



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2017 – 04:53 PM EST

PDB ID : 1F4A
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-ORTHORHOMBIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : unknown
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

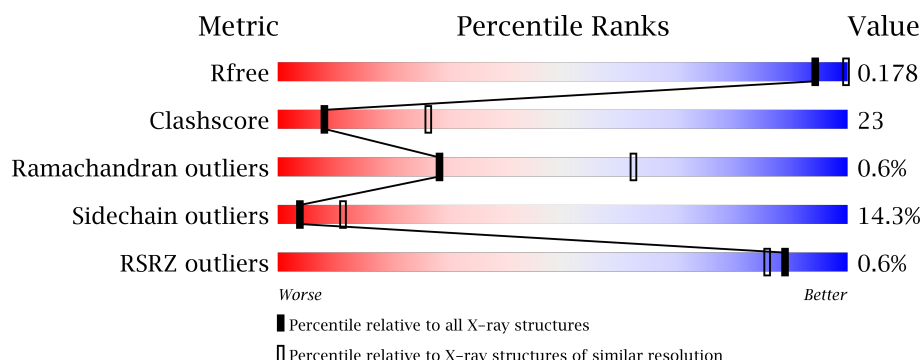
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Mol	Chain	Length	Quality of chain
1	A	1021	<div> <div> <div>0.1%</div> <div>49%</div> <div>38%</div> <div>11%</div> <div>0.1%</div> </div> </div>
1	B	1021	<div> <div>49%</div> <div>38%</div> <div>11%</div> <div>0.1%</div> </div>
1	C	1021	<div> <div>49%</div> <div>38%</div> <div>11%</div> <div>0.1%</div> </div>
1	D	1021	<div> <div>0.1%</div> <div>49%</div> <div>38%</div> <div>11%</div> <div>0.1%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34424 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	B	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	C	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	D	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	365	Total	O	0	0
			365	365		
3	B	366	Total	O	0	0
			366	366		
3	C	367	Total	O	0	0
			367	367		
3	D	366	Total	O	0	0
			366	366		

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 ($\text{RSRZ} > 2$). 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.

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

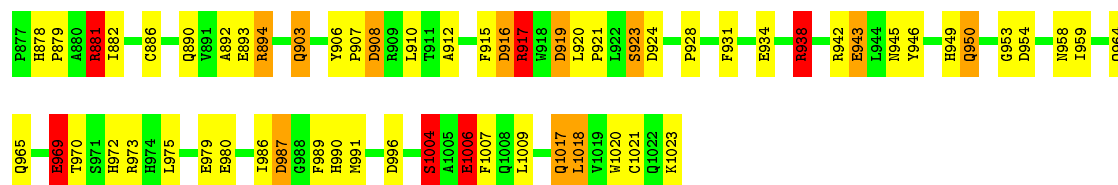
49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

Chain A: ■ ■ ■ ■

49% ■ ■ ■ ■ 38% ■ ■ ■ ■ 11%

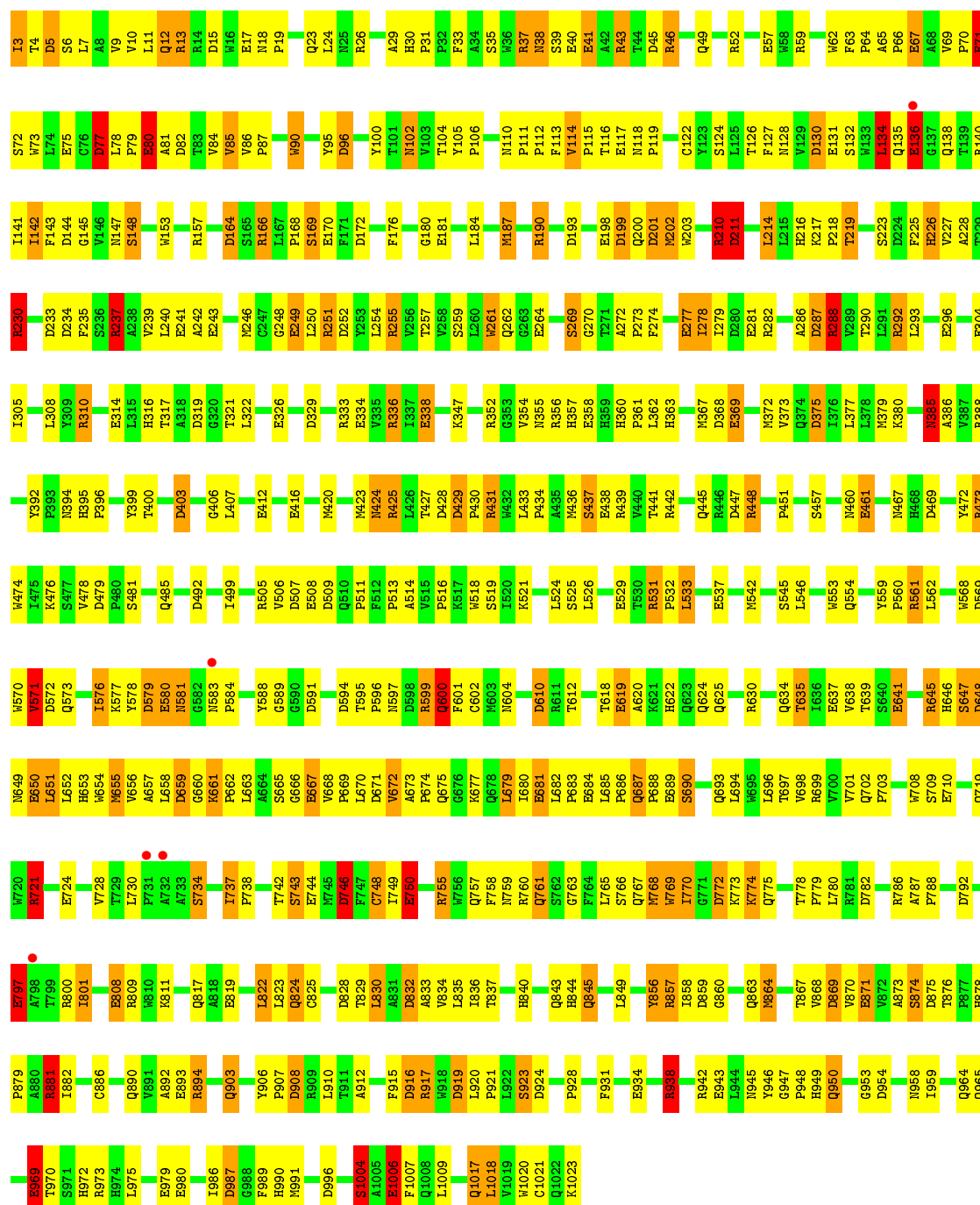
Chain A: ■ ■ ■ ■

49% ■ ■



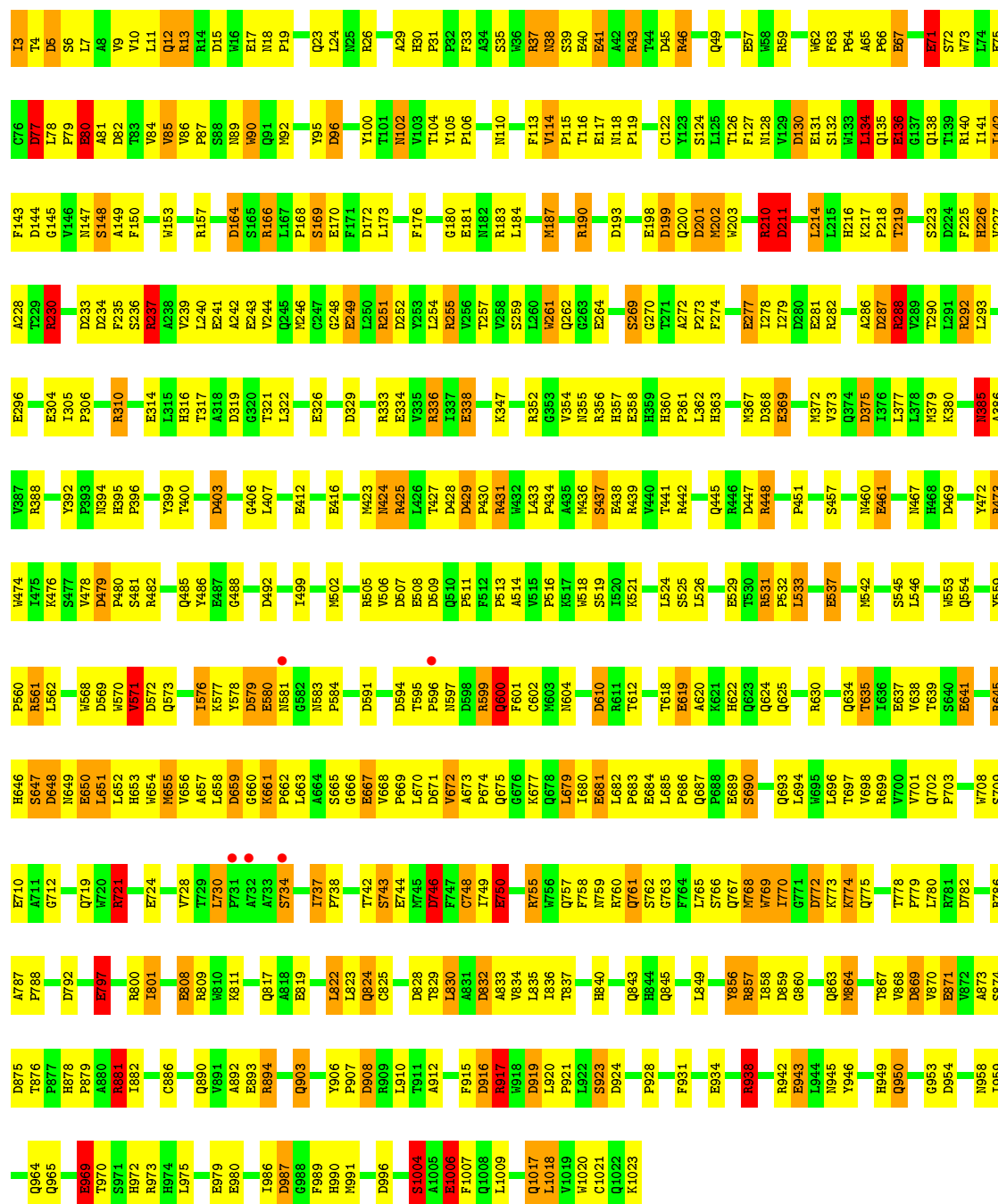
• Molecule 1: BETA-GALACTOSIDASE

Chain B: 49% 38% 11%



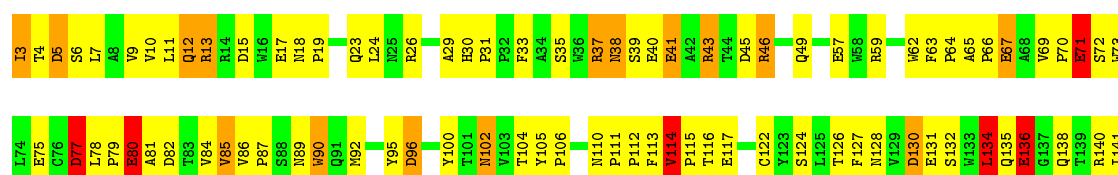
• Molecule 1: BETA-GALACTOSIDASE

Chain C: 



• Molecule 1: BETA-GALACTOSIDASE

Chain D: 



E969	H878	E797	V720	L651	D569	R473	R388	E304	T229	I142
E970	P879	R800	R721	L652	H570	H474	Y392	L305	R230	F143
S971	A880	I801	E724	H653	Y571	I475	Y393	L308	D233	D144
H972	R881	E808	V728	H654	D572	K476	N394	R310	D234	G145
R973	L882	E809	V729	M655	Q573	S477	H395	E314	P235	N147
H974	C886	R809	L730	A656	I576	D479	P396	L315	S236	S148
L975	Q890	H810	P731	L657	K577	P480	Y399	H316	R237	A149
E979	H891	K811	A732	L658	Y578	S481	T400	T317	A238	F150
E980	A892	Q817	A733	G660	D579	Q485	Y399	E241	E242	W153
E983	E893	A818	S734	K661	E580	D492	D403	A318	E243	R157
R894	E819	L663	I737	P662	H581	D492	L407	G320	E243	
Q903	L822	A664	P738	S665	N583	T499	E412	L322		D164
Y906	L823	G666	T742	G666	P584	R505	E416	E326	M246	S165
P907	Q824	E667	S743	E667	D591	V506	H416	E326	C247	R166
D908	C825	V668	E744	V668	D594	D507	T417	D329	Q248	L167
R909	D828	P669	H745	P669	T595	E508	H418		E249	P168
G909	L829	L670	D746	L670	P596	D509	G419		L250	S169
L910	L830	V672	F747	V672	N597	Q510	M423	R333	R252	E170
T911	A831	A673	C748	A673	D598	P611	E424	E334	F171	D172
A912	D832	P674	I749	P674	R599	F512	R425	V335	L254	
F915	A833	Q675	E750	Q675	Q600	P513	R425	R335	R255	F176
D916	V834	G676	R755	G676	F601	A514	L436	T337	V256	
R918	L835	Q678	H756	Q678	G602	P515	T427	E338	T257	G180
E918	L836	H756	Q757	H756	N603	P516	D428		V258	E181
D919	T837	Q757	F758	L680	N604	H517	D429	R347	S259	
P921	H840	N759	N759	I680	D610	H518	P430	R352	W261	L184
L922	Q843	Q761	R760	E881	R611	T520	H431	G353	Q262	H187
S923	H844	S762	Q761	E884	T612	R521	L433	V354	G263	
D924	Q845	G763	G763	L685	T618	L524	P434	R356	E264	R190
P928	L849	F764	F764	P686	E619	S525	A435	R357	S269	D193
F931	L849	L765	S766	Q687	A620	L526	S437	E358	G270	
E934	K854	Q767	Q767	P688	K621	E529	E438	R359	T271	E198
Y856	T855	H768	H768	E889	H622	T530	R439	H360	A272	D199
R857	Y856	N769	N769	P689	Q623	H531	V440	P361	P273	Q200
I770	R857	I770	I770	R698	Q624	P532	T441	L362	F274	D201
I858	L858	Q771	Q771	R699	Q625	L533	R442	H363	E277	M202
D859	Q860	D772	D772	V700	R630	L533	Q445	R367	L278	W203
Q860	Q860	K773	K773	V638	T634	E537	R446	D368	L278	R210
Q863	Q863	Q774	Q774	V639	T634	N542	D447	E369	D280	D211
M864	M864	Q775	Q775	E641	T636	L546	R448		E281	
T867	T867	T776	T776	E641	E637	S545	P451	R372	R282	L214
V868	V868	P779	P779	V701	V638	L546	S457	Q374	A286	L215
V870	V870	L780	L780	Q702	V639	N553	N460	D375	D287	H216
E871	E871	D782	D782	P703	E641	Q554	E461	L377	P218	K217
V872	V872	R786	R786	W708	E641	Q554	E461	L378	V289	T219
A873	A873	A787	A787	S709	R645	Y559	N467	K379	L291	S223
S874	S874	F788	F788	E710	H646	P560	H468	K380	R292	D224
D875	D875	G712	G712	A711	S647	R561	D469		L293	F225
T876	T876	D792	D792	G712	D648	L562	A386		E296	H226
P877	P877			Q719	N649	N568	Y472			V227
					E650					A228

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.40 Å 173.40 Å 204.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.97 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.5 (24.97-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.80 Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.167 , 0.198 0.149 , 0.178	Depositor DCC
R_{free} test set	1590 reflections (1.53%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 100.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34424	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.08	52/8515 (0.6%)	1.61	173/11615 (1.5%)
1	B	1.08	52/8515 (0.6%)	1.61	175/11615 (1.5%)
1	C	1.08	52/8515 (0.6%)	1.61	174/11615 (1.5%)
1	D	1.08	52/8515 (0.6%)	1.61	176/11615 (1.5%)
All	All	1.08	208/34060 (0.6%)	1.61	698/46460 (1.5%)

All (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	CD-OE2	9.53	1.36	1.25
1	C	75	GLU	CD-OE2	9.53	1.36	1.25
1	D	75	GLU	CD-OE2	9.49	1.36	1.25
1	B	75	GLU	CD-OE2	9.46	1.36	1.25
1	D	710	GLU	CD-OE2	7.62	1.34	1.25
1	B	710	GLU	CD-OE2	7.61	1.34	1.25
1	A	710	GLU	CD-OE2	7.61	1.34	1.25
1	C	710	GLU	CD-OE2	7.61	1.34	1.25
1	B	136	GLU	CD-OE2	7.46	1.33	1.25
1	D	136	GLU	CD-OE2	7.44	1.33	1.25
1	A	181	GLU	CD-OE2	7.44	1.33	1.25
1	C	181	GLU	CD-OE2	7.43	1.33	1.25
1	D	181	GLU	CD-OE2	7.43	1.33	1.25
1	D	264	GLU	CD-OE2	7.43	1.33	1.25
1	A	136	GLU	CD-OE2	7.42	1.33	1.25
1	B	181	GLU	CD-OE2	7.41	1.33	1.25
1	B	40	GLU	CD-OE2	7.41	1.33	1.25
1	A	508	GLU	CD-OE2	7.40	1.33	1.25
1	A	264	GLU	CD-OE2	7.39	1.33	1.25
1	A	681	GLU	CD-OE2	7.38	1.33	1.25
1	B	264	GLU	CD-OE2	7.38	1.33	1.25
1	C	264	GLU	CD-OE2	7.38	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	508	GLU	CD-OE2	7.38	1.33	1.25
1	B	508	GLU	CD-OE2	7.37	1.33	1.25
1	C	681	GLU	CD-OE2	7.37	1.33	1.25
1	B	681	GLU	CD-OE2	7.36	1.33	1.25
1	C	40	GLU	CD-OE2	7.36	1.33	1.25
1	C	136	GLU	CD-OE2	7.36	1.33	1.25
1	D	40	GLU	CD-OE2	7.36	1.33	1.25
1	A	40	GLU	CD-OE2	7.35	1.33	1.25
1	C	508	GLU	CD-OE2	7.35	1.33	1.25
1	D	681	GLU	CD-OE2	7.34	1.33	1.25
1	B	314	GLU	CD-OE2	7.32	1.33	1.25
1	C	943	GLU	CD-OE2	7.26	1.33	1.25
1	A	314	GLU	CD-OE2	7.25	1.33	1.25
1	A	943	GLU	CD-OE2	7.24	1.33	1.25
1	C	314	GLU	CD-OE2	7.24	1.33	1.25
1	B	943	GLU	CD-OE2	7.22	1.33	1.25
1	D	314	GLU	CD-OE2	7.21	1.33	1.25
1	D	943	GLU	CD-OE2	7.18	1.33	1.25
1	C	369	GLU	CD-OE2	7.11	1.33	1.25
1	B	369	GLU	CD-OE2	7.07	1.33	1.25
1	A	797	GLU	CD-OE2	7.05	1.33	1.25
1	C	797	GLU	CD-OE2	7.04	1.33	1.25
1	D	369	GLU	CD-OE2	7.04	1.33	1.25
1	B	797	GLU	CD-OE2	7.04	1.33	1.25
1	A	369	GLU	CD-OE2	7.03	1.33	1.25
1	D	797	GLU	CD-OE2	7.02	1.33	1.25
1	C	979	GLU	CD-OE2	6.94	1.33	1.25
1	D	979	GLU	CD-OE2	6.92	1.33	1.25
1	A	650	GLU	CD-OE2	6.88	1.33	1.25
1	A	979	GLU	CD-OE2	6.87	1.33	1.25
1	D	650	GLU	CD-OE2	6.85	1.33	1.25
1	B	650	GLU	CD-OE2	6.85	1.33	1.25
1	C	650	GLU	CD-OE2	6.82	1.33	1.25
1	D	969	GLU	CD-OE2	6.81	1.33	1.25
1	C	750	GLU	CD-OE2	6.79	1.33	1.25
1	A	326	GLU	CD-OE2	6.77	1.33	1.25
1	B	979	GLU	CD-OE2	6.77	1.33	1.25
1	B	326	GLU	CD-OE2	6.76	1.33	1.25
1	A	969	GLU	CD-OE2	6.76	1.33	1.25
1	D	326	GLU	CD-OE2	6.76	1.33	1.25
1	D	724	GLU	CD-OE2	6.76	1.33	1.25
1	C	969	GLU	CD-OE2	6.75	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	750	GLU	CD-OE2	6.75	1.33	1.25
1	C	326	GLU	CD-OE2	6.75	1.33	1.25
1	B	969	GLU	CD-OE2	6.74	1.33	1.25
1	B	724	GLU	CD-OE2	6.73	1.33	1.25
1	C	724	GLU	CD-OE2	6.73	1.33	1.25
1	B	198	GLU	CD-OE2	6.72	1.33	1.25
1	A	724	GLU	CD-OE2	6.72	1.33	1.25
1	B	750	GLU	CD-OE2	6.69	1.33	1.25
1	D	241	GLU	CD-OE2	6.68	1.32	1.25
1	A	198	GLU	CD-OE2	6.67	1.32	1.25
1	C	198	GLU	CD-OE2	6.66	1.32	1.25
1	C	241	GLU	CD-OE2	6.66	1.32	1.25
1	A	241	GLU	CD-OE2	6.66	1.32	1.25
1	D	198	GLU	CD-OE2	6.65	1.32	1.25
1	D	750	GLU	CD-OE2	6.64	1.32	1.25
1	B	241	GLU	CD-OE2	6.61	1.32	1.25
1	C	338	GLU	CD-OE2	6.55	1.32	1.25
1	A	338	GLU	CD-OE2	6.50	1.32	1.25
1	B	338	GLU	CD-OE2	6.50	1.32	1.25
1	D	338	GLU	CD-OE2	6.45	1.32	1.25
1	A	461	GLU	CD-OE2	6.38	1.32	1.25
1	C	438	GLU	CD-OE2	6.37	1.32	1.25
1	B	461	GLU	CD-OE2	6.35	1.32	1.25
1	D	461	GLU	CD-OE2	6.35	1.32	1.25
1	B	438	GLU	CD-OE2	6.34	1.32	1.25
1	A	438	GLU	CD-OE2	6.34	1.32	1.25
1	C	461	GLU	CD-OE2	6.32	1.32	1.25
1	B	296	GLU	CD-OE2	6.32	1.32	1.25
1	D	438	GLU	CD-OE2	6.32	1.32	1.25
1	A	296	GLU	CD-OE2	6.31	1.32	1.25
1	D	296	GLU	CD-OE2	6.30	1.32	1.25
1	C	296	GLU	CD-OE2	6.26	1.32	1.25
1	C	249	GLU	CD-OE2	6.22	1.32	1.25
1	A	249	GLU	CD-OE2	6.21	1.32	1.25
1	D	249	GLU	CD-OE2	6.21	1.32	1.25
1	B	537	GLU	CD-OE2	6.20	1.32	1.25
1	A	744	GLU	CD-OE2	6.20	1.32	1.25
1	D	744	GLU	CD-OE2	6.19	1.32	1.25
1	B	744	GLU	CD-OE2	6.19	1.32	1.25
1	C	637	GLU	CD-OE2	6.17	1.32	1.25
1	C	808	GLU	CD-OE2	6.17	1.32	1.25
1	C	744	GLU	CD-OE2	6.17	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	808	GLU	CD-OE2	6.16	1.32	1.25
1	B	637	GLU	CD-OE2	6.15	1.32	1.25
1	C	537	GLU	CD-OE2	6.15	1.32	1.25
1	A	808	GLU	CD-OE2	6.14	1.32	1.25
1	C	57	GLU	CD-OE2	6.14	1.32	1.25
1	A	637	GLU	CD-OE2	6.14	1.32	1.25
1	D	537	GLU	CD-OE2	6.14	1.32	1.25
1	D	808	GLU	CD-OE2	6.14	1.32	1.25
1	A	537	GLU	CD-OE2	6.14	1.32	1.25
1	B	249	GLU	CD-OE2	6.12	1.32	1.25
1	D	57	GLU	CD-OE2	6.12	1.32	1.25
1	A	57	GLU	CD-OE2	6.10	1.32	1.25
1	B	57	GLU	CD-OE2	6.10	1.32	1.25
1	D	637	GLU	CD-OE2	6.10	1.32	1.25
1	D	667	GLU	CD-OE2	6.08	1.32	1.25
1	D	641	GLU	CD-OE2	6.05	1.32	1.25
1	D	281	GLU	CD-OE2	6.04	1.32	1.25
1	A	667	GLU	CD-OE2	6.03	1.32	1.25
1	C	667	GLU	CD-OE2	6.03	1.32	1.25
1	A	641	GLU	CD-OE2	6.03	1.32	1.25
1	B	641	GLU	CD-OE2	6.00	1.32	1.25
1	B	80	GLU	CD-OE2	6.00	1.32	1.25
1	C	80	GLU	CD-OE2	5.99	1.32	1.25
1	B	667	GLU	CD-OE2	5.99	1.32	1.25
1	D	80	GLU	CD-OE2	5.99	1.32	1.25
1	A	80	GLU	CD-OE2	5.97	1.32	1.25
1	A	281	GLU	CD-OE2	5.97	1.32	1.25
1	C	641	GLU	CD-OE2	5.96	1.32	1.25
1	C	281	GLU	CD-OE2	5.96	1.32	1.25
1	B	281	GLU	CD-OE2	5.94	1.32	1.25
1	C	871	GLU	CD-OE2	5.90	1.32	1.25
1	C	41	GLU	CD-OE2	5.89	1.32	1.25
1	A	871	GLU	CD-OE2	5.88	1.32	1.25
1	D	871	GLU	CD-OE2	5.88	1.32	1.25
1	D	41	GLU	CD-OE2	5.87	1.32	1.25
1	A	41	GLU	CD-OE2	5.84	1.32	1.25
1	B	871	GLU	CD-OE2	5.84	1.32	1.25
1	B	41	GLU	CD-OE2	5.83	1.32	1.25
1	B	334	GLU	CD-OE2	5.77	1.31	1.25
1	A	334	GLU	CD-OE2	5.74	1.31	1.25
1	D	334	GLU	CD-OE2	5.73	1.31	1.25
1	C	334	GLU	CD-OE2	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	GLU	CD-OE2	5.55	1.31	1.25
1	C	71	GLU	CD-OE2	5.52	1.31	1.25
1	A	71	GLU	CD-OE2	5.50	1.31	1.25
1	D	71	GLU	CD-OE2	5.48	1.31	1.25
1	B	619	GLU	CD-OE2	5.45	1.31	1.25
1	B	1006	GLU	CD-OE2	5.42	1.31	1.25
1	A	619	GLU	CD-OE2	5.41	1.31	1.25
1	C	1006	GLU	CD-OE2	5.39	1.31	1.25
1	C	619	GLU	CD-OE2	5.39	1.31	1.25
1	C	412	GLU	CD-OE2	5.39	1.31	1.25
1	D	1006	GLU	CD-OE2	5.38	1.31	1.25
1	D	131	GLU	CD-OE2	5.37	1.31	1.25
1	B	412	GLU	CD-OE2	5.36	1.31	1.25
1	A	1006	GLU	CD-OE2	5.36	1.31	1.25
1	B	131	GLU	CD-OE2	5.36	1.31	1.25
1	D	980	GLU	CD-OE2	5.36	1.31	1.25
1	D	580	GLU	CD-OE2	5.35	1.31	1.25
1	D	619	GLU	CD-OE2	5.35	1.31	1.25
1	A	412	GLU	CD-OE2	5.33	1.31	1.25
1	C	131	GLU	CD-OE2	5.33	1.31	1.25
1	A	17	GLU	CD-OE2	5.32	1.31	1.25
1	D	412	GLU	CD-OE2	5.31	1.31	1.25
1	A	131	GLU	CD-OE2	5.31	1.31	1.25
1	A	277	GLU	CD-OE2	5.31	1.31	1.25
1	B	277	GLU	CD-OE2	5.31	1.31	1.25
1	A	980	GLU	CD-OE2	5.30	1.31	1.25
1	A	580	GLU	CD-OE2	5.30	1.31	1.25
1	D	117	GLU	CD-OE2	5.30	1.31	1.25
1	C	17	GLU	CD-OE2	5.30	1.31	1.25
1	D	17	GLU	CD-OE2	5.29	1.31	1.25
1	B	17	GLU	CD-OE2	5.29	1.31	1.25
1	A	934	GLU	CD-OE2	5.29	1.31	1.25
1	C	580	GLU	CD-OE2	5.28	1.31	1.25
1	C	277	GLU	CD-OE2	5.28	1.31	1.25
1	A	117	GLU	CD-OE2	5.28	1.31	1.25
1	D	277	GLU	CD-OE2	5.28	1.31	1.25
1	B	934	GLU	CD-OE2	5.27	1.31	1.25
1	C	980	GLU	CD-OE2	5.27	1.31	1.25
1	B	893	GLU	CD-OE2	5.27	1.31	1.25
1	B	580	GLU	CD-OE2	5.27	1.31	1.25
1	A	684	GLU	CD-OE2	5.27	1.31	1.25
1	B	980	GLU	CD-OE2	5.27	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	689	GLU	CD-OE2	5.26	1.31	1.25
1	D	934	GLU	CD-OE2	5.26	1.31	1.25
1	A	893	GLU	CD-OE2	5.26	1.31	1.25
1	C	117	GLU	CD-OE2	5.26	1.31	1.25
1	C	934	GLU	CD-OE2	5.26	1.31	1.25
1	B	689	GLU	CD-OE2	5.25	1.31	1.25
1	C	893	GLU	CD-OE2	5.24	1.31	1.25
1	D	684	GLU	CD-OE2	5.23	1.31	1.25
1	D	689	GLU	CD-OE2	5.22	1.31	1.25
1	A	689	GLU	CD-OE2	5.22	1.31	1.25
1	C	819	GLU	CD-OE2	5.21	1.31	1.25
1	B	819	GLU	CD-OE2	5.21	1.31	1.25
1	C	684	GLU	CD-OE2	5.21	1.31	1.25
1	B	684	GLU	CD-OE2	5.20	1.31	1.25
1	D	893	GLU	CD-OE2	5.20	1.31	1.25
1	B	117	GLU	CD-OE2	5.20	1.31	1.25
1	A	819	GLU	CD-OE2	5.19	1.31	1.25
1	D	819	GLU	CD-OE2	5.16	1.31	1.25

All (698) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	809[A]	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	B	809[B]	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	809[A]	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	A	809[B]	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	D	809[A]	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	D	809[B]	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	C	809[A]	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	C	809[B]	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	C	881	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	D	881	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	C	881	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	A	881	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	D	881	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	A	881	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	B	881	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	B	881	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	A	531	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	531	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	D	531	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	C	531	ARG	NE-CZ-NH1	10.71	125.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	385	ASN	CB-CA-C	-10.44	89.51	110.40
1	A	385	ASN	CB-CA-C	-10.44	89.52	110.40
1	B	385	ASN	CB-CA-C	-10.44	89.53	110.40
1	C	385	ASN	CB-CA-C	-10.43	89.54	110.40
1	D	507	ASP	CB-CG-OD2	-10.36	108.97	118.30
1	C	507	ASP	CB-CG-OD2	-10.34	109.00	118.30
1	A	507	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	B	507	ASP	CB-CG-OD2	-10.26	109.07	118.30
1	C	356	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	13	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	C	13	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	D	13	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	A	356	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	B	356	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	B	13	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	D	356	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	D	237	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	D	591	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	C	591	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	A	237	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	B	237	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	C	237	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	591	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	D	439	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	439	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	B	439	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	B	591	ASP	CB-CG-OD2	-9.48	109.77	118.30
1	C	439	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	C	249	GLU	N-CA-CB	9.26	127.27	110.60
1	A	249	GLU	N-CA-CB	9.24	127.24	110.60
1	B	249	GLU	N-CA-CB	9.24	127.23	110.60
1	D	249	GLU	N-CA-CB	9.22	127.20	110.60
1	D	509	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	A	509	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	B	509	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	C	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	C	424	ASN	CB-CA-C	-9.11	92.18	110.40
1	B	424	ASN	CB-CA-C	-9.11	92.19	110.40
1	A	424	ASN	CB-CA-C	-9.10	92.20	110.40
1	D	424	ASN	CB-CA-C	-9.10	92.20	110.40
1	C	938	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	938	ARG	NE-CZ-NH2	-8.81	115.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	938	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	B	429	ASP	CB-CG-OD1	8.80	126.22	118.30
1	D	938	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	429	ASP	CB-CG-OD1	8.74	126.17	118.30
1	C	429	ASP	CB-CG-OD1	8.74	126.16	118.30
1	D	429	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	210	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	C	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	D	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	C	509	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	509	ASP	CB-CG-OD1	8.46	125.92	118.30
1	A	509	ASP	CB-CG-OD1	8.43	125.89	118.30
1	B	509	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	233	ASP	CB-CG-OD1	8.23	125.70	118.30
1	A	233	ASP	CB-CG-OD1	8.22	125.70	118.30
1	D	233	ASP	CB-CG-OD1	8.20	125.68	118.30
1	C	233	ASP	CB-CG-OD1	8.19	125.67	118.30
1	B	130	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	D	226	HIS	CB-CA-C	-8.16	94.08	110.40
1	C	226	HIS	CB-CA-C	-8.16	94.08	110.40
1	A	130	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	B	226	HIS	CB-CA-C	-8.15	94.10	110.40
1	A	226	HIS	CB-CA-C	-8.14	94.11	110.40
1	D	287	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	A	287	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	B	287	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	C	130	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	C	287	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	130	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	479	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	479	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	B	479	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	C	479	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	B	211	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	211	ASP	CB-CG-OD1	7.97	125.48	118.30
1	A	211	ASP	CB-CG-OD1	7.96	125.47	118.30
1	B	828	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	C	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	828	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	D	792	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	828	ASP	CB-CG-OD2	-7.92	111.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	828	ASP	CB-CG-OD2	-7.92	111.18	118.30
1	B	792	ASP	CB-CG-OD2	-7.91	111.19	118.30
1	A	792	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	C	792	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	D	13	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	13	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	C	13	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	385	ASN	N-CA-CB	-7.77	96.62	110.60
1	B	385	ASN	N-CA-CB	-7.77	96.62	110.60
1	D	288	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	D	385	ASN	N-CA-CB	-7.76	96.63	110.60
1	C	385	ASN	N-CA-CB	-7.76	96.63	110.60
1	C	310	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	310	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	C	648	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	13	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	659	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	648	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	C	659	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	B	310	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	648	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	D	648	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	310	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	832	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	B	659	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	A	288	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	B	288	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	C	288	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	D	659	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	D	832	ASP	CB-CG-OD1	7.64	125.17	118.30
1	B	832	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	832	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	832	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	832	ASP	CB-CG-OD1	7.61	125.15	118.30
1	D	479	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	479	ASP	CB-CG-OD1	7.61	125.15	118.30
1	C	479	ASP	CB-CG-OD1	7.60	125.14	118.30
1	C	832	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	832	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	B	479	ASP	CB-CG-OD1	7.59	125.14	118.30
1	B	639	THR	CA-CB-CG2	-7.47	101.94	112.40
1	C	639	THR	CA-CB-CG2	-7.46	101.95	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431[A]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	431[B]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	252	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	A	639	THR	CA-CB-CG2	-7.45	101.97	112.40
1	D	639	THR	CA-CB-CG2	-7.44	101.98	112.40
1	B	199	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	D	252	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	252	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	448	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	199	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	199	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	B	252	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	211	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	B	431[A]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	431[B]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	431[A]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	431[B]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	1004	SER	N-CA-CB	7.36	121.55	110.50
1	C	1004	SER	N-CA-CB	7.36	121.54	110.50
1	C	211	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	1004	SER	N-CA-CB	7.36	121.53	110.50
1	B	211	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	A	211	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	D	199	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	1004	SER	N-CA-CB	7.33	121.50	110.50
1	A	448	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	403	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	403	ASP	CB-CG-OD1	7.29	124.86	118.30
1	C	448	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	448	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	C	403	ASP	CB-CG-OD1	7.27	124.84	118.30
1	C	431[A]	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	C	431[B]	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	403	ASP	CB-CG-OD1	7.25	124.83	118.30
1	D	96	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	648	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	96	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	924	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	924	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	336	ARG	NE-CZ-NH1	7.19	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	924	ASP	CB-CG-OD1	7.18	124.77	118.30
1	D	924	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	126	THR	CA-CB-CG2	-7.17	102.36	112.40
1	C	924	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	A	924	ASP	CB-CG-OD1	7.16	124.75	118.30
1	C	648	ASP	CB-CG-OD1	7.16	124.74	118.30
1	D	924	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	126	THR	CA-CB-CG2	-7.15	102.39	112.40
1	C	126	THR	CA-CB-CG2	-7.15	102.39	112.40
1	D	126	THR	CA-CB-CG2	-7.14	102.40	112.40
1	B	924	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	648	ASP	CB-CG-OD1	7.14	124.72	118.30
1	C	336	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	336	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	336	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	648	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	B	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	C	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	C	252	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	746	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	C	356	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	553	TRP	CA-CB-CG	-7.06	100.28	113.70
1	A	252	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	746	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	C	746	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	252	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	746	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	D	400	THR	CA-CB-CG2	-7.01	102.59	112.40
1	B	252	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	859	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	400	THR	CA-CB-CG2	-6.97	102.64	112.40
1	C	400	THR	CA-CB-CG2	-6.97	102.64	112.40
1	D	356	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	356	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	859	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	233	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	233	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	287	ASP	CB-CG-OD1	6.95	124.55	118.30
1	C	591	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	859	ASP	CB-CG-OD1	6.94	124.55	118.30
1	B	400	THR	CA-CB-CG2	-6.94	102.68	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	C	233	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	287	ASP	CB-CG-OD1	6.93	124.53	118.30
1	A	591	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	429	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	859	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	569	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	C	96	ASP	CB-CG-OD1	6.91	124.52	118.30
1	D	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	591	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	403	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	859	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	859	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	287	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	859	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	569	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	429	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	D	96	ASP	CB-CG-OD1	6.87	124.49	118.30
1	A	356	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	C	859	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	569	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	429	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	B	591	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	96	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	429	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	B	569	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	D	403	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	881	ARG	CD-NE-CZ	6.82	133.14	123.60
1	A	403	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	C	881	ARG	CD-NE-CZ	6.81	133.13	123.60
1	D	881	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	881	ARG	CD-NE-CZ	6.80	133.12	123.60
1	B	96	ASP	CB-CG-OD1	6.79	124.42	118.30
1	C	403	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	C	659	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	375	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	659	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	571	VAL	CB-CA-C	-6.65	98.77	111.40
1	B	375	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	C	375	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	571	VAL	CB-CA-C	-6.63	98.80	111.40
1	D	571	VAL	CB-CA-C	-6.63	98.81	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	571	VAL	CB-CA-C	-6.62	98.83	111.40
1	A	375	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	D	672	VAL	CB-CA-C	-6.60	98.86	111.40
1	C	672	VAL	CB-CA-C	-6.60	98.86	111.40
1	B	424	ASN	N-CA-CB	-6.59	98.74	110.60
1	D	659	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	424	ASN	N-CA-CB	-6.58	98.75	110.60
1	A	424	ASN	N-CA-CB	-6.58	98.75	110.60
1	A	672	VAL	CB-CA-C	-6.58	98.89	111.40
1	C	424	ASN	N-CA-CB	-6.57	98.77	110.60
1	B	672	VAL	CB-CA-C	-6.57	98.92	111.40
1	C	507	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	166	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	507	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	507	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	166	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	507	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	166	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	919	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	15	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	15	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	C	919	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	D	15	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	15	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	919	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	15	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	166	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	875	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	15	ASP	CB-CG-OD1	6.43	124.08	118.30
1	C	5	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	875	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	A	15	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	875	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	5	ASP	CB-CG-OD1	6.40	124.06	118.30
1	C	600	GLN	N-CA-CB	6.39	122.10	110.60
1	B	600	GLN	N-CA-CB	6.39	122.10	110.60
1	B	919	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	5	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	938	ARG	N-CA-CB	6.38	122.09	110.60
1	D	5	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	875	ASP	CB-CG-OD2	-6.38	112.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	938	ARG	N-CA-CB	6.38	122.08	110.60
1	B	15	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	600	GLN	N-CA-CB	6.37	122.07	110.60
1	D	938	ARG	N-CA-CB	6.37	122.07	110.60
1	D	750	GLU	N-CA-CB	6.37	122.06	110.60
1	C	938	ARG	N-CA-CB	6.37	122.06	110.60
1	C	750	GLU	N-CA-CB	6.36	122.05	110.60
1	B	750	GLU	N-CA-CB	6.35	122.03	110.60
1	D	319	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	D	600	GLN	N-CA-CB	6.35	122.02	110.60
1	A	750	GLU	N-CA-CB	6.34	122.01	110.60
1	B	319	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	319	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	782	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	782	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	782	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	319	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	782	ASP	CB-CG-OD1	6.27	123.94	118.30
1	C	908	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	439	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	439	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	651	LEU	CB-CA-C	-6.25	98.31	110.20
1	B	651	LEU	CB-CA-C	-6.25	98.32	110.20
1	D	651	LEU	CB-CA-C	-6.25	98.32	110.20
1	D	428	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	D	439	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	651	LEU	CB-CA-C	-6.23	98.36	110.20
1	C	439	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	938	ARG	CG-CD-NE	-6.22	98.73	111.80
1	A	428	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	938	ARG	CG-CD-NE	-6.21	98.76	111.80
1	B	428	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	938	ARG	CG-CD-NE	-6.20	98.78	111.80
1	D	938	ARG	CG-CD-NE	-6.19	98.80	111.80
1	A	908	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	954	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	428	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	572	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	D	572	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	908	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	172	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	B	431[A]	ARG	NE-CZ-NH2	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431[B]	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	572	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	D	954	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	572	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	954	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	772	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	908	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	172	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	431[A]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	431[B]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	954	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	431[A]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	431[B]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	172	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	172	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	772	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	772	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	569	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	336	ARG	CB-CA-C	-6.07	98.27	110.40
1	C	772	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	D	336	ARG	CB-CA-C	-6.05	98.30	110.40
1	A	336	ARG	CB-CA-C	-6.05	98.30	110.40
1	B	336	ARG	CB-CA-C	-6.05	98.31	110.40
1	C	431[A]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	431[B]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	679	LEU	CA-CB-CG	-6.03	101.44	115.30
1	A	679	LEU	CA-CB-CG	-6.01	101.48	115.30
1	D	679	LEU	CA-CB-CG	-6.00	101.50	115.30
1	B	679	LEU	CA-CB-CG	-6.00	101.51	115.30
1	A	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	C	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	C	569	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	A	142	ILE	CB-CA-C	-5.97	99.66	111.60
1	B	142	ILE	CB-CA-C	-5.97	99.67	111.60
1	C	45	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	136	GLU	CB-CA-C	-5.97	98.47	110.40
1	C	142	ILE	CB-CA-C	-5.96	99.67	111.60
1	D	569	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	569	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	B	45	ASP	CB-CG-OD2	-5.95	112.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	142	ILE	CB-CA-C	-5.95	99.70	111.60
1	C	908	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	5	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	908	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	908	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	5	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	199	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	1018	LEU	CB-CA-C	-5.89	99.01	110.20
1	A	1018	LEU	CB-CA-C	-5.88	99.02	110.20
1	B	43	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	199	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	769	TRP	CB-CA-C	-5.88	98.65	110.40
1	B	908	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	D	769	TRP	CB-CA-C	-5.87	98.65	110.40
1	A	5	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	C	769	TRP	CB-CA-C	-5.87	98.66	110.40
1	A	199	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	199	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	1018	LEU	CB-CA-C	-5.86	99.06	110.20
1	C	82	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	1018	LEU	CB-CA-C	-5.85	99.08	110.20
1	B	769	TRP	CB-CA-C	-5.85	98.70	110.40
1	D	77	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	C	423	MET	C-N-CA	5.84	136.29	121.70
1	A	82	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	423	MET	C-N-CA	5.82	136.24	121.70
1	D	82	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	77	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	77	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	144	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	423	MET	C-N-CA	5.80	136.21	121.70
1	D	423	MET	C-N-CA	5.80	136.21	121.70
1	B	954	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	610	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	D	130	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	368	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	77	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	130	ASP	CB-CG-OD1	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	610	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	134	LEU	N-CA-CB	5.78	121.97	110.40
1	C	134	LEU	N-CA-CB	5.78	121.97	110.40
1	D	134	LEU	N-CA-CB	5.78	121.97	110.40
1	D	954	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	144	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	43	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	130	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	134	LEU	N-CA-CB	5.78	121.96	110.40
1	C	987	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	130	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	77	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	77	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	610	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	239	VAL	CA-CB-CG2	-5.77	102.25	110.90
1	C	239	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	D	144	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	792	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	610	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	43	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	954	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	C	954	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	239	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	C	144	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	368	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	987	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	368	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	368	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	43	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	792	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	292	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	792	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	469	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	239	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	D	987	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	987	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	469	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	792	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	230	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	469	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	230	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	164	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	144	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	469	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	164	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	635	THR	CA-CB-CG2	-5.66	104.47	112.40
1	D	635	THR	CA-CB-CG2	-5.66	104.48	112.40
1	A	144	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	635	THR	CA-CB-CG2	-5.66	104.48	112.40
1	C	45	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	164	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	635	THR	CA-CB-CG2	-5.64	104.50	112.40
1	D	230	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	164	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	164	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	164	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	144	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	288	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	A	164	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	288	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	B	288	ARG	CD-NE-CZ	-5.62	115.72	123.60
1	D	45	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	772	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	45	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	594	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	45	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	288	ARG	CD-NE-CZ	-5.61	115.74	123.60
1	B	210	ARG	N-CA-CB	5.61	120.69	110.60
1	A	210	ARG	N-CA-CB	5.61	120.69	110.60
1	D	210	ARG	N-CA-CB	5.60	120.68	110.60
1	A	594	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	C	210	ARG	N-CA-CB	5.59	120.67	110.60
1	C	292	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	230	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	772	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	164	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	772	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	594	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	916	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	594	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	C	916	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	292	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	492	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	772	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	492	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	292	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	292	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	828	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	916	ASP	CB-CG-OD1	5.53	123.27	118.30
1	C	492	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	D	492	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	916	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	987	ASP	CB-CG-OD2	-5.50	113.34	118.30
1	B	292	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	292	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	561	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	561	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	987	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	987	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	987	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	C	829	THR	CA-CB-CG2	-5.47	104.74	112.40
1	B	829	THR	CA-CB-CG2	-5.47	104.74	112.40
1	A	829	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	829	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	671	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	561	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	917	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	561	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	447	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	C	447	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	863	GLN	CB-CA-C	-5.42	99.56	110.40
1	D	863	GLN	CB-CA-C	-5.42	99.56	110.40
1	A	863	GLN	CB-CA-C	-5.41	99.57	110.40
1	A	917	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	863	GLN	CB-CA-C	-5.41	99.58	110.40
1	D	447	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	447	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	319	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	506	VAL	CA-CB-CG1	-5.38	102.82	110.90
1	A	671	ASP	CB-CG-OD1	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	THR	CA-CB-CG2	-5.38	104.88	112.40
1	A	219	THR	CA-CB-CG2	-5.37	104.88	112.40
1	A	506	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	C	219	THR	CA-CB-CG2	-5.37	104.89	112.40
1	B	748	CYS	N-CA-CB	5.36	120.25	110.60
1	C	506	VAL	CA-CB-CG1	-5.36	102.86	110.90
1	C	671	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	506	VAL	CA-CB-CG1	-5.35	102.87	110.90
1	C	917	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	782	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	319	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	219	THR	CA-CB-CG2	-5.34	104.92	112.40
1	D	748	CYS	N-CA-CB	5.34	120.20	110.60
1	A	748	CYS	N-CA-CB	5.33	120.20	110.60
1	B	671	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	748	CYS	N-CA-CB	5.33	120.19	110.60
1	B	319	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	579	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	319	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	980	GLU	N-CA-CB	5.31	120.16	110.60
1	D	579	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	917	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	782	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	C	782	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	C	980	GLU	N-CA-CB	5.29	120.12	110.60
1	A	980	GLU	N-CA-CB	5.29	120.12	110.60
1	D	261	TRP	CB-CA-C	-5.29	99.82	110.40
1	B	579	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	386	ALA	N-CA-CB	-5.29	102.70	110.10
1	D	980	GLU	N-CA-CB	5.28	120.11	110.60
1	D	782	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	386	ALA	N-CA-CB	-5.28	102.71	110.10
1	B	261	TRP	CB-CA-C	-5.28	99.84	110.40
1	C	386	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	261	TRP	CB-CA-C	-5.27	99.87	110.40
1	A	579	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	261	TRP	CB-CA-C	-5.26	99.87	110.40
1	A	386	ALA	N-CA-CB	-5.26	102.73	110.10
1	A	269	SER	N-CA-CB	5.24	118.36	110.50
1	C	916	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	C	329	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	201	ASP	CB-CG-OD2	-5.22	113.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	572	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	269	SER	N-CA-CB	5.21	118.31	110.50
1	A	329	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	C	599	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	916	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	710	GLU	CB-CA-C	-5.20	100.00	110.40
1	D	269	SER	N-CA-CB	5.20	118.30	110.50
1	A	710	GLU	CB-CA-C	-5.19	100.01	110.40
1	D	710	GLU	CB-CA-C	-5.19	100.02	110.40
1	C	710	GLU	CB-CA-C	-5.19	100.03	110.40
1	B	104	THR	CA-CB-CG2	-5.18	105.14	112.40
1	C	269	SER	N-CA-CB	5.18	118.27	110.50
1	C	572	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	104	THR	CA-CB-CG2	-5.17	105.16	112.40
1	C	671	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	248	GLY	C-N-CA	-5.17	108.77	121.70
1	D	329	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	201	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	46	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	518	TRP	CB-CA-C	-5.17	100.07	110.40
1	A	248	GLY	C-N-CA	-5.16	108.79	121.70
1	D	671	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	C	46	ARG	C-N-CD	-5.16	109.25	120.60
1	C	201	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	248	GLY	C-N-CA	-5.16	108.80	121.70
1	D	104	THR	CA-CB-CG2	-5.16	105.18	112.40
1	A	864	MET	N-CA-CB	5.16	119.88	110.60
1	A	599	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	916	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	671	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	518	TRP	CB-CA-C	-5.15	100.10	110.40
1	D	46	ARG	C-N-CD	-5.15	109.27	120.60
1	D	518	TRP	CB-CA-C	-5.15	100.09	110.40
1	C	248	GLY	C-N-CA	-5.15	108.82	121.70
1	C	864	MET	N-CA-CB	5.15	119.87	110.60
1	A	46	ARG	C-N-CD	-5.15	109.28	120.60
1	A	572	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	201	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	599	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	572	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	610	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	864	MET	N-CA-CB	5.14	119.85	110.60
1	D	903[A]	GLN	N-CA-CB	5.14	119.85	110.60
1	D	903[B]	GLN	N-CA-CB	5.14	119.85	110.60
1	B	864	MET	N-CA-CB	5.14	119.85	110.60
1	C	104	THR	CA-CB-CG2	-5.14	105.21	112.40
1	B	193	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	518	TRP	CB-CA-C	-5.13	100.13	110.40
1	B	903[A]	GLN	N-CA-CB	5.13	119.84	110.60
1	B	903[B]	GLN	N-CA-CB	5.13	119.84	110.60
1	A	903[A]	GLN	N-CA-CB	5.13	119.83	110.60
1	A	903[B]	GLN	N-CA-CB	5.13	119.83	110.60
1	C	903[A]	GLN	N-CA-CB	5.13	119.83	110.60
1	C	903[B]	GLN	N-CA-CB	5.13	119.83	110.60
1	D	651	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	B	651	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	46	ARG	C-N-CD	-5.12	109.34	120.60
1	B	671	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	916	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	237	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	193	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	651	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	193	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	651	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	B	599	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	610	ASP	CB-CG-OD1	5.08	122.88	118.30
1	D	310	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	610	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	610	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	46	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	193	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	310	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	721	ARG	N-CA-CB	5.05	119.69	110.60
1	D	363	HIS	CA-CB-CG	-5.05	105.02	113.60
1	D	721	ARG	N-CA-CB	5.04	119.68	110.60
1	A	721	ARG	N-CA-CB	5.04	119.67	110.60
1	C	919	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	363	HIS	CA-CB-CG	-5.03	105.05	113.60
1	B	721	ARG	N-CA-CB	5.03	119.66	110.60
1	A	919	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	363	HIS	CA-CB-CG	-5.02	105.06	113.60
1	C	869	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	869	ASP	CB-CG-OD2	-5.02	113.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	919	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	363	HIS	CA-CB-CG	-5.01	105.08	113.60
1	A	237	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	D	114	VAL	CA-CB-CG1	5.01	118.41	110.90
1	B	919	ASP	CB-CG-OD1	5.00	122.80	118.30
1	B	420	MET	CG-SD-CE	-5.00	92.19	100.20

There are no chirality outliers.

There are no planarity outliers.

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	8238	0	7824	394	0
1	B	8238	0	7824	374	0
1	C	8238	0	7824	379	0
1	D	8238	0	7824	374	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	365	0	0	10	0
3	B	366	0	0	10	0
3	C	367	0	0	10	0
3	D	366	0	0	10	0
All	All	34424	0	31296	1496	0

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

All (1496) 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:B:427:THR:HA	1:B:436:MET:HE1	1.21	1.11
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.34	1.09
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.09
1:C:427:THR:HA	1:C:436:MET:HE1	1.28	1.08
1:A:427:THR:HA	1:A:436:MET:HE1	1.32	1.07
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.34	1.06
1:D:427:THR:HA	1:D:436:MET:HE1	1.35	1.05
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.39	1.05
1:D:693:GLN:HG2	1:D:721:ARG:HD3	1.39	1.04
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.39	1.03
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.39	1.01
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.44	0.99
1:C:597:ASN:HD22	1:C:599:ARG:H	1.11	0.98
1:D:597:ASN:HD22	1:D:599:ARG:H	1.11	0.98
1:C:597:ASN:ND2	1:C:599:ARG:H	1.65	0.95
1:B:38:ASN:ND2	1:B:41:GLU:H	1.66	0.94
1:A:38:ASN:ND2	1:A:41:GLU:H	1.66	0.94
1:A:597:ASN:ND2	1:A:599:ARG:H	1.65	0.94
1:D:597:ASN:ND2	1:D:599:ARG:H	1.65	0.94
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.34	0.93
1:B:427:THR:HA	1:B:436:MET:CE	1.99	0.93
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.34	0.93
1:C:38:ASN:ND2	1:C:41:GLU:H	1.66	0.93
1:B:597:ASN:ND2	1:B:599:ARG:H	1.65	0.92
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.34	0.92
1:D:38:ASN:ND2	1:D:41:GLU:H	1.66	0.92
1:C:427:THR:HA	1:C:436:MET:CE	1.99	0.92
1:A:427:THR:HA	1:A:436:MET:CE	1.99	0.92
1:B:597:ASN:HD22	1:B:599:ARG:H	1.11	0.92
1:D:427:THR:HA	1:D:436:MET:CE	1.99	0.91
1:A:597:ASN:HD22	1:A:599:ARG:H	1.11	0.91
1:D:255:ARG:HH11	1:D:255:ARG:HG2	1.34	0.89
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.58	0.86
1:A:734:SER:HB3	1:A:860:GLY:HA3	1.57	0.86
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.57	0.86
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.58	0.85
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.58	0.85
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.58	0.85
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.57	0.85
1:D:856:TYR:HB3	1:D:864:MET:CE	2.07	0.85
1:A:856:TYR:HB3	1:A:864:MET:CE	2.07	0.84
1:C:856:TYR:HB3	1:C:864:MET:CE	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.57	0.84
1:B:856:TYR:HB3	1:B:864:MET:CE	2.07	0.83
1:D:734:SER:CB	1:D:860:GLY:HA3	2.08	0.83
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.94	0.83
1:B:734:SER:CB	1:B:860:GLY:HA3	2.08	0.82
1:A:734:SER:CB	1:A:860:GLY:HA3	2.09	0.82
1:C:654:TRP:NE1	1:C:666:GLY:HA3	1.94	0.82
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	1.98	0.82
1:B:654:TRP:NE1	1:B:666:GLY:HA3	1.94	0.82
1:C:734:SER:CB	1:C:860:GLY:HA3	2.09	0.82
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	1.98	0.82
1:A:654:TRP:NE1	1:A:666:GLY:HA3	1.94	0.81
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.11	0.81
1:A:830:LEU:CD2	1:A:835:LEU:HB2	2.11	0.81
1:C:830:LEU:CD2	1:C:835:LEU:HB2	2.11	0.81
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	1.98	0.81
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	1.98	0.80
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.11	0.80
1:C:134:LEU:N	1:C:134:LEU:HD12	1.97	0.80
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.97	0.80
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.97	0.80
1:A:134:LEU:HD12	1:A:134:LEU:N	1.97	0.79
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.97	0.79
1:B:77:ASP:O	1:B:78:LEU:HD23	1.83	0.79
1:D:436:MET:HE1	1:D:467:ASN:HD22	1.46	0.79
1:C:77:ASP:O	1:C:78:LEU:HD23	1.83	0.79
1:B:134:LEU:N	1:B:134:LEU:HD12	1.97	0.78
1:D:77:ASP:O	1:D:78:LEU:HD23	1.83	0.78
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.65	0.78
1:A:77:ASP:O	1:A:78:LEU:HD23	1.83	0.78
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.97	0.77
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:B:9:VAL:O	1:B:12:GLN:HB3	1.85	0.77
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.65	0.77
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.99	0.77
1:D:134:LEU:N	1:D:134:LEU:HD12	1.97	0.77
1:A:11:LEU:HD21	1:A:187:MET:CE	2.15	0.77
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.66	0.77
1:B:928:PRO:HB2	1:B:973:ARG:NH1	1.99	0.77
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	1.85	0.77
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:928:PRO:HB2	1:D:973:ARG:NH1	1.99	0.77
1:D:9:VAL:O	1:D:12:GLN:HB3	1.85	0.76
1:B:11:LEU:HD21	1:B:187:MET:CE	2.15	0.76
1:D:11:LEU:HD21	1:D:187:MET:CE	2.15	0.76
1:A:9:VAL:O	1:A:12:GLN:HB3	1.85	0.76
1:C:9:VAL:O	1:C:12:GLN:HB3	1.85	0.76
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.14	0.76
1:C:11:LEU:HD21	1:C:187:MET:CE	2.15	0.76
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.14	0.76
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.49	0.76
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.76
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.68	0.76
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	1.85	0.76
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.75
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.68	0.75
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.14	0.75
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.68	0.75
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.35	0.75
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.85	0.75
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.68	0.75
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.68	0.74
1:C:38:ASN:HD22	1:C:41:GLU:H	1.35	0.74
1:A:38:ASN:HD22	1:A:41:GLU:H	1.35	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.69	0.74
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.74
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.14	0.74
1:D:655:MET:HG3	1:D:656:VAL:N	2.03	0.74
1:C:436:MET:HE1	1:C:467:ASN:HD22	1.53	0.73
1:D:579:ASP:OD1	1:D:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.53	0.73
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.70	0.73
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.70	0.73
1:B:237:ARG:HB3	1:B:237:ARG:HH11	1.54	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.71	0.73
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.02	0.73
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.89	0.72
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.70	0.72
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.54	0.72
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.72
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.71	0.72
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.35	0.72
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.35	0.72
1:B:3:ILE:HG13	1:B:4:THR:N	2.04	0.72
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.71	0.72
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.71	0.72
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.71	0.72
1:D:380:LYS:HE2	3:D:4077:HOH:O	1.90	0.72
1:D:3:ILE:HG13	1:D:4:THR:N	2.04	0.72
1:A:652:LEU:HD11	1:A:698:VAL:HB	1.71	0.72
1:D:436:MET:CE	1:D:467:ASN:HD22	2.03	0.72
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.55	0.72
1:B:237:ARG:CB	1:B:237:ARG:HH11	2.02	0.72
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.35	0.72
1:A:436:MET:CE	1:A:467:ASN:HD22	2.03	0.71
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.71
1:C:655:MET:HG3	1:C:656:VAL:N	2.03	0.71
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.55	0.71
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.72	0.71
1:A:3:ILE:HG13	1:A:4:THR:N	2.04	0.71
1:B:38:ASN:HD22	1:B:41:GLU:H	1.35	0.71
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.55	0.71
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.02	0.71
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.71
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.71	0.71
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.71	0.71
1:C:3:ILE:HG13	1:C:4:THR:N	2.04	0.71
1:C:436:MET:CE	1:C:467:ASN:HD22	2.03	0.71
1:B:380:LYS:HE2	3:B:4134:HOH:O	1.90	0.71
1:B:436:MET:CE	1:B:467:ASN:HD22	2.03	0.71
1:C:380:LYS:HE2	3:C:4174:HOH:O	1.90	0.71
1:C:650:GLU:HB3	1:C:670:LEU:HD12	1.73	0.71
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.73	0.70
1:B:11:LEU:HD21	1:B:187:MET:HE3	1.72	0.70
1:C:836:ILE:N	1:C:836:ILE:HD13	2.07	0.69
1:D:38:ASN:HD22	1:D:41:GLU:H	1.35	0.69
1:A:655:MET:HG3	1:A:656:VAL:N	2.03	0.69
1:C:11:LEU:HD21	1:C:187:MET:HE3	1.74	0.69
1:A:380:LYS:HE2	3:A:4077:HOH:O	1.90	0.69
1:A:836:ILE:N	1:A:836:ILE:HD13	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.73	0.69
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.69
1:D:836:ILE:N	1:D:836:ILE:HD13	2.07	0.69
1:B:655:MET:HG3	1:B:656:VAL:N	2.03	0.69
1:B:836:ILE:HD13	1:B:836:ILE:N	2.07	0.69
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.73	0.68
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.68
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.92	0.68
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.73	0.68
1:C:255:ARG:NH1	1:C:255:ARG:HG2	2.07	0.68
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.91	0.68
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.91	0.68
1:B:35:SER:OG	1:B:37:ARG:NH1	2.27	0.68
1:C:923:SER:HB3	3:C:4345:HOH:O	1.94	0.68
1:D:35:SER:OG	1:D:37:ARG:NH1	2.27	0.68
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.68
1:A:923:SER:HB3	3:A:4380:HOH:O	1.94	0.67
1:D:923:SER:HB3	3:D:4380:HOH:O	1.94	0.67
1:D:211:ASP:OD1	1:D:211:ASP:N	2.27	0.67
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.76	0.67
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.07	0.67
1:D:856:TYR:CD2	1:D:864:MET:HE1	2.29	0.67
1:D:965:GLN:O	1:D:969:GLU:HG3	1.94	0.67
1:B:965:GLN:O	1:B:969:GLU:HG3	1.94	0.67
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.67
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.77	0.67
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.91	0.67
1:C:965:GLN:O	1:C:969:GLU:HG3	1.94	0.67
1:A:211:ASP:N	1:A:211:ASP:OD1	2.27	0.67
1:A:35:SER:OG	1:A:37:ARG:NH1	2.27	0.67
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.28	0.66
1:B:255:ARG:NH1	1:B:255:ARG:HG2	2.07	0.66
1:C:375:ASP:O	1:C:379:MET:HG3	1.95	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.77	0.66
1:D:11:LEU:HD21	1:D:187:MET:HE3	1.76	0.66
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.77	0.66
1:A:965:GLN:O	1:A:969:GLU:HG3	1.94	0.66
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.66
1:A:7:LEU:N	1:A:71:GLU:OE2	2.28	0.66
1:B:824:GLN:HG3	1:B:825:CYS:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:SER:HB3	3:B:4305:HOH:O	1.94	0.66
1:B:856:TYR:CD2	1:B:864:MET:HE1	2.31	0.66
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.77	0.66
1:D:824:GLN:HG3	1:D:825:CYS:N	2.11	0.66
1:A:856:TYR:HB3	1:A:864:MET:HE1	1.77	0.66
1:B:7:LEU:N	1:B:71:GLU:OE2	2.28	0.66
1:D:59:ARG:NH2	1:D:81:ALA:O	2.28	0.66
1:B:59:ARG:NH2	1:B:81:ALA:O	2.28	0.66
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.77	0.66
1:A:375:ASP:O	1:A:379:MET:HG3	1.95	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.27	0.65
1:C:30:HIS:HB2	1:C:31:PRO:HD2	1.77	0.65
1:C:824:GLN:HG3	1:C:825:CYS:N	2.11	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.28	0.65
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.30	0.65
1:D:7:LEU:N	1:D:71:GLU:OE2	2.28	0.65
1:D:856:TYR:HD2	1:D:864:MET:HE1	1.61	0.65
1:B:375:ASP:O	1:B:379:MET:HG3	1.95	0.65
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.77	0.65
1:C:210:ARG:HD3	3:C:4138:HOH:O	1.97	0.65
1:D:375:ASP:O	1:D:379:MET:HG3	1.95	0.65
1:A:824:GLN:HG3	1:A:825:CYS:N	2.10	0.65
1:B:742:THR:HG22	1:B:743:SER:N	2.12	0.65
1:B:775:GLN:OE1	1:B:890:GLN:NE2	2.30	0.65
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.30	0.65
1:D:742:THR:HG22	1:D:743:SER:N	2.12	0.65
1:A:742:THR:HG22	1:A:743:SER:N	2.12	0.64
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.64
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.77	0.64
1:C:742:THR:HG22	1:C:743:SER:N	2.12	0.64
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.79	0.64
1:A:210:ARG:HD3	3:A:4036:HOH:O	1.97	0.64
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.30	0.64
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.62	0.64
1:D:856:TYR:HB3	1:D:864:MET:HE1	1.78	0.64
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:D:499:ILE:HB	1:D:533:LEU:HB2	1.79	0.64
1:B:210:ARG:HD3	3:B:4098:HOH:O	1.97	0.64
1:B:797:GLU:O	1:B:801:ILE:HD12	1.98	0.64
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.77	0.64
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.97	0.64
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.81	0.63
1:A:287:ASP:CG	1:D:425:ARG:HH22	2.00	0.63
1:A:835:LEU:C	1:A:836:ILE:HD13	2.19	0.63
1:B:835:LEU:C	1:B:836:ILE:HD13	2.19	0.63
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.81	0.63
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.81	0.63
1:B:746:ASP:HA	1:B:760:ARG:CG	2.22	0.63
1:C:746:ASP:HA	1:C:760:ARG:CG	2.22	0.63
1:C:797:GLU:O	1:C:801:ILE:HD12	1.98	0.63
1:B:649:ASN:OD1	1:B:703:PRO:HD2	1.99	0.63
1:B:66:PRO:HD2	1:B:67:GLU:HG2	1.81	0.63
1:A:66:PRO:HD2	1:A:67:GLU:HG2	1.81	0.63
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.63
1:C:211:ASP:OD1	1:C:211:ASP:N	2.27	0.63
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.81	0.63
1:D:649:ASN:OD1	1:D:703:PRO:HD2	1.99	0.63
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.81	0.62
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.34	0.62
1:A:797:GLU:O	1:A:801:ILE:HD12	1.98	0.62
1:D:746:ASP:HA	1:D:760:ARG:CG	2.22	0.62
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.07	0.62
1:A:649:ASN:OD1	1:A:703:PRO:HD2	1.99	0.62
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.34	0.62
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.34	0.62
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.81	0.62
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.34	0.62
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.99	0.62
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.81	0.62
1:C:835:LEU:C	1:C:836:ILE:HD13	2.19	0.62
1:A:906:TYR:HB3	1:A:907:PRO:HD2	1.81	0.62
1:C:767:GLN:HG3	1:C:768:MET:N	2.15	0.62
1:A:767:GLN:HG3	1:A:768:MET:N	2.15	0.62
1:D:835:LEU:C	1:D:836:ILE:HD13	2.19	0.62
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.81	0.62
1:C:778:THR:CG2	1:C:779:PRO:HD2	2.30	0.62
1:D:797:GLU:O	1:D:801:ILE:HD12	1.98	0.62
1:B:767:GLN:HG3	1:B:768:MET:N	2.15	0.61
1:D:66:PRO:HD2	1:D:67:GLU:HG2	1.81	0.61
1:A:778:THR:CG2	1:A:779:PRO:HD2	2.30	0.61
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:HD12	1:B:824:GLN:N	2.16	0.61
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.81	0.61
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.81	0.61
1:C:928:PRO:O	1:C:973:ARG:NH1	2.33	0.61
1:A:651:LEU:HD12	1:A:669:PRO:HA	1.83	0.61
1:B:856:TYR:HD2	1:B:864:MET:HE1	1.63	0.61
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.01	0.61
1:A:928:PRO:O	1:A:973:ARG:NH1	2.34	0.61
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.83	0.61
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.30	0.61
1:C:651:LEU:HD12	1:C:669:PRO:HA	1.83	0.61
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.81	0.61
1:B:928:PRO:O	1:B:973:ARG:NH1	2.34	0.61
1:D:928:PRO:O	1:D:973:ARG:NH1	2.34	0.61
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.83	0.60
1:D:102:ASN:ND2	1:D:201:ASP:HB2	2.16	0.60
1:D:778:THR:CG2	1:D:779:PRO:HD2	2.30	0.60
1:D:822:LEU:HD12	1:D:824:GLN:N	2.16	0.60
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.16	0.60
1:A:822:LEU:HD12	1:A:824:GLN:N	2.16	0.60
1:B:822:LEU:HD11	1:B:824:GLN:O	2.01	0.60
1:C:595:THR:HG23	1:C:596:PRO:HA	1.82	0.60
1:D:822:LEU:HD11	1:D:824:GLN:O	2.01	0.60
1:A:610:ASP:OD2	1:A:612:THR:HG23	2.01	0.60
1:C:102:ASN:ND2	1:C:201:ASP:HB2	2.16	0.60
1:C:822:LEU:HD11	1:C:824:GLN:O	2.01	0.60
1:C:870:VAL:HG12	1:C:871:GLU:N	2.16	0.60
1:D:595:THR:HG23	1:D:596:PRO:HA	1.82	0.60
1:A:595:THR:HG23	1:A:596:PRO:HA	1.82	0.60
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.16	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.84	0.60
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.31	0.60
1:B:595:THR:HG23	1:B:596:PRO:HA	1.82	0.60
1:B:80:GLU:CD	1:B:80:GLU:H	2.01	0.60
1:B:734:SER:HB3	1:B:860:GLY:CA	2.30	0.60
1:C:822:LEU:HD12	1:C:824:GLN:N	2.16	0.60
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.36	0.60
1:C:511:PRO:HA	1:C:516:PRO:HB3	1.84	0.60
1:C:734:SER:HB3	1:C:860:GLY:CA	2.30	0.60
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.60
1:A:282:ARG:HD3	1:D:418:HIS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD12	1:D:669:PRO:HA	1.83	0.60
1:A:128:ASN:HA	1:A:180:GLY:O	2.02	0.60
1:B:610:ASP:OD2	1:B:612:THR:HG23	2.01	0.60
1:B:651:LEU:HD12	1:B:669:PRO:HA	1.83	0.60
1:C:128:ASN:HA	1:C:180:GLY:O	2.02	0.60
1:A:830:LEU:HD21	1:A:835:LEU:HB2	1.84	0.59
1:A:734:SER:HB3	1:A:860:GLY:CA	2.30	0.59
1:B:870:VAL:HG12	1:B:871:GLU:N	2.16	0.59
1:D:227:VAL:HG13	1:D:240:LEU:HD11	1.83	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.84	0.59
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.02	0.59
1:C:759:ASN:OD1	1:C:761:GLN:N	2.35	0.59
1:D:734:SER:HB3	1:D:860:GLY:CA	2.30	0.59
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.83	0.59
1:A:759:ASN:OD1	1:A:761:GLN:N	2.35	0.59
1:A:822:LEU:HD11	1:A:824:GLN:O	2.01	0.59
1:C:610:ASP:OD2	1:C:612:THR:HG23	2.01	0.59
1:D:701:VAL:HG12	1:D:702:GLN:N	2.17	0.59
1:D:767:GLN:HG3	1:D:768:MET:N	2.15	0.59
1:A:696:LEU:HD12	1:A:697:THR:N	2.18	0.59
1:A:870:VAL:HG12	1:A:871:GLU:N	2.16	0.59
1:B:696:LEU:HD12	1:B:697:THR:N	2.18	0.59
1:D:128:ASN:HA	1:D:180:GLY:O	2.02	0.59
1:A:505:ARG:HG2	1:A:996:ASP:OD2	2.02	0.59
1:D:696:LEU:HD12	1:D:697:THR:N	2.18	0.59
1:B:128:ASN:HA	1:B:180:GLY:O	2.02	0.59
1:A:282:ARG:HH12	1:D:419:GLY:C	2.06	0.59
1:D:505:ARG:HG2	1:D:996:ASP:OD2	2.02	0.59
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.84	0.59
1:D:870:VAL:HG12	1:D:871:GLU:N	2.16	0.59
1:A:701:VAL:HG12	1:A:702:GLN:N	2.17	0.58
1:B:336:ARG:NH2	1:B:338:GLU:OE1	2.36	0.58
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.31	0.58
1:C:696:LEU:HD12	1:C:697:THR:N	2.17	0.58
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.84	0.58
1:B:6:SER:HB2	1:B:71:GLU:OE2	2.04	0.58
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.19	0.58
1:C:473:ARG:HD3	1:C:473:ARG:O	2.04	0.58
1:C:533:LEU:HD12	1:C:533:LEU:C	2.24	0.58
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.36	0.58
1:B:511:PRO:HA	1:B:516:PRO:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.39	0.58
1:B:473:ARG:HD3	1:B:473:ARG:O	2.04	0.58
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.36	0.58
1:A:473:ARG:O	1:A:473:ARG:HD3	2.04	0.58
1:A:62:TRP:CD1	1:A:95:TYR:HB3	2.39	0.58
1:B:701:VAL:HG12	1:B:702:GLN:N	2.17	0.58
1:B:737:ILE:HG13	1:B:738:PRO:N	2.17	0.58
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.68	0.58
1:D:336:ARG:NH2	1:D:338:GLU:OE1	2.36	0.58
1:D:473:ARG:O	1:D:473:ARG:HD3	2.04	0.58
1:D:737:ILE:HG13	1:D:738:PRO:N	2.17	0.58
1:A:769:TRP:NE1	1:A:774:LYS:HG3	2.19	0.58
1:B:759:ASN:OD1	1:B:761:GLN:N	2.35	0.57
1:C:701:VAL:HG12	1:C:702:GLN:N	2.17	0.57
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.19	0.57
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.04	0.57
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.57
1:A:533:LEU:C	1:A:533:LEU:HD12	2.24	0.57
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.86	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.57
1:B:533:LEU:HD12	1:B:533:LEU:C	2.24	0.57
1:C:618:THR:HG22	1:C:912:ALA:HB1	1.86	0.57
1:D:618:THR:HG22	1:D:912:ALA:HB1	1.86	0.57
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.04	0.57
1:A:6:SER:HB2	1:A:71:GLU:OE2	2.03	0.57
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.39	0.57
1:C:737:ILE:HG13	1:C:738:PRO:N	2.17	0.57
1:C:769:TRP:NE1	1:C:774:LYS:HG3	2.19	0.57
1:D:80:GLU:H	1:D:80:GLU:CD	2.01	0.57
1:C:830:LEU:HD21	1:C:835:LEU:HB2	1.84	0.57
1:A:737:ILE:HG13	1:A:738:PRO:N	2.17	0.57
1:B:460:ASN:ND2	1:B:461:GLU:HG2	2.20	0.57
1:B:618:THR:HG22	1:B:912:ALA:HB1	1.86	0.57
1:C:134:LEU:H	1:C:134:LEU:HD12	1.69	0.57
1:C:62:TRP:CD1	1:C:95:TYR:HB3	2.39	0.57
1:D:533:LEU:HD12	1:D:533:LEU:C	2.24	0.57
1:C:26:ARG:HD2	1:C:169:SER:HA	1.87	0.57
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.04	0.57
1:D:140:ARG:NH1	1:D:170:GLU:OE1	2.31	0.57
1:D:316:HIS:HD2	1:D:317:THR:O	1.87	0.57
1:A:597:ASN:HD22	1:A:599:ARG:N	1.94	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:HD3	3:C:4137:HOH:O	2.05	0.57
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.40	0.57
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.57
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.40	0.57
1:A:419:GLY:C	1:D:282:ARG:HH12	2.08	0.57
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.87	0.57
1:B:26:ARG:HD2	1:B:169:SER:HA	1.87	0.57
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.57
1:B:763:GLY:HA3	1:B:822:LEU:HD21	1.87	0.57
1:C:460:ASN:ND2	1:C:461:GLU:HG2	2.20	0.57
1:C:6:SER:HB2	1:C:71:GLU:OE2	2.03	0.57
1:A:460:ASN:ND2	1:A:461:GLU:HG2	2.20	0.57
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.40	0.56
1:A:166:ARG:HD3	3:A:4035:HOH:O	2.05	0.56
1:A:457:SER:HA	1:A:485:GLN:O	2.06	0.56
1:B:166:ARG:HD3	3:B:4097:HOH:O	2.05	0.56
1:B:834:VAL:HG12	1:B:835:LEU:N	2.19	0.56
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.20	0.56
1:C:763:GLY:HA3	1:C:822:LEU:HD21	1.87	0.56
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.41	0.56
1:B:18:ASN:OD1	1:B:19:PRO:HD2	2.06	0.56
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.05	0.56
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.87	0.56
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.06	0.56
1:A:26:ARG:HD2	1:A:169:SER:HA	1.87	0.56
1:C:834:VAL:HG12	1:C:835:LEU:N	2.19	0.56
1:D:166:ARG:HD3	3:D:4035:HOH:O	2.05	0.56
1:D:38:ASN:HD21	1:D:41:GLU:H	1.53	0.56
1:D:457:SER:HA	1:D:485:GLN:O	2.06	0.56
1:A:304:GLU:C	1:A:305:ILE:HG13	2.26	0.56
1:A:531:ARG:O	1:A:561:ARG:NH1	2.39	0.56
1:A:834:VAL:HG12	1:A:835:LEU:N	2.19	0.56
1:B:531:ARG:O	1:B:561:ARG:NH1	2.39	0.56
1:C:457:SER:HA	1:C:485:GLN:O	2.06	0.56
1:D:834:VAL:HG12	1:D:835:LEU:N	2.19	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.05	0.56
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.36	0.56
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.40	0.56
1:D:134:LEU:H	1:D:134:LEU:HD12	1.69	0.56
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.06	0.56
1:A:80:GLU:H	1:A:80:GLU:CD	2.01	0.56
1:B:457:SER:HA	1:B:485:GLN:O	2.05	0.56
1:C:316:HIS:HD2	1:C:317:THR:O	1.88	0.56
1:C:833:ALA:HB1	1:C:858:ILE:O	2.06	0.56
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.05	0.56
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.36	0.56
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.71	0.56
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.04	0.55
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.74	0.55
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.39	0.55
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.41	0.55
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.22	0.55
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.42	0.55
1:A:833:ALA:HB1	1:A:858:ILE:O	2.06	0.55
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.42	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.36	0.55
1:B:134:LEU:H	1:B:134:LEU:HD12	1.69	0.55
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.22	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.53	0.55
1:B:833:ALA:HB1	1:B:858:ILE:O	2.06	0.55
1:C:304:GLU:C	1:C:305:ILE:HG13	2.26	0.55
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.22	0.55
1:C:531:ARG:O	1:C:561:ARG:NH1	2.39	0.55
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.31	0.55
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.42	0.55
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.06	0.55
1:D:304:GLU:C	1:D:305:ILE:HG13	2.26	0.55
1:B:304:GLU:C	1:B:305:ILE:HG13	2.26	0.55
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.55
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.41	0.55
1:A:942:ARG:HA	1:A:953:GLY:O	2.07	0.55
1:C:942:ARG:HA	1:C:953:GLY:O	2.07	0.55
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.36	0.55
1:C:786:ARG:HA	1:C:964:GLN:OE1	2.07	0.55
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	0.55
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.89	0.55
1:D:833:ALA:HB1	1:D:858:ILE:O	2.06	0.55
1:C:577:LYS:O	1:C:584:PRO:HA	2.06	0.54
1:D:531:ARG:O	1:D:561:ARG:NH1	2.39	0.54
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.89	0.54
1:C:749:ILE:O	1:C:755:ARG:HG3	2.07	0.54
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.11	0.54
1:A:749:ILE:O	1:A:755:ARG:HG3	2.08	0.54
1:B:942:ARG:HA	1:B:953:GLY:O	2.07	0.54
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.42	0.54
1:B:786:ARG:HA	1:B:964:GLN:OE1	2.07	0.54
1:B:894:ARG:NH1	1:B:919:ASP:OD1	2.34	0.54
1:D:26:ARG:HD2	1:D:169:SER:HA	1.87	0.54
1:A:746:ASP:HA	1:A:760:ARG:CG	2.22	0.54
1:B:79:PRO:N	1:B:80:GLU:OE2	2.41	0.54
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.74	0.54
1:D:79:PRO:N	1:D:80:GLU:OE2	2.41	0.54
1:D:942:ARG:HA	1:D:953:GLY:O	2.07	0.54
1:A:134:LEU:HD12	1:A:134:LEU:H	1.69	0.54
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.11	0.54
1:C:79:PRO:N	1:C:80:GLU:OE2	2.41	0.54
1:D:759:ASN:OD1	1:D:761:GLN:N	2.35	0.54
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.22	0.54
1:A:418:HIS:O	1:D:282:ARG:HD3	2.08	0.54
1:A:79:PRO:N	1:A:80:GLU:OE2	2.41	0.54
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.38	0.54
1:B:29:ALA:HA	3:B:4295:HOH:O	2.07	0.54
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.89	0.54
1:D:38:ASN:ND2	1:D:41:GLU:N	2.48	0.54
1:D:749:ILE:O	1:D:755:ARG:HG3	2.08	0.54
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.38	0.54
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.11	0.54
1:C:38:ASN:HD21	1:C:41:GLU:H	1.53	0.54
1:C:80:GLU:H	1:C:80:GLU:CD	2.01	0.54
1:D:29:ALA:HA	3:D:4347:HOH:O	2.07	0.54
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.54
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.38	0.54
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.91	0.54
1:C:903[A]:GLN:HB2	3:C:4239:HOH:O	2.08	0.54
1:D:786:ARG:HA	1:D:964:GLN:OE1	2.07	0.54
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.89	0.53
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.38	0.53
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.11	0.53
1:B:749:ILE:O	1:B:755:ARG:HG3	2.07	0.53
1:A:29:ALA:HA	3:A:4347:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:HIS:HD2	1:A:392:TYR:OH	1.91	0.53
1:A:903[A]:GLN:HB2	3:A:4157:HOH:O	2.09	0.53
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.09	0.53
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.38	0.53
1:B:1017:GLN:O	1:B:1018:LEU:HD23	2.09	0.53
1:B:742:THR:HG22	1:B:743:SER:H	1.74	0.53
1:C:110:ASN:O	1:C:113:PHE:N	2.39	0.53
1:C:6:SER:OG	1:C:9:VAL:HB	2.09	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:C:894:ARG:NH1	1:C:919:ASP:OD1	2.34	0.53
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.92	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.94	0.53
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.11	0.53
1:D:696:LEU:HD12	1:D:697:THR:H	1.74	0.53
1:A:959:ILE:O	1:A:959:ILE:HG23	2.09	0.53
1:B:597:ASN:HD22	1:B:599:ARG:N	1.94	0.53
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.44	0.53
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.38	0.53
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.52
1:A:6:SER:OG	1:A:9:VAL:HB	2.09	0.52
1:C:29:ALA:HA	3:C:4335:HOH:O	2.07	0.52
1:C:416:GLU:OE1	1:C:461:GLU:HG3	2.09	0.52
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.09	0.52
1:C:1017:GLN:O	1:C:1018:LEU:HD23	2.09	0.52
1:C:696:LEU:HD12	1:C:697:THR:H	1.74	0.52
1:C:959:ILE:O	1:C:959:ILE:HG23	2.09	0.52
1:D:742:THR:HG22	1:D:743:SER:H	1.74	0.52
1:A:416:GLU:OE1	1:A:461:GLU:HG3	2.09	0.52
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.39	0.52
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.09	0.52
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.25	0.52
1:A:696:LEU:HD12	1:A:697:THR:H	1.74	0.52
1:B:959:ILE:O	1:B:959:ILE:HG23	2.09	0.52
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.09	0.52
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.09	0.52
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.10	0.52
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.74	0.52
1:B:696:LEU:HD12	1:B:697:THR:H	1.74	0.52
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.44	0.52
1:A:749:ILE:N	1:A:749:ILE:HD12	2.25	0.52
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ILE:N	1:C:749:ILE:HD12	2.25	0.52
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.10	0.52
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.91	0.52
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.72	0.52
1:A:742:THR:HG22	1:A:743:SER:H	1.74	0.52
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.52
1:D:1017:GLN:O	1:D:1018:LEU:HD23	2.09	0.52
1:D:749:ILE:N	1:D:749:ILE:HD12	2.25	0.52
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.38	0.52
1:B:903[A]:GLN:HB2	3:B:4199:HOH:O	2.08	0.52
1:D:110:ASN:O	1:D:113:PHE:N	2.39	0.52
1:B:130:ASP:OD2	1:B:132:SER:OG	2.28	0.52
1:B:770:ILE:HG22	1:B:770:ILE:O	2.10	0.52
1:D:130:ASP:OD2	1:D:132:SER:OG	2.28	0.52
1:D:148:SER:HB3	1:D:190:ARG:O	2.10	0.52
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.43	0.52
1:D:6:SER:OG	1:D:9:VAL:HB	2.09	0.52
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.44	0.51
1:B:6:SER:OG	1:B:9:VAL:HB	2.09	0.51
1:C:742:THR:HG22	1:C:743:SER:H	1.74	0.51
1:D:542:MET:HA	1:D:604:ASN:HA	1.92	0.51
1:B:148:SER:HB3	1:B:190:ARG:O	2.10	0.51
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.92	0.51
1:B:749:ILE:HD12	1:B:749:ILE:N	2.25	0.51
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.10	0.51
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.44	0.51
1:B:808:GLU:HA	1:B:808:GLU:OE1	2.10	0.51
1:C:542:MET:HA	1:C:604:ASN:HA	1.92	0.51
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.11	0.51
1:B:416:GLU:OE1	1:B:461:GLU:HG3	2.09	0.51
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.10	0.51
1:D:959:ILE:O	1:D:959:ILE:HG23	2.09	0.51
1:A:251:ARG:NH1	1:A:251:ARG:HG2	2.25	0.51
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.10	0.51
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.51
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.41	0.51
1:A:130:ASP:OD2	1:A:132:SER:OG	2.28	0.51
1:A:531:ARG:HB3	1:A:532:PRO:HD2	1.92	0.51
1:A:808:GLU:HA	1:A:808:GLU:OE1	2.10	0.51
1:C:38:ASN:ND2	1:C:41:GLU:N	2.48	0.51
1:D:230:ARG:CG	1:D:230:ARG:HH11	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:903[A]:GLN:HB2	3:D:4157:HOH:O	2.08	0.51
1:A:26:ARG:CD	1:A:169:SER:HB3	2.41	0.51
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.14	0.51
1:B:822:LEU:HD12	1:B:824:GLN:H	1.76	0.51
1:C:148:SER:HB3	1:C:190:ARG:O	2.10	0.51
1:A:254:LEU:O	1:A:255:ARG:NH1	2.44	0.51
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.41	0.51
1:A:894:ARG:HD3	1:A:919:ASP:OD1	2.11	0.51
1:C:597:ASN:HD22	1:C:599:ARG:N	1.94	0.51
1:B:254:LEU:O	1:B:255:ARG:NH1	2.44	0.51
1:B:26:ARG:CD	1:B:169:SER:HB3	2.41	0.51
1:A:38:ASN:ND2	1:A:41:GLU:N	2.48	0.51
1:A:770:ILE:HG22	1:A:770:ILE:O	2.10	0.50
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.41	0.50
1:C:26:ARG:CD	1:C:169:SER:HB3	2.41	0.50
1:C:95:TYR:N	1:C:95:TYR:CD1	2.79	0.50
1:D:254:LEU:O	1:D:255:ARG:NH1	2.44	0.50
1:D:894:ARG:NH1	1:D:919:ASP:OD1	2.34	0.50
1:A:134:LEU:N	1:A:134:LEU:CD1	2.73	0.50
1:A:282:ARG:CG	1:D:423:MET:HB2	2.42	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.92	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.50
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.92	0.50
1:D:65:ALA:HB1	1:D:66:PRO:CD	2.41	0.50
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.47	0.50
1:A:836:ILE:HG22	1:A:837:THR:N	2.26	0.50
1:D:822:LEU:HD12	1:D:824:GLN:H	1.76	0.50
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.41	0.50
1:A:38:ASN:HD21	1:A:41:GLU:H	1.53	0.50
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.50
1:B:134:LEU:CD1	1:B:134:LEU:N	2.73	0.50
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.24	0.50
1:D:770:ILE:O	1:D:770:ILE:HG22	2.10	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.50
1:D:26:ARG:CD	1:D:169:SER:HB3	2.41	0.50
1:A:230:ARG:CG	1:A:230:ARG:HH11	2.24	0.50
1:A:542:MET:HA	1:A:604:ASN:HA	1.92	0.50
1:A:662:PRO:C	1:A:663:LEU:HD23	2.32	0.50
1:B:662:PRO:C	1:B:663:LEU:HD23	2.32	0.50
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.47	0.50
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.47	0.50
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.41	0.50
1:B:882:ILE:O	1:B:882:ILE:HG22	2.12	0.50
1:A:652:LEU:HD12	1:A:699:ARG:O	2.12	0.50
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.50
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.47	0.50
1:B:433:LEU:O	1:B:437:SER:HB3	2.12	0.50
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.47	0.50
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.50
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.16	0.50
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.47	0.50
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.47	0.50
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.50
1:B:894:ARG:HD3	1:B:919:ASP:OD1	2.11	0.50
1:C:662:PRO:C	1:C:663:LEU:HD23	2.32	0.50
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.47	0.50
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.11	0.50
1:D:95:TYR:N	1:D:95:TYR:CD1	2.79	0.50
1:C:433:LEU:O	1:C:437:SER:HB3	2.12	0.49
1:A:148:SER:HB3	1:A:190:ARG:O	2.10	0.49
1:C:254:LEU:O	1:C:255:ARG:NH1	2.44	0.49
1:C:30:HIS:ND1	1:C:31:PRO:O	2.40	0.49
1:C:822:LEU:HD12	1:C:824:GLN:H	1.76	0.49
1:A:12:GLN:HG3	1:A:13:ARG:N	2.27	0.49
1:A:638:VAL:O	1:A:677:LYS:HA	2.12	0.49
1:A:822:LEU:HD12	1:A:824:GLN:H	1.76	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.49
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.16	0.49
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.48	0.49
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.42	0.49
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:D:882:ILE:O	1:D:882:ILE:HG22	2.12	0.49
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.43	0.49
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.41	0.49
1:B:638:VAL:O	1:B:677:LYS:HA	2.12	0.49
1:B:763:GLY:CA	1:B:822:LEU:HD21	2.42	0.49
1:C:153:TRP:HA	1:C:157:ARG:O	2.13	0.49
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.43	0.49
1:C:595:THR:HG23	1:C:596:PRO:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:VAL:O	1:C:677:LYS:HA	2.12	0.49
1:C:770:ILE:O	1:C:770:ILE:HG22	2.10	0.49
1:D:12:GLN:HG3	1:D:13:ARG:N	2.27	0.49
1:D:595:THR:HG23	1:D:596:PRO:CA	2.43	0.49
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.49
1:A:153:TRP:HA	1:A:157:ARG:O	2.13	0.49
1:A:95:TYR:N	1:A:95:TYR:CD1	2.79	0.49
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.16	0.49
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.48	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:B:652:LEU:HD12	1:B:699:ARG:O	2.12	0.49
1:A:110:ASN:O	1:A:113:PHE:N	2.39	0.49
1:A:200:GLN:N	1:A:200:GLN:OE1	2.44	0.49
1:C:660:GLY:O	1:C:662:PRO:HD3	2.13	0.49
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.42	0.49
1:D:660:GLY:O	1:D:662:PRO:HD3	2.13	0.49
1:A:660:GLY:O	1:A:662:PRO:HD3	2.13	0.49
1:B:12:GLN:HG3	1:B:13:ARG:N	2.27	0.49
1:C:143:PHE:N	1:C:143:PHE:CD1	2.81	0.49
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.47	0.49
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.49
1:C:130:ASP:OD2	1:C:132:SER:OG	2.28	0.49
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.48	0.49
1:C:830:LEU:HD22	1:C:835:LEU:HB2	1.95	0.49
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.41	0.49
1:C:938:ARG:NH2	3:C:4307:HOH:O	2.45	0.49
1:D:652:LEU:HD12	1:D:699:ARG:O	2.12	0.49
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.39	0.49
1:B:595:THR:HG23	1:B:596:PRO:CA	2.43	0.49
1:B:938:ARG:NH2	3:B:4267:HOH:O	2.45	0.49
1:C:134:LEU:N	1:C:134:LEU:CD1	2.73	0.49
1:D:662:PRO:C	1:D:663:LEU:HD23	2.32	0.49
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.42	0.49
1:D:836:ILE:HG22	1:D:837:THR:N	2.26	0.49
1:A:143:PHE:N	1:A:143:PHE:CD1	2.81	0.48
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.48
1:A:651:LEU:HA	1:A:651:LEU:HD12	1.46	0.48
1:B:646:HIS:O	1:B:648:ASP:N	2.47	0.48
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.48	0.48
1:C:835:LEU:CD1	1:C:857:ARG:HB2	2.43	0.48
1:C:836:ILE:HG22	1:C:837:THR:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.48
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.16	0.48
1:C:882:ILE:HG22	1:C:882:ILE:O	2.12	0.48
1:A:787:ALA:HA	1:A:788:PRO:HD3	1.66	0.48
1:C:12:GLN:HG3	1:C:13:ARG:N	2.27	0.48
1:C:652:LEU:HD12	1:C:699:ARG:O	2.12	0.48
1:D:143:PHE:CD1	1:D:143:PHE:N	2.81	0.48
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.48
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.43	0.48
1:B:597:ASN:ND2	1:B:599:ARG:N	2.48	0.48
1:B:651:LEU:HD12	1:B:651:LEU:HA	1.46	0.48
1:B:660:GLY:O	1:B:662:PRO:HD3	2.13	0.48
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.44	0.48
1:B:835:LEU:CD1	1:B:857:ARG:HB2	2.43	0.48
1:D:433:LEU:O	1:D:437:SER:HB3	2.12	0.48
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.65	0.48
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.96	0.48
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.97	0.48
1:D:651:LEU:HD12	1:D:651:LEU:HA	1.46	0.48
1:A:595:THR:HG23	1:A:596:PRO:CA	2.43	0.48
1:A:651:LEU:HD23	1:A:653[A]:HIS:HE1	1.79	0.48
1:B:257:THR:OG1	1:B:316:HIS:HE1	1.97	0.48
1:C:646:HIS:O	1:C:648:ASP:N	2.46	0.48
1:C:651:LEU:HD23	1:C:653[A]:HIS:HE1	1.79	0.48
1:D:251:ARG:HH11	1:D:251:ARG:HG2	1.79	0.48
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.96	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.40	0.48
1:A:513:PRO:O	1:A:514:ALA:HB3	2.14	0.48
1:A:597:ASN:ND2	1:A:599:ARG:N	2.48	0.48
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.14	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:A:646:HIS:O	1:A:648:ASP:N	2.46	0.48
1:A:894:ARG:NH1	1:A:919:ASP:OD1	2.34	0.48
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.14	0.48
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.62	0.48
1:C:856:TYR:HD2	1:C:864:MET:CE	2.27	0.48
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.97	0.48
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.43	0.48
1:B:143:PHE:CD1	1:B:143:PHE:N	2.81	0.48
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HD3	1:B:169:SER:HB3	1.96	0.48
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.44	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:A:30:HIS:ND1	1:A:31:PRO:O	2.40	0.47
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.49	0.47
1:B:67:GLU:H	1:B:67:GLU:HG2	1.15	0.47
1:B:970:THR:CG2	1:B:975:LEU:HB2	2.44	0.47
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.47
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.47	0.47
1:A:668:VAL:HA	1:A:669:PRO:HD3	1.66	0.47
1:A:701:VAL:CG1	1:A:702:GLN:N	2.77	0.47
1:C:742:THR:CG2	1:C:743:SER:N	2.77	0.47
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.43	0.47
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:C:210:ARG:NH1	1:C:358:GLU:OE1	2.47	0.47
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.47
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.62	0.47
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.44	0.47
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.95	0.47
1:A:292:ARG:C	1:A:293:LEU:HD23	2.35	0.47
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.62	0.47
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.47
1:A:830:LEU:HD22	1:A:835:LEU:HB2	1.95	0.47
1:A:882:ILE:O	1:A:882:ILE:HG22	2.12	0.47
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.48	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
1:D:210:ARG:NH1	1:D:358:GLU:OE1	2.47	0.47
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.14	0.47
1:A:18:ASN:HA	1:A:19:PRO:HD3	1.56	0.47
1:A:856:TYR:HD2	1:A:864:MET:CE	2.27	0.47
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.44	0.47
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.79	0.47
1:C:701:VAL:CG1	1:C:702:GLN:N	2.77	0.47
1:A:423:MET:HB2	1:D:282:ARG:CG	2.43	0.47
1:D:635:THR:OG1	1:D:681:GLU:HG3	2.15	0.47
1:D:651:LEU:HD23	1:D:653[A]:HIS:HE1	1.79	0.47
1:A:26:ARG:HD3	1:A:169:SER:HB3	1.96	0.47
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.97	0.47
1:B:110:ASN:O	1:B:113:PHE:N	2.39	0.47
1:B:651:LEU:HD23	1:B:653[A]:HIS:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.97	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.97	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.14	0.47
1:B:701:VAL:CG1	1:B:702:GLN:N	2.78	0.47
1:C:214:LEU:HA	1:C:214:LEU:HD23	1.61	0.47
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.44	0.47
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.97	0.47
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.43	0.47
1:D:830:LEU:HD22	1:D:835:LEU:HB2	1.95	0.47
1:D:938:ARG:NH2	3:D:4279:HOH:O	2.45	0.47
1:C:513:PRO:O	1:C:514:ALA:HB3	2.14	0.47
1:C:661:LYS:HA	1:C:662:PRO:HD2	1.71	0.47
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.44	0.47
1:A:261:TRP:N	1:A:261:TRP:CD1	2.83	0.47
1:A:80:GLU:OE2	1:A:80:GLU:N	2.29	0.47
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.62	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.77	0.47
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.47
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.47
1:C:292:ARG:C	1:C:293:LEU:HD23	2.35	0.47
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.79	0.47
1:A:849:LEU:HD23	1:A:849:LEU:N	2.30	0.47
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.47
1:B:830:LEU:HD22	1:B:835:LEU:HB2	1.95	0.47
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.50	0.47
1:B:200:GLN:OE1	1:B:200:GLN:N	2.44	0.46
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.43	0.46
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.50	0.46
1:A:419:GLY:C	1:D:282:ARG:NH1	2.68	0.46
1:A:282:ARG:NH1	1:D:419:GLY:C	2.68	0.46
1:D:441:THR:HG22	1:D:474:TRP:CH2	2.50	0.46
1:D:573:GLN:HB2	1:D:602:CYS:O	2.14	0.46
1:D:701:VAL:CG1	1:D:702:GLN:N	2.77	0.46
1:B:292:ARG:C	1:B:293:LEU:HD23	2.35	0.46
1:B:513:PRO:O	1:B:514:ALA:HB3	2.14	0.46
1:B:573:GLN:HB2	1:B:602:CYS:O	2.14	0.46
1:B:95:TYR:CD1	1:B:95:TYR:N	2.79	0.46
1:C:234:ASP:O	1:C:235:PHE:HB2	2.15	0.46
1:C:635:THR:OG1	1:C:681:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ARG:HG2	1:D:230:ARG:HH11	1.81	0.46
1:D:234:ASP:O	1:D:235:PHE:HB2	2.15	0.46
1:D:292:ARG:C	1:D:293:LEU:HD23	2.35	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.81	0.46
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.97	0.46
1:A:429:ASP:OD1	1:A:431[A]:ARG:HG3	2.16	0.46
1:B:202:MET:HE3	1:B:357:HIS:CD2	2.50	0.46
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.16	0.46
1:D:834:VAL:CG1	1:D:835:LEU:N	2.79	0.46
1:B:226:HIS:CD2	1:B:226:HIS:N	2.83	0.46
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.82	0.46
1:B:429:ASP:OD1	1:B:431[A]:ARG:HG3	2.16	0.46
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.46
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.53	0.46
1:C:226:HIS:CD2	1:C:226:HIS:N	2.83	0.46
1:C:227:VAL:HG12	1:C:228:ALA:N	2.31	0.46
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.63	0.46
1:D:261:TRP:N	1:D:261:TRP:CD1	2.83	0.46
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.51	0.46
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.36	0.46
1:B:234:ASP:O	1:B:235:PHE:HB2	2.15	0.46
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.50	0.46
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.80	0.46
1:C:11:LEU:CD2	1:C:187:MET:HE3	2.45	0.46
1:C:84:VAL:HG13	1:C:85:VAL:N	2.31	0.46
1:D:200:GLN:N	1:D:200:GLN:OE1	2.44	0.46
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.69	0.46
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.97	0.46
1:A:742:THR:CG2	1:A:743:SER:N	2.77	0.46
1:B:166:ARG:HG3	1:B:392:TYR:CG	2.51	0.46
1:B:254:LEU:C	1:B:255:ARG:HG2	2.36	0.46
1:B:261:TRP:N	1:B:261:TRP:CD1	2.83	0.46
1:C:261:TRP:CD1	1:C:261:TRP:N	2.83	0.46
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.46
1:C:620:ALA:O	1:C:624:GLN:HG3	2.16	0.46
1:D:597:ASN:ND2	1:D:599:ARG:N	2.48	0.46
1:D:630:ARG:HB3	1:D:630:ARG:HE	1.31	0.46
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.78	0.46
1:B:620:ALA:O	1:B:624:GLN:HG3	2.16	0.46
1:B:635:THR:OG1	1:B:681:GLU:HG3	2.15	0.46
1:B:849:LEU:N	1:B:849:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.16	0.46
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.51	0.46
1:D:227:VAL:HG12	1:D:228:ALA:N	2.31	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.46
1:A:679:LEU:HD23	1:A:679:LEU:HA	1.13	0.46
1:B:111:PRO:HA	1:B:112:PRO:HA	1.57	0.46
1:B:369:GLU:O	1:B:373:VAL:HG23	2.16	0.46
1:B:742:THR:CG2	1:B:743:SER:N	2.77	0.46
1:B:834:VAL:CG1	1:B:835:LEU:N	2.79	0.46
1:B:856:TYR:HD2	1:B:864:MET:CE	2.27	0.46
1:C:141:ILE:CG1	1:C:142:ILE:N	2.79	0.46
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.36	0.46
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.80	0.46
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.46
1:D:701:VAL:O	1:D:703:PRO:HD3	2.16	0.46
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.31	0.46
1:A:881:ARG:HD3	1:A:987:ASP:CG	2.36	0.46
1:B:701:VAL:O	1:B:703:PRO:HD3	2.16	0.46
1:C:441:THR:HG22	1:C:474:TRP:CH2	2.50	0.46
1:D:254:LEU:C	1:D:255:ARG:HG2	2.36	0.46
1:D:658:LEU:O	1:D:659:ASP:C	2.54	0.46
1:D:870:VAL:CG1	1:D:871:GLU:N	2.79	0.46
1:A:141:ILE:CG1	1:A:142:ILE:N	2.79	0.46
1:A:369:GLU:O	1:A:373:VAL:HG23	2.16	0.46
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.31	0.46
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.51	0.46
1:B:168:PRO:O	1:B:442:ARG:NH2	2.48	0.46
1:B:870:VAL:CG1	1:B:871:GLU:N	2.79	0.46
1:B:881:ARG:HD3	1:B:987:ASP:CG	2.36	0.46
1:D:84:VAL:HG13	1:D:85:VAL:N	2.31	0.46
1:A:234:ASP:O	1:A:235:PHE:HB2	2.15	0.45
1:A:254:LEU:C	1:A:255:ARG:HG2	2.36	0.45
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.45
1:B:3:ILE:HD12	1:B:3:ILE:O	2.16	0.45
1:C:230:ARG:HG2	1:C:230:ARG:HH11	1.81	0.45
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.36	0.45
1:C:834:VAL:CG1	1:C:835:LEU:N	2.79	0.45
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.52	0.45
1:D:856:TYR:HD2	1:D:864:MET:CE	2.27	0.45
1:A:226:HIS:N	1:A:226:HIS:CD2	2.83	0.45
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HD12	1:A:3:ILE:O	2.16	0.45
1:A:441:THR:HG22	1:A:474:TRP:CH2	2.50	0.45
1:A:658:LEU:O	1:A:659:ASP:C	2.54	0.45
1:A:938:ARG:NH2	3:A:4279:HOH:O	2.45	0.45
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.53	0.45
1:B:38:ASN:ND2	1:B:41:GLU:HG3	2.31	0.45
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.36	0.45
1:B:80:GLU:N	1:B:80:GLU:OE2	2.29	0.45
1:C:242:ALA:O	1:C:290:THR:HA	2.16	0.45
1:C:701:VAL:O	1:C:703:PRO:HD3	2.16	0.45
1:D:226:HIS:N	1:D:226:HIS:CD2	2.83	0.45
1:D:369:GLU:O	1:D:373:VAL:HG23	2.16	0.45
1:D:881:ARG:HD3	1:D:987:ASP:CG	2.36	0.45
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.52	0.45
1:D:945:ASN:OD1	1:D:950:GLN:HB2	2.16	0.45
1:A:1018:LEU:HD23	1:A:1018:LEU:HA	1.53	0.45
1:A:227:VAL:HG12	1:A:228:ALA:N	2.31	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.16	0.45
1:A:834:VAL:CG1	1:A:835:LEU:N	2.79	0.45
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.45
1:B:757:GLN:HG2	1:B:758:PHE:N	2.31	0.45
1:B:832:ASP:N	1:B:832:ASP:OD1	2.50	0.45
1:C:230:ARG:CG	1:C:230:ARG:NH1	2.79	0.45
1:C:369:GLU:O	1:C:373:VAL:HG23	2.16	0.45
1:D:531:ARG:CB	1:D:532:PRO:HD2	2.46	0.45
1:A:202:MET:HE3	1:A:357:HIS:CD2	2.52	0.45
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.61	0.45
1:A:242:ALA:O	1:A:290:THR:HA	2.16	0.45
1:A:524:LEU:HB2	3:A:4198:HOH:O	2.16	0.45
1:A:620:ALA:O	1:A:624:GLN:HG3	2.16	0.45
1:A:84:VAL:HG13	1:A:85:VAL:N	2.31	0.45
1:B:141:ILE:CG1	1:B:142:ILE:N	2.79	0.45
1:B:242:ALA:O	1:B:290:THR:HA	2.16	0.45
1:B:352:ARG:O	1:B:385:ASN:HB2	2.17	0.45
1:B:531:ARG:CB	1:B:532:PRO:HD2	2.46	0.45
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.39	0.45
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.79	0.45
1:C:67:GLU:HG2	1:C:67:GLU:H	1.15	0.45
1:C:80:GLU:OE2	1:C:80:GLU:N	2.29	0.45
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.45
1:D:3:ILE:O	1:D:3:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:ALA:O	1:D:624:GLN:HG3	2.16	0.45
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.45	0.45
1:A:352:ARG:O	1:A:385:ASN:HB2	2.17	0.45
1:A:559:TYR:HA	1:A:560:PRO:HD2	1.85	0.45
1:A:915:PHE:O	1:A:916:ASP:HB2	2.17	0.45
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.45
1:B:679:LEU:HD23	1:B:679:LEU:HA	1.13	0.45
1:C:38:ASN:ND2	1:C:41:GLU:HG3	2.32	0.45
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.45
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.45	0.45
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.36	0.45
1:B:227:VAL:HG12	1:B:228:ALA:N	2.31	0.45
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.50	0.45
1:B:650:GLU:HA	1:B:701:VAL:O	2.17	0.45
1:D:111:PRO:HA	1:D:112:PRO:HA	1.56	0.45
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.51	0.45
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.45
1:A:945:ASN:OD1	1:A:950:GLN:HB2	2.16	0.45
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.95	0.45
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.69	0.45
1:C:524:LEU:HB2	3:C:4262:HOH:O	2.16	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.45
1:C:650:GLU:HA	1:C:701:VAL:O	2.17	0.45
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.80	0.45
1:D:38:ASN:ND2	1:D:41:GLU:HG3	2.32	0.45
1:D:757:GLN:HG2	1:D:758:PHE:N	2.31	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:B:84:VAL:HG13	1:B:85:VAL:N	2.31	0.45
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.99	0.45
1:B:894:ARG:NH2	1:B:921:PRO:HD3	2.31	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.16	0.45
1:C:730:LEU:H	1:C:730:LEU:HG	1.41	0.45
1:C:832:ASP:OD1	1:C:832:ASP:N	2.49	0.45
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.80	0.45
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.69	0.45
1:B:255:ARG:NH1	1:B:255:ARG:CG	2.79	0.45
1:B:915:PHE:O	1:B:916:ASP:HB2	2.17	0.45
1:C:849:LEU:N	1:C:849:LEU:HD23	2.30	0.45
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	2.16	0.45
1:D:524:LEU:HB2	3:D:4198:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:CD1	1:A:399:TYR:N	2.85	0.45
1:A:77:ASP:C	1:A:78:LEU:HD23	2.37	0.45
1:B:230:ARG:HG2	1:B:230:ARG:HH11	1.81	0.45
1:B:599:ARG:HB2	1:B:600:GLN:H	1.54	0.45
1:C:77:ASP:C	1:C:78:LEU:HD23	2.37	0.45
1:C:945:ASN:OD1	1:C:950:GLN:HB2	2.16	0.45
1:D:441:THR:HG22	1:D:474:TRP:CZ3	2.52	0.45
1:D:832:ASP:N	1:D:832:ASP:OD1	2.50	0.45
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.99	0.44
1:B:38:ASN:ND2	1:B:41:GLU:N	2.48	0.44
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.61	0.44
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.44
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.44
1:C:352:ARG:O	1:C:385:ASN:HB2	2.17	0.44
1:C:399:TYR:N	1:C:399:TYR:CD1	2.85	0.44
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.99	0.44
1:D:1018:LEU:HA	1:D:1018:LEU:HD23	1.53	0.44
1:D:230:ARG:NH1	1:D:230:ARG:CG	2.79	0.44
1:D:352:ARG:O	1:D:385:ASN:HB2	2.17	0.44
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.44
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.52	0.44
1:A:531:ARG:CB	1:A:532:PRO:HD2	2.46	0.44
1:A:78:LEU:HB3	1:A:80:GLU:OE2	2.18	0.44
1:B:136:GLU:O	1:B:216:HIS:HE1	2.01	0.44
1:C:18:ASN:HA	1:C:19:PRO:HD3	1.56	0.44
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.51	0.44
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.44
1:C:668:VAL:HA	1:C:669:PRO:HD3	1.66	0.44
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.31	0.44
1:D:141:ILE:CG1	1:D:142:ILE:N	2.79	0.44
1:D:650:GLU:HA	1:D:701:VAL:O	2.17	0.44
1:A:230:ARG:CG	1:A:230:ARG:NH1	2.79	0.44
1:A:708:TRP:N	1:A:708:TRP:CD1	2.85	0.44
1:A:870:VAL:CG1	1:A:871:GLU:N	2.79	0.44
1:A:989:PHE:CD1	1:A:989:PHE:N	2.86	0.44
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.52	0.44
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.36	0.44
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.52	0.44
1:C:316:HIS:HB2	1:C:321:THR:O	2.16	0.44
1:C:870:VAL:CG1	1:C:871:GLU:N	2.79	0.44
1:C:881:ARG:HD3	1:C:987:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:849:LEU:HD23	1:D:849:LEU:N	2.30	0.44
1:A:136:GLU:O	1:A:216:HIS:HE1	2.01	0.44
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.36	0.44
1:B:143:PHE:O	1:B:168:PRO:HA	2.17	0.44
1:B:77:ASP:C	1:B:78:LEU:HD23	2.37	0.44
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.44
1:C:708:TRP:N	1:C:708:TRP:CD1	2.85	0.44
1:D:708:TRP:CD1	1:D:708:TRP:N	2.85	0.44
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.99	0.44
1:A:63:PHE:N	1:A:63:PHE:CD1	2.86	0.44
1:A:650:GLU:HA	1:A:701:VAL:O	2.17	0.44
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.52	0.44
1:B:947:GLY:HA3	1:B:948:PRO:HD2	1.89	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.51	0.44
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.78	0.44
1:C:989:PHE:CD1	1:C:989:PHE:N	2.86	0.44
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.00	0.44
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.18	0.44
1:D:77:ASP:C	1:D:78:LEU:HD23	2.38	0.44
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.61	0.44
1:A:168:PRO:O	1:A:442:ARG:NH2	2.48	0.44
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.83	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.18	0.44
1:C:79:PRO:HB2	1:C:80:GLU:HG3	2.00	0.44
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.56	0.44
1:D:242:ALA:O	1:D:290:THR:HA	2.16	0.44
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.51	0.44
1:B:399:TYR:N	1:B:399:TYR:CD1	2.85	0.44
1:B:524:LEU:HB2	3:B:4222:HOH:O	2.16	0.44
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.53	0.44
1:C:63:PHE:N	1:C:63:PHE:CD1	2.86	0.44
1:D:136:GLU:O	1:D:216:HIS:HE1	2.01	0.44
1:B:30:HIS:CE1	1:B:33:PHE:CD1	3.06	0.44
1:B:78:LEU:HB3	1:B:80:GLU:OE2	2.18	0.44
1:C:441:THR:HG22	1:C:474:TRP:CZ3	2.52	0.44
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.44
1:A:441:THR:HG22	1:A:474:TRP:CZ3	2.52	0.44
1:B:11:LEU:CD2	1:B:187:MET:HE3	2.44	0.44
1:C:136:GLU:O	1:C:216:HIS:HE1	2.01	0.44
1:D:134:LEU:N	1:D:134:LEU:CD1	2.73	0.44
1:D:989:PHE:CD1	1:D:989:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:HIS:HB2	1:A:321:THR:O	2.16	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.43
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.18	0.43
1:C:145:GLY:HA3	1:C:210:ARG:HG3	2.00	0.43
1:C:915:PHE:O	1:C:916:ASP:HB2	2.17	0.43
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.36	0.43
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.48	0.43
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.06	0.43
1:A:3:ILE:C	1:A:5:ASP:H	2.22	0.43
1:B:630:ARG:HB3	1:B:630:ARG:HE	1.31	0.43
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.51	0.43
1:B:748:CYS:C	1:B:749:ILE:HD12	2.39	0.43
1:B:989:PHE:CD1	1:B:989:PHE:N	2.86	0.43
1:C:255:ARG:NH1	1:C:255:ARG:CG	2.79	0.43
1:C:597:ASN:ND2	1:C:599:ARG:N	2.48	0.43
1:D:30:HIS:CE1	1:D:33:PHE:CD1	3.06	0.43
1:D:79:PRO:HB2	1:D:80:GLU:HG3	2.00	0.43
1:D:915:PHE:O	1:D:916:ASP:HB2	2.17	0.43
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.52	0.43
1:A:742:THR:CG2	1:A:743:SER:H	2.31	0.43
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.59	0.43
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.53	0.43
1:C:3:ILE:C	1:C:5:ASP:H	2.22	0.43
1:C:634:GLN:NE2	1:C:682:LEU:O	2.51	0.43
1:D:145:GLY:HA3	1:D:210:ARG:HG3	2.00	0.43
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.43
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.36	0.43
1:A:285:TYR:OH	1:D:424:ASN:HB3	2.19	0.43
1:A:881:ARG:HD3	1:A:987:ASP:OD2	2.17	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:B:433:LEU:HB3	1:B:434:PRO:HD3	2.00	0.43
1:B:682:LEU:HA	1:B:683:PRO:HD3	1.91	0.43
1:C:168:PRO:O	1:C:442:ARG:NH2	2.48	0.43
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.43
1:C:657:ALA:O	1:C:694:LEU:HD12	2.18	0.43
1:D:399:TYR:N	1:D:399:TYR:CD1	2.85	0.43
1:D:881:ARG:HD3	1:D:987:ASP:OD2	2.18	0.43
1:A:143:PHE:O	1:A:168:PRO:HA	2.17	0.43
1:A:67:GLU:H	1:A:67:GLU:HG2	1.15	0.43
1:A:79:PRO:HB2	1:A:80:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:HA3	1:B:210:ARG:HG3	2.00	0.43
1:B:742:THR:CG2	1:B:743:SER:H	2.31	0.43
1:B:79:PRO:HB2	1:B:80:GLU:HG3	2.00	0.43
1:D:11:LEU:CD2	1:D:187:MET:HE3	2.48	0.43
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.82	0.43
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.51	0.43
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.84	0.43
1:B:118:ASN:HA	1:B:119:PRO:HD2	1.61	0.43
1:B:657:ALA:O	1:B:694:LEU:HD12	2.18	0.43
1:C:176:PHE:CD1	1:C:176:PHE:N	2.87	0.43
1:C:217:LYS:HB3	1:C:218:PRO:HD2	2.00	0.43
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.57	0.43
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.69	0.43
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.39	0.43
1:D:657:ALA:O	1:D:694:LEU:HD12	2.18	0.43
1:D:748:CYS:C	1:D:749:ILE:HD12	2.39	0.43
1:A:77:ASP:HA	3:A:4132:HOH:O	2.19	0.43
1:A:822:LEU:HD12	1:A:823:LEU:N	2.34	0.43
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.95	0.43
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.77	0.43
1:C:200:GLN:OE1	1:C:200:GLN:N	2.44	0.43
1:C:30:HIS:CE1	1:C:33:PHE:CD1	3.06	0.43
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.82	0.43
1:C:630:ARG:HE	1:C:630:ARG:HB3	1.31	0.43
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.45	0.43
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.13	0.43
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.53	0.43
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.66	0.43
1:A:217:LYS:HB3	1:A:218:PRO:HD2	2.00	0.43
1:A:630:ARG:HE	1:A:630:ARG:HB3	1.31	0.43
1:A:634:GLN:NE2	1:A:682:LEU:O	2.51	0.43
1:A:730:LEU:H	1:A:730:LEU:HG	1.41	0.43
1:A:748:CYS:C	1:A:749:ILE:HD12	2.39	0.43
1:B:708:TRP:CD1	1:B:708:TRP:N	2.85	0.43
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.80	0.43
1:D:354:VAL:HG22	1:D:355:ASN:N	2.34	0.43
1:D:910:LEU:HD12	1:D:910:LEU:C	2.39	0.43
1:A:105:TYR:HB3	1:A:106:PRO:HD2	2.01	0.43
1:A:251:ARG:CG	1:A:251:ARG:HH11	2.32	0.43
1:A:257:THR:HA	1:A:270:GLY:O	2.19	0.43
1:A:687:GLN:HA	1:A:688:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:CG1	1:B:240:LEU:HD11	2.48	0.43
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.32	0.43
1:B:634:GLN:NE2	1:B:682:LEU:O	2.51	0.43
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.43
1:C:734:SER:HB2	1:C:860:GLY:HA3	1.95	0.43
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.43
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.38	0.43
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.89	0.43
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.54	0.43
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.43
1:B:30:HIS:ND1	1:B:31:PRO:O	2.40	0.43
1:B:622:HIS:HD2	1:B:625:GLN:OE1	2.02	0.43
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.43
1:C:234:ASP:OD1	1:C:236:SER:OG	2.31	0.43
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.81	0.43
1:C:840:HIS:ND1	1:C:840:HIS:N	2.67	0.43
1:D:105:TYR:HB3	1:D:106:PRO:HD2	2.01	0.43
1:D:257:THR:HA	1:D:270:GLY:O	2.19	0.43
1:D:622:HIS:HD2	1:D:625:GLN:OE1	2.02	0.43
1:A:11:LEU:CD2	1:A:187:MET:HE3	2.45	0.42
1:A:145:GLY:HA3	1:A:210:ARG:HG3	2.01	0.42
1:A:354:VAL:HG22	1:A:355:ASN:N	2.34	0.42
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.53	0.42
1:A:635:THR:HA	1:A:680:ILE:O	2.19	0.42
1:A:822:LEU:HD13	1:A:822:LEU:HA	1.79	0.42
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.77	0.42
1:B:257:THR:HA	1:B:270:GLY:O	2.19	0.42
1:B:77:ASP:HA	3:B:4178:HOH:O	2.19	0.42
1:B:910:LEU:C	1:B:910:LEU:HD12	2.39	0.42
1:C:187:MET:O	1:C:187:MET:HG3	2.19	0.42
1:D:634:GLN:NE2	1:D:682:LEU:O	2.51	0.42
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.82	0.42
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.54	0.42
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.66	0.42
1:D:217:LYS:HB3	1:D:218:PRO:HD2	2.00	0.42
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	0.42
1:A:225:PHE:HA	1:A:243:GLU:O	2.19	0.42
1:A:657:ALA:O	1:A:694:LEU:HD12	2.18	0.42
1:B:635:THR:HA	1:B:680:ILE:O	2.19	0.42
1:C:183:ARG:HD3	1:C:183:ARG:HH11	1.55	0.42
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:MET:HB3	1:C:372:MET:CE	2.50	0.42
1:D:187:MET:HG3	1:D:187:MET:O	2.19	0.42
1:A:622:HIS:HD2	1:A:625:GLN:OE1	2.02	0.42
1:B:278:ILE:HD12	1:B:278:ILE:HA	1.88	0.42
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.42
1:C:227:VAL:CG1	1:C:240:LEU:HD11	2.48	0.42
1:C:576:ILE:HD13	1:C:584:PRO:HB2	2.02	0.42
1:C:822:LEU:HD12	1:C:823:LEU:N	2.34	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.73	0.42
1:D:782:ASP:OD1	1:D:854:LYS:NZ	2.52	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:A:282:ARG:NH1	1:D:418:HIS:O	2.52	0.42
1:B:227:VAL:CG1	1:B:228:ALA:N	2.83	0.42
1:B:52[A]:ARG:HH11	1:B:52[A]:ARG:HD3	1.65	0.42
1:B:737:ILE:HA	1:B:738:PRO:HD3	1.78	0.42
1:C:635:THR:HA	1:C:680:ILE:O	2.19	0.42
1:D:576:ILE:HD13	1:D:584:PRO:HB2	2.02	0.42
1:A:187:MET:HG3	1:A:187:MET:O	2.19	0.42
1:A:255:ARG:CG	1:A:255:ARG:NH1	2.79	0.42
1:A:367:MET:HB3	1:A:372:MET:CE	2.50	0.42
1:A:858:ILE:HG12	1:A:864:MET:HB3	2.02	0.42
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.42
1:C:274:PHE:HB3	1:C:286:ALA:O	2.20	0.42
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.54	0.42
1:C:742:THR:CG2	1:C:743:SER:H	2.31	0.42
1:D:367:MET:HB3	1:D:372:MET:CE	2.50	0.42
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.91	0.42
1:A:274:PHE:HB3	1:A:286:ALA:O	2.20	0.42
1:B:105:TYR:HB3	1:B:106:PRO:HD2	2.01	0.42
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.84	0.42
1:C:479:ASP:HA	1:C:480:PRO:HD2	1.73	0.42
1:C:77:ASP:HA	3:C:4218:HOH:O	2.19	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.61	0.42
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.54	0.42
1:A:910:LEU:HD12	1:A:910:LEU:C	2.39	0.42
1:B:685:LEU:CB	1:B:686:PRO:HD2	2.38	0.42
1:B:822:LEU:HD12	1:B:823:LEU:N	2.34	0.42
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.78	0.42
1:C:354:VAL:HG22	1:C:355:ASN:N	2.34	0.42
1:C:622:HIS:HD2	1:C:625:GLN:OE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:GLN:HG2	1:C:758:PHE:N	2.31	0.42
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.66	0.42
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.32	0.42
1:D:274:PHE:HB3	1:D:286:ALA:O	2.20	0.42
1:D:822:LEU:HD12	1:D:823:LEU:N	2.34	0.42
1:D:835:LEU:HA	1:D:835:LEU:HD12	1.90	0.42
1:A:424:ASN:HD22	1:A:424:ASN:HA	1.40	0.42
1:B:11:LEU:N	1:B:11:LEU:HD23	2.35	0.42
1:B:217:LYS:HB3	1:B:218:PRO:HD2	2.01	0.42
1:B:274:PHE:HB3	1:B:286:ALA:O	2.20	0.42
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.80	0.42
1:C:251:ARG:CG	1:C:251:ARG:HH11	2.32	0.42
1:C:63:PHE:CB	1:C:64:PRO:CD	2.98	0.42
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.54	0.42
1:D:635:THR:HA	1:D:680:ILE:O	2.19	0.42
1:D:840:HIS:ND1	1:D:840:HIS:N	2.67	0.42
1:D:858:ILE:HG12	1:D:864:MET:HB3	2.02	0.42
1:A:11:LEU:N	1:A:11:LEU:HD23	2.35	0.42
1:A:441:THR:O	1:A:445:GLN:HG3	2.20	0.42
1:A:474:TRP:CZ2	1:A:478:VAL:HG21	2.55	0.42
1:B:124:SER:HA	1:B:184:LEU:O	2.20	0.42
1:B:3:ILE:C	1:B:5:ASP:H	2.22	0.42
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.42
1:C:472:TYR:O	1:C:476:LYS:HG2	2.20	0.42
1:C:474:TRP:CZ2	1:C:478:VAL:HG21	2.55	0.42
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.46	0.42
1:C:856:TYR:CD1	1:C:856:TYR:N	2.88	0.42
1:C:910:LEU:HD12	1:C:910:LEU:C	2.39	0.42
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.84	0.42
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.75	0.42
1:D:856:TYR:CD1	1:D:856:TYR:N	2.88	0.42
1:A:111:PRO:HA	1:A:112:PRO:HA	1.56	0.41
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.46	0.41
1:A:856:TYR:N	1:A:856:TYR:CD1	2.88	0.41
1:B:262:GLN:HG2	1:B:262:GLN:O	2.19	0.41
1:B:576:ILE:HD13	1:B:584:PRO:HB2	2.02	0.41
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.41
1:A:176:PHE:CD1	1:A:176:PHE:N	2.87	0.41
1:A:721:ARG:HE	1:B:874:SER:CB	2.32	0.41
1:A:757:GLN:HG2	1:A:758:PHE:N	2.31	0.41
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PHE:N	1:B:176:PHE:CD1	2.87	0.41
1:B:288:ARG:HD3	1:B:288:ARG:HH11	1.48	0.41
1:C:105:TYR:HB3	1:C:106:PRO:HD2	2.01	0.41
1:C:227:VAL:CG1	1:C:228:ALA:N	2.83	0.41
1:C:395:HIS:HA	1:C:396:PRO:HD3	1.83	0.41
1:C:599:ARG:HB2	1:C:600:GLN:H	1.54	0.41
1:D:141:ILE:HG12	1:D:142:ILE:N	2.35	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.55	0.41
1:D:559:TYR:HB2	1:D:562:LEU:CD1	2.47	0.41
1:A:141:ILE:HG12	1:A:142:ILE:N	2.35	0.41
1:A:524:LEU:O	1:A:561:ARG:NH2	2.50	0.41
1:B:23:GLN:HG2	3:B:4413:HOH:O	2.20	0.41
1:C:141:ILE:HG12	1:C:142:ILE:N	2.35	0.41
1:C:262:GLN:O	1:C:262:GLN:HG2	2.19	0.41
1:C:578:TYR:HA	1:C:583:ASN:O	2.20	0.41
1:C:858:ILE:HG12	1:C:864:MET:HB3	2.02	0.41
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.86	0.41
1:D:835:LEU:HD12	1:D:857:ARG:HB2	2.03	0.41
1:A:23:GLN:HG2	3:A:7533:HOH:O	2.20	0.41
1:A:63:PHE:CB	1:A:64:PRO:CD	2.98	0.41
1:A:682:LEU:HA	1:A:683:PRO:HD3	1.91	0.41
1:A:835:LEU:HD12	1:A:857:ARG:HB2	2.03	0.41
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.56	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.90	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.86	0.41
1:B:41:GLU:HG2	1:B:46:ARG:NH1	2.35	0.41
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.85	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.58	0.41
1:D:41:GLU:HG2	1:D:46:ARG:NH1	2.35	0.41
1:D:524:LEU:O	1:D:561:ARG:NH2	2.50	0.41
1:D:742:THR:CG2	1:D:743:SER:H	2.32	0.41
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.55	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.54	0.41
1:B:63:PHE:CB	1:B:64:PRO:CD	2.98	0.41
1:B:822:LEU:HA	1:B:822:LEU:HD13	1.79	0.41
1:D:124:SER:HA	1:D:184:LEU:O	2.20	0.41
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.86	0.41
1:D:352:ARG:NH2	1:D:641:GLU:OE1	2.54	0.41
1:D:77:ASP:HA	3:D:4132:HOH:O	2.19	0.41
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.88	0.41
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.41
1:B:367:MET:HB3	1:B:372:MET:CE	2.50	0.41
1:B:649:ASN:O	1:B:702:GLN:HG3	2.21	0.41
1:B:856:TYR:CD1	1:B:856:TYR:N	2.88	0.41
1:C:11:LEU:HD23	1:C:11:LEU:N	2.35	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
1:A:278:ILE:HA	1:A:278:ILE:HD12	1.88	0.41
1:A:380:LYS:HE3	1:A:406:GLY:O	2.21	0.41
1:A:578:TYR:HA	1:A:583:ASN:O	2.20	0.41
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.54	0.41
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.45	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:B:655:MET:O	1:B:696:LEU:HD12	2.21	0.41
1:B:69:VAL:HG13	1:B:70:PRO:HD2	2.03	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.56	0.41
1:C:26:ARG:HD2	1:C:169:SER:HB3	2.02	0.41
1:C:41:GLU:HG2	1:C:46:ARG:NH1	2.35	0.41
1:C:559:TYR:HB2	1:C:562:LEU:CD1	2.47	0.41
1:C:649:ASN:O	1:C:702:GLN:HG3	2.21	0.41
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.91	0.41
1:C:970:THR:HG22	1:C:972:HIS:O	2.21	0.41
1:D:63:PHE:CB	1:D:64:PRO:CD	2.98	0.41
1:A:227:VAL:CG1	1:A:228:ALA:N	2.83	0.41
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.38	0.41
1:A:840:HIS:N	1:A:840:HIS:ND1	2.67	0.41
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.36	0.41
1:A:949:HIS:CD2	1:A:1020:TRP:NE1	2.79	0.41
1:C:441:THR:O	1:C:445:GLN:HG3	2.20	0.41
1:C:511:PRO:HA	1:C:516:PRO:CB	2.51	0.41
1:D:26:ARG:HD2	1:D:169:SER:HB3	2.02	0.41
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.56	0.41
1:A:282:ARG:HG3	1:D:423:MET:HB2	2.03	0.41
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.36	0.41
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.56	0.41
1:A:262:GLN:HG2	1:A:262:GLN:O	2.19	0.41
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.35	0.41
1:A:649:ASN:O	1:A:702:GLN:HG3	2.21	0.41
1:A:778:THR:HG22	1:A:779:PRO:N	2.35	0.41
1:B:858:ILE:HG12	1:B:864:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:HA	1:C:306:PRO:HD2	1.88	0.41
1:C:524:LEU:O	1:C:561:ARG:NH2	2.50	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.41
1:C:652:LEU:O	1:C:667:GLU:HA	2.20	0.41
1:D:11:LEU:N	1:D:11:LEU:HD23	2.35	0.41
1:D:655:MET:O	1:D:696:LEU:HD12	2.21	0.41
1:D:649:ASN:O	1:D:702:GLN:HG3	2.21	0.41
1:D:778:THR:CG2	1:D:779:PRO:CD	2.99	0.41
1:D:778:THR:HG22	1:D:779:PRO:N	2.35	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.41
1:A:63:PHE:HB3	1:A:64:PRO:CD	2.45	0.41
1:A:655:MET:O	1:A:696:LEU:HD12	2.21	0.41
1:A:970:THR:HG22	1:A:972:HIS:O	2.21	0.41
1:B:105:TYR:HA	1:B:106:PRO:HD3	1.91	0.41
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.55	0.41
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.81	0.41
1:B:778:THR:HG22	1:B:779:PRO:N	2.35	0.41
1:C:380:LYS:HE3	1:C:406:GLY:O	2.21	0.41
1:C:835:LEU:HD12	1:C:857:ARG:HB2	2.03	0.41
1:D:114:VAL:HA	1:D:115:PRO:HD3	1.77	0.41
1:D:168:PRO:O	1:D:442:ARG:NH2	2.48	0.41
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.54	0.41
1:A:161:TYR:OH	1:A:163:GLN:NE2	2.50	0.41
1:A:26:ARG:HD2	1:A:169:SER:HB3	2.02	0.41
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.75	0.41
1:A:868:VAL:HG12	1:A:869:ASP:N	2.36	0.41
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.23	0.41
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.19	0.41
1:B:588:TYR:O	1:B:589:GLY:C	2.59	0.41
1:B:868:VAL:HG12	1:B:869:ASP:N	2.36	0.41
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.84	0.41
1:C:778:THR:HG22	1:C:779:PRO:N	2.35	0.41
1:D:176:PHE:N	1:D:176:PHE:CD1	2.87	0.41
1:D:578:TYR:HA	1:D:583:ASN:O	2.21	0.41
1:D:970:THR:HG22	1:D:972:HIS:O	2.21	0.41
1:A:149:ALA:O	1:A:150:PHE:HB3	2.21	0.40
1:A:576:ILE:HD13	1:A:584:PRO:HB2	2.02	0.40
1:B:141:ILE:HG12	1:B:142:ILE:N	2.35	0.40
1:B:26:ARG:HD2	1:B:169:SER:HB3	2.02	0.40
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.56	0.40
1:B:840:HIS:ND1	1:B:840:HIS:N	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ARG:NH2	1:C:641:GLU:OE1	2.54	0.40
1:D:69:VAL:HG13	1:D:70:PRO:HD2	2.03	0.40
1:A:272:ALA:CB	1:A:273:PRO:CD	2.99	0.40
1:A:278:ILE:HD13	1:A:278:ILE:N	2.37	0.40
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.54	0.40
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.61	0.40
1:B:380:LYS:HE3	1:B:406:GLY:O	2.21	0.40
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.42	0.40
1:B:658:LEU:HG	1:B:661:LYS:HZ2	1.86	0.40
1:C:149:ALA:O	1:C:150:PHE:HB3	2.21	0.40
1:C:23:GLN:HG2	3:C:4454:HOH:O	2.20	0.40
1:C:762:SER:C	1:C:822:LEU:HD23	2.42	0.40
1:D:23:GLN:HG2	3:D:7533:HOH:O	2.20	0.40
1:A:502:MET:HA	1:A:537:GLU:O	2.22	0.40
1:A:588:TYR:O	1:A:589:GLY:C	2.59	0.40
1:B:272:ALA:CB	1:B:273:PRO:CD	2.99	0.40
1:B:780:LEU:HD12	1:B:780:LEU:HA	1.89	0.40
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.86	0.40
1:C:502:MET:HA	1:C:537:GLU:O	2.22	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.21	0.40
1:D:149:ALA:O	1:D:150:PHE:HB3	2.21	0.40
1:D:3:ILE:C	1:D:5:ASP:H	2.22	0.40
1:A:147:ASN:HA	1:A:148:SER:HA	1.65	0.40
1:A:244:VAL:O	1:A:288:ARG:HA	2.22	0.40
1:A:762:SER:C	1:A:822:LEU:HD23	2.42	0.40
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.55	0.40
1:B:578:TYR:HA	1:B:583:ASN:O	2.21	0.40
1:B:970:THR:HG22	1:B:972:HIS:O	2.21	0.40
1:C:128:ASN:HD22	1:C:180:GLY:C	2.25	0.40
1:C:38:ASN:HD21	1:C:41:GLU:N	2.17	0.40
1:C:65:ALA:CB	1:C:66:PRO:CD	3.00	0.40
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.48	0.40
1:D:702:GLN:O	1:D:712:GLY:N	2.50	0.40
1:D:868:VAL:HG12	1:D:869:ASP:N	2.36	0.40
1:D:89:ASN:O	1:D:92:MET:HB2	2.22	0.40
1:A:100:TYR:O	1:A:597:ASN:HB2	2.22	0.40
1:A:128:ASN:HD22	1:A:180:GLY:C	2.25	0.40
1:B:844:HIS:ND1	1:B:845:GLN:HG2	2.36	0.40
1:B:90:TRP:CD1	1:B:90:TRP:C	2.95	0.40
1:C:244:VAL:O	1:C:288:ARG:HA	2.22	0.40
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:TYR:HA	1:C:560:PRO:HD2	1.86	0.40
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.42	0.40
1:C:702:GLN:O	1:C:712:GLY:N	2.50	0.40
1:C:868:VAL:HG12	1:C:869:ASP:N	2.36	0.40
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.54	0.40
1:D:237:ARG:NH1	1:D:237:ARG:CB	2.79	0.40
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	28	62
1	B	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	28	62
1	C	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	28	62
1	D	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	28	62
All	All	4104/4084 (100%)	3812 (93%)	268 (6%)	24 (1%)	28	62

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	B	647	SER
1	C	647	SER
1	D	647	SER
1	A	77	ASP
1	A	601	PHE
1	B	77	ASP
1	B	601	PHE

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Mol	Chain	Res	Type
1	C	77	ASP
1	C	601	PHE
1	D	77	ASP
1	D	601	PHE
1	A	164	ASP
1	B	164	ASP
1	C	164	ASP
1	D	164	ASP
1	A	690	SER
1	B	690	SER
1	C	690	SER
1	D	690	SER
1	A	10	VAL
1	B	10	VAL
1	C	10	VAL
1	D	10	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	880/873 (101%)	755 (86%)	125 (14%)	4	12
1	B	880/873 (101%)	755 (86%)	125 (14%)	4	12
1	C	880/873 (101%)	755 (86%)	125 (14%)	4	12
1	D	880/873 (101%)	755 (86%)	125 (14%)	4	12
All	All	3520/3492 (101%)	3020 (86%)	500 (14%)	4	12

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	12	GLN
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN

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Mol	Chain	Res	Type
1	A	39	SER
1	A	49	GLN
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	80	GLU
1	A	85	VAL
1	A	90	TRP
1	A	102	ASN
1	A	114	VAL
1	A	116	THR
1	A	134	LEU
1	A	135	GLN
1	A	136	GLU
1	A	138	GLN
1	A	148	SER
1	A	169	SER
1	A	187	MET
1	A	190	ARG
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	214	LEU
1	A	219	THR
1	A	223	SER
1	A	230	ARG
1	A	237	ARG
1	A	246	MET
1	A	249	GLU
1	A	251	ARG
1	A	255	ARG
1	A	259	SER
1	A	269	SER
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	282	ARG
1	A	288	ARG
1	A	310	ARG
1	A	322	LEU
1	A	333	ARG
1	A	347	LYS

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Mol	Chain	Res	Type
1	A	385	ASN
1	A	394	ASN
1	A	424	ASN
1	A	425	ARG
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	481	SER
1	A	519	SER
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	529	GLU
1	A	533	LEU
1	A	545	SER
1	A	546	LEU
1	A	554	GLN
1	A	571	VAL
1	A	576	ILE
1	A	580	GLU
1	A	581	ASN
1	A	600	GLN
1	A	645	ARG
1	A	647	SER
1	A	655	MET
1	A	661	LYS
1	A	665	SER
1	A	672	VAL
1	A	675	GLN
1	A	687	GLN
1	A	690	SER
1	A	719	GLN
1	A	721	ARG
1	A	728	VAL
1	A	730	LEU
1	A	734	SER
1	A	737	ILE
1	A	743	SER
1	A	746	ASP
1	A	750	GLU
1	A	755	ARG
1	A	761	GLN

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	766	SER
1	A	768	MET
1	A	770	ILE
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	797	GLU
1	A	800	ARG
1	A	801	ILE
1	A	811	LYS
1	A	817	GLN
1	A	822	LEU
1	A	824	GLN
1	A	830	LEU
1	A	843	GLN
1	A	845	GLN
1	A	856	TYR
1	A	857	ARG
1	A	867	THR
1	A	874	SER
1	A	881	ARG
1	A	894	ARG
1	A	917	ARG
1	A	923	SER
1	A	931	PHE
1	A	938	ARG
1	A	950	GLN
1	A	958	ASN
1	A	969	GLU
1	A	986	ILE
1	A	991	MET
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1023	LYS
1	B	3	ILE
1	B	12	GLN
1	B	24	LEU
1	B	37	ARG
1	B	38	ASN
1	B	39	SER

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Mol	Chain	Res	Type
1	B	49	GLN
1	B	67	GLU
1	B	71	GLU
1	B	72	SER
1	B	80	GLU
1	B	85	VAL
1	B	90	TRP
1	B	102	ASN
1	B	114	VAL
1	B	116	THR
1	B	134	LEU
1	B	135	GLN
1	B	136	GLU
1	B	138	GLN
1	B	148	SER
1	B	169	SER
1	B	187	MET
1	B	190	ARG
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	214	LEU
1	B	219	THR
1	B	223	SER
1	B	230	ARG
1	B	237	ARG
1	B	246	MET
1	B	249	GLU
1	B	251	ARG
1	B	255	ARG
1	B	259	SER
1	B	269	SER
1	B	277	GLU
1	B	278	ILE
1	B	279	ILE
1	B	282	ARG
1	B	288	ARG
1	B	310	ARG
1	B	322	LEU
1	B	333	ARG
1	B	347	LYS
1	B	385	ASN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	424	ASN
1	B	425	ARG
1	B	437	SER
1	B	448	ARG
1	B	473	ARG
1	B	481	SER
1	B	519	SER
1	B	521	LYS
1	B	525	SER
1	B	526	LEU
1	B	529	GLU
1	B	533	LEU
1	B	545	SER
1	B	546	LEU
1	B	554	GLN
1	B	571	VAL
1	B	576	ILE
1	B	580	GLU
1	B	581	ASN
1	B	600	GLN
1	B	645	ARG
1	B	647	SER
1	B	655	MET
1	B	661	LYS
1	B	665	SER
1	B	672	VAL
1	B	675	GLN
1	B	687	GLN
1	B	690	SER
1	B	719	GLN
1	B	721	ARG
1	B	728	VAL
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	743	SER
1	B	746	ASP
1	B	750	GLU
1	B	755	ARG
1	B	761	GLN
1	B	765	LEU

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Mol	Chain	Res	Type
1	B	766	SER
1	B	768	MET
1	B	770	ILE
1	B	772	ASP
1	B	773	LYS
1	B	774	LYS
1	B	797	GLU
1	B	800	ARG
1	B	801	ILE
1	B	811	LYS
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN
1	B	830	LEU
1	B	843	GLN
1	B	845	GLN
1	B	856	TYR
1	B	857	ARG
1	B	867	THR
1	B	874	SER
1	B	881	ARG
1	B	894	ARG
1	B	917	ARG
1	B	923	SER
1	B	931	PHE
1	B	938	ARG
1	B	950	GLN
1	B	958	ASN
1	B	969	GLU
1	B	986	ILE
1	B	991	MET
1	B	1004	SER
1	B	1006	GLU
1	B	1017	GLN
1	B	1023	LYS
1	C	3	ILE
1	C	12	GLN
1	C	24	LEU
1	C	37	ARG
1	C	38	ASN
1	C	39	SER
1	C	49	GLN

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Mol	Chain	Res	Type
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	85	VAL
1	C	90	TRP
1	C	102	ASN
1	C	114	VAL
1	C	116	THR
1	C	134	LEU
1	C	135	GLN
1	C	136	GLU
1	C	138	GLN
1	C	148	SER
1	C	169	SER
1	C	187	MET
1	C	190	ARG
1	C	202	MET
1	C	210	ARG
1	C	211	ASP
1	C	214	LEU
1	C	219	THR
1	C	223	SER
1	C	230	ARG
1	C	237	ARG
1	C	246	MET
1	C	249	GLU
1	C	251	ARG
1	C	255	ARG
1	C	259	SER
1	C	269	SER
1	C	277	GLU
1	C	278	ILE
1	C	279	ILE
1	C	282	ARG
1	C	288	ARG
1	C	310	ARG
1	C	322	LEU
1	C	333	ARG
1	C	347	LYS
1	C	385	ASN
1	C	394	ASN

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Mol	Chain	Res	Type
1	C	424	ASN
1	C	425	ARG
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	481	SER
1	C	519	SER
1	C	521	LYS
1	C	525	SER
1	C	526	LEU
1	C	529	GLU
1	C	533	LEU
1	C	545	SER
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	576	ILE
1	C	580	GLU
1	C	581	ASN
1	C	600	GLN
1	C	645	ARG
1	C	647	SER
1	C	655	MET
1	C	661	LYS
1	C	665	SER
1	C	672	VAL
1	C	675	GLN
1	C	687	GLN
1	C	690	SER
1	C	719	GLN
1	C	721	ARG
1	C	728	VAL
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	743	SER
1	C	746	ASP
1	C	750	GLU
1	C	755	ARG
1	C	761	GLN
1	C	765	LEU
1	C	766	SER

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Mol	Chain	Res	Type
1	C	768	MET
1	C	770	ILE
1	C	772	ASP
1	C	773	LYS
1	C	774	LYS
1	C	797	GLU
1	C	800	ARG
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN
1	C	822	LEU
1	C	824	GLN
1	C	830	LEU
1	C	843	GLN
1	C	845	GLN
1	C	856	TYR
1	C	857	ARG
1	C	867	THR
1	C	874	SER
1	C	881	ARG
1	C	894	ARG
1	C	917	ARG
1	C	923	SER
1	C	931	PHE
1	C	938	ARG
1	C	950	GLN
1	C	958	ASN
1	C	969	GLU
1	C	986	ILE
1	C	991	MET
1	C	1004	SER
1	C	1006	GLU
1	C	1017	GLN
1	C	1023	LYS
1	D	3	ILE
1	D	12	GLN
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	49	GLN
1	D	67	GLU

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Mol	Chain	Res	Type
1	D	71	GLU
1	D	72	SER
1	D	80	GLU
1	D	85	VAL
1	D	90	TRP
1	D	102	ASN
1	D	114	VAL
1	D	116	THR
1	D	134	LEU
1	D	135	GLN
1	D	136	GLU
1	D	138	GLN
1	D	148	SER
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	214	LEU
1	D	219	THR
1	D	223	SER
1	D	230	ARG
1	D	237	ARG
1	D	246	MET
1	D	249	GLU
1	D	251	ARG
1	D	255	ARG
1	D	259	SER
1	D	269	SER
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	282	ARG
1	D	288	ARG
1	D	310	ARG
1	D	322	LEU
1	D	333	ARG
1	D	347	LYS
1	D	385	ASN
1	D	394	ASN
1	D	424	ASN

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Mol	Chain	Res	Type
1	D	425	ARG
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	481	SER
1	D	519	SER
1	D	521	LYS
1	D	525	SER
1	D	526	LEU
1	D	529	GLU
1	D	533	LEU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	576	ILE
1	D	580	GLU
1	D	581	ASN
1	D	600	GLN
1	D	645	ARG
1	D	647	SER
1	D	655	MET
1	D	661	LYS
1	D	665	SER
1	D	672	VAL
1	D	675	GLN
1	D	687	GLN
1	D	690	SER
1	D	719	GLN
1	D	721	ARG
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	743	SER
1	D	746	ASP
1	D	750	GLU
1	D	755	ARG
1	D	761	GLN
1	D	765	LEU
1	D	766	SER
1	D	768	MET

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Mol	Chain	Res	Type
1	D	770	ILE
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	797	GLU
1	D	800	ARG
1	D	801	ILE
1	D	811	LYS
1	D	817	GLN
1	D	822	LEU
1	D	824	GLN
1	D	830	LEU
1	D	843	GLN
1	D	845	GLN
1	D	856	TYR
1	D	857	ARG
1	D	867	THR
1	D	874	SER
1	D	881	ARG
1	D	894	ARG
1	D	917	ARG
1	D	923	SER
1	D	931	PHE
1	D	938	ARG
1	D	950	GLN
1	D	958	ASN
1	D	969	GLU
1	D	986	ILE
1	D	991	MET
1	D	1004	SER
1	D	1006	GLU
1	D	1017	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	50	GLN
1	A	102	ASN
1	A	128	ASN
1	A	163	GLN

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Mol	Chain	Res	Type
1	A	216	HIS
1	A	226	HIS
1	A	316	HIS
1	A	357	HIS
1	A	385	ASN
1	A	424	ASN
1	A	467	ASN
1	A	554	GLN
1	A	581	ASN
1	A	597	ASN
1	A	604	ASN
1	A	622	HIS
1	A	624	GLN
1	A	634	GLN
1	A	817	GLN
1	A	890	GLN
1	A	949	HIS
1	A	990	HIS
1	A	1017	GLN
1	B	38	ASN
1	B	50	GLN
1	B	102	ASN
1	B	128	ASN
1	B	163	GLN
1	B	216	HIS
1	B	226	HIS
1	B	316	HIS
1	B	357	HIS
1	B	385	ASN
1	B	424	ASN
1	B	467	ASN
1	B	554	GLN
1	B	581	ASN
1	B	597	ASN
1	B	604	ASN
1	B	622	HIS
1	B	624	GLN
1	B	634	GLN
1	B	817	GLN
1	B	890	GLN
1	B	949	HIS
1	B	990	HIS

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Mol	Chain	Res	Type
1	B	1017	GLN
1	C	38	ASN
1	C	50	GLN
1	C	102	ASN
1	C	128	ASN
1	C	216	HIS
1	C	226	HIS
1	C	316	HIS
1	C	357	HIS
1	C	385	ASN
1	C	424	ASN
1	C	467	ASN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	604	ASN
1	C	622	HIS
1	C	624	GLN
1	C	634	GLN
1	C	817	GLN
1	C	890	GLN
1	C	949	HIS
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN
1	D	50	GLN
1	D	102	ASN
1	D	128	ASN
1	D	216	HIS
1	D	226	HIS
1	D	316	HIS
1	D	357	HIS
1	D	385	ASN
1	D	424	ASN
1	D	467	ASN
1	D	554	GLN
1	D	581	ASN
1	D	597	ASN
1	D	604	ASN
1	D	622	HIS
1	D	624	GLN
1	D	634	GLN

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Mol	Chain	Res	Type
1	D	817	GLN
1	D	890	GLN
1	D	949	HIS
1	D	990	HIS
1	D	1017	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1021/1021 (100%)	-0.81	8 (0%) 86 81	8, 29, 70, 100	19 (1%)
1	B	1021/1021 (100%)	-0.80	5 (0%) 90 88	8, 29, 70, 100	19 (1%)
1	C	1021/1021 (100%)	-0.84	5 (0%) 90 88	8, 29, 70, 100	19 (1%)
1	D	1021/1021 (100%)	-0.81	6 (0%) 89 86	8, 29, 70, 100	19 (1%)
All	All	4084/4084 (100%)	-0.81	24 (0%) 89 86	8, 29, 71, 100	76 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	732	ALA	4.5
1	A	732	ALA	4.1
1	C	581	ASN	3.6
1	A	581	ASN	3.4
1	A	801	ILE	3.2
1	A	730	LEU	3.0
1	B	732	ALA	3.0
1	C	732	ALA	2.8
1	A	734	SER	2.8
1	A	733	ALA	2.7
1	D	730	LEU	2.5
1	D	733	ALA	2.5
1	B	583	ASN	2.4
1	C	596	PRO	2.4
1	B	798	ALA	2.3
1	A	729	THR	2.2
1	D	734	SER	2.2
1	C	734	SER	2.1
1	B	731	PRO	2.1
1	B	136	GLU	2.1
1	D	731	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	731	PRO	2.0
1	A	582	GLY	2.0
1	D	582	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	D	3002	1/1	0.96	0.12	1.95	31,31,31,31	0
2	MG	B	3002	1/1	0.94	0.11	1.60	31,31,31,31	0
2	MG	A	3002	1/1	0.98	0.11	0.98	31,31,31,31	0
2	MG	C	3002	1/1	0.96	0.12	0.97	31,31,31,31	0
2	MG	B	3001	1/1	0.99	0.06	-1.48	28,28,28,28	0
2	MG	C	3001	1/1	0.99	0.04	-2.05	28,28,28,28	0
2	MG	A	3001	1/1	0.96	0.08	-2.15	28,28,28,28	0
2	MG	D	3001	1/1	0.99	0.06	-2.52	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.