



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:09 am GMT

PDB ID : 1CE8
Title : CARBAMOYL PHOSPHATE SYNTHETASE FROM ESCHERICHIS COLI
WITH COMPLEXED WITH THE ALLOSTERIC LIGAND IMP
Authors : Thoden, J.B.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-03-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

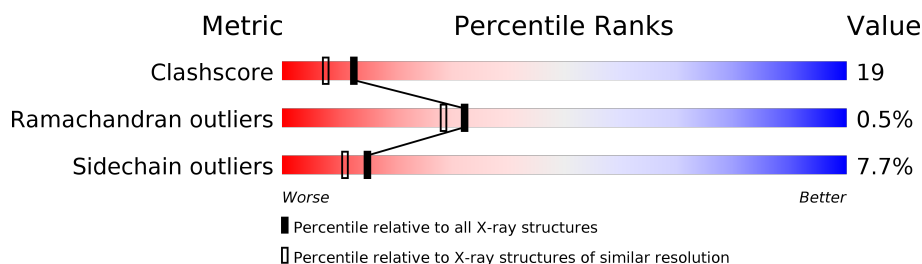
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	
1	C	1073	
1	E	1073	
1	G	1073	
2	B	382	
2	D	382	
2	F	382	

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Mol	Chain	Length	Quality of chain
2	H	382	<div><div></div><div>35%</div><div>51%</div><div>12%</div><div>..</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48888 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 PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	8	0
			8198	5143	1427	1583	45			
1	C	1058	Total	C	N	O	S	0	1	0
			8167	5125	1426	1571	45			
1	E	1058	Total	C	N	O	S	0	12	0
			8232	5165	1444	1578	45			
1	G	1058	Total	C	N	O	S	0	2	0
			8170	5128	1424	1573	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	SEQUENCE CONFLICT	UNP P00968
C	46	ASN	LEU	SEQUENCE CONFLICT	UNP P00968
E	46	ASN	LEU	SEQUENCE CONFLICT	UNP P00968
G	46	ASN	LEU	SEQUENCE CONFLICT8	UNP P00968

- Molecule 2 is a protein called PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	1	0
			2902	1829	512	551	10			
2	D	379	Total	C	N	O	S	0	1	0
			2899	1828	509	551	11			
2	F	379	Total	C	N	O	S	0	1	0
			2900	1828	510	552	10			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	SEQUENCE CONFLICT	UNP P0A6F1
D	183	GLN	GLU	SEQUENCE CONFLICT	UNP P0A6F1
F	183	GLN	GLU	SEQUENCE CONFLICT	UNP P0A6F1
H	183	GLN	GLU	SEQUENCE CONFLICT8	UNP P0A6F1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	A	6	Total K 6 6	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

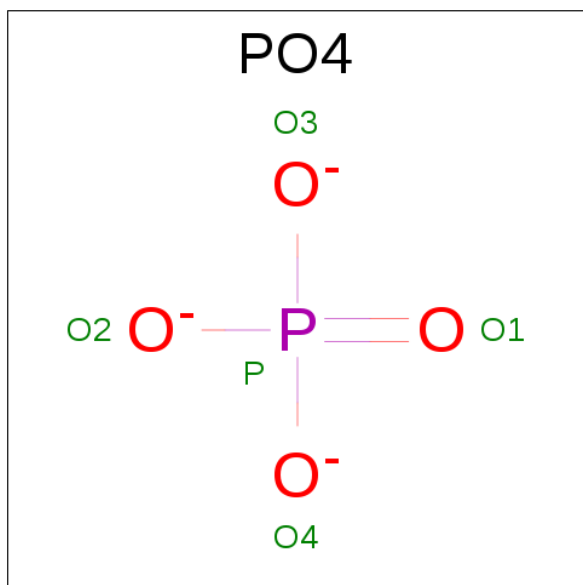
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	3	Total Cl 3 3	0	0

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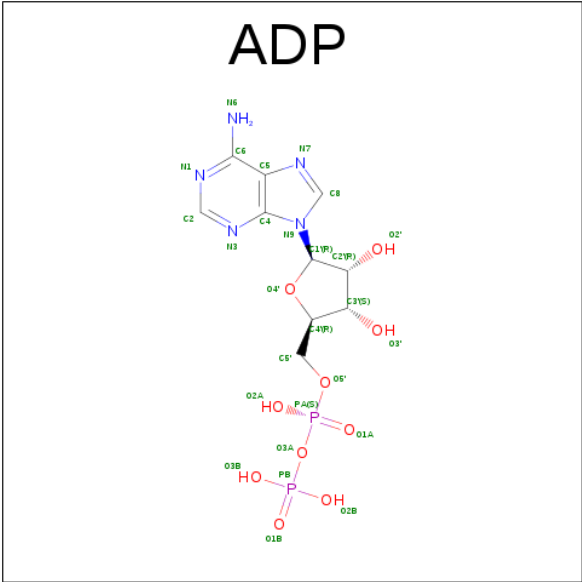
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	C	3	Total	Cl	0	0
			3	3		
5	E	3	Total	Cl	0	0
			3	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



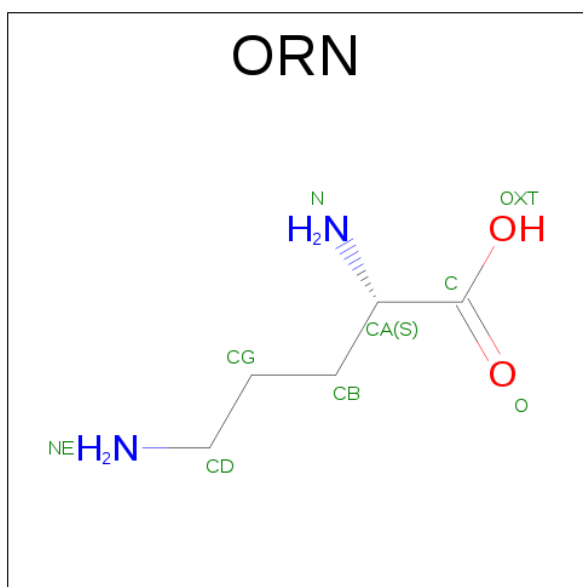
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



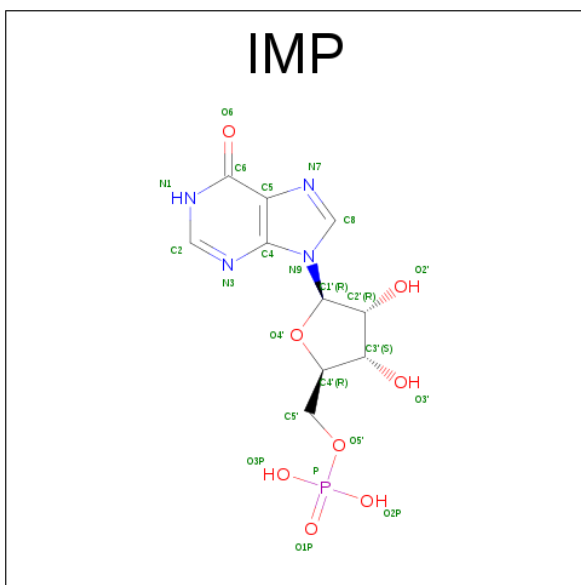
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



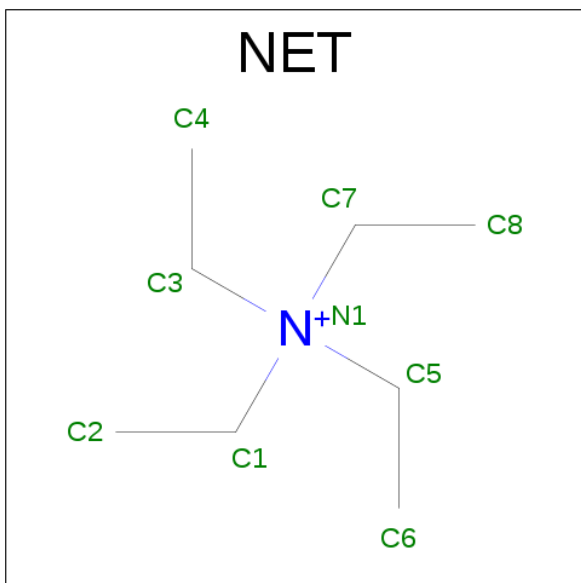
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
9	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N 9 8 1	0	0
10	C	1	Total C N 9 8 1	0	0
10	E	1	Total C N 9 8 1	0	0
10	G	1	Total C N 9 8 1	0	0

- Molecule 11 is water.

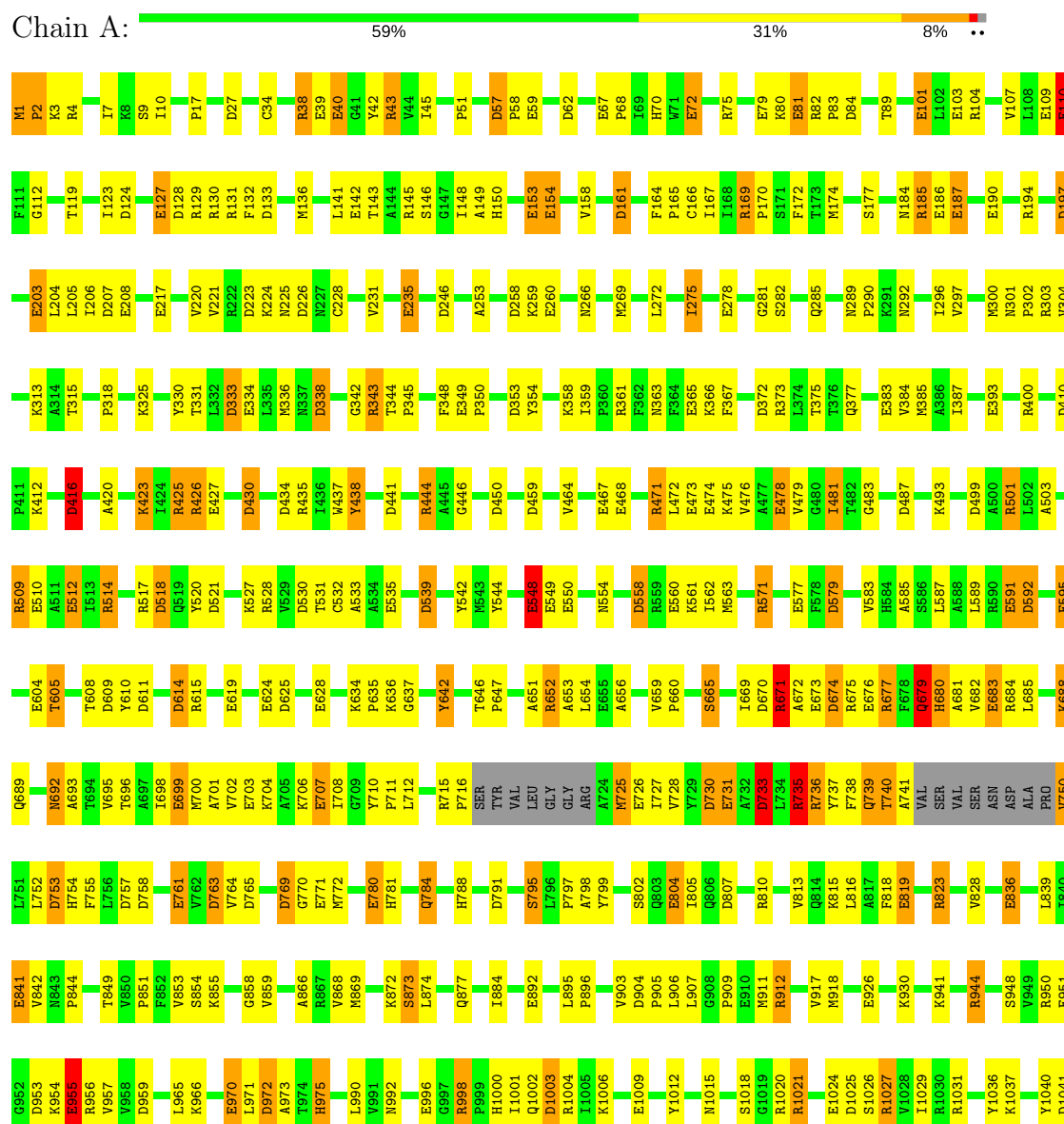
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	842	Total O 842 842	0	0
11	B	190	Total O 190 190	0	0
11	C	732	Total O 732 732	0	0
11	D	193	Total O 193 193	0	0
11	E	939	Total O 939 939	0	0
11	F	233	Total O 233 233	0	0
11	G	743	Total O 743 743	0	0
11	H	165	Total O 165 165	0	0

3 Residue-property plots

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

Note EDS was not executed.


• Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)



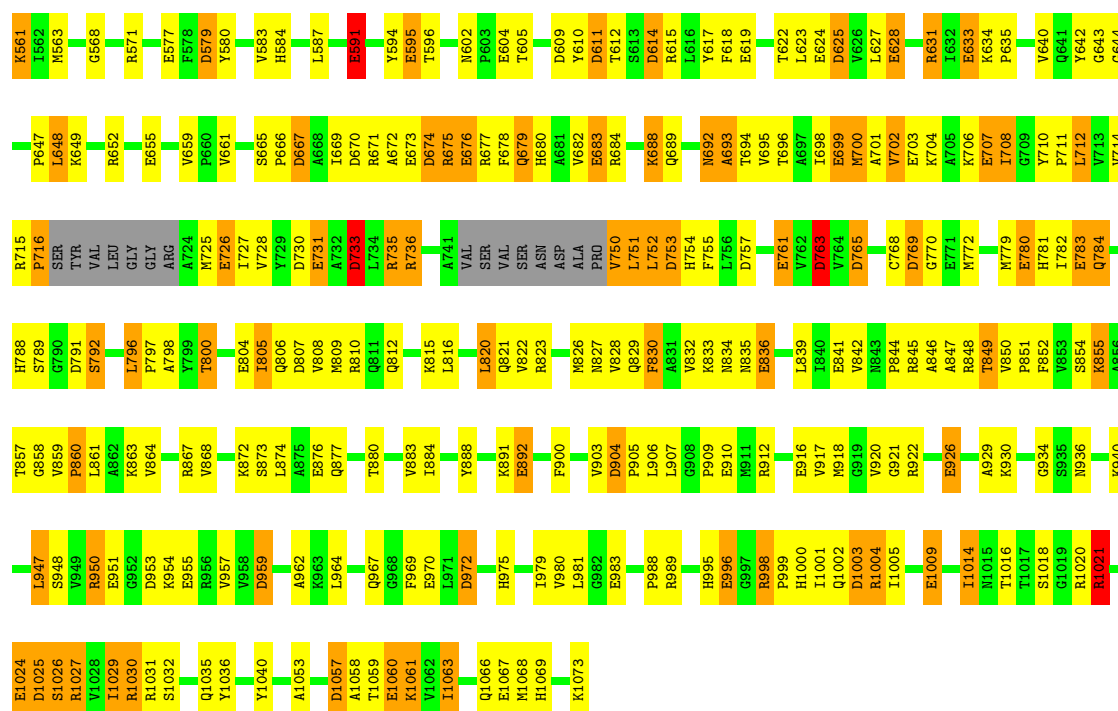


D121	V221	G343	E467	R559	D667	L734	D807	R912	I1029
D124	R222	G342	V470	E560	A668	R735	V808	E926	A1030
E127	K223	R343	R471	K561	I669	R736	M809	E1031	S1032
D128	K224	T344	L472	N563	D670	R737	Q811	K940	F738
R129	D226	P345	E473	R573	R671	Q739	Q812	K941	Q739
R130	N227	E349	E474	E577	E673	R740	V813	R944	D1041
	C228		K475	E578	D674	A741	K815	A945	T1042
D133	E235	T352	E478	E579	R675	VAL	K816	A946	D1043
I139	N236	D353	F578	D579	R676	SER	F818	L947	L1044
I148	E250	V356	F488	Y580	F678	SER	E819	S948	A1051
L141	A251	T357	F489	H584	Q679	ASN	F830	R950	L1054
E142	P252	K358	R490	E591	H680	ASP	A831	E951	D1057
		I359		D592	E683	ALA	V832	K954	K1061
I139	V250	N363	K493	E604	L685	PRO	K833	E955	Y1062
I148	D258	F364	R494	T605			E836	R956	V1063
H150	E260	E365	D499		K688	L752	V837	V957	S1064
T151	R265	D372	R509	T608	Q689	D753	Y838	R958	E1067
M152	N266	R373	E512	T609	T694	H754	L839	D959	K224
E153	A267	E383	T513	Y610	V695	L756	I840	L960	L37
E154	S268	E383	R514	D611	T696	D757	E841	A961	M1068
V158	A270	E393	R515		A697	D758	F844	A962	H1069
D161	V271	R400	K515	D614	E698	A759	R845	K963	A1070
V162	E274	E403	L516	R615	V699	V761	R848	Q967	Q1071
F164	I275	E403	D518	F618	T700	V762	K858	E970	K1073
P165	E278	D410	Q519	E619	A701	V764	V871	L971	
			Y520	T622	V702	D765	M772	D972	
I168	S282	S414	D521	E624	K704		K863	H975	
R169	V288	L415	H523	E625	K706	D769	R867	R998	
M174	N289	D416	K527		E707	E770	K872	H1000	
S177	P290	P413	D630	E628	I708	M773	S873	I1001	
R185	G293	E419	T531	R631	G709	M779	E876	Q1002	
E186	R294	A420	E535	K634	L712	E780	Q877	D1003	
E187	E299	T422	F536	K635	R715	H781	E882	R1004	
F188	P302	L423	R425	V636	P716	L782	V890	E1009	
E189	R306	K424	T540	G637	SER	E783	K891	Y1010	
I191		R426	A541	Y642	TYR	Q784	P896	T1011	
D197	K313	L428	Y542	G644	VAL	A785	L895	Y1012	
E203	P318	D434	M543	G645	GLY	G790	K899	I1013	
T206	T331	Y438	Y544	T646	ARG	D791	G1018	S1018	
D207	L332	E507	E548	P647	A724	S795	G1019	G1019	
E208	D333	L447	E549	L648	M725	L796	R1020	R1020	
Y213	E334	D459	E550	B652	E726		V903	R1021	
K214	L355	R460	E551		I727		D904	A1022	
E215	M336	V464	N554	E655	V728		P905	I1023	
V220	T340		P555	P660			L907	E1024	
			S556		E731		E910	D1025	
			T567		A732		M911	S1026	
			D558		D733			R1027	
								V1028	

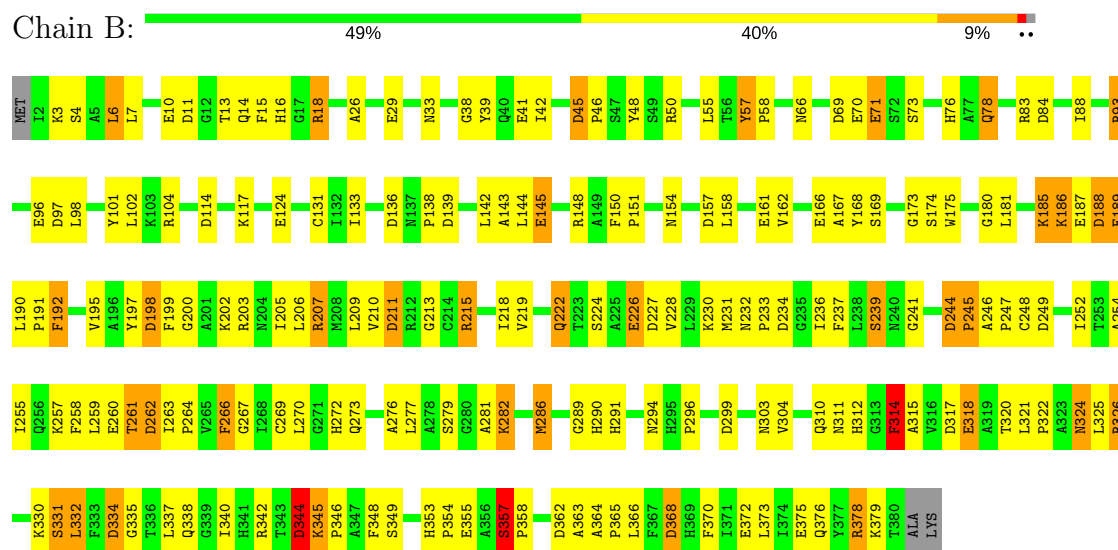
● Molecule 1: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain G: 

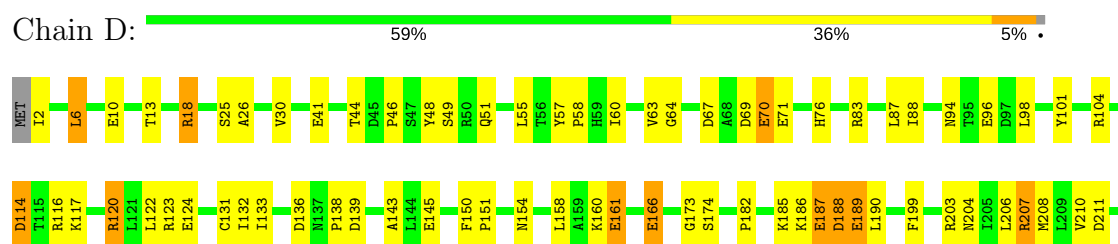
M1	Q93	R194	E278	T390	D487
P2	L100	D197	P290	E403	F488
K3	E101	L198	R294	F409	L489
T5	L102	S199	E297	D410	Q491
D6	E103	P200	K202	F411	L492
I7	R104	T201	N301	K412	K493
K8	L108	E203	P302	V413	R494
S9	E109	L204	S306	S414	
L1044	E110	L205	S307	D417	F497
A1051	A118	T206	S308	P418	A498
L1054	D121	D207	K313	E419	D499
D1057	E215	E208	E420	L502	A500
K1061	D124	Y216	A421	R509	R501
V1062	K125	E217	T422	E510	
S1064	A126	M218	K423	A511	
E1067	D223	K224	I424	E512	
M1068	K225	R129	R425	R513	
H1069	D226	R130	R426	R514	
A1070	N227	D133	E427	K515	
Q1071	C228	Y134	D430	L516	
K1073	E235	K138	R430	R517	
	N236	L141	D434	D518	
	F237	G147	R435	D521	
	M240	I148	I436		
	H243	E153	W437	V525	
	T244	E154	Y438	K527	
	G245	V158	I439	R528	
	S247	D161	A440	V529	
	I248	E164	A442	D530	
	A253	F164	F443	A534	
	P165	P166	A444	E535	
	I167	E260	G445	D539	
	M174	Y261	T456	T540	
	G180	M264	R457	A541	
	Y183	R265	I458	M542	
	R184	K259	V464	M543	
	R185	E260	E467	Y544	
	E186	Y261	L469	Y547	
	E187	M264	A370	E548	
	F188	R265	K371	E549	
	E190	E274	D372	E550	
		E275	Y183	C551	
		E276	T375	E552	
		E277	T376	A553	
		E278	Q377	N554	
		E279	E383	P555	
		E280	E386	D558	
		E281	V479	R559	
		E282	G480	E560	

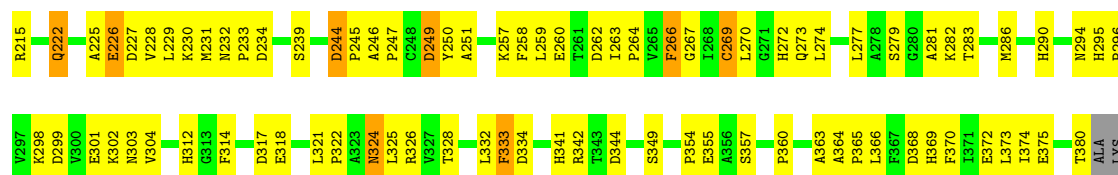


• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)



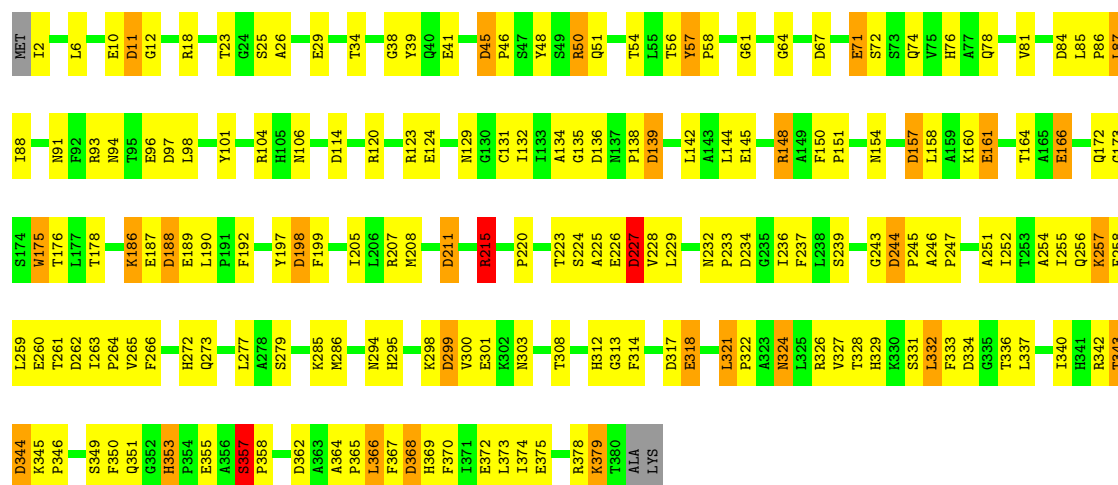
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)





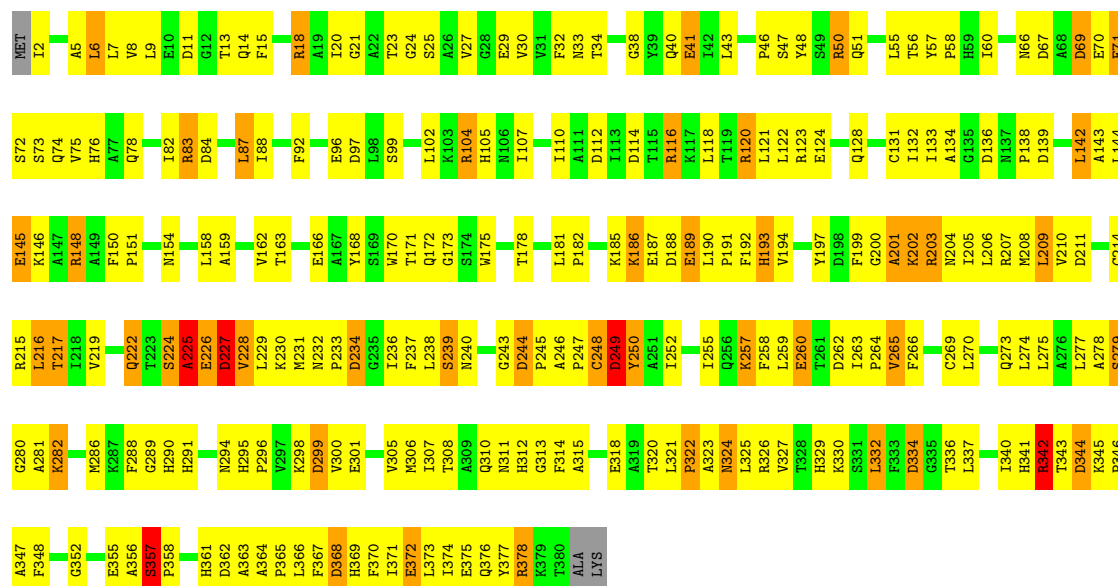
• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain F: 51% 40% 8% ..



• Molecule 2: PROTEIN (CARBAMOYL-PHOSPHATE SYNTHASE)

Chain H: 35% 51% 12% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.10Å 163.90Å 331.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.193 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48888	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, K, MN, ORN, IMP, NET, PO4

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	1.03	66/8356 (0.8%)	1.41	138/11295 (1.2%)
1	C	1.04	78/8297 (0.9%)	1.41	118/11216 (1.1%)
1	E	1.04	72/8406 (0.9%)	1.45	135/11358 (1.2%)
1	G	1.04	78/8304 (0.9%)	1.48	144/11225 (1.3%)
2	B	0.92	17/2968 (0.6%)	1.41	55/4030 (1.4%)
2	D	0.94	17/2965 (0.6%)	1.38	42/4026 (1.0%)
2	F	0.95	15/2966 (0.5%)	1.44	49/4028 (1.2%)
2	H	1.00	18/2957 (0.6%)	1.54	55/4016 (1.4%)
All	All	1.02	361/45219 (0.8%)	1.44	736/61194 (1.2%)

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
2	B	0	2
2	H	0	2
All	All	0	4

All (361) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	841	GLU	CD-OE1	-13.34	1.10	1.25
2	H	227	ASP	CG-OD2	9.15	1.46	1.25
2	D	166	GLU	CD-OE2	9.14	1.35	1.25
2	B	372	GLU	CD-OE2	8.34	1.34	1.25
2	H	166	GLU	CD-OE2	8.31	1.34	1.25
1	G	560	GLU	CD-OE1	8.26	1.34	1.25
1	G	676	GLU	CD-OE1	8.05	1.34	1.25
1	C	1024	GLU	CD-OE1	8.04	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	GLU	CD-OE1	7.79	1.34	1.25
2	B	226	GLU	CD-OE1	7.72	1.34	1.25
1	G	512	GLU	CD-OE1	7.65	1.34	1.25
1	C	703	GLU	CD-OE1	7.65	1.34	1.25
1	G	474	GLU	CD-OE1	7.56	1.33	1.25
2	H	145	GLU	CD-OE1	7.52	1.33	1.25
1	E	577	GLU	CD-OE1	7.51	1.33	1.25
2	H	187	GLU	CD-OE1	7.48	1.33	1.25
2	F	226	GLU	CD-OE1	7.48	1.33	1.25
1	E	655	GLU	CD-OE1	7.46	1.33	1.25
1	C	59	GLU	CD-OE1	7.46	1.33	1.25
1	G	703	GLU	CD-OE1	7.41	1.33	1.25
2	H	70	GLU	CD-OE1	7.41	1.33	1.25
1	A	187	GLU	CD-OE2	7.39	1.33	1.25
1	C	535	GLU	CD-OE1	7.39	1.33	1.25
1	A	109	GLU	CD-OE1	7.33	1.33	1.25
1	G	683	GLU	CD-OE1	7.23	1.33	1.25
1	C	910	GLU	CD-OE2	7.22	1.33	1.25
2	F	166	GLU	CD-OE2	7.21	1.33	1.25
2	F	187	GLU	CD-OE1	7.20	1.33	1.25
2	H	71	GLU	CD-OE2	7.17	1.33	1.25
1	A	474	GLU	CD-OE1	7.17	1.33	1.25
2	H	189	GLU	CD-OE1	7.14	1.33	1.25
1	C	109	GLU	CD-OE1	7.14	1.33	1.25
1	A	683	GLU	CD-OE2	7.13	1.33	1.25
1	C	673	GLU	CD-OE1	7.13	1.33	1.25
1	C	707	GLU	CD-OE1	7.12	1.33	1.25
1	A	72	GLU	CD-OE2	7.12	1.33	1.25
1	C	474	GLU	CD-OE1	7.11	1.33	1.25
1	G	59	GLU	CD-OE1	7.11	1.33	1.25
1	A	217	GLU	CD-OE2	7.10	1.33	1.25
1	A	676	GLU	CD-OE1	7.03	1.33	1.25
2	F	372	GLU	CD-OE1	7.03	1.33	1.25
1	G	1009	GLU	CD-OE1	7.02	1.33	1.25
1	C	67	GLU	CD-OE1	7.02	1.33	1.25
1	A	512	GLU	CD-OE1	7.01	1.33	1.25
1	E	819	GLU	CD-OE1	6.99	1.33	1.25
2	B	166	GLU	CD-OE1	6.98	1.33	1.25
1	E	478	GLU	CD-OE2	6.97	1.33	1.25
1	A	110	GLU	CD-OE2	6.97	1.33	1.25
1	E	628	GLU	CD-OE1	6.96	1.33	1.25
1	G	628	GLU	CD-OE1	6.96	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLU	CD-OE1	6.95	1.33	1.25
2	B	318	GLU	CD-OE2	6.95	1.33	1.25
1	C	676	GLU	CD-OE1	6.94	1.33	1.25
1	E	110	GLU	CD-OE1	6.93	1.33	1.25
1	G	278	GLU	CD-OE2	6.93	1.33	1.25
1	C	187	GLU	CD-OE2	6.92	1.33	1.25
1	E	190	GLU	CD-OE1	6.90	1.33	1.25
1	G	655	GLU	CD-OE1	6.86	1.33	1.25
1	A	841	GLU	CD-OE2	6.84	1.33	1.25
1	G	1024	GLU	CD-OE1	6.84	1.33	1.25
1	E	703	GLU	CD-OE1	6.83	1.33	1.25
1	C	365	GLU	CD-OE1	6.83	1.33	1.25
1	C	1009	GLU	CD-OE1	6.82	1.33	1.25
1	E	841	GLU	CD-OE2	6.82	1.33	1.25
2	B	10	GLU	CD-OE1	6.81	1.33	1.25
1	A	836	GLU	CD-OE1	6.80	1.33	1.25
1	E	910	GLU	CD-OE2	6.78	1.33	1.25
2	F	96	GLU	CD-OE2	6.78	1.33	1.25
1	C	699	GLU	CD-OE1	6.75	1.33	1.25
1	G	707	GLU	CD-OE1	6.75	1.33	1.25
1	E	619	GLU	CD-OE1	6.74	1.33	1.25
2	D	375	GLU	CD-OE2	6.72	1.33	1.25
1	G	804	GLU	CD-OE2	6.71	1.33	1.25
1	G	876	GLU	CD-OE2	6.71	1.33	1.25
1	E	707	GLU	CD-OE1	6.70	1.33	1.25
2	D	226	GLU	CD-OE1	6.69	1.33	1.25
1	A	79	GLU	CD-OE2	6.68	1.32	1.25
1	C	591	GLU	CD-OE1	6.68	1.32	1.25
2	F	301	GLU	CD-OE1	6.68	1.32	1.25
1	C	110	GLU	CD-OE1	6.64	1.32	1.25
1	C	955	GLU	CD-OE1	6.63	1.32	1.25
2	H	375	GLU	CD-OE2	6.62	1.32	1.25
2	B	145	GLU	CD-OE1	6.61	1.32	1.25
1	C	403	GLU	CD-OE2	6.59	1.32	1.25
1	G	591	GLU	CD-OE1	6.57	1.32	1.25
1	A	39	GLU	CD-OE1	6.56	1.32	1.25
1	A	707	GLU	CD-OE1	6.54	1.32	1.25
1	C	154	GLU	CD-OE1	6.54	1.32	1.25
1	E	153	GLU	CD-OE1	6.54	1.32	1.25
1	G	153	GLU	CD-OE1	6.54	1.32	1.25
1	C	189	GLU	CD-OE2	6.53	1.32	1.25
1	C	101	GLU	CD-OE1	6.53	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	GLU	CD-OE1	6.53	1.32	1.25
2	D	187	GLU	CD-OE1	6.53	1.32	1.25
1	A	154	GLU	CD-OE1	6.52	1.32	1.25
1	G	783	GLU	CD-OE1	6.52	1.32	1.25
1	E	731	GLU	CD-OE1	6.50	1.32	1.25
1	C	836	GLU	CD-OE2	6.50	1.32	1.25
1	C	468	GLU	CD-OE1	6.50	1.32	1.25
2	F	189	GLU	CD-OE2	6.50	1.32	1.25
2	B	161	GLU	CD-OE2	6.48	1.32	1.25
1	G	208	GLU	CD-OE1	6.48	1.32	1.25
1	E	780	GLU	CD-OE1	6.47	1.32	1.25
1	G	577	GLU	CD-OE1	6.47	1.32	1.25
1	C	512	GLU	CD-OE2	6.46	1.32	1.25
1	G	1060	GLU	CD-OE2	6.45	1.32	1.25
1	A	473	GLU	CD-OE1	6.45	1.32	1.25
1	C	876	GLU	CD-OE2	6.45	1.32	1.25
1	G	619	GLU	CD-OE1	6.44	1.32	1.25
1	A	591	GLU	CD-OE1	6.43	1.32	1.25
1	G	190	GLU	CD-OE1	6.43	1.32	1.25
1	G	841	GLU	CD-OE2	6.43	1.32	1.25
2	D	70	GLU	CD-OE1	6.42	1.32	1.25
2	D	301	GLU	CD-OE1	6.42	1.32	1.25
1	G	1067	GLU	CD-OE1	6.41	1.32	1.25
1	E	970	GLU	CD-OE1	6.40	1.32	1.25
1	C	780	GLU	CD-OE1	6.40	1.32	1.25
1	A	260	GLU	CD-OE1	6.39	1.32	1.25
1	A	235	GLU	CD-OE1	6.38	1.32	1.25
1	A	365	GLU	CD-OE1	6.38	1.32	1.25
1	C	655	GLU	CD-OE2	6.37	1.32	1.25
1	E	127	GLU	CD-OE1	6.35	1.32	1.25
2	F	145	GLU	CD-OE1	6.35	1.32	1.25
1	C	804	GLU	CD-OE1	6.34	1.32	1.25
1	C	771	GLU	CD-OE1	6.33	1.32	1.25
1	C	726	GLU	CD-OE1	6.33	1.32	1.25
1	E	419	GLU	CD-OE1	6.32	1.32	1.25
1	A	1024	GLU	CD-OE1	6.32	1.32	1.25
1	A	334	GLU	CD-OE2	6.30	1.32	1.25
2	D	189	GLU	CD-OE2	6.29	1.32	1.25
2	D	372	GLU	CD-OE2	6.29	1.32	1.25
1	G	926	GLU	CD-OE1	6.29	1.32	1.25
1	E	699	GLU	CD-OE1	6.28	1.32	1.25
1	C	334	GLU	CD-OE2	6.27	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	GLU	CD-OE1	6.27	1.32	1.25
1	E	215	GLU	CD-OE1	6.27	1.32	1.25
1	C	217	GLU	CD-OE2	6.26	1.32	1.25
1	C	186	GLU	CD-OE2	6.26	1.32	1.25
1	C	731	GLU	CD-OE1	6.26	1.32	1.25
1	E	365	GLU	CD-OE1	6.26	1.32	1.25
2	H	372	GLU	CD-OE1	6.25	1.32	1.25
1	G	215	GLU	CD-OE1	6.25	1.32	1.25
1	C	624	GLU	CD-OE1	6.25	1.32	1.25
2	F	260	GLU	CD-OE2	6.25	1.32	1.25
1	E	761	GLU	CD-OE1	6.24	1.32	1.25
1	C	926	GLU	CD-OE1	6.24	1.32	1.25
1	A	955	GLU	CD-OE1	6.23	1.32	1.25
1	E	676	GLU	CD-OE1	6.22	1.32	1.25
2	D	161	GLU	CD-OE2	6.22	1.32	1.25
1	G	552	GLU	CD-OE2	6.22	1.32	1.25
1	C	190	GLU	CD-OE1	6.21	1.32	1.25
1	E	624	GLU	CD-OE1	6.21	1.32	1.25
2	B	260	GLU	CD-OE2	6.21	1.32	1.25
1	G	109	GLU	CD-OE1	6.21	1.32	1.25
1	A	970	GLU	CD-OE1	6.20	1.32	1.25
1	A	996	GLU	CD-OE2	6.20	1.32	1.25
1	C	892	GLU	CD-OE2	6.20	1.32	1.25
2	H	41	GLU	CD-OE1	6.18	1.32	1.25
1	E	427	GLU	CD-OE2	6.18	1.32	1.25
1	G	510	GLU	CD-OE1	6.18	1.32	1.25
1	C	278	GLU	CD-OE2	6.17	1.32	1.25
1	A	731	GLU	CD-OE1	6.15	1.32	1.25
1	G	478[A]	GLU	CD-OE2	6.14	1.32	1.25
1	G	478[B]	GLU	CD-OE2	6.14	1.32	1.25
2	H	96	GLU	CD-OE2	6.14	1.32	1.25
1	C	72	GLU	CD-OE2	6.13	1.32	1.25
1	A	468	GLU	CD-OE1	6.13	1.32	1.25
1	C	81	GLU	CD-OE1	6.12	1.32	1.25
1	E	103	GLU	CD-OE1	6.12	1.32	1.25
1	E	804	GLU	CD-OE2	6.12	1.32	1.25
1	A	892	GLU	CD-OE2	6.12	1.32	1.25
1	G	836	GLU	CD-OE1	6.11	1.32	1.25
1	E	72	GLU	CD-OE2	6.10	1.32	1.25
1	E	836	GLU	CD-OE2	6.09	1.32	1.25
1	C	478	GLU	CD-OE2	6.09	1.32	1.25
1	A	535	GLU	CD-OE1	6.08	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	GLU	CD-OE2	6.08	1.32	1.25
1	E	154	GLU	CD-OE1	6.07	1.32	1.25
2	F	375	GLU	CD-OE2	6.06	1.32	1.25
1	G	79	GLU	CD-OE2	6.05	1.32	1.25
1	C	951	GLU	CD-OE2	6.05	1.32	1.25
1	A	560	GLU	CD-OE2	6.05	1.32	1.25
1	A	771	GLU	CD-OE2	6.04	1.32	1.25
1	E	25	GLU	CD-OE1	6.04	1.32	1.25
1	G	427	GLU	CD-OE2	6.04	1.32	1.25
1	A	819	GLU	CD-OE1	6.04	1.32	1.25
1	E	467	GLU	CD-OE1	6.04	1.32	1.25
1	G	951	GLU	CD-OE2	6.03	1.32	1.25
1	A	804	GLU	CD-OE1	6.03	1.32	1.25
1	E	550	GLU	CD-OE1	6.01	1.32	1.25
1	G	467	GLU	CD-OE1	6.00	1.32	1.25
1	A	208	GLU	CD-OE1	5.99	1.32	1.25
2	F	318	GLU	CD-OE2	5.99	1.32	1.25
1	A	127	GLU	CD-OE1	5.99	1.32	1.25
1	A	549	GLU	CD-OE2	5.98	1.32	1.25
1	G	334	GLU	CD-OE2	5.97	1.32	1.25
1	E	683	GLU	CD-OE2	5.97	1.32	1.25
1	E	882	GLU	CD-OE2	5.97	1.32	1.25
2	B	187	GLU	CD-OE1	5.95	1.32	1.25
2	D	10	GLU	CD-OE1	5.95	1.32	1.25
1	E	955	GLU	CD-OE1	5.94	1.32	1.25
1	C	467	GLU	CD-OE1	5.94	1.32	1.25
1	E	187	GLU	CD-OE2	5.93	1.32	1.25
2	D	41	GLU	CD-OE1	5.93	1.32	1.25
1	C	419	GLU	CD-OE2	5.93	1.32	1.25
1	C	39	GLU	CD-OE1	5.92	1.32	1.25
2	B	70	GLU	CD-OE1	5.91	1.32	1.25
1	E	208	GLU	CD-OE1	5.91	1.32	1.25
1	E	771[A]	GLU	CD-OE2	5.91	1.32	1.25
1	E	771[B]	GLU	CD-OE2	5.91	1.32	1.25
1	G	633	GLU	CD-OE1	5.91	1.32	1.25
1	C	153	GLU	CD-OE1	5.91	1.32	1.25
1	C	841	GLU	CD-OE2	5.90	1.32	1.25
1	A	548	GLU	CD-OE1	5.90	1.32	1.25
2	B	189	GLU	CD-OE2	5.89	1.32	1.25
1	E	673	GLU	CD-OE1	5.89	1.32	1.25
1	E	560	GLU	CD-OE1	5.89	1.32	1.25
1	C	79	GLU	CD-OE2	5.89	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	GLU	CD-OE2	5.88	1.32	1.25
1	G	780	GLU	CD-OE2	-5.88	1.19	1.25
1	G	996	GLU	CD-OE2	5.88	1.32	1.25
1	A	604	GLU	CD-OE1	5.86	1.32	1.25
1	G	186	GLU	CD-OE2	5.86	1.32	1.25
1	G	260	GLU	CD-OE1	5.86	1.32	1.25
1	A	951	GLU	CD-OE2	5.86	1.32	1.25
2	H	225	ALA	C-O	-5.86	1.12	1.23
1	G	349	GLU	CD-OE2	5.86	1.32	1.25
2	D	355	GLU	CD-OE1	5.86	1.32	1.25
2	D	96	GLU	CD-OE2	5.85	1.32	1.25
2	D	145	GLU	CD-OE1	5.84	1.32	1.25
1	C	203	GLU	CD-OE2	5.84	1.32	1.25
1	G	673	GLU	CD-OE1	5.83	1.32	1.25
1	C	383	GLU	CD-OE2	5.82	1.32	1.25
1	G	726	GLU	CD-OE1	5.81	1.32	1.25
1	A	383	GLU	CD-OE2	5.79	1.32	1.25
1	A	103	GLU	CD-OE1	5.79	1.32	1.25
1	G	365	GLU	CD-OE1	5.79	1.32	1.25
1	G	699	GLU	CD-OE1	5.79	1.32	1.25
1	C	549	GLU	CD-OE2	5.78	1.32	1.25
1	A	699	GLU	CD-OE1	5.78	1.32	1.25
1	A	761	GLU	CD-OE1	5.78	1.32	1.25
1	C	633	GLU	CD-OE1	5.78	1.32	1.25
1	C	819	GLU	CD-OE1	5.77	1.32	1.25
1	E	951	GLU	CD-OE2	5.77	1.31	1.25
1	C	1067	GLU	CD-OE1	5.77	1.31	1.25
1	G	72	GLU	CD-OE2	5.75	1.31	1.25
1	C	473	GLU	CD-OE1	5.75	1.31	1.25
1	G	916	GLU	CD-OE2	5.75	1.31	1.25
1	A	153	GLU	CD-OE1	5.73	1.31	1.25
1	A	59	GLU	CD-OE1	5.73	1.31	1.25
1	G	970	GLU	CD-OE1	5.73	1.31	1.25
1	G	595	GLU	CD-OE1	5.72	1.31	1.25
2	H	29	GLU	CD-OE1	5.72	1.31	1.25
2	B	29	GLU	CD-OE1	5.71	1.31	1.25
1	C	215	GLU	CD-OE1	5.71	1.31	1.25
1	C	683	GLU	CD-OE2	5.70	1.31	1.25
1	G	110	GLU	CD-OE1	5.70	1.31	1.25
1	G	189	GLU	CD-OE2	5.69	1.31	1.25
1	E	349	GLU	CD-OE2	5.68	1.31	1.25
2	F	124	GLU	CD-OE1	5.65	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1060	GLU	CD-OE1	5.64	1.31	1.25
1	G	535	GLU	CD-OE1	5.64	1.31	1.25
1	E	591[A]	GLU	CD-OE1	5.64	1.31	1.25
1	E	591[B]	GLU	CD-OE1	5.64	1.31	1.25
2	H	226	GLU	CD-OE1	5.63	1.31	1.25
1	A	101	GLU	CD-OE1	5.62	1.31	1.25
1	G	473	GLU	CD-OE1	5.62	1.31	1.25
2	H	301	GLU	CD-OE1	5.61	1.31	1.25
1	C	550	GLU	CD-OE1	5.60	1.31	1.25
1	C	970	GLU	CD-OE1	5.59	1.31	1.25
1	E	726	GLU	CD-OE1	5.59	1.31	1.25
1	E	203	GLU	CD-OE2	5.58	1.31	1.25
2	B	375	GLU	CD-OE2	5.58	1.31	1.25
1	C	996	GLU	CD-OE2	5.58	1.31	1.25
1	E	260	GLU	CD-OE1	5.57	1.31	1.25
2	D	260	GLU	CD-OE2	5.56	1.31	1.25
1	E	926	GLU	CD-OE1	5.56	1.31	1.25
1	A	1060	GLU	CD-OE2	5.56	1.31	1.25
2	B	71	GLU	CD-OE2	5.55	1.31	1.25
2	D	318	GLU	CD-OE2	5.54	1.31	1.25
1	G	403	GLU	CD-OE2	5.54	1.31	1.25
1	C	260	GLU	CD-OE2	5.54	1.31	1.25
2	B	96	GLU	CD-OE2	5.53	1.31	1.25
1	G	624	GLU	CD-OE1	5.53	1.31	1.25
1	G	731	GLU	CD-OE1	5.53	1.31	1.25
1	E	235	GLU	CD-OE1	5.52	1.31	1.25
1	E	109	GLU	CD-OE1	5.52	1.31	1.25
1	G	217	GLU	CD-OE2	5.52	1.31	1.25
1	G	103	GLU	CD-OE1	5.50	1.31	1.25
1	G	761	GLU	CD-OE1	5.49	1.31	1.25
2	H	318	GLU	CD-OE2	5.48	1.31	1.25
2	F	148	ARG	N-CA	-5.48	1.35	1.46
1	G	39	GLU	CD-OE1	5.47	1.31	1.25
1	G	274	GLU	CD-OE1	5.47	1.31	1.25
1	E	474	GLU	CD-OE1	5.46	1.31	1.25
1	C	577	GLU	CD-OE1	5.46	1.31	1.25
1	A	40	GLU	CD-OE1	5.46	1.31	1.25
1	G	67	GLU	CD-OE1	5.43	1.31	1.25
1	C	219	GLU	CD-OE1	5.43	1.31	1.25
1	C	916	GLU	CD-OE2	5.41	1.31	1.25
1	G	892	GLU	CD-OE2	5.41	1.31	1.25
1	A	1009	GLU	CD-OE1	5.41	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	512	GLU	CD-OE1	5.41	1.31	1.25
2	D	124	GLU	CD-OE1	5.41	1.31	1.25
1	E	882	GLU	CD-OE1	-5.41	1.19	1.25
1	G	40	GLU	CD-OE1	5.39	1.31	1.25
1	G	983	GLU	CD-OE2	5.37	1.31	1.25
1	G	550	GLU	CD-OE1	5.37	1.31	1.25
1	A	393	GLU	CD-OE1	5.36	1.31	1.25
1	C	274	GLU	CD-OE1	5.36	1.31	1.25
1	E	299	GLU	CD-OE2	5.36	1.31	1.25
1	E	59	GLU	CD-OE1	5.36	1.31	1.25
1	A	1067	GLU	CD-OE1	5.32	1.31	1.25
1	A	203	GLU	CD-OE2	5.32	1.31	1.25
1	A	780	GLU	CD-OE2	-5.32	1.19	1.25
1	C	552	GLU	CD-OE2	5.31	1.31	1.25
1	A	595	GLU	CD-OE1	5.30	1.31	1.25
1	C	604	GLU	CD-OE1	5.29	1.31	1.25
1	E	548	GLU	CD-OE1	5.29	1.31	1.25
1	G	25	GLU	CD-OE1	5.28	1.31	1.25
1	A	926	GLU	CD-OE1	5.26	1.31	1.25
1	C	154	GLU	CD-OE2	-5.25	1.19	1.25
1	G	154	GLU	CD-OE1	5.25	1.31	1.25
1	G	910	GLU	CD-OE2	5.24	1.31	1.25
2	B	41	GLU	CD-OE1	5.24	1.31	1.25
1	C	127	GLU	CD-OE1	5.23	1.31	1.25
1	G	468	GLU	CD-OE1	5.23	1.31	1.25
1	A	81	GLU	CD-OE1	5.21	1.31	1.25
1	A	190	GLU	CD-OE1	5.20	1.31	1.25
2	F	71	GLU	CD-OE2	5.18	1.31	1.25
1	E	1024	GLU	CD-OE1	5.17	1.31	1.25
1	A	624	GLU	CD-OE1	5.17	1.31	1.25
1	E	101	GLU	CD-OE1	5.16	1.31	1.25
2	H	124	GLU	CD-OE2	5.16	1.31	1.25
1	E	535	GLU	CD-OE1	5.15	1.31	1.25
2	H	260	GLU	CD-OE2	5.14	1.31	1.25
1	C	510	GLU	CD-OE1	5.14	1.31	1.25
1	G	187	GLU	CD-OE2	5.13	1.31	1.25
1	C	103	GLU	CD-OE1	5.11	1.31	1.25
1	A	628	GLU	CD-OE1	5.11	1.31	1.25
1	C	299	GLU	CD-OE1	-5.11	1.20	1.25
1	A	619	GLU	CD-OE1	5.10	1.31	1.25
1	A	673	GLU	CD-OE1	5.09	1.31	1.25
1	E	393	GLU	CD-OE1	5.09	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	127	GLU	CD-OE1	5.08	1.31	1.25
2	B	124	GLU	CD-OE1	5.07	1.31	1.25
1	E	403	GLU	CD-OE2	5.06	1.31	1.25
1	E	274	GLU	CD-OE1	5.06	1.31	1.25
1	E	189	GLU	CD-OE2	5.05	1.31	1.25
1	G	549	GLU	CD-OE2	5.04	1.31	1.25
1	E	549	GLU	CD-OE2	5.03	1.31	1.25
1	G	419	GLU	CD-OE1	5.03	1.31	1.25
1	A	427	GLU	CD-OE2	5.02	1.31	1.25
1	C	882	GLU	CD-OE2	5.02	1.31	1.25
2	F	71	GLU	CD-OE1	-5.02	1.20	1.25
1	C	983	GLU	CD-OE2	5.01	1.31	1.25
1	E	876	GLU	CD-OE2	5.01	1.31	1.25
1	E	473	GLU	CD-OE1	5.01	1.31	1.25
1	G	780	GLU	CD-OE1	5.00	1.31	1.25
1	E	142	GLU	CD-OE2	5.00	1.31	1.25
1	E	278	GLU	CD-OE2	5.00	1.31	1.25

All (736) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	ASP	CB-CG-OD2	-15.41	104.43	118.30
2	H	249	ASP	CB-CG-OD1	-15.06	104.74	118.30
2	F	120	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	E	642	TYR	CB-CG-CD1	13.16	128.89	121.00
1	E	438	TYR	CB-CG-CD1	13.10	128.86	121.00
2	H	250	TYR	CB-CG-CD2	13.00	128.80	121.00
1	E	82[A]	ARG	NE-CZ-NH2	-12.51	114.05	120.30
1	E	82[B]	ARG	NE-CZ-NH2	-12.51	114.05	120.30
1	E	438	TYR	CB-CG-CD2	-12.04	113.78	121.00
1	E	642	TYR	CB-CG-CD2	-11.62	114.03	121.00
1	C	400	ARG	NE-CZ-NH1	11.25	125.93	120.30
2	B	286	MET	CG-SD-CE	-10.91	82.75	100.20
2	B	357	SER	O-C-N	-10.74	100.69	121.10
1	G	848	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	944	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	E	38	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	E	129	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	C	194	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	C	84	ASP	CB-CG-OD1	-10.00	109.30	118.30
2	H	357	SER	O-C-N	-9.98	102.13	121.10
2	F	357	SER	O-C-N	-9.98	102.14	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	579	ASP	CB-CG-OD1	-9.95	109.34	118.30
1	A	129	ARG	NE-CZ-NH1	9.89	125.25	120.30
2	F	120	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	G	530	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	G	434	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	G	223	ASP	CB-CG-OD2	-9.46	109.78	118.30
1	G	425	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	677	ARG	NE-CZ-NH1	9.39	125.00	120.30
2	F	97	ASP	CB-CG-OD1	-9.30	109.93	118.30
1	G	667	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	G	579	ASP	CB-CG-OD1	-9.18	110.04	118.30
2	B	262	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	E	609	ASP	CB-CG-OD2	-9.00	110.20	118.30
2	H	211	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	C	514	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	G	6	ASP	CB-CG-OD1	-8.95	110.25	118.30
1	G	438	TYR	CB-CG-CD1	-8.93	115.64	121.00
1	A	226	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	C	258	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	C	194	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	C	361	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	C	129	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	D	234	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	A	625	ASP	CB-CG-OD2	8.75	126.18	118.30
1	C	133	ASP	CB-CG-OD1	-8.72	110.45	118.30
2	H	250	TYR	CG-CD2-CE2	8.70	128.26	121.30
1	G	223	ASP	CB-CG-OD1	8.69	126.12	118.30
1	C	372	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	E	265	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	1004	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	G	625	ASP	CB-CG-OD2	8.57	126.01	118.30
2	H	342	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	B	227	ASP	CB-CG-OD2	-8.50	110.65	118.30
2	F	368	ASP	CB-CG-OD2	8.48	125.93	118.30
2	H	227	ASP	CB-CG-OD1	8.48	125.93	118.30
2	H	299	ASP	CB-CG-OD2	8.47	125.92	118.30
1	A	625	ASP	CB-CG-OD1	-8.45	110.70	118.30
1	C	450	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	G	43	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	G	372	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	C	43	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	B	314	PHE	CB-CA-C	-8.40	93.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	791	ASP	CB-CG-OD1	8.39	125.85	118.30
1	G	757	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	G	130	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	G	133	ASP	CB-CG-OD1	-8.33	110.80	118.30
2	H	262	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	1003	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	C	1004	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	G	265	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	G	959	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	G	226	ASP	CB-CG-OD1	-8.16	110.96	118.30
1	C	121	ASP	CB-CG-OD2	8.15	125.63	118.30
2	H	299	ASP	CB-CG-OD1	-8.12	110.99	118.30
1	G	530	ASP	CB-CG-OD1	8.10	125.59	118.30
2	B	262	ASP	CB-CG-OD1	8.09	125.58	118.30
1	C	674	ASP	CB-CG-OD1	-8.08	111.03	118.30
1	E	487	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	G	43	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	E	223	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	C	400	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	G	765	ASP	CB-CG-OD2	7.98	125.48	118.30
1	G	258	ASP	CB-CG-OD2	-7.97	111.12	118.30
2	D	211	ASP	CB-CG-OD1	7.97	125.47	118.30
1	C	223	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	E	128	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	G	124	ASP	CB-CG-OD1	-7.91	111.18	118.30
2	F	157	ASP	CB-CG-OD2	7.91	125.42	118.30
1	G	444	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	E	6	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	A	518	ASP	CB-CG-OD2	-7.88	111.21	118.30
2	D	334	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	E	43	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	B	249	ASP	CB-CG-OD1	-7.86	111.23	118.30
1	C	514	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	C	753	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	C	128	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	592	ASP	CB-CG-OD1	-7.79	111.29	118.30
2	H	139	ASP	CB-CG-OD1	7.79	125.31	118.30
2	D	211	ASP	CB-CG-OD2	-7.76	111.31	118.30
2	H	67	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	C	614	ASP	CB-CG-OD1	-7.75	111.33	118.30
2	F	148	ARG	N-CA-CB	-7.74	96.68	110.60
1	G	246	ASP	CB-CG-OD1	-7.73	111.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	810	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	G	614	ASP	CB-CG-OD1	-7.70	111.37	118.30
2	B	211	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	733	ASP	CB-CG-OD1	7.69	125.22	118.30
1	G	434	ASP	CB-CG-OD1	7.68	125.21	118.30
1	E	38	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	C	579	ASP	CB-CG-OD2	7.67	125.20	118.30
1	G	183	TYR	CB-CG-CD1	-7.66	116.40	121.00
2	H	225	ALA	CB-CA-C	-7.66	98.61	110.10
1	A	670	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	E	129	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	F	317	ASP	CB-CG-OD1	-7.65	111.41	118.30
2	B	317	ASP	CB-CG-OD2	7.65	125.19	118.30
1	C	539	ASP	CB-CG-OD1	-7.65	111.42	118.30
1	C	131	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	D	83	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	E	791	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	C	104	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	361	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	43	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	129	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	677	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	F	97	ASP	CB-CG-OD2	7.57	125.11	118.30
1	C	121	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	E	223	ASP	CB-CG-OD1	7.54	125.08	118.30
2	D	207	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	E	1057	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	E	609	ASP	CB-CG-OD1	7.50	125.05	118.30
1	G	333	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	G	959	ASP	CB-CG-OD1	7.49	125.04	118.30
1	G	625	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	E	579	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	343	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	E	514	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	E	487	ASP	CB-CG-OD1	7.45	125.00	118.30
2	D	120	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	E	400	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	B	198	ASP	CB-CG-OD2	7.44	125.00	118.30
2	F	50	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	H	116	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	C	226	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	C	128	ASP	CB-CG-OD2	-7.39	111.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	471	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	133	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	G	757	ASP	CB-CG-OD2	7.37	124.93	118.30
2	D	18	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	G	807	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	E	410	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	C	972	ASP	CB-CG-OD2	-7.34	111.69	118.30
2	B	207	ARG	NE-CZ-NH1	7.31	123.96	120.30
2	D	326	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	F	262	ASP	CB-CG-OD2	-7.30	111.73	118.30
2	H	116	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	G	471	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	258	ASP	CB-CG-OD1	7.27	124.84	118.30
2	D	326	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	E	197	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	E	494	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	E	121	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	62	ASP	CB-CG-OD1	7.21	124.79	118.30
2	H	368	ASP	CB-CG-OD1	-7.21	111.81	118.30
2	H	378	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	518	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	807	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	C	6	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	A	128	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	43	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	G	124	ASP	CB-CG-OD2	7.16	124.75	118.30
1	C	609	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	G	667	ASP	CB-CG-OD2	7.15	124.73	118.30
1	C	450	ASP	CB-CG-OD2	7.14	124.73	118.30
2	D	136	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	372	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	E	517	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	904	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	558	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	G	133	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	733	ASP	CB-CG-OD2	-7.08	111.92	118.30
2	H	84	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	303	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	G	521	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	G	386	ALA	N-CA-CB	7.07	120.00	110.10
1	A	131	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	592	ASP	CB-CG-OD2	7.05	124.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	357	SER	CA-C-N	7.04	136.80	117.10
1	G	128	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	E	1041	ASP	CB-CG-OD1	-7.03	111.97	118.30
2	F	139	ASP	CB-CG-OD2	-7.03	111.98	118.30
2	H	262	ASP	CB-CG-OD1	7.01	124.61	118.30
1	G	372	ASP	CB-CG-OD1	6.99	124.59	118.30
1	G	642	TYR	CB-CG-CD1	6.98	125.19	121.00
1	E	614	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	G	84	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	C	104	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	E	372	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	C	124	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	E	84	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	E	769	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	G	306	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	E	490[A]	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	E	490[B]	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	757	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	G	438	TYR	CB-CG-CD2	6.91	125.14	121.00
1	E	128	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	769	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	G	1030	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	733	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	333	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	G	769	ASP	CB-CG-OD1	-6.87	112.11	118.30
1	A	614	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	G	104	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	D	67	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	G	631	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	G	765	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	C	84	ASP	CB-CG-OD2	6.82	124.44	118.30
1	G	735	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	E	733	ASP	CB-CG-OD2	-6.79	112.18	118.30
1	E	956	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	E	684	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	E	124	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	G	128	ASP	CB-CG-OD1	6.77	124.39	118.30
1	G	121	ASP	CB-CG-OD1	-6.76	112.21	118.30
1	G	674	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	G	258	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	124	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	A	614	ASP	CB-CG-OD2	6.75	124.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	ASP	CB-CG-OD1	6.75	124.38	118.30
1	E	757	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	471	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	F	262	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	521	ASP	CB-CG-OD1	-6.74	112.24	118.30
1	C	521	ASP	CB-CG-OD1	-6.73	112.25	118.30
1	E	121	ASP	CB-CG-OD1	-6.72	112.25	118.30
2	D	234	ASP	CB-CG-OD1	6.72	124.35	118.30
1	G	443	PHE	CB-CG-CD1	-6.71	116.10	120.80
2	F	161	GLU	OE1-CD-OE2	6.69	131.33	123.30
2	D	136	ASP	CB-CG-OD1	-6.69	112.28	118.30
2	F	188	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	674	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	791	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	A	410	ASP	CB-CG-OD1	-6.67	112.30	118.30
2	F	84	ASP	CB-CG-OD1	6.66	124.29	118.30
2	F	188	ASP	CB-CG-OD1	-6.65	112.32	118.30
1	G	614	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	27	ASP	CB-CG-OD2	6.63	124.27	118.30
1	E	434	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	A	430	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	G	594	TYR	CB-CA-C	-6.61	97.19	110.40
1	E	161	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	615	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	715	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	139	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	972	ASP	CB-CG-OD1	6.59	124.23	118.30
1	G	642	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	H	97	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	E	530	ASP	CB-CG-OD1	6.57	124.22	118.30
2	H	357	SER	CA-C-N	6.57	135.50	117.10
1	A	410	ASP	CB-CG-OD2	6.56	124.20	118.30
2	F	11	ASP	CB-CG-OD2	6.53	124.18	118.30
1	G	226	ASP	CB-CG-OD2	6.53	124.18	118.30
1	C	499	ASP	CB-CG-OD2	6.53	124.17	118.30
1	C	667	ASP	CB-CG-OD1	-6.53	112.43	118.30
1	A	27	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	128	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	H	139	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	124	ASP	CB-CG-OD2	6.50	124.15	118.30
1	G	1057	ASP	CB-CG-OD1	-6.50	112.45	118.30
2	D	69	ASP	CB-CG-OD1	-6.50	112.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	ASP	CB-CG-OD1	6.50	124.14	118.30
2	B	368	ASP	CB-CG-OD1	-6.50	112.45	118.30
2	F	227	ASP	CB-CG-OD2	-6.49	112.46	118.30
2	H	136	ASP	CB-CG-OD1	-6.49	112.46	118.30
2	B	368	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	579	ASP	CB-CG-OD1	-6.49	112.46	118.30
1	C	769	ASP	CB-CG-OD1	-6.47	112.47	118.30
2	B	266	PHE	CB-CG-CD2	-6.47	116.27	120.80
2	B	136	ASP	CB-CG-OD1	-6.46	112.49	118.30
2	B	198	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	571	ARG	CD-NE-CZ	-6.45	114.58	123.60
1	E	667	ASP	CB-CG-OD1	-6.44	112.50	118.30
2	H	211	ASP	CB-CG-OD1	6.43	124.09	118.30
1	G	246	ASP	CB-CG-OD2	6.43	124.09	118.30
2	H	67	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	674	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	F	357	SER	CA-C-N	6.41	135.06	117.10
2	D	344	ASP	CB-CG-OD2	6.41	124.07	118.30
1	E	999	PRO	N-CA-C	-6.41	95.44	112.10
2	B	18	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	F	139	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	1021	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	425	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	518	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	1025	ASP	CB-CG-OD2	6.39	124.05	118.30
1	G	670	ASP	CB-CG-OD2	6.39	124.05	118.30
1	E	6	ASP	CB-CG-OD2	6.38	124.05	118.30
2	H	69	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	558	ASP	CB-CG-OD1	-6.38	112.56	118.30
2	B	344	ASP	CB-CG-OD1	-6.38	112.56	118.30
2	D	69	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	670	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	E	426	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	27	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	A	807	ASP	CB-CG-OD2	6.34	124.01	118.30
2	B	227	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	579	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	459	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	438	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	A	769	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	592	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	E	4	ARG	NE-CZ-NH1	6.29	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	426	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	E	614	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	609	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	173	THR	N-CA-CB	6.27	122.22	110.30
2	H	228	VAL	CA-CB-CG1	-6.27	101.49	110.90
2	F	57	TYR	CA-CB-CG	-6.27	101.49	113.40
2	F	317	ASP	CB-CG-OD2	6.27	123.94	118.30
1	G	338	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	C	361	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	716	PRO	N-CA-CB	6.26	110.82	103.30
1	G	735	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	G	791	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	C	207	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	G	6	ASP	CB-CG-OD2	6.25	123.92	118.30
1	G	499	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	E	471	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	499	ASP	CB-CG-OD1	-6.23	112.69	118.30
2	B	211	ASP	CB-CG-OD1	6.23	123.90	118.30
2	D	262	ASP	CB-CG-OD1	6.22	123.90	118.30
2	F	50	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	1021[A]	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	1021[B]	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	G	539	ASP	CB-CG-OD1	-6.22	112.71	118.30
1	A	104	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	F	114	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	C	733	ASP	CB-CG-OD1	6.21	123.89	118.30
1	E	334	GLU	CB-CA-C	-6.21	97.99	110.40
1	E	509	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	B	69	ASP	CB-CG-OD1	-6.20	112.72	118.30
2	H	368	ASP	CB-CG-OD2	6.19	123.88	118.30
1	E	124	ASP	CB-CG-OD1	6.19	123.87	118.30
2	D	244	ASP	CB-CG-OD1	-6.18	112.74	118.30
2	F	378	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	F	234	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	G	1004	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	E	791	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	791	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	124	ASP	CB-CG-OD2	6.15	123.83	118.30
1	C	444	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	736	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	950	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	757	ASP	CB-CG-OD2	6.14	123.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	342	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	G	733	ASP	CB-CG-OD2	-6.13	112.78	118.30
2	F	123	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	E	999	PRO	N-CA-CB	6.13	110.65	103.30
1	G	716	PRO	N-CA-CB	6.12	110.64	103.30
2	B	266	PHE	CB-CG-CD1	6.12	125.08	120.80
1	E	831	ALA	N-CA-CB	6.11	118.65	110.10
2	B	45	ASP	CB-CG-OD2	6.10	123.79	118.30
1	G	487	ASP	CB-CG-OD1	6.10	123.79	118.30
1	E	539	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	E	530	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	A	539	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	D	262	ASP	CB-CG-OD2	-6.08	112.82	118.30
1	A	416[A]	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	416[B]	ASP	CB-CG-OD2	-6.07	112.83	118.30
2	F	344	ASP	CB-CG-OD1	-6.07	112.83	118.30
2	D	139	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	736	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	E	611	ASP	CB-CG-OD2	6.07	123.76	118.30
1	G	65	TYR	CB-CG-CD1	6.07	124.64	121.00
2	D	83	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	B	188	ASP	CB-CG-OD2	6.06	123.76	118.30
1	E	625	ASP	CB-CG-OD2	6.06	123.75	118.30
1	E	544	TYR	CB-CG-CD2	6.05	124.63	121.00
1	G	75	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	571	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	G	410	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	C	539	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	84	ASP	CB-CG-OD1	-6.04	112.87	118.30
2	F	198	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	194	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	130	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	E	959	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	753	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	F	120	ARG	CD-NE-CZ	6.02	132.03	123.60
1	E	258	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	265	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	F	45	ASP	CB-CG-OD1	-6.01	112.89	118.30
2	B	84	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	444	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	D	249	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	A	904	ASP	CB-CG-OD1	-5.99	112.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	E	807	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	C	226	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	667	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	139	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	333	ASP	CB-CG-OD1	5.99	123.69	118.30
2	B	136	ASP	CB-CG-OD2	5.98	123.68	118.30
1	E	226	ASP	CB-CG-OD2	5.98	123.68	118.30
1	E	557	THR	CA-CB-CG2	-5.98	104.03	112.40
2	B	362	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	C	763	ASP	CB-CG-OD1	-5.97	112.92	118.30
2	D	120	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	H	234	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	471	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	D	18	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	671	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	1004	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	758	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	956	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	F	67	ASP	CB-CG-OD1	-5.94	112.95	118.30
2	F	215	ARG	N-CA-CB	5.94	121.29	110.60
2	B	18	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	H	250	TYR	CD1-CG-CD2	-5.93	111.37	117.90
1	E	769	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	249	ASP	CB-CG-OD2	5.93	123.64	118.30
2	H	250	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	C	133	ASP	CB-CG-OD2	5.91	123.62	118.30
1	G	609	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	499	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	1004	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	E	757	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	763	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	E	959	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	G	674	ASP	CB-CG-OD1	5.89	123.60	118.30
2	F	148	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	G	441	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	E	169	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	G	501	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	226	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	161	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	904	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	684	ARG	NE-CZ-NH1	5.87	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	D	227	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	E	571	ARG	CB-CA-C	-5.86	98.68	110.40
1	A	459	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	E	416	ASP	CB-CG-OD2	-5.84	113.04	118.30
2	F	211	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	42	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	C	959	ASP	CB-CG-OD1	5.83	123.54	118.30
1	G	579	ASP	CB-CG-OD2	5.82	123.54	118.30
2	B	317	ASP	CB-CG-OD1	-5.81	113.07	118.30
2	B	69	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	223	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	G	416	ASP	CB-CG-OD2	5.79	123.51	118.30
1	G	609	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	G	769	ASP	CB-CG-OD2	5.79	123.51	118.30
2	D	344	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	C	758	ASP	CB-CG-OD2	5.79	123.51	118.30
1	G	1027	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	530	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	1003	ASP	CB-CG-OD2	5.78	123.50	118.30
1	E	625	ASP	CB-CG-OD1	-5.77	113.10	118.30
2	F	344	ASP	CB-CG-OD2	5.77	123.50	118.30
1	E	353	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	611	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	E	521	ASP	CB-CG-OD2	5.76	123.48	118.30
2	D	114	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	C	410	ASP	CB-CG-OD1	5.75	123.48	118.30
2	B	97	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	E	306	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	D	13	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	735	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	G	611	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	E	1010	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	528	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	615	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	H	136	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	459	ASP	CB-CG-OD2	5.74	123.46	118.30
2	B	39	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	H	299	ASP	N-CA-C	-5.73	95.52	111.00
2	B	157	ASP	CB-CG-OD2	5.73	123.46	118.30
2	H	50	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	670	ASP	CB-CG-OD1	-5.73	113.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	670	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	430	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	6	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	615	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	G	559	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	1025	ASP	CB-CG-OD1	-5.71	113.17	118.30
2	D	139	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	161	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	609	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	1030	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	373	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	416	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	450	ASP	CB-CG-OD1	-5.68	113.18	118.30
1	A	416[A]	ASP	CB-CG-OD1	5.68	123.42	118.30
1	A	416[B]	ASP	CB-CG-OD1	5.68	123.42	118.30
2	H	234	ASP	CB-CG-OD1	5.68	123.41	118.30
1	G	972	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	H	188	ASP	CB-CG-OD2	5.68	123.41	118.30
1	E	373	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	E	521	ASP	CB-CG-OD1	-5.66	113.21	118.30
2	H	193	HIS	N-CA-CB	5.66	120.79	110.60
2	F	211	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	B	244	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	207	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	430	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	A	499	ASP	CB-CG-OD1	-5.65	113.22	118.30
2	B	244	ASP	CB-CG-OD2	5.64	123.38	118.30
2	H	112	ASP	CB-CG-OD2	5.64	123.37	118.30
2	B	215[A]	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	B	215[B]	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	333	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	G	261	TYR	CB-CG-CD2	-5.63	117.62	121.00
2	F	353	HIS	CA-CB-CG	-5.63	104.03	113.60
1	A	959	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	C	912	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	E	258	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	698	ILE	N-CA-CB	-5.62	97.87	110.80
1	C	807	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	H	244	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	652	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	H	326	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	609	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	441	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	E	82[A]	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	E	82[B]	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	C	161	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	E	904	ASP	CB-CG-OD1	-5.59	113.27	118.30
2	D	188	ASP	CB-CG-OD1	-5.59	113.27	118.30
2	D	368	ASP	CB-CG-OD1	-5.58	113.27	118.30
2	D	317	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	E	733	ASP	CB-CG-OD1	5.57	123.31	118.30
1	G	675	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	372	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	434	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	E	542	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	753	ASP	CB-CG-OD1	5.57	123.31	118.30
1	E	1025	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	129	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	344	ASP	CB-CG-OD2	5.56	123.30	118.30
1	G	185	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	372	ASP	CB-CG-OD1	5.55	123.30	118.30
1	G	57	ASP	CB-CG-OD2	5.55	123.30	118.30
1	G	1027	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	1057	ASP	CB-CG-OD2	5.54	123.29	118.30
1	E	539	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	487	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	E	353	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	G	615	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	G	807	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	1003	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	410	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	757	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	1057	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	438	TYR	CA-CB-CG	-5.52	102.91	113.40
1	E	197	ASP	CB-CG-OD1	5.52	123.27	118.30
2	F	372	GLU	CB-CA-C	-5.51	99.39	110.40
1	A	611	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	715	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	400	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	F	234	ASP	CB-CG-OD1	5.49	123.24	118.30
2	H	97	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	435	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	C	161	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	197	ASP	CB-CG-OD2	-5.49	113.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	43	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	45	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	C	521	ASP	CB-CG-OD2	5.48	123.23	118.30
1	G	81	GLU	CG-CD-OE2	5.48	129.25	118.30
2	B	84	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	C	223	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	530	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	E	520	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	246	ASP	CB-CG-OD1	-5.46	113.39	118.30
2	F	11	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	G	972	ASP	CB-CG-OD1	5.46	123.21	118.30
1	G	1003	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	197	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	1057	ASP	CB-CG-OD2	5.45	123.20	118.30
2	H	322	PRO	N-CA-C	-5.44	97.95	112.10
1	A	131	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	G	273	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	953	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	A	973	ALA	N-CA-CB	5.43	117.71	110.10
1	E	592	ASP	CB-CG-OD2	5.43	123.19	118.30
2	H	250	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	C	154	GLU	CB-CG-CD	5.43	128.85	114.20
1	G	129	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	G	330	TYR	CG-CD1-CE1	5.43	125.64	121.30
1	G	57	ASP	C-N-CD	-5.42	108.67	120.60
2	D	10	GLU	N-CA-CB	-5.42	100.84	110.60
1	E	558	ASP	CB-CG-OD1	-5.42	113.43	118.30
1	E	867	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	G	194	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	E	520	TYR	CB-CA-C	-5.41	99.58	110.40
1	E	765	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	A	223	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	642	TYR	CB-CG-CD1	5.40	124.24	121.00
1	C	998	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	G	571	ARG	CB-CA-C	-5.40	99.61	110.40
1	A	434	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	758	ASP	CB-CG-OD2	5.38	123.15	118.30
1	G	27	ASP	CB-CG-OD2	5.38	123.15	118.30
1	C	416	ASP	CB-CG-OD1	-5.37	113.46	118.30
1	C	487	ASP	CB-CG-OD2	-5.37	113.46	118.30
2	H	344	ASP	CB-CG-OD1	-5.37	113.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	39	TYR	CB-CG-CD1	5.37	124.22	121.00
1	E	133	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	E	972	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	G	796	LEU	C-N-CD	-5.36	108.80	120.60
1	C	625	ASP	CB-CG-OD1	-5.36	113.48	118.30
2	F	198	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	E	716	PRO	N-CA-CB	5.35	109.72	103.30
2	B	93	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	614	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	944	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	E	674	ASP	CB-CG-OD2	5.34	123.10	118.30
1	G	65	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	E	185	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	D	114	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	848	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	F	227	ASP	CB-CG-OD1	5.33	123.10	118.30
1	G	830	PHE	CB-CG-CD2	5.32	124.52	120.80
1	G	730	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	333	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	518	ASP	CB-CG-OD1	-5.31	113.52	118.30
2	H	188	ASP	CB-CG-OD1	-5.31	113.53	118.30
1	G	540	THR	CA-CB-CG2	-5.30	104.98	112.40
2	B	57	TYR	CA-CB-CG	-5.30	103.33	113.40
1	G	521	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	38	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	1025	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	266	PHE	CB-CG-CD2	-5.29	117.10	120.80
2	B	83	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	H	120	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	B	362	ASP	CB-CG-OD2	5.28	123.05	118.30
1	G	694	THR	CA-CB-CG2	-5.28	105.01	112.40
2	H	357	SER	N-CA-CB	5.28	118.42	110.50
1	G	1025	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	353	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	E	674	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	E	765	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	501	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	207	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	G	501	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	57	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	G	753	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	343	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	338	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	312	HIS	CG-CD2-NE2	-5.24	99.25	109.20
1	G	84	ASP	CB-CG-OD2	5.24	123.01	118.30
2	F	136	ASP	CB-CG-OD2	5.23	123.01	118.30
2	H	334	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	333	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	769	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	226	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	D	188	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	631	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	D	269	CYS	CB-CA-C	5.21	120.83	110.40
2	B	372	GLU	N-CA-CB	-5.21	101.22	110.60
2	F	299	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	670	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	97	ASP	CB-CG-OD2	5.21	122.99	118.30
2	D	368	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	1012	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	E	417	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	C	758	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	F	244	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	E	459	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	G	333	ASP	CB-CG-OD1	5.20	122.97	118.30
1	G	953	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	F	362	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	E	904	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	823	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	G	675	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	H	237	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	A	605	THR	N-CA-C	5.18	124.99	111.00
1	G	161	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	G	441	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	1030	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	520	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	G	197	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	G	430	ASP	CB-CG-OD1	-5.17	113.65	118.30
2	B	326	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	F	368	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	C	1057	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	338	ASP	CB-CG-OD1	-5.15	113.66	118.30
2	B	50	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	SER	N-CA-CB	5.13	118.20	110.50
1	E	27	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	763	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	G	558	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	972	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	558	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	509	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	220	VAL	CB-CA-C	-5.12	101.68	111.40
1	C	677	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	353	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	514	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	D	101	TYR	CB-CG-CD1	5.10	124.06	121.00
1	G	539	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	169	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	361	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	G	1021	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	246	ASP	CB-CG-OD1	-5.08	113.73	118.30
2	H	18	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	E	611	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	G	998	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	558	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	C	757	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	E	517	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	G	736	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	765	ASP	CB-CG-OD2	5.06	122.85	118.30
1	G	430	ASP	CB-CG-OD2	5.06	122.85	118.30
2	H	83	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	953	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	618	PHE	CB-CG-CD1	5.04	124.33	120.80
1	E	579	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	265	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	E	758	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	152	MET	N-CA-CB	5.02	119.64	110.60
1	A	953	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	67	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	670	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	133	ASP	CB-CG-OD2	5.01	122.81	118.30
2	H	314	PHE	CB-CG-CD2	-5.01	117.29	120.80
1	C	237	PHE	CB-CG-CD2	-5.01	117.29	120.80
1	G	611	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	1041	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	258	ASP	CB-CG-OD2	-5.00	113.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	558	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	314	PHE	Mainchain
2	B	357	SER	Peptide
2	H	250	TYR	Sidechain
2	H	357	SER	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	8198	0	8215	275	1
1	C	8167	0	8201	242	0
1	E	8232	0	8274	251	0
1	G	8170	0	8204	343	0
2	B	2902	0	2872	145	0
2	D	2899	0	2868	95	0
2	F	2900	0	2867	118	1
2	H	2895	0	2863	230	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	6	0	0	0	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3	0	0	1	0
5	G	3	0	0	2	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	2	0
7	C	54	0	24	1	0
7	E	54	0	24	5	0
7	G	54	0	24	5	0
8	A	18	0	22	4	0
8	C	18	0	22	3	0
8	E	18	0	21	4	0
8	G	18	0	22	4	0
9	A	23	0	11	1	0
9	C	23	0	11	1	0
9	E	23	0	11	2	0
9	G	23	0	11	1	0
10	A	9	0	20	0	0
10	C	9	0	20	0	0
10	E	9	0	20	3	0
10	G	9	0	20	1	0
11	A	842	0	0	26	1
11	B	190	0	0	3	0
11	C	732	0	0	12	0
11	D	193	0	0	3	0
11	E	939	0	0	30	0
11	F	233	0	0	4	1
11	G	743	0	0	19	0
11	H	165	0	0	4	0
All	All	48888	0	44671	1666	2

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 19.

All (1666) 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:A:130[B]:ARG:CZ	1:A:130[B]:ARG:NH2	1.70	1.49
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.26	1.16
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.06	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.13	1.06
1:A:130[B]:ARG:CZ	1:A:130[B]:ARG:NH1	2.18	1.05
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.39	1.04
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.04
2:H:227:ASP:HA	2:H:230:LYS:HD2	1.41	1.02
1:A:554:ASN:HD22	8:A:5014:ORN:HD3	1.19	1.01
1:E:784:GLN:NE2	1:E:784:GLN:H	1.58	0.99
2:H:236:ILE:HD12	2:H:263:ILE:HG21	1.43	0.98
1:G:554:ASN:HD22	8:G:5074:ORN:HD3	1.30	0.97
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.80	0.95
2:D:222:GLN:H	2:D:222:GLN:HE21	1.05	0.94
1:A:682:VAL:HG11	1:A:689:GLN:HE21	1.33	0.93
2:B:261:THR:HG21	2:B:263:ILE:HG13	1.49	0.92
1:A:710:TYR:HA	1:A:712:LEU:HD12	1.50	0.92
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.50	0.92
1:G:1001:ILE:HD13	1:G:1029:ILE:HB	1.51	0.91
1:G:1027:ARG:NH1	1:G:1031:ARG:HD2	1.85	0.91
2:H:324:ASN:HD22	2:H:324:ASN:H	1.17	0.90
1:G:708:ILE:HG23	1:G:754:HIS:HB2	1.52	0.90
1:G:1063:ILE:HD13	1:G:1068:MET:HG3	1.51	0.90
1:E:571:ARG:HH21	1:E:645[B]:GLN:HE21	1.16	0.89
1:A:554:ASN:ND2	8:A:5014:ORN:HD3	1.87	0.89
1:G:1001:ILE:CD1	1:G:1029:ILE:HB	2.03	0.89
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.54	0.89
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.09	0.88
2:H:322:PRO:CB	2:H:324:ASN:HD21	1.85	0.88
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.08	0.88
1:A:784:GLN:HE21	1:A:784:GLN:H	1.21	0.87
2:H:342:ARG:HH11	2:H:342:ARG:HG3	1.39	0.87
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.54	0.87
2:H:150:PHE:CD1	2:H:151:PRO:HD2	2.09	0.87
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.56	0.86
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.90	0.86
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.10	0.85
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.04	0.85
2:F:322:PRO:HG2	2:F:324:ASN:HD21	1.39	0.84
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.58	0.84
2:B:261:THR:HG22	2:B:263:ILE:H	1.43	0.83
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.13	0.83
10:E:5053:NET:H42	10:E:5053:NET:H22	1.61	0.83
1:G:708:ILE:CG2	1:G:712:LEU:HD11	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1001:ILE:CD1	1:E:1029:ILE:HB	2.09	0.82
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.61	0.82
1:E:784:GLN:HE21	1:E:784:GLN:H	1.25	0.82
2:D:228:VAL:HA	2:D:231:MET:HE2	1.59	0.81
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.62	0.81
2:H:324:ASN:HD22	2:H:324:ASN:N	1.75	0.81
2:H:7:LEU:HD23	2:H:15:PHE:CD1	2.16	0.81
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.46	0.81
2:B:261:THR:CG2	2:B:263:ILE:H	1.95	0.80
1:E:1001:ILE:HG13	1:E:1002:GLN:N	1.95	0.80
2:B:286:MET:HE1	2:B:315:ALA:HB2	1.64	0.79
1:C:784:GLN:H	1:C:784:GLN:HE21	1.31	0.79
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.65	0.79
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.65	0.79
1:E:228:CYS:O	1:E:269:MET:HE1	1.82	0.79
2:H:228:VAL:HG11	2:H:258:PHE:CE1	2.18	0.79
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.65	0.78
2:F:215:ARG:HG3	2:F:215:ARG:HH11	1.49	0.78
2:F:236:ILE:HB	2:F:265:VAL:HG22	1.64	0.78
1:E:6:ASP:OD1	1:E:7:ILE:HG13	1.83	0.78
1:A:225:ASN:ND2	1:A:331:THR:HG21	1.99	0.78
1:A:784:GLN:NE2	1:A:784:GLN:H	1.80	0.78
2:H:236:ILE:HD12	2:H:263:ILE:CG2	2.14	0.77
2:D:370:PHE:O	2:D:374:ILE:HG13	1.84	0.77
1:E:1020:ARG:HH21	1:E:1023:ILE:HG21	1.50	0.77
1:E:679:GLN:O	1:E:683:GLU:HG3	1.84	0.77
1:G:769:ASP:HB3	1:G:874:LEU:HD12	1.66	0.77
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.68	0.76
2:H:133:ILE:HD12	2:H:143:ALA:CB	2.12	0.76
1:C:905:PRO:HB2	1:C:1040:TYR:OH	1.85	0.76
2:H:321:LEU:HD23	2:H:325:LEU:O	1.86	0.76
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.51	0.76
1:A:313:LYS:HE2	1:A:608:THR:O	1.84	0.76
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.68	0.76
1:C:845:ARG:HG3	1:C:845:ARG:HH11	1.50	0.76
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.14	0.76
1:E:872:LYS:HD3	1:E:877:GLN:HG2	1.67	0.76
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.20	0.76
2:F:300:VAL:HG22	2:F:328:THR:O	1.87	0.75
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.67	0.75
1:G:480:GLY:HA3	11:G:5615:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:LYS:HE3	11:E:5750:HOH:O	1.86	0.75
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.68	0.75
1:E:1020:ARG:NH2	1:E:1023:ILE:HG21	2.02	0.75
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.51	0.75
1:C:318:PRO:HG3	1:C:610:TYR:OH	1.87	0.75
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.67	0.74
1:E:79:GLU:O	1:E:82[B]:ARG:NH1	2.18	0.74
1:E:151:THR:OG1	1:E:154:GLU:HG3	1.87	0.74
1:C:873:SER:O	1:C:877:GLN:HG3	1.86	0.74
2:D:222:GLN:N	2:D:222:GLN:HE21	1.85	0.74
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.68	0.74
1:G:708:ILE:HG22	1:G:712:LEU:HD11	1.69	0.74
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.23	0.73
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.87	0.73
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.87	0.73
1:A:130[B]:ARG:NH1	1:A:130[B]:ARG:HD2	2.03	0.73
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.70	0.73
2:H:367:PHE:O	2:H:371:ILE:HG12	1.88	0.73
2:H:209:LEU:HD22	2:H:216:LEU:CD2	2.18	0.73
1:E:905:PRO:HB2	1:E:1040:TYR:OH	1.89	0.72
2:H:186:LYS:O	2:H:189:GLU:HB2	1.89	0.72
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.88	0.72
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.72	0.72
1:G:4:ARG:HD3	1:G:7:ILE:HD12	1.70	0.72
2:B:38:GLY:HA3	2:B:358:PRO:HB3	1.69	0.72
1:A:130[B]:ARG:NH2	1:A:130[B]:ARG:NE	2.38	0.72
1:E:873:SER:O	1:E:877:GLN:HG3	1.89	0.72
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.54	0.72
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.71	0.72
2:H:32:PHE:O	2:H:291:HIS:HB2	1.90	0.71
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.90	0.71
2:H:313:GLY:HA3	11:H:3579:HOH:O	1.90	0.71
2:H:74:GLN:HB3	11:H:3855:HOH:O	1.90	0.71
1:G:784:GLN:NE2	1:G:784:GLN:H	1.87	0.71
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.15	0.71
2:H:369:HIS:O	2:H:373:LEU:HG	1.90	0.71
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.90	0.71
1:A:1054:LEU:HD23	11:A:5359:HOH:O	1.90	0.71
1:G:810:ARG:HG3	1:G:810:ARG:HH11	1.54	0.71
2:H:275:LEU:O	2:H:279:SER:HB2	1.91	0.71
1:G:921:GLY:HA3	1:G:926:GLU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLU:HB2	2:B:117:LYS:HD2	1.72	0.71
2:B:322:PRO:HB2	2:B:324:ASN:ND2	2.05	0.70
1:E:563:MET:CE	1:E:635:PRO:HG3	2.21	0.70
2:H:205:ILE:HG12	2:H:355:GLU:HG3	1.74	0.70
1:C:975:HIS:HD1	1:E:975:HIS:HD1	0.81	0.70
2:F:322:PRO:CG	2:F:324:ASN:HD21	2.03	0.70
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.21	0.70
1:A:1069:HIS:HA	1:A:1072:ILE:HD12	1.74	0.70
2:H:342:ARG:HB2	2:H:347:ALA:HB3	1.74	0.70
1:E:313:LYS:HE2	1:E:608:THR:O	1.91	0.70
1:A:475:LYS:O	1:A:479:VAL:HG22	1.92	0.70
1:A:873:SER:O	1:A:877:GLN:HG3	1.91	0.70
1:C:696:THR:HB	1:C:700:MET:SD	2.32	0.70
1:E:139:ILE:HD11	1:E:141:LEU:HD12	1.72	0.70
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.55	0.70
1:E:150:HIS:ND1	11:E:5507:HOH:O	2.25	0.69
1:C:482:THR:HG23	11:C:5556:HOH:O	1.92	0.69
1:E:685:LEU:HD22	1:E:815:LYS:HB3	1.72	0.69
1:C:860:PRO:HB2	1:C:863:LYS:HG3	1.74	0.69
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.93	0.69
2:H:173:GLY:O	2:H:207:ARG:HG2	1.92	0.69
2:H:41:GLU:HB3	2:H:358:PRO:HD3	1.74	0.69
1:G:860:PRO:O	1:G:864:VAL:HG23	1.92	0.69
2:F:313:GLY:HA3	11:F:3076:HOH:O	1.92	0.69
1:E:1026:SER:O	1:E:1029:ILE:HG22	1.93	0.69
1:G:365:GLU:HG2	1:G:366:LYS:N	2.07	0.69
1:G:784:GLN:HE21	1:G:784:GLN:H	1.40	0.69
2:H:193:HIS:NE2	2:H:217:THR:HB	2.08	0.69
1:A:358:LYS:HE3	11:A:5399:HOH:O	1.92	0.69
1:E:222[B]:ARG:NH2	1:E:278:GLU:HG2	2.07	0.69
2:H:369:HIS:CE1	2:H:373:LEU:HD21	2.28	0.69
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.20	0.69
1:A:1:MET:HB3	1:A:224:LYS:CE	2.23	0.68
2:B:173:GLY:O	2:B:207:ARG:HG2	1.93	0.68
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.08	0.68
2:H:222:GLN:H	2:H:222:GLN:HE21	1.41	0.68
1:G:873:SER:O	1:G:877:GLN:HG3	1.93	0.68
2:H:361:HIS:HA	11:H:3881:HOH:O	1.93	0.68
1:A:702:VAL:HG13	1:A:731:GLU:HG3	1.76	0.68
1:G:1021:ARG:HH11	1:G:1021:ARG:HG2	1.58	0.68
2:F:279:SER:O	2:F:322:PRO:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:O	1:A:471:ARG:HG2	1.92	0.68
1:C:930:LYS:HE3	11:C:5088:HOH:O	1.93	0.68
1:E:728:VAL:HG13	1:E:733:ASP:CB	2.08	0.68
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.59	0.68
1:E:554:ASN:HD22	8:E:5054:ORN:HD3	1.59	0.68
1:E:761:GLU:HB3	1:E:781:HIS:ND1	2.09	0.68
2:D:215:ARG:HH11	2:D:215:ARG:HG3	1.59	0.68
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.28	0.68
1:C:865:ALA:O	1:C:869:MET:HG3	1.94	0.67
1:G:708:ILE:HG21	1:G:712:LEU:HD11	1.75	0.67
2:B:46:PRO:HA	2:B:76:HIS:CG	2.30	0.67
1:E:1001:ILE:HG13	1:E:1002:GLN:H	1.56	0.67
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.77	0.67
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.12	0.67
1:G:154:GLU:O	1:G:158:VAL:HG23	1.94	0.67
1:G:699:GLU:HA	1:G:702:VAL:CG2	2.24	0.67
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.76	0.67
1:C:313:LYS:HE2	1:C:608:THR:O	1.94	0.67
1:E:751:LEU:O	1:E:752:LEU:HD12	1.94	0.67
2:B:353:HIS:HB3	2:B:355:GLU:OE1	1.95	0.67
1:G:947:LEU:N	1:G:947:LEU:HD12	2.09	0.67
2:H:83:ARG:HD2	2:H:83:ARG:O	1.95	0.67
1:E:891:LYS:NZ	11:E:5694:HOH:O	2.28	0.67
2:F:370:PHE:O	2:F:374:ILE:HG13	1.94	0.67
2:F:369:HIS:O	2:F:373:LEU:HG	1.95	0.67
2:B:186:LYS:O	2:B:189:GLU:HB2	1.95	0.66
2:F:324:ASN:HD22	2:F:324:ASN:N	1.90	0.66
1:C:679:GLN:O	1:C:683:GLU:HG3	1.95	0.66
1:E:158:VAL:HG11	1:E:206:ILE:HB	1.77	0.66
1:E:667:ASP:OD1	1:E:677:ARG:NH2	2.28	0.66
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.59	0.66
1:G:1057:ASP:HB3	1:G:1060:GLU:HB2	1.77	0.66
1:G:525:VAL:HG22	1:G:548:GLU:H	1.60	0.66
1:A:1063:ILE:HD13	1:A:1068:MET:HG3	1.78	0.66
1:G:509:ARG:HB2	1:G:512:GLU:HG3	1.77	0.66
1:C:698:ILE:H	1:C:698:ILE:HD12	1.61	0.66
1:E:652[B]:ARG:HG3	11:E:5628:HOH:O	1.94	0.66
2:F:23:THR:HG23	2:F:134:ALA:O	1.96	0.66
2:H:342:ARG:NH1	2:H:342:ARG:HG3	2.06	0.66
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.78	0.66
1:E:998:ARG:HB3	1:E:999:PRO:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:ILE:HG12	2:H:377:TYR:OH	1.96	0.66
1:G:17:PRO:HG3	1:G:917:VAL:CG1	2.26	0.66
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.18	0.66
1:G:464:VAL:HG21	2:H:88:ILE:HG12	1.78	0.65
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.23	0.65
2:H:40:GLN:NE2	2:H:66:ASN:O	2.28	0.65
2:B:299:ASP:O	2:B:303:ASN:N	2.30	0.65
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.12	0.65
1:G:559:ARG:HH11	1:G:595:GLU:HA	1.61	0.65
1:E:715:ARG:CG	1:E:725:MET:HE1	2.26	0.65
1:A:696:THR:HB	1:A:700:MET:SD	2.36	0.65
1:A:708:ILE:CG2	1:A:754:HIS:HB2	2.26	0.65
1:G:666:PRO:HA	1:G:669:ILE:HD12	1.79	0.65
1:G:43:ARG:NH2	1:G:81:GLU:OE1	2.30	0.65
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.26	0.65
2:B:261:THR:CG2	2:B:263:ILE:HG13	2.25	0.65
1:E:947:LEU:N	1:E:947:LEU:HD12	2.12	0.65
1:G:833:LYS:O	1:G:836:GLU:HB2	1.96	0.65
1:G:930:LYS:NZ	1:G:1058:ALA:O	2.30	0.65
2:H:266:PHE:HB2	2:H:370:PHE:CD1	2.31	0.65
1:E:863:LYS:HE2	11:E:5733:HOH:O	1.95	0.65
2:H:247:PRO:O	2:H:249:ASP:N	2.30	0.65
1:A:112:GLY:HA2	11:A:5423:HOH:O	1.95	0.65
1:G:648:LEU:HD13	1:G:845:ARG:HD3	1.78	0.65
2:H:60:ILE:HB	2:H:82:ILE:HD13	1.79	0.65
2:B:190:LEU:O	2:B:215[B]:ARG:NH2	2.29	0.65
1:E:784:GLN:HE21	1:E:784:GLN:N	1.94	0.65
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.78	0.65
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.77	0.65
1:C:321:LYS:NZ	1:C:611:ASP:OD2	2.29	0.65
1:G:1027:ARG:HH11	1:G:1031:ARG:HD2	1.60	0.65
2:H:123:ARG:HA	2:H:288:PHE:CD2	2.32	0.65
2:H:321:LEU:HD23	2:H:325:LEU:HB3	1.79	0.65
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.43	0.64
1:A:9:SER:OG	1:A:83:PRO:HA	1.98	0.64
1:C:715:ARG:NH2	7:C:5027:ADP:O1A	2.30	0.64
1:C:523:HIS:HB3	1:C:524:PRO:HD2	1.78	0.64
2:F:38:GLY:HA3	2:F:358:PRO:HB3	1.80	0.64
1:A:426:ARG:HD2	1:A:426:ARG:C	2.18	0.64
1:C:784:GLN:H	1:C:784:GLN:NE2	1.95	0.64
1:E:417:ASP:OD2	1:E:423:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:THR:HG22	1:C:423:LYS:HG3	1.79	0.64
2:D:182:PRO:HB2	11:D:1950:HOH:O	1.96	0.64
1:G:331:THR:OG1	1:G:334:GLU:HG3	1.97	0.64
1:A:844:PRO:HD2	11:A:5463:HOH:O	1.97	0.64
1:C:1026:SER:O	1:C:1029:ILE:HG22	1.97	0.64
1:E:1000:HIS:CD2	1:E:1002:GLN:HB3	2.33	0.64
1:G:1027:ARG:HH12	1:G:1031:ARG:HD2	1.63	0.64
1:A:671:ARG:HD3	11:A:5564:HOH:O	1.98	0.64
2:B:272:HIS:ND1	2:B:349:SER:OG	2.30	0.64
1:C:708:ILE:CG2	1:C:754:HIS:HB2	2.27	0.64
2:F:205:ILE:HG21	2:F:237:PHE:CZ	2.32	0.64
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.15	0.64
1:A:228:CYS:SG	1:A:269:MET:HG2	2.37	0.64
1:E:715:ARG:NH2	7:E:5047:ADP:O1A	2.29	0.64
1:E:959:ASP:O	1:E:963:LYS:HG3	1.97	0.64
2:F:252:ILE:O	2:F:256:GLN:HG3	1.97	0.64
2:F:286:MET:HE2	2:F:314:PHE:O	1.98	0.64
2:H:334:ASP:OD1	2:H:336:THR:HG23	1.98	0.64
1:E:1073:LYS:HD2	1:E:1073:LYS:N	2.13	0.64
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.80	0.63
1:E:903:VAL:O	1:E:905:PRO:HD3	1.99	0.63
1:E:998:ARG:CB	1:E:999:PRO:HA	2.27	0.63
1:E:685:LEU:HD11	1:E:819:GLU:HG2	1.81	0.63
2:B:335:GLY:HA2	11:B:5198:HOH:O	1.96	0.63
1:E:8:LYS:HE3	11:E:5452:HOH:O	1.99	0.63
2:H:324:ASN:O	2:H:342:ARG:HD2	1.98	0.63
2:H:264:PRO:HD3	2:H:377:TYR:CD1	2.34	0.63
1:C:704:LYS:O	1:C:707:GLU:HB2	1.98	0.63
2:F:225:ALA:O	2:F:229:LEU:HG	1.98	0.63
2:B:45:ASP:HB3	2:B:48:TYR:HD2	1.64	0.63
1:C:1024:GLU:HG3	11:C:5748:HOH:O	1.98	0.63
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.79	0.63
2:F:322:PRO:HG2	2:F:324:ASN:ND2	2.13	0.63
1:G:769:ASP:CB	1:G:874:LEU:HD12	2.29	0.63
1:G:954:LYS:O	1:G:957:VAL:HG12	1.99	0.63
2:H:363:ALA:C	2:H:365:PRO:HD2	2.19	0.63
1:A:154:GLU:HA	11:A:5142:HOH:O	1.99	0.63
1:A:289:ASN:OD1	1:A:290:PRO:HD2	1.98	0.63
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.33	0.63
1:E:535:GLU:HG2	1:E:536:PHE:CE2	2.34	0.62
1:E:571:ARG:HH21	1:E:645[B]:GLN:NE2	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:PRO:HA	2:F:76:HIS:CG	2.33	0.62
1:E:267:ALA:O	1:E:271:VAL:HG23	1.99	0.62
2:D:228:VAL:HA	2:D:231:MET:CE	2.30	0.62
1:A:930:LYS:HE3	11:A:5068:HOH:O	1.99	0.62
1:G:130:ARG:HG3	1:G:148:ILE:HG13	1.81	0.62
2:H:248:CYS:O	2:H:252:ILE:HG13	1.99	0.62
2:B:218:ILE:N	2:B:218:ILE:HD13	2.13	0.62
2:B:273:GLN:NE2	2:B:314:PHE:O	2.32	0.62
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.81	0.62
1:C:1:MET:HA	1:C:224:LYS:CE	2.30	0.62
1:C:59:GLU:HG3	1:C:60:MET:HE2	1.82	0.62
1:C:698:ILE:HG13	1:C:738:PHE:CD2	2.34	0.62
1:A:1026:SER:O	1:A:1029:ILE:HG22	1.99	0.62
2:B:255:ILE:HA	2:B:258:PHE:CD2	2.35	0.62
1:E:363:ASN:ND2	1:E:365:GLU:OE2	2.31	0.62
1:G:715:ARG:NH2	7:G:5067:ADP:O1A	2.32	0.62
2:H:41:GLU:HB2	2:H:358:PRO:HG3	1.80	0.62
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.45	0.62
2:H:224:SER:OG	2:H:226:GLU:HB2	1.99	0.62
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.35	0.61
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.64	0.61
2:H:34:THR:HA	2:H:56:THR:OG1	2.00	0.61
1:A:654:LEU:O	1:A:659:VAL:HG23	2.00	0.61
1:C:353:ASP:OD2	2:D:116:ARG:HD2	1.99	0.61
1:C:695:VAL:CG1	1:C:701:ALA:HB2	2.21	0.61
1:E:418:PRO:HD2	11:E:5587:HOH:O	2.00	0.61
1:E:795:SER:HB2	1:E:890:VAL:HG22	1.82	0.61
1:G:805:ILE:HG22	1:G:806:GLN:N	2.15	0.61
1:C:698:ILE:N	1:C:698:ILE:HD12	2.16	0.61
1:G:596:THR:O	1:G:614:ASP:HB2	2.01	0.61
2:B:71:GLU:O	2:B:203:ARG:HG3	1.99	0.61
2:H:281:ALA:HA	2:H:320:THR:O	2.01	0.61
1:A:145:ARG:HH12	1:A:161:ASP:CG	2.04	0.61
1:A:426:ARG:HD3	11:A:5504:HOH:O	2.00	0.61
2:B:299:ASP:HB3	2:B:304:VAL:HG22	1.81	0.61
2:F:364:ALA:N	2:F:365:PRO:HD2	2.15	0.61
1:E:460:ARG:HG3	11:E:5326:HOH:O	2.01	0.61
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.00	0.61
1:G:699:GLU:HA	1:G:702:VAL:HG21	1.82	0.61
1:G:678:PHE:CZ	1:G:842:VAL:HG23	2.35	0.61
2:H:193:HIS:O	2:H:234:ASP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:ILE:HD13	1:C:1029:ILE:HB	1.83	0.61
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.36	0.61
1:G:1:MET:HG3	1:G:225:ASN:HD21	1.66	0.61
1:G:704:LYS:O	1:G:707:GLU:HB2	2.01	0.61
2:H:266:PHE:HD2	2:H:370:PHE:CD2	2.18	0.61
2:D:222:GLN:H	2:D:222:GLN:NE2	1.88	0.61
1:C:863:LYS:O	1:C:867:ARG:HG3	2.00	0.60
1:E:43:ARG:NH2	1:E:81:GLU:OE1	2.29	0.60
1:A:998:ARG:HG2	1:A:1003:ASP:OD2	2.00	0.60
1:A:1001:ILE:HD13	1:A:1029:ILE:HB	1.82	0.60
1:A:682:VAL:HG11	1:A:689:GLN:NE2	2.11	0.60
1:C:35:LYS:O	1:C:39:GLU:HB2	2.00	0.60
1:G:950:ARG:HG3	1:G:1016:THR:OG1	2.02	0.60
1:G:24:CYS:HB2	1:G:604:GLU:HB3	1.84	0.60
1:G:9:SER:N	1:G:84:ASP:OD2	2.32	0.60
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.36	0.60
2:H:240:ASN:HA	2:H:270:LEU:H	1.67	0.60
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.82	0.60
2:H:374:ILE:O	2:H:377:TYR:HB3	2.01	0.60
2:B:353:HIS:HB3	2:B:355:GLU:CD	2.22	0.60
2:F:34:THR:HA	2:F:56:THR:OG1	2.01	0.60
2:H:33:ASN:HA	2:H:291:HIS:O	2.01	0.60
2:B:150:PHE:CD1	2:B:151:PRO:HD2	2.37	0.60
1:G:644:GLY:O	1:G:647:PRO:HD2	2.01	0.60
1:G:67:GLU:HB3	1:G:68:PRO:HD2	1.82	0.60
2:H:197:TYR:HA	2:H:219:VAL:HG22	1.84	0.60
2:H:365:PRO:HA	2:H:368:ASP:OD2	2.01	0.60
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.84	0.60
1:G:780:GLU:OE2	1:G:800:THR:HG23	2.02	0.60
2:H:144:LEU:O	2:H:148:ARG:HG3	2.01	0.60
1:A:583:VAL:O	1:A:587:LEU:HG	2.00	0.60
1:E:1:MET:HA	1:E:224:LYS:CE	2.32	0.60
1:G:40:GLU:HG2	1:G:325:LYS:HE2	1.84	0.60
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.83	0.60
2:B:11:ASP:OD1	2:B:13:THR:HB	2.02	0.59
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.23	0.59
2:D:26:ALA:O	2:D:131:CYS:HA	2.02	0.59
1:G:417:ASP:OD2	1:G:423:LYS:NZ	2.28	0.59
2:H:73:SER:HA	2:H:203:ARG:NH2	2.16	0.59
2:H:286:MET:HB2	2:H:313:GLY:O	2.03	0.59
1:A:679:GLN:O	1:A:683:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:HG2	1:C:296:ILE:HG12	1.84	0.59
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.37	0.59
2:D:298:LYS:HB2	2:D:332:LEU:HD11	1.84	0.59
2:F:324:ASN:H	2:F:324:ASN:HD22	1.50	0.59
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.67	0.59
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.03	0.59
1:G:1:MET:CG	1:G:225:ASN:HD21	2.15	0.59
2:H:322:PRO:O	2:H:325:LEU:N	2.35	0.59
2:H:46:PRO:HG2	2:H:201:ALA:O	2.03	0.59
1:A:698:ILE:O	1:A:702:VAL:HG23	2.03	0.59
1:A:710:TYR:HA	1:A:712:LEU:CD1	2.26	0.59
1:E:757:ASP:HB2	11:E:5978:HOH:O	2.03	0.59
1:E:941[A]:LYS:NZ	11:E:5448:HOH:O	2.32	0.59
1:G:883:VAL:C	1:G:884:ILE:HG12	2.23	0.59
2:H:142:LEU:O	2:H:146:LYS:HG3	2.02	0.59
2:H:228:VAL:HG11	2:H:258:PHE:CZ	2.38	0.59
2:H:263:ILE:HA	2:H:377:TYR:CE1	2.38	0.59
1:A:1000:HIS:CD2	1:A:1002:GLN:HB3	2.38	0.59
2:B:205:ILE:O	2:B:209:LEU:HG	2.02	0.59
2:B:192:PHE:O	2:B:215[B]:ARG:HG2	2.03	0.59
2:B:365:PRO:HA	2:B:368:ASP:OD2	2.02	0.59
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.37	0.59
1:G:623:LEU:O	1:G:627:LEU:HG	2.03	0.59
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.03	0.59
2:H:208:MET:SD	2:H:355:GLU:HA	2.42	0.59
1:A:682:VAL:CG1	1:A:689:GLN:HE21	2.10	0.58
1:A:349:GLU:O	2:B:294:ASN:HB2	2.02	0.58
2:H:142:LEU:HD12	2:H:142:LEU:O	2.03	0.58
1:A:130[B]:ARG:NH1	1:A:130[B]:ARG:CD	2.66	0.58
2:B:326:ARG:O	2:B:326:ARG:HG3	2.01	0.58
1:E:1004:ARG:O	1:E:1009[B]:GLU:HG3	2.03	0.58
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.38	0.58
1:G:998:ARG:CB	1:G:999:PRO:HA	2.33	0.58
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.15	0.58
1:G:423:LYS:HB3	11:G:5599:HOH:O	2.04	0.58
1:G:698:ILE:O	1:G:702:VAL:HG23	2.03	0.58
2:H:249:ASP:OD1	2:H:249:ASP:N	2.28	0.58
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.85	0.58
1:E:954:LYS:NZ	9:E:5052:IMP:O3P	2.29	0.58
1:E:715:ARG:NE	1:E:725:MET:HE1	2.19	0.58
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ARG:O	1:A:738:PHE:N	2.36	0.58
1:C:728:VAL:HG13	1:C:733:ASP:HB3	1.86	0.58
1:G:550:GLU:OE1	2:H:120:ARG:NH2	2.30	0.58
1:G:563:MET:CE	1:G:635:PRO:HG3	2.34	0.58
1:G:751:LEU:O	1:G:752:LEU:HD13	2.03	0.58
1:G:765:ASP:OD1	1:G:827:ASN:ND2	2.30	0.58
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.35	0.58
2:F:224:SER:OG	2:F:227:ASP:HB2	2.02	0.58
2:F:334:ASP:OD1	2:F:336:THR:HG23	2.03	0.58
2:H:78:GLN:NE2	2:H:78:GLN:HA	2.19	0.58
1:A:780:GLU:HG2	1:A:799:TYR:CE1	2.38	0.58
1:G:167:ILE:HD12	1:G:167:ILE:N	2.19	0.58
1:G:225:ASN:ND2	1:G:331:THR:HG21	2.18	0.58
1:A:674:ASP:HB3	1:A:677:ARG:HB2	1.85	0.57
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.86	0.57
1:C:561:LYS:HE2	11:C:5569:HOH:O	2.04	0.57
1:E:704:LYS:O	1:E:707:GLU:HB2	2.04	0.57
1:G:223:ASP:OD1	1:G:227:ASN:HB2	2.04	0.57
2:B:286:MET:CE	2:B:315:ALA:HB2	2.34	0.57
2:B:66:ASN:HB3	2:B:93:ARG:O	2.04	0.57
1:C:426:ARG:C	1:C:426:ARG:HD3	2.24	0.57
1:C:951:GLU:O	1:C:954:LYS:HB2	2.04	0.57
2:H:236:ILE:CD1	2:H:263:ILE:HG21	2.28	0.57
2:D:244:ASP:OD1	2:D:245:PRO:HD2	2.05	0.57
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.86	0.57
2:B:232:ASN:N	2:B:233:PRO:HD3	2.20	0.57
2:B:279:SER:O	2:B:322:PRO:HG3	2.04	0.57
2:H:133:ILE:CG2	2:H:138:PRO:HB3	2.34	0.57
1:C:730:ASP:OD1	1:C:733:ASP:HB2	2.04	0.57
2:D:150:PHE:CD1	2:D:151:PRO:HD2	2.39	0.57
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.85	0.57
1:G:9:SER:OG	1:G:83:PRO:HA	2.04	0.57
1:C:906:LEU:HD13	1:C:1030:ARG:CD	2.34	0.57
2:H:244:ASP:OD1	2:H:245:PRO:HD2	2.05	0.57
1:A:740:THR:HG22	1:A:741:ALA:N	2.20	0.57
2:H:228:VAL:HA	2:H:231:MET:CE	2.35	0.57
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.87	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.85	0.57
2:B:324:ASN:O	2:B:342:ARG:HD2	2.05	0.57
1:E:153:GLU:HB3	11:E:5512:HOH:O	2.05	0.57
1:G:591:GLU:HG3	1:G:591:GLU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:679:GLN:HG2	1:G:683:GLU:OE1	2.04	0.57
1:G:708:ILE:CG2	1:G:754:HIS:HB2	2.28	0.57
1:G:490:ARG:HD3	11:G:5750:HOH:O	2.04	0.57
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.85	0.57
1:E:726:GLU:HG2	1:E:727:ILE:N	2.19	0.57
2:H:232:ASN:N	2:H:233:PRO:HD3	2.19	0.57
2:H:342:ARG:NH2	2:H:344:ASP:OD2	2.37	0.57
1:A:51:PRO:HG3	1:A:918:MET:HB2	1.86	0.56
1:G:118:ALA:HA	11:G:5712:HOH:O	2.05	0.56
1:G:218:MET:HE3	1:G:264:MET:HB3	1.87	0.56
1:G:998:ARG:HB3	1:G:999:PRO:HA	1.87	0.56
1:G:905:PRO:HB2	1:G:1040:TYR:HH	1.69	0.56
1:G:704:LYS:O	1:G:708:ILE:HD12	2.05	0.56
1:C:698:ILE:H	1:C:698:ILE:CD1	2.18	0.56
2:F:157:ASP:OD2	11:F:3087:HOH:O	2.17	0.56
2:F:164:THR:O	2:F:220:PRO:HG3	2.06	0.56
1:C:51:PRO:HG3	1:C:918:MET:HB2	1.87	0.56
2:F:215:ARG:NH1	2:F:215:ARG:HG3	2.18	0.56
2:D:71:GLU:O	2:D:203:ARG:HG3	2.05	0.56
2:H:286:MET:N	2:H:313:GLY:O	2.27	0.56
1:A:412:LYS:HG2	1:A:438:TYR:CZ	2.41	0.56
1:G:185:ARG:NH2	11:G:5523:HOH:O	2.38	0.56
1:E:644:GLY:O	1:E:647:PRO:HD2	2.06	0.56
1:G:682:VAL:HG11	1:G:689:GLN:HE21	1.71	0.56
1:A:651:ALA:HB3	11:A:5560:HOH:O	2.05	0.56
1:A:954:LYS:O	1:A:957:VAL:HG12	2.06	0.56
1:C:525:VAL:HB	1:C:551:CYS:HA	1.87	0.56
1:C:757:ASP:O	1:C:833:LYS:HE3	2.05	0.56
2:F:286:MET:HE3	2:F:313:GLY:C	2.26	0.56
1:G:267:ALA:O	1:G:271:VAL:HG23	2.05	0.56
1:G:410:ASP:OD1	1:G:501:ARG:NH1	2.39	0.56
1:G:79:GLU:O	1:G:82:ARG:NE	2.38	0.56
1:C:481:ILE:HG13	1:C:481:ILE:O	2.06	0.56
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.06	0.56
2:H:206:LEU:O	2:H:210:VAL:HG23	2.06	0.56
1:C:548:GLU:OE2	2:D:114:ASP:HA	2.06	0.56
1:E:716:PRO:HA	1:E:750:VAL:HG22	1.87	0.56
1:A:1:MET:HB3	1:A:224:LYS:HE3	1.87	0.56
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.86	0.56
1:C:954:LYS:O	1:C:957:VAL:HG12	2.06	0.56
1:C:9:SER:OG	1:C:83:PRO:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82[B]:ARG:HE	1:E:111:PHE:HD1	1.52	0.56
1:G:998:ARG:HA	1:G:999:PRO:C	2.26	0.56
1:C:349:GLU:O	2:D:294:ASN:HB2	2.06	0.55
1:C:494:ARG:HG3	1:C:547:TYR:HB3	1.88	0.55
1:C:967:GLN:HG3	1:C:1054:LEU:CD1	2.33	0.55
1:G:559:ARG:HD2	1:G:595:GLU:HB2	1.89	0.55
1:G:698:ILE:N	1:G:698:ILE:HD12	2.20	0.55
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.89	0.55
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.36	0.55
1:C:905:PRO:HB2	1:C:1040:TYR:HH	1.71	0.55
1:E:228:CYS:C	1:E:269:MET:HE1	2.27	0.55
2:H:228:VAL:HG12	2:H:229:LEU:N	2.15	0.55
1:A:514:ARG:HD3	11:A:5539:HOH:O	2.06	0.55
2:B:45:ASP:HB3	2:B:48:TYR:CD2	2.41	0.55
1:G:850:VAL:O	1:G:854:SER:N	2.37	0.55
1:A:970:GLU:O	1:A:971:LEU:HD23	2.07	0.55
2:B:299:ASP:HB3	2:B:304:VAL:CG2	2.37	0.55
1:C:630:VAL:HG11	1:C:659:VAL:HG22	1.87	0.55
1:E:38:ARG:HG2	11:E:5462:HOH:O	2.06	0.55
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.41	0.55
1:G:907:LEU:HD11	8:G:5071:ORN:HD3	1.89	0.55
2:B:290:HIS:NE2	2:B:334:ASP:OD2	2.36	0.55
1:E:1020:ARG:HH21	1:E:1023:ILE:CG2	2.19	0.55
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.88	0.55
1:A:184:ASN:OD1	1:A:187:GLU:HG3	2.07	0.55
1:C:845:ARG:NH1	1:C:845:ARG:HG3	2.21	0.55
1:G:436:ILE:HG22	11:G:5277:HOH:O	2.07	0.55
1:G:554:ASN:ND2	8:G:5074:ORN:HD3	2.12	0.55
2:H:344:ASP:C	2:H:345:LYS:HG2	2.25	0.55
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.88	0.55
2:F:41:GLU:HB3	2:F:358:PRO:HD3	1.88	0.55
1:G:417:ASP:OD1	1:G:418:PRO:HD2	2.06	0.55
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.37	0.55
2:H:252:ILE:HD13	2:H:277:LEU:HB3	1.89	0.55
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.88	0.54
1:G:135:ALA:HB1	1:G:274:GLU:CG	2.37	0.54
1:G:10:ILE:HD12	1:G:42:TYR:HB3	1.89	0.54
2:H:265:VAL:HG12	2:H:347:ALA:HA	1.89	0.54
1:A:730:ASP:OD1	1:A:733:ASP:HB2	2.07	0.54
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.07	0.54
1:E:563:MET:HE1	1:E:635:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:GLU:HB3	11:G:5520:HOH:O	2.05	0.54
1:A:646:THR:HB	1:A:647:PRO:HD3	1.89	0.54
1:C:1027:ARG:HD3	1:C:1031:ARG:HD3	1.88	0.54
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.88	0.54
1:A:702:VAL:CG1	1:A:731:GLU:HG3	2.37	0.54
2:B:228:VAL:O	2:B:231:MET:HB2	2.07	0.54
2:F:251:ALA:O	2:F:255:ILE:HD12	2.07	0.54
1:G:1026:SER:O	1:G:1029:ILE:HG22	2.07	0.54
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.88	0.54
1:A:343:ARG:NH2	1:A:539:ASP:OD2	2.40	0.54
1:C:490:ARG:HG3	1:C:522:LEU:HD13	1.88	0.54
1:E:419:GLU:O	1:E:422:THR:HB	2.07	0.54
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.08	0.54
1:G:710:TYR:OH	1:G:731:GLU:HA	2.08	0.54
2:H:259:LEU:HD22	2:H:342:ARG:NH1	2.22	0.54
1:A:367:PHE:HB3	1:A:903:VAL:HG21	1.88	0.54
2:D:44:THR:HG21	2:D:70:GLU:HG2	1.89	0.54
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.26	0.54
1:E:559[A]:ARG:NH1	11:E:5624:HOH:O	2.37	0.54
1:A:45:ILE:HD13	1:A:81:GLU:HB3	1.90	0.54
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.54
1:A:75:ARG:HD2	1:A:107:VAL:HG22	1.90	0.54
1:A:764:VAL:HG11	1:A:813:VAL:HG21	1.88	0.54
1:A:955:GLU:HB2	11:A:5594:HOH:O	2.07	0.54
1:C:1000:HIS:CD2	1:C:1002:GLN:HB3	2.43	0.54
1:G:259:LYS:HE2	2:H:69:ASP:OD1	2.07	0.54
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.42	0.54
2:H:321:LEU:CD2	2:H:325:LEU:HB3	2.37	0.54
2:H:46:PRO:HD3	2:H:72:SER:HB3	1.90	0.54
1:A:186:GLU:HB2	11:A:5469:HOH:O	2.08	0.54
1:A:143:THR:HA	1:A:296:ILE:HG23	1.89	0.54
1:A:637:GLY:HA2	1:A:660:PRO:O	2.08	0.54
2:B:185:LYS:NZ	11:B:5146:HOH:O	2.39	0.54
1:E:561:LYS:HB2	1:E:635:PRO:HA	1.89	0.54
2:F:324:ASN:O	2:F:342:ARG:HD2	2.07	0.54
1:G:763:ASP:HB3	1:G:779:MET:HE1	1.89	0.54
2:H:226:GLU:C	2:H:228:VAL:H	2.11	0.54
2:H:364:ALA:N	2:H:365:PRO:HD2	2.23	0.54
1:A:906:LEU:O	1:A:912:ARG:NH2	2.30	0.54
1:C:104:ARG:HH11	1:C:104:ARG:HG3	1.73	0.54
2:F:286:MET:HE1	2:F:312:HIS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:HD22	8:A:5014:ORN:CD	2.05	0.53
8:E:5051:ORN:HB3	11:E:5697:HOH:O	2.07	0.53
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.42	0.53
1:E:907:LEU:HD11	8:E:5051:ORN:HD3	1.89	0.53
1:G:1027:ARG:HG2	1:G:1027:ARG:HH11	1.73	0.53
1:G:782:ILE:N	1:G:782:ILE:HD12	2.21	0.53
1:C:4:ARG:CD	1:C:7:ILE:HD12	2.37	0.53
1:E:648:LEU:HD13	1:E:845:ARG:HD3	1.91	0.53
2:F:342:ARG:NE	2:F:344:ASP:OD1	2.39	0.53
1:G:712:LEU:HD12	1:G:754:HIS:HA	1.90	0.53
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.90	0.53
1:C:920:VAL:O	1:C:930:LYS:HD3	2.08	0.53
1:E:554:ASN:HD22	8:E:5054:ORN:CD	2.22	0.53
1:G:58:PRO:HA	1:G:1066:GLN:NE2	2.23	0.53
2:H:266:PHE:CD2	2:H:370:PHE:CD2	2.97	0.53
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.39	0.53
2:B:324:ASN:HD22	2:B:325:LEU:N	2.06	0.53
1:C:282:SER:OG	1:C:302:PRO:HA	2.09	0.53
1:C:699:GLU:HA	1:C:702:VAL:HG23	1.91	0.53
1:C:421:LEU:HD22	1:G:421:LEU:HD13	1.90	0.53
1:G:863:LYS:HE2	11:G:5696:HOH:O	2.07	0.53
1:A:146:SER:HB2	1:A:205:LEU:HD11	1.91	0.53
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.43	0.53
1:E:358:LYS:HG2	1:E:359:ILE:N	2.22	0.53
2:F:41:GLU:HB2	2:F:358:PRO:HG3	1.90	0.53
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.89	0.53
1:E:715:ARG:HG3	1:E:725:MET:HE1	1.91	0.53
1:E:757:ASP:O	1:E:833:LYS:NZ	2.35	0.53
1:G:103:GLU:HB2	1:G:108:LEU:HD12	1.90	0.53
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.09	0.53
2:H:355:GLU:OE1	2:H:355:GLU:N	2.33	0.53
1:A:868:VAL:HA	1:A:872:LYS:O	2.08	0.53
2:B:226:GLU:O	2:B:230:LYS:HG3	2.09	0.53
1:C:941:LYS:NZ	1:C:1056:ALA:O	2.33	0.53
1:C:419:GLU:O	1:C:422:THR:HG22	2.08	0.53
2:D:174:SER:O	2:D:182:PRO:HD3	2.08	0.53
1:E:509:ARG:HH11	1:E:512:GLU:HG3	1.73	0.53
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.43	0.53
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.09	0.53
1:E:343:ARG:NH1	1:E:539:ASP:OD2	2.37	0.53
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:SER:HB3	11:G:5484:HOH:O	2.08	0.53
1:G:698:ILE:O	1:G:701:ALA:HB3	2.08	0.53
1:C:104:ARG:NH2	11:C:5648:HOH:O	2.35	0.53
1:G:53:THR:O	1:G:855:LYS:NZ	2.42	0.53
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.43	0.53
1:A:167:ILE:N	1:A:167:ILE:HD12	2.24	0.52
1:A:1:MET:H2	1:A:2:PRO:CD	2.22	0.52
1:A:275:ILE:HD13	1:A:275:ILE:N	2.23	0.52
2:B:244:ASP:OD1	2:B:245:PRO:HD2	2.09	0.52
1:E:772:MET:HA	1:E:818:PHE:HZ	1.74	0.52
1:G:344:THR:OG1	11:G:5810:HOH:O	2.19	0.52
1:G:805:ILE:O	1:G:808:VAL:N	2.42	0.52
1:G:769:ASP:CG	1:G:874:LEU:HD12	2.30	0.52
2:H:274:LEU:O	2:H:277:LEU:N	2.39	0.52
1:A:1:MET:N	1:A:2:PRO:HD3	2.24	0.52
1:A:585:ALA:HB2	1:A:642:TYR:CE2	2.43	0.52
2:B:73:SER:HA	2:B:203:ARG:NH2	2.24	0.52
2:B:337:LEU:HD12	2:B:338:GLN:N	2.25	0.52
1:C:822:VAL:O	1:C:823:ARG:HD3	2.10	0.52
2:F:173:GLY:O	2:F:207:ARG:HG2	2.08	0.52
1:G:135:ALA:HB1	1:G:274:GLU:HG2	1.90	0.52
1:G:166:CYS:C	1:G:167:ILE:HD12	2.29	0.52
1:A:712:LEU:O	1:A:727:ILE:HA	2.09	0.52
2:F:186:LYS:HB3	2:F:188:ASP:OD1	2.09	0.52
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.92	0.52
2:D:225:ALA:O	2:D:228:VAL:HB	2.10	0.52
2:D:277:LEU:CD2	2:D:283:THR:HG23	2.35	0.52
1:C:907:LEU:HD11	8:C:5031:ORN:HD3	1.92	0.52
2:F:299:ASP:O	2:F:303:ASN:N	2.42	0.52
2:F:318:GLU:HA	2:F:321:LEU:HD13	1.91	0.52
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.44	0.52
1:G:679:GLN:O	1:G:682:VAL:HB	2.09	0.52
1:G:833:LYS:O	1:G:834:ASN:HB2	2.08	0.52
2:H:257:LYS:O	2:H:260:GLU:HB2	2.09	0.52
2:H:342:ARG:CB	2:H:347:ALA:HB3	2.37	0.52
1:A:680:HIS:HB3	11:A:5749:HOH:O	2.09	0.52
1:A:446:GLY:O	1:E:447:LEU:HD23	2.10	0.52
1:G:929:ALA:HB2	1:G:1053:ALA:HB1	1.90	0.52
2:D:259:LEU:HD13	2:D:342:ARG:NH1	2.25	0.52
2:F:232:ASN:N	2:F:233:PRO:HD3	2.25	0.52
1:A:849:THR:O	1:A:853:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HD11	8:A:5011:ORN:HD3	1.92	0.52
2:B:228:VAL:HA	2:B:231:MET:CE	2.40	0.52
2:B:71:GLU:OE2	2:B:357:SER:OG	2.27	0.52
1:E:571:ARG:NH2	1:E:645[B]:GLN:HE21	1.98	0.52
2:F:364:ALA:O	2:F:367:PHE:HB2	2.09	0.52
1:G:436:ILE:HG23	1:G:437:TRP:CE3	2.45	0.52
2:H:290:HIS:ND1	2:H:312:HIS:NE2	2.57	0.52
1:A:420:ALA:HA	1:A:423:LYS:HD2	1.92	0.52
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.91	0.52
2:F:144:LEU:O	2:F:148:ARG:HB2	2.10	0.52
2:H:286:MET:CE	2:H:315:ALA:HB2	2.40	0.52
2:H:295:HIS:O	2:H:308:THR:N	2.39	0.52
2:H:259:LEU:HD22	2:H:342:ARG:HH12	1.75	0.52
1:A:708:ILE:HG23	1:A:754:HIS:HB2	1.91	0.52
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.58	0.52
1:E:799:TYR:HD1	1:E:799:TYR:H	1.57	0.52
2:F:285:LYS:NZ	11:F:3075:HOH:O	2.43	0.52
1:G:634:LYS:N	1:G:635:PRO:HD3	2.25	0.52
1:G:863:LYS:O	1:G:867:ARG:HG3	2.09	0.52
1:A:708:ILE:HG22	1:A:754:HIS:HB2	1.91	0.51
2:B:286:MET:SD	2:B:289:GLY:HA2	2.50	0.51
1:C:1001:ILE:HG13	1:C:1002:GLN:H	1.75	0.51
1:C:648:LEU:HD13	1:C:845:ARG:HD2	1.92	0.51
1:E:554:ASN:N	1:E:555:PRO:HD3	2.25	0.51
1:E:680:HIS:HB3	11:E:5910:HOH:O	2.09	0.51
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.92	0.51
1:A:1:MET:HB3	1:A:224:LYS:HE2	1.92	0.51
1:E:698:ILE:CD1	1:E:698:ILE:N	2.74	0.51
1:G:230:ILE:H	1:G:349:GLU:HG2	1.75	0.51
2:B:228:VAL:HA	2:B:231:MET:HE2	1.92	0.51
1:C:331:THR:OG1	1:C:334:GLU:OE2	2.29	0.51
1:A:493:LYS:HE2	1:A:517:ARG:HD3	1.93	0.51
2:B:286:MET:HE3	2:B:314:PHE:N	2.26	0.51
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.40	0.51
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.93	0.51
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.11	0.51
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.30	0.51
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.92	0.51
1:A:682:VAL:HG21	1:A:689:GLN:NE2	2.25	0.51
1:A:698:ILE:N	1:A:698:ILE:HD12	2.25	0.51
1:C:209:SER:OG	1:C:211:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:CD1	1:C:837:VAL:HG23	2.40	0.51
1:E:82[B]:ARG:NE	1:E:111:PHE:CD1	2.78	0.51
1:G:58:PRO:HA	1:G:1066:GLN:HE21	1.75	0.51
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.92	0.51
2:H:60:ILE:HB	2:H:82:ILE:CD1	2.40	0.51
1:E:1001:ILE:HD12	1:E:1029:ILE:HB	1.90	0.51
1:E:213:TRP:CZ3	1:E:289:ASN:HB2	2.46	0.51
1:E:784:GLN:NE2	1:E:784:GLN:N	2.41	0.51
2:F:135:GLY:O	2:F:138:PRO:HD3	2.10	0.51
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.40	0.51
1:G:692:ASN:N	1:G:692:ASN:HD22	2.08	0.51
1:G:796:LEU:HD23	1:G:797:PRO:N	2.26	0.51
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.40	0.51
1:A:941:LYS:HG2	1:A:1054:LEU:HD22	1.92	0.51
1:G:643:GLY:HA3	1:G:647:PRO:HG3	1.93	0.51
1:E:101:GLU:OE1	1:E:104:ARG:NH2	2.38	0.51
1:E:755:PHE:CE1	7:E:5047:ADP:C2	2.99	0.51
1:E:24:CYS:HB2	1:E:604:GLU:HB3	1.93	0.51
2:F:172:GLN:HG2	2:F:173:GLY:N	2.26	0.51
2:F:350:PHE:CG	2:F:366:LEU:HD21	2.46	0.51
1:G:828:VAL:CG1	1:G:839:LEU:HD11	2.40	0.51
1:A:10:ILE:CD1	1:A:42:TYR:HB3	2.41	0.51
1:A:10:ILE:HD12	1:A:42:TYR:HB3	1.93	0.51
1:A:692:ASN:ND2	1:A:692:ASN:N	2.59	0.51
1:C:734:LEU:O	1:C:734:LEU:HD12	2.11	0.51
1:C:878:GLY:HA2	11:C:5590:HOH:O	2.10	0.51
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.51
1:E:470:VAL:O	1:E:474:GLU:HG3	2.11	0.51
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.46	0.51
2:H:202:LYS:NZ	2:H:356:ALA:O	2.40	0.51
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.31	0.51
2:B:191:PRO:HD2	2:B:213:GLY:O	2.11	0.51
1:G:667:ASP:O	1:G:677:ARG:NH2	2.44	0.51
1:A:164:PHE:HB3	1:A:165:PRO:HA	1.92	0.50
1:A:710:TYR:CD2	1:A:712:LEU:HD13	2.46	0.50
1:A:89:THR:O	1:A:304:VAL:HG22	2.12	0.50
1:C:959:ASP:O	1:C:963:LYS:HG3	2.11	0.50
1:C:986:ILE:O	1:C:988:PRO:HD3	2.12	0.50
2:F:259:LEU:O	2:F:345:LYS:HE3	2.11	0.50
1:G:699:GLU:HA	1:G:702:VAL:HG23	1.93	0.50
1:A:737:TYR:O	1:A:740:THR:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLU:HB3	11:A:5774:HOH:O	2.10	0.50
1:C:464:VAL:HG21	2:D:88:ILE:HG12	1.92	0.50
1:E:493:LYS:HE2	1:E:517:ARG:HD3	1.91	0.50
1:G:158:VAL:O	1:G:161:ASP:HB3	2.10	0.50
1:G:692:ASN:H	1:G:692:ASN:HD22	1.60	0.50
1:G:698:ILE:CD1	1:G:698:ILE:H	2.24	0.50
1:A:659:VAL:CG1	1:A:660:PRO:HD2	2.41	0.50
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.75	0.50
2:B:133:ILE:HG22	2:B:138:PRO:HB3	1.93	0.50
1:E:514:ARG:HD3	11:E:5606:HOH:O	2.10	0.50
2:H:46:PRO:HA	2:H:76:HIS:CG	2.46	0.50
1:A:132:PHE:O	1:A:136:MET:HG2	2.11	0.50
1:A:665:SER:O	1:A:669:ILE:HG13	2.12	0.50
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.46	0.50
2:B:26:ALA:O	2:B:131:CYS:HA	2.11	0.50
1:E:1:MET:O	1:E:334:GLU:OE2	2.29	0.50
2:F:173:GLY:C	2:F:207:ARG:HG2	2.32	0.50
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.93	0.50
1:G:755:PHE:CE1	7:G:5067:ADP:C2	2.99	0.50
1:G:868:VAL:HA	1:G:872:LYS:O	2.11	0.50
1:G:349:GLU:O	2:H:294:ASN:HB2	2.11	0.50
1:A:561:LYS:HE3	11:A:5830:HOH:O	2.10	0.50
1:A:563:MET:SD	1:A:635:PRO:HG3	2.52	0.50
1:A:671:ARG:NH2	1:A:819:GLU:O	2.45	0.50
2:B:192:PHE:O	2:B:215[A]:ARG:HG2	2.10	0.50
1:E:523:HIS:HB2	11:E:5996:HOH:O	2.12	0.50
1:E:863:LYS:O	1:E:867:ARG:HG3	2.11	0.50
2:F:272:HIS:HA	2:F:349:SER:CB	2.41	0.50
2:H:255:ILE:HA	2:H:258:PHE:CD2	2.47	0.50
1:A:755:PHE:CE1	7:A:5007:ADP:C2	3.00	0.50
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.50
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.93	0.50
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.41	0.50
1:G:470:VAL:O	1:G:474:GLU:HG3	2.12	0.50
1:G:692:ASN:ND2	1:G:692:ASN:H	2.10	0.50
1:G:845:ARG:NH1	1:G:846:ALA:O	2.44	0.50
1:A:344:THR:HB	1:A:345:PRO:HD2	1.92	0.50
1:A:813:VAL:HG22	1:A:828:VAL:HG21	1.93	0.50
2:D:215:ARG:NH1	2:D:215:ARG:HG3	2.25	0.50
1:E:945:ALA:HA	1:E:1012:TYR:O	2.11	0.50
2:F:45:ASP:HB3	2:F:48:TYR:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:ILE:HG22	1:G:540:THR:OG1	2.12	0.50
1:G:812:GLN:O	1:G:816:LEU:HD12	2.11	0.50
1:C:40:GLU:HA	1:C:40:GLU:OE1	2.12	0.50
1:E:150:HIS:HB2	11:E:5507:HOH:O	2.11	0.50
2:F:273:GLN:HE21	2:F:351:GLN:HE22	1.59	0.50
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.26	0.50
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.94	0.50
1:A:412:LYS:HG2	1:A:438:TYR:CE2	2.47	0.50
1:A:948:SER:O	1:A:1015:ASN:HA	2.11	0.50
1:A:348:PHE:HB3	2:B:296:PRO:HG3	1.94	0.50
1:C:64:THR:O	1:C:1065:VAL:HG23	2.11	0.50
2:D:328:THR:HG21	2:D:341:HIS:HB2	1.93	0.50
2:H:123:ARG:HA	2:H:288:PHE:CE2	2.47	0.50
2:H:290:HIS:HB3	2:H:310:GLN:CB	2.42	0.50
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.93	0.49
1:C:152:MET:HG3	1:C:152:MET:O	2.10	0.49
1:E:814:GLN:NE2	11:E:5378:HOH:O	2.45	0.49
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.92	0.49
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.47	0.49
2:H:277:LEU:HD23	2:H:281:ALA:O	2.12	0.49
1:A:698:ILE:CD1	1:A:698:ILE:H	2.24	0.49
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.42	0.49
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.12	0.49
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.93	0.49
1:G:427:GLU:HG3	1:G:438:TYR:CE2	2.47	0.49
1:G:68:PRO:HB3	1:G:934:GLY:CA	2.41	0.49
2:H:162:VAL:HG23	2:H:200:GLY:HA3	1.95	0.49
2:H:348:PHE:HZ	2:H:370:PHE:HB2	1.77	0.49
1:E:759:ALA:O	1:E:784:GLN:HB2	2.12	0.49
1:A:679:GLN:HA	1:A:689:GLN:HE22	1.77	0.49
1:C:554:ASN:N	1:C:555:PRO:HD3	2.27	0.49
2:D:185:LYS:HE2	2:D:189:GLU:HB3	1.95	0.49
2:D:173:GLY:O	2:D:207:ARG:HG2	2.13	0.49
2:D:286[A]:MET:HE1	2:D:314:PHE:O	2.12	0.49
2:H:23:THR:HG22	2:H:24:GLY:N	2.27	0.49
2:H:290:HIS:HB3	2:H:310:GLN:HB3	1.95	0.49
1:A:285:GLN:HB3	11:A:5606:HOH:O	2.12	0.49
2:B:337:LEU:HD12	2:B:338:GLN:H	1.78	0.49
1:C:103:GLU:HB2	1:C:108:LEU:HD12	1.93	0.49
1:C:59:GLU:HG3	1:C:60:MET:CE	2.42	0.49
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:THR:O	1:C:304:VAL:HG22	2.13	0.49
1:E:509:ARG:HH11	1:E:512:GLU:CG	2.25	0.49
1:E:715:ARG:HB2	1:E:751:LEU:HB2	1.94	0.49
2:F:223:THR:HG22	2:F:228:VAL:HG23	1.94	0.49
2:H:159:ALA:O	2:H:163:THR:HB	2.13	0.49
1:A:954:LYS:NZ	9:A:5012:IMP:O3P	2.36	0.49
2:B:236:ILE:HD13	2:B:258:PHE:CE1	2.48	0.49
1:C:220:VAL:HG12	1:C:221:VAL:N	2.26	0.49
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.93	0.49
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.12	0.49
1:C:554:ASN:OD1	8:C:5034:ORN:HD3	2.12	0.49
2:H:266:PHE:HB2	2:H:370:PHE:CE1	2.47	0.49
2:H:305:VAL:HG12	2:H:306:MET:N	2.28	0.49
2:H:342:ARG:CG	2:H:347:ALA:HB3	2.43	0.49
2:B:7:LEU:HD23	2:B:15:PHE:CD1	2.47	0.49
1:C:490:ARG:HB3	1:C:490:ARG:CZ	2.28	0.49
2:D:199:PHE:HB3	2:D:270:LEU:HD23	1.95	0.49
1:C:265:ARG:NH1	2:D:360:PRO:HB3	2.28	0.49
1:E:1001:ILE:HD13	1:E:1029:ILE:HB	1.92	0.49
1:E:49:SER:O	1:E:51:PRO:HD3	2.13	0.49
1:E:652[B]:ARG:NH2	11:E:5846:HOH:O	2.45	0.49
1:E:715:ARG:HG3	1:E:725:MET:CE	2.43	0.49
1:G:148:ILE:HD13	1:G:204:LEU:O	2.12	0.49
1:G:755:PHE:CD1	7:G:5067:ADP:C2	3.00	0.49
2:H:172:GLN:O	2:H:207:ARG:HA	2.12	0.49
2:H:228:VAL:HG11	2:H:258:PHE:HE1	1.74	0.49
2:H:342:ARG:NE	2:H:344:ASP:OD1	2.46	0.49
1:C:1003:ASP:O	1:C:1007:ASN:ND2	2.45	0.49
1:C:637:GLY:HA2	1:C:660:PRO:O	2.12	0.49
1:C:676:GLU:O	1:C:680:HIS:HB2	2.12	0.49
1:E:420:ALA:HA	1:E:423:LYS:HG3	1.95	0.49
1:E:799:TYR:CD2	1:E:800:THR:HG23	2.48	0.49
1:G:559:ARG:HH12	1:G:614:ASP:CG	2.16	0.49
1:G:5:THR:O	1:G:8:LYS:NZ	2.41	0.49
1:C:1:MET:HA	1:C:224:LYS:NZ	2.28	0.49
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.95	0.49
1:E:677:ARG:O	1:E:680:HIS:HB2	2.12	0.49
1:E:998:ARG:HA	1:E:999:PRO:C	2.26	0.49
1:G:947:LEU:HA	1:G:1014:ILE:HG23	1.95	0.49
1:G:1021:ARG:HD2	1:G:1025:ASP:OD2	2.12	0.49
1:G:534:ALA:O	2:H:123:ARG:NH1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:780:GLU:OE1	1:G:798:ALA:HB1	2.13	0.49
1:A:1027:ARG:O	1:A:1031:ARG:HG3	2.13	0.48
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.94	0.48
1:C:770:GLY:HA2	1:C:823:ARG:NH1	2.28	0.48
2:D:321:LEU:HG	2:D:325:LEU:HB3	1.95	0.48
2:D:298:LYS:CB	2:D:332:LEU:HD11	2.42	0.48
1:G:579:ASP:OD2	1:G:605:THR:HB	2.13	0.48
2:H:327:VAL:HG13	2:H:337:LEU:HD11	1.95	0.48
2:H:48:TYR:CE2	2:H:311:ASN:ND2	2.82	0.48
1:A:636:LYS:HE3	11:A:5551:HOH:O	2.13	0.48
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.28	0.48
2:D:190:LEU:HB2	2:D:215:ARG:HB3	1.96	0.48
1:E:941[B]:LYS:HE3	1:E:1054:LEU:O	2.13	0.48
1:G:198:LEU:O	1:G:200:PRO:HD3	2.13	0.48
1:G:763:ASP:HB3	1:G:779:MET:CE	2.43	0.48
1:G:370:ALA:HB2	1:G:900:PHE:HB3	1.96	0.48
1:C:361:ARG:CZ	1:C:571:ARG:HG2	2.43	0.48
1:C:66:ILE:HG21	1:C:918:MET:HB3	1.95	0.48
1:C:708:ILE:HG23	1:C:754:HIS:HB2	1.96	0.48
2:H:173:GLY:C	2:H:207:ARG:HG2	2.33	0.48
2:H:263:ILE:HG12	2:H:377:TYR:CZ	2.48	0.48
2:F:86:PRO:HA	11:F:2588:HOH:O	2.13	0.48
1:G:73:VAL:O	1:G:77:ILE:HG13	2.13	0.48
2:H:255:ILE:HG22	2:H:278:ALA:CB	2.42	0.48
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.40	0.48
1:E:313:LYS:HE2	1:E:608:THR:C	2.33	0.48
1:G:659:VAL:O	1:G:661:VAL:HG23	2.13	0.48
1:C:288:VAL:O	1:C:290:PRO:HD3	2.14	0.48
1:C:250:VAL:HA	1:C:356:VAL:O	2.14	0.48
1:C:975:HIS:O	1:C:979:ILE:HG12	2.13	0.48
1:E:9:SER:OG	1:E:83:PRO:HA	2.13	0.48
2:F:85:LEU:HD12	2:F:86:PRO:HD2	1.95	0.48
1:G:768:CYS:HB3	1:G:822:VAL:HG12	1.96	0.48
1:A:851:PRO:O	1:A:854:SER:HB2	2.13	0.48
2:B:71:GLU:C	2:B:203:ARG:HG3	2.33	0.48
2:B:222:GLN:H	2:B:222:GLN:HE21	1.61	0.48
1:C:225:ASN:ND2	1:C:331:THR:HG21	2.28	0.48
1:C:780:GLU:OE1	1:C:799:TYR:N	2.46	0.48
1:E:667:ASP:O	1:E:677:ARG:NH2	2.46	0.48
2:F:98:LEU:O	2:F:101:TYR:HB3	2.13	0.48
1:E:349:GLU:O	2:F:294:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:688:LYS:NZ	1:G:836:GLU:OE1	2.44	0.48
1:A:1:MET:N	1:A:2:PRO:CD	2.77	0.48
1:A:772:MET:HA	1:A:818:PHE:HZ	1.78	0.48
2:B:364:ALA:N	2:B:365:PRO:HD2	2.29	0.48
1:C:257:THR:HG22	2:D:63:VAL:HG21	1.96	0.48
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.14	0.48
1:E:809:MET:O	1:E:813:VAL:HG23	2.12	0.48
2:F:379:LYS:HB3	2:F:379:LYS:HE2	1.46	0.48
1:G:64:THR:CB	1:G:1066:GLN:HE22	2.25	0.48
2:B:218:ILE:HG22	2:B:219:VAL:N	2.28	0.48
2:D:206:LEU:O	2:D:210:VAL:HG23	2.13	0.48
2:D:246:ALA:HB3	2:D:247:PRO:HD3	1.96	0.48
1:A:107:VAL:O	1:A:110:GLU:HB2	2.14	0.48
1:A:423:LYS:NZ	11:A:5823:HOH:O	2.45	0.48
1:C:992:ASN:O	1:C:1000:HIS:HA	2.14	0.48
1:C:101:GLU:O	1:C:105:GLN:HG2	2.13	0.48
2:D:225:ALA:O	2:D:229:LEU:HG	2.14	0.48
2:D:295:HIS:CE1	2:D:333:PHE:HD2	2.31	0.48
1:G:964:LEU:O	1:G:969:PHE:HB2	2.14	0.48
2:H:194:VAL:O	2:H:216:LEU:HA	2.13	0.48
2:H:8:VAL:HG22	2:H:14:GLN:HG2	1.96	0.48
2:B:252:ILE:HD13	2:B:277:LEU:HB3	1.95	0.47
1:A:464:VAL:HG21	2:B:88:ILE:HG12	1.96	0.47
1:C:868:VAL:HA	1:C:872:LYS:O	2.14	0.47
1:E:1063:ILE:HG12	1:E:1064:SER:N	2.27	0.47
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.65	0.47
1:G:68:PRO:HB3	1:G:934:GLY:HA2	1.96	0.47
2:H:224:SER:C	2:H:226:GLU:H	2.16	0.47
1:A:692:ASN:HD22	1:A:692:ASN:N	2.13	0.47
2:D:369:HIS:O	2:D:373:LEU:HG	2.14	0.47
1:E:164:PHE:HB3	1:E:165:PRO:HA	1.96	0.47
1:G:552:GLU:OE2	2:H:116:ARG:NE	2.36	0.47
2:H:286:MET:SD	2:H:289:GLY:HA2	2.54	0.47
2:H:343:THR:OG1	2:H:344:ASP:N	2.46	0.47
1:A:43:ARG:NH1	11:A:5640:HOH:O	2.46	0.47
1:A:738:PHE:HZ	1:A:750:VAL:HG11	1.80	0.47
2:B:261:THR:CG2	2:B:262:ASP:N	2.78	0.47
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.77	0.47
1:C:229:ILE:O	1:C:229:ILE:HG13	2.14	0.47
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.95	0.47
2:D:173:GLY:C	2:D:207:ARG:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.31	0.47
1:G:93:GLN:HG2	5:G:5076:CL:CL	2.51	0.47
1:G:676:GLU:O	1:G:680:HIS:ND1	2.47	0.47
1:A:221:VAL:HA	1:A:281:GLY:HA2	1.97	0.47
1:A:45:ILE:HD13	1:A:81:GLU:CB	2.43	0.47
1:C:375:THR:HG23	1:C:377:GLN:H	1.79	0.47
1:C:554:ASN:ND2	11:C:5322:HOH:O	2.47	0.47
2:D:226:GLU:O	2:D:230:LYS:HG3	2.14	0.47
1:E:958:VAL:O	1:E:961:ALA:HB3	2.15	0.47
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.96	0.47
2:H:73:SER:HA	2:H:203:ARG:HH22	1.79	0.47
1:A:119:THR:O	1:A:123:ILE:HG13	2.14	0.47
2:D:364:ALA:N	2:D:365:PRO:HD2	2.30	0.47
1:E:158:VAL:O	1:E:162:VAL:HG13	2.15	0.47
1:G:138:LYS:HE2	11:G:5508:HOH:O	2.15	0.47
1:A:478:GLU:HG3	11:A:5534:HOH:O	2.13	0.47
2:B:269:CYS:O	2:B:272:HIS:HB3	2.14	0.47
1:E:340:THR:O	1:E:343:ARG:HB2	2.15	0.47
1:G:796:LEU:HD23	1:G:796:LEU:C	2.35	0.47
2:H:25:SER:HA	2:H:132:ILE:O	2.14	0.47
1:A:358:LYS:HG2	1:A:359:ILE:N	2.29	0.47
1:A:653:ALA:O	1:A:656:ALA:HB3	2.15	0.47
2:B:142:LEU:O	2:B:145:GLU:HB3	2.15	0.47
1:E:670:ASP:HB2	11:E:5438:HOH:O	2.15	0.47
1:G:330:TYR:HD1	1:G:334:GLU:OE1	1.97	0.47
1:G:959:ASP:O	1:G:962:ALA:HB3	2.14	0.47
2:H:20:ILE:O	2:H:99:SER:OG	2.28	0.47
2:B:261:THR:HG23	2:B:262:ASP:N	2.30	0.47
2:D:286[A]:MET:HE1	2:D:312:HIS:ND1	2.30	0.47
1:E:785:ALA:HB1	7:E:5047:ADP:C2	2.49	0.47
1:G:347:SER:O	1:G:348:PHE:HB3	2.15	0.47
1:G:240:MET:HE3	7:G:5060:ADP:C4	2.50	0.47
2:H:280:GLY:HA3	2:H:322:PRO:HG3	1.95	0.47
2:H:57:TYR:CE1	2:H:58:PRO:HD2	2.47	0.47
1:A:45:ILE:CD1	1:A:81:GLU:HB3	2.44	0.47
2:B:266:PHE:HB3	2:B:370:PHE:CD1	2.50	0.47
2:B:331:SER:O	2:B:335:GLY:HA2	2.15	0.47
2:B:264:PRO:HB3	2:B:373:LEU:HB3	1.95	0.47
1:C:946:LEU:C	1:C:947:LEU:HD12	2.36	0.47
2:D:354:PRO:HB3	2:D:363:ALA:O	2.15	0.47
1:E:103:GLU:HG3	1:E:104:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ILE:HG22	1:E:11:LEU:N	2.30	0.47
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.45	0.47
2:F:342:ARG:HA	2:F:342:ARG:HD2	1.69	0.47
1:G:659:VAL:O	1:G:661:VAL:N	2.48	0.47
2:H:209:LEU:HB3	2:H:216:LEU:HD21	1.97	0.47
1:G:290:PRO:O	2:H:92:PHE:HB3	2.15	0.47
1:A:698:ILE:HG22	1:A:699:GLU:N	2.30	0.47
1:A:802:SER:O	1:A:805:ILE:HG22	2.14	0.47
2:B:197:TYR:HB3	2:B:199:PHE:CZ	2.50	0.47
2:D:133:ILE:HD12	2:D:143:ALA:CB	2.28	0.47
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.50	0.47
2:F:272:HIS:HA	2:F:349:SER:HB2	1.96	0.47
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	1.96	0.47
1:G:810:ARG:HG3	1:G:810:ARG:NH1	2.22	0.47
2:H:190:LEU:HB2	2:H:215:ARG:HB3	1.96	0.47
1:C:176:GLY:HA3	1:C:377:GLN:HA	1.96	0.46
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.37	0.46
2:H:290:HIS:ND1	2:H:312:HIS:CE1	2.84	0.46
1:A:975:HIS:HD1	1:G:975:HIS:HD1	0.72	0.46
2:D:270:LEU:O	2:D:274:LEU:HG	2.15	0.46
1:E:1067:GLU:O	1:E:1071:GLN:HG3	2.15	0.46
1:E:946:LEU:HB3	1:E:1013:ILE:HG12	1.96	0.46
2:F:29:GLU:HA	2:F:129:ASN:HA	1.97	0.46
1:G:141:LEU:HB3	1:G:297:VAL:HG21	1.97	0.46
2:H:370:PHE:O	2:H:374:ILE:HG13	2.15	0.46
1:A:441:ASP:OD1	1:A:444:ARG:NH1	2.44	0.46
1:C:490:ARG:HG3	1:C:522:LEU:CD1	2.45	0.46
1:C:534:ALA:HB1	2:D:120:ARG:HG2	1.97	0.46
1:C:769:ASP:OD1	1:C:771:GLU:HB3	2.16	0.46
1:E:76:LYS:NZ	11:E:5748:HOH:O	2.42	0.46
1:E:805:ILE:HD12	1:E:832:VAL:HG11	1.97	0.46
1:G:1021:ARG:CG	1:G:1021:ARG:HH11	2.27	0.46
1:G:164:PHE:HB3	1:G:165:PRO:HA	1.97	0.46
1:G:7:ILE:HD13	1:G:85:ALA:HB2	1.95	0.46
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.67	0.46
2:H:361:HIS:CD2	2:H:361:HIS:N	2.80	0.46
1:A:1:MET:HA	1:A:224:LYS:NZ	2.30	0.46
2:D:246:ALA:N	2:D:247:PRO:HD2	2.30	0.46
2:D:296:PRO:HB2	2:D:332:LEU:HB2	1.97	0.46
2:D:272:HIS:HA	2:D:349:SER:CB	2.46	0.46
1:E:130:ARG:HD2	11:E:5490:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ARG:NH1	7:E:5040:ADP:O2A	2.45	0.46
1:E:643:GLY:HA3	1:E:647:PRO:HG3	1.97	0.46
2:F:175:TRP:CG	2:F:176:THR:N	2.84	0.46
2:F:41:GLU:CB	2:F:358:PRO:HG3	2.44	0.46
1:G:1:MET:N	1:G:2:PRO:CD	2.79	0.46
1:G:74:VAL:O	1:G:77:ILE:N	2.48	0.46
1:G:783:GLU:HB2	1:G:792:SER:HB3	1.98	0.46
1:G:883:VAL:O	1:G:884:ILE:HG12	2.15	0.46
1:A:472:LEU:O	1:A:476:VAL:HG23	2.16	0.46
1:A:57:ASP:HA	1:A:58:PRO:HD3	1.78	0.46
1:A:679:GLN:HG2	1:A:689:GLN:OE1	2.14	0.46
2:B:206:LEU:O	2:B:210:VAL:HG23	2.16	0.46
1:E:1063:ILE:HD13	1:E:1068:MET:HG3	1.97	0.46
1:E:9:SER:OG	1:E:84:ASP:N	2.46	0.46
1:G:10:ILE:HD13	1:G:37:LEU:HD13	1.96	0.46
1:G:640:VAL:HG23	1:G:640:VAL:O	2.14	0.46
2:H:298:LYS:O	2:H:329:HIS:HA	2.14	0.46
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.98	0.46
1:A:728:VAL:HB	1:A:733:ASP:HB3	1.98	0.46
1:A:780:GLU:HB3	1:A:798:ALA:HA	1.97	0.46
1:E:490[B]:ARG:NH1	1:E:494:ARG:HD2	2.31	0.46
1:G:236:ASN:OD1	1:G:244:THR:HG22	2.15	0.46
1:G:554:ASN:N	1:G:555:PRO:HD3	2.31	0.46
1:E:420:ALA:O	1:E:423:LYS:HG3	2.16	0.46
1:E:799:TYR:CD1	1:E:799:TYR:N	2.83	0.46
1:G:580:TYR:CE1	1:G:584:HIS:CE1	3.04	0.46
1:G:628:GLU:OE1	1:G:628:GLU:HA	2.15	0.46
1:A:130[B]:ARG:HE	1:A:130[B]:ARG:HB3	1.38	0.46
1:C:921:GLY:HA3	1:C:926:GLU:HB3	1.98	0.46
2:D:225:ALA:HA	2:D:258:PHE:CZ	2.50	0.46
1:E:222[A]:ARG:NE	1:E:226:ASP:OD1	2.39	0.46
2:H:168:TYR:N	2:H:168:TYR:CD1	2.83	0.46
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.98	0.46
1:A:698:ILE:CD1	1:A:698:ILE:N	2.79	0.46
2:B:246:ALA:N	2:B:247:PRO:CD	2.79	0.46
1:C:1001:ILE:HG13	1:C:1002:GLN:N	2.31	0.46
1:G:695:VAL:CG1	1:G:696:THR:N	2.79	0.46
2:H:181:LEU:HA	2:H:182:PRO:HD3	1.73	0.46
1:A:127:GLU:HB2	1:A:172:PHE:CE1	2.51	0.46
1:A:141:LEU:HB3	1:A:297:VAL:HG21	1.98	0.46
1:C:947:LEU:N	1:C:947:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:PRO:HD3	1:E:352:ILE:HD11	1.98	0.46
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.46
1:E:947:LEU:N	1:E:947:LEU:CD1	2.79	0.46
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.63	0.46
1:G:301:ASN:HA	1:G:302:PRO:HD3	1.81	0.46
1:G:93:GLN:HB3	10:G:5073:NET:H22	1.96	0.46
1:G:698:ILE:HD12	1:G:698:ILE:H	1.80	0.46
1:G:891:LYS:HG2	1:G:892:GLU:N	2.29	0.46
2:H:228:VAL:HA	2:H:231:MET:HE2	1.97	0.46
1:C:948:SER:OG	9:C:5032:IMP:H8	2.16	0.45
1:C:930:LYS:NZ	1:C:1058:ALA:O	2.48	0.45
1:E:509:ARG:NH1	1:E:512:GLU:CG	2.80	0.45
1:E:509:ARG:NH1	1:E:512:GLU:HG3	2.31	0.45
1:E:750:VAL:O	1:E:750:VAL:HG12	2.16	0.45
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.96	0.45
1:G:698:ILE:N	1:G:698:ILE:CD1	2.79	0.45
1:G:768:CYS:O	1:G:822:VAL:O	2.34	0.45
1:A:423:LYS:HB3	11:A:5517:HOH:O	2.15	0.45
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.99	0.45
1:A:780:GLU:HG2	1:A:799:TYR:HE1	1.81	0.45
2:F:322:PRO:CB	2:F:324:ASN:ND2	2.79	0.45
2:H:209:LEU:HD23	2:H:214:CYS:SG	2.56	0.45
2:H:21:GLY:HA3	2:H:107:ILE:O	2.17	0.45
1:A:231:VAL:O	1:A:350:PRO:HG2	2.16	0.45
2:B:282:LYS:HG2	2:B:320:THR:HG21	1.97	0.45
2:B:98:LEU:O	2:B:102:LEU:HG	2.17	0.45
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.16	0.45
1:C:782:ILE:HD12	1:C:782:ILE:N	2.31	0.45
1:C:868:VAL:HG23	1:C:877:GLN:HE22	1.81	0.45
1:E:1:MET:HA	1:E:224:LYS:NZ	2.31	0.45
1:E:580:TYR:CE1	1:E:584:HIS:CE1	3.05	0.45
1:G:860:PRO:HB2	1:G:863:LYS:HB2	1.99	0.45
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.98	0.45
1:A:481:ILE:HG13	1:A:481:ILE:O	2.17	0.45
1:A:816:LEU:HD11	1:A:839:LEU:HD21	1.99	0.45
1:C:674:ASP:HB3	1:C:677:ARG:HB2	1.98	0.45
2:D:49:SER:HA	2:D:76:HIS:O	2.17	0.45
1:E:708:ILE:CG2	1:E:754:HIS:HB2	2.47	0.45
2:F:12:GLY:HA2	2:F:144:LEU:CD1	2.47	0.45
2:F:295:HIS:O	2:F:308:THR:N	2.46	0.45
1:G:583:VAL:HG13	1:G:612:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:LEU:HD12	2:H:87:LEU:HA	1.80	0.45
1:A:425:ARG:HD3	11:A:5280:HOH:O	2.16	0.45
1:A:854:SER:HA	1:A:859:VAL:O	2.17	0.45
1:C:906:LEU:HD13	1:C:1030:ARG:HD3	1.99	0.45
1:E:694:THR:CG2	1:E:695:VAL:N	2.80	0.45
2:F:46:PRO:HA	2:F:76:HIS:CB	2.47	0.45
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.43	0.45
1:G:726:GLU:HG3	1:G:727:ILE:N	2.32	0.45
2:H:281:ALA:C	2:H:282:LYS:HG2	2.37	0.45
1:A:197:ASP:OD2	1:A:1037:LYS:HE3	2.17	0.45
1:C:950:ARG:HB3	11:C:5613:HOH:O	2.16	0.45
2:F:228:VAL:HG11	2:F:258:PHE:CZ	2.52	0.45
2:F:324:ASN:HA	2:F:343:THR:OG1	2.17	0.45
2:F:350:PHE:CG	2:F:366:LEU:CD2	2.99	0.45
1:G:710:TYR:HA	1:G:711:PRO:C	2.37	0.45
1:G:903:VAL:HG12	1:G:904:ASP:N	2.32	0.45
1:A:548:GLU:HG2	2:B:114:ASP:CG	2.37	0.45
2:B:190:LEU:HA	2:B:191:PRO:HD3	1.77	0.45
2:B:181:LEU:HD13	2:B:207:ARG:NH2	2.32	0.45
2:B:232:ASN:N	2:B:233:PRO:CD	2.79	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
2:B:46:PRO:HG2	2:B:200:GLY:O	2.16	0.45
2:D:6:LEU:O	2:D:132:ILE:HA	2.16	0.45
2:D:264:PRO:HB3	2:D:373:LEU:HB3	1.98	0.45
2:D:46:PRO:HA	2:D:76:HIS:CG	2.51	0.45
1:E:830:PHE:CE1	1:E:839:LEU:CD1	2.99	0.45
1:G:383:GLU:OE2	1:G:604:GLU:OE2	2.34	0.45
1:G:258:ASP:OD2	2:H:358:PRO:HA	2.17	0.45
2:H:373:LEU:HD23	2:H:373:LEU:N	2.31	0.45
1:A:142:GLU:CG	1:A:143:THR:N	2.80	0.45
2:B:266:PHE:HB3	2:B:370:PHE:CE1	2.52	0.45
1:C:782:ILE:N	1:C:782:ILE:CD1	2.79	0.45
2:D:324:ASN:HD22	2:D:324:ASN:N	2.14	0.45
1:E:1061:LYS:HE3	11:E:5652:HOH:O	2.16	0.45
10:E:5053:NET:H42	10:E:5053:NET:C2	2.32	0.45
1:G:716:PRO:HA	1:G:750:VAL:CG2	2.47	0.45
1:G:725:MET:HG3	1:G:909:PRO:HB2	1.98	0.45
2:H:225:ALA:O	2:H:229:LEU:HG	2.17	0.45
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.82	0.45
2:H:51:GLN:O	2:H:78:GLN:N	2.46	0.45
1:A:412:LYS:HD3	1:A:437:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:PRO:HG2	2:B:324:ASN:ND2	2.25	0.45
2:D:269:CYS:O	2:D:272:HIS:HB3	2.16	0.45
2:F:91:ASN:OD1	2:F:93:ARG:HB2	2.17	0.45
1:G:1020:ARG:O	1:G:1024:GLU:HG3	2.17	0.45
2:H:170:TRP:HB3	2:H:216:LEU:HD12	1.98	0.45
2:H:290:HIS:CB	2:H:310:GLN:HB3	2.47	0.45
2:H:334:ASP:CG	2:H:336:THR:HG23	2.37	0.45
2:B:162:VAL:HG12	2:B:162:VAL:O	2.17	0.45
1:C:1027:ARG:HG3	1:C:1027:ARG:NH1	2.32	0.45
1:C:695:VAL:CG1	1:C:696:THR:N	2.80	0.45
1:C:735:ARG:HH11	1:C:735:ARG:HG2	1.82	0.45
1:C:992:ASN:HB2	1:C:999:PRO:O	2.16	0.45
1:E:18:ILE:HD12	1:E:23:ALA:C	2.37	0.45
2:F:244:ASP:OD1	2:F:245:PRO:HD2	2.17	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.80	0.45
1:G:471:ARG:HD2	11:G:5606:HOH:O	2.17	0.45
1:G:494:ARG:HG3	1:G:547:TYR:CB	2.47	0.45
1:G:816:LEU:O	1:G:820:LEU:HD12	2.17	0.45
2:H:290:HIS:HB2	2:H:312:HIS:NE2	2.32	0.45
1:A:366:LYS:NZ	1:A:911:MET:O	2.44	0.44
2:B:45:ASP:O	2:B:76:HIS:HB2	2.17	0.44
1:C:1:MET:N	1:C:2:PRO:CD	2.79	0.44
1:C:735:ARG:HG2	1:C:735:ARG:NH1	2.31	0.44
1:E:282:SER:OG	1:E:302:PRO:HA	2.17	0.44
1:G:325:LYS:HB3	1:G:330:TYR:CD2	2.52	0.44
1:G:6:ASP:N	1:G:6:ASP:OD1	2.49	0.44
1:G:859:VAL:O	1:G:861:LEU:N	2.50	0.44
2:H:142:LEU:C	2:H:142:LEU:HD12	2.36	0.44
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.42	0.44
2:H:322:PRO:O	2:H:324:ASN:N	2.49	0.44
2:H:327:VAL:HG11	2:H:330:LYS:HD2	1.98	0.44
2:H:75:VAL:HG12	2:H:75:VAL:O	2.17	0.44
1:A:726:GLU:HG3	1:A:727:ILE:H	1.82	0.44
2:B:324:ASN:N	2:B:324:ASN:HD22	2.15	0.44
2:D:204:ASN:O	2:D:208:MET:HG3	2.17	0.44
1:E:250:VAL:HA	1:E:356:VAL:O	2.18	0.44
1:E:840:ILE:O	1:E:841:GLU:HB3	2.17	0.44
2:H:286:MET:HE1	2:H:315:ALA:HB2	1.97	0.44
2:H:327:VAL:HG13	2:H:337:LEU:CD1	2.48	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:1:MET:H2	1:A:2:PRO:HD3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ALA:O	2:B:281:ALA:HB3	2.17	0.44
2:B:318:GLU:HA	2:B:321:LEU:HD13	1.98	0.44
1:C:944:ARG:O	1:C:1010:TYR:HA	2.17	0.44
1:C:1044:LEU:HA	1:C:1044:LEU:HD12	1.76	0.44
1:C:734:LEU:C	1:C:734:LEU:HD12	2.36	0.44
1:C:784:GLN:HA	11:C:5592:HOH:O	2.16	0.44
2:D:228:VAL:O	2:D:231:MET:HB2	2.17	0.44
2:D:322:PRO:HD2	2:D:325:LEU:HD12	1.98	0.44
1:E:956:ARG:CB	1:E:1044:LEU:HD21	2.48	0.44
1:E:426:ARG:HD3	1:E:426:ARG:C	2.37	0.44
1:G:375:THR:HG23	1:G:377:GLN:H	1.82	0.44
1:E:225:ASN:ND2	1:E:331:THR:HG21	2.33	0.44
1:E:1:MET:N	1:E:2:PRO:CD	2.80	0.44
1:E:697:ALA:HB3	1:E:700:MET:HB2	2.00	0.44
2:F:286:MET:CE	2:F:312:HIS:ND1	2.80	0.44
1:G:224:LYS:HG2	11:G:5551:HOH:O	2.18	0.44
1:G:456:THR:HB	1:G:458:ILE:HG13	1.99	0.44
1:G:543:MET:HE1	1:G:617:TYR:CZ	2.53	0.44
1:G:712:LEU:HD12	1:G:712:LEU:HA	1.74	0.44
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.60	0.44
2:H:217:THR:HG21	2:H:231:MET:SD	2.58	0.44
1:A:585:ALA:HB2	1:A:642:TYR:CD2	2.52	0.44
1:A:788:HIS:HD2	1:A:909:PRO:O	2.00	0.44
1:C:358:LYS:HG2	1:C:359:ILE:N	2.32	0.44
1:C:726:GLU:OE2	1:C:1020:ARG:HD2	2.17	0.44
1:E:652[B]:ARG:NH1	11:E:5630:HOH:O	2.51	0.44
2:F:164:THR:N	2:F:198:ASP:OD2	2.51	0.44
2:F:208:MET:O	2:F:211:ASP:HB2	2.17	0.44
2:F:337:LEU:HD21	2:F:340:ILE:CG2	2.47	0.44
2:H:23:THR:HG23	2:H:134:ALA:O	2.16	0.44
2:H:71:GLU:C	2:H:203:ARG:HG3	2.37	0.44
1:C:1000:HIS:NE2	1:C:1002:GLN:HB3	2.32	0.44
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.72	0.44
1:E:1027:ARG:HG2	1:E:1031:ARG:HG3	1.99	0.44
1:E:1:MET:CA	1:E:224:LYS:NZ	2.81	0.44
1:E:561:LYS:HE3	11:E:5895:HOH:O	2.16	0.44
1:G:235:GLU:HB2	1:G:253:ALA:HA	1.99	0.44
2:H:30:VAL:HG12	2:H:122:LEU:HD11	2.00	0.44
1:A:259:LYS:NZ	11:A:5677:HOH:O	2.51	0.44
1:A:739:GLN:CG	1:A:740:THR:N	2.79	0.44
1:C:712:LEU:HA	1:C:712:LEU:HD12	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:GLU:CG	1:C:727:ILE:N	2.80	0.44
1:E:425:ARG:HD3	11:E:5322:HOH:O	2.18	0.44
1:E:948:SER:OG	9:E:5052:IMP:H5'2	2.17	0.44
1:E:796:LEU:C	1:E:796:LEU:HD23	2.38	0.44
2:F:160:LYS:HE3	2:F:161:GLU:OE2	2.18	0.44
2:F:246:ALA:N	2:F:247:PRO:HD2	2.33	0.44
2:F:54:THR:HA	2:F:81:VAL:HB	2.00	0.44
1:G:409:PHE:O	1:G:444:ARG:NH2	2.46	0.44
1:G:440:ALA:O	1:G:444:ARG:HG3	2.18	0.44
1:A:313:LYS:HA	1:A:313:LYS:HD2	1.78	0.44
2:B:13:THR:HG22	2:B:15:PHE:CE1	2.53	0.44
2:B:71:GLU:HG3	2:B:202:LYS:HE3	2.00	0.44
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.52	0.44
1:C:423:LYS:H	1:C:423:LYS:HG3	1.43	0.44
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.81	0.44
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.66	0.44
2:H:270:LEU:HA	2:H:273:GLN:OE1	2.17	0.44
2:B:175:TRP:CD1	2:B:180:GLY:HA2	2.52	0.44
2:B:188:ASP:OD1	2:B:189:GLU:N	2.51	0.44
2:B:248:CYS:O	2:B:252:ILE:HG13	2.18	0.44
2:D:286[A]:MET:CE	2:D:312:HIS:ND1	2.81	0.44
1:G:1027:ARG:HG2	1:G:1027:ARG:NH1	2.32	0.44
1:G:103:GLU:HA	1:G:108:LEU:HD12	1.99	0.44
2:H:48:TYR:CZ	2:H:311:ASN:ND2	2.86	0.44
1:A:634:LYS:N	1:A:635:PRO:HD3	2.33	0.43
2:B:277:LEU:HD23	2:B:281:ALA:O	2.18	0.43
2:B:342:ARG:NE	2:B:344:ASP:OD1	2.33	0.43
1:C:922:ARG:NH2	1:C:1060:GLU:OE1	2.40	0.43
1:C:335:LEU:HB2	1:C:346:ALA:HB3	2.00	0.43
1:C:1042:THR:N	8:C:5031:ORN:O	2.44	0.43
1:C:698:ILE:N	1:C:698:ILE:CD1	2.80	0.43
1:E:475:LYS:HD3	1:E:488:PHE:CZ	2.53	0.43
1:G:692:ASN:N	1:G:692:ASN:ND2	2.64	0.43
2:H:310:GLN:HE22	2:H:352:GLY:CA	2.31	0.43
1:A:10:ILE:HD11	1:A:42:TYR:CD2	2.52	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.90	0.43
1:A:373:ARG:NH1	1:A:430:ASP:O	2.44	0.43
1:A:726:GLU:OE2	1:A:1020:ARG:HD2	2.17	0.43
1:C:105:GLN:HA	1:C:105:GLN:NE2	2.33	0.43
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.29	0.43
1:G:822:VAL:HG11	1:G:826:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:O	1:A:281:GLY:HA2	2.18	0.43
1:A:509:ARG:O	1:A:512:GLU:HB2	2.18	0.43
1:A:532:CYS:O	1:A:533:ALA:HB3	2.18	0.43
2:B:254:ALA:O	2:B:257:LYS:HB2	2.18	0.43
2:B:46:PRO:HA	2:B:76:HIS:CB	2.47	0.43
1:E:57:ASP:HA	1:E:58:PRO:HD3	1.67	0.43
1:G:475:LYS:HD3	1:G:488:PHE:CZ	2.53	0.43
1:G:561:LYS:NZ	1:G:633:GLU:O	2.45	0.43
1:G:699:GLU:CA	1:G:702:VAL:HG23	2.48	0.43
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.99	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.99	0.43
2:D:267:GLY:O	2:D:349:SER:HB2	2.18	0.43
1:E:1004:ARG:HA	1:E:1009[B]:GLU:HG3	2.00	0.43
1:E:213:TRP:CH2	1:E:289:ASN:HB2	2.52	0.43
2:F:266:PHE:HB2	2:F:370:PHE:CD1	2.53	0.43
1:G:543:MET:CE	1:G:617:TYR:CZ	3.02	0.43
2:H:171:THR:HB	2:H:185:LYS:O	2.19	0.43
2:B:138:PRO:HA	11:B:5177:HOH:O	2.18	0.43
2:B:199:PHE:O	2:B:241:GLY:HA3	2.19	0.43
1:C:130:ARG:HG3	1:C:148:ILE:HG13	2.00	0.43
1:C:1:MET:N	1:C:2:PRO:HD2	2.33	0.43
1:C:472:LEU:O	1:C:476:VAL:HG23	2.18	0.43
1:C:560:GLU:OE2	1:C:636:LYS:NZ	2.30	0.43
1:E:1:MET:N	1:E:2:PRO:HD2	2.33	0.43
1:E:733:ASP:O	1:E:736:ARG:HB3	2.18	0.43
2:F:158:LEU:HD12	2:F:243:GLY:N	2.34	0.43
1:G:475:LYS:O	1:G:479:VAL:HG13	2.19	0.43
1:G:920:VAL:O	1:G:930:LYS:HD3	2.19	0.43
1:A:527:LYS:HB2	1:A:544:TYR:CE1	2.54	0.43
2:B:259:LEU:HD23	2:B:259:LEU:HA	1.78	0.43
1:G:700:MET:CE	1:G:704:LYS:HD3	2.49	0.43
1:G:857:THR:OG1	1:G:859:VAL:HB	2.18	0.43
2:H:232:ASN:N	2:H:233:PRO:CD	2.82	0.43
1:A:185:ARG:NH2	11:A:5455:HOH:O	2.49	0.43
1:A:579:ASP:OD2	1:A:605:THR:HB	2.18	0.43
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.64	0.43
1:E:1051:ALA:O	1:E:1054:LEU:HB2	2.19	0.43
2:F:26:ALA:O	2:F:131:CYS:HA	2.18	0.43
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.83	0.43
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.49	0.43
2:F:57:TYR:CD1	2:F:58:PRO:CD	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:906:LEU:HD13	1:G:1030:ARG:HD3	1.99	0.43
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.54	0.43
1:A:866:ALA:HA	1:A:869:MET:HE2	2.00	0.43
1:C:202:LYS:HG2	1:C:202:LYS:O	2.18	0.43
1:C:648:LEU:HD13	1:C:845:ARG:CD	2.49	0.43
1:C:958:VAL:HG13	1:C:986:ILE:HD12	2.01	0.43
2:D:364:ALA:N	2:D:365:PRO:CD	2.82	0.43
1:E:941[B]:LYS:HE2	11:E:5448:HOH:O	2.19	0.43
1:E:946:LEU:C	1:E:947:LEU:HD12	2.39	0.43
1:E:951:GLU:OE1	1:E:951:GLU:HA	2.17	0.43
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.54	0.43
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.01	0.43
2:F:353:HIS:ND1	2:F:355:GLU:OE2	2.48	0.43
1:G:339:ILE:HG22	1:G:540:THR:CB	2.49	0.43
1:G:364:PHE:CE1	1:G:372:ASP:HA	2.54	0.43
1:G:922:ARG:CZ	1:G:1061:LYS:HD2	2.48	0.43
1:G:936:ASN:HB2	11:G:5111:HOH:O	2.17	0.43
1:G:995:HIS:CE1	1:G:996:GLU:HG3	2.53	0.43
2:H:342:ARG:CG	2:H:342:ARG:HH11	2.20	0.43
1:A:164:PHE:CB	1:A:165:PRO:HA	2.48	0.43
1:A:384:VAL:HG22	1:A:385:MET:N	2.34	0.43
1:A:4:ARG:CZ	1:A:7:ILE:HD11	2.48	0.43
1:A:589:LEU:HA	1:A:592:ASP:HB2	2.01	0.43
1:A:659:VAL:HG12	1:A:660:PRO:HD2	2.00	0.43
2:B:185:LYS:HD3	2:B:190:LEU:HD21	2.01	0.43
1:C:1031:ARG:HB3	1:C:1031:ARG:HE	1.50	0.43
1:E:804:GLU:O	1:E:808:VAL:HG23	2.18	0.43
1:G:5:THR:CG2	1:G:6:ASP:N	2.82	0.43
2:H:199:PHE:CE2	2:H:238:LEU:HB3	2.50	0.43
1:A:158:VAL:O	1:A:161:ASP:HB3	2.19	0.43
2:B:175:TRP:HB2	2:B:181:LEU:CD2	2.48	0.43
2:B:266:PHE:HA	2:B:348:PHE:O	2.19	0.43
1:C:416:ASP:O	1:C:418:PRO:HD3	2.19	0.43
1:C:509:ARG:O	1:C:512:GLU:HB2	2.19	0.43
1:G:1014:ILE:O	1:G:1014:ILE:HG23	2.19	0.43
1:G:390:THR:HB	11:G:5332:HOH:O	2.19	0.43
1:G:548:GLU:HG2	2:H:114:ASP:OD2	2.18	0.43
1:A:142:GLU:HG2	1:A:143:THR:N	2.33	0.42
1:A:169:ARG:HA	1:A:170:PRO:HD3	1.81	0.42
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.90	0.42
2:B:363:ALA:C	2:B:365:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLU:HA	1:C:101:GLU:OE1	2.19	0.42
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.18	0.42
1:C:712:LEU:HD12	1:C:754:HIS:HA	2.01	0.42
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.34	0.42
1:C:66:ILE:CG2	1:C:918:MET:HB3	2.49	0.42
2:D:25:SER:HA	2:D:132:ILE:O	2.19	0.42
1:E:150:HIS:NE2	1:E:203:GLU:HG3	2.34	0.42
1:E:755:PHE:CD1	7:E:5047:ADP:C2	3.07	0.42
2:F:318:GLU:HG2	2:F:318:GLU:O	2.18	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.77	0.42
1:A:769:ASP:OD2	1:A:874:LEU:HB2	2.19	0.42
2:F:324:ASN:ND2	2:F:324:ASN:N	2.63	0.42
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.54	0.42
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.54	0.42
1:G:502:LEU:HD23	1:G:502:LEU:HA	1.67	0.42
1:G:695:VAL:HG12	1:G:696:THR:N	2.34	0.42
1:G:850:VAL:HB	1:G:851:PRO:CD	2.49	0.42
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.19	0.42
1:A:164:PHE:HA	1:A:165:PRO:C	2.39	0.42
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.86	0.42
1:E:697:ALA:HA	1:E:698:ILE:HD13	2.02	0.42
2:F:229:LEU:HA	2:F:229:LEU:HD23	1.68	0.42
2:F:342:ARG:HB3	2:F:345:LYS:H	1.84	0.42
1:G:103:GLU:HG3	1:G:104:ARG:N	2.31	0.42
1:G:1063:ILE:CD1	1:G:1068:MET:HG3	2.36	0.42
1:G:17:PRO:HG3	1:G:917:VAL:HG13	2.01	0.42
1:G:674:ASP:HB3	1:G:677:ARG:HB2	2.02	0.42
2:H:337:LEU:HA	2:H:337:LEU:HD12	1.58	0.42
1:A:755:PHE:CD1	7:A:5007:ADP:C2	3.08	0.42
1:A:695:VAL:HG11	1:A:701:ALA:N	2.35	0.42
2:B:199:PHE:HB3	2:B:270:LEU:HD23	2.02	0.42
1:C:740:THR:H	1:C:740:THR:HG23	1.52	0.42
1:E:644:GLY:O	1:E:648:LEU:HB2	2.19	0.42
2:F:365:PRO:HA	2:F:368:ASP:OD2	2.19	0.42
1:G:354:TYR:OH	1:G:529:VAL:HG13	2.19	0.42
1:G:53:THR:OG1	1:G:56:THR:HG23	2.19	0.42
1:G:810:ARG:NH1	1:G:810:ARG:CG	2.79	0.42
1:G:847:ALA:C	1:G:849:THR:H	2.23	0.42
2:B:344:ASP:OD2	2:B:345:LYS:HG2	2.19	0.42
1:C:868:VAL:HG23	1:C:877:GLN:NE2	2.35	0.42
1:C:534:ALA:O	2:D:123:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:637:GLY:HA2	1:E:660:PRO:O	2.20	0.42
1:E:895:LEU:HA	1:E:896:PRO:HD3	1.81	0.42
2:F:71:GLU:O	2:F:72:SER:HB3	2.20	0.42
1:G:622:THR:OG1	1:G:625:ASP:OD2	2.28	0.42
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.80	0.42
1:G:82:ARG:N	1:G:83:PRO:HD3	2.33	0.42
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.73	0.42
1:C:780:GLU:OE1	1:C:798:ALA:HB1	2.20	0.42
2:D:249:ASP:OD1	2:D:250:TYR:N	2.53	0.42
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.19	0.42
2:F:50:ARG:H	2:F:78[B]:GLN:NE2	2.18	0.42
1:G:294:ARG:HD2	5:G:5077:CL:CL	2.57	0.42
1:G:809:MET:HB3	1:G:830:PHE:CE2	2.55	0.42
2:H:118:LEU:O	2:H:121:LEU:HB3	2.20	0.42
2:H:199:PHE:HD2	2:H:239:SER:O	2.03	0.42
2:H:71:GLU:OE2	2:H:204:ASN:HB2	2.20	0.42
1:A:1:MET:HA	1:A:224:LYS:HZ2	1.85	0.42
1:A:681:ALA:O	1:A:685:LEU:HG	2.19	0.42
1:A:700:MET:O	1:A:704:LYS:HB2	2.19	0.42
2:B:342:ARG:HA	2:B:342:ARG:HD2	1.76	0.42
1:C:713:VAL:O	1:C:713:VAL:HG12	2.19	0.42
1:C:770:GLY:CA	1:C:823:ARG:NH1	2.82	0.42
2:D:299:ASP:O	2:D:303:ASN:N	2.50	0.42
1:E:142:GLU:OE2	1:E:294:ARG:NH2	2.53	0.42
1:E:93:GLN:HG2	5:E:5056:CL:CL	2.57	0.42
2:F:273:GLN:O	2:F:277:LEU:HG	2.19	0.42
2:F:300:VAL:HG22	2:F:328:THR:C	2.37	0.42
2:F:333:PHE:HD1	2:F:333:PHE:HA	1.65	0.42
1:G:534:ALA:HB1	2:H:120:ARG:HG2	2.02	0.42
2:H:280:GLY:CA	2:H:322:PRO:HG3	2.50	0.42
2:H:78:GLN:NE2	2:H:78:GLN:CA	2.80	0.42
1:A:278[A]:GLU:HG2	11:A:5637:HOH:O	2.20	0.42
1:A:9:SER:HA	1:A:43:ARG:O	2.20	0.42
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.81	0.42
2:B:286:MET:CE	2:B:315:ALA:N	2.83	0.42
1:C:956:ARG:NH2	1:C:1048:PHE:CD2	2.88	0.42
1:C:32:GLN:OE1	1:C:320:ALA:HB3	2.19	0.42
2:D:132:ILE:HG21	2:D:132:ILE:HD13	1.84	0.42
1:E:622:THR:OG1	1:E:625:ASP:OD2	2.33	0.42
1:G:100:LEU:HD12	1:G:100:LEU:N	2.35	0.42
1:G:243:HIS:CD2	7:G:5060:ADP:H5'2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:ARG:HG3	1:G:547:TYR:HB2	2.02	0.42
1:G:65:TYR:CG	1:G:77:ILE:HD13	2.55	0.42
2:H:322:PRO:C	2:H:324:ASN:ND2	2.73	0.42
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.50	0.42
1:C:237:PHE:HB3	1:C:248:ILE:O	2.19	0.42
2:D:245:PRO:HG3	2:D:273:GLN:OE1	2.20	0.42
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.86	0.42
1:E:540:THR:HG22	1:E:541:ALA:N	2.35	0.42
1:E:708:ILE:HG23	1:E:754:HIS:HB2	2.01	0.42
2:F:298:LYS:O	2:F:329:HIS:HA	2.20	0.42
1:G:782:ILE:CD1	1:G:782:ILE:N	2.83	0.42
1:A:375:THR:HG23	1:A:377:GLN:H	1.85	0.42
1:A:646:THR:HB	1:A:647:PRO:CD	2.49	0.42
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.35	0.42
1:C:167:ILE:HD12	1:C:167:ILE:N	2.35	0.42
1:C:699:GLU:HA	1:C:702:VAL:CG2	2.49	0.42
2:D:133:ILE:HG22	2:D:138:PRO:HB3	2.02	0.42
1:E:103:GLU:HG2	11:E:5484:HOH:O	2.19	0.42
2:H:9:LEU:HD12	2:H:13:THR:HB	2.02	0.42
1:A:148:ILE:CG2	1:A:149:ALA:N	2.82	0.41
1:A:501:ARG:HD2	1:A:501:ARG:HH11	1.73	0.41
1:A:770:GLY:CA	1:A:823:ARG:CZ	2.98	0.41
1:A:688:LYS:HE3	1:A:836:GLU:OE2	2.19	0.41
2:B:78:GLN:NE2	2:B:78:GLN:HA	2.35	0.41
1:C:494:ARG:HA	1:C:547:TYR:HB2	2.01	0.41
1:C:726:GLU:HG3	1:C:727:ILE:H	1.85	0.41
1:E:383:GLU:OE2	1:E:604:GLU:OE2	2.37	0.41
10:E:5053:NET:H31	10:E:5053:NET:H63	1.83	0.41
2:H:186:LYS:HB2	2:H:189:GLU:HG3	2.01	0.41
2:H:233:PRO:HD2	2:H:263:ILE:HD11	2.01	0.41
1:A:166:CYS:C	1:A:167:ILE:HD12	2.40	0.41
1:A:354:TYR:CD1	1:A:387:ILE:HG23	2.56	0.41
1:A:770:GLY:HA2	1:A:823:ARG:CZ	2.50	0.41
2:B:345:LYS:HB3	2:B:346:PRO:HD2	2.02	0.41
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.00	0.41
1:C:513:ILE:HG23	1:C:513:ILE:HD12	1.75	0.41
1:C:702:VAL:CG1	1:C:731:GLU:HG3	2.50	0.41
1:C:83:PRO:O	1:C:113:VAL:HG22	2.20	0.41
1:E:783:GLU:HG3	1:E:1043:THR:HG21	2.03	0.41
1:E:694:THR:O	1:E:695:VAL:HG23	2.20	0.41
1:G:108:LEU:HB2	11:G:5174:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:LEU:O	1:G:497:PHE:HD2	2.03	0.41
1:G:680:HIS:O	1:G:684:ARG:N	2.51	0.41
1:A:795:SER:OG	1:A:797:PRO:O	2.35	0.41
1:A:944:ARG:HD3	1:A:972:ASP:OD1	2.20	0.41
2:B:190:LEU:HD23	2:B:213:GLY:HA2	2.02	0.41
2:B:322:PRO:HD2	2:B:325:LEU:HD12	2.02	0.41
1:C:11:LEU:HA	1:C:45:ILE:O	2.21	0.41
1:C:1:MET:O	1:C:329:GLY:O	2.38	0.41
1:C:504:LYS:HE2	11:C:5562:HOH:O	2.19	0.41
1:C:71:TRP:CD2	1:C:105:GLN:HG3	2.55	0.41
1:C:726:GLU:OE2	1:C:736:ARG:NH2	2.53	0.41
1:C:891:LYS:HG2	1:C:892:GLU:N	2.35	0.41
2:D:160:LYS:HE3	2:D:161:GLU:OE2	2.20	0.41
1:E:464:VAL:HG21	2:F:88:ILE:HG12	2.01	0.41
1:G:1035:GLN:HG2	1:G:1036:TYR:CD2	2.55	0.41
1:G:980:VAL:HG13	11:G:5678:HOH:O	2.19	0.41
2:H:295:HIS:HA	2:H:296:PRO:HD3	1.87	0.41
1:A:170:PRO:HG2	1:A:177:SER:O	2.20	0.41
2:B:167:ALA:O	2:B:168:TYR:HB3	2.20	0.41
2:D:279:SER:O	2:D:322:PRO:HG3	2.20	0.41
2:F:45:ASP:HB3	2:F:48:TYR:CD2	2.54	0.41
1:G:135:ALA:HB1	1:G:274:GLU:HG3	2.01	0.41
1:G:470:VAL:O	1:G:473:GLU:HB2	2.21	0.41
1:G:321:LYS:NZ	1:G:611:ASP:OD2	2.46	0.41
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.34	0.41
2:H:30:VAL:HB	2:H:128:GLN:O	2.20	0.41
1:A:712:LEU:HD23	1:A:752:LEU:HG	2.03	0.41
1:A:82:ARG:N	1:A:83:PRO:CD	2.84	0.41
2:B:190:LEU:HB2	2:B:215[B]:ARG:HB3	2.02	0.41
2:B:267:GLY:O	2:B:349:SER:HB2	2.20	0.41
1:C:646:THR:HB	1:C:647:PRO:HD3	2.02	0.41
2:D:87:LEU:HD23	2:D:87:LEU:HA	1.69	0.41
1:E:168:ILE:HD12	1:E:191:ILE:HG21	2.01	0.41
2:F:322:PRO:CB	2:F:324:ASN:HD21	2.32	0.41
2:F:87:LEU:HA	2:F:87:LEU:HD12	1.74	0.41
1:G:101:GLU:HG3	11:G:5486:HOH:O	2.20	0.41
1:G:514:ARG:HG3	1:G:517:ARG:NH2	2.35	0.41
2:H:342:ARG:HA	2:H:342:ARG:HD2	1.77	0.41
1:A:1044:LEU:HA	1:A:1044:LEU:HD12	1.98	0.41
1:A:130[B]:ARG:HH11	1:A:130[B]:ARG:HD2	1.81	0.41
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LEU:HA	1:A:896:PRO:HD3	1.86	0.41
2:B:33:ASN:HB3	2:B:55:LEU:HD23	2.03	0.41
1:C:230:ILE:HG13	1:C:265:ARG:HG3	2.03	0.41
1:C:431:ALA:HB2	1:C:435:ARG:HD3	2.02	0.41
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.88	0.41
2:D:232:ASN:N	2:D:233:PRO:HD3	2.35	0.41
1:E:763:ASP:O	1:E:779:MET:HE3	2.21	0.41
1:E:773:VAL:HG21	1:E:814:GLN:HA	2.02	0.41
1:G:763:ASP:OD1	1:G:829:GLN:HG2	2.20	0.41
2:H:128:GLN:NE2	11:H:4033:HOH:O	2.49	0.41
2:H:197:TYR:OH	2:H:228:VAL:HG21	2.21	0.41
1:A:634:LYS:N	1:A:635:PRO:CD	2.84	0.41
1:A:710:TYR:CB	1:A:711:PRO:HA	2.47	0.41
1:A:725:MET:SD	1:A:909:PRO:HB2	2.60	0.41
2:B:291:HIS:HA	2:B:310:GLN:O	2.20	0.41
1:C:141:LEU:HA	1:C:141:LEU:HD23	1.89	0.41
1:C:213:TRP:CH2	1:C:289:ASN:HB2	2.56	0.41
1:C:639:ILE:HG23	1:C:641:GLN:OE1	2.21	0.41
1:E:1004:ARG:CA	1:E:1009[B]:GLU:HG3	2.50	0.41
1:E:1031:ARG:HB3	1:E:1031:ARG:HE	1.76	0.41
1:E:10:ILE:HD12	1:E:42:TYR:HB3	2.03	0.41
1:E:530:ASP:O	1:E:531:THR:OG1	2.29	0.41
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.28	0.41
8:G:5074:ORN:OXT	2:H:120:ARG:NH1	2.54	0.41
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.71	0.41
2:H:296:PRO:HA	2:H:306:MET:O	2.21	0.41
1:A:740:THR:CG2	1:A:741:ALA:N	2.83	0.41
1:A:80:LYS:HG2	1:A:80:LYS:O	2.20	0.41
2:B:101:TYR:O	2:B:104:ARG:HB3	2.19	0.41
1:C:145[A]:ARG:NH2	11:C:5474:HOH:O	2.53	0.41
1:C:423:LYS:HE3	11:C:5542:HOH:O	2.21	0.41
1:C:447:LEU:HD23	1:G:446:GLY:O	2.20	0.41
1:C:59:GLU:CG	1:C:60:MET:CE	2.99	0.41
2:D:120:ARG:HD2	11:D:1337:HOH:O	2.20	0.41
2:D:250:TYR:CD2	2:D:251:ALA:N	2.89	0.41
1:E:1:MET:CA	1:E:224:LYS:HZ1	2.33	0.41
1:E:579:ASP:OD2	1:E:605:THR:HB	2.21	0.41
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.29	0.41
1:E:715:ARG:CD	1:E:725:MET:HE1	2.50	0.41
1:G:634:LYS:N	1:G:635:PRO:CD	2.81	0.41
1:G:680:HIS:O	1:G:683:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:852:PHE:HE1	1:G:918:MET:HG3	1.85	0.41
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.56	0.41
1:A:170:PRO:HA	1:A:204:LEU:HD23	2.03	0.41
2:B:236:ILE:HD13	2:B:258:PHE:CD1	2.56	0.41
2:B:246:ALA:HB3	2:B:247:PRO:CD	2.49	0.41
2:B:354:PRO:HA	2:B:363:ALA:HB3	2.03	0.41
1:C:944:ARG:HB3	1:C:1009:GLU:O	2.20	0.41
1:C:385:MET:HG2	1:C:386:ALA:N	2.35	0.41
1:C:589:LEU:O	1:C:594:TYR:HB2	2.21	0.41
2:D:186:LYS:HB2	2:D:189:GLU:CD	2.40	0.41
1:E:289:ASN:O	1:E:293:GLY:N	2.51	0.41
1:E:710:TYR:HB3	1:E:711:PRO:HA	2.03	0.41
1:E:738:PHE:O	1:E:741:ALA:HB3	2.21	0.41
1:G:468:GLU:OE1	2:H:87:LEU:HD21	2.20	0.41
1:G:888:TYR:O	1:G:920:VAL:HA	2.20	0.41
2:H:290:HIS:O	2:H:311:ASN:HA	2.21	0.41
2:H:48:TYR:HA	2:H:51:GLN:NE2	2.35	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CE2	2.56	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CZ	2.55	0.41
1:A:828:VAL:HG13	1:A:842:VAL:HG22	2.03	0.41
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.87	0.41
1:C:1001:ILE:HD13	1:C:1029:ILE:CB	2.49	0.41
1:C:395:LEU:HD21	1:C:409:PHE:HZ	1.86	0.41
1:C:665:SER:O	1:C:669:ILE:HG13	2.21	0.41
2:D:55:LEU:HD13	2:D:60:ILE:HD12	2.01	0.41
2:F:254:ALA:O	2:F:257:LYS:HB2	2.21	0.41
1:G:147:GLY:HA3	1:G:158:VAL:HG13	2.03	0.41
1:G:805:ILE:C	1:G:808:VAL:H	2.23	0.41
2:H:225:ALA:HA	2:H:258:PHE:CE1	2.56	0.41
2:H:33:ASN:HB3	2:H:55:LEU:HD23	2.03	0.41
2:H:48:TYR:O	2:H:51:GLN:HB2	2.21	0.41
1:C:494:ARG:HG3	1:C:547:TYR:CB	2.51	0.41
1:C:765:ASP:OD2	1:C:849:THR:OG1	2.31	0.41
2:D:302:LYS:HB2	2:D:304:VAL:HG22	2.02	0.41
1:E:608:THR:HB	1:E:618:PHE:CE2	2.56	0.41
1:E:648:LEU:CD1	1:E:845:ARG:HD3	2.51	0.41
1:G:1063:ILE:HG23	1:G:1063:ILE:O	2.21	0.41
1:G:339:ILE:HG12	11:G:5306:HOH:O	2.20	0.41
1:G:493:LYS:HD2	1:G:493:LYS:HA	1.69	0.41
1:G:568:GLY:O	1:G:602:ASN:HB2	2.21	0.41
1:G:65:TYR:OH	1:G:81:GLU:OE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:PRO:HG2	2:H:263:ILE:CD1	2.51	0.41
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.22	0.40
1:A:34:CYS:O	1:A:38:ARG:HB3	2.21	0.40
2:B:48:TYR:CZ	2:B:311:ASN:ND2	2.89	0.40
1:E:288:VAL:O	1:E:290:PRO:HD3	2.21	0.40
2:F:25:SER:HA	2:F:132:ILE:O	2.21	0.40
1:G:76:LYS:HE2	1:G:1059:THR:O	2.21	0.40
1:G:516:LEU:HA	1:G:516:LEU:HD12	1.73	0.40
2:B:237:PHE:CZ	2:B:239:SER:HA	2.56	0.40
1:C:152:MET:SD	1:C:189:GLU:HA	2.61	0.40
1:C:695:VAL:HG12	1:C:696:THR:N	2.35	0.40
1:C:772:MET:HE1	1:C:880:THR:HG22	2.03	0.40
1:C:770:GLY:HA3	1:C:823:ARG:CZ	2.51	0.40
1:C:550:GLU:HB3	2:D:117:LYS:HB2	2.04	0.40
1:E:688:LYS:HD3	1:E:838:TYR:CE2	2.56	0.40
1:G:1021:ARG:NH1	1:G:1021:ARG:HG2	2.32	0.40
2:H:307:ILE:O	2:H:362:ASP:HB2	2.20	0.40
2:H:43:LEU:HB3	2:H:75:VAL:HG13	2.03	0.40
1:A:266:ASN:ND2	11:A:5484:HOH:O	2.54	0.40
2:B:144:LEU:HD21	2:B:148:ARG:HH21	1.85	0.40
2:B:174:SER:HB2	2:B:211:ASP:OD2	2.21	0.40
2:B:246:ALA:N	2:B:247:PRO:HD2	2.36	0.40
2:B:6:LEU:HD12	2:B:16:HIS:ND1	2.36	0.40
1:C:431:ALA:HB2	1:C:435:ARG:CZ	2.51	0.40
1:C:82:ARG:HA	1:C:82:ARG:HD2	1.78	0.40
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.79	0.40
1:E:93:GLN:HB2	1:E:174:MET:HG2	2.04	0.40
1:E:772:MET:HB3	1:E:772:MET:HE3	1.76	0.40
1:E:830:PHE:CD1	1:E:839:LEU:CD1	3.04	0.40
1:E:838:TYR:N	1:E:838:TYR:CD1	2.89	0.40
1:G:1026:SER:HB2	1:G:1030:ARG:NH1	2.32	0.40
1:G:948:SER:OG	9:G:5072:IMP:H5'2	2.22	0.40
2:H:258:PHE:C	2:H:260:GLU:H	2.24	0.40
1:A:595:GLU:HA	1:A:614:ASP:OD2	2.21	0.40
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.36	0.40
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.21	0.40
1:C:367:PHE:CE1	1:C:912:ARG:HG2	2.57	0.40
1:C:471:ARG:HH21	1:C:474:GLU:CD	2.25	0.40
1:C:53:THR:OG1	1:C:56:THR:HG23	2.22	0.40
1:C:554:ASN:N	1:C:555:PRO:CD	2.85	0.40
1:C:687:LEU:HA	1:C:687:LEU:HD12	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:VAL:HG12	2:D:122:LEU:HD11	2.04	0.40
2:D:281:ALA:HB2	2:D:321:LEU:HD12	2.03	0.40
1:E:344:THR:HB	1:E:345:PRO:HD2	2.03	0.40
1:E:177:SER:OG	1:E:899:LYS:NZ	2.54	0.40
1:G:847:ALA:O	1:G:850:VAL:HG23	2.21	0.40
2:H:102:LEU:HA	2:H:102:LEU:HD23	1.89	0.40
2:H:73:SER:CA	2:H:203:ARG:NH2	2.85	0.40
2:B:190:LEU:HB2	2:B:215[A]:ARG:HB3	2.03	0.40
1:C:1027:ARG:O	1:C:1031:ARG:HG3	2.22	0.40
1:C:944:ARG:HD3	1:C:972:ASP:OD1	2.21	0.40
2:D:173:GLY:O	2:D:182:PRO:HG2	2.22	0.40
2:D:290:HIS:HA	11:D:1444:HOH:O	2.22	0.40
2:D:98:LEU:HD12	2:D:98:LEU:O	2.22	0.40
1:E:101:GLU:OE1	1:E:101:GLU:HA	2.22	0.40
1:E:420:ALA:HA	1:E:423:LYS:HD2	2.04	0.40
1:E:646:THR:HB	1:E:647:PRO:HD3	2.01	0.40
1:E:648:LEU:HD12	11:E:5366:HOH:O	2.21	0.40
1:G:237:PHE:HB3	1:G:248:ILE:O	2.22	0.40
2:H:121:LEU:HD12	2:H:121:LEU:O	2.21	0.40
2:H:305:VAL:CG1	2:H:306:MET:N	2.85	0.40
2:H:60:ILE:HG13	2:H:82:ILE:CG2	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130[B]:ARG:NH1	11:F:3079:HOH:O[3_545]	1.65	0.55
2:F:10:GLU:OE1	11:A:5434:HOH:O[3_555]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1060/1073 (99%)	1010 (95%)	46 (4%)	4 (0%)	38	35
1	C	1053/1073 (98%)	1002 (95%)	48 (5%)	3 (0%)	44	44
1	E	1064/1073 (99%)	1011 (95%)	50 (5%)	3 (0%)	44	44
1	G	1054/1073 (98%)	981 (93%)	67 (6%)	6 (1%)	28	24
2	B	378/382 (99%)	358 (95%)	18 (5%)	2 (0%)	32	28
2	D	378/382 (99%)	362 (96%)	16 (4%)	0	100	100
2	F	378/382 (99%)	360 (95%)	17 (4%)	1 (0%)	44	44
2	H	377/382 (99%)	341 (90%)	27 (7%)	9 (2%)	7	2
All	All	5742/5820 (99%)	5425 (94%)	289 (5%)	28 (0%)	32	28

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	357	SER
1	C	368	ALA
2	F	357	SER
2	H	201	ALA
2	H	248	CYS
2	H	323	ALA
2	H	357	SER
1	A	679	GLN
1	C	2	PRO
1	C	698	ILE
1	G	558	ASP
1	G	702	VAL
1	E	975	HIS
1	G	821	GLN
2	H	11	ASP
2	H	243	GLY
2	H	269	CYS
1	A	975	HIS
1	A	1027	ARG
1	G	693	ALA
1	G	788	HIS
2	H	47	SER
2	B	245	PRO
1	E	88	PRO
1	G	860	PRO
2	H	225	ALA
1	A	2	PRO

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Mol	Chain	Res	Type
1	E	702	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	873/878 (99%)	814 (93%)	59 (7%)	18	15
1	C	866/878 (99%)	813 (94%)	53 (6%)	22	18
1	E	877/878 (100%)	811 (92%)	66 (8%)	16	12
1	G	867/878 (99%)	788 (91%)	79 (9%)	11	7
2	B	309/310 (100%)	281 (91%)	28 (9%)	11	7
2	D	309/310 (100%)	292 (94%)	17 (6%)	25	22
2	F	309/310 (100%)	280 (91%)	29 (9%)	10	6
2	H	308/310 (99%)	272 (88%)	36 (12%)	6	3
All	All	4718/4752 (99%)	4351 (92%)	367 (8%)	15	11

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	38	ARG
1	A	110	GLU
1	A	153	GLU
1	A	174	MET
1	A	185	ARG
1	A	275	ILE
1	A	300	MET
1	A	333	ASP
1	A	338	ASP
1	A	363	ASN
1	A	416[A]	ASP
1	A	416[B]	ASP
1	A	423	LYS

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Mol	Chain	Res	Type
1	A	426	ARG
1	A	481	ILE
1	A	518	ASP
1	A	542	TYR
1	A	548	GLU
1	A	558	ASP
1	A	562	ILE
1	A	571	ARG
1	A	591	GLU
1	A	652	ARG
1	A	665	SER
1	A	671	ARG
1	A	675	ARG
1	A	679	GLN
1	A	680	HIS
1	A	684	ARG
1	A	688	LYS
1	A	692	ASN
1	A	706	LYS
1	A	707	GLU
1	A	725	MET
1	A	733	ASP
1	A	735	ARG
1	A	736	ARG
1	A	739	GLN
1	A	740	THR
1	A	750	VAL
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	795	SER
1	A	815	LYS
1	A	841	GLU
1	A	855	LYS
1	A	873	SER
1	A	884	ILE
1	A	912	ARG
1	A	950	ARG
1	A	955	GLU
1	A	966	LYS
1	A	998	ARG
1	A	1006	LYS

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Mol	Chain	Res	Type
1	A	1018	SER
1	A	1021	ARG
1	A	1063	ILE
2	B	3	LYS
2	B	4	SER
2	B	6	LEU
2	B	14	GLN
2	B	18	ARG
2	B	78	GLN
2	B	154	ASN
2	B	169	SER
2	B	185	LYS
2	B	186	LYS
2	B	192	PHE
2	B	222	GLN
2	B	224	SER
2	B	239	SER
2	B	261	THR
2	B	282	LYS
2	B	324	ASN
2	B	330	LYS
2	B	331	SER
2	B	332	LEU
2	B	340	ILE
2	B	344	ASP
2	B	345	LYS
2	B	357	SER
2	B	366	LEU
2	B	376	GLN
2	B	378	ARG
2	B	379	LYS
1	C	1	MET
1	C	3	LYS
1	C	4	ARG
1	C	5	THR
1	C	8	LYS
1	C	88	PRO
1	C	103	GLU
1	C	109	GLU
1	C	152	MET
1	C	174	MET
1	C	185	ARG

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Mol	Chain	Res	Type
1	C	236	ASN
1	C	275	ILE
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	416	ASP
1	C	422	THR
1	C	478	GLU
1	C	481	ILE
1	C	490	ARG
1	C	509	ARG
1	C	571	ARG
1	C	648	LEU
1	C	671	ARG
1	C	675	ARG
1	C	680	HIS
1	C	687	LEU
1	C	704	LYS
1	C	706	LYS
1	C	712	LEU
1	C	751	LEU
1	C	758	ASP
1	C	763	ASP
1	C	772	MET
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	815	LYS
1	C	855	LYS
1	C	880	THR
1	C	891	LYS
1	C	912	ARG
1	C	950	ARG
1	C	1002	GLN
1	C	1018	SER
1	C	1027	ARG
1	C	1064	SER
1	C	1073	LYS

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Mol	Chain	Res	Type
2	D	2	ILE
2	D	6	LEU
2	D	18	ARG
2	D	104	ARG
2	D	154	ASN
2	D	166	GLU
2	D	188	ASP
2	D	222	GLN
2	D	239	SER
2	D	257	LYS
2	D	263	ILE
2	D	282	LYS
2	D	324	ASN
2	D	333	PHE
2	D	357	SER
2	D	366	LEU
2	D	380	THR
1	E	1	MET
1	E	8	LYS
1	E	55	MET
1	E	58	PRO
1	E	133	ASP
1	E	174	MET
1	E	185	ARG
1	E	220	VAL
1	E	236	ASN
1	E	275	ILE
1	E	363	ASN
1	E	414	SER
1	E	416	ASP
1	E	423	LYS
1	E	426	ARG
1	E	428	LEU
1	E	509	ARG
1	E	515	LYS
1	E	518	ASP
1	E	542	TYR
1	E	548	GLU
1	E	556	SER
1	E	558	ASP
1	E	571	ARG
1	E	634[A]	LYS

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Mol	Chain	Res	Type
1	E	634[B]	LYS
1	E	648	LEU
1	E	652[A]	ARG
1	E	652[B]	ARG
1	E	671	ARG
1	E	675	ARG
1	E	688	LYS
1	E	689	GLN
1	E	698	ILE
1	E	706	LYS
1	E	711	PRO
1	E	712	LEU
1	E	731	GLU
1	E	733	ASP
1	E	735	ARG
1	E	736	ARG
1	E	739	GLN
1	E	751	LEU
1	E	753	ASP
1	E	763	ASP
1	E	772	MET
1	E	784	GLN
1	E	789	SER
1	E	795	SER
1	E	805	ILE
1	E	811	GLN
1	E	815	LYS
1	E	839	LEU
1	E	845	ARG
1	E	912	ARG
1	E	940	LYS
1	E	947	LEU
1	E	950	ARG
1	E	957	VAL
1	E	967	GLN
1	E	972	ASP
1	E	1000	HIS
1	E	1018	SER
1	E	1031	ARG
1	E	1061	LYS
1	E	1073	LYS
2	F	2	ILE

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Mol	Chain	Res	Type
2	F	6	LEU
2	F	11	ASP
2	F	18	ARG
2	F	74	GLN
2	F	87	LEU
2	F	104	ARG
2	F	106	ASN
2	F	154	ASN
2	F	166	GLU
2	F	175	TRP
2	F	178	THR
2	F	186	LYS
2	F	190	LEU
2	F	192	PHE
2	F	215	ARG
2	F	227	ASP
2	F	239	SER
2	F	257	LYS
2	F	261	THR
2	F	321	LEU
2	F	324	ASN
2	F	326	ARG
2	F	331	SER
2	F	332	LEU
2	F	343	THR
2	F	357	SER
2	F	366	LEU
2	F	379	LYS
1	G	1	MET
1	G	4	ARG
1	G	8	LYS
1	G	35[A]	LYS
1	G	35[B]	LYS
1	G	43	ARG
1	G	101	GLU
1	G	104	ARG
1	G	153	GLU
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	207	ASP
1	G	228	CYS

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Mol	Chain	Res	Type
1	G	275	ILE
1	G	313	LYS
1	G	338	ASP
1	G	343	ARG
1	G	353	ASP
1	G	363	ASN
1	G	412	LYS
1	G	414	SER
1	G	416	ASP
1	G	518	ASP
1	G	542	TYR
1	G	548	GLU
1	G	558	ASP
1	G	561	LYS
1	G	587	LEU
1	G	591	GLU
1	G	631	ARG
1	G	648	LEU
1	G	649	LYS
1	G	652	ARG
1	G	665	SER
1	G	671	ARG
1	G	675	ARG
1	G	679	GLN
1	G	688	LYS
1	G	692	ASN
1	G	700	MET
1	G	706	LYS
1	G	708	ILE
1	G	712	LEU
1	G	733	ASP
1	G	735	ARG
1	G	736	ARG
1	G	750	VAL
1	G	751	LEU
1	G	752	LEU
1	G	753	ASP
1	G	763	ASP
1	G	772	MET
1	G	784	GLN
1	G	789	SER
1	G	792	SER

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Mol	Chain	Res	Type
1	G	800	THR
1	G	805	ILE
1	G	815	LYS
1	G	820	LEU
1	G	835	ASN
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	912	ARG
1	G	940	LYS
1	G	947	LEU
1	G	950	ARG
1	G	955	GLU
1	G	967	GLN
1	G	1014	ILE
1	G	1018	SER
1	G	1021	ARG
1	G	1026	SER
1	G	1029	ILE
1	G	1032	SER
1	G	1061	LYS
1	G	1063	ILE
1	G	1073	LYS
2	H	2	ILE
2	H	6	LEU
2	H	18	ARG
2	H	50	ARG
2	H	87	LEU
2	H	104	ARG
2	H	142	LEU
2	H	145	GLU
2	H	148	ARG
2	H	154	ASN
2	H	178	THR
2	H	186	LYS
2	H	192	PHE
2	H	202	LYS
2	H	209	LEU
2	H	216	LEU
2	H	217	THR
2	H	222	GLN
2	H	224	SER

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Mol	Chain	Res	Type
2	H	227	ASP
2	H	239	SER
2	H	249	ASP
2	H	257	LYS
2	H	265	VAL
2	H	279	SER
2	H	282	LYS
2	H	300	VAL
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	342	ARG
2	H	357	SER
2	H	366	LEU
2	H	372	GLU
2	H	376	GLN
2	H	378	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	519	GLN
1	A	554	ASN
1	A	689	GLN
1	A	692	ASN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	834	ASN
1	A	835	ASN
1	A	942	HIS
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1071	GLN
2	B	76	HIS

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Mol	Chain	Res	Type
2	B	78	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
2	B	353	HIS
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	645	GLN
1	C	784	GLN
1	C	803	GLN
1	C	812	GLN
1	C	834	ASN
1	C	835	ASN
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1007	ASN
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	78	GLN
2	D	106	ASN
2	D	154	ASN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN
1	E	266	ASN
1	E	457	ASN
1	E	554	ASN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	814	GLN
1	E	834	ASN
1	E	835	ASN
1	E	967	GLN
1	E	987	ASN

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Mol	Chain	Res	Type
1	E	992	ASN
1	E	995	HIS
1	E	1000	HIS
1	E	1035	GLN
1	E	1071	GLN
2	F	51	GLN
2	F	74	GLN
2	F	105	HIS
2	F	154	ASN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	225	ASN
1	G	457	ASN
1	G	519	GLN
1	G	554	ASN
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN
1	G	877	GLN
1	G	936	ASN
1	G	942	HIS
1	G	967	GLN
1	G	987	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1069	HIS
1	G	1071	GLN
2	H	51	GLN
2	H	76	HIS
2	H	78	GLN
2	H	105	HIS
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 52 are monoatomic - leaving 28 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$
7	ADP	A	5000	3	25,29,29	1.16	4 (16%)	24,45,45	1.18	2 (8%)
6	PO4	A	5006	3,4	4,4,4	1.66	1 (25%)	6,6,6	1.12	0
7	ADP	A	5007	3,4	25,29,29	1.15	2 (8%)	24,45,45	1.03	1 (4%)
8	ORN	A	5011	-	3,8,8	0.52	0	2,9,9	0.30	0
9	IMP	A	5012	-	21,25,25	1.64	6 (28%)	22,38,38	1.45	4 (18%)
10	NET	A	5013	-	8,8,8	0.67	0	10,10,10	0.58	0
8	ORN	A	5014	-	3,8,8	0.48	0	2,9,9	0.10	0
7	ADP	C	5020	3	25,29,29	1.32	5 (20%)	24,45,45	1.38	4 (16%)
6	PO4	C	5026	3,4	4,4,4	2.07	2 (50%)	6,6,6	0.76	0
7	ADP	C	5027	3,4	25,29,29	1.40	4 (16%)	24,45,45	1.08	2 (8%)
8	ORN	C	5031	-	3,8,8	0.37	0	2,9,9	0.35	0
9	IMP	C	5032	-	21,25,25	1.57	4 (19%)	22,38,38	1.42	4 (18%)
10	NET	C	5033	-	8,8,8	0.59	0	10,10,10	0.49	0
8	ORN	C	5034	-	3,8,8	0.57	0	2,9,9	0.24	0
7	ADP	E	5040	3	25,29,29	1.10	2 (8%)	24,45,45	1.16	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	E	5046	3,4	4,4,4	2.33	3 (75%)	6,6,6	0.55	0
7	ADP	E	5047	3,4	25,29,29	1.34	5 (20%)	24,45,45	1.17	3 (12%)
8	ORN	E	5051	-	3,8,8	0.48	0	2,9,9	0.29	0
9	IMP	E	5052	-	21,25,25	1.36	4 (19%)	22,38,38	2.09	5 (22%)
10	NET	E	5053	-	8,8,8	0.79	0	10,10,10	0.36	0
8	ORN	E	5054	-	3,8,8	0.41	0	2,9,9	1.23	0
7	ADP	G	5060	3	25,29,29	1.16	2 (8%)	24,45,45	1.30	3 (12%)
6	PO4	G	5066	3,4	4,4,4	1.48	1 (25%)	6,6,6	0.85	0
7	ADP	G	5067	3,4	25,29,29	1.39	5 (20%)	24,45,45	1.33	3 (12%)
8	ORN	G	5071	-	3,8,8	0.37	0	2,9,9	0.14	0
9	IMP	G	5072	-	21,25,25	1.37	4 (19%)	22,38,38	1.73	6 (27%)
10	NET	G	5073	-	8,8,8	0.67	0	10,10,10	0.47	0
8	ORN	G	5074	-	3,8,8	0.47	0	2,9,9	0.78	0

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
7	ADP	A	5000	3	-	0/12/32/32	0/3/3/3
6	PO4	A	5006	3,4	-	0/0/0/0	0/0/0/0
7	ADP	A	5007	3,4	-	0/12/32/32	0/3/3/3
8	ORN	A	5011	-	-	0/4/8/8	0/0/0/0
9	IMP	A	5012	-	-	0/6/26/26	0/3/3/3
10	NET	A	5013	-	-	0/12/12/12	0/0/0/0
8	ORN	A	5014	-	-	0/4/8/8	0/0/0/0
7	ADP	C	5020	3	-	0/12/32/32	0/3/3/3
6	PO4	C	5026	3,4	-	0/0/0/0	0/0/0/0
7	ADP	C	5027	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	5031	-	-	0/4/8/8	0/0/0/0
9	IMP	C	5032	-	-	0/6/26/26	0/3/3/3
10	NET	C	5033	-	-	0/12/12/12	0/0/0/0
8	ORN	C	5034	-	-	0/4/8/8	0/0/0/0
7	ADP	E	5040	3	-	0/12/32/32	0/3/3/3
6	PO4	E	5046	3,4	-	0/0/0/0	0/0/0/0
7	ADP	E	5047	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	5051	-	-	0/4/8/8	0/0/0/0
9	IMP	E	5052	-	-	0/6/26/26	0/3/3/3
10	NET	E	5053	-	-	0/12/12/12	0/0/0/0
8	ORN	E	5054	-	-	0/4/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	G	5060	3	-	0/12/32/32	0/3/3/3
6	PO4	G	5066	3,4	-	0/0/0/0	0/0/0/0
7	ADP	G	5067	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	5071	-	-	0/4/8/8	0/0/0/0
9	IMP	G	5072	-	-	0/6/26/26	0/3/3/3
10	NET	G	5073	-	-	0/12/12/12	0/0/0/0
8	ORN	G	5074	-	-	0/4/8/8	0/0/0/0

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5020	ADP	O4'-C1'	-3.40	1.36	1.41
7	G	5067	ADP	O4'-C1'	-3.27	1.36	1.41
6	E	5046	PO4	P-O2	-3.16	1.43	1.54
9	A	5012	IMP	O4'-C1'	-2.80	1.37	1.41
6	C	5026	PO4	P-O4	-2.74	1.44	1.54
9	E	5052	IMP	P-O3P	-2.69	1.43	1.54
6	E	5046	PO4	P-O3	-2.62	1.45	1.54
9	C	5032	IMP	O4'-C1'	-2.48	1.37	1.41
6	C	5026	PO4	P-O2	-2.46	1.45	1.54
6	A	5006	PO4	P-O2	-2.40	1.45	1.54
9	E	5052	IMP	O4'-C1'	-2.34	1.38	1.41
9	G	5072	IMP	O4'-C1'	-2.27	1.38	1.41
7	E	5047	ADP	O4'-C1'	-2.27	1.38	1.41
9	A	5012	IMP	P-O3P	-2.22	1.45	1.54
7	A	5000	ADP	C4-N3	-2.18	1.32	1.35
6	E	5046	PO4	P-O4	-2.18	1.46	1.54
7	G	5060	ADP	C2'-C1'	-2.09	1.50	1.53
6	G	5066	PO4	P-O2	-2.01	1.47	1.54
7	A	5000	ADP	PB-O3A	2.01	1.63	1.60
7	C	5020	ADP	PB-O3A	2.03	1.63	1.60
7	A	5007	ADP	O2'-C2'	2.06	1.47	1.43
9	E	5052	IMP	O2'-C2'	2.06	1.47	1.43
9	C	5032	IMP	O2'-C2'	2.07	1.47	1.43
7	E	5047	ADP	O2'-C2'	2.11	1.47	1.43
7	C	5020	ADP	C2-N1	2.14	1.37	1.33
7	G	5067	ADP	C2-N1	2.19	1.38	1.33
7	G	5067	ADP	O2'-C2'	2.20	1.48	1.43
9	A	5012	IMP	O3'-C3'	2.27	1.48	1.43
9	A	5012	IMP	C2-N1	2.28	1.38	1.33
7	A	5000	ADP	O2'-C2'	2.33	1.48	1.43
9	G	5072	IMP	O3'-C3'	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	5040	ADP	O3'-C3'	2.38	1.48	1.43
9	G	5072	IMP	O2'-C2'	2.42	1.48	1.43
7	E	5047	ADP	C2-N1	2.48	1.38	1.33
9	A	5012	IMP	C6-N1	2.49	1.37	1.33
7	C	5027	ADP	C2-N1	2.49	1.38	1.33
7	E	5047	ADP	O3'-C3'	2.57	1.48	1.43
7	A	5000	ADP	O3'-C3'	2.58	1.48	1.43
7	C	5020	ADP	O3'-C3'	2.59	1.48	1.43
9	C	5032	IMP	O3'-C3'	2.62	1.49	1.43
7	G	5067	ADP	O3'-C3'	2.68	1.49	1.43
9	G	5072	IMP	O6-C6	2.70	1.31	1.24
7	A	5007	ADP	O3'-C3'	2.82	1.49	1.43
7	C	5020	ADP	O2'-C2'	2.88	1.49	1.43
9	E	5052	IMP	O6-C6	3.01	1.32	1.24
7	C	5027	ADP	O2'-C2'	3.02	1.49	1.43
7	E	5040	ADP	PB-O3A	3.06	1.65	1.60
7	G	5060	ADP	O3'-C3'	3.29	1.50	1.43
7	C	5027	ADP	O3'-C3'	3.32	1.50	1.43
7	G	5067	ADP	PB-O3A	3.55	1.65	1.60
7	C	5027	ADP	PB-O3A	3.74	1.66	1.60
9	C	5032	IMP	O6-C6	4.02	1.34	1.24
9	A	5012	IMP	O6-C6	4.08	1.34	1.24
7	E	5047	ADP	PB-O3A	4.15	1.66	1.60

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	5052	IMP	O3P-P-O5'	-6.32	89.90	106.73
9	G	5072	IMP	O3P-P-O5'	-3.41	97.67	106.73
9	C	5032	IMP	O3P-P-O5'	-3.04	98.66	106.73
9	E	5052	IMP	C6-C5-C4	-2.97	117.89	120.84
9	G	5072	IMP	C6-C5-C4	-2.89	117.97	120.84
7	C	5020	ADP	N6-C6-N1	-2.45	113.91	118.77
9	A	5012	IMP	C6-C5-C4	-2.31	118.55	120.84
7	A	5000	ADP	C2'-C3'-C4'	-2.23	98.28	102.62
7	C	5020	ADP	C2'-C3'-C4'	-2.14	98.45	102.62
9	A	5012	IMP	O3P-P-O5'	-2.03	101.33	106.73
9	E	5052	IMP	C4-C5-N7	2.06	111.40	109.41
9	C	5032	IMP	O2'-C2'-C3'	2.08	118.49	111.83
9	C	5032	IMP	C2-N1-C6	2.15	119.50	115.91
9	G	5072	IMP	O3P-P-O2P	2.29	116.87	107.61
7	G	5060	ADP	C5-C6-N6	2.31	125.18	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	5020	ADP	O3'-C3'-C2'	2.32	119.25	111.83
9	C	5032	IMP	O3'-C3'-C2'	2.36	119.38	111.83
7	E	5047	ADP	C5-C6-N6	2.39	125.33	120.47
7	E	5047	ADP	O3'-C3'-C2'	2.41	119.54	111.83
7	C	5027	ADP	O2'-C2'-C3'	2.48	119.77	111.83
7	A	5007	ADP	O2'-C2'-C3'	2.56	120.02	111.83
9	E	5052	IMP	O3'-C3'-C2'	2.58	120.10	111.83
9	G	5072	IMP	O3'-C3'-C2'	2.60	120.16	111.83
7	C	5027	ADP	C5-C6-N6	2.66	125.90	120.47
7	E	5047	ADP	O2'-C2'-C3'	2.67	120.40	111.83
9	A	5012	IMP	O2P-P-O5'	2.71	113.93	106.73
7	G	5067	ADP	C5-C6-N6	2.73	126.03	120.47
7	G	5067	ADP	O3'-C3'-C2'	2.76	120.68	111.83
7	G	5067	ADP	O2'-C2'-C3'	2.79	120.78	111.83
7	E	5040	ADP	C5-C6-N6	2.80	126.18	120.47
7	E	5040	ADP	O3'-C3'-C2'	2.81	120.82	111.83
9	G	5072	IMP	C4-C5-N7	2.94	112.25	109.41
7	G	5060	ADP	O2'-C2'-C3'	2.95	121.29	111.83
9	G	5072	IMP	O2'-C2'-C3'	2.99	121.40	111.83
9	A	5012	IMP	O3'-C3'-C2'	3.03	121.55	111.83
7	A	5000	ADP	C5-C6-N6	3.14	126.86	120.47
7	G	5060	ADP	O3'-C3'-C2'	3.29	122.37	111.83
9	E	5052	IMP	O2'-C2'-C3'	3.70	123.67	111.83
7	C	5020	ADP	C5-C6-N6	4.18	129.00	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	5007	ADP	2	0
8	A	5011	ORN	1	0
9	A	5012	IMP	1	0
8	A	5014	ORN	3	0
7	C	5027	ADP	1	0
8	C	5031	ORN	2	0
9	C	5032	IMP	1	0
8	C	5034	ORN	1	0
7	E	5040	ADP	1	0
7	E	5047	ADP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	5051	ORN	2	0
9	E	5052	IMP	2	0
10	E	5053	NET	3	0
8	E	5054	ORN	2	0
7	G	5060	ADP	2	0
7	G	5067	ADP	3	0
8	G	5071	ORN	1	0
9	G	5072	IMP	1	0
10	G	5073	NET	1	0
8	G	5074	ORN	3	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.