49
1:D:728:LYS:HE2	1:D:762:ALA:HB1	1.95	0.49
1:D:917:MET:CG	1:D:944:VAL:CG2	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:OD2	1:A:422:TYR:CE1	2.65	0.48
1:B:99:ILE:HG23	1:B:127:PHE:HA	1.95	0.48
1:B:395:ILE:CD1	1:B:1086:ARG:O	2.59	0.48
1:C:59:LEU:O	1:C:60:ASP:HB3	2.13	0.48
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.28	0.48
1:A:385:ASN:O	1:A:387:PHE:N	2.46	0.48
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.95	0.48
1:D:506:ASN:HD22	4:D:1201:BTI:H92	1.78	0.48
1:D:509:ILE:HD13	1:D:1074:ARG:HD3	1.96	0.48
1:A:329:VAL:CG2	1:A:348:GLN:OE1	2.61	0.48
1:B:772:THR:HG22	1:B:783:TYR:CZ	2.48	0.48
1:C:191:LEU:HA	1:C:237:ARG:HA	1.95	0.48
1:C:615:ALA:HA	1:C:619:LEU:HB2	1.95	0.48
1:D:412:GLY:O	1:D:413:PHE:HB3	2.14	0.48
1:D:587:MET:HA	1:D:590:ILE:HD11	1.95	0.48
1:A:435:SER:OG	1:A:438:GLN:HB2	2.14	0.48
1:A:469:LYS:HD2	1:A:469:LYS:HA	1.58	0.48
1:A:784:LYS:HD3	1:A:784:LYS:O	2.12	0.48
1:B:258:VAL:HB	1:B:364:GLN:OE1	2.13	0.48
1:C:924:ASN:O	1:C:925:ASP:CB	2.60	0.48
1:D:397:TYR:HA	1:D:451:ARG:O	2.13	0.48
1:D:504:ILE:CG2	1:D:1042:MET:HG3	2.44	0.48
1:D:1071:ASN:HB3	1:D:1073:ASN:HD22	1.79	0.48
1:D:1089:ILE:CG2	1:D:1090:LYS:N	2.76	0.48
1:A:38:LYS:HB3	1:A:38:LYS:HE2	1.61	0.48
1:A:364:GLN:HA	1:A:367:ILE:HG13	1.94	0.48
1:B:565:LEU:HD11	1:B:598:PHE:HE2	1.79	0.48
1:B:802:SER:OG	1:B:809:SER:HB2	2.14	0.48
1:B:1049:GLU:C	1:B:1050:ILE:HG13	2.38	0.48
1:C:578:LEU:HD12	1:C:801:MET:HE1	1.96	0.48
1:C:580:THR:HB	1:C:614:VAL:HG21	1.94	0.48
1:C:798:VAL:O	1:C:799:ALA:C	2.57	0.48
1:C:938:LEU:O	1:C:939:ASP:O	2.32	0.48
1:C:1019:GLN:HA	1:C:1022:GLN:NE2	2.28	0.48
1:D:590:ILE:HG13	1:D:837:TYR:CE2	2.48	0.48
1:A:78:TYR:CE2	1:C:1081:ASN:HA	2.49	0.48
1:B:287:LEU:O	1:B:291:ILE:HG13	2.14	0.48
1:C:152:LYS:HE2	1:C:324:GLU:OE2	2.13	0.48
1:C:278:ALA:CB	1:C:335:ILE:CG2	2.91	0.48
1:C:756:ILE:O	1:C:760:LYS:HB2	2.14	0.48
1:D:429:LEU:HD23	1:D:443:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:O	1:A:94:GLU:CG	2.58	0.48
1:A:871:TYR:HE1	1:A:891:LYS:CD	2.25	0.48
1:B:580:THR:HG21	1:B:610:ALA:HB3	1.96	0.48
1:C:360:ILE:O	1:C:362:MET:N	2.46	0.48
1:C:715:ARG:HH21	1:C:865:GLU:CD	2.21	0.48
1:D:983:GLU:HA	1:D:983:GLU:OE2	2.13	0.48
1:D:1065:ILE:HG23	1:D:1076:ILE:HG13	1.95	0.48
1:A:791:VAL:O	1:A:822:ARG:NH2	2.37	0.48
1:A:960:ASN:OD1	1:A:960:ASN:C	2.57	0.48
1:A:1003:THR:HG22	1:A:1006:ASP:OD2	2.14	0.48
1:C:570:PHE:O	1:C:574:HIS:HE1	1.96	0.48
1:D:664:GLN:O	1:D:668:LYS:HG3	2.14	0.48
1:D:869:GLY:O	1:D:870:GLN:C	2.57	0.48
1:B:465:VAL:HG12	1:B:466:MET:HE2	1.94	0.48
1:C:399:SER:CB	1:C:450:MET:HE3	2.43	0.48
1:D:164:LEU:HD12	1:D:165:PRO:HD2	1.96	0.48
1:B:284:SER:OG	1:B:287:LEU:HB2	2.14	0.48
1:B:537:ILE:C	1:B:538(A):SER:H	2.22	0.48
1:D:118:TYR:CZ	1:D:331:VAL:HG22	2.49	0.48
1:D:647:ASN:HD22	1:D:647:ASN:C	2.22	0.48
1:A:156:ARG:NH1	1:A:167:ILE:O	2.47	0.47
1:A:313:LEU:CD2	1:A:323:ILE:HD11	2.39	0.47
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.96	0.47
1:C:438:GLN:HA	1:C:441:GLU:HG2	1.97	0.47
1:D:66:ILE:HB	1:D:86:VAL:HG23	1.96	0.47
1:D:896:ARG:HD2	1:D:928:GLU:OE2	2.13	0.47
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.95	0.47
1:B:817:LEU:O	1:B:818:ASN:C	2.58	0.47
1:C:661:LYS:HZ1	1:C:1004:GLU:HB3	1.79	0.47
1:D:1075:THR:HG22	1:D:1077:TYR:CE1	2.49	0.47
1:A:1003:THR:CG2	1:A:1006:ASP:H	2.24	0.47
1:B:831:MET:O	1:B:832:GLU:C	2.56	0.47
1:C:738:LEU:HD21	1:C:759:LEU:HD13	1.97	0.47
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.79	0.47
1:D:743:MET:HE3	1:D:907:VAL:HG13	1.95	0.47
1:B:286:THR:O	1:B:290:ARG:CG	2.62	0.47
1:B:396:ALA:HB3	1:B:453:ARG:HB2	1.96	0.47
1:B:652:LYS:HG3	1:B:653:ASN:N	2.29	0.47
1:D:593:LYS:O	1:D:597:VAL:HG23	2.15	0.47
1:D:883:LEU:O	1:D:886:ARG:HG2	2.15	0.47
1:A:189:PHE:CE2	1:A:208:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LEU:HD21	1:B:826:THR:CG2	2.44	0.47
1:B:871:TYR:CD1	1:B:871:TYR:C	2.92	0.47
1:C:381:GLU:O	1:C:383:PRO:HD3	2.15	0.47
1:C:622:ASN:HD22	1:C:623:PRO:N	2.11	0.47
1:C:644:ARG:HA	1:C:677:PHE:CE1	2.49	0.47
1:D:720:LEU:HD21	1:D:758:GLU:CG	2.37	0.47
1:A:193:ILE:O	1:A:193:ILE:CG2	2.60	0.47
1:A:263:ARG:HH21	1:A:330:GLN:HE21	1.63	0.47
1:A:979:GLY:O	1:A:981:TYR:N	2.47	0.47
1:B:36:GLN:O	1:B:36:GLN:HG2	2.15	0.47
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.80	0.47
1:B:414:GLN:OE1	1:D:1082:GLY:O	2.32	0.47
1:B:519:ARG:CB	1:B:520:PRO:CD	2.90	0.47
1:B:556:TRP:O	1:B:560:GLN:NE2	2.43	0.47
1:B:740:ILE:HD11	1:B:759:LEU:CD1	2.44	0.47
1:B:864:HIS:HD2	1:B:866:MET:H	1.63	0.47
1:C:902:GLY:O	1:C:903:ASP:HB3	2.15	0.47
1:D:351:VAL:C	1:D:353:ALA:H	2.22	0.47
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.95	0.47
1:A:239:ILE:CD1	1:A:315:SER:HB3	2.44	0.47
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.97	0.47
1:B:59:LEU:HD22	1:B:350:LEU:HD21	1.97	0.47
1:B:394:ILE:O	1:B:414:GLN:O	2.33	0.47
1:C:130:ARG:NH1	1:C:133:GLU:OE1	2.47	0.47
1:C:814:TYR:CZ	1:C:828:ILE:HG13	2.49	0.47
1:C:1035:THR:N	1:C:1036:PRO:CD	2.77	0.47
1:D:760:LYS:CD	1:D:768:ILE:HD12	2.44	0.47
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.65	0.47
1:B:867:PRO:O	1:B:870:GLN:HB2	2.14	0.47
1:D:712:ASN:OD1	1:D:714:GLU:HG2	2.15	0.47
1:A:325:VAL:CG1	1:A:326:ASN:N	2.77	0.47
1:A:853:ASP:OD2	1:A:853:ASP:N	2.41	0.47
1:A:879:LYS:O	1:A:881:LEU:N	2.48	0.47
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.70	0.47
1:C:760:LYS:NZ	1:C:792:ASP:OD2	2.46	0.47
1:D:54:ARG:O	1:D:58:GLU:HG3	2.15	0.47
1:D:938:LEU:O	1:D:939:ASP:HB3	2.14	0.47
1:D:947:PHE:C	1:D:949:LYS:H	2.23	0.47
1:A:871:TYR:C	1:A:871:TYR:CD2	2.92	0.46
1:B:129:ARG:O	1:B:133:GLU:HG3	2.15	0.46
1:B:501:LEU:CD1	1:B:1085:ARG:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:GLU:C	1:C:519:ARG:H	2.23	0.46
1:D:565:LEU:HD23	1:D:824:LEU:HD11	1.96	0.46
1:A:272:GLN:CD	1:A:272:GLN:H	2.14	0.46
1:B:465:VAL:HG22	1:B:487:LEU:CD2	2.45	0.46
1:B:540:GLY:N	1:B:543:GLN:HE21	2.06	0.46
1:C:320:PHE:C	1:C:320:PHE:CD2	2.94	0.46
1:C:407:LEU:HD21	1:C:429:LEU:HD13	1.96	0.46
1:C:803:GLY:O	1:C:804:LEU:C	2.57	0.46
1:C:922:VAL:C	1:C:924:ASN:N	2.55	0.46
1:A:174:ILE:HB	1:A:179:LEU:HD13	1.97	0.46
1:A:440:GLU:O	1:A:440:GLU:HG2	2.15	0.46
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.23	0.46
1:A:879:LYS:C	1:A:881:LEU:N	2.74	0.46
1:B:459:ILE:N	1:B:460:PRO:HD2	2.30	0.46
1:C:399:SER:HA	1:C:450:MET:HE3	1.96	0.46
1:C:866:MET:HG2	1:C:894:TYR:CE2	2.50	0.46
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.63	0.46
1:D:647:ASN:O	1:D:649:VAL:N	2.47	0.46
1:A:798:VAL:O	1:A:799:ALA:C	2.59	0.46
1:A:879:LYS:O	1:A:882:GLY:N	2.42	0.46
1:A:1035:THR:HB	1:A:1036:PRO:HD3	1.98	0.46
1:B:703:THR:C	1:B:704:ILE:HD13	2.40	0.46
1:C:688:VAL:O	1:C:689:ALA:C	2.57	0.46
1:C:949:LYS:HD2	1:C:971:GLN:OE1	2.15	0.46
1:D:388:MET:HE2	1:D:388:MET:HA	1.97	0.46
1:D:490:ILE:H	1:D:490:ILE:HD12	1.80	0.46
1:D:543:GLN:HE21	1:D:636:ASN:HA	1.76	0.46
1:A:551:LYS:HE3	1:A:551:LYS:HA	1.97	0.46
1:A:780:LEU:O	1:A:781:LEU:C	2.57	0.46
1:A:826:THR:CG2	1:A:831:MET:HE2	2.44	0.46
1:B:360:ILE:O	1:B:361:ASN:C	2.58	0.46
1:C:578:LEU:HD22	1:C:845:TYR:HB3	1.98	0.46
1:D:624:TRP:CD2	1:D:1005:GLN:HG2	2.51	0.46
1:A:175:LYS:O	1:A:176:SER:C	2.59	0.46
1:A:503:TYR:O	1:A:505:GLY:N	2.49	0.46
1:B:268:GLN:HB3	1:B:273:LYS:HA	1.96	0.46
1:B:433:ALA:C	1:B:435:SER:H	2.23	0.46
1:B:846:SER:HA	1:B:849:GLU:HG2	1.97	0.46
1:C:403:PHE:O	1:C:404:GLY:C	2.58	0.46
1:D:56:ALA:O	1:D:59:LEU:N	2.38	0.46
1:D:56:ALA:HB1	1:D:61:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:874:LEU:O	1:D:887:PHE:HE1	1.99	0.46
1:A:840:THR:O	1:A:843:THR:HB	2.15	0.46
1:B:622:ASN:HD22	1:B:624:TRP:H	1.62	0.46
1:B:1065:ILE:CG2	1:B:1074:ARG:HD3	2.45	0.46
1:C:504:ILE:CG2	1:C:1042:MET:HG3	2.46	0.46
1:C:517:GLU:C	1:C:519:ARG:N	2.73	0.46
1:D:917:MET:HE3	1:D:940:PHE:HD2	1.80	0.46
1:D:991:ARG:O	1:D:995:GLU:HB2	2.15	0.46
1:B:38:LYS:HA	1:B:38:LYS:HD2	1.76	0.46
1:B:367:ILE:O	1:B:367:ILE:HG22	2.15	0.46
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.97	0.46
1:B:896:ARG:HD2	1:B:928:GLU:OE2	2.15	0.46
1:C:154:LYS:O	1:C:155:ALA:C	2.58	0.46
1:C:568:THR:OG1	1:C:807:GLN:HG3	2.16	0.46
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.98	0.46
1:C:921:MET:O	1:C:926:LEU:N	2.47	0.46
1:D:66:ILE:HG13	1:D:86:VAL:HG21	1.97	0.46
1:D:149:PHE:CE2	1:D:325:VAL:HG21	2.51	0.46
1:D:708:GLY:HA2	1:D:715:ARG:NH1	2.30	0.46
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.46	0.46
1:A:395:ILE:HD12	1:A:1086:ARG:HB2	1.98	0.46
1:A:715:ARG:O	1:A:715:ARG:NE	2.47	0.46
1:C:479:LYS:O	1:C:480:PHE:C	2.58	0.46
1:D:828:ILE:HD12	1:D:829:GLU:H	1.80	0.46
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.45	0.46
1:B:331:VAL:HG23	1:B:332:GLU:OE2	2.15	0.46
1:C:87:GLY:HA3	1:C:90:LEU:HB2	1.98	0.46
1:C:274:VAL:HG12	1:C:275:VAL:HG23	1.98	0.46
1:C:431:THR:HG21	1:C:443:MET:HA	1.97	0.46
1:C:606:MET:CE	1:C:607:TRP:HB2	2.45	0.46
1:C:897:VAL:HG12	1:C:914:VAL:HG13	1.98	0.46
1:D:290:ARG:NE	1:D:320:PHE:HE1	2.13	0.46
1:D:743:MET:HG3	1:D:907:VAL:CG1	2.46	0.46
1:B:310:VAL:HG22	1:B:325:VAL:HG22	1.98	0.45
1:B:437:LYS:HE3	1:B:437:LYS:HA	1.97	0.45
1:C:473:SER:OG	1:C:474:GLY:N	2.49	0.45
1:A:53:PHE:CZ	1:A:65:ALA:HB2	2.52	0.45
1:A:329:VAL:CG2	1:A:348:GLN:NE2	2.80	0.45
1:A:870:GLN:OE1	1:A:911:SER:HB2	2.16	0.45
1:B:650:GLY:HA2	1:B:1013:TYR:CE1	2.51	0.45
1:C:995:GLU:CG	1:C:1002:VAL:CG2	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ILE:O	1:D:312:PHE:HB2	2.16	0.45
1:A:208:ARG:HG3	1:A:208:ARG:O	2.16	0.45
1:A:453:ARG:HG3	1:A:453:ARG:NH1	2.31	0.45
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.26	0.45
1:C:837:TYR:CZ	1:C:841:VAL:HG21	2.52	0.45
1:D:1080:MET:O	1:D:1081:ASN:C	2.58	0.45
1:A:94:GLU:HA	1:A:97:LEU:HD12	1.98	0.45
1:A:335:ILE:HD11	1:A:374:ILE:O	2.17	0.45
1:A:647:ASN:HA	1:A:659:ILE:HD11	1.99	0.45
1:A:704:ILE:HD12	1:A:738:LEU:HD11	1.99	0.45
1:B:391:THR:HG22	1:B:392:GLY:N	2.31	0.45
1:B:395:ILE:CG1	1:B:396:ALA:N	2.79	0.45
1:B:1032:LEU:HD13	1:B:1052:ILE:HA	1.99	0.45
1:C:606:MET:HE3	1:C:607:TRP:N	2.32	0.45
1:C:864:HIS:CD2	1:C:866:MET:H	2.33	0.45
1:D:299:MET:HB3	1:D:304:TYR:HB3	1.99	0.45
1:D:337:GLU:HG2	1:D:344:ILE:CD1	2.46	0.45
1:A:43:ALA:HA	1:A:66:ILE:HD13	1.99	0.45
1:B:338:MET:HE3	1:B:338:MET:HB2	1.80	0.45
1:C:215:ASP:CB	1:C:219:ARG:HH22	2.29	0.45
1:C:304:TYR:OH	1:C:327:PRO:HA	2.16	0.45
1:C:690:ASN:O	1:C:694:GLN:HG2	2.16	0.45
1:D:738:LEU:HD12	1:D:739:ALA:N	2.32	0.45
1:A:516:VAL:O	1:A:517:GLU:C	2.59	0.45
1:A:590:ILE:O	1:A:591:ALA:C	2.60	0.45
1:A:641:MET:HE3	1:A:674:PHE:HE1	1.76	0.45
1:B:481:ILE:HD12	1:B:481:ILE:H	1.82	0.45
1:B:1042:MET:HE3	1:B:1062:LEU:HD12	1.99	0.45
1:C:87:GLY:C	1:C:89:ASP:N	2.74	0.45
1:C:380:THR:HG22	1:C:426:LEU:HD11	1.99	0.45
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.81	0.45
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.51	0.45
1:A:237:ARG:NH1	1:A:237:ARG:CG	2.71	0.45
1:A:259:HIS:CD2	1:A:296:ILE:HD13	2.52	0.45
1:A:708:GLY:HA2	1:A:715:ARG:NH1	2.32	0.45
1:A:1065:ILE:N	1:A:1065:ILE:HD12	2.32	0.45
1:B:257:ILE:HD12	1:B:300:GLU:OE1	2.16	0.45
1:B:402:GLY:H	1:B:405:VAL:HG21	1.82	0.45
1:B:846:SER:HA	1:B:849:GLU:CG	2.46	0.45
1:C:1069:ASP:OD2	1:C:1073:ASN:O	2.34	0.45
1:D:425:LEU:C	1:D:425:LEU:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:THR:O	1:A:976:ALA:HB2	2.16	0.45
1:A:1017:TYR:CZ	1:A:1021:ILE:HD13	2.52	0.45
1:B:164:LEU:HB3	1:B:165:PRO:HD2	1.98	0.45
1:B:400:SER:OG	1:B:401:GLY:N	2.50	0.45
1:B:627:LEU:HD12	1:B:627:LEU:O	2.17	0.45
1:B:867:PRO:O	1:B:868:GLY:C	2.59	0.45
1:C:731:GLU:OE1	1:C:763:VAL:HB	2.17	0.45
1:D:292:CYS:O	1:D:293:ASP:C	2.60	0.45
1:D:331:VAL:HG12	1:D:375:GLN:HE22	1.82	0.45
1:A:533:SER:O	1:A:537:ILE:HG12	2.17	0.45
1:A:1068:PRO:HD3	1:A:1074:ARG:HE	1.81	0.45
1:B:871:TYR:O	1:B:871:TYR:HD1	1.97	0.45
1:B:960:ASN:O	1:B:961:LYS:C	2.60	0.45
1:C:261:PHE:CD1	1:C:369:THR:HG22	2.52	0.45
1:C:811:ASN:OD1	1:C:832:GLU:OE1	2.35	0.45
1:D:245:ILE:HG21	1:D:283:LEU:HD11	1.99	0.45
1:D:276:GLU:CD	1:D:377:ARG:HH22	2.25	0.45
1:D:1076:ILE:HD13	1:D:1089:ILE:HD13	1.93	0.45
1:A:65:ALA:O	1:A:83:SER:HA	2.17	0.45
1:A:90:LEU:HD21	1:A:94:GLU:HG3	2.00	0.45
1:A:181:LYS:O	1:A:182:GLU:HB3	2.17	0.45
1:A:643:LEU:CD1	1:A:648:ALA:HA	2.47	0.45
1:A:866:MET:HE2	1:A:871:TYR:N	2.32	0.45
1:C:721:GLU:N	1:C:721:GLU:CD	2.74	0.45
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.82	0.44
1:A:212:GLU:N	1:A:213:LEU:HD23	2.32	0.44
1:A:1058:LEU:HD22	1:A:1080:MET:SD	2.58	0.44
1:B:646:SER:HB3	1:B:685:GLN:NE2	2.26	0.44
1:C:145:HIS:HE1	1:C:302:ILE:O	1.99	0.44
1:C:524:TYR:CD2	1:C:843:THR:HG22	2.51	0.44
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.52	0.44
1:D:938:LEU:O	1:D:939:ASP:CB	2.62	0.44
1:B:239:ILE:CG2	1:B:313:LEU:HD21	2.47	0.44
1:B:960:ASN:HD22	1:B:963:LEU:H	1.65	0.44
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.32	0.44
1:C:807:GLN:H	1:C:807:GLN:HG2	1.62	0.44
1:D:296:ILE:O	1:D:300:GLU:CB	2.60	0.44
1:A:213:LEU:N	1:A:213:LEU:CD2	2.80	0.44
1:A:259:HIS:HD2	1:A:296:ILE:HD13	1.83	0.44
1:B:54:ARG:O	1:B:55:ALA:C	2.60	0.44
1:B:796:THR:HB	1:B:810:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ARG:HA	1:C:701:GLU:HB3	2.00	0.44
1:C:1035:THR:N	1:C:1036:PRO:HD2	2.32	0.44
1:D:526:LEU:HD23	1:D:526:LEU:HA	1.84	0.44
1:D:926:LEU:HD12	1:D:926:LEU:HA	1.84	0.44
1:A:920:TYR:CE1	1:A:939:ASP:O	2.71	0.44
1:B:98:ASN:C	1:B:98:ASN:HD22	2.25	0.44
1:B:907:VAL:O	1:B:911:SER:CB	2.48	0.44
1:C:622:ASN:ND2	1:C:624:TRP:N	2.60	0.44
1:B:261:PHE:HE1	1:B:367:ILE:O	2.00	0.44
1:B:403:PHE:HE2	1:D:337:GLU:HB3	1.83	0.44
1:C:432:HIS:CG	1:C:433:ALA:N	2.84	0.44
1:C:631:ARG:HA	1:C:631:ARG:HD3	1.76	0.44
1:D:162:ALA:O	1:D:163:ASP:HB2	2.18	0.44
1:D:266:SER:HA	1:D:478:THR:HG22	2.00	0.44
1:D:772:THR:HG23	1:D:773:HIS:N	2.33	0.44
1:A:362:MET:HE1	1:A:367:ILE:HD13	1.97	0.44
1:A:551:LYS:O	1:A:555:GLU:HG2	2.17	0.44
1:B:70:GLU:HG3	1:B:92:PRO:HB3	1.99	0.44
1:B:311:GLU:CD	1:B:326:ASN:HD21	2.26	0.44
1:C:700:SER:H	1:C:736:HIS:CD2	2.29	0.44
1:D:476:TYR:C	1:D:476:TYR:CD2	2.95	0.44
1:D:643:LEU:O	1:D:676:ILE:HA	2.18	0.44
1:D:875:SER:OG	1:D:887:PHE:CE2	2.69	0.44
1:A:179:LEU:CG	1:A:217:PHE:HE2	2.29	0.44
1:A:267:VAL:HG22	1:A:480:PHE:HD2	1.83	0.44
1:A:760:LYS:HG2	1:A:768:ILE:HD12	1.99	0.44
1:B:704:ILE:CD1	1:B:730:LEU:HD11	2.48	0.44
1:C:71:ASP:C	1:C:73:SER:H	2.25	0.44
1:C:193:ILE:HG12	1:C:235:ILE:HB	2.00	0.44
1:C:518:LYS:O	1:C:519:ARG:O	2.36	0.44
1:D:485:PRO:C	1:D:487:LEU:N	2.75	0.44
1:D:588:ILE:HD13	1:D:588:ILE:HA	1.62	0.44
1:A:869:GLY:O	1:A:871:TYR:N	2.51	0.44
1:B:717(A):ILE:HB	1:B:718:TYR:CD1	2.52	0.44
1:C:347:THR:O	1:C:348:GLN:C	2.60	0.44
1:C:403:PHE:CD1	1:C:403:PHE:C	2.95	0.44
1:D:328:ARG:HD3	1:D:329:VAL:O	2.18	0.44
1:D:935:GLY:CA	1:D:966:VAL:HG13	2.37	0.44
1:A:87:GLY:O	1:A:89:ASP:N	2.51	0.44
1:A:286:THR:O	1:A:289:GLN:N	2.51	0.44
1:A:490:ILE:H	1:A:490:ILE:HG13	1.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HD3	1:B:335:ILE:HG22	2.00	0.44
1:B:302:ILE:C	1:B:303:LYS:HG2	2.43	0.44
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.52	0.44
1:C:622:ASN:ND2	1:C:622:ASN:C	2.74	0.44
1:C:641:MET:HE3	1:C:641:MET:HB2	1.60	0.44
1:D:702:GLY:O	1:D:738:LEU:HD12	2.18	0.44
1:A:48:ILE:HG13	1:A:118:TYR:CE2	2.53	0.43
1:B:1080:MET:CE	1:B:1085:ARG:NH2	2.81	0.43
1:C:571:ARG:NH2	1:C:605:GLU:OE1	2.50	0.43
1:C:631:ARG:HD3	1:C:631:ARG:O	2.18	0.43
1:D:627:LEU:O	1:D:631:ARG:HB2	2.17	0.43
1:D:744:ALA:HB3	1:D:746:LEU:HG	1.99	0.43
1:D:818:ASN:N	1:D:818:ASN:HD22	2.15	0.43
1:A:38:LYS:N	1:A:112:ASP:OD1	2.47	0.43
1:A:40:LEU:HD23	1:A:40:LEU:C	2.43	0.43
1:A:219:ARG:HA	1:A:219:ARG:NE	2.21	0.43
1:A:252:ASP:HA	1:A:351:VAL:HG13	2.00	0.43
1:A:563:VAL:HG11	1:A:794:ILE:HD12	1.98	0.43
1:A:724:VAL:O	1:A:725:LYS:C	2.61	0.43
1:B:521:LYS:HB3	1:B:1043:ARG:NH2	2.33	0.43
1:D:264:ASP:HB2	1:D:280:SER:HA	1.99	0.43
1:D:1054:LYS:O	1:D:1054:LYS:HG3	2.18	0.43
1:A:239:ILE:CD1	1:A:315:SER:CB	2.95	0.43
1:A:799:ALA:N	1:A:811:ASN:ND2	2.67	0.43
1:B:59:LEU:O	1:B:60:ASP:HB2	2.18	0.43
1:B:107:LYS:C	1:B:109:ALA:H	2.26	0.43
1:B:814:TYR:CE2	1:B:828:ILE:HG21	2.53	0.43
1:B:891:LYS:HB2	1:B:891:LYS:HE3	1.85	0.43
1:C:150:GLY:O	1:C:151:ASP:HB2	2.18	0.43
1:C:210:GLU:C	1:C:212:GLU:N	2.74	0.43
1:C:427:VAL:HG21	1:C:450:MET:HE1	2.00	0.43
1:C:878:ALA:O	1:C:883:LEU:C	2.61	0.43
1:D:363:GLN:C	1:D:365:LYS:N	2.75	0.43
1:D:814:TYR:CZ	1:D:828:ILE:HG13	2.54	0.43
1:D:877:GLN:O	1:D:878:ALA:C	2.60	0.43
1:A:820:PHE:HB3	1:A:821:PRO:HD3	1.99	0.43
1:B:163:ASP:O	1:B:164:LEU:HD23	2.18	0.43
1:B:746:LEU:HA	1:B:746:LEU:HD23	1.74	0.43
1:C:563:VAL:HG23	1:C:823:HIS:O	2.18	0.43
1:C:643:LEU:HD23	1:C:676:ILE:HG12	1.99	0.43
1:D:288:ARG:HA	1:D:291:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:871:TYR:C	1:D:871:TYR:CD2	2.95	0.43
1:A:825:ARG:O	1:A:826:THR:HB	2.17	0.43
1:B:1051:GLU:OE1	1:B:1057:ARG:NH1	2.51	0.43
1:C:169:GLY:HA3	1:C:236:GLU:HA	2.00	0.43
1:C:193:ILE:CG1	1:C:235:ILE:HB	2.48	0.43
1:C:322:PHE:CD1	1:C:322:PHE:C	2.97	0.43
1:C:986:ASP:C	1:C:986:ASP:OD1	2.61	0.43
1:D:246:GLU:HB3	1:D:311:GLU:HA	2.00	0.43
1:D:640:GLN:HG3	1:D:673:VAL:CB	2.49	0.43
1:D:743:MET:CE	1:D:905:VAL:HG13	2.48	0.43
1:D:1042:MET:CE	1:D:1062:LEU:HB2	2.30	0.43
1:A:381:GLU:HA	1:A:388:MET:O	2.18	0.43
1:A:550:PRO:O	1:A:551:LYS:C	2.61	0.43
1:C:66:ILE:HB	1:C:86:VAL:CG2	2.49	0.43
1:C:358:GLU:OE1	1:C:358:GLU:HA	2.19	0.43
1:C:374:ILE:HG22	1:C:443:MET:CE	2.47	0.43
1:D:164:LEU:HA	1:D:165:PRO:HD2	1.89	0.43
1:D:363:GLN:C	1:D:365:LYS:H	2.27	0.43
1:D:1042:MET:HB2	1:D:1062:LEU:HD12	2.00	0.43
1:A:147:ASP:OD2	1:A:154:LYS:HE3	2.19	0.43
1:A:636:ASN:OD1	1:A:636:ASN:N	2.52	0.43
1:B:55:ALA:O	1:B:58:GLU:HB2	2.19	0.43
1:B:879:LYS:C	1:B:881:LEU:H	2.25	0.43
1:D:289:GLN:NE2	1:D:289:GLN:CA	2.76	0.43
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.84	0.43
1:D:891:LYS:HB2	1:D:891:LYS:HE2	1.78	0.43
1:B:994:LEU:HD23	1:B:994:LEU:HA	1.88	0.43
1:C:87:GLY:HA2	1:C:101:ARG:NH1	2.33	0.43
1:C:438:GLN:HA	1:C:441:GLU:CG	2.49	0.43
1:C:519:ARG:HG3	1:C:520:PRO:O	2.17	0.43
1:D:491:GLN:H	1:D:491:GLN:HG2	1.73	0.43
1:D:948:PHE:CD1	1:D:967:ILE:HD13	2.54	0.43
1:A:45:ARG:HA	1:A:76:HIS:CD2	2.54	0.43
1:A:563:VAL:HG21	1:A:787:ILE:HG12	2.01	0.43
1:A:747:LEU:O	1:A:747:LEU:HG	2.18	0.43
1:B:128:ALA:O	1:B:131:CYS:HB2	2.19	0.43
1:B:292:CYS:O	1:B:293:ASP:C	2.61	0.43
1:B:320:PHE:O	1:B:321:PHE:CD1	2.72	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.19	0.43
1:C:543:GLN:H	1:C:543:GLN:HG2	1.59	0.43
1:D:479:LYS:HG2	1:D:482:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:837:TYR:CZ	1:D:841:VAL:HG21	2.53	0.43
1:D:1008:ILE:HD12	1:D:1008:ILE:HA	1.85	0.43
1:A:207:VAL:CG1	1:A:213:LEU:HD22	2.49	0.43
1:A:509:ILE:HD11	1:A:1065:ILE:HG21	2.00	0.43
1:B:350:LEU:C	1:B:352:ALA:N	2.76	0.43
1:B:368:THR:CG2	1:B:369:THR:N	2.81	0.43
1:B:881:LEU:HD21	1:B:923:GLN:OE1	2.19	0.43
1:B:919:LEU:HD12	1:B:919:LEU:HA	1.87	0.43
1:C:311:GLU:HB2	1:C:324:GLU:HB3	2.01	0.43
1:C:396:ALA:HB3	1:C:453:ARG:HB2	2.00	0.43
1:C:655:PRO:HG2	1:C:985:VAL:HG23	2.01	0.43
1:A:184:ALA:CB	1:A:185:GLU:OE2	2.60	0.42
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.83	0.42
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.42
1:A:650:GLY:HA2	1:A:1013:TYR:CE1	2.53	0.42
1:A:717:ASN:C	1:A:717(A):ILE:HD12	2.44	0.42
1:A:970:GLY:O	1:A:971:GLN:C	2.61	0.42
1:B:944:VAL:O	1:B:948:PHE:HD1	2.02	0.42
1:C:215:ASP:HB2	1:C:219:ARG:HH12	1.84	0.42
1:C:443:MET:HE3	1:C:466:MET:HE3	2.01	0.42
1:C:459:ILE:N	1:C:460:PRO:CD	2.82	0.42
1:C:1014:PRO:O	1:C:1018:GLU:HG2	2.18	0.42
1:D:314:VAL:O	1:D:314:VAL:HG12	2.19	0.42
1:D:437:LYS:HD3	1:D:441:GLU:OE1	2.19	0.42
1:D:994:LEU:O	1:D:998:GLN:HG3	2.19	0.42
1:D:1052:ILE:HG22	1:D:1053:ASP:N	2.24	0.42
1:D:1069:ASP:OD2	1:D:1069:ASP:C	2.62	0.42
1:A:445:ARG:CZ	1:C:54:ARG:HG2	2.48	0.42
1:A:818:ASN:N	1:A:818:ASN:HD22	2.16	0.42
1:A:869:GLY:O	1:A:872:SER:N	2.51	0.42
1:A:873:ASN:C	1:A:875:SER:N	2.74	0.42
1:B:403:PHE:CD1	1:B:403:PHE:C	2.97	0.42
1:B:814:TYR:OH	1:B:828:ILE:HG12	2.19	0.42
1:B:908:THR:HA	1:B:909:PRO:HA	1.69	0.42
1:C:617:ASN:C	1:C:617:ASN:HD22	2.27	0.42
1:C:908:THR:HA	1:C:909:PRO:HA	1.77	0.42
1:D:532:VAL:HG12	1:D:537:ILE:HD12	2.01	0.42
1:A:325:VAL:HG12	1:A:326:ASN:N	2.34	0.42
1:A:916:ASP:OD1	1:A:943:SER:OG	2.32	0.42
1:B:156:ARG:HH21	1:B:166:VAL:HB	1.84	0.42
1:B:162:ALA:HB2	1:B:301:ASN:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ILE:HD12	1:B:481:ILE:N	2.34	0.42
1:C:644:ARG:O	1:C:645:ALA:C	2.61	0.42
1:C:940:PHE:HB3	1:C:941:PRO:CD	2.46	0.42
1:D:67:TYR:CD1	1:D:77:ARG:HG3	2.55	0.42
1:D:129:ARG:O	1:D:130:ARG:C	2.62	0.42
1:D:142:HIS:H	1:D:145:HIS:CD2	2.35	0.42
1:D:338:MET:CE	1:D:430:SER:HB3	2.49	0.42
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.33	0.42
1:A:278:ALA:CB	1:A:335:ILE:CG2	2.95	0.42
1:D:952:ILE:HD12	1:D:952:ILE:HA	1.80	0.42
1:A:564:LEU:O	1:A:793:ILE:HA	2.19	0.42
1:A:581:ARG:HA	1:A:581:ARG:HD3	1.77	0.42
1:A:843:THR:C	1:A:845:TYR:H	2.27	0.42
1:B:118:TYR:CD1	1:B:118:TYR:C	2.98	0.42
1:B:335:ILE:CG2	1:B:336:THR:N	2.77	0.42
1:B:503:TYR:CD1	1:B:503:TYR:C	2.97	0.42
1:B:631:ARG:HA	1:B:631:ARG:HD3	1.46	0.42
1:B:1008:ILE:N	1:B:1008:ILE:CD1	2.72	0.42
1:D:444:VAL:CG2	1:D:466:MET:HB2	2.49	0.42
1:D:470:LYS:HB3	1:D:480:PHE:HE1	1.85	0.42
1:D:481:ILE:HG22	1:D:482:GLU:N	2.34	0.42
1:D:583:ARG:NH1	1:D:1035:THR:HA	2.34	0.42
1:D:1013:TYR:O	1:D:1014:PRO:C	2.63	0.42
1:D:1089:ILE:HG22	1:D:1090:LYS:N	2.33	0.42
1:A:43:ALA:HA	1:A:66:ILE:HD11	2.01	0.42
1:A:651:TYR:CE1	1:A:652:LYS:HG2	2.54	0.42
1:A:991:ARG:HG3	1:A:995:GLU:HG3	2.01	0.42
1:B:613:ASP:O	1:B:617:ASN:HB2	2.18	0.42
1:B:960:ASN:HD22	1:B:963:LEU:HB3	1.84	0.42
1:B:1062:LEU:C	1:B:1062:LEU:HD23	2.45	0.42
1:D:65:ALA:O	1:D:83:SER:HA	2.19	0.42
1:A:231:SER:O	1:A:232:GLU:HG3	2.19	0.42
1:B:433:ALA:C	1:B:435:SER:N	2.78	0.42
1:B:1044:ASN:OD1	1:D:1067:GLU:HG3	2.20	0.42
1:C:198:GLY:HA3	1:C:228:PHE:CE2	2.55	0.42
1:C:647:ASN:O	1:C:648:ALA:HB3	2.20	0.42
1:D:318:ASP:O	1:D:319:GLU:CB	2.67	0.42
1:D:470:LYS:HB3	1:D:480:PHE:CE1	2.54	0.42
1:D:584:THR:O	1:D:585:LYS:C	2.61	0.42
1:A:457:THR:OG1	1:A:459:ILE:HD12	2.20	0.42
1:A:519:ARG:HD2	1:A:522:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:GLY:O	1:A:833:SER:HB3	2.20	0.42
1:C:71:ASP:C	1:C:73:SER:N	2.77	0.42
1:C:567:ASP:HB2	1:C:598:PHE:CZ	2.55	0.42
1:D:364:GLN:OE1	1:D:364:GLN:O	2.37	0.42
1:A:873:ASN:O	1:A:875:SER:N	2.53	0.42
1:B:388:MET:HA	1:B:389:PRO:HD3	1.83	0.42
1:D:52:ILE:C	1:D:54:ARG:N	2.77	0.42
1:D:897:VAL:CG1	1:D:914:VAL:HG13	2.50	0.42
1:B:72:LYS:O	1:B:77:ARG:HD3	2.19	0.42
1:C:191:LEU:HD23	1:C:237:ARG:CA	2.42	0.42
1:D:543:GLN:O	1:D:547:GLU:HG2	2.20	0.42
1:D:613:ASP:HB2	1:D:1013:TYR:CE2	2.54	0.42
1:D:693:VAL:HG11	1:D:700:SER:HB3	2.00	0.42
1:A:880:SER:O	1:A:880:SER:OG	2.34	0.41
1:B:557:VAL:C	1:B:559:LYS:H	2.28	0.41
1:B:869:GLY:O	1:B:870:GLN:C	2.61	0.41
1:C:67:TYR:O	1:C:85:LEU:HD12	2.20	0.41
1:C:495:ASP:HB2	1:C:499:LYS:HG3	2.02	0.41
1:C:820:PHE:O	1:C:821:PRO:C	2.63	0.41
1:C:1070:GLU:H	1:C:1070:GLU:HG3	1.60	0.41
1:D:129:ARG:O	1:D:131:CYS:N	2.53	0.41
1:D:331:VAL:HG13	1:D:428:LYS:HE2	2.02	0.41
1:D:638:LEU:HD22	1:D:672:ASP:HB3	2.02	0.41
1:D:946:SER:O	1:D:951:GLU:HB2	2.20	0.41
1:A:378:ILE:HB	1:A:427:VAL:HG23	2.02	0.41
1:B:380:THR:HG23	1:B:426:LEU:HD11	2.02	0.41
1:C:1008:ILE:H	1:C:1008:ILE:HG13	1.65	0.41
1:D:679:SER:HA	1:D:907:VAL:CG2	2.49	0.41
1:D:731:GLU:HB2	1:D:766:LEU:HD22	2.03	0.41
1:A:250:ILE:HD11	1:A:260:LEU:HD11	2.03	0.41
1:B:256:ASN:C	1:B:257:ILE:HG13	2.46	0.41
1:B:719:THR:HG22	1:B:721:GLU:H	1.85	0.41
1:C:187:ALA:O	1:C:188:GLY:C	2.63	0.41
1:D:121:LEU:HB3	1:D:127:PHE:CD2	2.55	0.41
1:D:487:LEU:HD12	1:D:487:LEU:HA	1.83	0.41
1:D:583:ARG:O	1:D:584:THR:C	2.63	0.41
1:B:925:ASP:O	1:B:926:LEU:HD13	2.21	0.41
1:C:119:GLY:N	1:C:122:SER:OG	2.52	0.41
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.91	0.41
1:C:809:SER:HB3	1:C:812:SER:HB2	2.03	0.41
1:D:783:TYR:O	1:D:784:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.86	0.41
1:A:832:GLU:O	1:A:836:HIS:CD2	2.74	0.41
1:A:942:GLU:O	1:A:946:SER:HB3	2.20	0.41
1:B:77:ARG:NH1	1:D:1059:ILE:CD1	2.83	0.41
1:B:265:CYS:O	1:B:268:GLN:NE2	2.54	0.41
1:B:715:ARG:HA	1:B:715:ARG:HD2	1.83	0.41
1:B:879:LYS:C	1:B:881:LEU:N	2.79	0.41
1:C:278:ALA:HB2	1:C:335:ILE:CG2	2.50	0.41
1:C:837:TYR:CE2	1:C:841:VAL:HG21	2.55	0.41
1:C:1007:ILE:O	1:C:1011:VAL:HG23	2.20	0.41
1:D:683:VAL:O	1:D:685:GLN:N	2.53	0.41
1:D:743:MET:HG3	1:D:907:VAL:HG13	2.02	0.41
1:D:1065:ILE:HG22	1:D:1066:SER:N	2.35	0.41
1:A:501:LEU:HD22	1:A:1078:TYR:CD1	2.56	0.41
1:A:880:SER:O	1:A:881:LEU:HD23	2.21	0.41
1:A:888:ASP:OD1	1:A:888:ASP:N	2.53	0.41
1:A:1023:THR:O	1:A:1026:GLN:N	2.52	0.41
1:B:391:THR:CG2	1:B:392:GLY:N	2.83	0.41
1:B:398:ARG:HH22	1:B:1085:ARG:HE	1.68	0.41
1:B:458:ASN:O	1:B:459:ILE:C	2.62	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.01	0.41
1:B:1075:THR:HG1	1:B:1088:TYR:HE2	1.67	0.41
1:C:213:LEU:O	1:C:214:GLU:C	2.62	0.41
1:C:444:VAL:CG2	1:C:466:MET:HB3	2.42	0.41
1:C:936:TYR:CZ	1:C:966:VAL:HG12	2.55	0.41
1:D:242:PRO:HB3	1:D:313:LEU:HG	2.03	0.41
1:A:362:MET:HE3	1:A:362:MET:HB3	1.51	0.41
1:A:593:LYS:O	1:A:597:VAL:HG23	2.21	0.41
1:A:1075:THR:HG22	1:A:1077:TYR:CE1	2.55	0.41
1:C:215:ASP:CB	1:C:219:ARG:NH2	2.84	0.41
1:C:565:LEU:HD22	1:C:598:PHE:HE2	1.85	0.41
1:C:955:PRO:HG2	1:C:958:GLY:CA	2.49	0.41
1:D:142:HIS:N	1:D:145:HIS:HD2	2.17	0.41
1:D:417:GLU:H	1:D:417:GLU:HG2	1.74	0.41
1:D:453:ARG:NH1	1:D:495:ASP:HB3	2.31	0.41
1:A:661:LYS:HZ1	1:A:1004:GLU:CD	2.28	0.41
1:B:402:GLY:H	1:B:405:VAL:CG2	2.34	0.41
1:B:1069:ASP:OD2	1:B:1071:ASN:HB2	2.21	0.41
1:C:550:PRO:HD2	1:C:551:LYS:H	1.85	0.41
1:C:558:LYS:HD3	1:C:765:ASP:O	2.20	0.41
1:C:773:HIS:HA	1:C:806:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:HB	1:A:234:TYR:HB2	2.03	0.41
1:A:192:MET:HG3	1:A:193:ILE:N	2.35	0.41
1:A:246:GLU:OE1	1:A:330:GLN:NE2	2.48	0.41
1:A:286:THR:O	1:A:287:LEU:C	2.63	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.71	0.41
1:A:828:ILE:O	1:A:829:GLU:C	2.64	0.41
1:A:924:ASN:HB2	1:A:926:LEU:HD22	2.02	0.41
1:A:955:PRO:O	1:A:956:VAL:C	2.64	0.41
1:B:101:ARG:O	1:B:105:VAL:HG23	2.20	0.41
1:B:908:THR:HG22	1:B:909:PRO:HA	2.03	0.41
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.77	0.41
1:C:486:GLU:O	1:C:486:GLU:HG2	2.20	0.41
1:C:622:ASN:HD22	1:C:624:TRP:N	2.11	0.41
1:C:758:GLU:O	1:C:762:ALA:HB2	2.20	0.41
1:C:1059:ILE:O	1:C:1080:MET:HA	2.21	0.41
1:C:1091:ASP:OD2	1:C:1092:GLU:N	2.54	0.41
1:D:712:ASN:HA	1:D:713:PRO:HD2	1.95	0.41
1:D:870:GLN:O	1:D:872:SER:N	2.53	0.41
1:D:883:LEU:O	1:D:886:ARG:N	2.53	0.41
1:D:908:THR:HA	1:D:909:PRO:HA	1.79	0.41
1:A:152:LYS:HD2	1:A:152:LYS:HA	1.75	0.41
1:B:525:GLU:HB3	1:B:840:THR:CG2	2.41	0.41
1:B:667:ALA:HB1	1:B:698:LYS:HE2	2.03	0.41
1:B:913:VAL:HG22	1:B:943:SER:O	2.21	0.41
1:B:991:ARG:NH1	1:B:1002:VAL:HG12	2.36	0.41
1:C:169:GLY:HA2	1:C:236:GLU:HA	2.03	0.41
1:C:219:ARG:HB2	1:C:219:ARG:HH11	1.86	0.41
1:C:370:LEU:O	1:C:432:HIS:HE1	2.04	0.41
1:C:440:GLU:HG3	1:C:472:THR:HG22	2.03	0.41
1:C:651:TYR:HD2	1:C:1013:TYR:CE2	2.38	0.41
1:D:296:ILE:O	1:D:296:ILE:HG23	2.21	0.41
1:D:414:GLN:HE21	1:D:414:GLN:HB3	1.74	0.41
1:D:876:GLN:O	1:D:877:GLN:C	2.63	0.41
1:A:41:LEU:HD23	1:A:42:VAL:N	2.36	0.40
1:A:212:GLU:C	1:A:213:LEU:HD23	2.46	0.40
1:A:817:LEU:O	1:A:818:ASN:C	2.64	0.40
1:B:56:ALA:O	1:B:59:LEU:N	2.55	0.40
1:B:245:ILE:CG2	1:B:246:GLU:N	2.82	0.40
1:B:352:ALA:C	1:B:354:GLY:H	2.28	0.40
1:B:780:LEU:HD13	1:C:778:ASN:HD21	1.85	0.40
1:C:631:ARG:HD3	1:C:631:ARG:C	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:PHE:HB2	1:D:606:MET:HB3	2.02	0.40
1:A:181:LYS:HE3	1:A:181:LYS:HA	2.03	0.40
1:A:206:ILE:H	1:A:206:ILE:HG13	1.59	0.40
1:A:717:ASN:HB3	1:A:717(A):ILE:HD12	2.03	0.40
1:B:363:GLN:OE1	1:B:363:GLN:CA	2.64	0.40
1:B:406:ARG:N	1:B:430:SER:O	2.38	0.40
1:B:756:ILE:HD13	1:B:756:ILE:HA	1.94	0.40
1:B:1053:ASP:HB3	1:B:1056:LYS:HG3	2.03	0.40
1:C:517:GLU:HB3	1:C:519:ARG:NE	2.36	0.40
1:D:337:GLU:HG2	1:D:344:ILE:HD12	2.03	0.40
1:D:712:ASN:OD1	1:D:712:ASN:C	2.65	0.40
1:D:998:GLN:O	1:D:999:GLN:O	2.39	0.40
1:A:399:SER:HB3	1:A:400:SER:H	1.52	0.40
1:A:516:VAL:O	1:A:518:LYS:N	2.55	0.40
1:A:812:SER:HB3	1:D:778:ASN:HD21	1.86	0.40
1:B:504:ILE:CG2	1:B:1042:MET:HG3	2.50	0.40
1:B:650:GLY:HA2	1:B:1013:TYR:CZ	2.57	0.40
1:C:343:ASP:CG	1:C:346:LYS:HB2	2.46	0.40
1:C:721:GLU:N	1:C:721:GLU:OE1	2.52	0.40
1:D:357:LEU:O	1:D:362:MET:HB2	2.21	0.40
1:D:1075:THR:HG22	1:D:1077:TYR:HE1	1.83	0.40
1:A:48:ILE:O	1:A:48:ILE:HD13	2.21	0.40
1:A:682:TRP:O	1:A:683:VAL:C	2.64	0.40
1:A:780:LEU:HD13	1:D:778:ASN:ND2	2.35	0.40
1:A:826:THR:HG21	1:A:831:MET:CE	2.50	0.40
1:A:952:ILE:O	1:A:952:ILE:HG22	2.21	0.40
1:B:769:HIS:CE1	1:B:793:ILE:HG21	2.55	0.40
1:C:90:LEU:HD12	1:C:90:LEU:HA	1.90	0.40
1:C:167:ILE:O	1:C:168:PRO:C	2.64	0.40
1:C:641:MET:HE2	1:C:642:LEU:O	2.21	0.40
1:C:652:LYS:HG3	1:C:653:ASN:N	2.36	0.40
1:D:142:HIS:O	1:D:145:HIS:HB2	2.21	0.40
1:D:250:ILE:HG21	1:D:347:THR:HG21	2.04	0.40
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.56	0.40
1:D:866:MET:CE	1:D:874:LEU:CD2	2.99	0.40
1:D:960:ASN:HD22	1:D:963:LEU:N	2.16	0.40
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.36	0.40
1:A:370:LEU:O	1:A:432:HIS:HE1	2.05	0.40
1:B:239:ILE:HG21	1:B:313:LEU:HD21	2.02	0.40
1:C:174:ILE:HG13	1:C:235:ILE:CG2	2.51	0.40
1:C:565:LEU:HD22	1:C:598:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:O	1:D:55:ALA:N	2.55	0.40
1:D:249:VAL:C	1:D:250:ILE:HG13	2.46	0.40
1:D:429:LEU:CD2	1:D:443:MET:SD	3.10	0.40
1:D:477:THR:HG23	1:D:479:LYS:HB2	2.02	0.40
1:D:722:TYR:CD2	1:D:722:TYR:C	2.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1048/1173 (89%)	907 (86%)	111 (11%)	30 (3%)	3	20
1	B	985/1173 (84%)	847 (86%)	117 (12%)	21 (2%)	5	27
1	C	1057/1173 (90%)	896 (85%)	113 (11%)	48 (4%)	2	12
1	D	985/1173 (84%)	842 (86%)	110 (11%)	33 (3%)	3	17
All	All	4075/4692 (87%)	3492 (86%)	451 (11%)	132 (3%)	3	18

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ALA
1	A	527	ALA
1	A	880	SER
1	A	999	GLN
1	B	94	GLU
1	B	95	SER
1	B	148	MET
1	B	166	VAL
1	B	414	GLN
1	B	522	PRO

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Mol	Chain	Res	Type
1	B	523	ASP
1	B	950	GLY
1	B	1001	PRO
1	C	151	ASP
1	C	168	PRO
1	C	211	SER
1	C	214	GLU
1	C	515	ASN
1	C	645	ALA
1	C	687	LYS
1	C	852	SER
1	C	883	LEU
1	C	885	GLU
1	C	887	PHE
1	C	923	GLN
1	C	925	ASP
1	C	939	ASP
1	C	978	PRO
1	C	1057	ARG
1	D	92	PRO
1	D	319	GLU
1	D	494	LEU
1	D	684	ASP
1	D	870	GLN
1	D	884	GLY
1	D	999	GLN
1	D	1084	ALA
1	A	99	ILE
1	A	177	TYR
1	A	182	GLU
1	A	220	ALA
1	A	517	GLU
1	A	649	VAL
1	A	868	GLY
1	A	870	GLN
1	A	876	GLN
1	A	976	ALA
1	B	147	ASP
1	B	495	ASP
1	B	648	ALA
1	C	92	PRO
1	C	169	GLY

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Mol	Chain	Res	Type
1	C	197	SER
1	C	208	ARG
1	C	361	ASN
1	C	518	LYS
1	C	931	VAL
1	C	960	ASN
1	C	969	LYS
1	C	974	LEU
1	D	130	ARG
1	D	161	LYS
1	D	303	LYS
1	D	306	ASN
1	D	317	GLY
1	D	318	ASP
1	D	478	THR
1	D	515	ASN
1	D	854	ILE
1	D	1001	PRO
1	A	88	SER
1	A	176	SER
1	A	223	GLU
1	A	270	ARG
1	A	386	ASP
1	A	551	LYS
1	A	874	LEU
1	A	884	GLY
1	C	88	SER
1	C	227	SER
1	C	270	ARG
1	C	648	ALA
1	C	935	GLY
1	D	271	HIS
1	D	414	GLN
1	D	648	ALA
1	D	876	GLN
1	D	886	ARG
1	A	186	GLU
1	A	192	MET
1	A	504	ILE
1	A	903	ASP
1	B	413	PHE
1	B	558	LYS

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Mol	Chain	Res	Type
1	B	617	ASN
1	B	925	ASP
1	C	124	ASN
1	C	199	GLY
1	C	282	GLY
1	C	489	ASP
1	C	980	GLU
1	C	1084	ALA
1	D	518	LYS
1	A	511	GLY
1	A	550	PRO
1	A	980	GLU
1	B	907	VAL
1	B	1002	VAL
1	C	354	GLY
1	C	760	LYS
1	C	941	PRO
1	C	981	TYR
1	D	53	PHE
1	D	70	GLU
1	D	878	ALA
1	A	229	GLY
1	B	86	VAL
1	C	519	ARG
1	C	924	ASN
1	D	160	ILE
1	D	649	VAL
1	B	1000	GLY
1	C	173	PRO
1	D	166	VAL
1	D	868	GLY
1	D	513	PRO
1	C	189	PHE
1	C	649	VAL
1	C	821	PRO
1	D	1052	ILE
1	B	828	ILE
1	C	932	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	908/1006 (90%)	712 (78%)	196 (22%)	1	6
1	B	856/1006 (85%)	712 (83%)	144 (17%)	2	11
1	C	910/1006 (90%)	703 (77%)	207 (23%)	1	5
1	D	856/1006 (85%)	704 (82%)	152 (18%)	2	10
All	All	3530/4024 (88%)	2831 (80%)	699 (20%)	1	8

All (699) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	38	LYS
1	A	40	LEU
1	A	44	ASN
1	A	48	ILE
1	A	60	ASP
1	A	62	SER
1	A	63	THR
1	A	66	ILE
1	A	72	LYS
1	A	77	ARG
1	A	90	LEU
1	A	97	LEU
1	A	99	ILE
1	A	108	GLN
1	A	122	SER
1	A	125	GLU
1	A	126	GLN
1	A	131	CYS
1	A	143	LEU
1	A	152	LYS
1	A	154	LYS
1	A	156	ARG
1	A	157	THR

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Mol	Chain	Res	Type
1	A	160	ILE
1	A	161	LYS
1	A	174	ILE
1	A	179	LEU
1	A	185	GLU
1	A	186	GLU
1	A	192	MET
1	A	193	ILE
1	A	194	LYS
1	A	196	THR
1	A	205	ARG
1	A	206	ILE
1	A	209	GLU
1	A	210	GLU
1	A	212	GLU
1	A	213	LEU
1	A	214	GLU
1	A	217	PHE
1	A	219	ARG
1	A	221	LYS
1	A	226	LYS
1	A	227	SER
1	A	230	ASN
1	A	233	VAL
1	A	235	ILE
1	A	237	ARG
1	A	239	ILE
1	A	241	ASN
1	A	249	VAL
1	A	269	ARG
1	A	271	HIS
1	A	272	GLN
1	A	287	LEU
1	A	288	ARG
1	A	296	ILE
1	A	303	LYS
1	A	306	ASN
1	A	313	LEU
1	A	315	SER
1	A	328	ARG
1	A	329	VAL
1	A	331	VAL

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Mol	Chain	Res	Type
1	A	334	THR
1	A	335	ILE
1	A	361	ASN
1	A	363	GLN
1	A	367	ILE
1	A	370	LEU
1	A	376	CYS
1	A	386	ASP
1	A	388	MET
1	A	391	THR
1	A	393	THR
1	A	417	GLU
1	A	423	ASP
1	A	425	LEU
1	A	427	VAL
1	A	428	LYS
1	A	430	SER
1	A	434	ILE
1	A	437	LYS
1	A	438	GLN
1	A	440	GLU
1	A	445	ARG
1	A	451	ARG
1	A	467	LYS
1	A	469	LYS
1	A	470	LYS
1	A	472	THR
1	A	482	GLU
1	A	486	GLU
1	A	487	LEU
1	A	490	ILE
1	A	491	GLN
1	A	494	LEU
1	A	496	ARG
1	A	500	THR
1	A	504	ILE
1	A	506	ASN
1	A	509	ILE
1	A	517	GLU
1	A	518	LYS
1	A	519	ARG
1	A	526	LEU

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Mol	Chain	Res	Type
1	A	528	SER
1	A	538(A)	SER
1	A	538(B)	PHE
1	A	539	SER
1	A	542	LYS
1	A	551	LYS
1	A	558	LYS
1	A	559	LYS
1	A	565	LEU
1	A	566	THR
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	599	LYS
1	A	607	TRP
1	A	613	ASP
1	A	628	GLU
1	A	631	ARG
1	A	632	LYS
1	A	641	MET
1	A	649	VAL
1	A	652	LYS
1	A	661	LYS
1	A	671	ILE
1	A	676	ILE
1	A	685	GLN
1	A	695	GLU
1	A	707	THR
1	A	710	ILE
1	A	714	GLU
1	A	715	ARG
1	A	719	THR
1	A	743	MET
1	A	750	LYS
1	A	754	GLU
1	A	759	LEU
1	A	760	LYS
1	A	766	LEU
1	A	775	THR
1	A	781	LEU
1	A	784	LYS
1	A	794	ILE

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Mol	Chain	Res	Type
1	A	809	SER
1	A	811	ASN
1	A	828	ILE
1	A	829	GLU
1	A	831	MET
1	A	853	ASP
1	A	855	LYS
1	A	863	GLN
1	A	872	SER
1	A	875	SER
1	A	876	GLN
1	A	881	LEU
1	A	886	ARG
1	A	897	VAL
1	A	904	ILE
1	A	906	LYS
1	A	907	VAL
1	A	908	THR
1	A	917	MET
1	A	919	LEU
1	A	925	ASP
1	A	926	LEU
1	A	927	ASP
1	A	928	GLU
1	A	939	ASP
1	A	943	SER
1	A	944	VAL
1	A	945	VAL
1	A	946	SER
1	A	961	LYS
1	A	962	ASP
1	A	966	VAL
1	A	968	LEU
1	A	985	VAL
1	A	992	GLU
1	A	999	GLN
1	A	1007	ILE
1	A	1008	ILE
1	A	1019	GLN
1	A	1021	ILE
1	A	1029	ASN
1	A	1031	SER

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Mol	Chain	Res	Type
1	A	1044	ASN
1	A	1062	LEU
1	A	1064	THR
1	A	1085	ARG
1	B	39	LYS
1	B	40	LEU
1	B	47	GLU
1	B	50	ILE
1	B	62	SER
1	B	70	GLU
1	B	74	SER
1	B	75	LEU
1	B	79	LYS
1	B	82	GLU
1	B	90	LEU
1	B	98	ASN
1	B	99	ILE
1	B	107	LYS
1	B	108	GLN
1	B	110	ASN
1	B	122	SER
1	B	129	ARG
1	B	143	LEU
1	B	153	VAL
1	B	156	ARG
1	B	160	ILE
1	B	161	LYS
1	B	163	ASP
1	B	166	VAL
1	B	167	ILE
1	B	258	VAL
1	B	268	GLN
1	B	269	ARG
1	B	275	VAL
1	B	277	VAL
1	B	287	LEU
1	B	288	ARG
1	B	296	ILE
1	B	299	MET
1	B	303	LYS
1	B	305	VAL
1	B	315	SER

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Mol	Chain	Res	Type
1	B	329	VAL
1	B	331	VAL
1	B	335	ILE
1	B	346	LYS
1	B	347	THR
1	B	357	LEU
1	B	357(A)	PHE
1	B	358	GLU
1	B	365	LYS
1	B	366	ASP
1	B	368	THR
1	B	375	GLN
1	B	376	CYS
1	B	399	SER
1	B	407	LEU
1	B	425	LEU
1	B	427	VAL
1	B	437	LYS
1	B	451	ARG
1	B	467	LYS
1	B	469	LYS
1	B	472	THR
1	B	486	GLU
1	B	490	ILE
1	B	494	LEU
1	B	496	ARG
1	B	498	THR
1	B	500	THR
1	B	516	VAL
1	B	518	LYS
1	B	523	ASP
1	B	526	LEU
1	B	533	SER
1	B	534	SER
1	B	535	SER
1	B	536	LYS
1	B	542	LYS
1	B	546	ASP
1	B	580	THR
1	B	588	ILE
1	B	599	LYS
1	B	607	TRP

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Mol	Chain	Res	Type
1	B	617	ASN
1	B	631	ARG
1	B	641	MET
1	B	649	VAL
1	B	664	GLN
1	B	685	GLN
1	B	704	ILE
1	B	707	THR
1	B	715	ARG
1	B	720	LEU
1	B	721	GLU
1	B	740	ILE
1	B	743	MET
1	B	750	LYS
1	B	760	LYS
1	B	768	ILE
1	B	775	THR
1	B	781	LEU
1	B	784	LYS
1	B	792	ASP
1	B	796	THR
1	B	809	SER
1	B	826	THR
1	B	828	ILE
1	B	839	SER
1	B	853	ASP
1	B	855	LYS
1	B	870	GLN
1	B	871	TYR
1	B	874	LEU
1	B	875	SER
1	B	876	GLN
1	B	879	LYS
1	B	881	LEU
1	B	888	ASP
1	B	891	LYS
1	B	906	LYS
1	B	907	VAL
1	B	908	THR
1	B	911	SER
1	B	916	ASP
1	B	919	LEU

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Mol	Chain	Res	Type
1	B	925	ASP
1	B	926	LEU
1	B	927	ASP
1	B	932	ILE
1	B	934	ASP
1	B	944	VAL
1	B	945	VAL
1	B	949	LYS
1	B	969	LYS
1	B	982	LEU
1	B	985	VAL
1	B	997	GLU
1	B	1003	THR
1	B	1008	ILE
1	B	1015	LYS
1	B	1016	VAL
1	B	1019	GLN
1	B	1023	THR
1	B	1024	ARG
1	B	1031	SER
1	B	1056	LYS
1	B	1087	ILE
1	C	36	GLN
1	C	37	ILE
1	C	44	ASN
1	C	70	GLU
1	C	73	SER
1	C	75	LEU
1	C	86	VAL
1	C	88	SER
1	C	90	LEU
1	C	94	GLU
1	C	97	LEU
1	C	99	ILE
1	C	100	GLU
1	C	103	ILE
1	C	108	GLN
1	C	110	ASN
1	C	122	SER
1	C	125	GLU
1	C	130	ARG
1	C	136	ILE

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Mol	Chain	Res	Type
1	C	139	ILE
1	C	143	LEU
1	C	147	ASP
1	C	164	LEU
1	C	170	THR
1	C	181	LYS
1	C	183	PHE
1	C	185	GLU
1	C	189	PHE
1	C	192	MET
1	C	193	ILE
1	C	196	THR
1	C	197	SER
1	C	202	LYS
1	C	206	ILE
1	C	207	VAL
1	C	210	GLU
1	C	211	SER
1	C	213	LEU
1	C	214	GLU
1	C	215	ASP
1	C	221	LYS
1	C	226	LYS
1	C	232	GLU
1	C	235	ILE
1	C	262	GLU
1	C	269	ARG
1	C	281	VAL
1	C	283	LEU
1	C	296	ILE
1	C	303	LYS
1	C	305	VAL
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	338	MET
1	C	362	MET
1	C	362(A)	PRO
1	C	365	LYS
1	C	366	ASP
1	C	369	THR
1	C	375	GLN

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Mol	Chain	Res	Type
1	C	378	ILE
1	C	379	THR
1	C	386	ASP
1	C	388	MET
1	C	414	GLN
1	C	418	ILE
1	C	423	ASP
1	C	425	LEU
1	C	427	VAL
1	C	428	LYS
1	C	435	SER
1	C	437	LYS
1	C	444	VAL
1	C	451	ARG
1	C	453	ARG
1	C	466	MET
1	C	467	LYS
1	C	468	ASN
1	C	469	LYS
1	C	470	LYS
1	C	473	SER
1	C	475	ASP
1	C	481	ILE
1	C	486	GLU
1	C	491	GLN
1	C	494	LEU
1	C	495	ASP
1	C	496	ARG
1	C	500	THR
1	C	502	GLU
1	C	509	ILE
1	C	515	ASN
1	C	516	VAL
1	C	518	LYS
1	C	519	ARG
1	C	521	LYS
1	C	526	LEU
1	C	528	SER
1	C	529	ILE
1	C	531	THR
1	C	534	SER
1	C	536	LYS

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Mol	Chain	Res	Type
1	C	538(A)	SER
1	C	538(B)	PHE
1	C	541	THR
1	C	542	LYS
1	C	543	GLN
1	C	544	LEU
1	C	559	LYS
1	C	563	VAL
1	C	580	THR
1	C	588	ILE
1	C	590	ILE
1	C	606	MET
1	C	607	TRP
1	C	628	GLU
1	C	629	ARG
1	C	631	ARG
1	C	632	LYS
1	C	637	VAL
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	653	ASN
1	C	660	HIS
1	C	661	LYS
1	C	679	SER
1	C	687	LYS
1	C	688	VAL
1	C	714	GLU
1	C	719	THR
1	C	743	MET
1	C	750	LYS
1	C	756	ILE
1	C	765	ASP
1	C	766	LEU
1	C	781	LEU
1	C	784	LYS
1	C	794	ILE
1	C	807	GLN
1	C	811	ASN
1	C	823	HIS
1	C	828	ILE
1	C	831	MET

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Mol	Chain	Res	Type
1	C	839	SER
1	C	843	THR
1	C	852	SER
1	C	853	ASP
1	C	855	LYS
1	C	861	ILE
1	C	863	GLN
1	C	870	GLN
1	C	871	TYR
1	C	881	LEU
1	C	883	LEU
1	C	886	ARG
1	C	887	PHE
1	C	888	ASP
1	C	889	GLU
1	C	890	VAL
1	C	891	LYS
1	C	892	ASP
1	C	904	ILE
1	C	906	LYS
1	C	907	VAL
1	C	912	LYS
1	C	914	VAL
1	C	923	GLN
1	C	924	ASN
1	C	926	LEU
1	C	928	GLU
1	C	929	GLN
1	C	934	ASP
1	C	937	LYS
1	C	945	VAL
1	C	946	SER
1	C	960	ASN
1	C	963	LEU
1	C	966	VAL
1	C	968	LEU
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	974	LEU
1	C	975	THR
1	C	977	ARG

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Mol	Chain	Res	Type
1	C	983	GLU
1	C	986	ASP
1	C	1002	VAL
1	C	1003	THR
1	C	1007	ILE
1	C	1008	ILE
1	C	1015	LYS
1	C	1029	ASN
1	C	1043	ARG
1	C	1044	ASN
1	C	1048	VAL
1	C	1049	GLU
1	C	1062	LEU
1	C	1063	GLU
1	C	1064	THR
1	C	1070	GLU
1	C	1085	ARG
1	C	1087	ILE
1	C	1090	LYS
1	D	36	GLN
1	D	37	ILE
1	D	44	ASN
1	D	60	ASP
1	D	66	ILE
1	D	70	GLU
1	D	75	LEU
1	D	77	ARG
1	D	82	GLU
1	D	102	ILE
1	D	105	VAL
1	D	108	GLN
1	D	126	GLN
1	D	137	LYS
1	D	139	ILE
1	D	157	THR
1	D	161	LYS
1	D	166	VAL
1	D	240	ASP
1	D	257	ILE
1	D	260	LEU
1	D	262	GLU
1	D	271	HIS

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Mol	Chain	Res	Type
1	D	273	LYS
1	D	287	LEU
1	D	288	ARG
1	D	289	GLN
1	D	296	ILE
1	D	300	GLU
1	D	302	ILE
1	D	305	VAL
1	D	306	ASN
1	D	313	LEU
1	D	323	ILE
1	D	329	VAL
1	D	335	ILE
1	D	337	GLU
1	D	346	LYS
1	D	358	GLU
1	D	361	ASN
1	D	362	MET
1	D	362(A)	PRO
1	D	364	GLN
1	D	375	GLN
1	D	377	ARG
1	D	394	ILE
1	D	403	PHE
1	D	405	VAL
1	D	417	GLU
1	D	424	SER
1	D	425	LEU
1	D	427	VAL
1	D	437	LYS
1	D	451	ARG
1	D	456	LYS
1	D	457	THR
1	D	467	LYS
1	D	470	LYS
1	D	476	TYR
1	D	477	THR
1	D	481	ILE
1	D	487	LEU
1	D	489	ASP
1	D	491	GLN
1	D	496	ARG

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Mol	Chain	Res	Type
1	D	498	THR
1	D	518	LYS
1	D	519	ARG
1	D	525	GLU
1	D	535	SER
1	D	537	ILE
1	D	538(A)	SER
1	D	538(B)	PHE
1	D	542	LYS
1	D	551	LYS
1	D	558	LYS
1	D	580	THR
1	D	581	ARG
1	D	588	ILE
1	D	590	ILE
1	D	607	TRP
1	D	613	ASP
1	D	620	LYS
1	D	622	ASN
1	D	631	ARG
1	D	644	ARG
1	D	647	ASN
1	D	649	VAL
1	D	671	ILE
1	D	679	SER
1	D	683	VAL
1	D	684	ASP
1	D	707	THR
1	D	715	ARG
1	D	717	ASN
1	D	717(A)	ILE
1	D	725	LYS
1	D	750	LYS
1	D	754	GLU
1	D	763	VAL
1	D	766	LEU
1	D	775	THR
1	D	781	LEU
1	D	784	LYS
1	D	791	VAL
1	D	798	VAL
1	D	807	GLN

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Mol	Chain	Res	Type
1	D	809	SER
1	D	811	ASN
1	D	828	ILE
1	D	843	THR
1	D	859	THR
1	D	863	GLN
1	D	866	MET
1	D	870	GLN
1	D	873	ASN
1	D	875	SER
1	D	881	LEU
1	D	885	GLU
1	D	897	VAL
1	D	906	LYS
1	D	907	VAL
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	938	LEU
1	D	945	VAL
1	D	946	SER
1	D	952	ILE
1	D	961	LYS
1	D	975	THR
1	D	977	ARG
1	D	983	GLU
1	D	999	GLN
1	D	1052	ILE
1	D	1053	ASP
1	D	1054	LYS
1	D	1056	LYS
1	D	1057	ARG
1	D	1058	LEU
1	D	1063	GLU
1	D	1064	THR
1	D	1065	ILE
1	D	1067	GLU
1	D	1070	GLU
1	D	1071	ASN
1	D	1077	TYR
1	D	1080	MET
1	D	1085	ARG

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Mol	Chain	Res	Type
1	D	1086	ARG
1	D	1087	ILE
1	D	1089	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	98	ASN
1	A	108	GLN
1	A	142	HIS
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	268	GLN
1	A	326	ASN
1	A	330	GLN
1	A	363	GLN
1	A	432	HIS
1	A	438	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	617	ASN
1	A	622	ASN
1	A	653	ASN
1	A	660	HIS
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	818	ASN
1	A	836	HIS
1	A	858	ASN
1	A	864	HIS
1	A	877	GLN
1	A	923	GLN
1	A	998	GLN
1	A	999	GLN
1	A	1005	GLN

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Mol	Chain	Res	Type
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	110	ASN
1	B	145	HIS
1	B	244	HIS
1	B	268	GLN
1	B	326	ASN
1	B	330	GLN
1	B	348	GLN
1	B	375	GLN
1	B	491	GLN
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	660	HIS
1	B	685	GLN
1	B	690	ASN
1	B	717	ASN
1	B	736	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	836	HIS
1	B	858	ASN
1	B	864	HIS
1	B	898	ASN
1	B	960	ASN
1	B	964	GLN
1	B	998	GLN
1	B	999	GLN
1	B	1005	GLN
1	B	1019	GLN
1	B	1025	ASN
1	B	1029	ASN

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Mol	Chain	Res	Type
1	B	1044	ASN
1	B	1071	ASN
1	B	1073	ASN
1	B	1081	ASN
1	B	1093	ASN
1	C	36	GLN
1	C	44	ASN
1	C	108	GLN
1	C	110	ASN
1	C	145	HIS
1	C	241	ASN
1	C	244	HIS
1	C	271	HIS
1	C	330	GLN
1	C	375	GLN
1	C	464	ASN
1	C	510	ASN
1	C	543	GLN
1	C	574	HIS
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN
1	C	736	HIS
1	C	778	ASN
1	C	811	ASN
1	C	818	ASN
1	C	864	HIS
1	C	870	GLN
1	C	898	ASN
1	C	929	GLN
1	C	1005	GLN
1	C	1019	GLN
1	C	1022	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1081	ASN
1	C	1083	GLN
1	D	44	ASN
1	D	126	GLN
1	D	145	HIS

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Mol	Chain	Res	Type
1	D	244	HIS
1	D	256	ASN
1	D	268	GLN
1	D	289	GLN
1	D	301	ASN
1	D	326	ASN
1	D	330	GLN
1	D	361	ASN
1	D	363	GLN
1	D	364	GLN
1	D	375	GLN
1	D	414	GLN
1	D	468	ASN
1	D	515	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	617	ASN
1	D	622	ASN
1	D	647	ASN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	864	HIS
1	D	870	GLN
1	D	873	ASN
1	D	929	GLN
1	D	960	ASN
1	D	999	GLN
1	D	1005	GLN
1	D	1019	GLN
1	D	1025	ASN
1	D	1073	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BTI	D	1201	-	15,16,16	1.82	2 (13%)	20,21,21	1.91	5 (25%)
2	ADP	A	1201	-	28,29,29	1.58	5 (17%)	43,45,45	1.73	7 (16%)

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	-	-	6/6/27/27	0/2/2/2
2	ADP	A	1201	-	-	3/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1201	BTI	O3-C3	5.12	1.34	1.23
2	A	1201	ADP	C5-C4	4.93	1.47	1.39
4	D	1201	BTI	C2-S1	-4.15	1.76	1.82
2	A	1201	ADP	PA-O3A	3.69	1.63	1.59
2	A	1201	ADP	C5-C6	2.82	1.48	1.41
2	A	1201	ADP	C8-N7	2.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ADP	C5-N7	-2.21	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	C5-C4-N3	-5.91	118.59	126.72
4	D	1201	BTI	C6-C5-N3	-5.04	106.68	113.18
2	A	1201	ADP	N3-C4-N9	4.45	134.74	127.17
2	A	1201	ADP	C2-N3-C4	3.59	120.61	111.83
2	A	1201	ADP	C4-C5-N7	-3.41	106.68	110.58
4	D	1201	BTI	C2-C4-N2	-3.15	110.00	113.34
4	D	1201	BTI	C5-C6-S1	3.01	110.21	106.06
2	A	1201	ADP	N3-C2-N1	-2.88	124.22	128.58
4	D	1201	BTI	C4-C2-S1	2.83	108.25	105.03
4	D	1201	BTI	C6-S1-C2	2.73	95.65	89.98
2	A	1201	ADP	C5-N7-C8	2.38	107.19	103.45
2	A	1201	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O1A
4	D	1201	BTI	C9-C10-C11-O11
4	D	1201	BTI	C11-C10-C9-C8
4	D	1201	BTI	S1-C2-C7-C8
4	D	1201	BTI	C4-C2-C7-C8
4	D	1201	BTI	C2-C7-C8-C9
4	D	1201	BTI	C7-C8-C9-C10
2	A	1201	ADP	C5'-O5'-PA-O3A
2	A	1201	ADP	C4'-C5'-O5'-PA

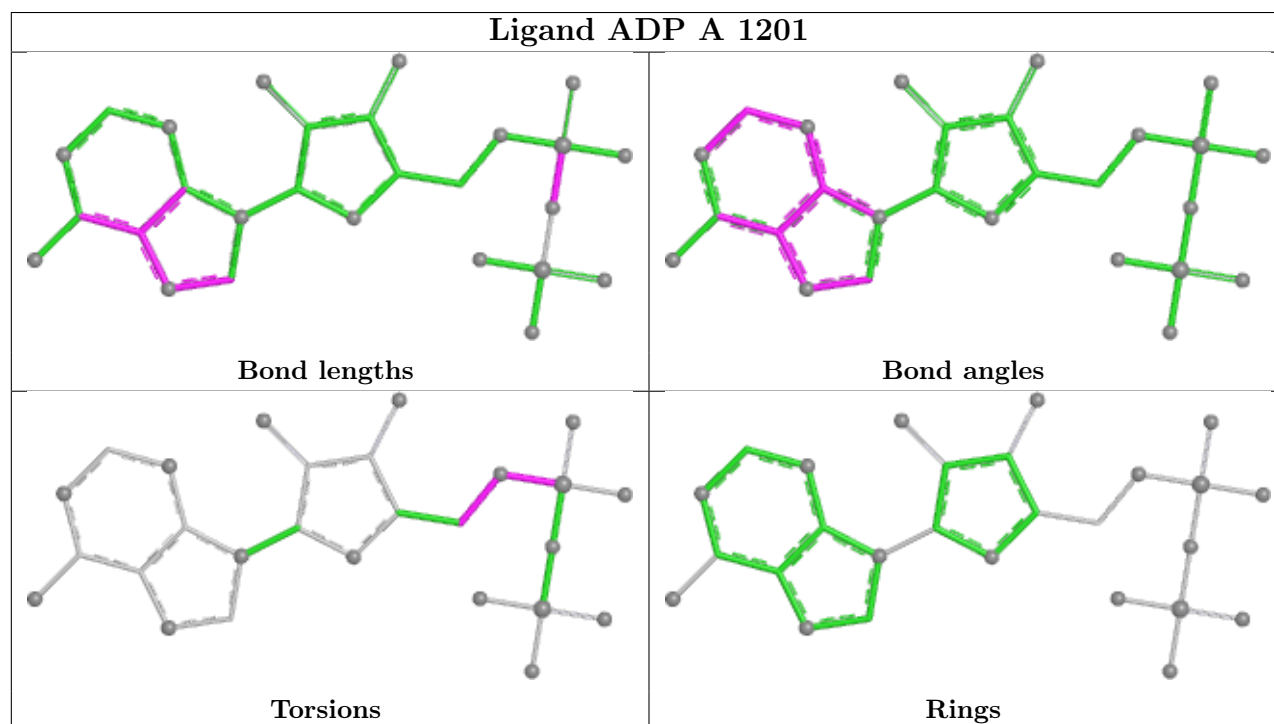
There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1052/1173 (89%)	-0.51	7 (0%)	84 66	36, 75, 131, 167	0
1	B	989/1173 (84%)	-0.35	4 (0%)	88 76	59, 105, 154, 233	0
1	C	1059/1173 (90%)	-0.34	9 (0%)	82 64	56, 101, 150, 197	0
1	D	989/1173 (84%)	-0.48	2 (0%)	91 83	41, 82, 173, 267	0
All	All	4089/4692 (87%)	-0.42	22 (0%)	87 72	36, 93, 151, 267	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	4.2
1	C	874	LEU	3.7
1	C	192	MET	3.7
1	A	189	PHE	3.4
1	A	224	ALA	3.4
1	C	875	SER	3.2
1	B	167	ILE	3.2
1	B	526	LEU	2.9
1	D	168	PRO	2.8
1	C	513	PRO	2.8
1	C	883	LEU	2.6
1	A	441	GLU	2.5
1	B	305	VAL	2.4
1	A	206	ILE	2.4
1	A	438	GLN	2.3
1	C	312	PHE	2.2
1	A	527	ALA	2.2
1	C	873	ASN	2.1
1	C	870	GLN	2.1
1	C	206	ILE	2.0
1	D	489	ASP	2.0
1	B	600	ASP	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](#)

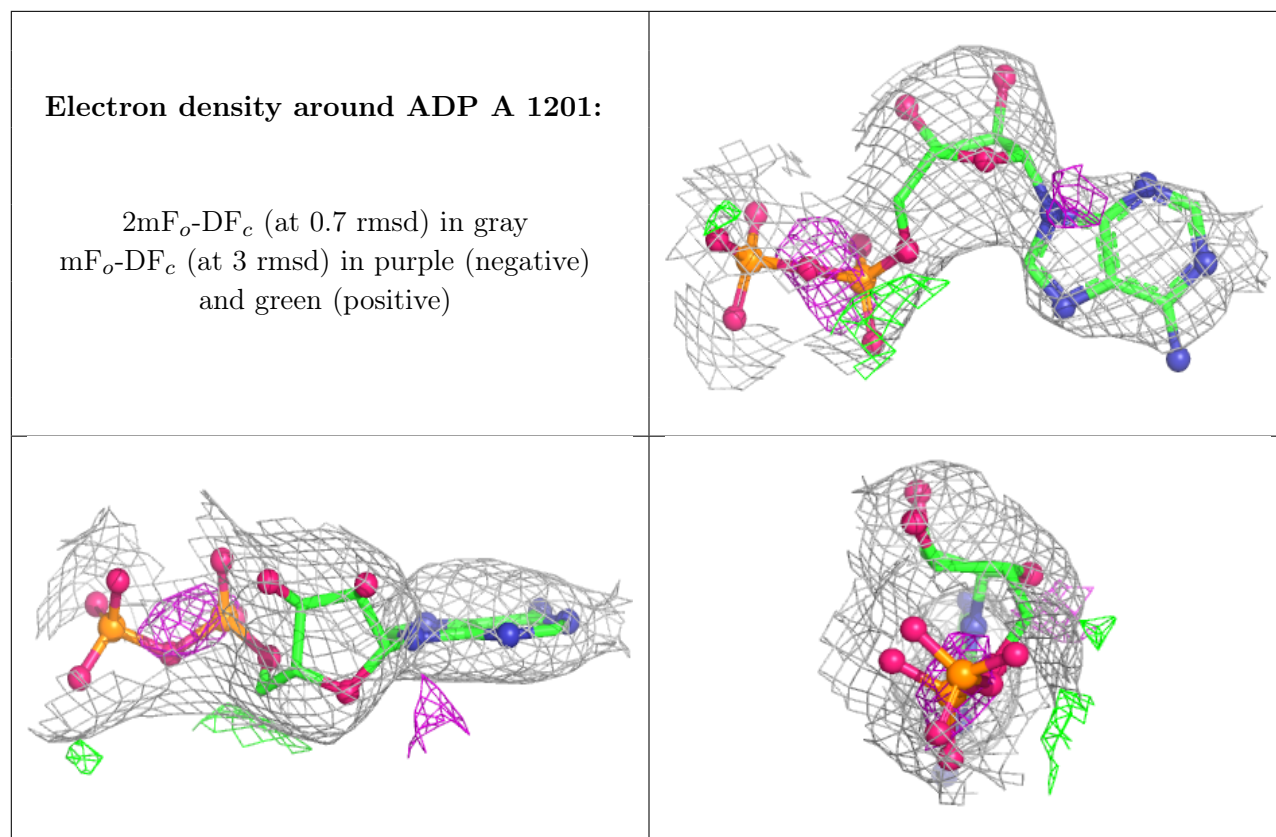
There are no oligosaccharides in this entry.

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	0.87	0.10	108,112,144,146	0
4	BTI	D	1201	15/15	0.87	0.14	128,133,136,136	0
3	MN	B	1201	1/1	0.97	0.04	108,108,108,108	0
3	MN	A	1202	1/1	0.97	0.08	83,83,83,83	0
3	MN	D	1202	1/1	0.98	0.05	79,79,79,79	0
3	MN	C	1201	1/1	0.98	0.07	105,105,105,105	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.